Selected Topics in Computational Quantum Physics
量子物理计算方法选讲

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Density Matrix Renormalization Group and Matrix Product States

- origin of Density Matrix Renormalization Group method (DMRG)

- many-body entanglement

- traditional DMRG method

- Matrix Product State (MPS) and Matrix Product Operator (MPO)

- MPS algorithms

- various applications

selected review articles:
U. Schollwock, arXiv: 1008.3477
N. Schuch, arXiv: 1306.5551.
F. Verstraete, J.I. Cirac, V. Murg, arXiv: 0907.2796.
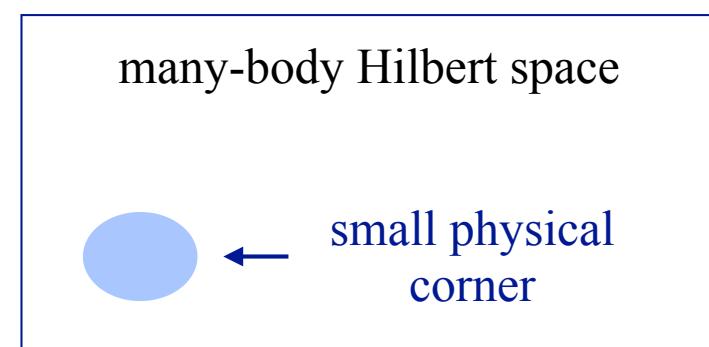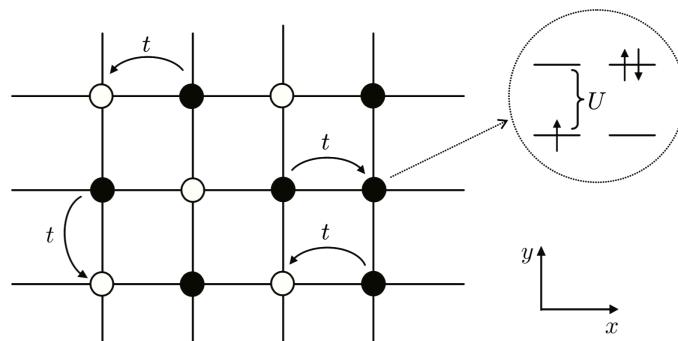
Physical corner of Hilbert space

- how can we describe quantum many-body ground states?

- general state of N spins

$$|\psi\rangle = \sum_{i_1,i_2,\cdots,i_N} C_{i_1,i_2,\cdots,i_N} |i_1, i_2, \cdots, i_N\rangle$$

exponentially large Hilbert space
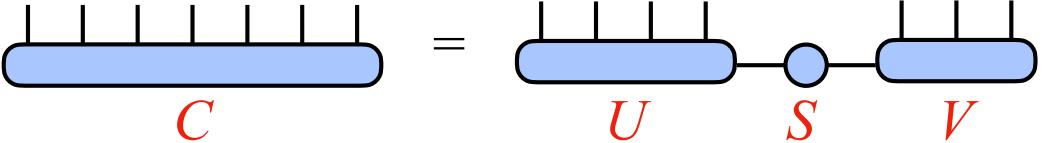
- but local Hamiltonian $\quad H = \sum_{\langle ij \rangle} h_{ij} \quad$ has only $O(N)$ parameters

ground state must live in a small physical corner of Hilbert space

- is there a nice way to describe states in the physical corner?

use entanglement structure

Many-body entanglement

- Schmidt decomposition
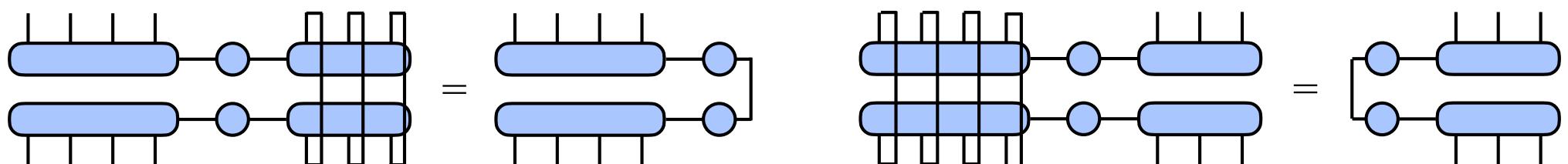
$$|\psi\rangle = \sum_{ij} C_{ij}|i\rangle_A|j\rangle_B = \sum_\alpha s_\alpha|u^\alpha\rangle_A|v^\alpha\rangle_B$$

- reduced density matrix

$$\rho_A = \mathrm{Tr}_B\rho = \sum_\alpha s_\alpha^2|u^\alpha\rangle_A{}_A\langle u^\alpha| \qquad\qquad \rho_B = \mathrm{Tr}_A\rho = \sum_\alpha s_\alpha^2|v^\alpha\rangle_B{}_B\langle v^\alpha|$$
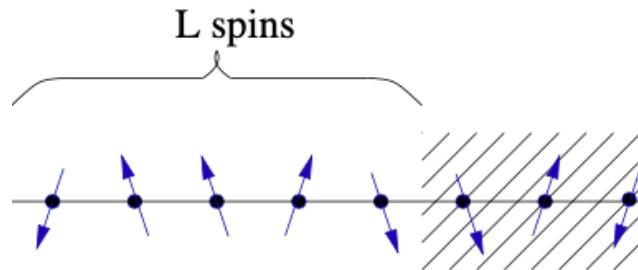
- Entanglement Entropy (EE) is a measure of the amount of entanglement

$$S = -\mathrm{Tr}[\rho_A\ln\rho_A] = -\mathrm{Tr}[\rho_B\ln\rho_B] = -\sum_\alpha s_\alpha^2\ln s_\alpha^2$$

- if there are totally D non-zero singular values s_α

  the maximum possible entanglement entropy is $\ln D$
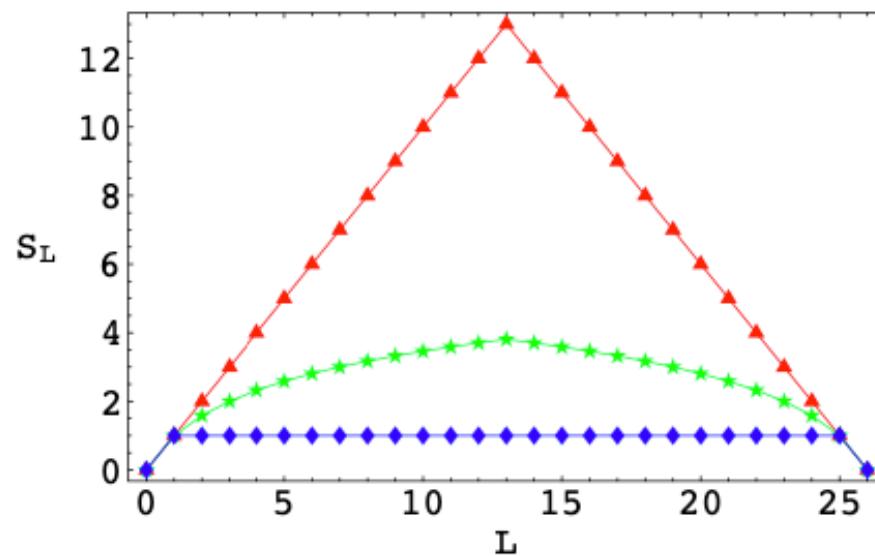
Entanglement structure

- we use von Neumann entropy as a measure of entanglement

L spins

$$S_L = -\,\mathrm{Tr}(\rho_L \log_2 \rho_L)$$

- S_L is upper bounded by $\quad S_L \leq \min(L, N-L)$

  since ρ_L is supported in a local space of dimension $\quad d_L = \min(2^L, 2^{N-L})$

