Matrix Product States

Ying-Jer Kao
Department of Physics
National Taiwan University

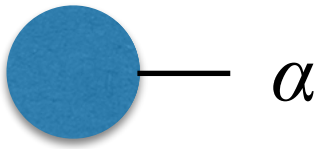
MOST 科技部
Ministry of Science and Technology

Graphical Representation

$$A = \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ \vdots \\ A_N \end{bmatrix}$$

vector

$$A_\alpha$$



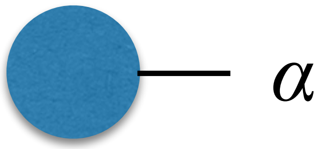
Graphical Representation

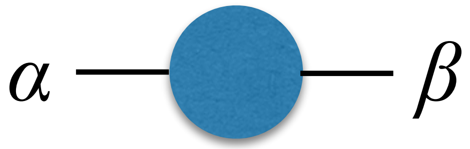
$$A = \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ \vdots \\ A_N \end{bmatrix} \quad B = \begin{bmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{m1} & \cdots & B_{mn} \end{bmatrix}$$

vector

matrix

$$A_\alpha \qquad B_{\alpha\beta}$$



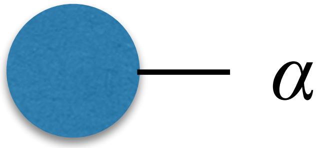


Graphical Representation

$$A = \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ \vdots \\ A_N \end{bmatrix} \quad B = \begin{bmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{m1} & \cdots & B_{mn} \end{bmatrix}$$

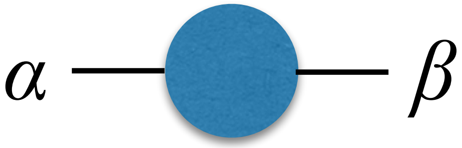
vector

A_α



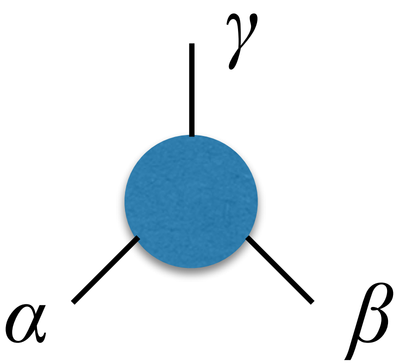
matrix

$B_{\alpha\beta}$



rank-3 tensor

$C_{\alpha\beta\gamma}$

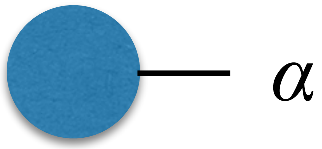


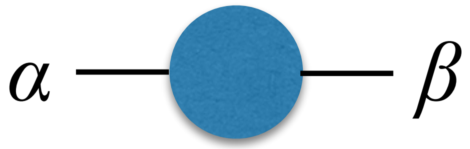
Graphical Representation

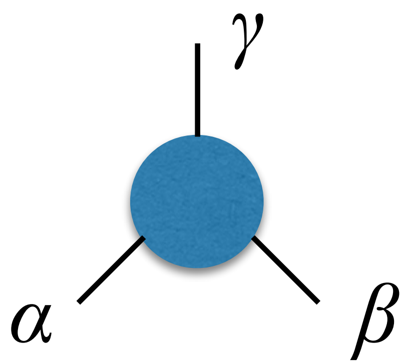
$$A = \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ \vdots \\ A_N \end{bmatrix} \quad B = \begin{bmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{m1} & \cdots & B_{mn} \end{bmatrix}$$

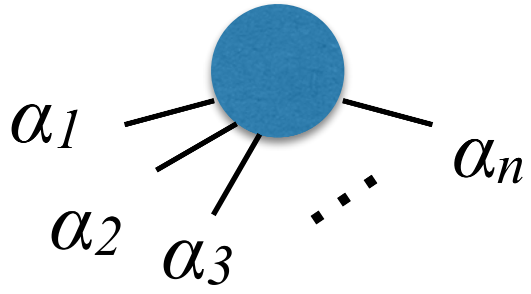
vector | matrix | rank-3 tensor | rank-*n* tensor

A_α $\quad$ $B_{\alpha\beta}$ $\quad$ $C_{\alpha\beta\gamma}$ $\quad$ $T_{\alpha_1\alpha_2\alpha_3\ldots\alpha_n}$









Graphical Representation

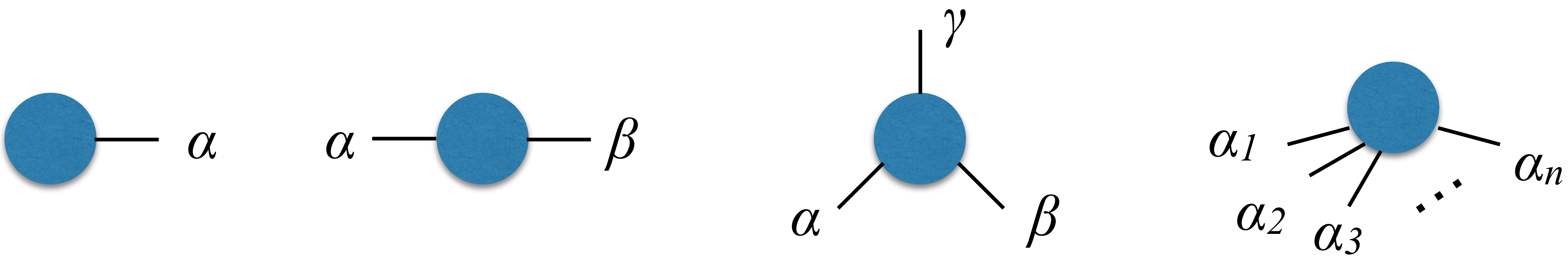
$$A = \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ \vdots \\ A_N \end{bmatrix} \quad B = \begin{bmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{m1} & \cdots & B_{mn} \end{bmatrix}$$

scalar

S

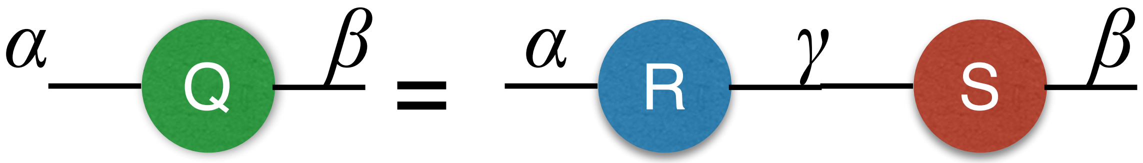
vector matrix rank-3 tensor rank-*n* tensor

A_α $B_{\alpha\beta}$ $C_{\alpha\beta\gamma}$ $T_{\alpha_1\alpha_2\alpha_3\ldots\alpha_n}$



Graphical Representation

product of tensors (matrices)

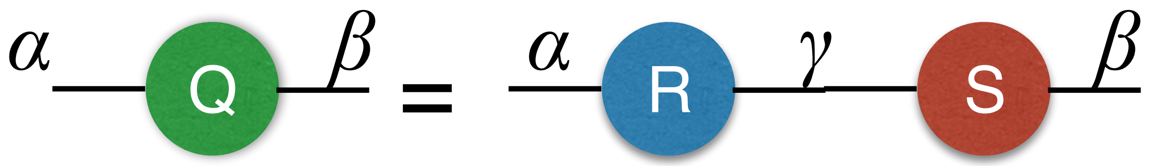


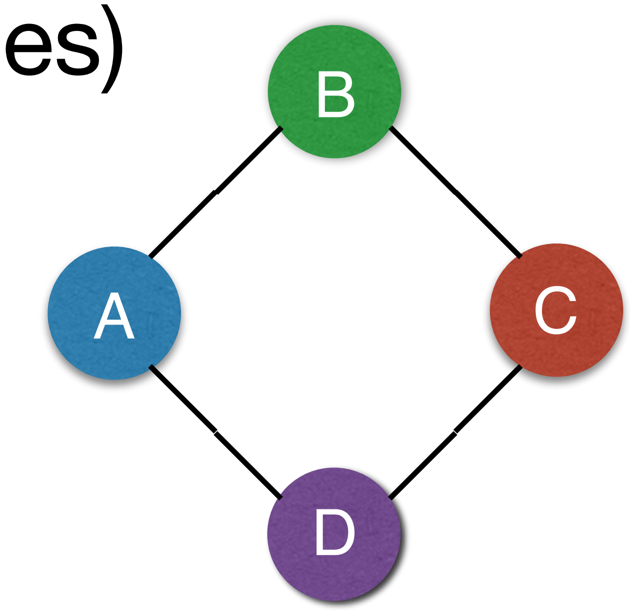
$$Q_{\alpha\beta} = \sum_{\gamma} R_{\alpha\gamma} S_{\gamma\beta}$$

- Internal lines are summed over
- External lines are external indices

Graphical Representation

product of tensors (matrices)



