計算科学における情報圧縮

Information Compression in Computational Science

2019.12.12

#10: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

Entanglement of information and matrix product states

理学系研究科　物理学専攻　大久保　毅

Department of Physics, **Tsuyoshi Okubo**

Outline

- Outline of tensor network decomposition
- Entanglement
    - Schmidt decomposition
    - Entanglement entropy and its area law
- Matrix product states
    - Matrix product states (MPS)
    - Canonical form
    - infinite MPS

Outline of tensor network decomposition

Classification of Information Compression by Memory Costs

Linear algebra for huge data: $\vec{v} \in \mathbb{C}^M$

(1) A matrix can be stored

Required memory~ $O(M^2)$

(2) Although a matrix cannot be stored, vectors can be stored

Required memory~ $O(M)$

(3) A vector cannot be stored

$\boxed{\text{Required memory} \ll O(M)}$

We try to approximate a vector in a compact form.

$M \sim a^N$ → Memory ~ $O(N^x)$

Exponential **Polynomial**

N :problem size (e.g. system size)

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).

(1) Almost all C_i are zero (or very small).

We store only a few finite elements $\{(i, C_i)\}$

E.g.

Fourier transformation $\vec{v} = \sum_{k=1}^{M} D_k \vec{f}_k$

If we can neglect larger wave numbers, we can efficiently approximate the vector with smaller number of coefficients.

Classical state $|\Psi\rangle = |01011\ldots00\rangle$

In this case, we know that only a specific C_i is non-zero.

We need only an integer corresponding to the non-zero element.

When we efficiently compress a vector?

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

(2) 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.

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

e.g.

$$|\phi_1\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$|\phi_1\rangle = |01\rangle - |10\rangle$$

structure: **"product state"**

independent elements: **small vectors**

Tensor network decomposition of a vector

Target: Exponentially large Hilbert space

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

+

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

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

Tensor network decomposition

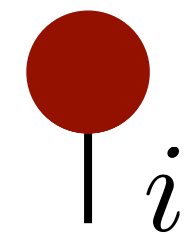
$$v_i = v_{i_1,i_2,\ldots,i_N} = \sum_{\{x\}} T^{(1)}[i_1]_{x_1,x_2,\ldots} T^{(2)}[i_2]_{x_1,x_3,\ldots} \cdots T^{(N)}[i_N]_{x_3,x_{100},\ldots}$$

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

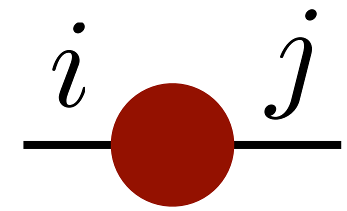
$T[i]_{x_1,x_2,\ldots}$: local tensor for "state" i

Graphical representations for tensor network

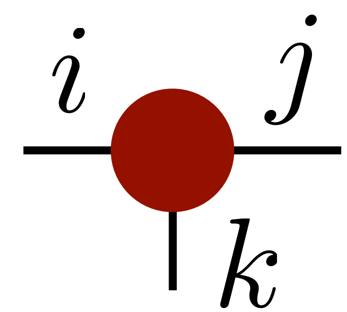
- Vector $\vec{v} : v_i$



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

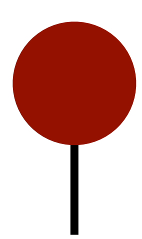
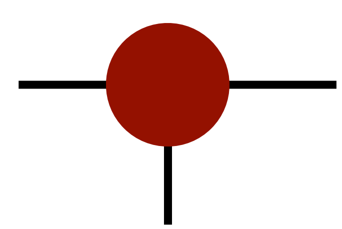


- Tensor $T : T_{i,j,k}$



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

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

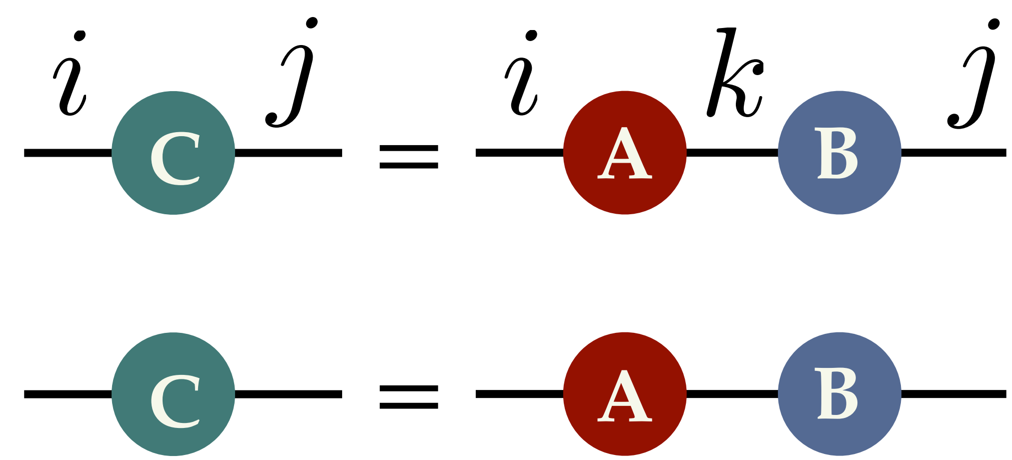
$\vec{v} =$  $T =$ 

Graphical representations for tensor network

Matrix product

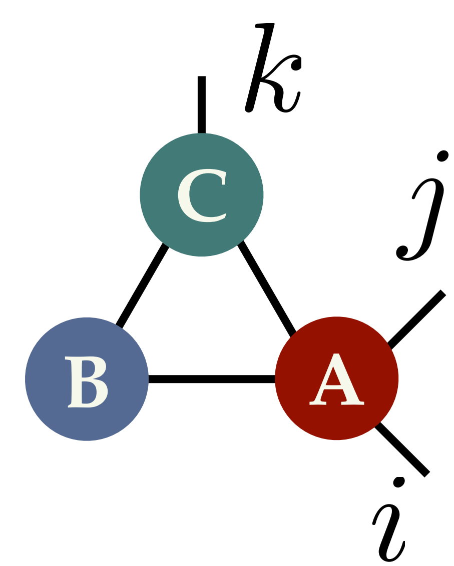
$$C_{i,j} = (AB)_{i,j} = \sum_k A_{i,k} B_{k,j}$$

$$C = AB$$



Generalization to tensors

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

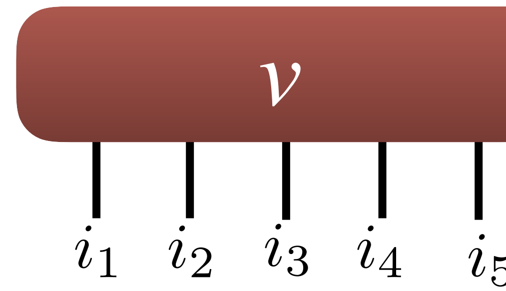


Contraction of a network = **Calculation of a lot of multiplications**

(縮約)

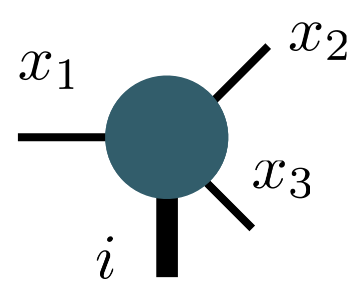
Graph for a tensor network decomposition

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



*Vector looks like a tensor

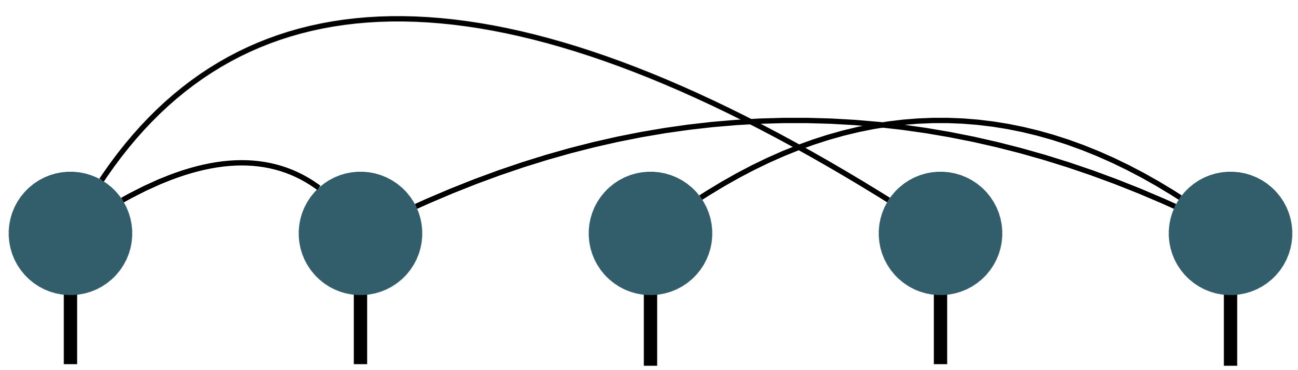
- Tensor $T[i]_{x_1,x_2,x_3}$



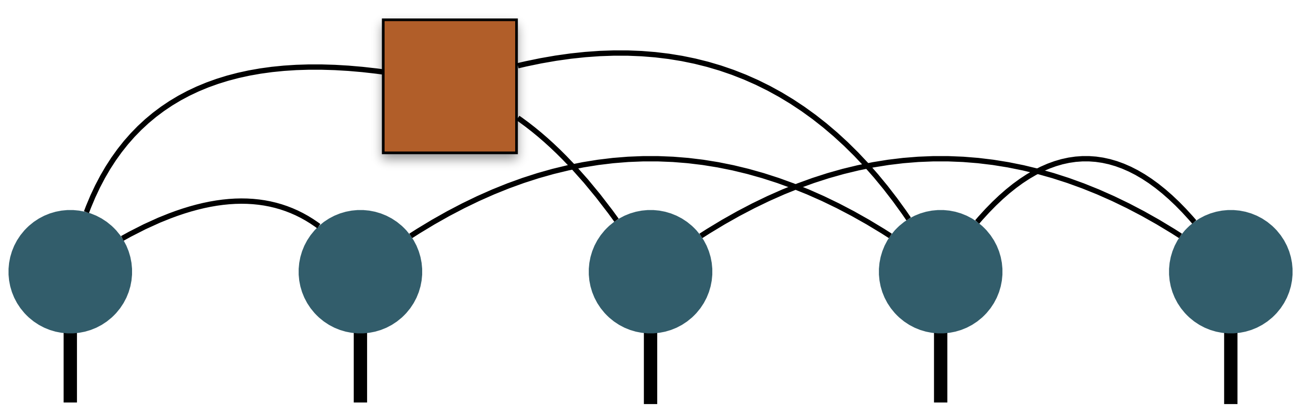
*We treat i as an index of the tensor.