- entropy S_L for some pure states with $N = 26$ spins

linear upper bound

logarithmic upper bound
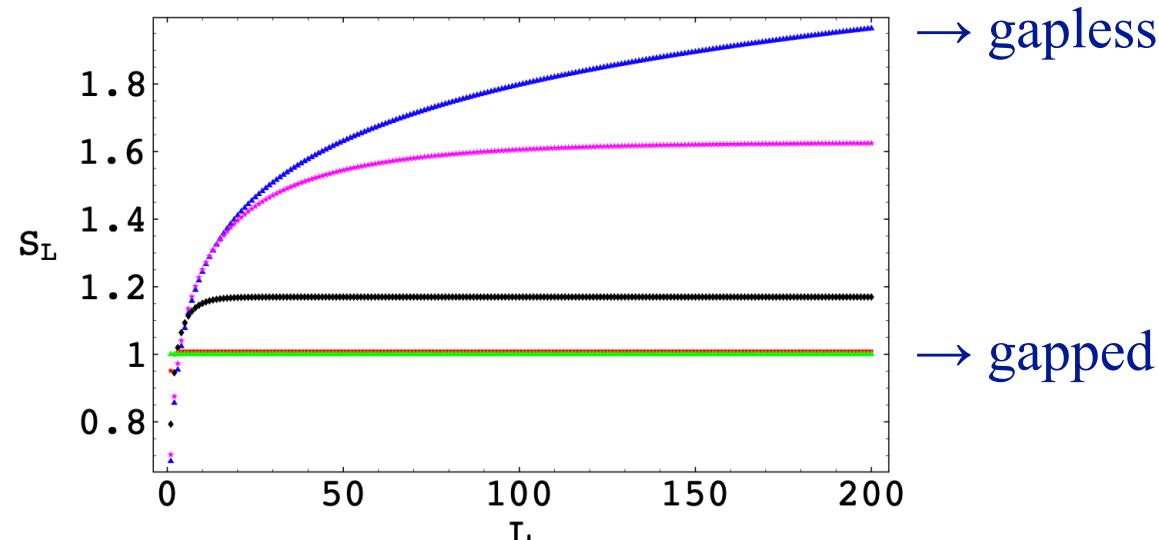
GHZ state $\dfrac{1}{\sqrt{2}}(|000\cdots 0\rangle + |111\cdots 1\rangle)$

Area law

- area law for ground states of gapped Hamiltonians

  the entropy of the reduced states of a block A scales like the length of its boundary ∂A


- gapped 1D system ground state $\quad S(\rho_L) \sim$ constant

  even for gapless 1D system ground state $\quad S(\rho_L) \sim \ln L$

J. I. Latorre, E. Rico, G. Vidal, Quant.Inf.Comput. 4, 48-92 (2004).

Construction of states satisfying area law

- area law suggests: the entanglement between two regions is located around the boundary
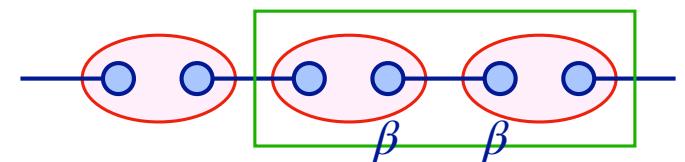
- we will construct an ansatz for quantum many-body systems which satisfies area law by construction

1. each site is composed of two virtual sites
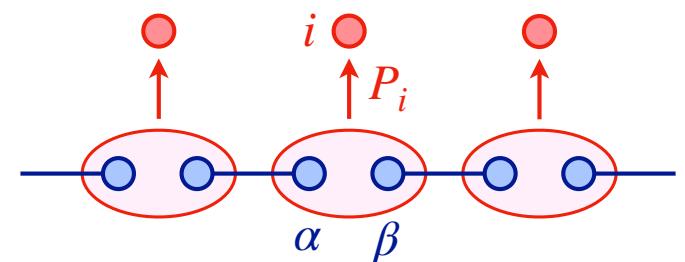
2. virtual sites are placed in maximally entangled states, area law is satisfied

$$|\omega_D\rangle = \sum_{\beta=1}^{D} |\beta, \beta\rangle$$

3. map virtual sites to physical sites by P

$$P_i = \sum_{i,\alpha,\beta} A_{i,\alpha,\beta}^{[i]} |i\rangle\langle\alpha, \beta|$$
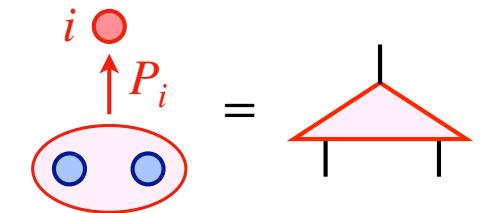
- total state is $\qquad |\psi\rangle = (P_1 \otimes P_2 \otimes \cdots \otimes P_N)|\omega_D\rangle^{\otimes N}$
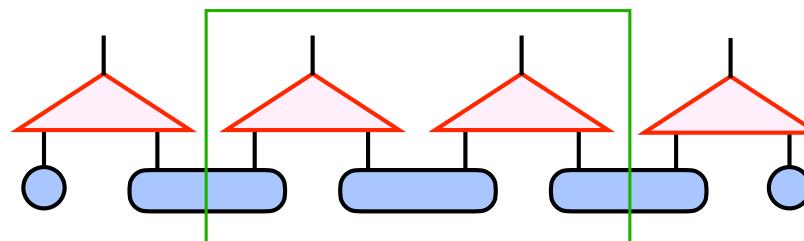
Area law is satisfied

- maximally entangled states and projectors
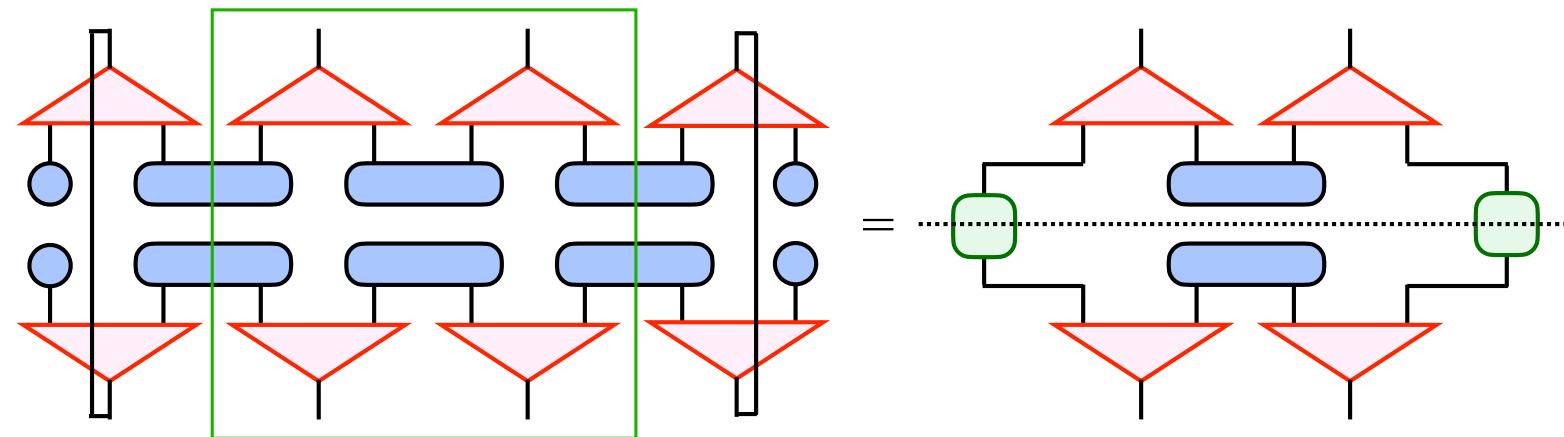
$$|\omega_D\rangle = \sum_{\beta=1}^{D} |\beta, \beta\rangle \quad = \quad = \mathbb{1}_{D \times D}$$

- we consider the entanglement between the two regions
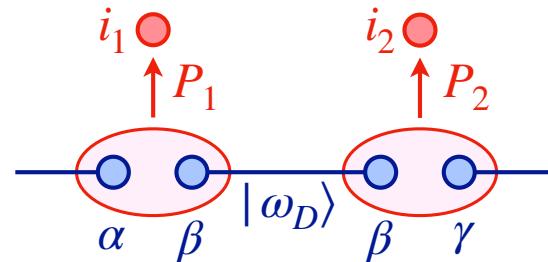
- the reduced density matrix is

- the dashed line cuts 2 bonds, each has dimension D

 the maximum possible entanglement entropy is $2\ln D$

Matrix Product State (MPS)

- two-site example

$$\sum_\beta A^{[1]}_{i_1,\alpha\beta} A^{[2]}_{i_2,\beta\gamma} = \alpha \underset{A^{[1]}}{\overset{i_1}{\square}} \overset{\beta}{\underset{A^{[2]}}{\overset{i_2}{\square}}} \gamma$$

$$P_1 \otimes P_2 |\omega_D\rangle = \left[\sum_{i_1\alpha\beta_1} A^{[1]}_{i_1,\alpha\beta_1} |i_1\rangle \langle\alpha\beta_1| \right] \left[\sum_{i_2\beta_2\gamma} A^{[2]}_{i_2,\beta_2\gamma} |i_2\rangle \langle\beta_2\gamma| \right] \left[\sum_\beta |\beta\beta\rangle \right]$$

$$= \sum_{i_1 i_2 \alpha\gamma} \left[\sum_\beta A^{[1]}_{i_1,\alpha\beta} A^{[2]}_{i_2,\beta\gamma} \right] |i_1 i_2\rangle \langle\alpha\gamma| = \sum_{i_1 i_2 \alpha\gamma} \left(A^{[1]}_{i_1} A^{[2]}_{i_2} \right)_{\alpha\gamma} |i_1 i_2\rangle \langle\alpha\gamma|$$

