Matrix product state, entanglement, and applications

Chia-Min Chung

National Sun Yat-sen University

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2022 summer school for physics and tensor-network methods in correlated systems

中山大學
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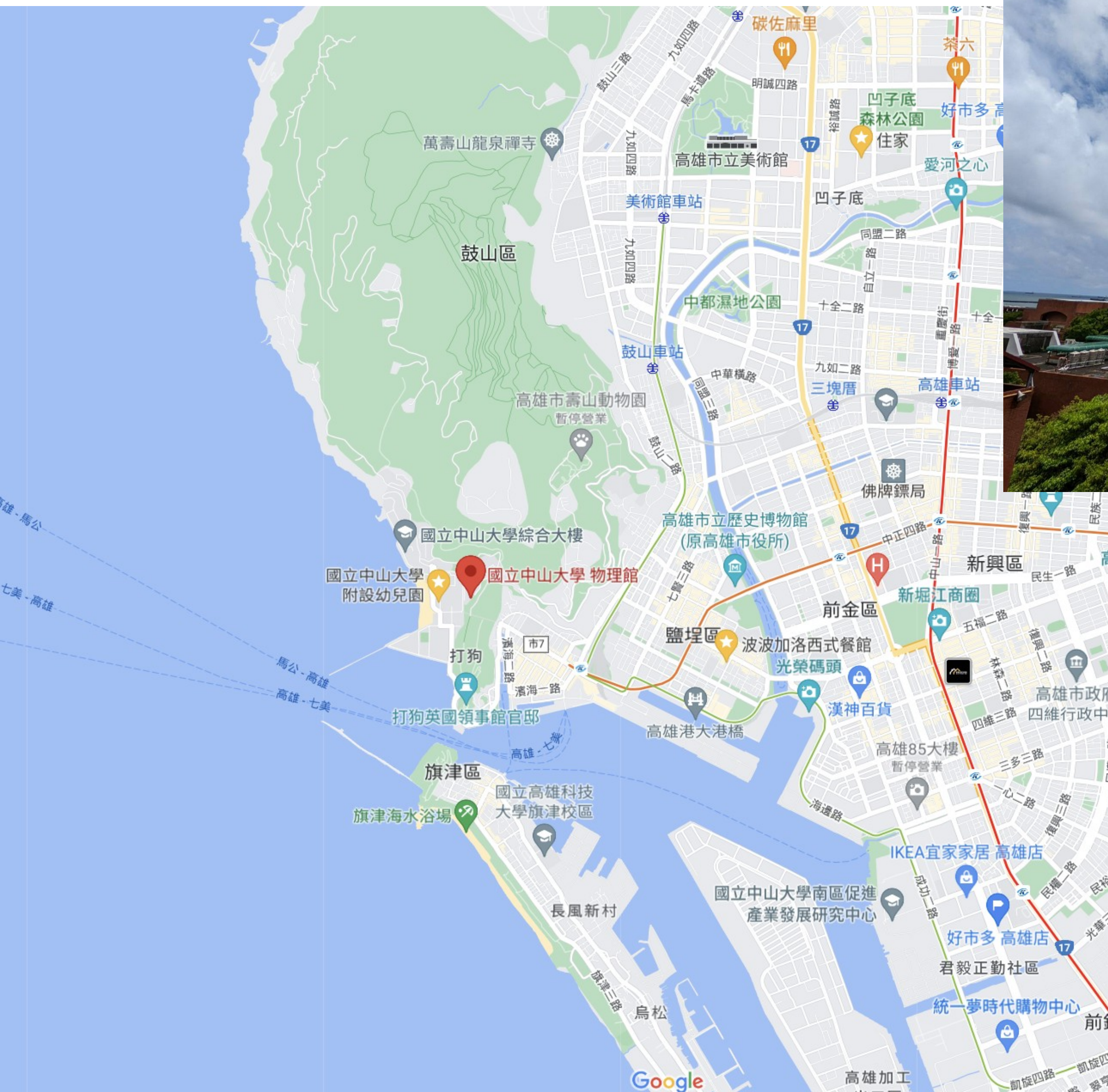


What is / why tensor network?

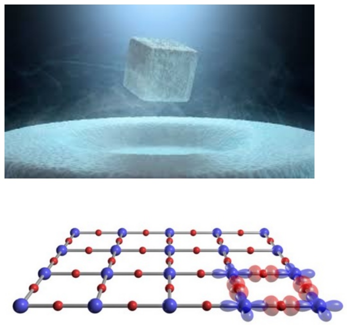
– a good approximation for a **many-body state**

What is a many-body state?

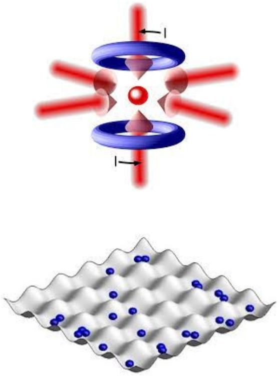
Ex: $\downarrow \uparrow \uparrow \uparrow \downarrow \downarrow$

$$
\begin{aligned}
\Psi &= \sum_{\{s_i\}} \psi_{s_1,s_2,\cdots,s_N} |s_1, s_2, \cdots, s_N\rangle \\
&= \psi_{0,0,0,\cdots} |\uparrow\uparrow\uparrow\cdots\rangle \\
&+ \psi_{1,0,0,\cdots} |\downarrow\uparrow\uparrow\cdots\rangle \\
&+ \psi_{0,1,0,\cdots} |\uparrow\downarrow\uparrow\cdots\rangle \\
&+ \cdots
\end{aligned}
$$

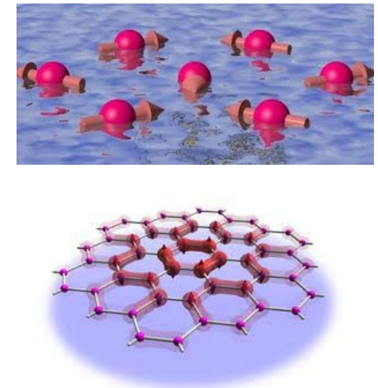
exponentially many...



strongly correlated electrons

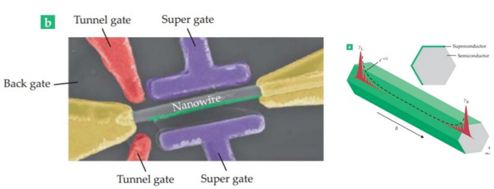


cold atoms

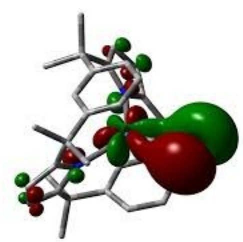


frustrated spins

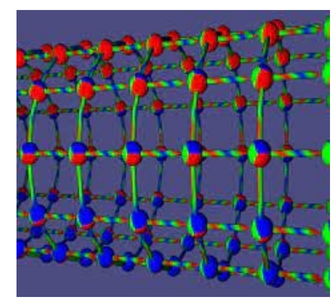
$$\Psi = \sum_{\{s_i\}} \psi_{s_1,s_2,\cdots,s_N} |s_1, s_2, \cdots, s_N\rangle$$



quantum devices



quantum chemistry

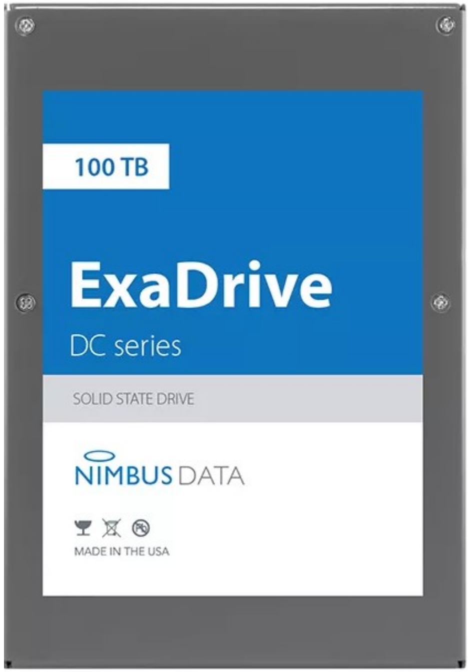


lattice gauge theory

Why is it important?

$$\Psi = \sum_{\{s_i\}} \psi_{s_1, s_2, \cdots, s_N} |s_1, s_2, \cdots, s_N\rangle$$

# of spins	Configurations	# of coef	Storage
1	$\uparrow, \downarrow$	2	16 bytes
2	$\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow$	4	32 bytes
10		1024	≈ 8 KB
30		≈ 10^8	≈ 130 MB
50		≈ 10^{14}	≈ 140 TB
100		≈ 10^{29}	≈ 10^{14} × 100 TB



Why is it important?

$$\Psi = \sum_{\{s_i\}} \psi_{s_1,s_2,\cdots,s_N} |s_1, s_2, \cdots, s_N\rangle$$

# of spins	Configurations		
1	$\uparrow, \downarrow$		
2	$\uparrow\uparrow, \uparrow\downarrow,$		
10			
30			
50			
100		≈ 1	TB

Why is it important?

$$\Psi = \sum_{\{s_i\}} \psi_{s_1,s_2,\cdots,s_N} |s_1, s_2, \cdots, s_N\rangle$$

# of spins	Configurations		
1	$\uparrow, \downarrow$		
2			
30			
50			
100		$\approx$	TB

We need a good approximation!