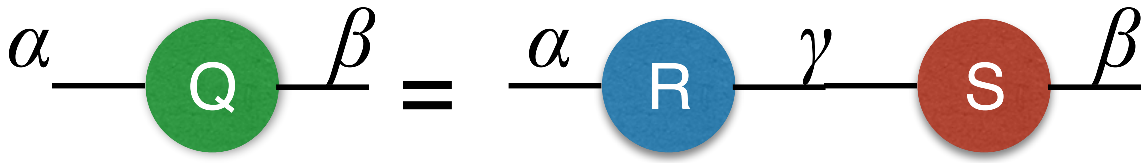


$$Q_{\alpha\beta} = \sum_{\gamma} R_{\alpha\gamma} S_{\gamma\beta}$$

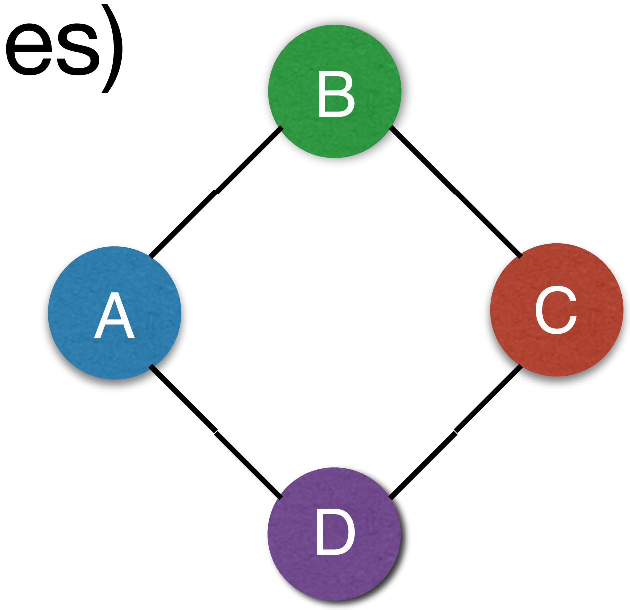
- Internal lines are summed over
- External lines are external indices

Graphical Representation

product of tensors (matrices)



$$Q_{\alpha\beta} = \sum_{\gamma} R_{\alpha\gamma} S_{\gamma\beta}$$

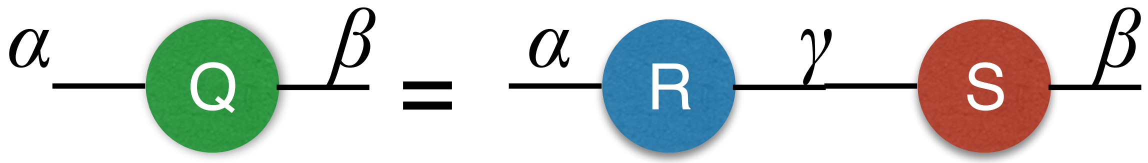


$$\mathrm{Tr}(ABCD)$$

- Internal lines are summed over
- External lines are external indices

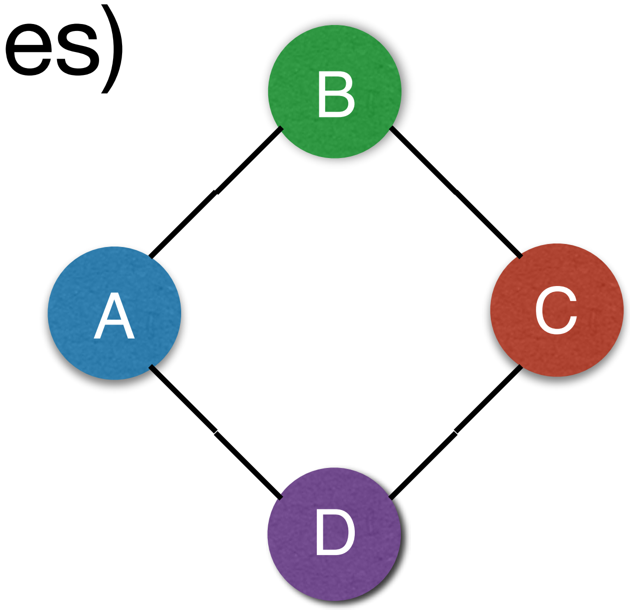
Graphical Representation

product of tensors (matrices)

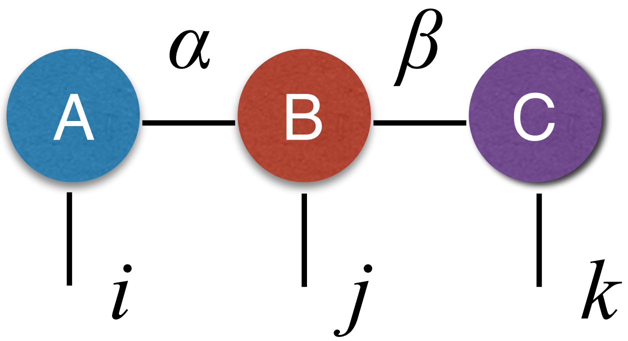


$$Q_{\alpha\beta} = \sum_{\gamma} R_{\alpha\gamma} S_{\gamma\beta}$$

- Internal lines are summed over
- External lines are external indices

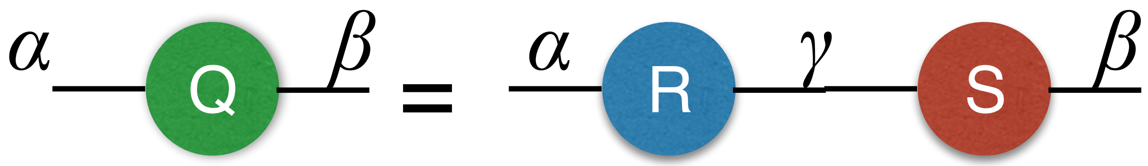


$$\mathrm{Tr}(ABCD)$$



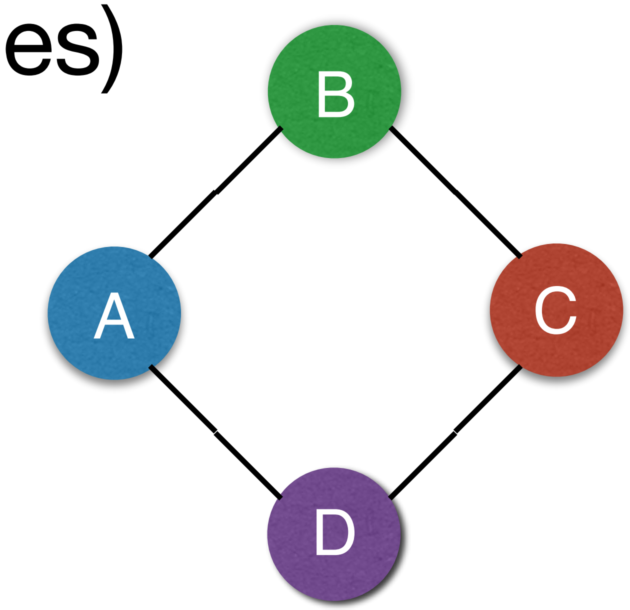
Graphical Representation

product of tensors (matrices)

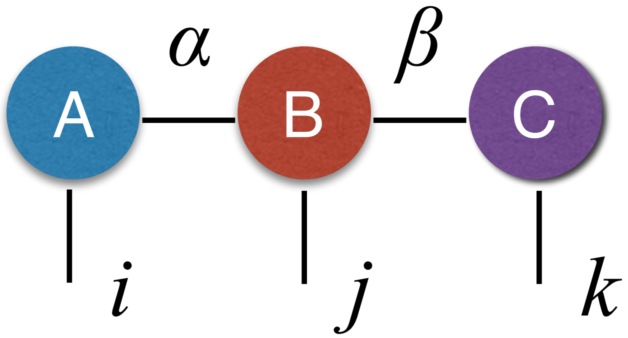


$$Q_{\alpha\beta} = \sum_{\gamma} R_{\alpha\gamma} S_{\gamma\beta}$$

- Internal lines are summed over
- External lines are external indices



$$\mathrm{Tr}(ABCD)$$



$$T_{ijk} = \sum_{\alpha\beta} A_{\alpha i} B_{\alpha\beta j} C_{\beta k}$$

Graphical Representation

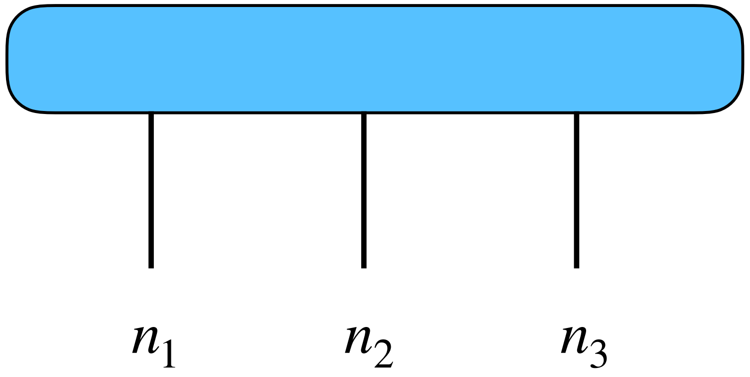
Wavefunction

$$|\Psi\rangle = \sum_{n_1 n_2 n_3} \Psi_{n_1 n_2 n_3} \left|n_1 n_2 n_3\right\rangle$$