- 1D ring example

$$|\Psi\rangle \equiv \quad \boxed{\overset{i_1 \quad i_2 \quad i_3 \quad \cdots \quad i_N}{c_{i_1,\ldots,i_N}}} \quad = \quad \overset{i_1}{\boxed{A^{[1]}}} \overset{\alpha}{} \overset{i_2}{\boxed{A^{[2]}}} \overset{\beta}{} \overset{i_3}{\boxed{A^{[3]}}} \text{------} \overset{i_N}{\boxed{A^{[N]}}}$$

$$|\Psi\rangle = \sum_{i_1,\cdots,i_N} c_{i_1,\cdots,i_N} |i_1,\cdots,i_N\rangle = (P_1 \otimes \cdots \otimes P_N)|\omega_D\rangle^{\otimes N} = \sum_{i_1,\cdots,i_N} \text{Tr}[A^{[1]}_{i_1} A^{[2]}_{i_2} \cdots A^{[N]}_{i_N}] |i_1,\cdots i_N\rangle$$

- the coefficient can be expressed as a product of matrices
  that's why it is called Matrix Product State (MPS)
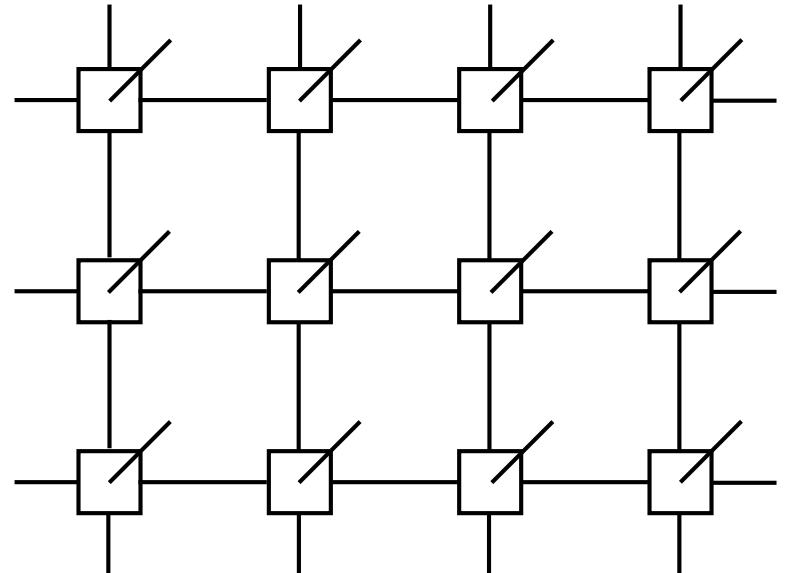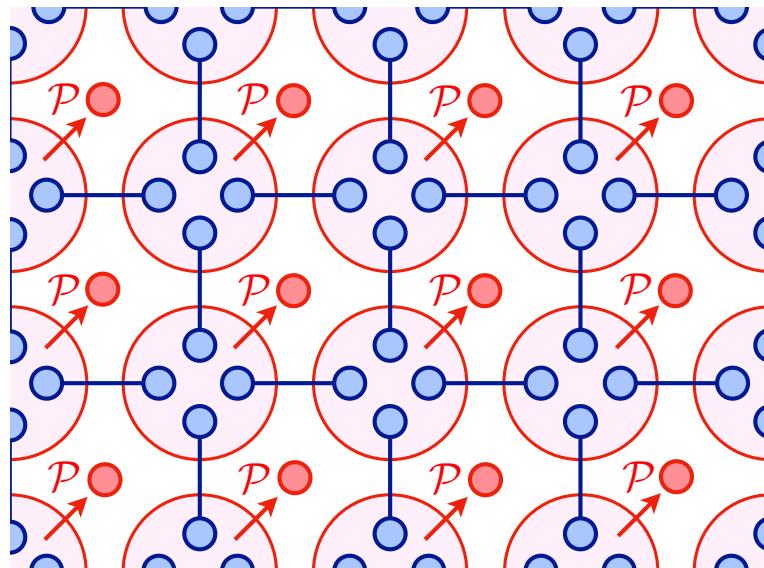
Projected Entangled-Pair States (PEPS)

- matrix product states → 1D Projected Entangled-Pair States (PEPS)

$$|\omega_D\rangle = \sum_{i=1}^{D} |i, i\rangle$$
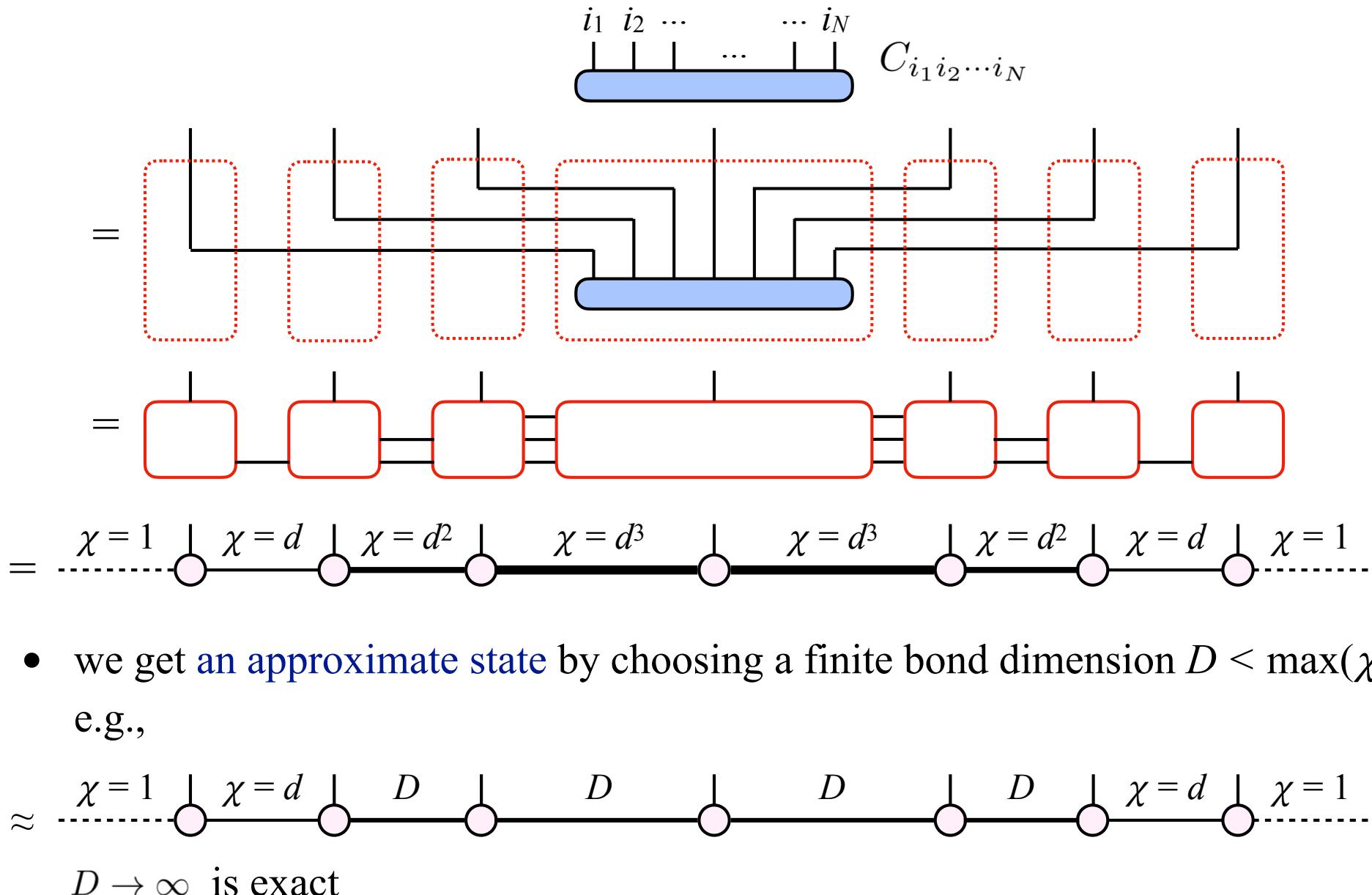
$$|\Psi\rangle = \sum_{i_1,\dots,i_N} c_{i_1\dots i_N} |i_1,\dots,i_N\rangle = (\mathcal{P}_1 \otimes \cdots \otimes \mathcal{P}_N)|\omega_D\rangle^{\otimes N} = \sum_{i_1,\dots,i_N} \text{tr}\big[A_{i_1}^{[1]} A_{i_2}^{[2]} \cdots A_{i_N}^{[N]}\big] |i_1,\dots,i_N\rangle$$