Many-body state as a tensor

Scalar C $$4$$

Vector V_i $$\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Matrix M_{ij} $$\begin{bmatrix} 2 & 1 \\ -1 & 4 \end{bmatrix}$$

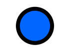
Tensor $T_{i,j,k,l}$

Many body state $\psi_{s_1,s_2,\cdots,s_N}$

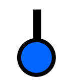
Many-body state as a tensor

Graphic notation

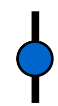
Scalar C 4



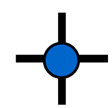
Vector V_i $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$



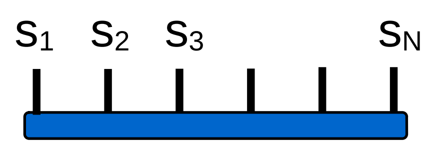
Matrix M_{ij} $\begin{bmatrix} 2 & 1 \\ -1 & 4 \end{bmatrix}$



Tensor $T_{i,j,k,l}$



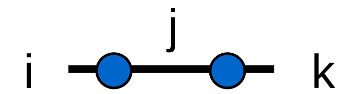
Many body state $\psi_{s_1,s_2,\cdots,s_N}$



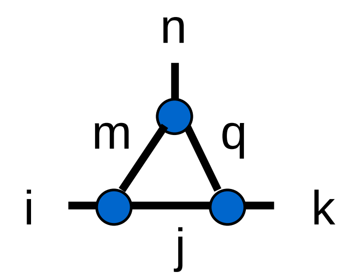
Graphical notation

Tensor contraction

$$M_{ik} = \sum_j A_{ij} B_{jk}$$



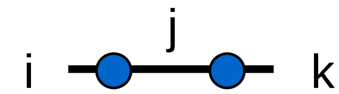
$$T_{ikn} = \sum_{jqm} A_{ijm} B_{jkq} C_{mqn}$$



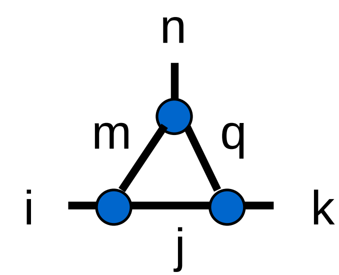
Graphical notation

Tensor contraction

$$M_{ik} = \sum_j A_{ij} B_{jk}$$



$$T_{ikn} = \sum_{jqm} A_{ijm} B_{jkq} C_{mqn}$$

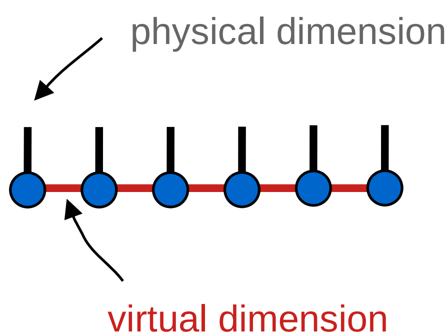


Matrix product state (MPS)

$\psi_{s_1, s_2, \cdots, s_N}$

Many body state

$\approx$



Matrix product state

Singular value decomposition (SVD)

Eigenvalue value decomposition

$$\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix} = \begin{bmatrix} & & \\ & U & \\ & & \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \end{bmatrix} \begin{bmatrix} & & \\ & U^\dagger & \\ & & \end{bmatrix}$$

$$U^\dagger U = U U^\dagger = 1$$

Singular value decomposition

$$\begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & A & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} \cdot & \cdot \\ \cdot & U \\ \cdot & \cdot \\ \cdot & \cdot \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & V^\dagger & \cdot & \cdot \end{bmatrix}$$

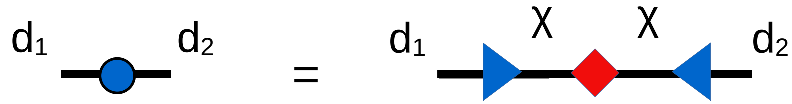
real & positive

$$U^\dagger U = 1, \quad V^\dagger V = 1$$

$$U U^\dagger \neq 1, \quad V V^\dagger \neq 1, \quad U^\dagger V \neq 1$$

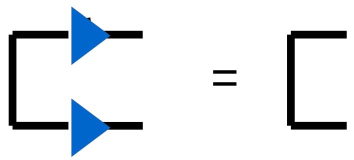
Singular value decomposition (SVD)

$$A = U \Sigma V^\dagger$$

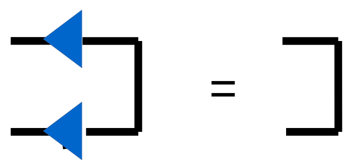


$\chi \leq \min(d_1, d_2)$

$$U^\dagger U = 1$$



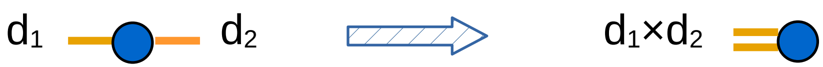
$$V^\dagger V = 1$$



Reshape between tensor and matrix

(just relabel the indices)

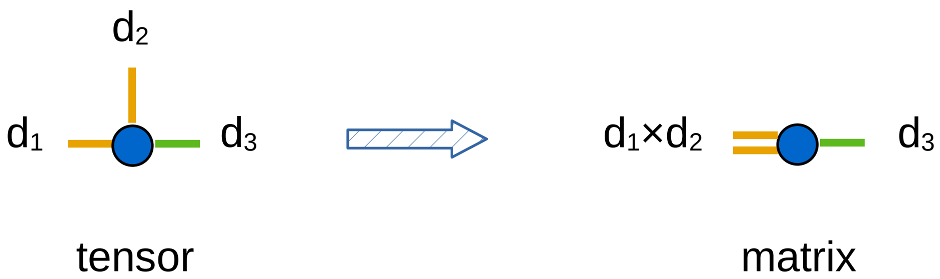
$$
\begin{array}{cc}
d_1 & \begin{bmatrix} a_{00} & a_{01} \\ a_{11} & a_{10} \end{bmatrix} \\
 & d_2
\end{array}
\Rightarrow
\begin{array}{c}
00 \to 0 \\
01 \to 1 \\
10 \to 2 \\
11 \to 3
\end{array}
\Rightarrow
\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} \; d_1 \times d_2
$$