Tensor network decomposition

$\vec{v} =$



$\vec{w} =$

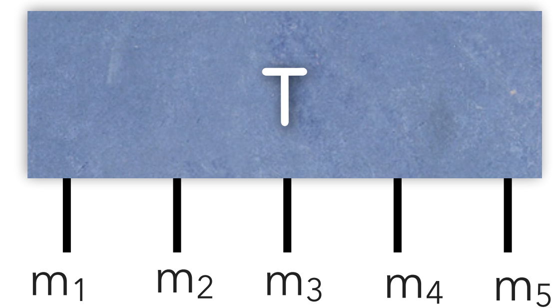


*We can consider tensors independent on i.

SVD of wave function?

Wave function: $|\Psi\rangle = \sum_{\{m_i=0,1\}} T_{m_1,m_2,\cdots,m_N} |m_1, m_2, \cdots, m_N\rangle$

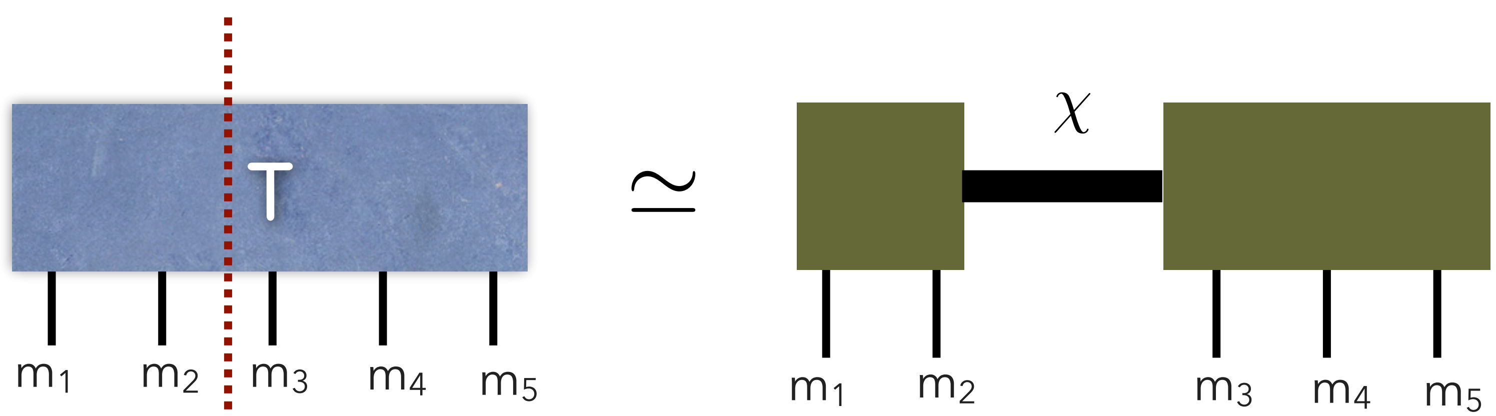
$T_{m_1,m_2,\cdots,m_N}$:N-leg tensor (or Vector)



We can consider it as a matrix by making two groups:

$T_{\{m_1,m_2,\cdots,m_M\},\{m_{M+1},\cdots,m_N\}}$

We can perform the low rank approximation of T.



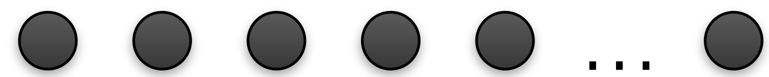
What does it mean?

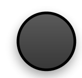
It is related to MPS

Entanglement（エンタングルメント）

N-qubit system (S=1/2 quantum spin system)

Example vector: Wave function of N-qubit systems



 takes two states $|0\rangle, |1\rangle$ $(|\uparrow\rangle, |\downarrow\rangle)$

$$
\begin{aligned}
|\Psi\rangle &= \sum_{\{i_1, i_2, \dots i_N\}} \Psi_{i_1 i_2 \dots i_N} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle \\
&= \sum_{\{i_1, i_2, \dots i_N\}} \Psi_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle
\end{aligned}
$$

Coefficients = vector: $\vec{\Psi} \in \mathbb{C}^{2^N}$

* Inner product: $\langle \Phi | \Psi \rangle = \vec{\Phi}^* \cdot \vec{\Psi}$

Schmidt decomposition

General vector: $\vec{x} \in \mathbb{V}_1 \otimes \mathbb{V}_2$

$$\dim\, \mathbb{V}_1 = n_1, \dim\, \mathbb{V}_2 = n_2$$
$$(n_1 \geq n_2)$$

Schmidt decomposition

There exists special basis which satisfies

$$\vec{x} = \sum_{i=1}^{n_2} \lambda_i \vec{u}_i \otimes \vec{v}_i$$

No off-diagonal coupling!

Orthonormal basis

$$\{\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_{n_1}\} \in \mathbb{V}_1$$
$$\{\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_{n_2}\} \in \mathbb{V}_2$$

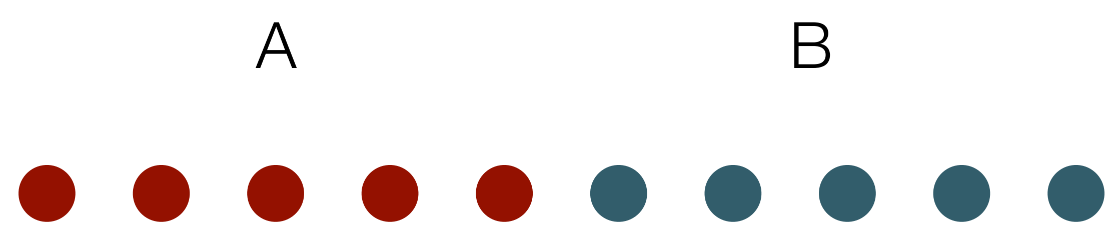
Schmidt coefficient $\lambda_i \geq 0$

Schmidt decomposition is unique.

Schmidt decomposition for a wave function

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

Schmidt decomposition

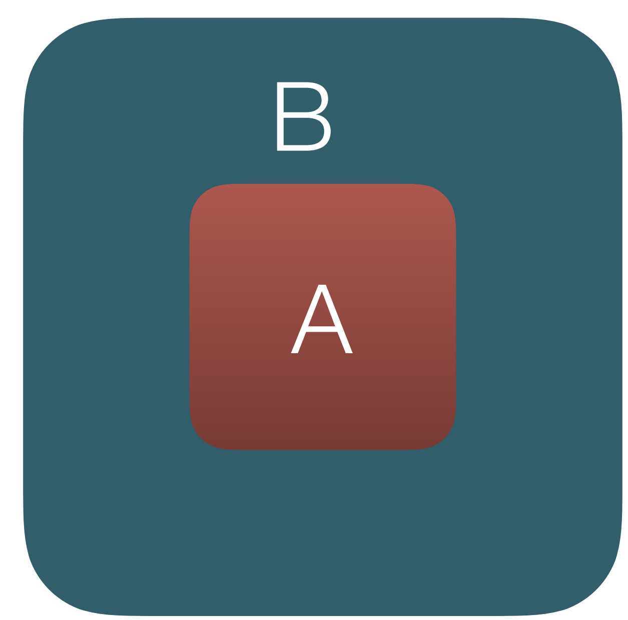


Divide system into two parts, A and B:

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

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

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



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

Schmidt coefficient: $\lambda_i \geq 0$

Relation between SVD and Schmidt decomposition

Singular value decomposition (SVD):

For a K × L matrix M,

$$M_{i,j} = \sum_m U_{i,m} \lambda_m V^\dagger_{m,j}$$

Singular values: $\lambda_m \geq 0$

Singular vectors:
$$\sum_m U_{i,m} U^\dagger_{m,j} = \delta_{i,j}$$
$$\sum_m V_{i,m} V^\dagger_{m,j} = \delta_{i,j}$$

Relation to the Schmidt decomposition:

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

$$|\alpha_m\rangle = \sum_i U_{i,m} |A_i\rangle$$
$$|\beta_m\rangle = \sum_j V^\dagger_{m,j} |B_j\rangle$$

$$\Rightarrow \quad \langle \alpha_i | \alpha_j \rangle = \langle \beta_i | \beta_j \rangle = \delta_{i,j}$$

By using SVD, we can perform Schmidt decomposition.

Partial trace and reduced density matrix

For $\vec{x} \in \mathbb{V}_1 \otimes \mathbb{V}_2$ $\quad \dim\ \mathbb{V}_1 = n_1, \dim\ \mathbb{V}_2 = n_2 \quad |\vec{x}| = 1$

Density matrix: $\rho \equiv \vec{x}\vec{x}^\dagger \quad (\rho_{ij} = x_i x_j^*)$

（密度行列）$(\rho = |x\rangle\langle x|)$ $\quad$ *Note: $\mathrm{rank}\ \rho = 1$

Orthonormal basis: $\{\vec{e}_1, \vec{e}_2, \ldots, \vec{e}_{n_1}\} \in \mathbb{V}_1 \quad \{\vec{f}_1, \vec{f}_2, \ldots, \vec{f}_{n_2}\} \in \mathbb{V}_2$

Basis for $\vec{x}$: $\vec{g}_{i_1,i_2} = \vec{e}_{i_1} \otimes \vec{f}_{i_2}$

Index: $i = (i_1, i_2)$

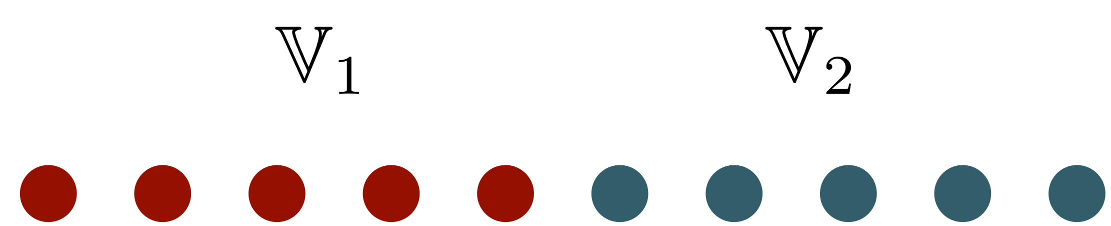
Reduced Density matrix:

（縮約密度行列）

$\rho_{\mathbb{V}_1} \equiv \mathrm{Tr}_{\mathbb{V}_2}\rho$: a positive-semidefinite square matrix in $\mathbb{V}_1$

*Note: generally, $\mathrm{rank}\ \rho_{\mathbb{V}_1} > 1$

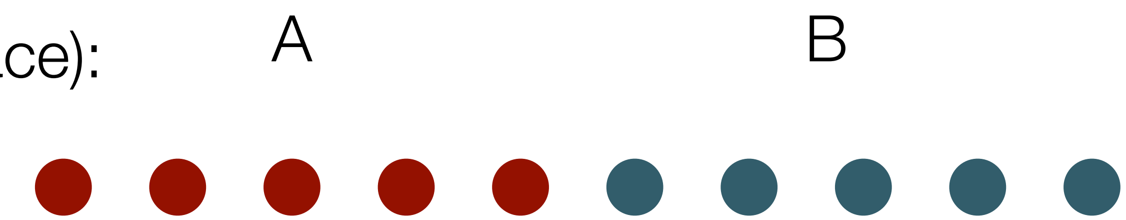
$$\boxed{(\rho_{\mathbb{V}_1})_{i_1,j_1} = \sum_{\underline{i_2}} \rho_{(i_1,\underline{i_2}),(j_1,\underline{i_2})}}$$