$$\left|n\right\rangle = \{|\uparrow\rangle, |\downarrow\rangle\}$$

$$\left|n\right\rangle = \{|0\rangle, |1\rangle, |2\rangle, \ldots\}$$

$$\psi_{n_1 n_2 n_3} =$$



rank-3 tensor

physical index

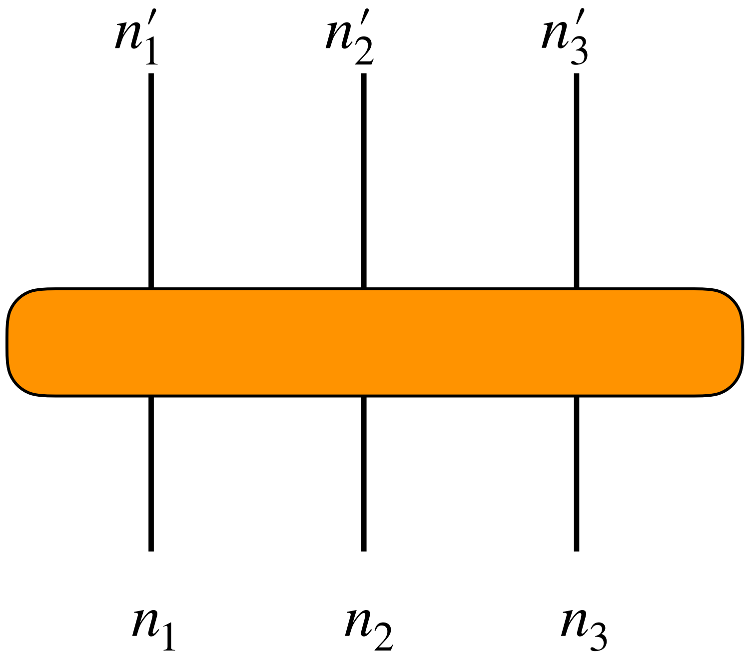
Graphical Representation

Operator

$$\hat{O} = \sum_{nn'} O^{n_1'n_2'n_3'}_{n_1n_2n_3} \left|n_1n_2n_3\right\rangle \left\langle n_1'n_2'n_3'\right|$$

physical index

$$O^{n_1'n_2'n_3'}_{n_1n_2n_3} =$$



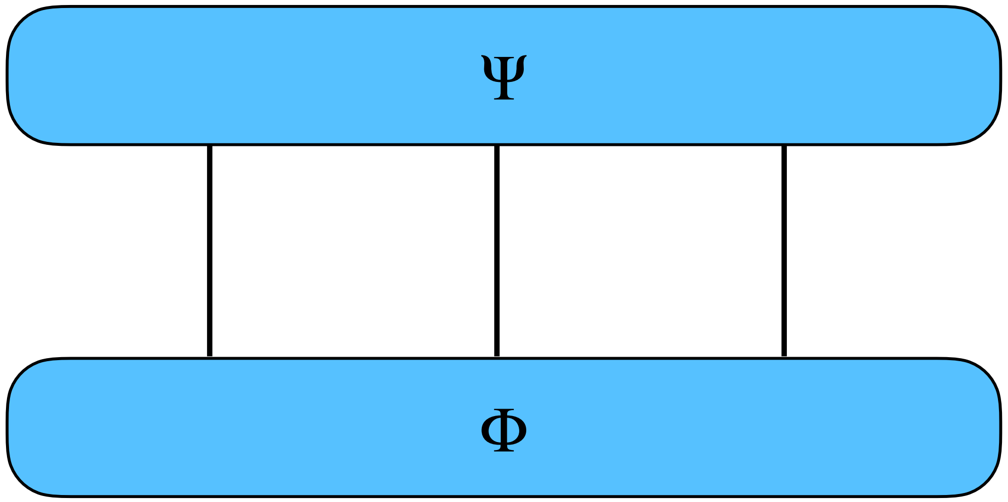
rank-6 tensor

physical index

Graphical Representation

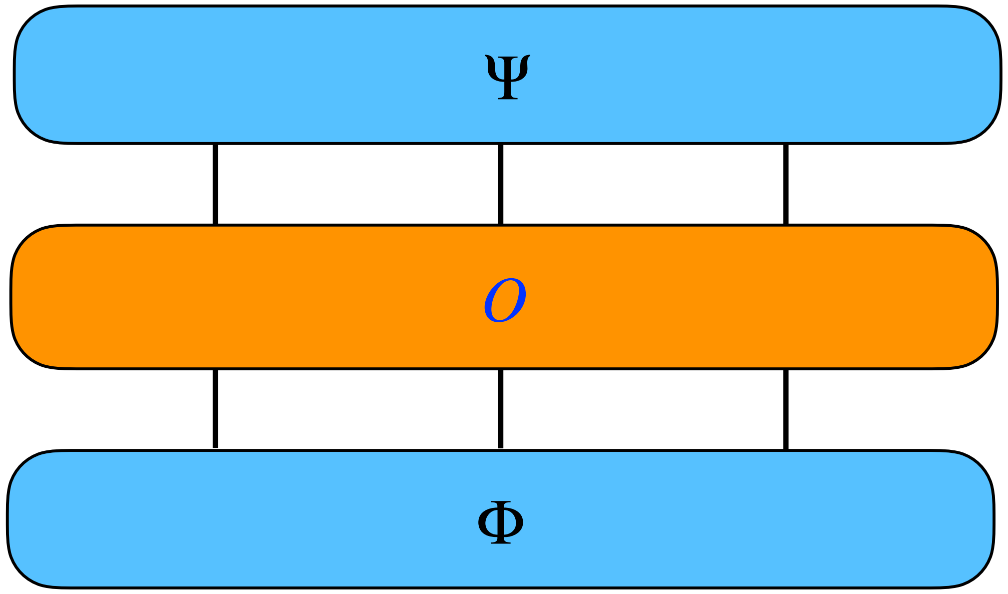
Overlap

$$\langle \Phi | \Psi \rangle = \sum_{n} \Phi^{n_1 n_2 n_3} \Psi_{n_1 n_2 n_3}$$

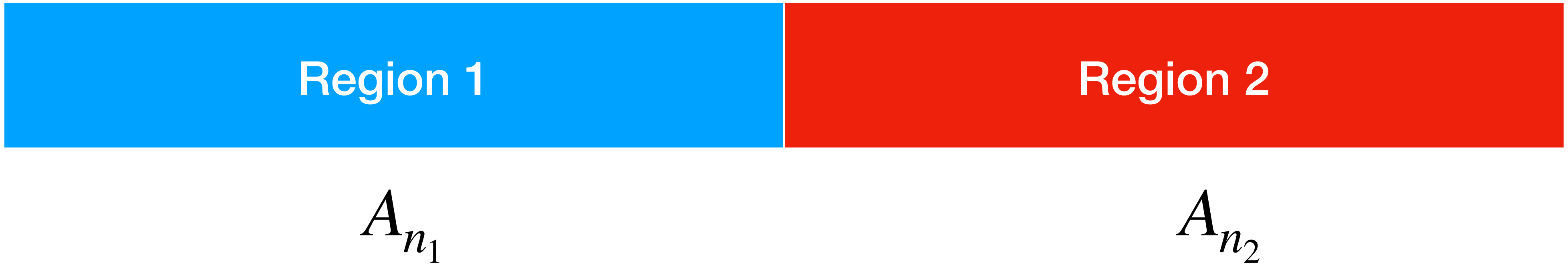


Expectation value

$$\langle \Phi | \hat{O} | \Psi \rangle = \sum_{n,n'} \Phi^{n_1' n_2' n_3'} O^{n_1 n_2 n_3}_{n_1' n_2' n_3'} \Psi_{n_1 n_2 n_3}$$



Entanglement

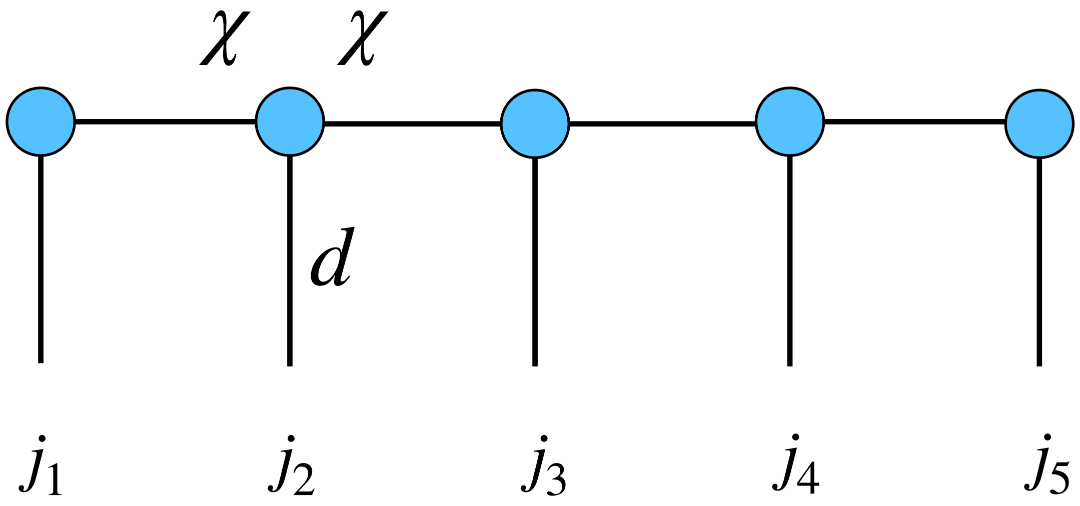


- Consider two parts of a system represented by A_{n_1} and A_{n_2}
  - If the two parts are not entangled: $\psi_{n_1 n_2} = A_{n_1} A_{n_2}$
  - If they are entangled: $\psi_{n_1 n_2} = \sum_i A^i_{n_1} A^i_{n_2}$
  - If the number of the terms in the sum is small, the two parts have low entanglement