matrix

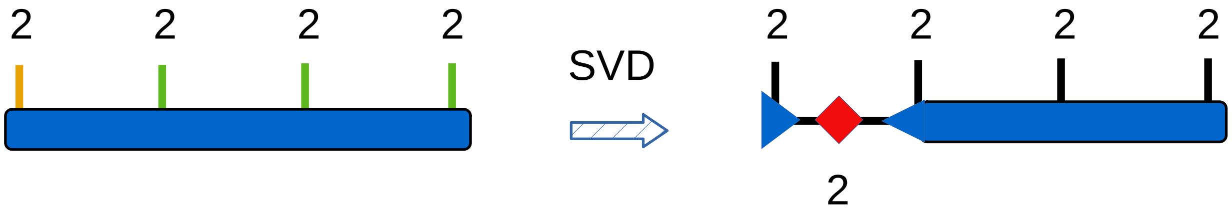
vector

Reshape between tensor and matrix

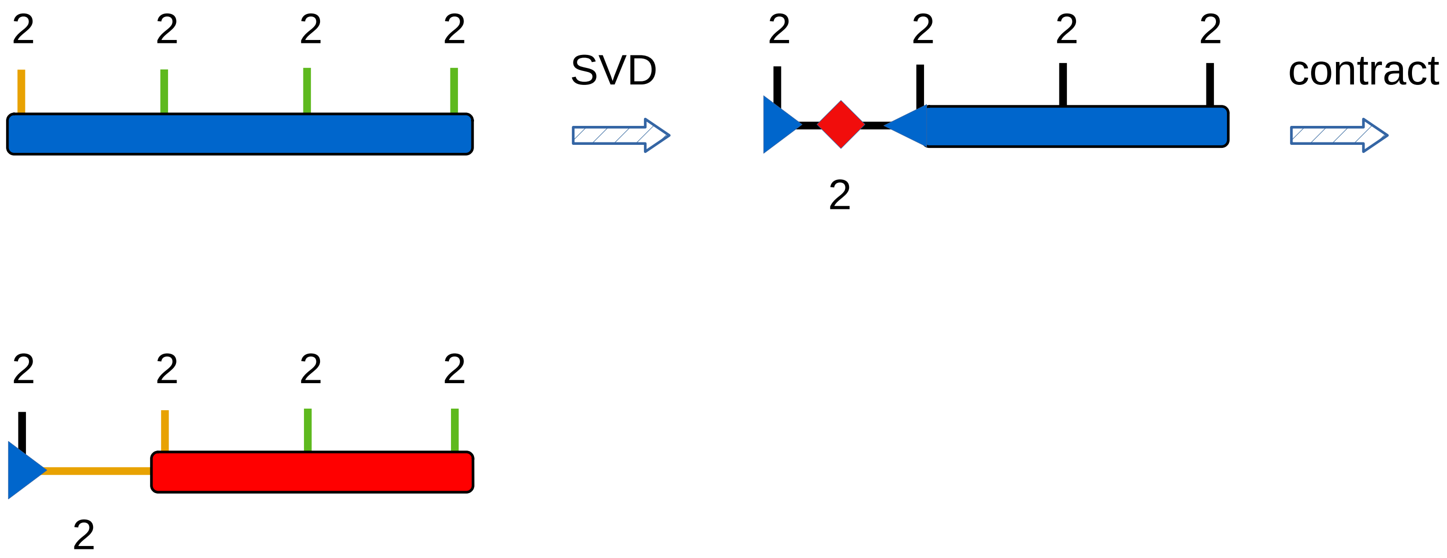


$\chi \leq \min(d_1 d_2, d_3)$

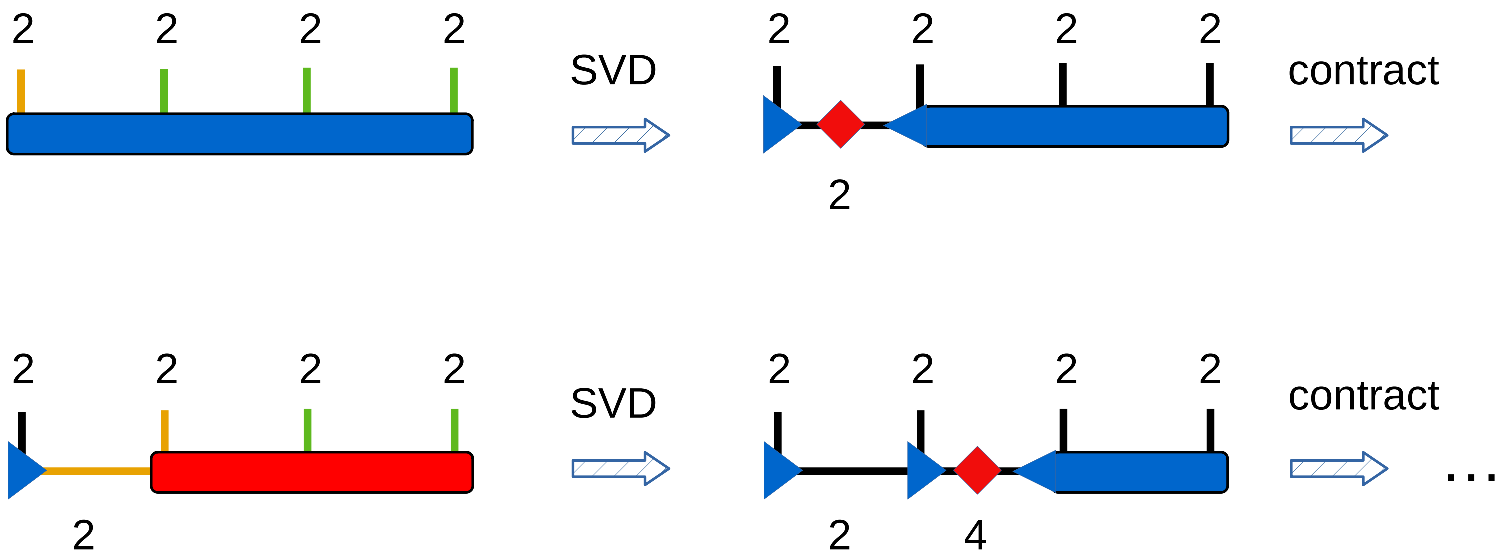
Transform a many-body state to an MPS



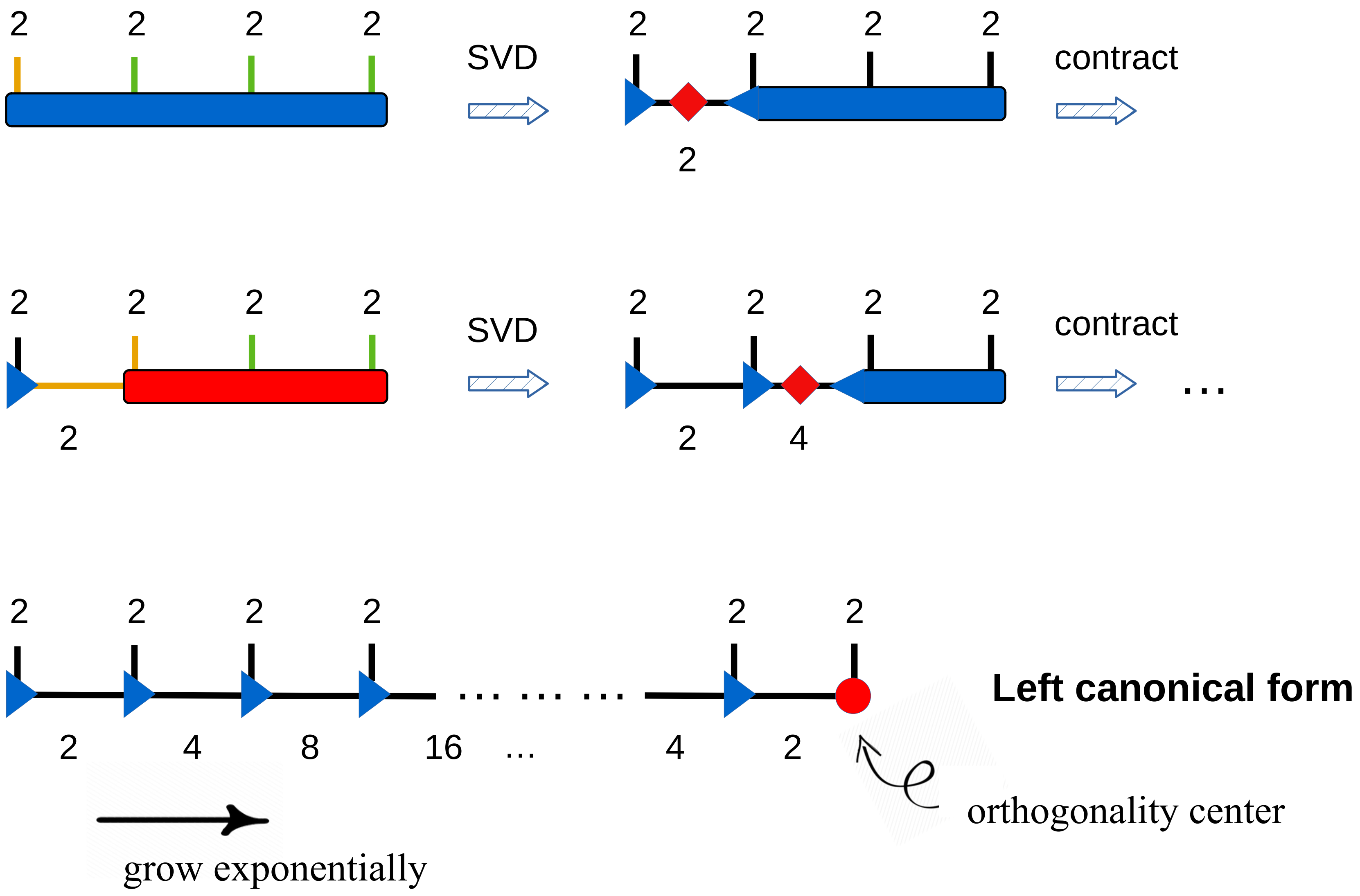
Transform a many-body state to an MPS



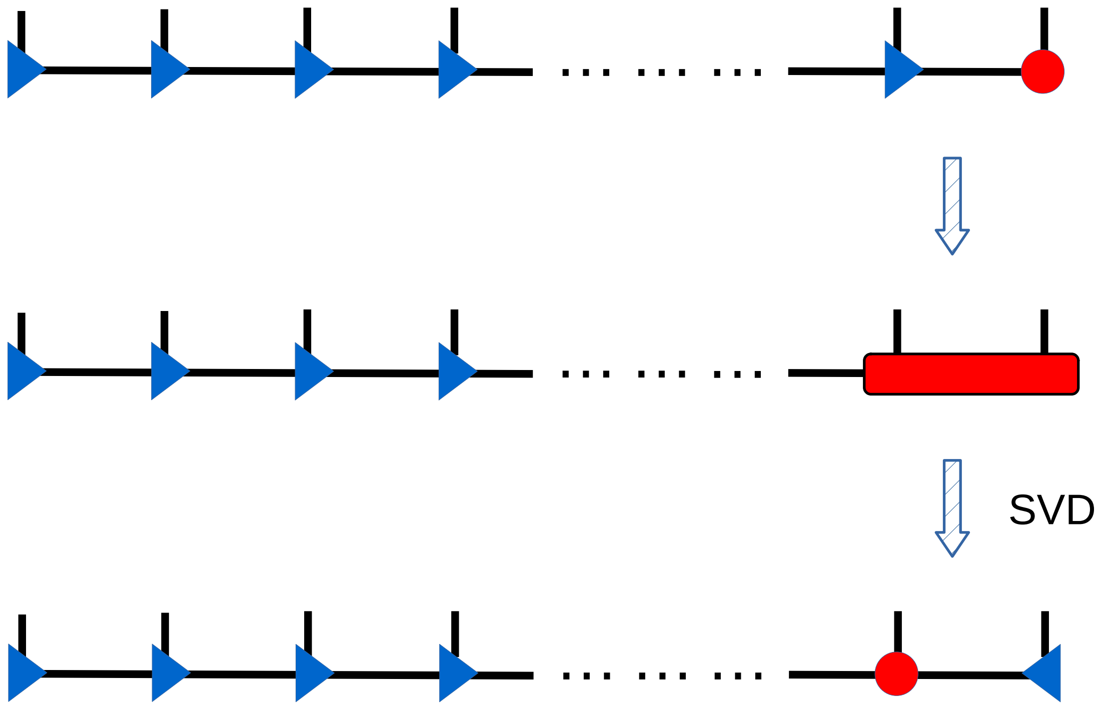
Transform a many-body state to an MPS



Transform a many-body state to an MPS

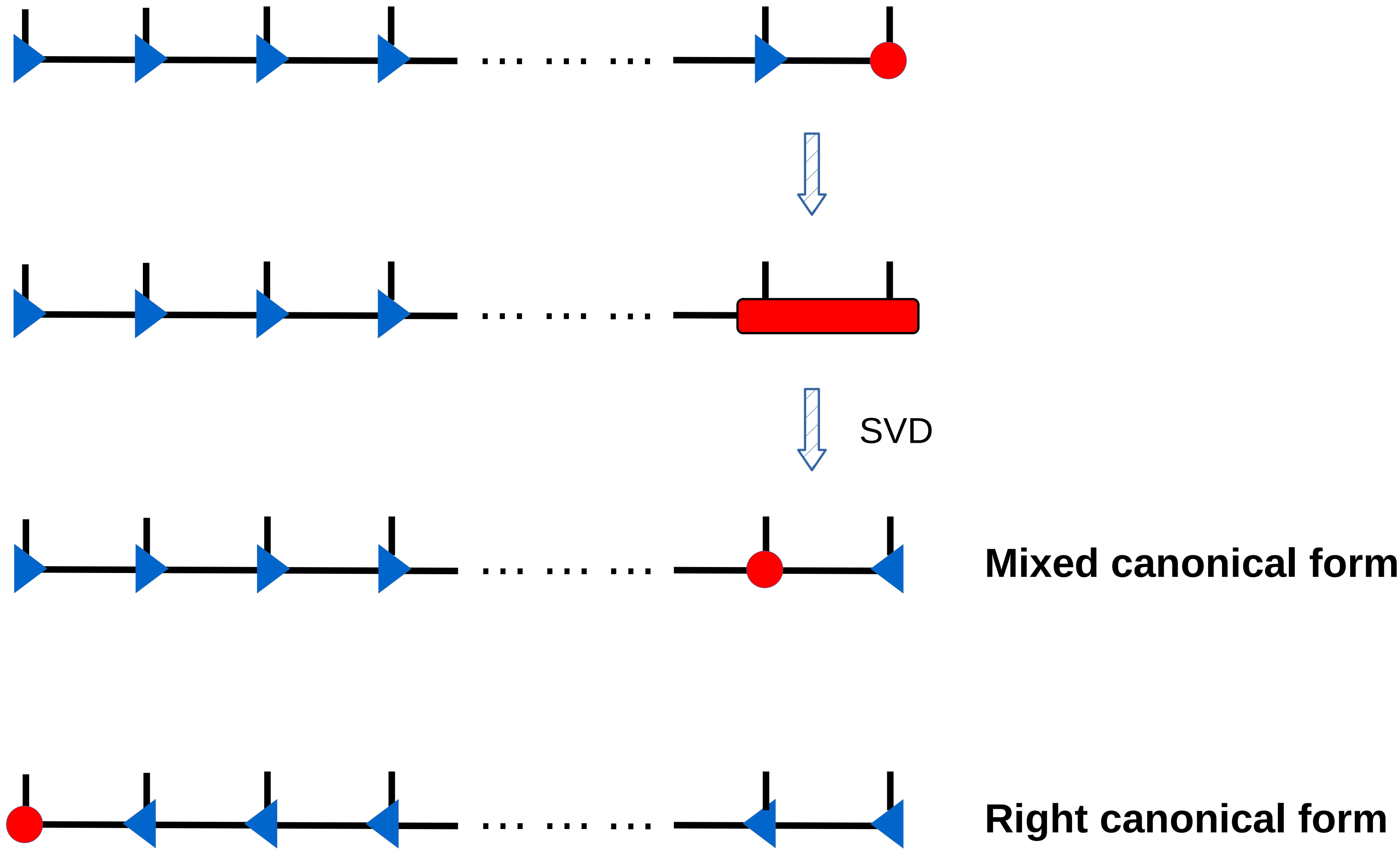


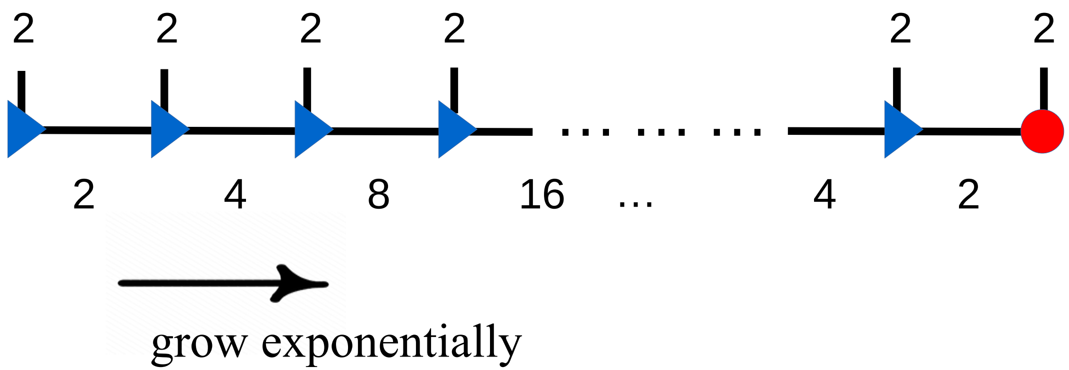
Move the orthogonality center



Mixed canonical form

Move the orthogonality center

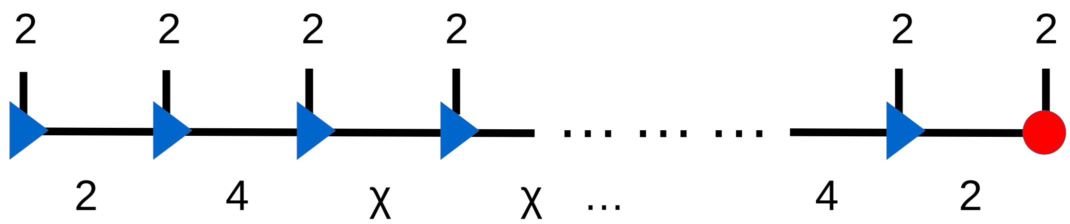




Not so useful

Restrict the bond (or virtual) dimension

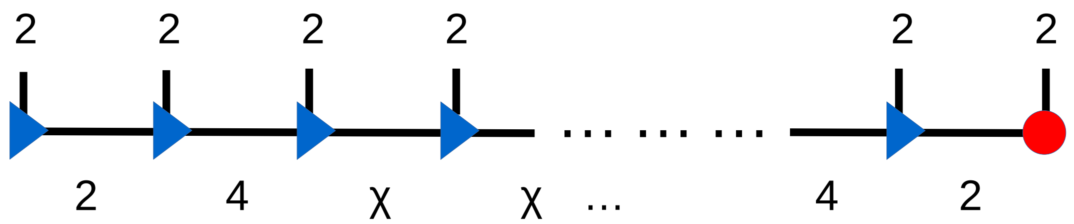