- generate to 2D → 2D Projected Entangled-Pair States (PEPS)

Approximating states as MPS

- given infinitely large bond dimensions, every state can be written as an MPS

$$i_1 \quad i_2 \quad \cdots \qquad \cdots \quad i_N$$

$$C_{i_1 i_2 \cdots i_N}$$

$$\chi = 1 \quad \chi = d \quad \chi = d^2 \quad \chi = d^3 \quad \chi = d^3 \quad \chi = d^2 \quad \chi = d \quad \chi = 1$$

- we get an approximate state by choosing a finite bond dimension $D < \max(\chi)$, e.g.,

$$\chi = 1 \quad \chi = d \quad D \quad D \quad D \quad D \quad \chi = d \quad \chi = 1$$

$D \to \infty$ is exact

Canonical form of MPS

- MPS has gauge degree of freedom, T_i and $\widetilde{T}_i$ represent the same state

$$|\psi\rangle = $$

T_1 T_2 T_3 T_4 T_5

$$= \quad X_1 \; X_1^{-1} \; X_2 \; X_2^{-1} \; X_3 \; X_3^{-1} \; X_4 \; X_4^{-1}$$

$$= \quad \widetilde{T}_1 \quad \widetilde{T}_2 \quad \widetilde{T}_3 \quad \widetilde{T}_4 \quad \widetilde{T}_5$$

- we may fix the gauge degree of freedom by introducing a canonical form of the MPS in which the bond index corresponds to the Schmidt decomposition

$$|\psi\rangle = $$

G_0 T_1 G_1 T_2 G_2 T_3 G_3 T_4 G_4 T_5 G_5

$$|u^\alpha\rangle_L \qquad S^\alpha \qquad |u^\alpha\rangle_R$$

satisfying

$$\begin{array}{ccc} G \quad T & & T_L \\ & = & \\ \mathbb{I} \quad G \quad T^* & & \mathbb{I} \quad T_L^* \end{array} = \mathbb{I}$$

left canonical condition

$$\begin{array}{ccc} T \quad G & & T_R \\ & = & \\ T^* \quad G \quad \mathbb{I} & & T_R^* \quad \mathbb{I} \end{array} = \mathbb{I}$$
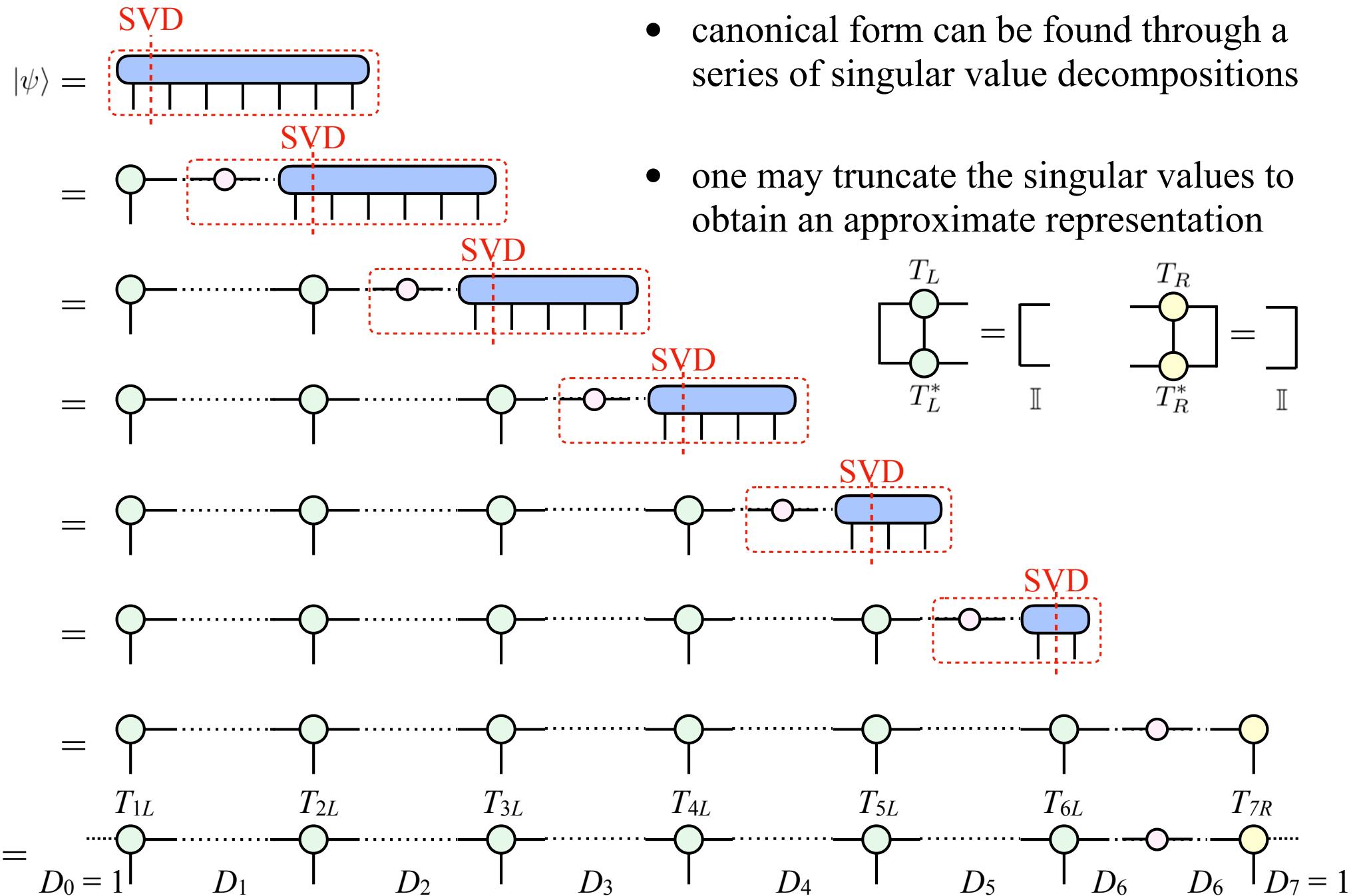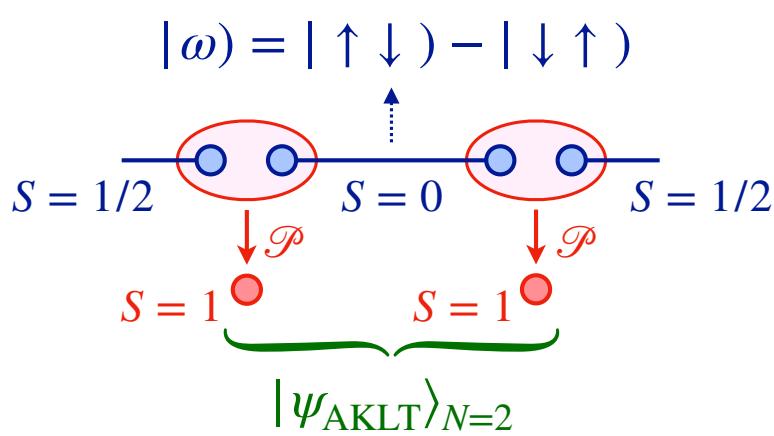
right canonical condition

Find canonical form using SVD

- canonical form can be found through a series of singular value decompositions

- one may truncate the singular values to obtain an approximate representation
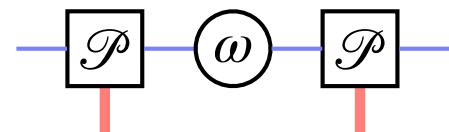
AKLT state

- the paradigmatic analytical MPS model is the so-called AKLT state named after Affleck, Kennedy, Lieb, and Tasaki

$$|\omega) = |\uparrow\downarrow) - |\downarrow\uparrow)$$

- from physical spins: $\quad 1 \otimes 1 = 0 \oplus 1 \oplus 2$

  from virtual spins: $\quad \frac{1}{2} \otimes 0 \otimes \frac{1}{2} = 0 \oplus 1$

- there is non-trivial constraint on $|\psi_{AKLT}\rangle_{N=2}$ arising from the AKLT construction

  $|\psi_{AKLT}\rangle_{N=2}$ cannot have spin 2

- AKLT state as MPS

$$|\omega) = |\uparrow\downarrow) - |\downarrow\uparrow)$$

$$\mathscr{P} = |+\rangle(\uparrow\uparrow| + |0\rangle\frac{(\uparrow\downarrow| + (\downarrow\uparrow|}{\sqrt{2}} + |-\rangle(\downarrow\downarrow|$$

- we may construct the parent Hamiltonian $\hat{H}$ of the AKLT state

$$\hat{H} = \sum_i \hat{\Pi}_i, \quad \hat{\Pi}_i|\psi_{AKLT}\rangle_{N=2} = 0, \quad \hat{H}|\psi_{AKLT}\rangle = 0$$

I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. 59, 799 (1987).