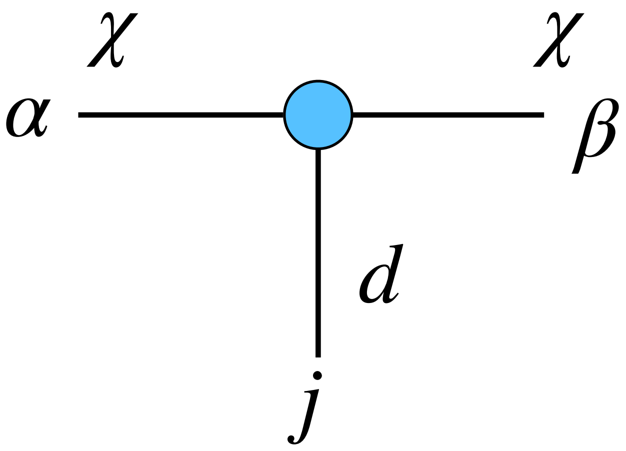
Matrix Product States

- If we keep only χ virtual bond dimensions , we have an approximate wave function in MPS
- Size of Hilbert space: $d^L \rightarrow \chi^2 dL$

$$\psi_{j_1,j_2,j_3,j_4,j_5} \approx$$

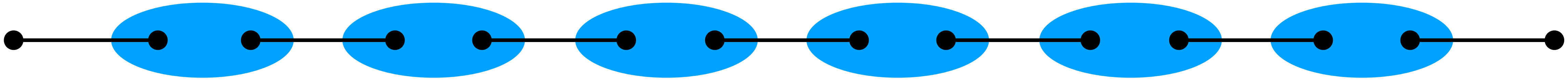


$$A^j_{\alpha\beta} =$$

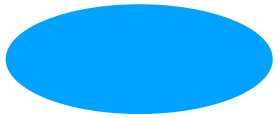


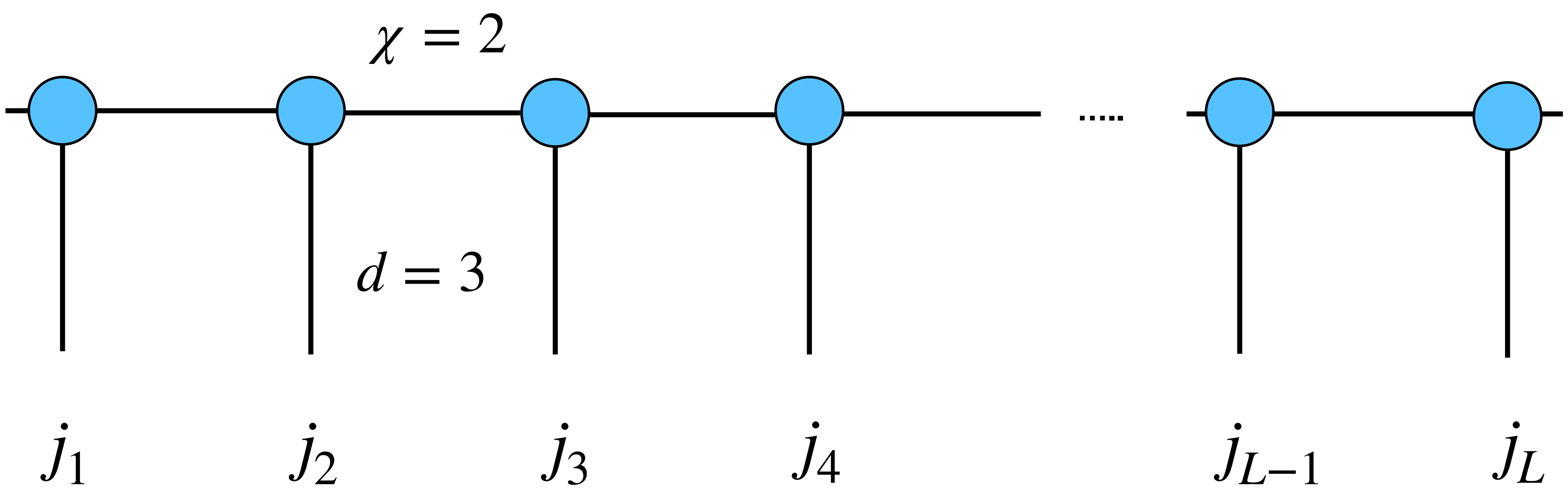
$$\left|\psi\right\rangle = \sum_{j_1,j_2,\ldots,j_L} A_1^{j_1} A_2^{j_2} \cdots A_L^{j_L} \left|j_1 j_2 \ldots j_L\right\rangle$$

AKLT state



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

 $= |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$



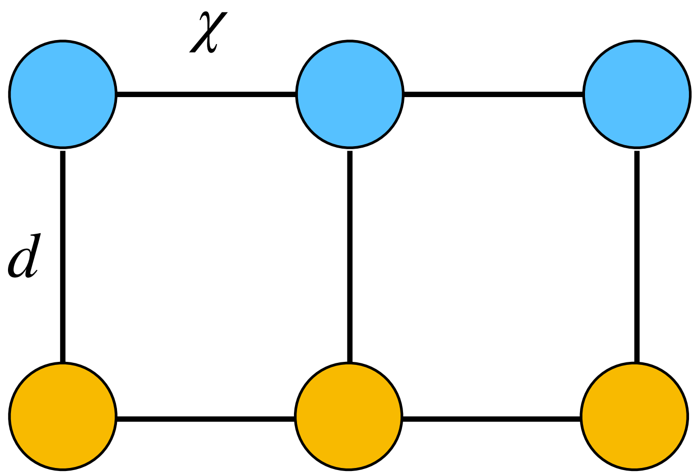
$$|\psi\rangle = \sum_{\{s\}} \mathrm{tr}\left[A^{s_1}A^{s_2}\ldots A^{s_N}\right]\left|s_1 s_2 \ldots s_N\right\rangle$$

$$A^+ = \begin{bmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix}, A^0 = \begin{bmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{bmatrix}, A^- = \begin{bmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{bmatrix}$$

MPS contraction

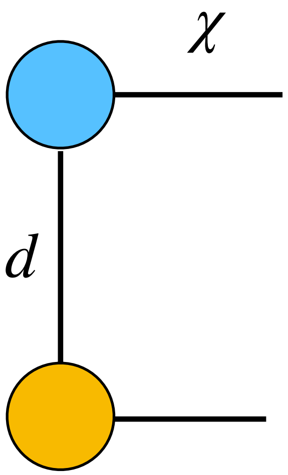
Overlap

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



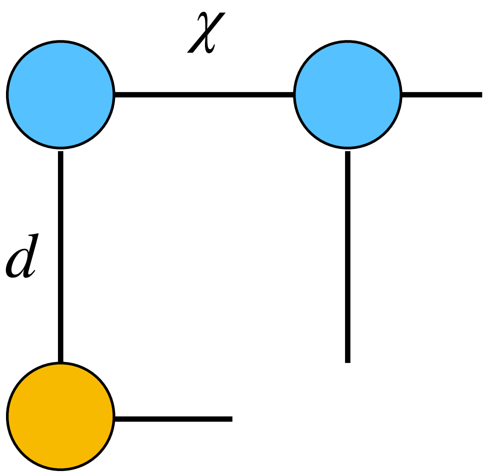
Efficient Contraction

(1)



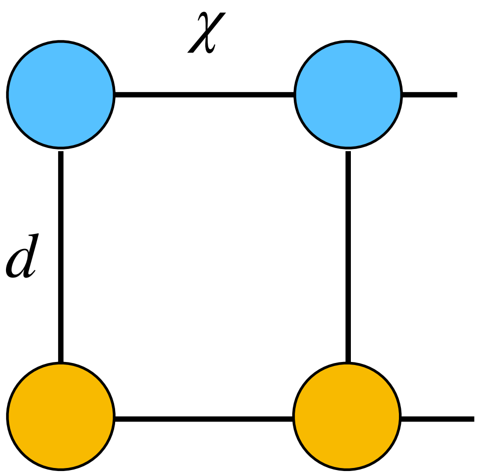
$O(\chi^2 d)$

(2)



$O(\chi^3 d)$

(3)



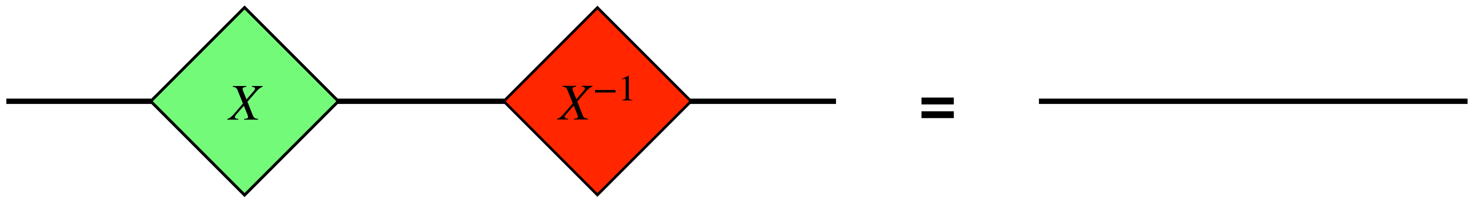
$O(\chi^3 d)$

Total cost: $O(\chi^3 dL)$

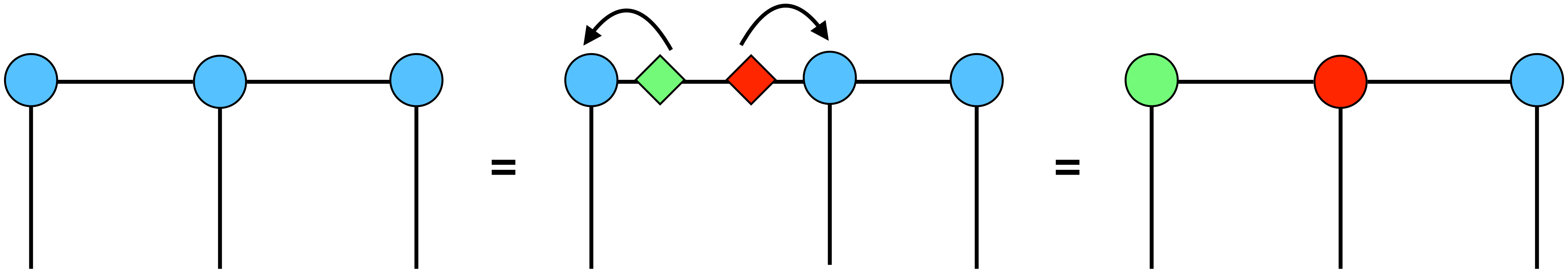
Gauge Choice

- MPS representation is not unique

$$XX^{-1} = I$$



insert gauge matrices



Entanglement

- A generic quantum state has a d^L dimensional Hilbert space
  $$|\psi\rangle = \sum_{j_1,j_2,\ldots,j_L} \psi_{j_1,j_2,\ldots,j_L} \left|j_1\right\rangle \left|j_2\right\rangle \ldots \left|j_L\right\rangle, j_n = 1\ldots d$$