Entanglement entropy

Entanglement entropy:

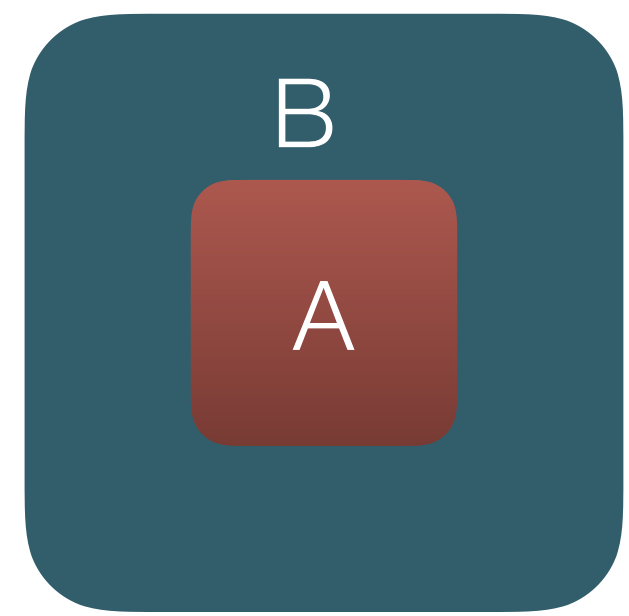
Reduced density matrix of a sub system (sub space):



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

Entanglement entropy = von Neumann entropy of ρ_A

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



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

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

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

$$\left(\sum_i \lambda_i^2 = 1\right)$$

Entanglement entropy is calculated through the spectrum of Schmidt coefficients.

(It also indicates $S = -\mathrm{Tr}(\rho_B \log \rho_B)$)

Intuition for EE

Entanglement entropy is related to spectrum of singular values.

$$S = -\mathrm{Tr}(\rho_A \log \rho_A) = -\sum_i \lambda_i^2 \log \lambda_i^2$$

Normalization: $(\sum_i \lambda_i^2 = 1)$

- $\mathrm{rank}\rho_A = 1$

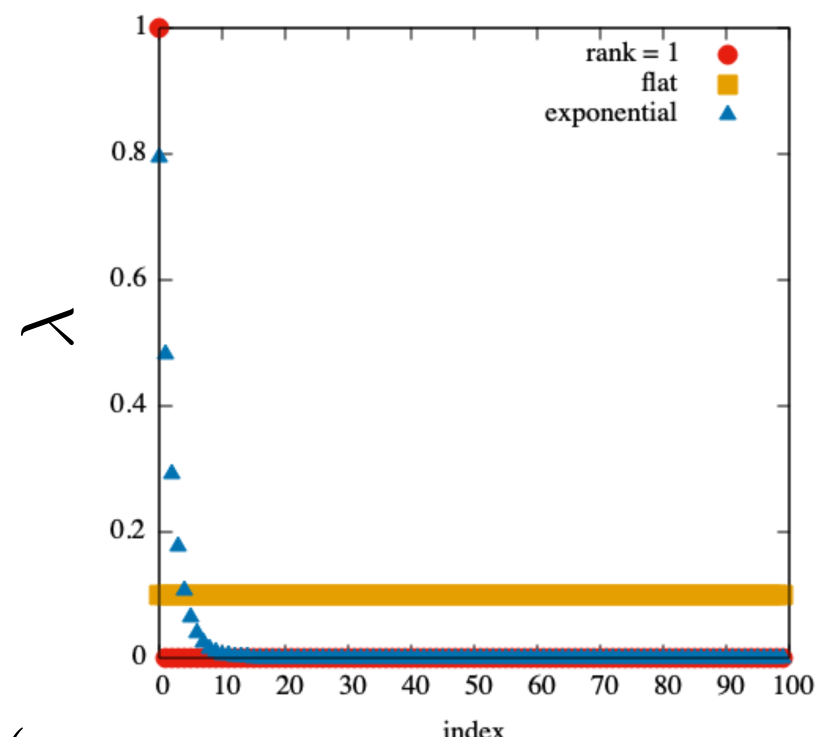
  $\lambda_1 = 1, \lambda_j = 0 \ (j \neq 1)$ ➡ $S = 0$

- Flat spectrum

  $\lambda_1 = \lambda_2 = \cdots = \lambda_n = \frac{1}{\sqrt{n}}$ ➡ $S = \log n$

- Exponential decay

  $\lambda_i \propto e^{-\alpha i}$ ➡ $S = 1 - \log 2\alpha \ (\alpha \ll 1, \alpha n \to \infty)$



Smaller exponent gives larger entropy.

Intuition for EE: two s=1/2 spins

A B

1. $|\Psi\rangle = |\uparrow\rangle \otimes |\downarrow\rangle$

A product state $\lambda = 1, \; S = 0$

Product state : S=0

2. $|\Psi\rangle = \frac{1}{2}\left(|\uparrow\rangle - |\downarrow\rangle\right) \otimes \left(|\uparrow\rangle - |\downarrow\rangle\right)$

Another product state $\lambda = 1 \;, \; S = 0$

3. $|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle\right)$

Spin singlet $\lambda_1 = \lambda_2 = \frac{1}{\sqrt{2}} \;, \quad S = \log 2$

Maximally entangled State

4. $|\Psi\rangle = \left(x|\uparrow\rangle \otimes |\downarrow\rangle + \sqrt{1-x^2}|\downarrow\rangle \otimes |\uparrow\rangle\right)$

Complicated state $\lambda_1 = |x|, \lambda_2 = \sqrt{1-x^2}$

$$S = x^2 \log x^2 + \sqrt{1-x^2} \log(1-x^2)$$

Large entanglement entropy ~ Large correlation between two parts

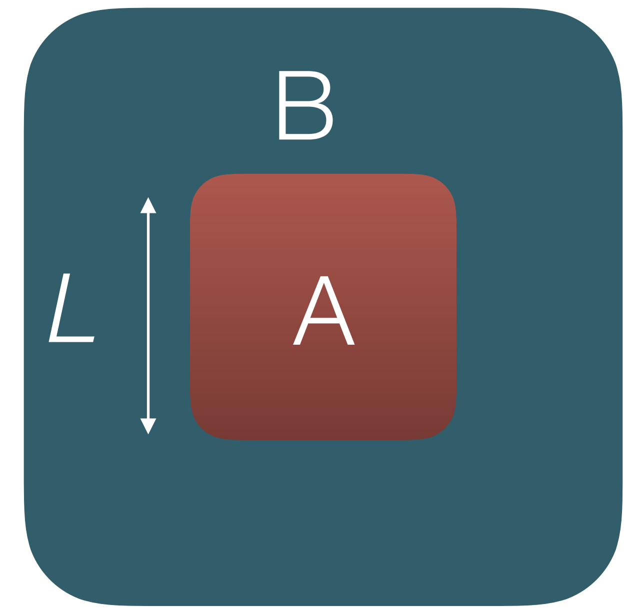
Area law of the entanglement entropy in physics

General wave functions (vector):

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

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

(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)

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

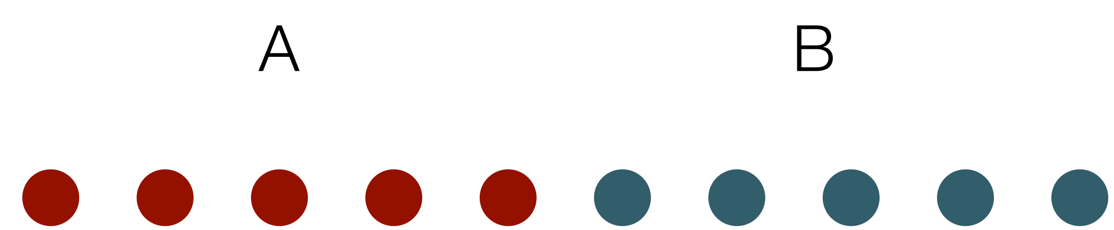
In the case of one-dimensional system:

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



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.

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

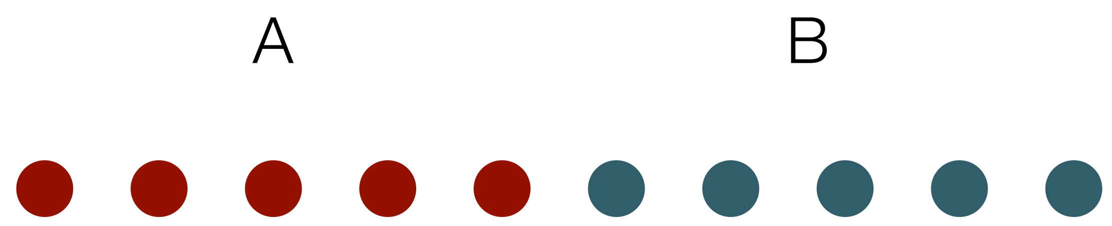
*Note: the ground state of this model is gapped