Parent Hamiltonian of the AKLT state

- the full parent Hamiltonian is a sum of local parent Hamiltonians

  each local parent Hamiltonian is a projector onto the $S_{ij} = 2$ subspace

$$H = \sum_{\langle i,j \rangle} h_{i,j}, \qquad h_{i,j} = \Pi^{S_{ij}=2}$$

since $|\psi_{\text{AKLT}}\rangle_{N=2}$ cannot have spin 2, we have $h_{i,j}|\psi_{\text{AKLT}}\rangle_{N=2} = 0$ and $H|\psi_{\text{AKLT}}\rangle = 0$

- for spin-1 chain, the projector $\Pi^{S_{ij}=2}$ satisfies

$$\Pi^{S_{ij}=2}|S_{ij} = 0\rangle = 0, \qquad \Pi^{S_{ij}=2}|S_{ij} = 1\rangle = 0, \qquad \Pi^{S_{ij}=2}|S_{ij} = 2\rangle = |S_{ij} = 2\rangle$$

- $\Pi^{S_{ij}=2}$ can be constructed as

$$\Pi^{S_{ij}=2} = \lambda[S_{ij}^2 - 0 \times (0 + 1)][S_{ij}^2 - 1 \times (1 + 1)]$$

$$\lambda[2 \times (2 + 1) - 0 \times (0 + 1)][2 \times (2 + 1) - 1 \times (1 + 1)] = 1 \quad \Rightarrow \lambda = \frac{1}{24}$$

$$S_{ij}^2 = (S_i + S_j)^2 = 2S_i \cdot S_j + 2 \times 1 \times (1 + 1) = 2S_i \cdot S_j + 4$$

- the local parent Hamiltonian becomes

$$\Pi^{S_{ij}=2} = \frac{1}{6}(S_i \cdot S_j)^2 + \frac{1}{2}S_i \cdot S_j + \frac{1}{3}$$

Parent Hamiltonian of MPS

- we block two sites

$$|\psi_{\mathrm{AKLT}}\rangle_{N=2} = $$ $$= |\mathbf{p}\rangle \mathbf{T}(\mathbf{v}|$$

- $\hat{T}$ is a map from the $D^2 = 4$ virtual space $|\mathbf{v})$ to the $d^2 = 9$ physical space $|\mathbf{p}\rangle$

  since $9 > 4$, there exists a null space that annihilates the physical state

- we calculate the inverse of $\hat{T}$ $$\hat{T}^{-1}\hat{T} = \hat{I} = |\mathbf{v})\mathbf{I}(\mathbf{v}|$$

- the local parent Hamiltonian is

$$\hat{\Pi}_{N=2} = $$

- this is because

$$\hat{\Pi}_{N=2}\hat{T} = $$ $$= 0$$

Non-Hermitian Parent Hamiltonian

- given $\langle L|$ and $|R\rangle$, find out a non-Hermitian H? such that $H|R\rangle = 0$, $\langle L|H = 0$

- $k = 2$ example

- we verify in a straightforward way
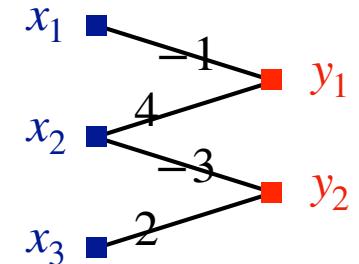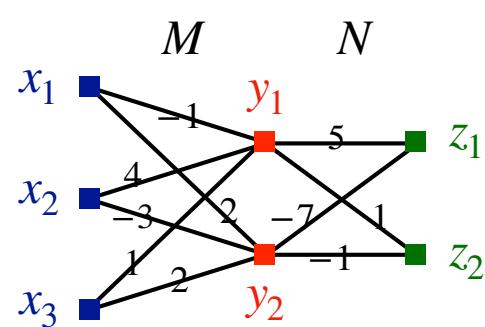
Viewing matrices as graphs

- every matrix corresponds to a graph
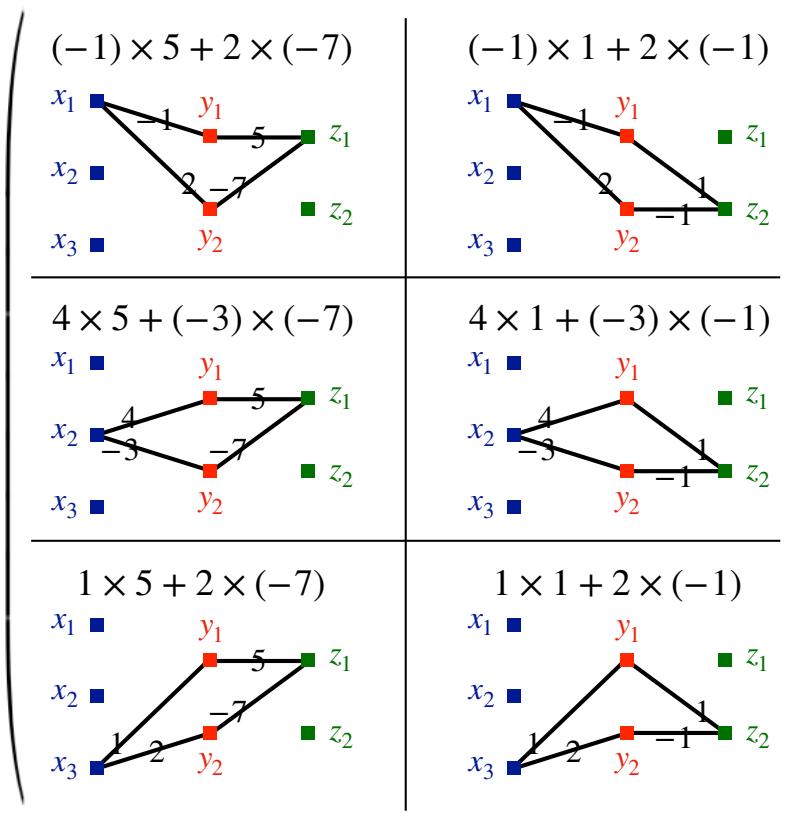
$$M = \begin{pmatrix} M(x_1, y_1) & M(x_1, y_2) \\ M(x_2, y_1) & M(x_2, y_2) \\ M(x_3, y_1) & M(x_3, y_2) \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \\ M_{31} & M_{32} \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 4 & -3 \\ 0 & 2 \end{pmatrix}$$

- matrix multiplication corresponds to traveling along paths

$$\begin{pmatrix} -1 & 2 \\ 4 & -3 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 5 & 1 \\ -7 & -1 \end{pmatrix} =$$

$(-1) \times 5 + 2 \times (-7)$ $\qquad$ $(-1) \times 1 + 2 \times (-1)$

$4 \times 5 + (-3) \times (-7)$ $\qquad$ $4 \times 1 + (-3) \times (-1)$

$1 \times 5 + 2 \times (-7)$ $\qquad$ $1 \times 1 + 2 \times (-1)$

$$= \begin{pmatrix} -19 & -3 \\ 41 & 7 \\ -9 & -1 \end{pmatrix}$$

https://www.math3ma.com

Viewing matrices as graphs

- symmetric matrices correspond to symmetric graphs

$$MM^\dagger \qquad\qquad M^\dagger M$$

- block matrices correspond to disconnected graphs
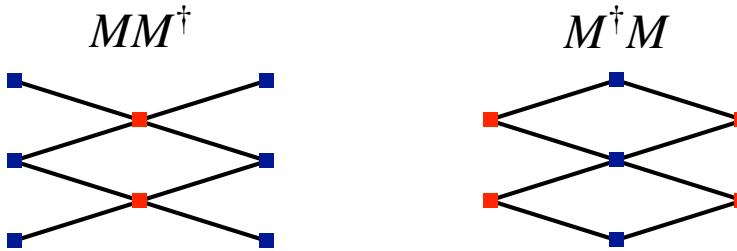
$$\begin{pmatrix} -1 & 2 \\ 4 & -3 \\ 1 & 2 \end{pmatrix} \oplus \begin{pmatrix} 5 & 1 \\ -7 & -1 \end{pmatrix} = \quad \oplus \quad = \begin{pmatrix} -1 & 2 & 0 & 0 \\ 4 & -3 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 0 & 0 & 5 & 1 \\ 0 & 0 & -7 & -1 \end{pmatrix} =$$
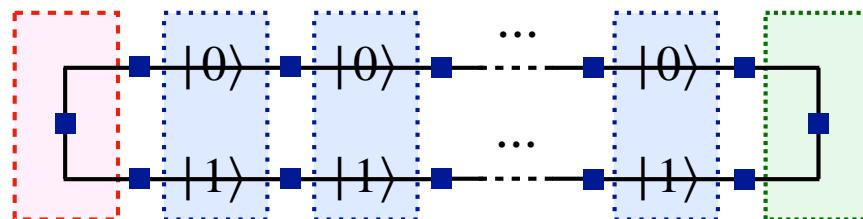
- singular value decomposition

$$M \qquad = \qquad U \quad S \quad V$$

States with exact matrix product form
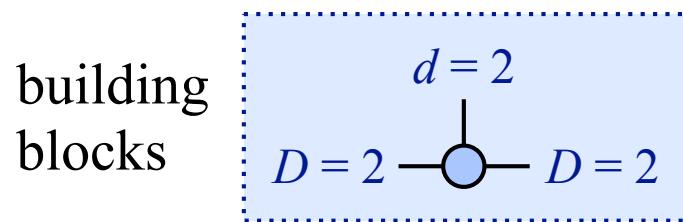
- matrix product state $\rightarrow$ matrix elements are physical states