- Decompose a state into a superposition of product states (Schmidt decomposition)

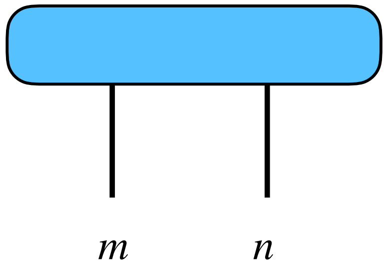
$$|\psi\rangle = \sum_{i,j} C_{i,j} |i\rangle_A \otimes |j\rangle_B = \sum_{\alpha} \lambda_\alpha |\alpha\rangle_A \otimes |\alpha\rangle_B$$

- Entanglement entropy $S = -\operatorname{tr}\rho_A \ln \rho_A = -\sum_{\alpha} \lambda_\alpha^2 \log \lambda_\alpha^2$

Schmidt Decomposition

- Schmidt Decomposition = Singular Value Decomposition

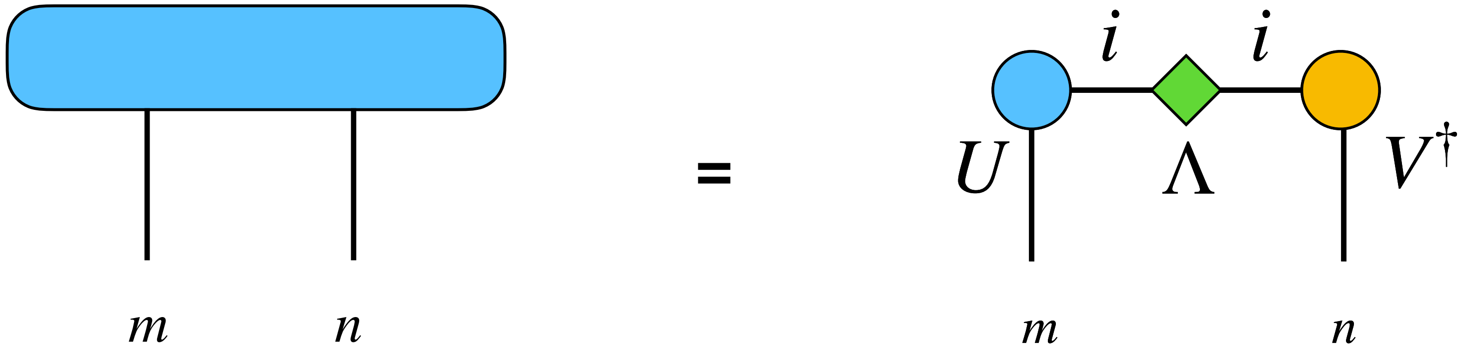
$\psi_{mn} =$



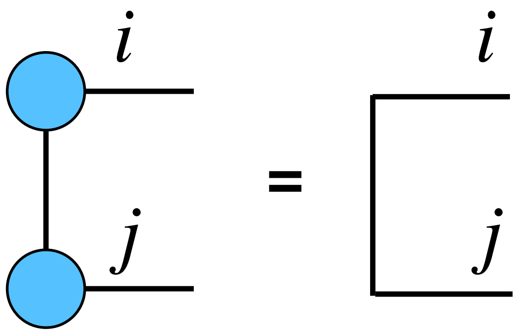
$m = \{j_1, j_2, \ldots, j_m\}$

$n = \{j_{m+1}, \ldots, j_L\}$

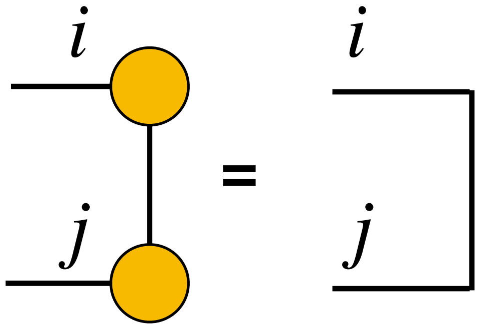
$$\psi_{mn} = \sum_i U_{mi} \Lambda_i V^*_{ni}$$



$$\sum_m U_{mi} U^*_{mj} = \delta_{ij}$$



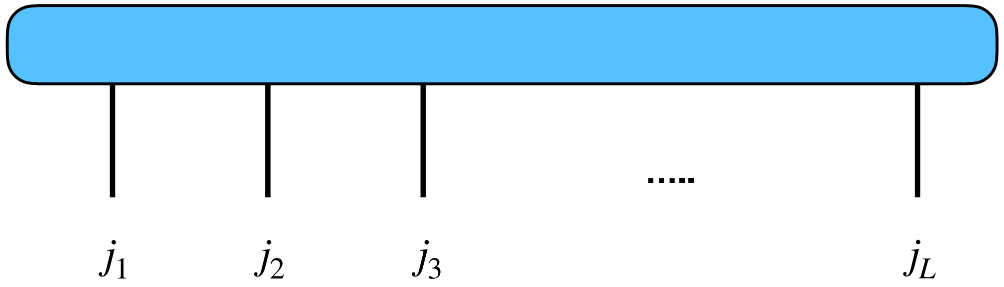
$$\sum_n V^*_{ni} V_{nj} = \delta_{ij}$$



Matrix Product States

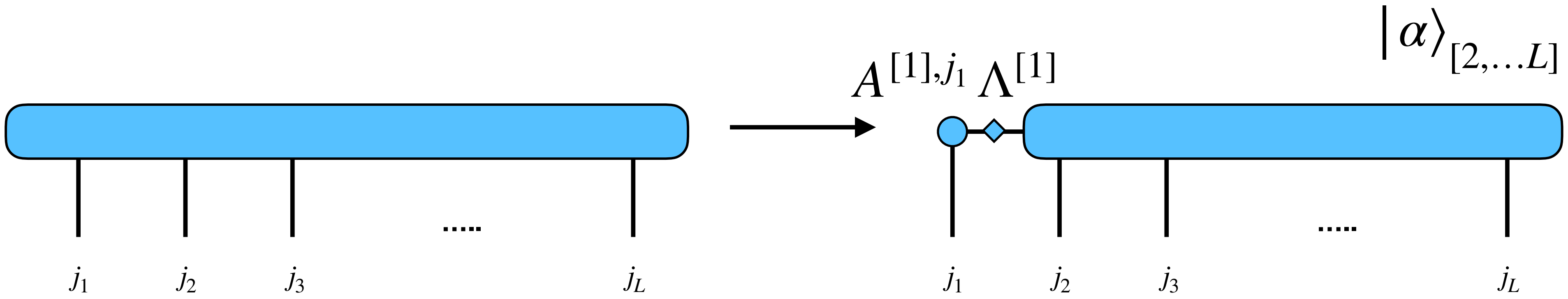
- Coefficient in a many-body wave function $\psi_{j_1,j_2,\ldots,j_L}$ is a rank-*L* tensor

$$\psi_{j_1,j_2,\ldots,j_L} =$$



- Successive Schmidt decompositions generate an MPS

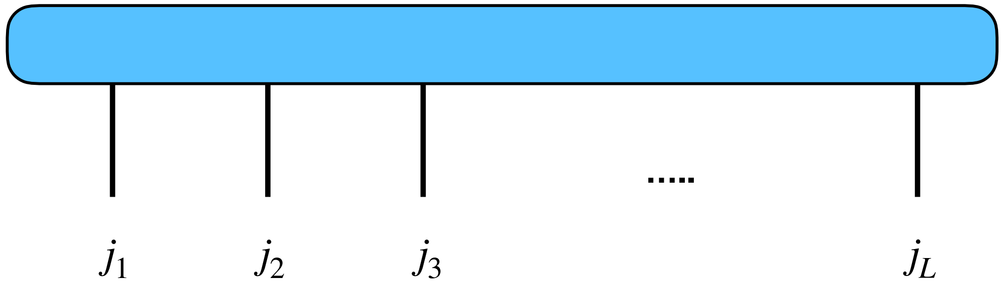
$$|\psi\rangle = \sum_{j_1=1}^{d} \sum_{\alpha=1}^{d} A_{\alpha}^{[1],j_1} \Lambda_{\alpha}^{[1]} \left|j_1\right\rangle \, |\alpha\rangle_{[2,\ldots L]}$$