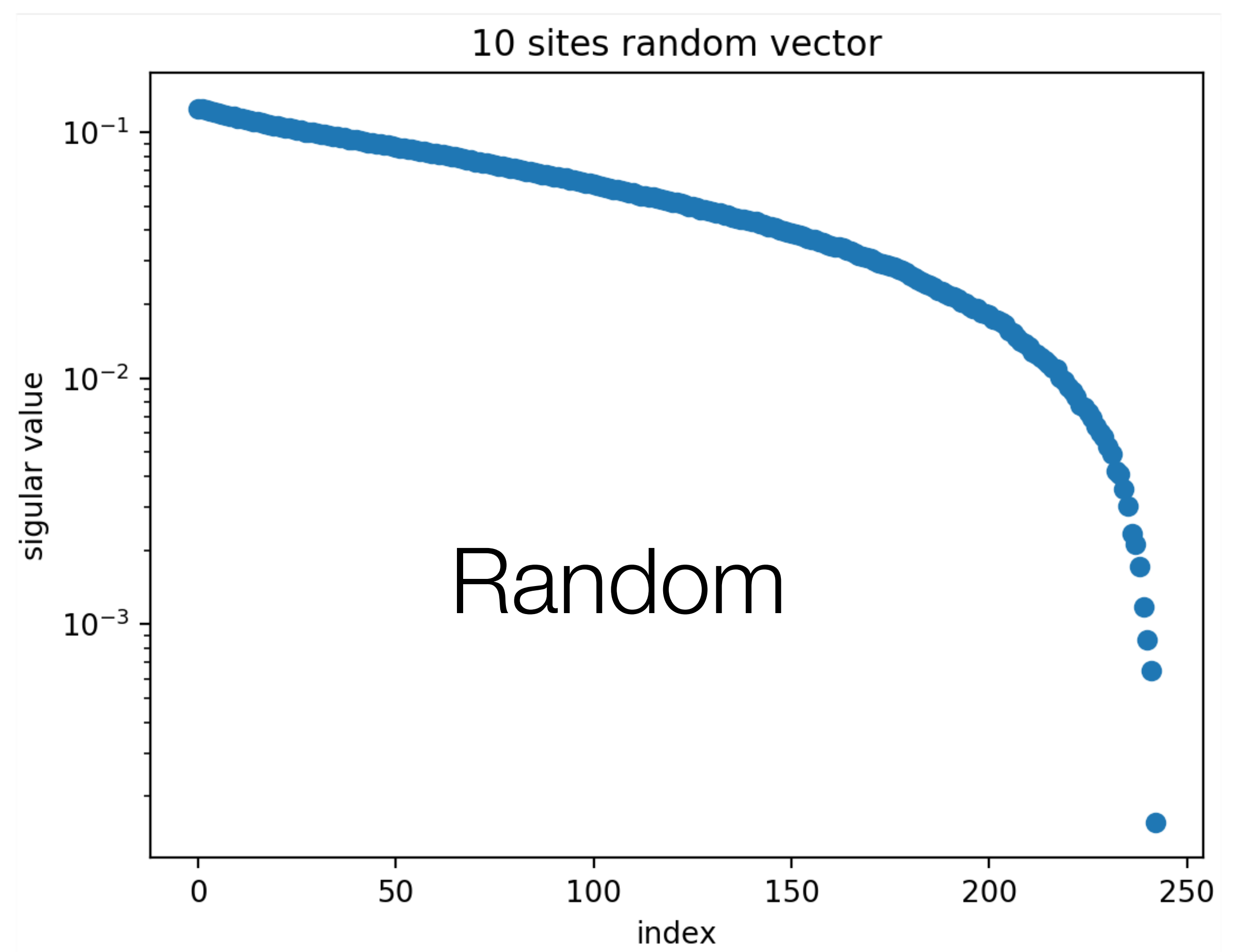
show help: *python Ex1-2.py -h*

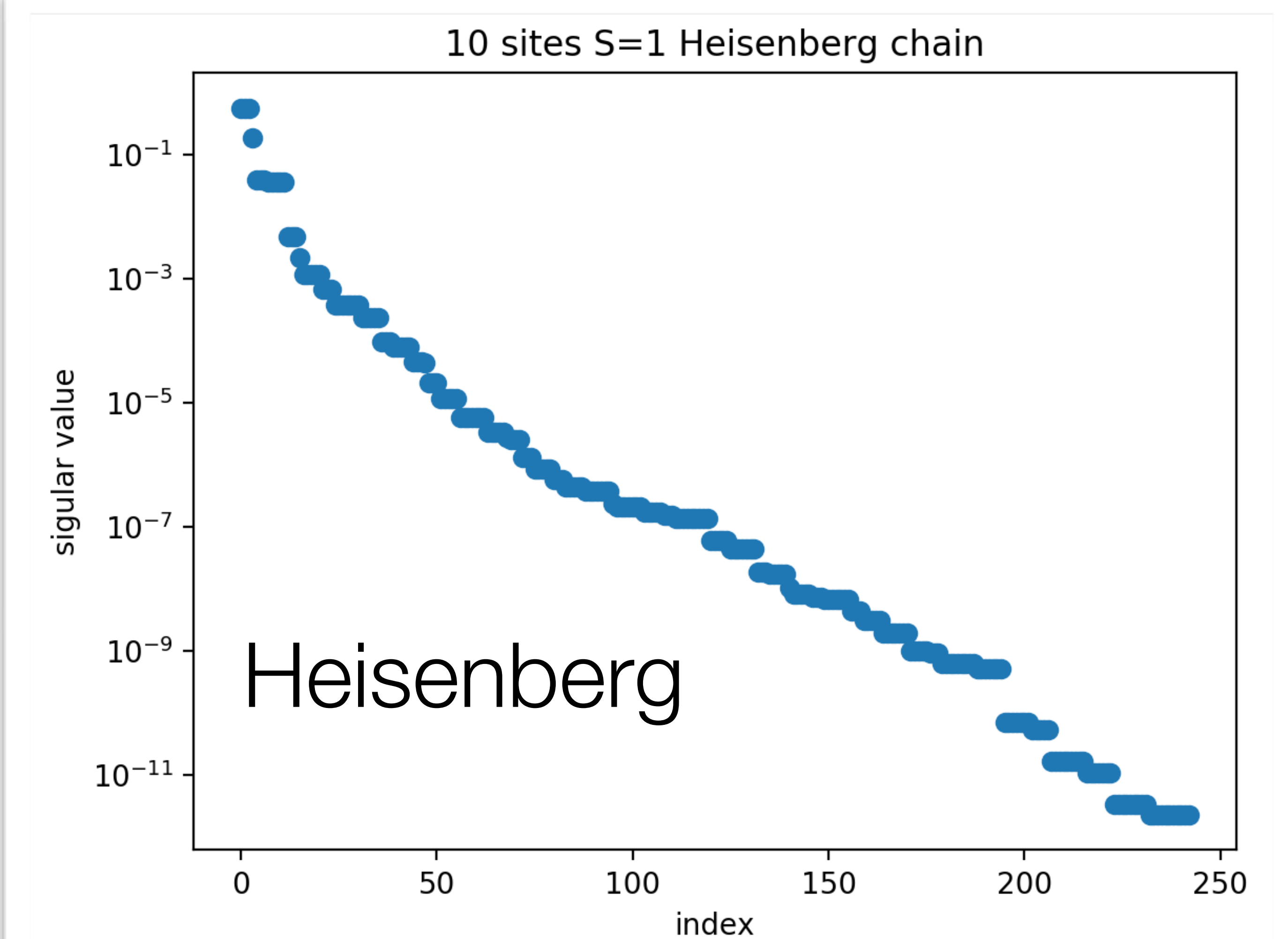
*** Try to simulate different system size "N"**
*** You can simulate other S by changing "m"**

Result: N=10 spectrum

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







Ground state wave function has lower entanglement!

Matrix product states（行列積状態）

Data compression of wave functions (vectors)

General wave function:

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

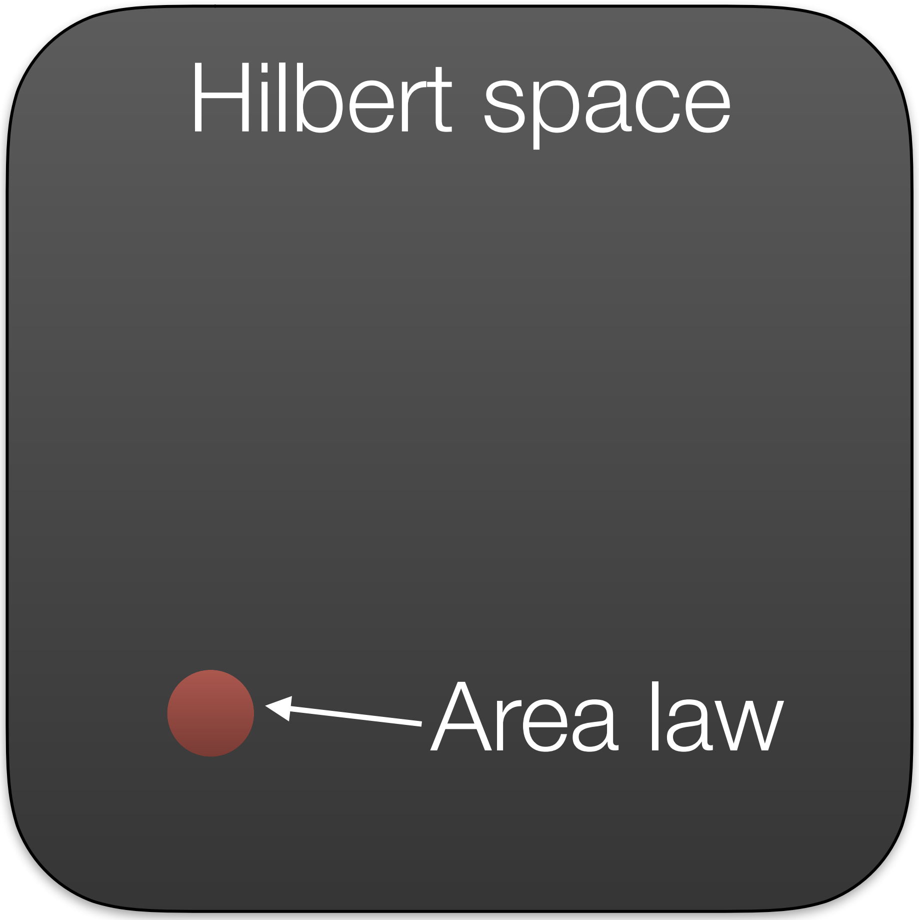
Coefficient vector can represent any points in the Hilbert space.

Ground states satisfy the area law.

In order to represent the ground state accurately, we might not need all of a^N elements.

Data compression by tensor decomposition:

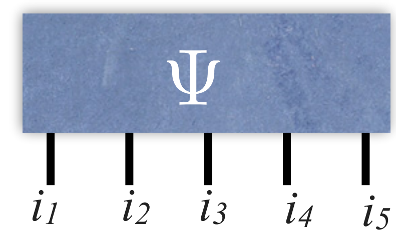
Tensor network states



Tensor network state

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

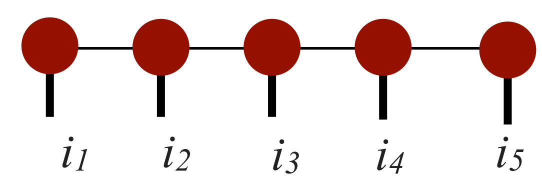
Vector (or N-rank tensor): $\Psi_{i_1 i_2 \dots i_N}$ =



# of Elements$=a^N$

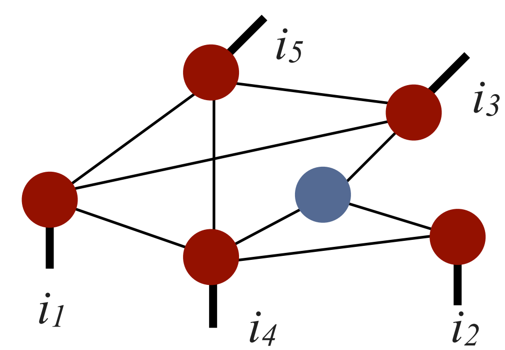
"Tensor network" decomposition

- 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

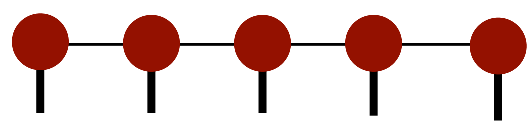
By choosing a "good" network, we can express G.S. wave function efficiently.