- GHZ state

$$|\psi\rangle = |00\cdots0\rangle + |11\cdots1\rangle = |0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle + |1\rangle \otimes |1\rangle \otimes \cdots \otimes |1\rangle$$
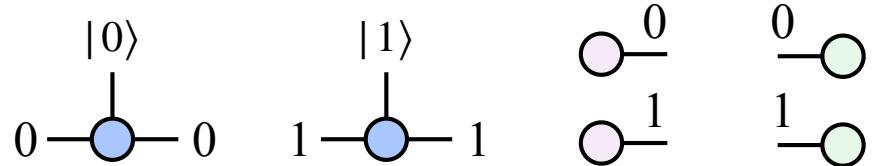
$$|\psi\rangle = \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} |0\rangle & 0 \\ 0 & |1\rangle \end{pmatrix} \begin{pmatrix} |0\rangle & 0 \\ 0 & |1\rangle \end{pmatrix} \cdots \begin{pmatrix} |0\rangle & 0 \\ 0 & |1\rangle \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$
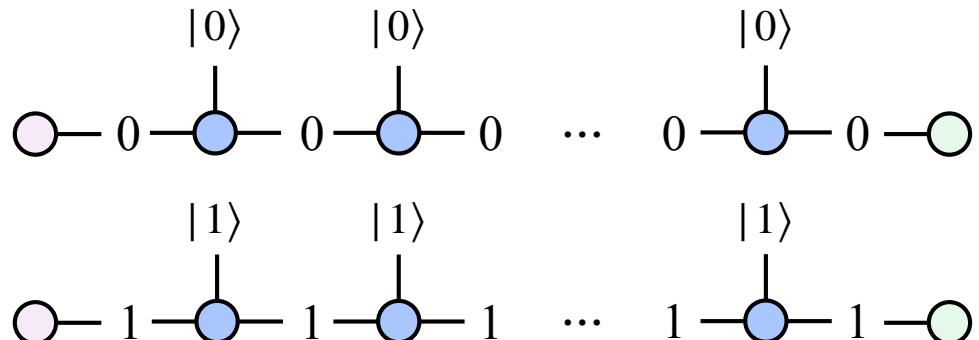
- we obtain a translational invariant matrix product state

physical dimension: $d = 2$, virtual dimension: $D = 2$
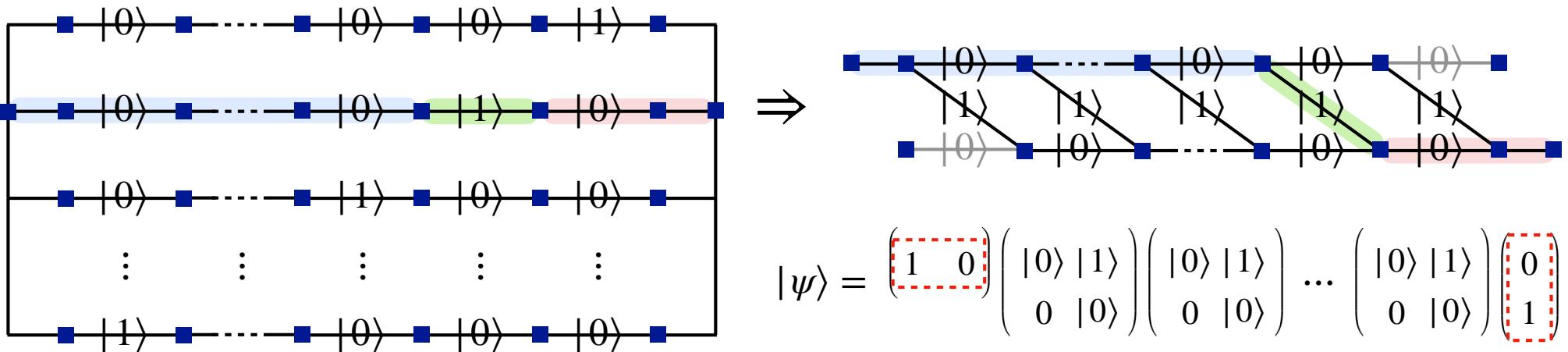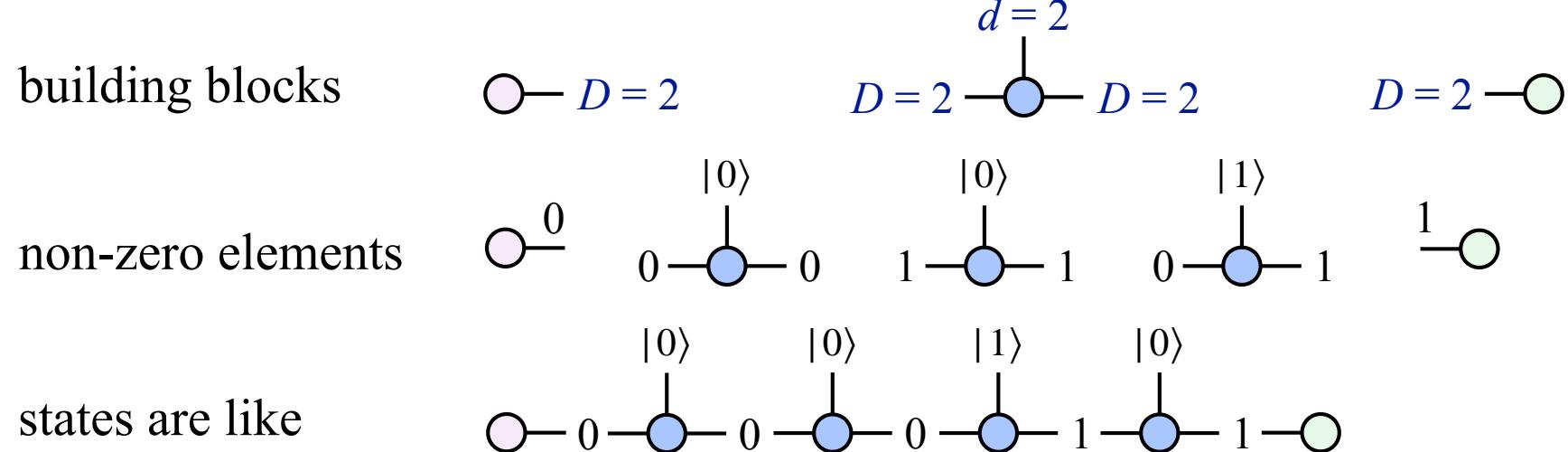
States with exact matrix product form

- W state $|\psi\rangle = |0\cdots001\rangle + |0\cdots010\rangle + |0\cdots100\rangle + \cdots + |1\cdots000\rangle$

- we may simplify the expression by combining like terms

$$|\psi\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} |0\rangle & |1\rangle \\ 0 & |0\rangle \end{pmatrix} \begin{pmatrix} |0\rangle & |1\rangle \\ 0 & |0\rangle \end{pmatrix} \cdots \begin{pmatrix} |0\rangle & |1\rangle \\ 0 & |0\rangle \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
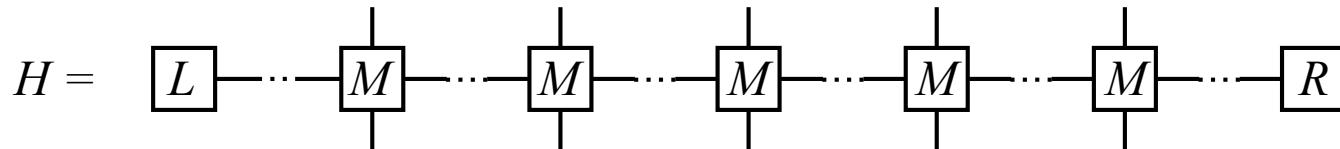
- we obtain a translational invariant matrix product state with $D = 2$
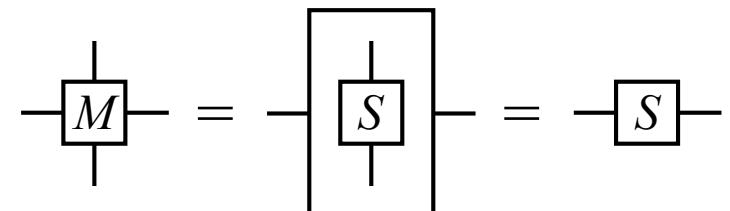
Matrix Product Operator (MPO)