In practice, restrict the maximal virtual dimension to χ



What dose it mean physically ...

Restrict the bond (or virtual) dimension

In practice, restrict the maximal virtual dimension to χ

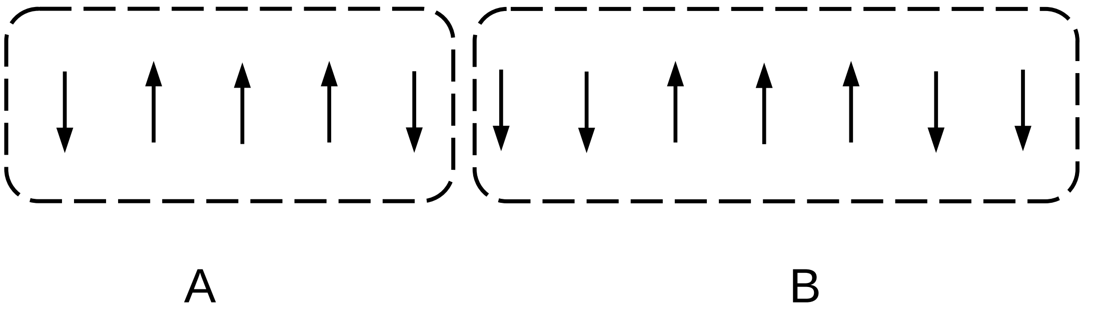


What dose it mean physically ...

Restrict the entanglement !

(Why …?)

Entanglement between two subsystems



Reduced density matrix

$$\rho_A = \mathrm{Tr}_B\,(\rho) = \mathrm{Tr}_B\,(|\psi\rangle\langle\psi|) = \sum_{\phi} \langle\phi|\psi\rangle\langle\psi|\phi\rangle$$

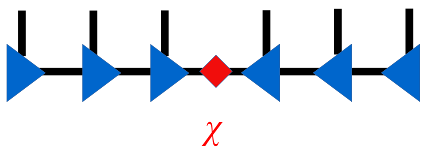
Entanglement entropy

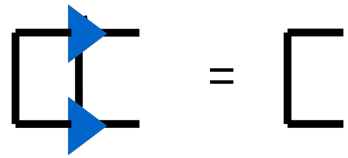
$$S_A = -\mathrm{Tr}(\rho_A \log \rho_A) \leq \log D$$

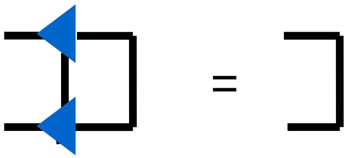