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

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

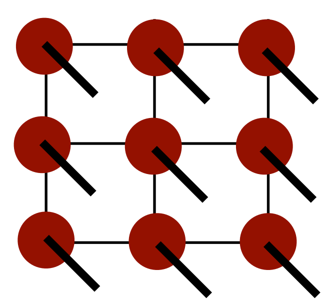
Examples of TNS

MPS:



Good for 1-d gapped systems

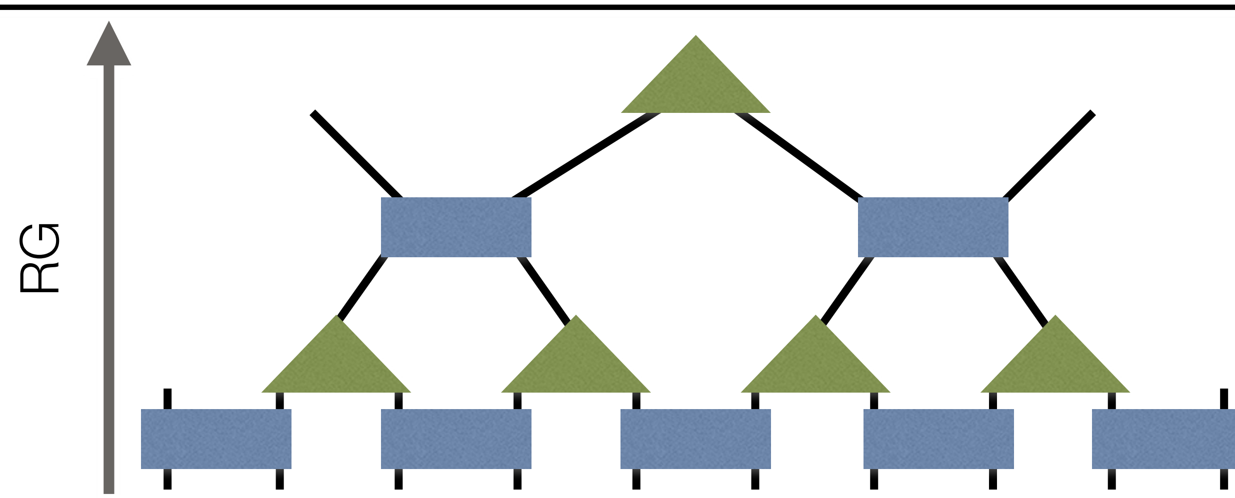
PEPS, TPS:



For higher dimensional systems

Extension of MPS

MERA:



Scale invariant systems

Matrix product state (MPS)

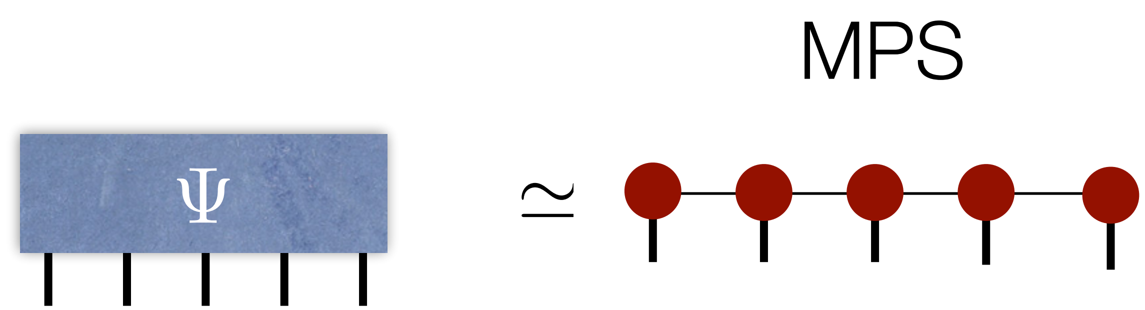
Good reviews:

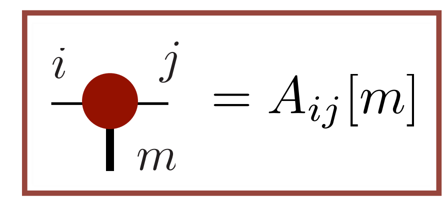
(U. Schollwöck, Annals. of Physics **326**, 96 (2011))
(R. Orús, Annals. of Physics **349**, 117 (2014))

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

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

$A[i]$: Matrix for state i





Note:

- MPS is called 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)

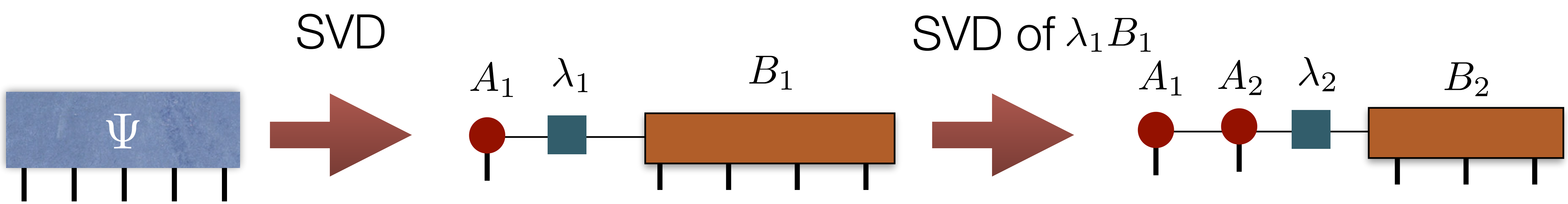
$$|\Psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots$$

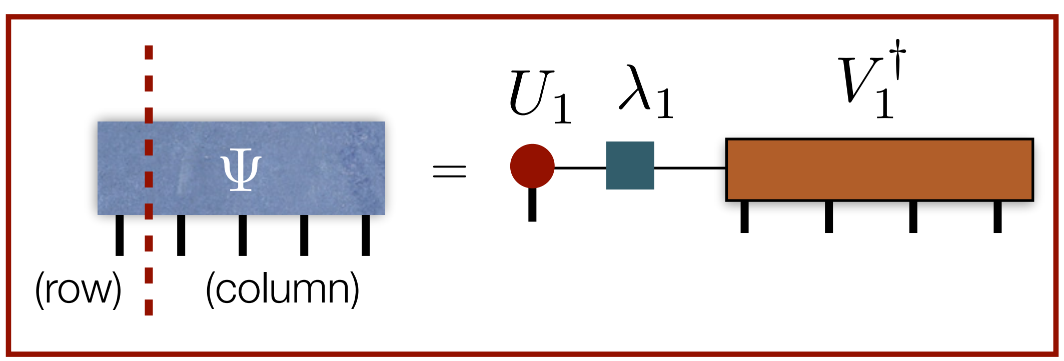
$$\Psi_{i_1 i_2 \dots i_N} = \phi_1[i_1] \phi_2[i_2] \cdots \phi_N[i_N]$$

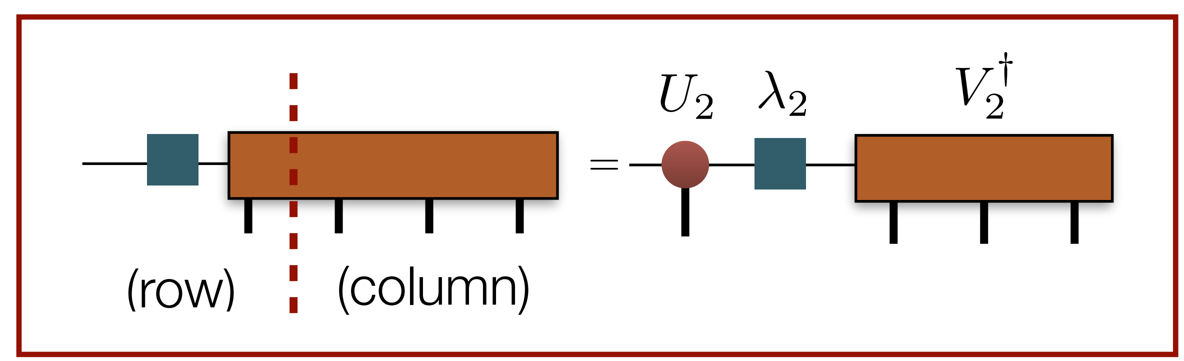
$$\phi_n[i] \equiv \langle i | \phi_i \rangle$$

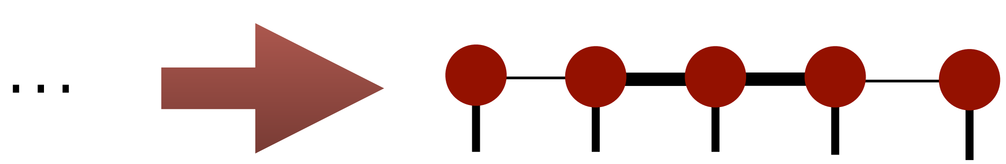
Matrix product state without approximation

General wave function (or vector) can be represented by MPS exactly through successive Schmidt decompositions







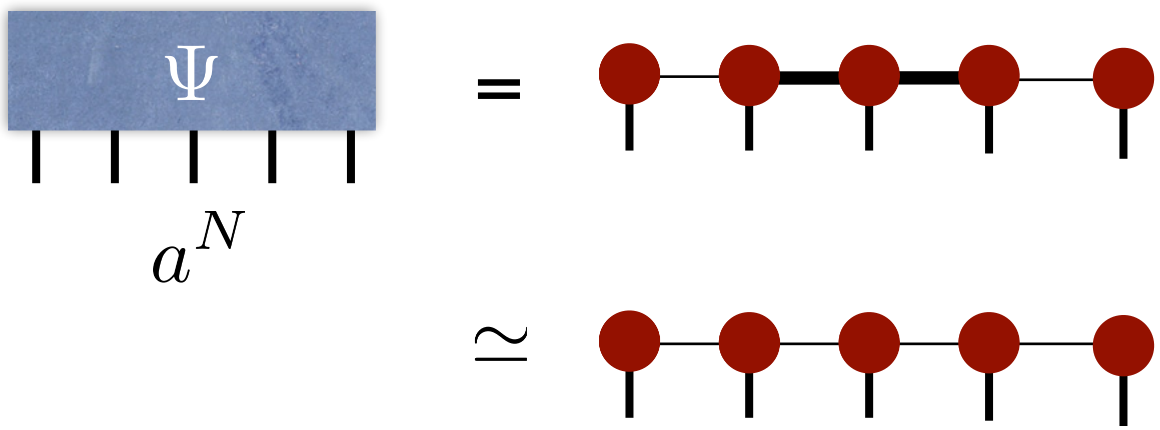


In this construction, the sizes of matrices depend on the position.