- 1D Hamiltonian can be written as an Matrix Product Operator (MPO)

  e.g., under Open Boundary Condition (OBC)

$$H = \boxed{L} - \cdots - \boxed{M} - \cdots - \boxed{M} - \cdots - \boxed{M} - \cdots - \boxed{M} - \cdots - \boxed{R}$$

  upper and lower bonds of M are physical bonds

  left and right bonds of M are virtual bonds

$$-\boxed{M}- \;=\; -\boxed{S}- \;=\; -\boxed{S}-$$

- we regard M as a matrix

  matrix product operator $\rightarrow$ matrix elements are physical operators

- example

$$H = \sum_j S_j^x S_{j+1}^x$$

- $N = 4$

  how to generate these three terms?
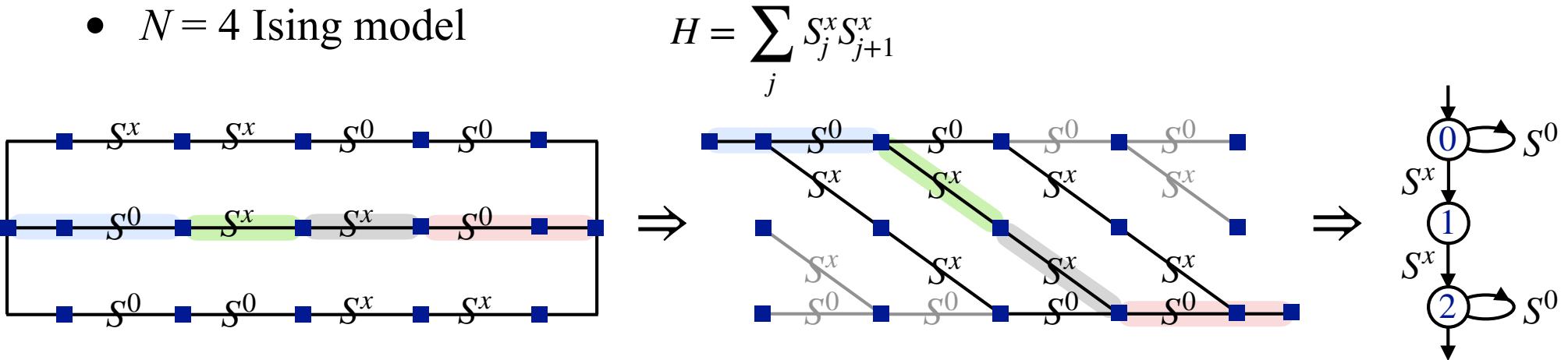
$$S_1^x S_2^x S_3^0 S_4^0 = \boxed{L} - ? - \boxed{S^x} - ? - \boxed{S^x} - ? - \boxed{S^0} - ? - \boxed{S^0} - ? - \boxed{R}$$

$$S_1^0 S_2^x S_3^x S_4^0 = \boxed{L} - ? - \boxed{S^0} - ? - \boxed{S^x} - ? - \boxed{S^x} - ? - \boxed{S^0} - ? - \boxed{R}$$

$$S_1^0 S_2^0 S_3^x S_4^x = \boxed{L} - ? - \boxed{S^0} - ? - \boxed{S^0} - ? - \boxed{S^x} - ? - \boxed{S^x} - ? - \boxed{R}$$

Matrix Product Operator (MPO)

- $N = 4$ Ising model

$$H = \sum_j S_j^x S_{j+1}^x$$
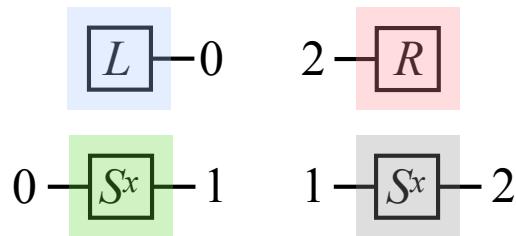
- MPO representation of the above Hamiltonian with $D_{\text{mpo}} = 3$

MPO

$$H = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} S^0 & S^x & 0 \\ 0 & 0 & S^x \\ 0 & 0 & S^0 \end{pmatrix} \begin{pmatrix} S^0 & S^x & 0 \\ 0 & 0 & S^x \\ 0 & 0 & S^0 \end{pmatrix} \begin{pmatrix} S^0 & S^x & 0 \\ 0 & 0 & S^x \\ 0 & 0 & S^0 \end{pmatrix} \begin{pmatrix} S^0 & S^x & 0 \\ 0 & 0 & S^x \\ 0 & 0 & S^0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

- building blocks
- full Hamiltonian

Finite automata for MPO

- transverse field Ising model

$$H = \sum_j \left(-S_j^z S_{j+1}^z + g S_j^x \right)$$
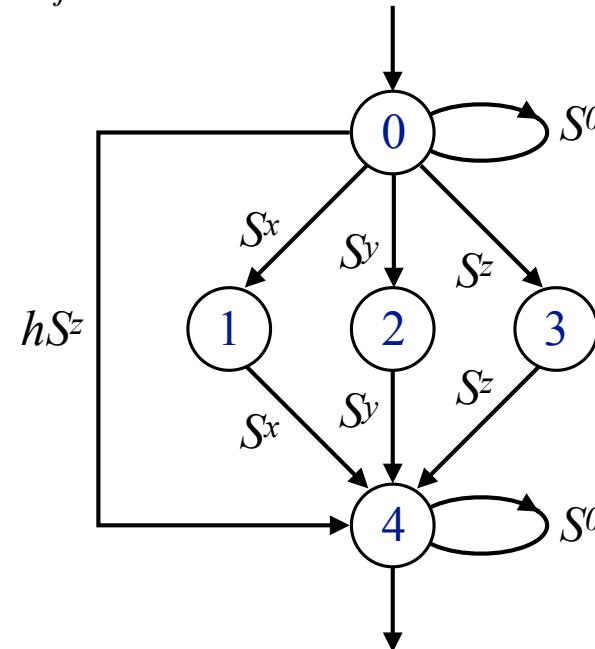
- Heisenberg model

$$H = \sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + S_j^z S_{j+1}^z + h S_j^z \right)$$

$$D_{\mathrm{mpo}} = 3 \quad \begin{array}{c|ccc} & 0 & 1 & 2 \\ \hline 0 & S^0 & -S^z & gS^x \\ 1 & 0 & 0 & S^z \\ 2 & 0 & 0 & S^0 \end{array}$$
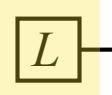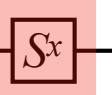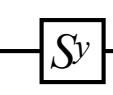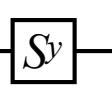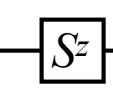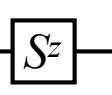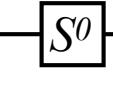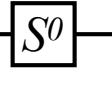
$$D_{\mathrm{mpo}} = 5 \quad \begin{array}{c|ccccc} & 0 & 1 & 2 & 3 & 4 \\ \hline 0 & S^0 & S^x & S^y & S^z & hS^z \\ 1 & 0 & 0 & 0 & 0 & S^x \\ 2 & 0 & 0 & 0 & 0 & S^y \\ 3 & 0 & 0 & 0 & 0 & S^z \\ 4 & 0 & 0 & 0 & 0 & S^0 \end{array}$$