Matrix Product States

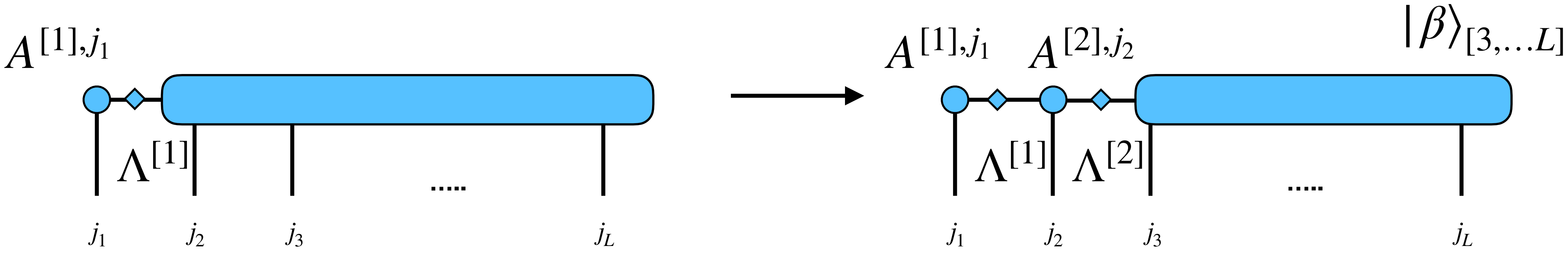
- Coefficient in a many-body wave function $\psi_{j_1,j_2,\dots,j_L}$ is a rank-*L* tensor

$\psi_{j_1,j_2,\dots,j_L} =$



- Successive Schmidt decompositions generate an MPS

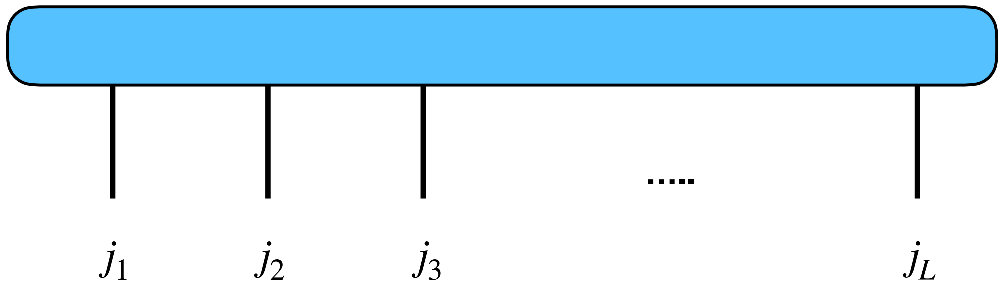
$$|\psi\rangle = \sum_{j_1,j_2}^{d}\sum_{\alpha=1}^{d}\sum_{\beta=1}^{d^2} A_{\alpha}^{[1]j_1}\Lambda_{\alpha}^{[1]}A_{\alpha\beta}^{[2]j_2}\Lambda_{\beta}^{[2]} \left|j_1\right\rangle \left|j_2\right\rangle |\beta\rangle_{[3,\dots L]}$$



Matrix Product States

- Coefficient in a many-body wave function $\psi_{j_1,j_2,\ldots,j_L}$ is a rank-*L* tensor

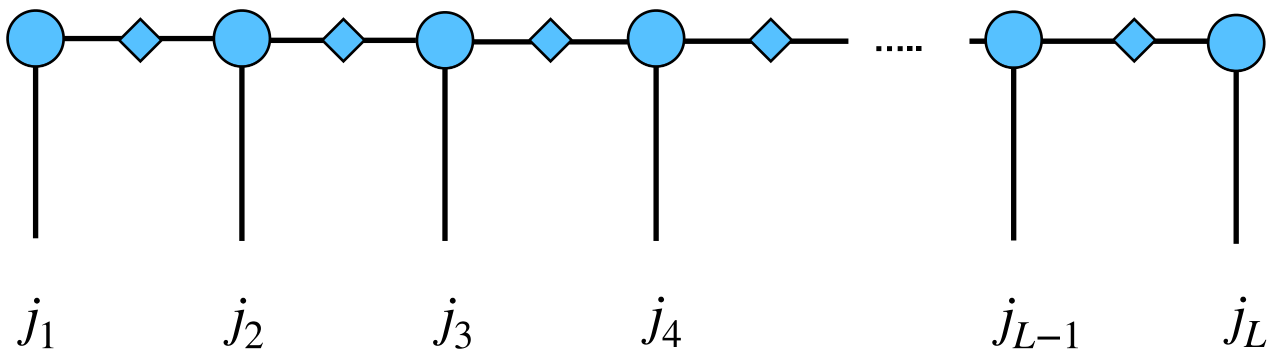
$$\psi_{j_1,j_2,\ldots,j_L} =$$



- Successive Schmidt decompositions generate an MPS

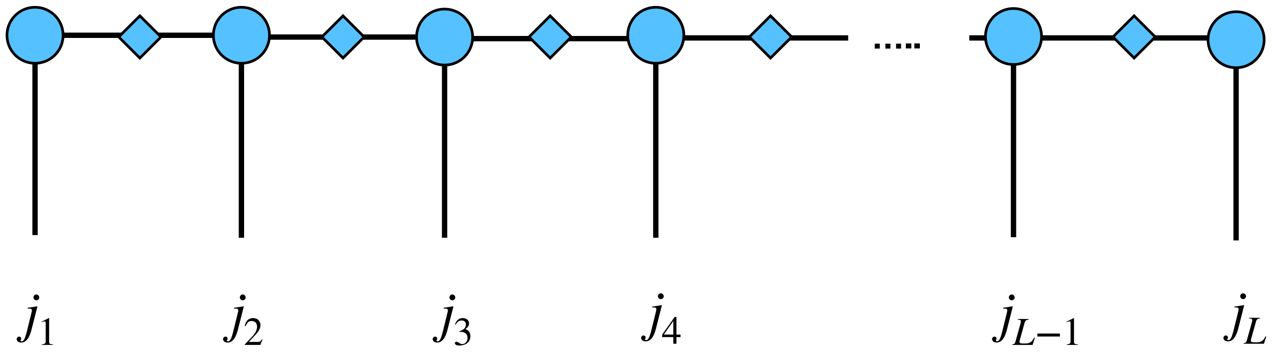
$$|\psi\rangle = \sum_{j_1,j_2,\ldots,j_L}^{d} \sum_{\alpha_1,\alpha_2,\ldots\alpha_L} A^{[1],j_1}_{\alpha_1} \Lambda^{[1]}_{\alpha_1} A^{[2],j_2}_{\alpha_1\alpha_2} \Lambda^{[2]}_{\alpha_2} \cdots \Lambda^{[L]}_{\alpha_L} A^{[L],j_L}_{\alpha_L} \left|j_1\right\rangle \left|j_2\right\rangle \cdots \left|j_L\right\rangle$$

Canonical Form



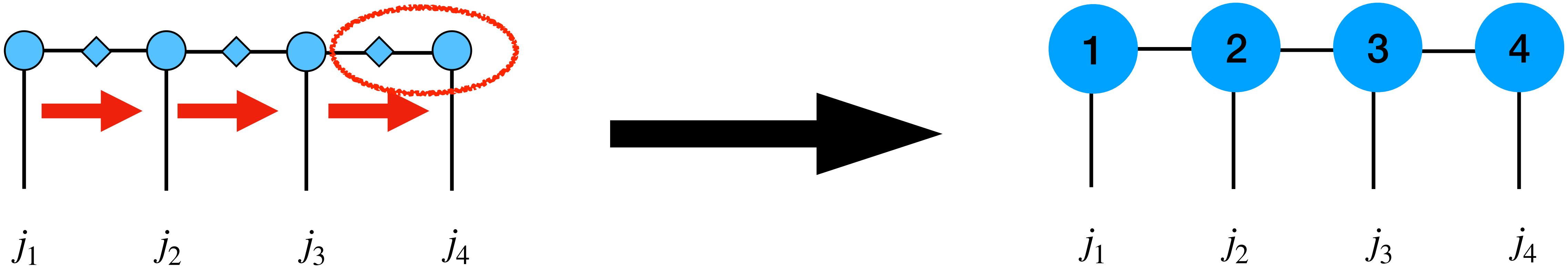
Canonical Forms

- Canonical Form (Vidal)