Ex: $\uparrow\downarrow$ $\qquad S_A = 0$

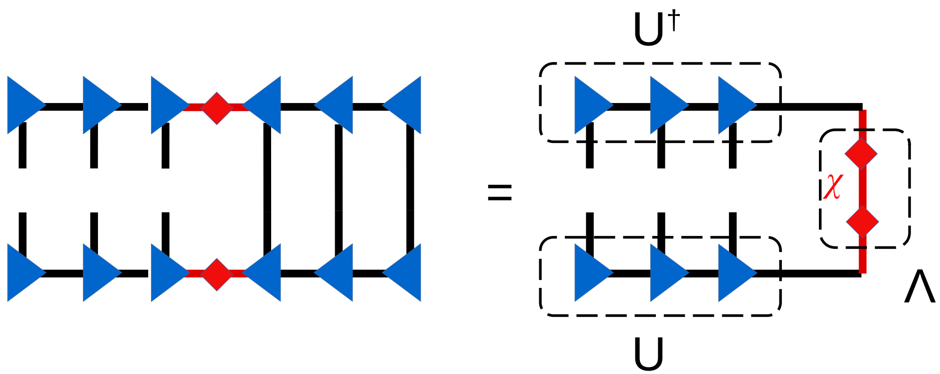
$\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) \qquad S_A = \log 2$

Orthogonal form and the reduce density matrix







$\rho_A =$ 

$= U\Lambda U^\dagger$

χ is also the dimension of ρ_{A}

$$S_A = -\mathrm{Tr}(\rho_A \log \rho_A) \le \log \chi$$

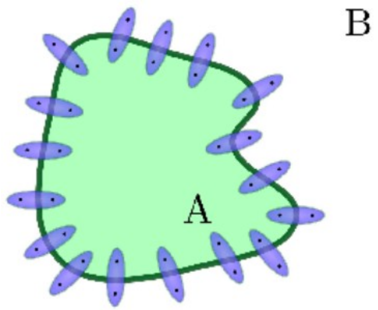
Why are the low-entanglement states important?

Area law

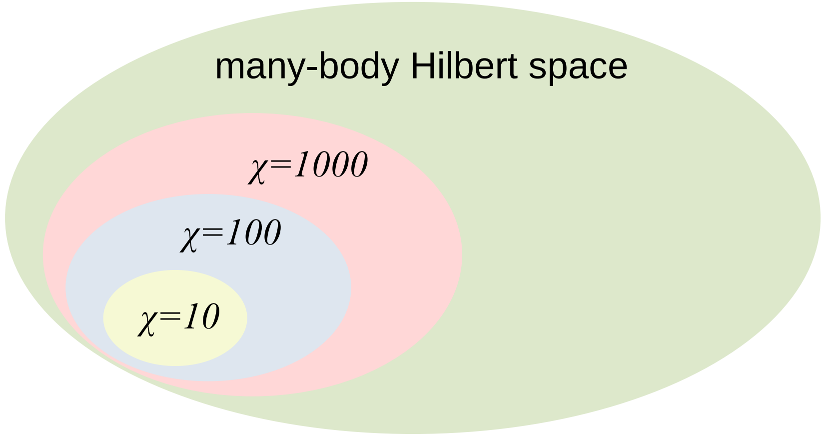
Gapped ground states of local Hamiltonians

$S_A \propto$ boundary

(Due to the local correlation)



MPS obeys 1D area law

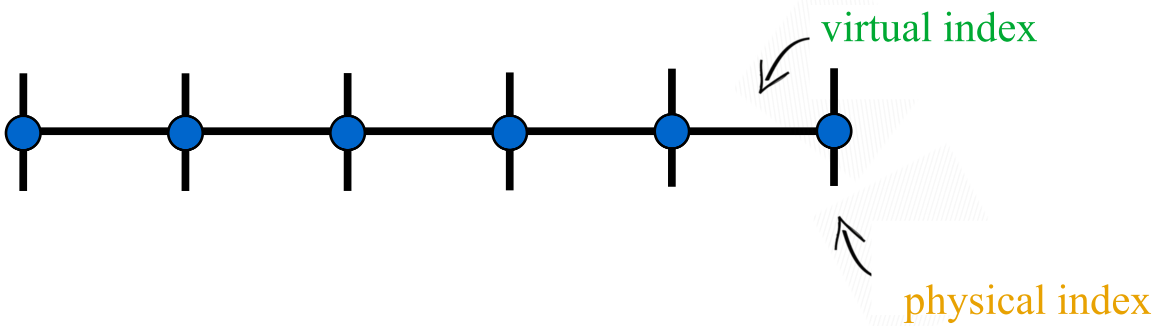


Volume law

In general, $S \propto$ volume

Ex: $\rho \propto e^{-\beta H}$

Matrix product operator (MPO)