MPO of Heisenberg model
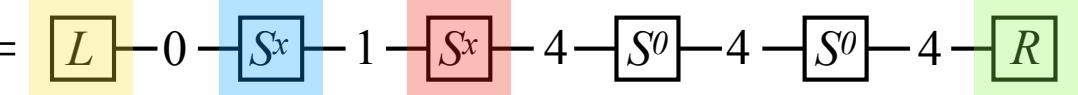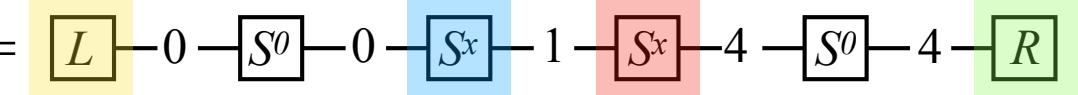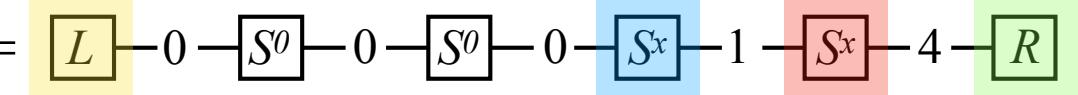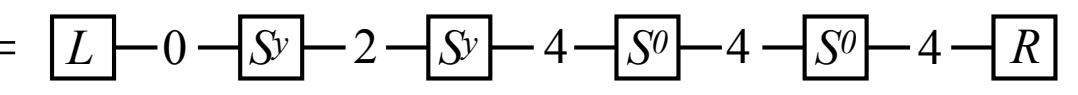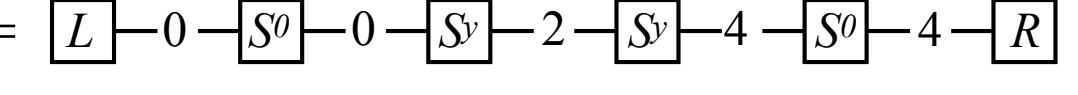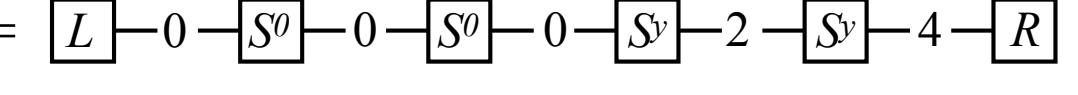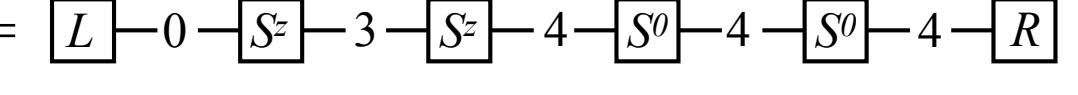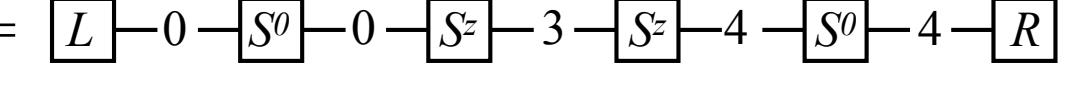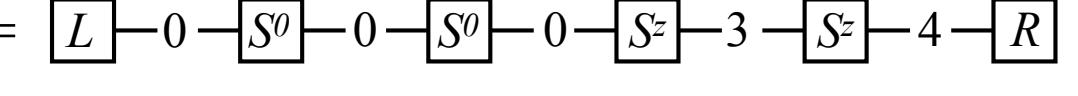
- $N = 4$, $D_{\mathrm{mpo}} = 5$

$$H = \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z \right)$$

- blocks

$$\boxed{L} - 0 \qquad 4 - \boxed{R}$$

$$0 - \boxed{S^x} - 1 \qquad 1 - \boxed{S^x} - 4$$

$$0 - \boxed{S^y} - 2 \qquad 2 - \boxed{S^y} - 4$$

$$0 - \boxed{S^z} - 3 \qquad 3 - \boxed{S^z} - 4$$

$$0 - \boxed{S^0} - 0 \qquad 4 - \boxed{S^0} - 4$$

- MPO

$$
\begin{array}{c|ccccc}
 & 0 & 1 & 2 & 3 & 4 \\
\hline
0 & S^0 & S^x & S^y & S^z & 0 \\
1 & 0 & 0 & 0 & 0 & S^x \\
2 & 0 & 0 & 0 & 0 & S^y \\
3 & 0 & 0 & 0 & 0 & S^z \\
4 & 0 & 0 & 0 & 0 & S^0 \\
\end{array}
$$

- full Hamiltonian

$$S_1^x S_2^x S_3^0 S_4^0 = \boxed{L} - 0 - \boxed{S^x} - 1 - \boxed{S^x} - 4 - \boxed{S^0} - 4 - \boxed{S^0} - 4 - \boxed{R}$$

$$S_1^0 S_2^x S_3^x S_4^0 = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^x} - 1 - \boxed{S^x} - 4 - \boxed{S^0} - 4 - \boxed{R}$$

$$S_1^0 S_2^0 S_3^x S_4^x = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^0} - 0 - \boxed{S^x} - 1 - \boxed{S^x} - 4 - \boxed{R}$$

$$S_1^y S_2^y S_3^0 S_4^0 = \boxed{L} - 0 - \boxed{S^y} - 2 - \boxed{S^y} - 4 - \boxed{S^0} - 4 - \boxed{S^0} - 4 - \boxed{R}$$

$$S_1^0 S_2^y S_3^y S_4^0 = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^y} - 2 - \boxed{S^y} - 4 - \boxed{S^0} - 4 - \boxed{R}$$

$$S_1^0 S_2^0 S_3^y S_4^y = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^0} - 0 - \boxed{S^y} - 2 - \boxed{S^y} - 4 - \boxed{R}$$

$$S_1^z S_2^z S_3^0 S_4^0 = \boxed{L} - 0 - \boxed{S^z} - 3 - \boxed{S^z} - 4 - \boxed{S^0} - 4 - \boxed{S^0} - 4 - \boxed{R}$$

$$S_1^0 S_2^z S_3^z S_4^0 = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^z} - 3 - \boxed{S^z} - 4 - \boxed{S^0} - 4 - \boxed{R}$$

$$S_1^0 S_2^0 S_3^z S_4^z = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^0} - 0 - \boxed{S^z} - 3 - \boxed{S^z} - 4 - \boxed{R}$$

MPO of transverse field Ising model

- $N = 4$, $D_{\mathrm{mpo}} = 3$

$$H = \sum_i \left(-S_i^z S_{i+1}^z + g S_i^x\right)$$

- blocks

- full Hamiltonian

$$\boxed{L} - 0 \qquad 2 - \boxed{R}$$

$$g\, S_1^x S_2^0 S_3^0 S_4^0 = \boxed{L} - 0 - \boxed{gS^x} - 2 - \boxed{S^0} - 2 - \boxed{S^0} - 2 - \boxed{S^0} - 2 - \boxed{R}$$

$$0 - \boxed{gS^x} - 2$$

$$g\, S_1^0 S_2^x S_3^0 S_4^0 = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{gS^x} - 2 - \boxed{S^0} - 2 - \boxed{S^0} - 2 - \boxed{R}$$

$$0 - \boxed{-S^z} - 1 \qquad 1 - \boxed{S^z} - 2$$

$$g\, S_1^0 S_2^0 S_3^x S_4^0 = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^0} - 0 - \boxed{gS^x} - 2 - \boxed{S^0} - 2 - \boxed{R}$$

$$0 - \boxed{S^0} - 0 \qquad 2 - \boxed{S^0} - 2$$

$$g\, S_1^0 S_2^0 S_3^0 S_4^x = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^0} - 0 - \boxed{S^0} - 0 - \boxed{gS^x} - 2 - \boxed{R}$$

- MPO

$$-S_1^z S_2^z S_3^0 S_4^0 = \boxed{L} - 0 - \boxed{-S^z} - 1 - \boxed{S^z} - 2 - \boxed{S^0} - 2 - \boxed{S^0} - 2 - \boxed{R}$$

$$
\begin{array}{c|ccc}
 & 0 & 1 & 2 \\
\hline
0 & S^0 & -S^z & gS^x \\
1 & 0 & 0 & S^z \\
2 & 0 & 0 & S^0
\end{array}
$$

$$-S_1^0 S_2^z S_3^z S_4^0 = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{-S^z} - 1 - \boxed{S^z} - 2 - \boxed{S^0} - 2 - \boxed{R}$$

$$-S_1^0 S_2^0 S_3^z S_4^z = \boxed{L} - 0 - \boxed{S^0} - 0 - \boxed{S^0} - 0 - \boxed{-S^z} - 1 - \boxed{S^z} - 2 - \boxed{R}$$

- questions:

how about next-nearest-neighbour terms?

how about periodic boundary condition?

Finite automata for MPO

- for an arbitrary Hamiltonian

$$H = \sum_i S_i$$

$$+ \sum_i A_i A'_{i+1} + \sum_i B_i B'_{i+1} + \sum_i C_i C'_{i+1} + \cdots$$

$$+ \sum_i A_i A''_{i+2} + \cdots$$

$$+ \sum_i A_i A'''_{i+3} + \cdots$$

(1) initial site $\boxed{0}$ and on-site term S

(2) add arrow and circle for each A_i, B_i, C_i, …

(3) add arrow and circle for each 2-body term, 3-body term, 4-body term …

(4) connect to the final site $\boxed{K}$