$\boxed{\text{Maximum bond dimension} = a^{N/2}}$

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

Matrix product state: Low rank approximation



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

a^N

Constant bond dimension = χ

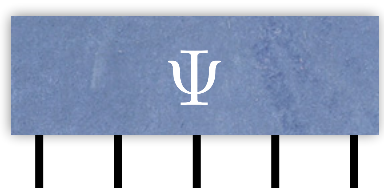
$\propto Na\chi^2$

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

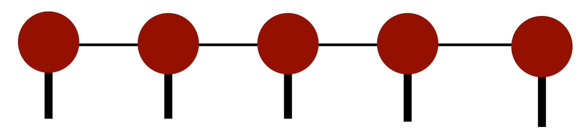
MPS is good for gapped 1d systems.

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

Upper bound of Entanglement entropy

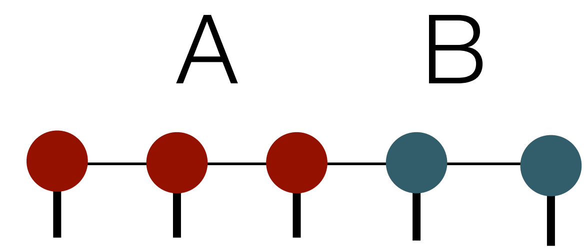


$\simeq$

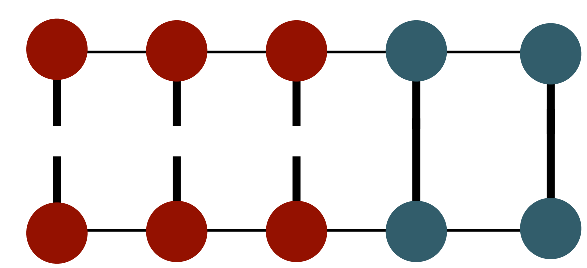


$\equiv |\tilde{\Psi}\rangle$:MPS with χ

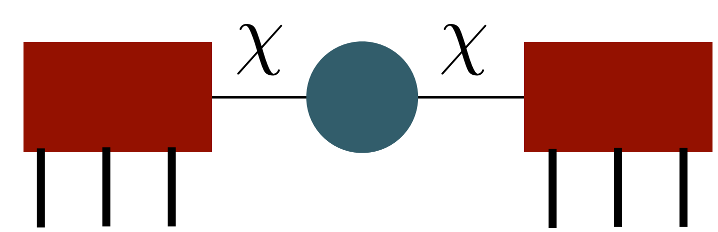
Reduced density matrix of region A:



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



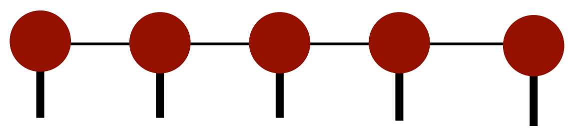
★ Structure of ρ_A:



$$\boxed{\begin{array}{l} \mathrm{rank}\ \rho_A \leq \chi \\ S_A = -\mathrm{Tr}\ \rho_A \log \rho_A \leq \log \chi \end{array}}$$

Required bond dimension in MPS representation

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



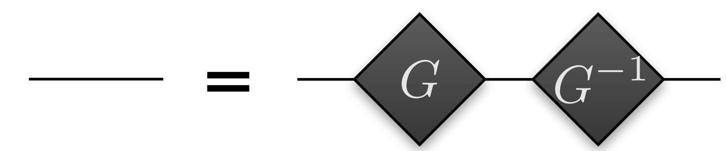
The upper bound is independent of the "length".

length of MPS ⇔ size of the problem

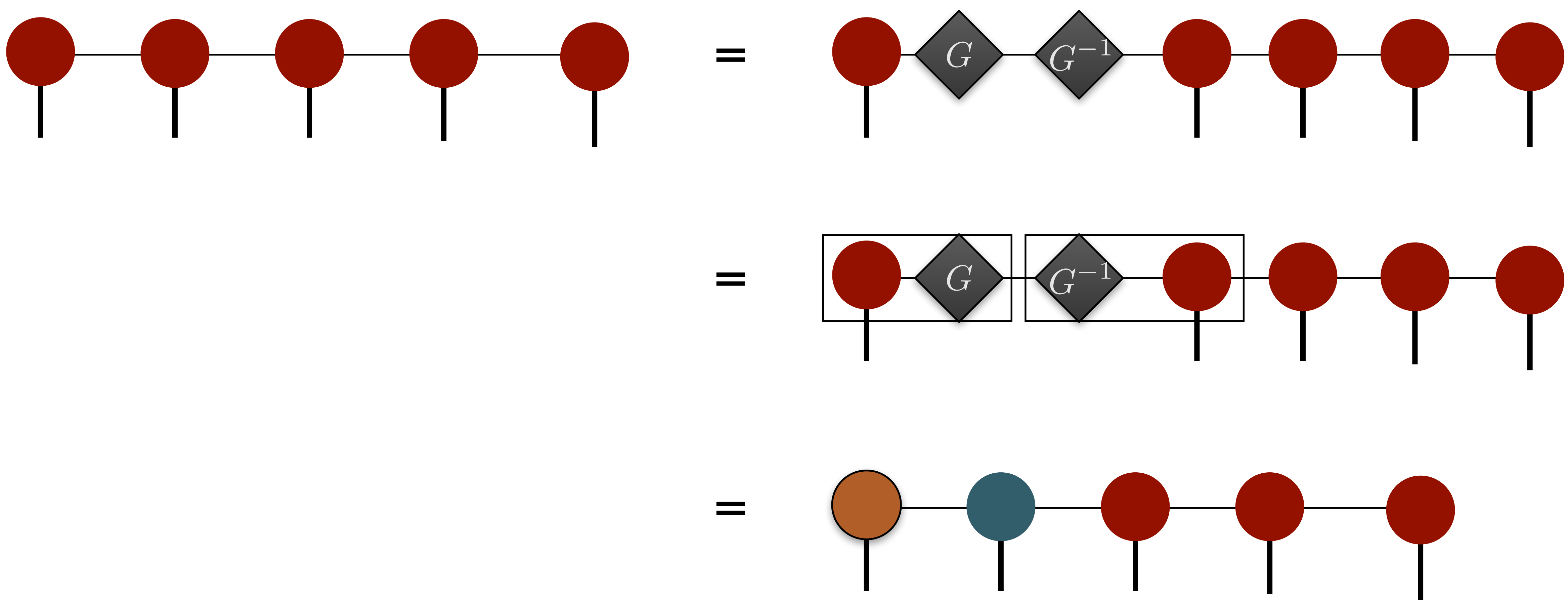
N $\qquad\qquad$ a^N

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

Gauge redundancy of MPS

MPS is not unique: gauge degree of freedom $I = GG^{-1}$ 

We can insert a pair of matrices GG^{-1} to MPS

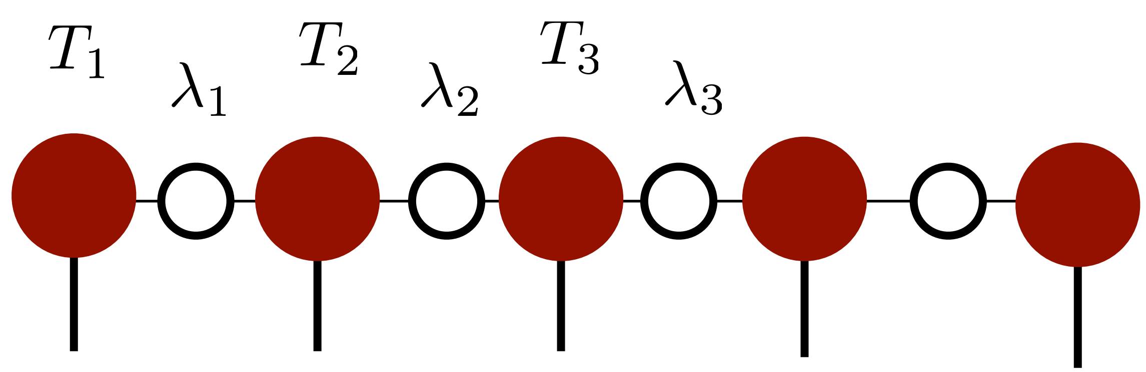


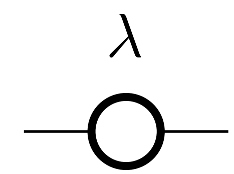
Gauge fix: Canonical form of MPS

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

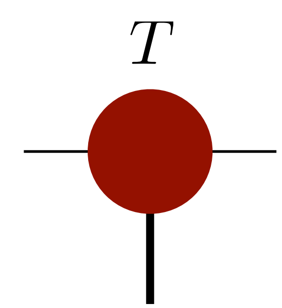
Canonical form of MPS: (Vidal canonical form)

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



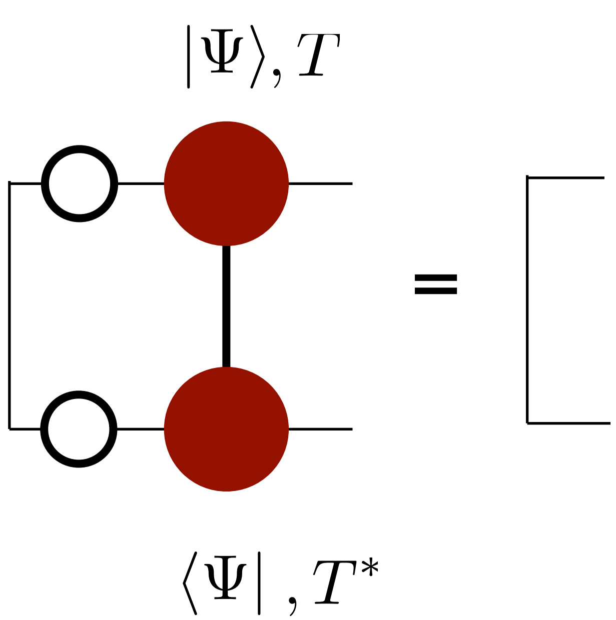


:Diagonal matrix corresponding to Schmidt coefficient

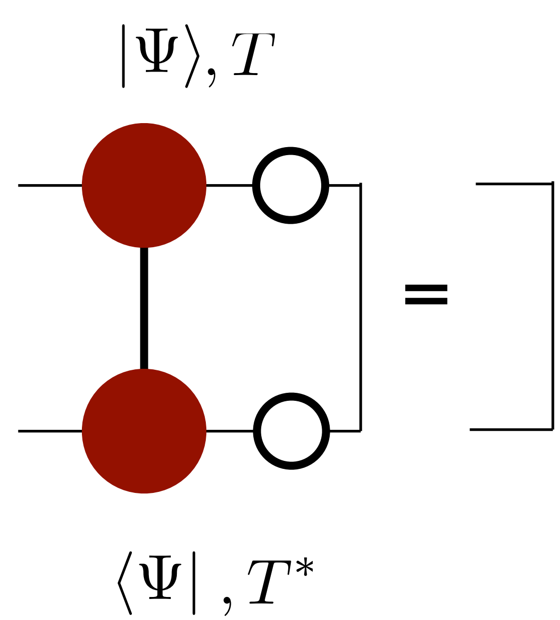


:Virtual indices corresponding to Schmidt basis

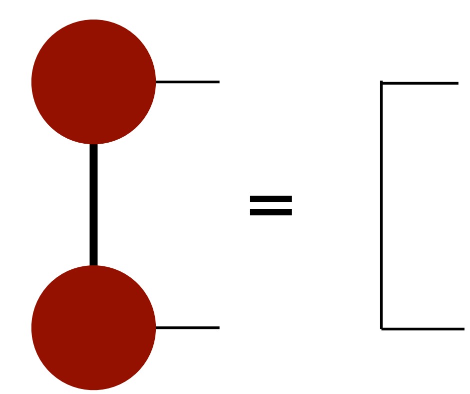
Left canonical condition:



Right canonical condition:



(Boundary)

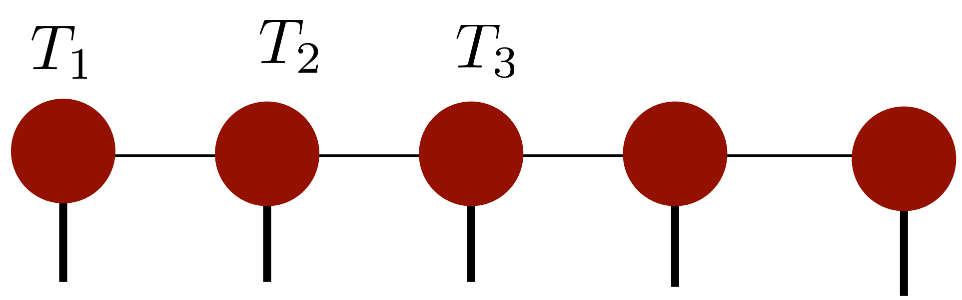


Canonical forms: Left and Right canonical forms

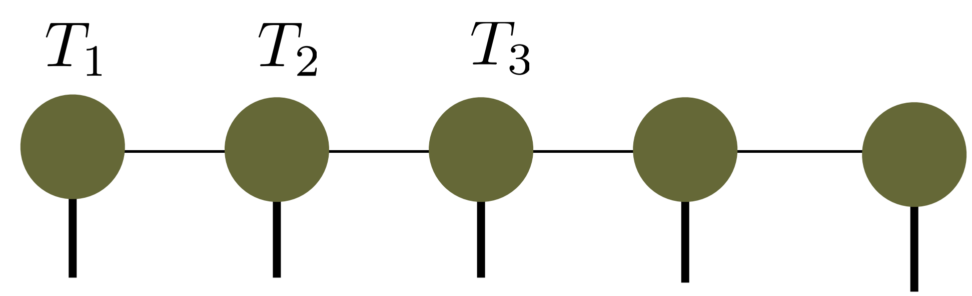
Ref. U. Schollwöck, Annals. of Physics **326**, 96 (2011)

Other "canonical" forms of MPS

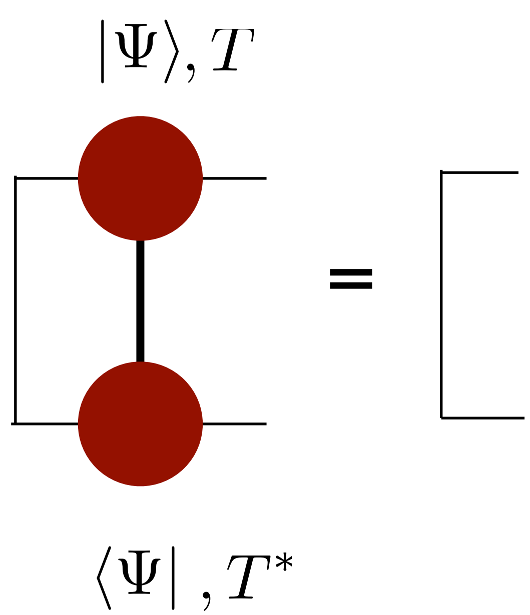
Left canonical form:

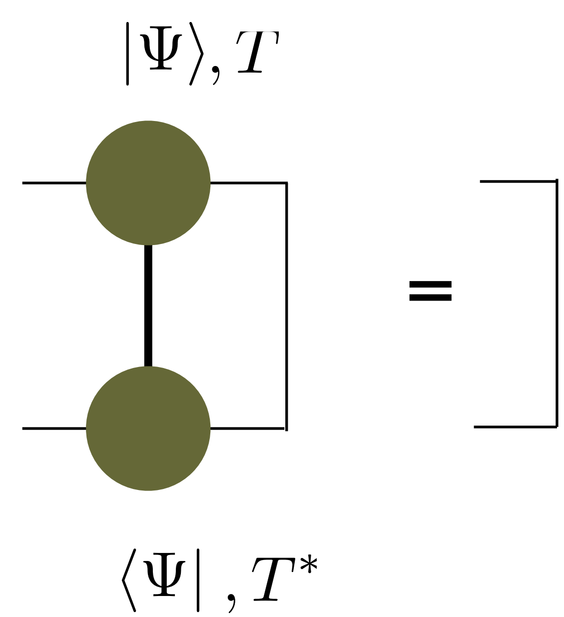


Right canonical form:



Satisfies (at least) left or canonical condition:

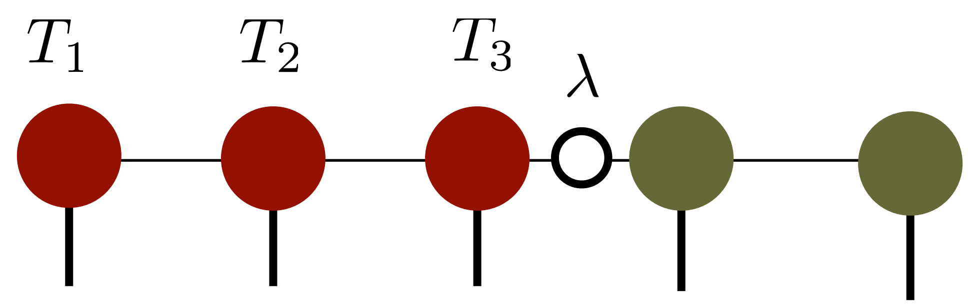




Canonical forms: Mixed canonical forms

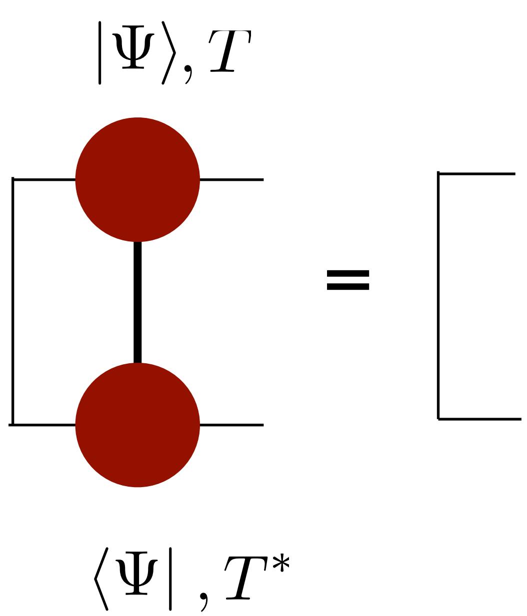
Ref. U. Schollwöck, Annals. of Physics **326**, 96 (2011)

Mixed canonical form:

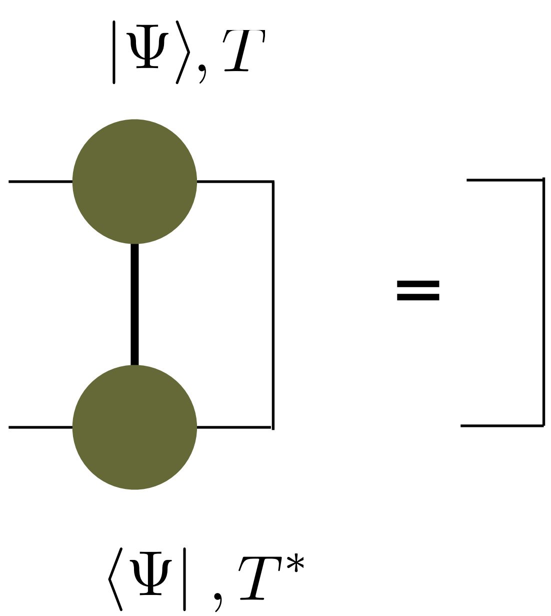


λ is identical with the Schmidt coefficient.

Left canonical condition:



Right canonical condition:

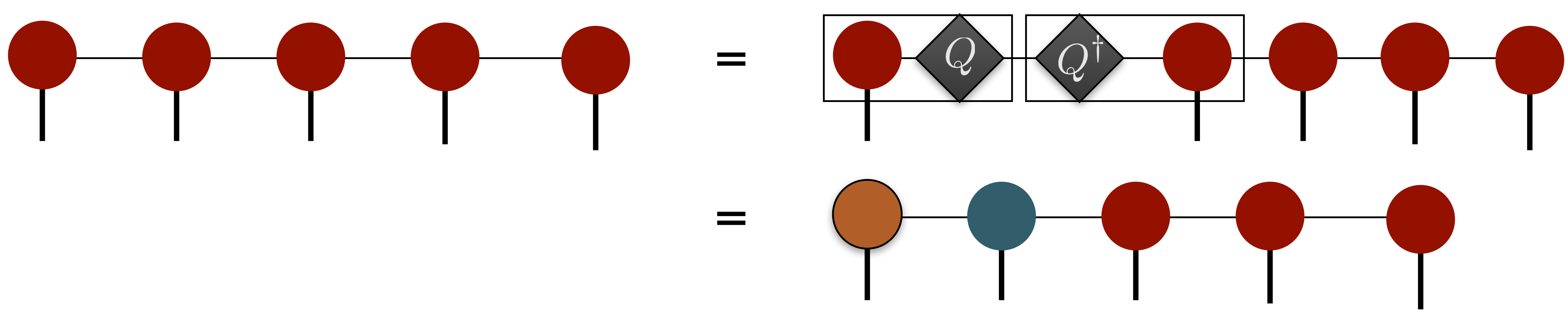


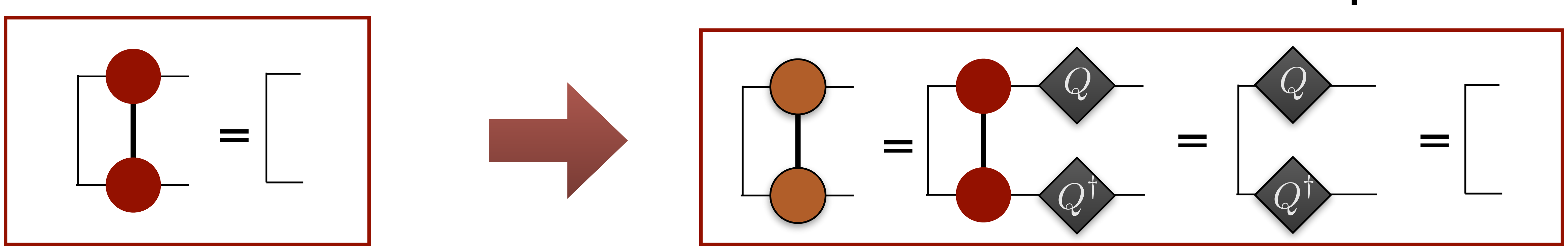
Canonical forms: Note

- Vidal canonical form is unique, up to trivial unitary transformation to virtual indices which keep the same diagonal matrix structure (Schmidt coefficients).