Ex: Transverse-field Ising model

$$\hat{H} = -\sum_{i=1}^{N-1} \hat{S}_i^x \hat{S}_{i+1}^x - h_z \sum_{i=1}^{N} \hat{S}_i^z, \qquad \hat{S}^z = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \hat{S}^x = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

physical dimension=2

$$\hat{H} = L_0 M_1 M_2 \cdots M_N R_0$$

$$L_0 = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}, \qquad M_i = \begin{bmatrix} \hat{I}_i & & \\ \hat{S}_i^x & 0 & \\ -h_z \hat{S}_i^z & -\hat{S}_i^x & \hat{I}_i \end{bmatrix}, \qquad R_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

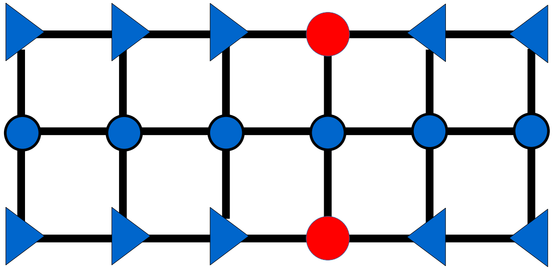
virtual dimension=3

Application:

Density Matrix Renormalization Group (DMRG)

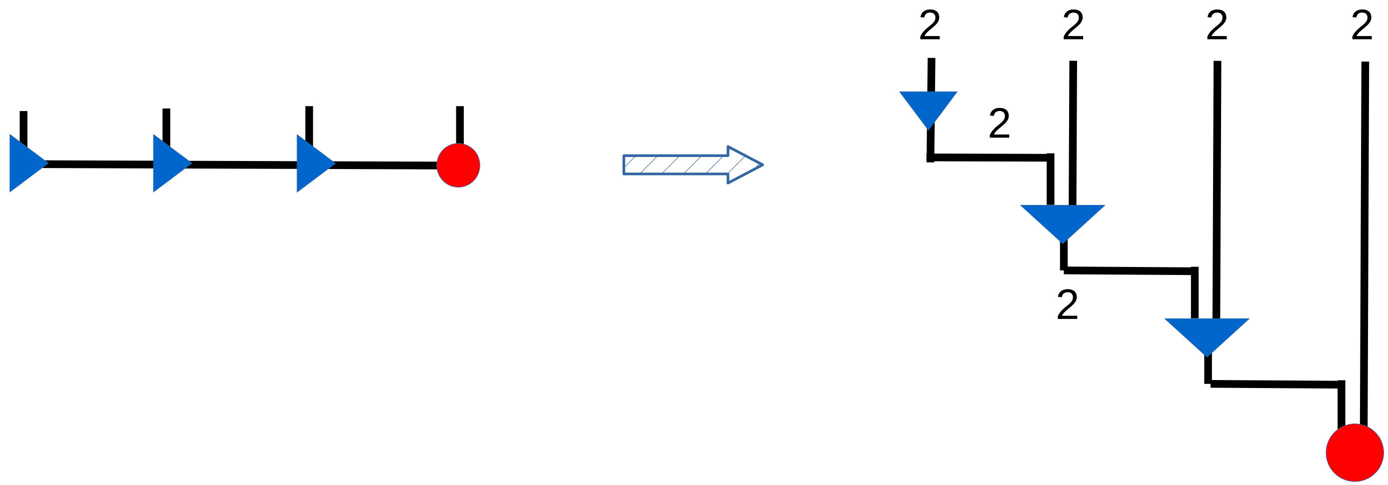
[Steven R. White, PRB (1992)]

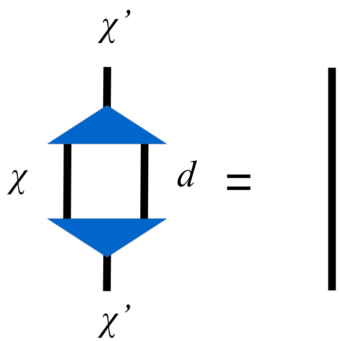
Variationally finding the ground state

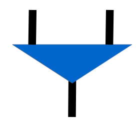
$\langle\psi|H|\psi\rangle =$ 

Optimize the MPS tensors one by one

Physical meaning of the orthogonal form

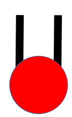




If $\chi' = \chi d$,  is a unitary (square) matrix

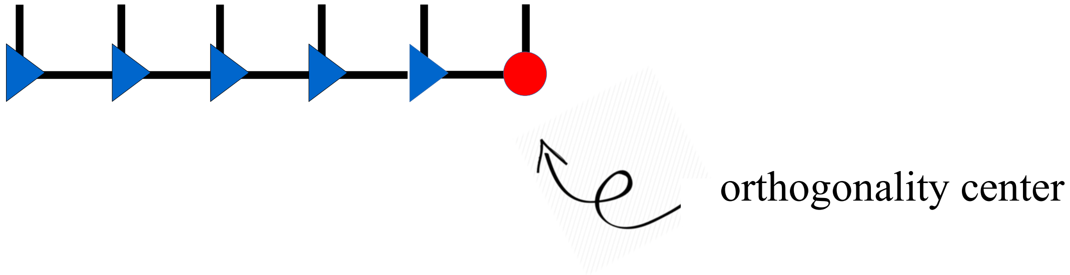
→ Rotation of basis

If $\chi' < \chi d$, ***Rotation*** + ***truncate*** basis

 is a wavefunction of the ***whole*** system in the reduced basis

DMRG algorithm

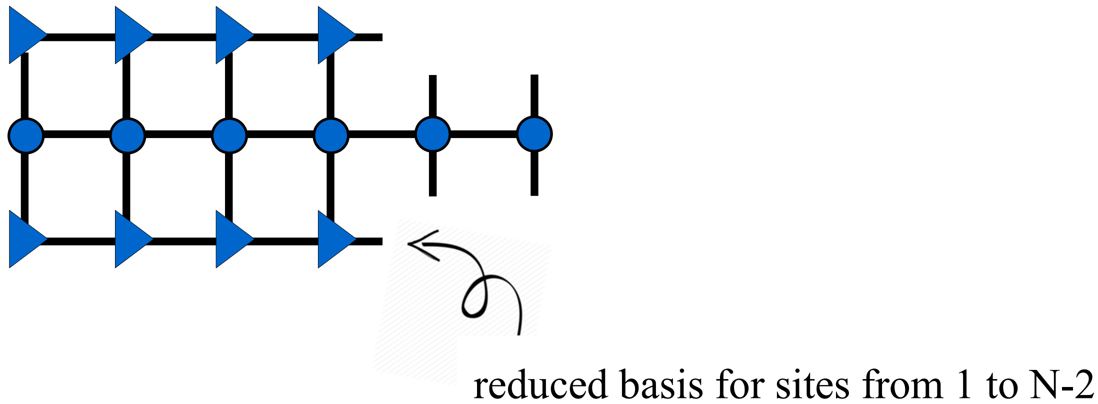
1. Prepare an initial MPS in the left canonical form



DMRG algorithm

2. Define the effective Hamiltonian

$$\hat{H}_{\rm eff} =$$



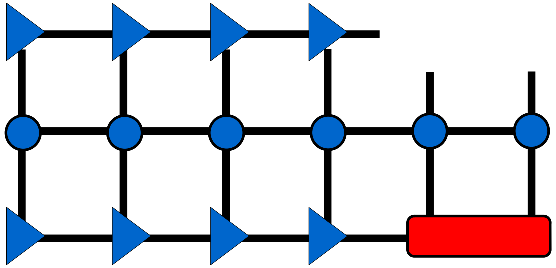
The Hamiltonian of the ***whole*** system