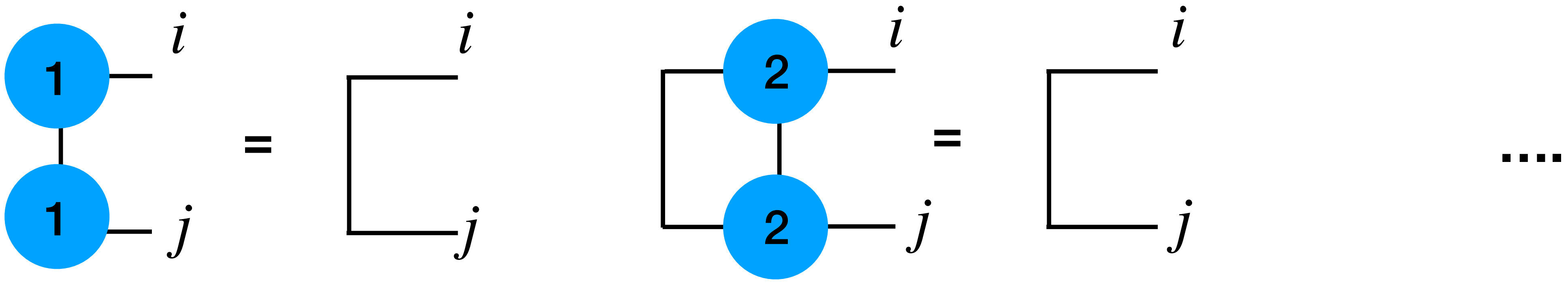


Absorb singular values into tensors

- Left Canonical Form

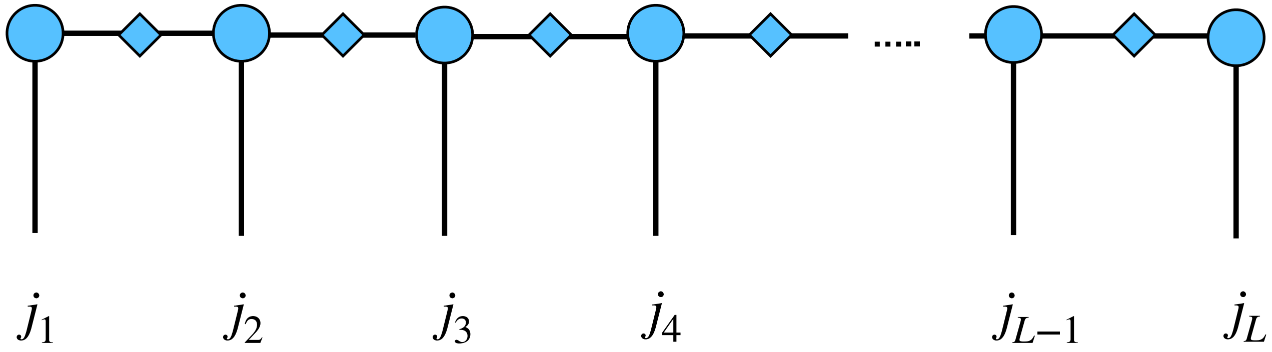


all tensors contract to identity matrix from **left**



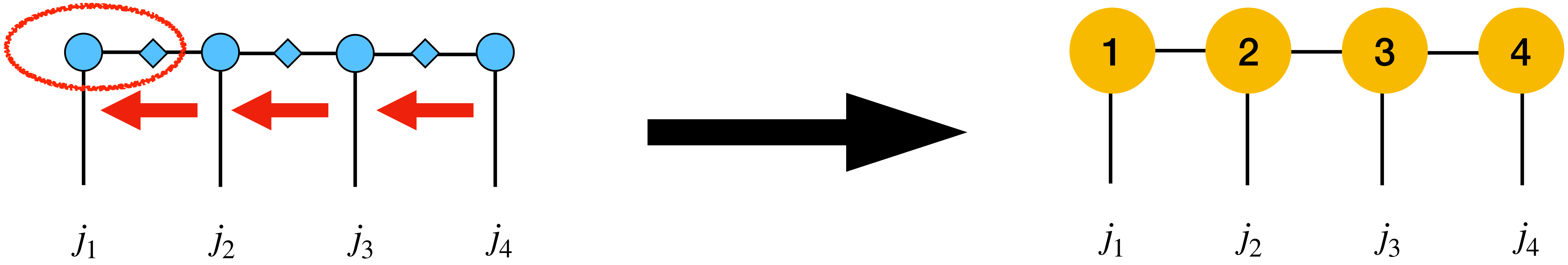
Canonical Forms

- Canonical Form (Vidal)

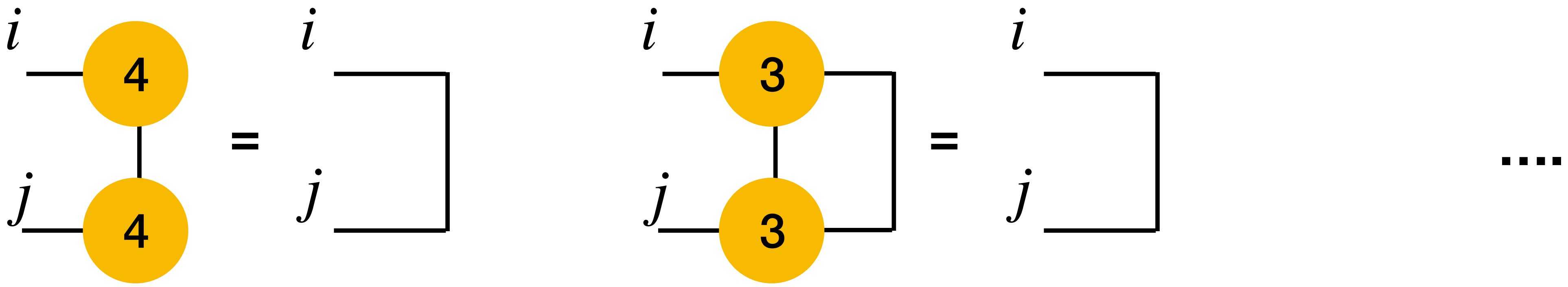


Absorb singular values into tensors

- Right Canonical Form

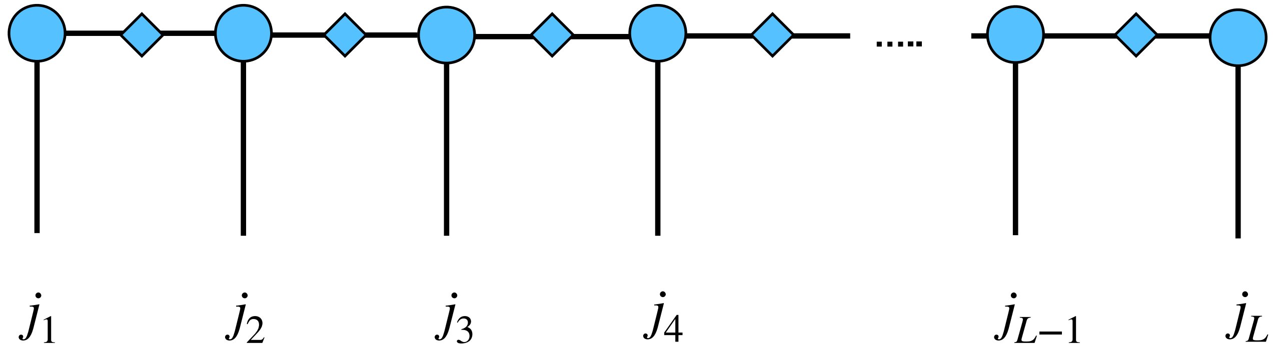


all tensors contract to identity matrix from **right**



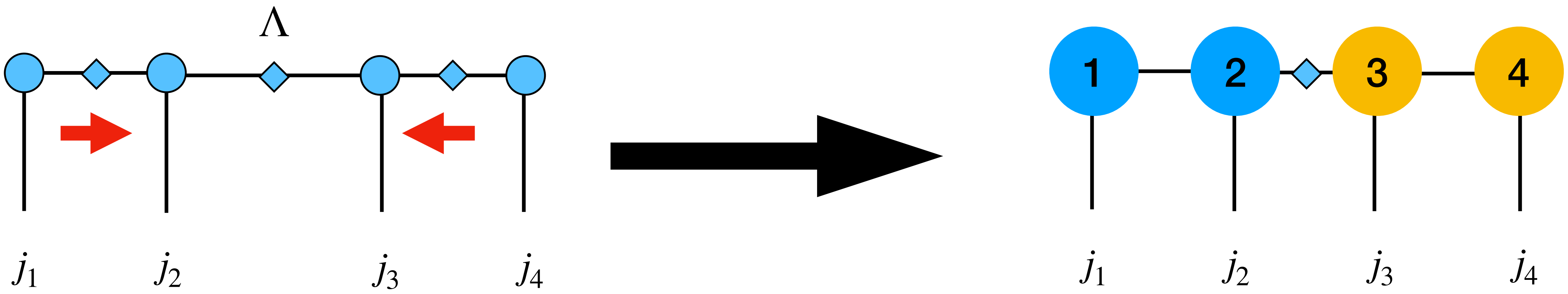
Canonical Forms

- Canonical Form (Vidal)