- Left, right and mixed canonical form is "not unique". Under general unitary transformation to virtual indices, it remains to satisfy the canonical condition

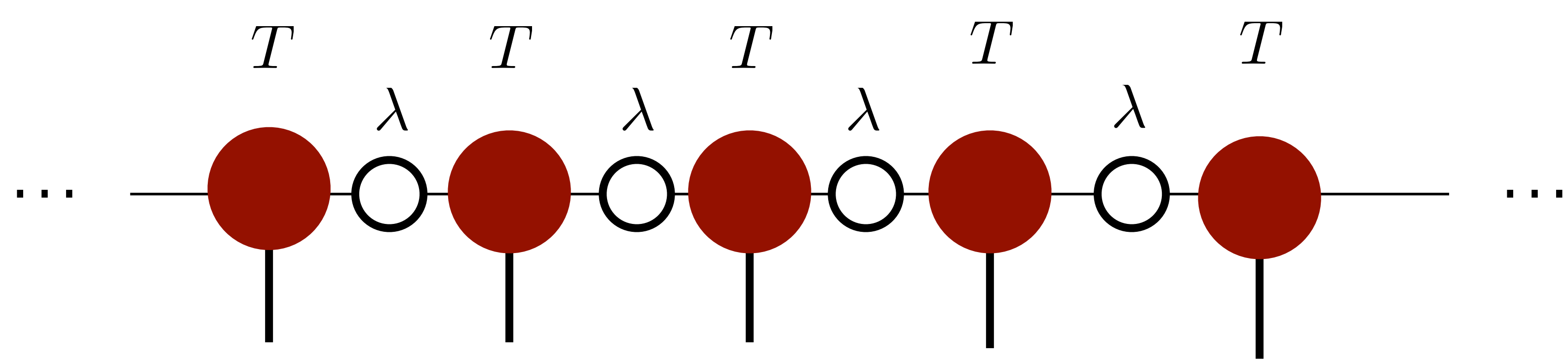
$$QQ^\dagger = Q^\dagger Q = I$$





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 and λ infinitely.

Translationally invariant system ➡ T and λ are independent of positions!

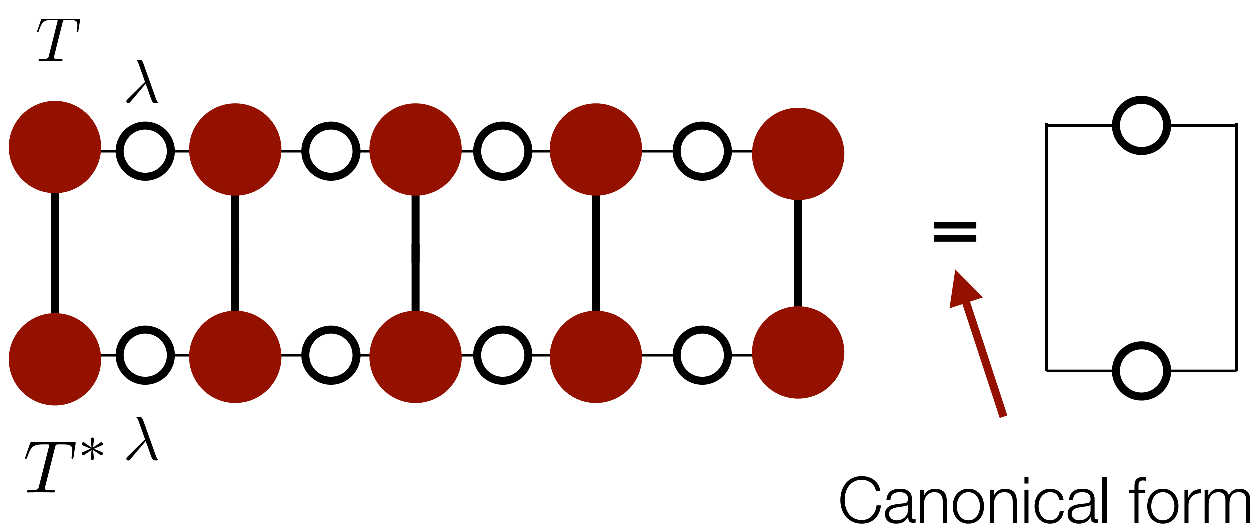
* Infinite MPS can be accurate when the EE satisfies the 1d area low (S~O(1)).

If the EE increases as increase the system size,
we may need infinitely large χ for infinite system.

(In practice, we can obtain a reasonable approximation with finite χ.)

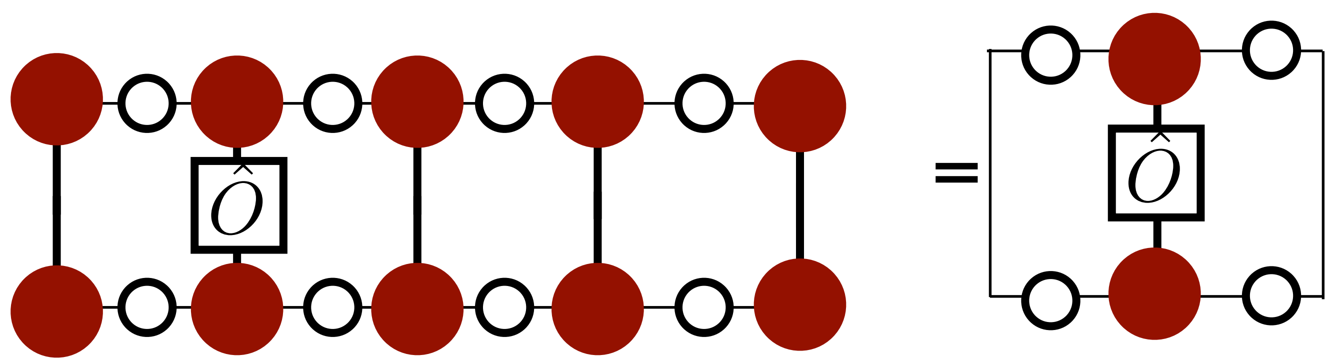
Calculation of expectation value

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



$= \sum_i \lambda_i^2 = 1$

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



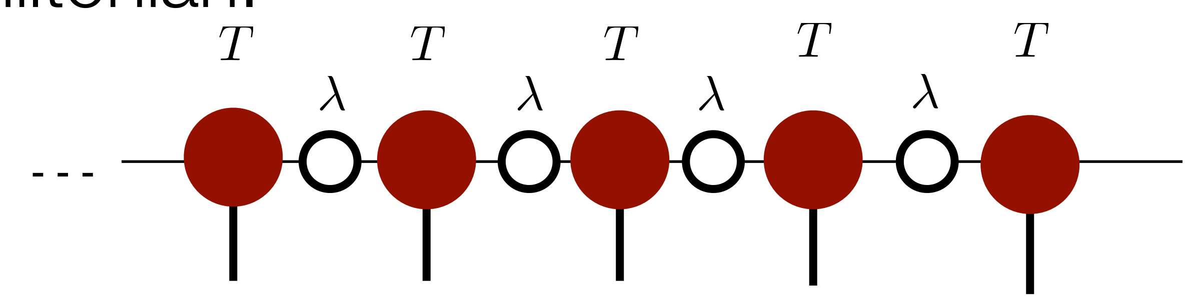
For iMPS, if it is in the (Vidal) canonical form,
the final graph is identical to the above finite system.

Example of iMPS: AKLT state

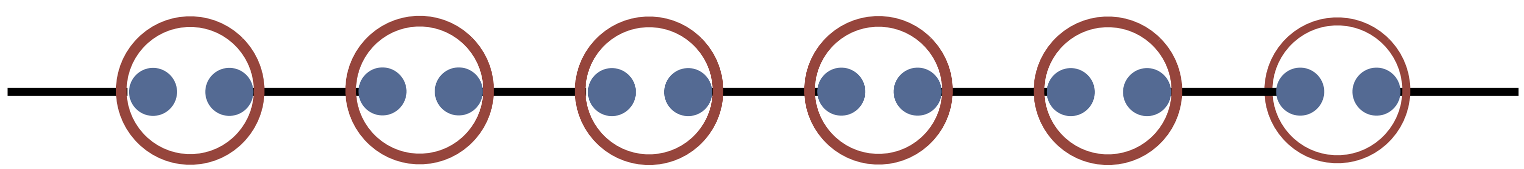
S=1 Affleck-Kennedy-Lieb-Tasaki (AKLT) Hamiltonian:

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \frac{J}{3} \sum_{\langle i,j \rangle} \left(\vec{S}_i \cdot \vec{S}_j \right)^2$$

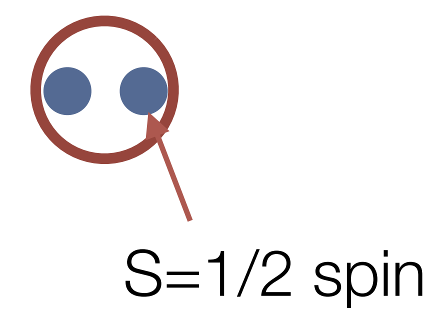
$$(J > 0)$$



The ground state of AKLT model:



S=1 spin:



χ=2 iMPS: (U. Schollwock, Annals. of Physics **326**, 96 (2011))

Spin singlet

$$T[S_z = 1] = \sqrt{\frac{4}{3}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$T[S_z = 0] = \sqrt{\frac{2}{3}} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \lambda = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$T[S_z = -1] = \sqrt{\frac{4}{3}} \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$$

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 *chi_max* and see energies

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

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

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.

Next week

1st: Huge data in modern physics

2nd: Information compression in modern physics

3rd: Review of linear algebra

4th: Singular value decomposition and low rank approximation

5th: Basics of sparse modeling

6th: Basics of Krylov subspace methods

7th: Information compression in materials science

8th: Accelerating data analysis: Application of sparse modeling

9th: Data compression: Application of Krylov subspace method

10th: Entanglement of information and matrix product states

11th: Application of MPS to eigenvalue problems (and machine learning)

12th: General tensor network representations

13th: Information compression by tensor network renormalization