in the reduced Hilbert space

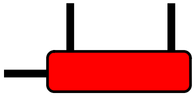
DMRG algorithm

3. Solve the ground state in the reduced Hilbert space

$$\hat{H}_{\text{eff}}|\phi\rangle = E_0|\phi\rangle$$



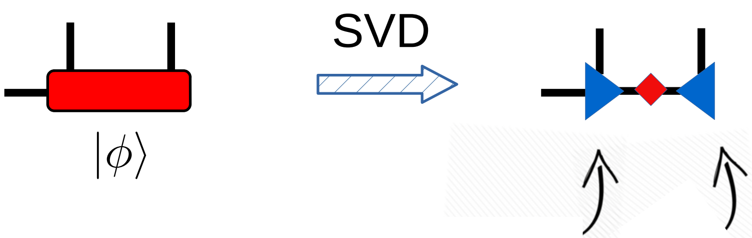
$$= \quad E_0$$



DMRG algorithm

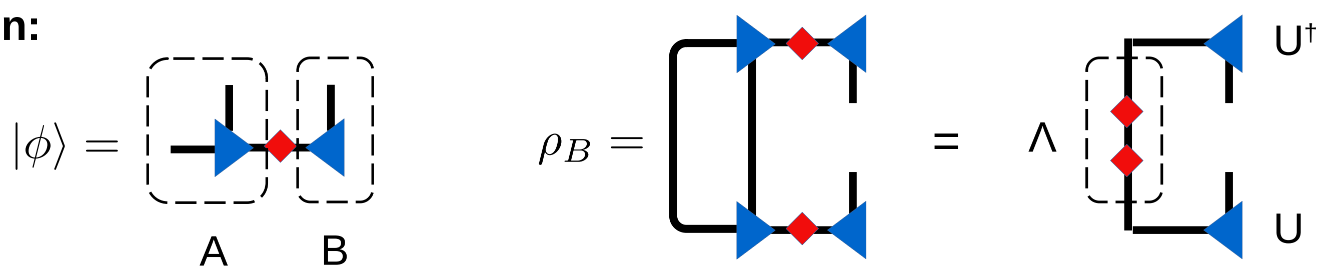
4. SVD on $|\phi\rangle$

Truncate the virtual dimension based on the singular values



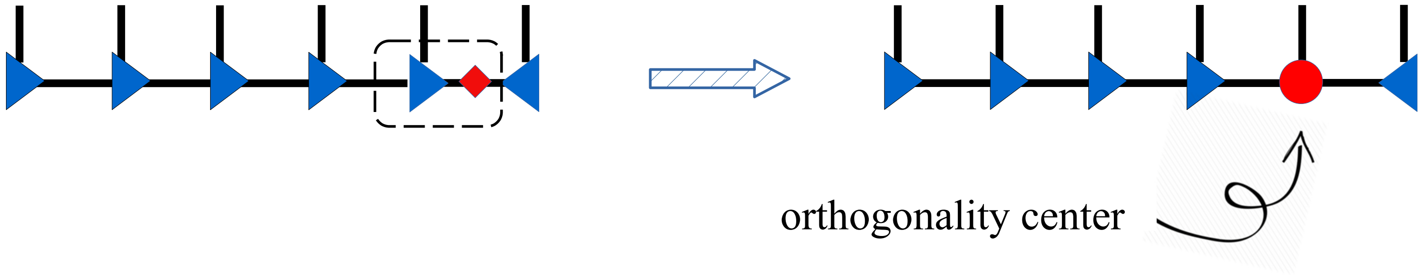
Rotate to the eigenbasis of $\rho_A \quad (\rho_B)$

Explain:

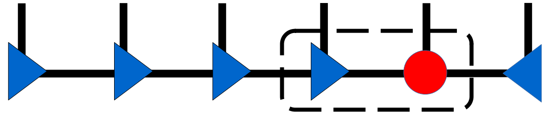


DMRG algorithm

5. Absorb the diagonal matrix to the left

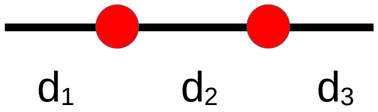


6. Optimize the next two sites   (and so on...)



Computational complexity

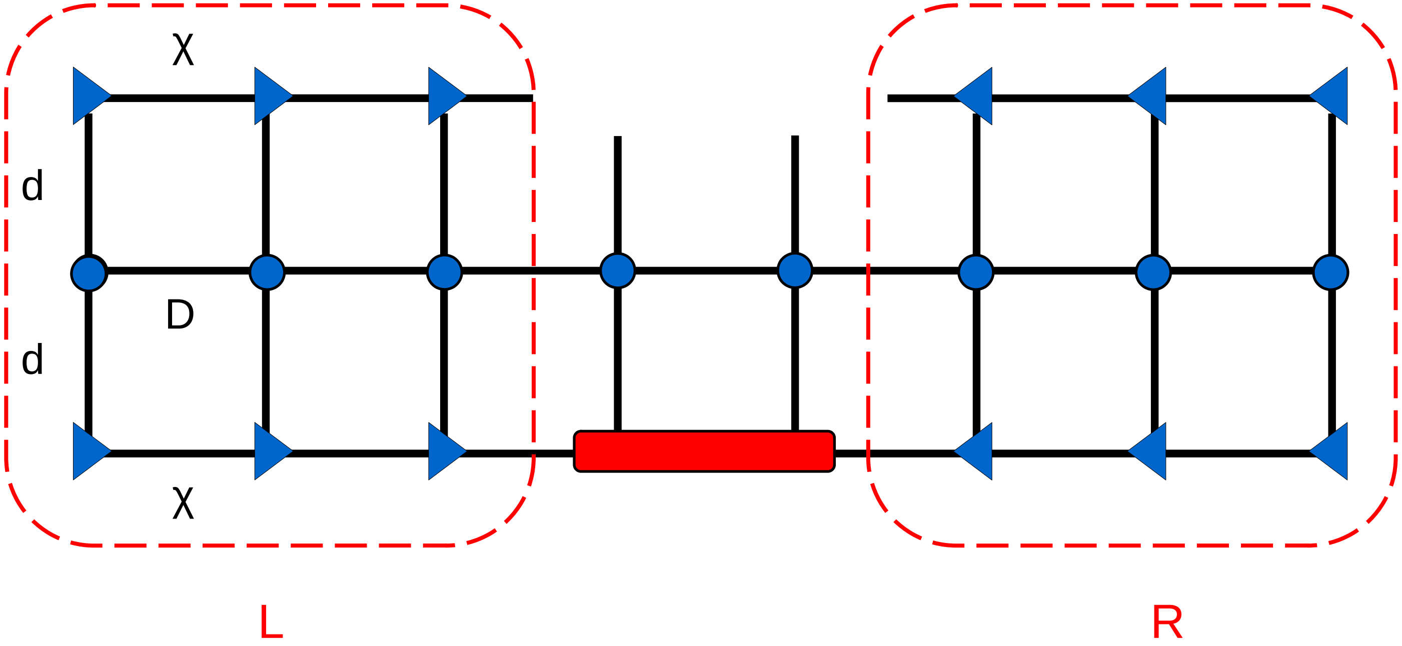
matrix multiplication



Complexity: $d_1 \times d_2 \times d_3$

(Number of real-number multiplications)

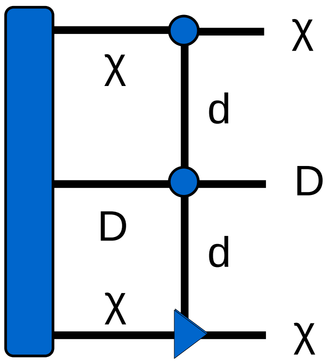
Computational complexity

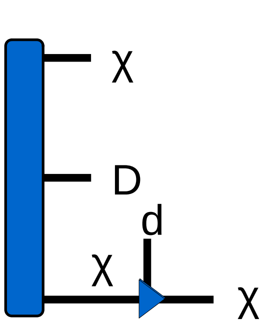


Complexity: ?

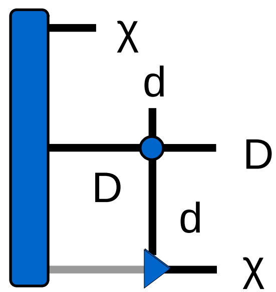
Computational complexity

L:

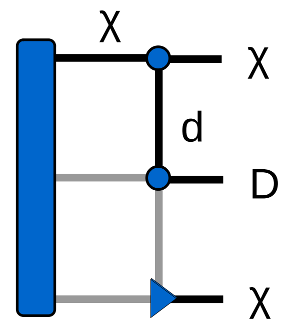




χ^3 d D



$\chi^2 d^2 D^2$



χ^3 d D

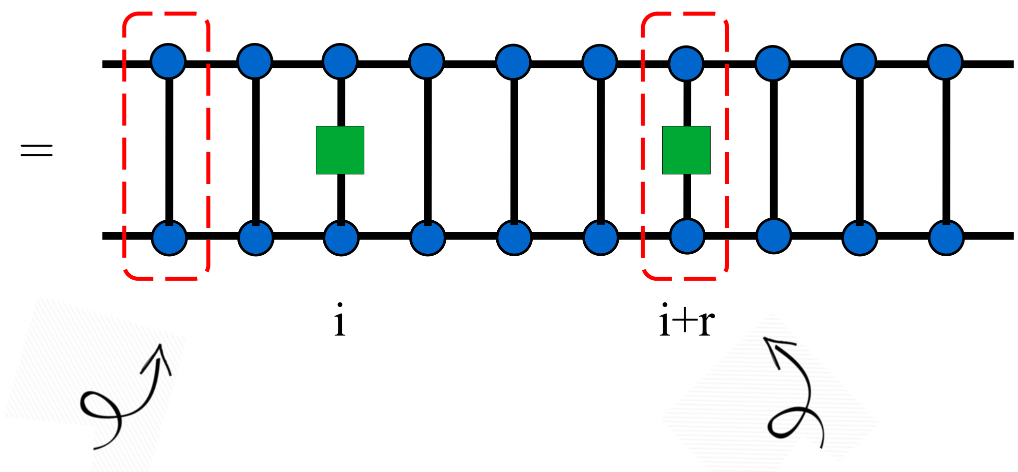
DMRG complexity $\propto L\,\chi^3$

Correlation function

$$C(r) = \langle O_i O_{i+r} \rangle - \langle O_i \rangle \langle O_{i+r} \rangle$$

Assume all the tensors are the same → uniform MPS (translational invariant)

$\langle O_i O_{i+r} \rangle =$



Transfer matrix E

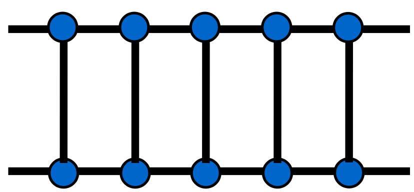
"Transfer matrix" E_O

$$\langle O_i O_{i+r} \rangle = \mathrm{Tr}\left(E^{\infty} \textcolor{green}{E_O} E^{r-1} \textcolor{green}{E_O} E^{\infty} \right)$$

Transfer matrix

$$E^{r} = \left[\begin{array}{c|c|c} \vec{v_1} & \vec{v_2} & \cdots \end{array}\right] \begin{bmatrix} \lambda_1^{r} & & \\ & \lambda_2^{r} & \\ & & \ddots \end{bmatrix} \left[\begin{array}{c} \vec{v_1} \\ \hline \vec{v_2} \\ \hline \vdots \end{array}\right]$$

$$\xrightarrow{r\to\infty} \quad \lambda_1^r \begin{bmatrix} \vec{v_1} \end{bmatrix} \begin{bmatrix} \quad \vec{v_1} \quad \end{bmatrix} = \lambda_1^r \, |v_1)(v_1|$$

$\langle\psi|\psi\rangle =$ Tr  $= \lim_{r\to\infty} \mathrm{Tr}(E^r) = \lim_{r\to\infty} \lambda_1^r = 1$

$\Rightarrow$ $\boxed{\lambda_1 = 1}$ (normalization condition)

Correlation function

For correlation function, we need to consider to the second order

$$\mathrm{E}^r \approx |v_1)(v_1| + \lambda_2^r \; |v_2)(v_2|$$

$$\begin{aligned}\langle O_i O_{i+r}\rangle &= \mathrm{Tr}\left(E^\infty E_O E^{r-1} E_O E^\infty\right) \\ &= (v_1|E_O\left[\; |v_1)(v_1| + \lambda_2^{r-1} \; |v_2)(v_2| \;\right]E_O|v_1) \\ &= \underbrace{(v_1|E_O|v_1)(v_1|E_O|v_1)}_{\langle O_i\rangle\langle O_{i+r}\rangle} + \lambda_2^{r-1} \; (v_1|E_O|v_2)(v_2|E_O|v_1)\end{aligned}$$

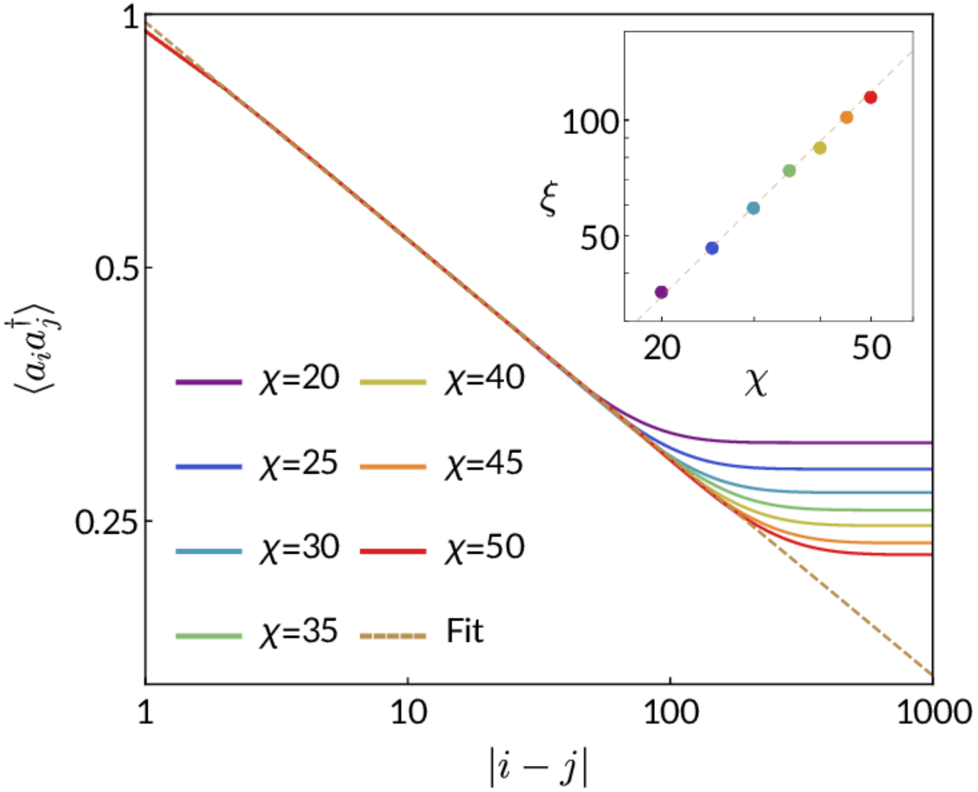
decay exponentially with r

$$C(r) = \langle O_i O_{i+r}\rangle - \langle O_i\rangle\langle O_{i+r}\rangle \propto e^{-r/\xi}$$

$$\xi \equiv -1/\log \lambda_2$$

$\boxed{\text{MPS has finite correlation length.}}$ (gapped ground state)

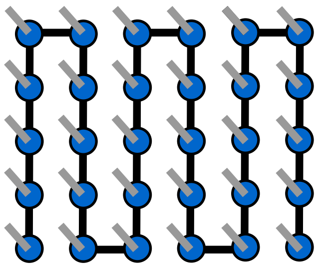
Correlation function



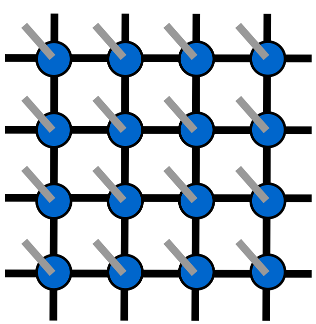
Other tensor networks

2D systems

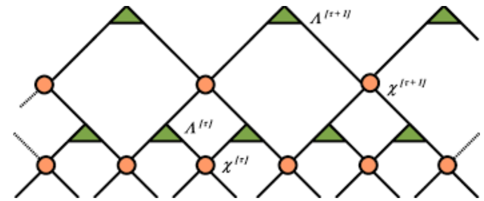
MPS



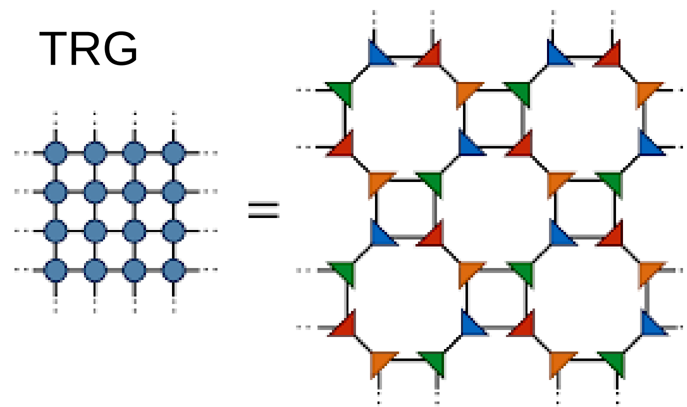
PEPS



MERA



TRG



and many others...

Thank you!

Measurement

On-site observable $\langle O_i \rangle$