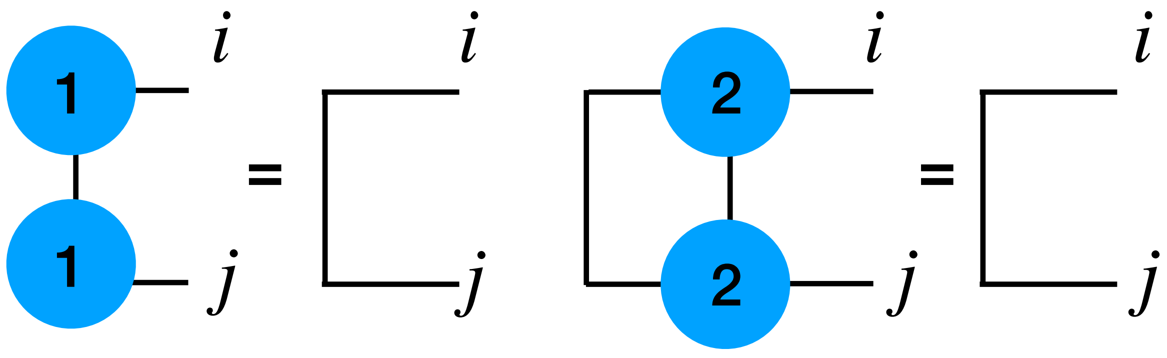


Absorb singular values into tensors

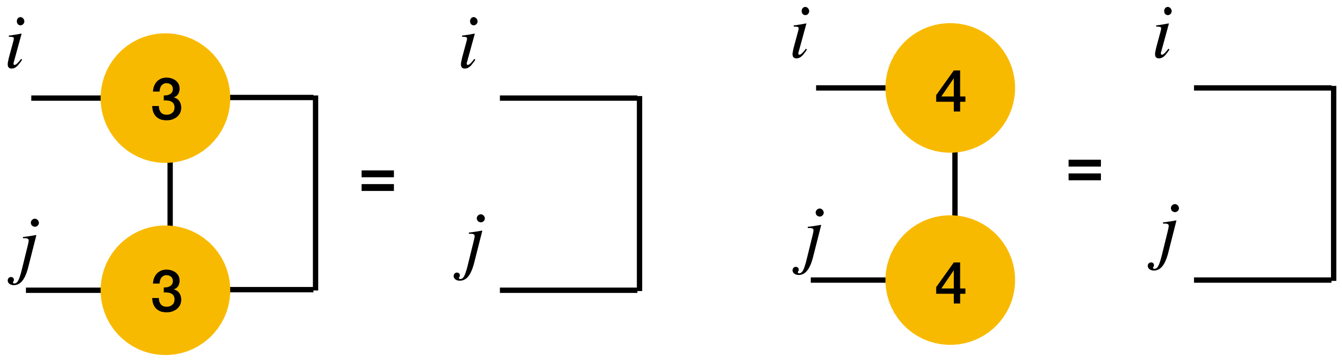
- Mixed Canonical Form (DMRG)



left canonical



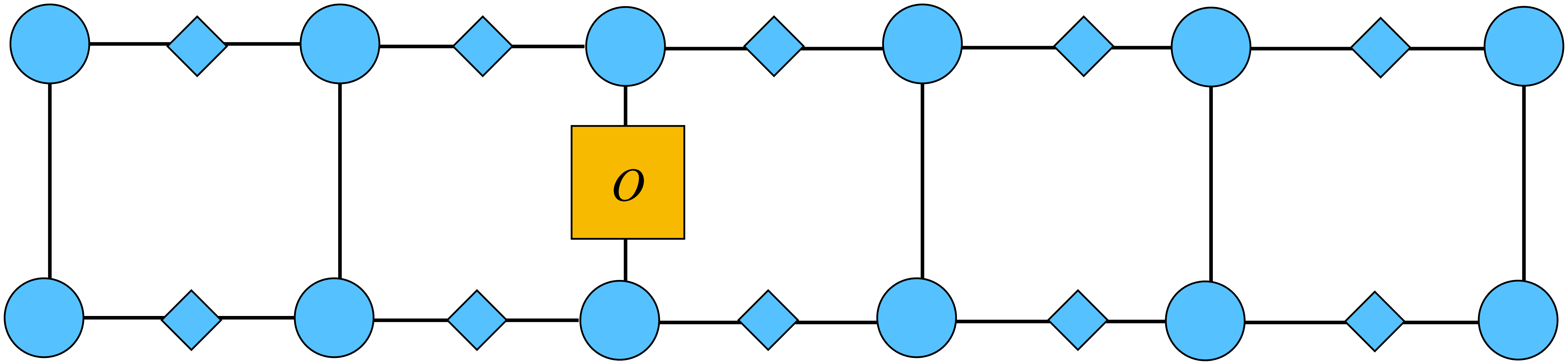
right canonical



MPS contraction

Expectation value

$$\langle \psi | O | \psi \rangle =$$



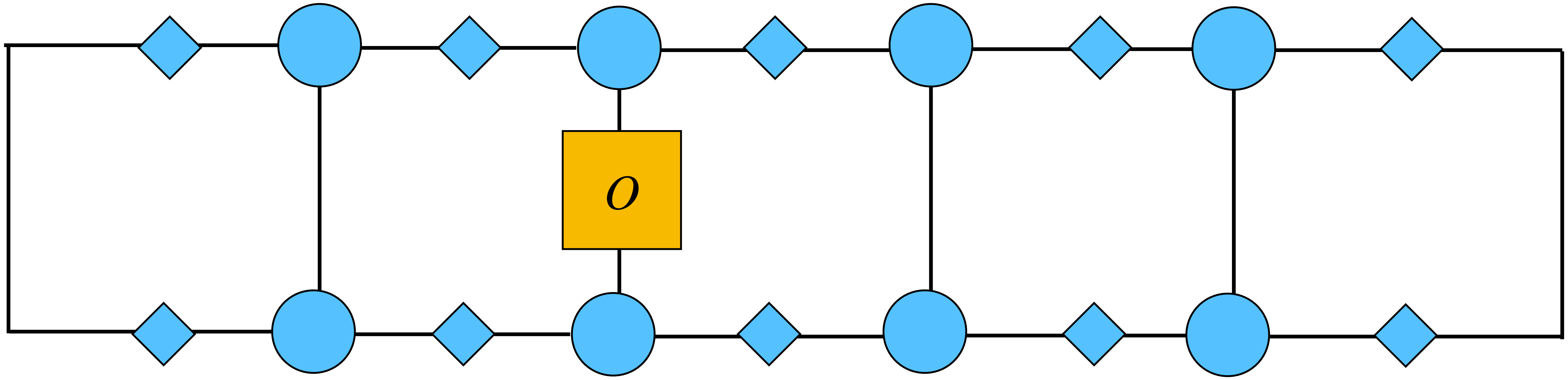
Left canonical

Right canonical

MPS contraction

Expectation value

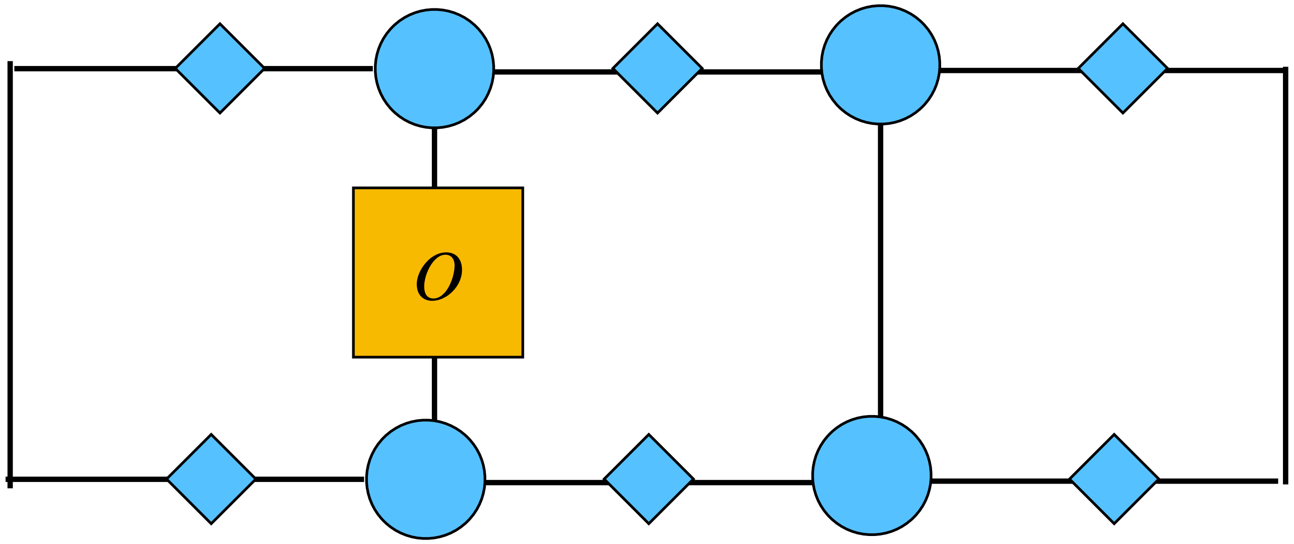
$\langle \psi \,|\, O \,|\, \psi \rangle =$



MPS contraction

Expectation value

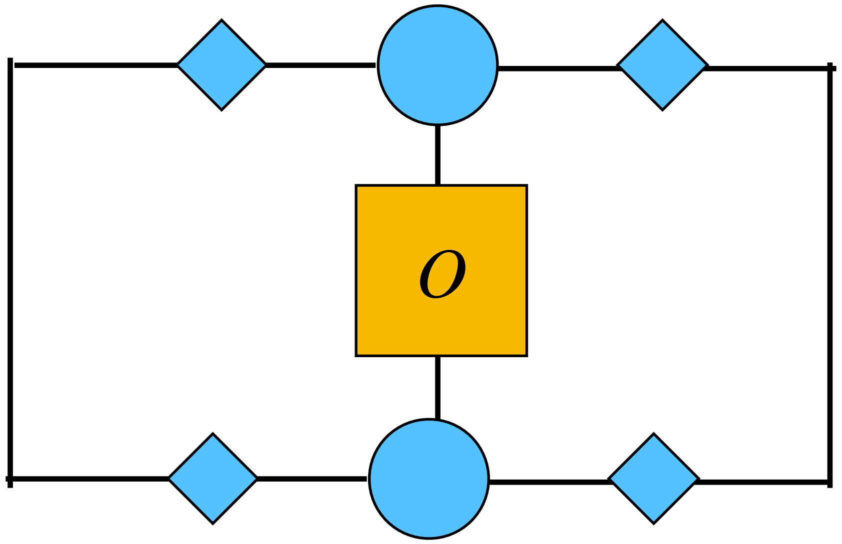
$\langle \psi | O | \psi \rangle =$



MPS contraction

Expectation value

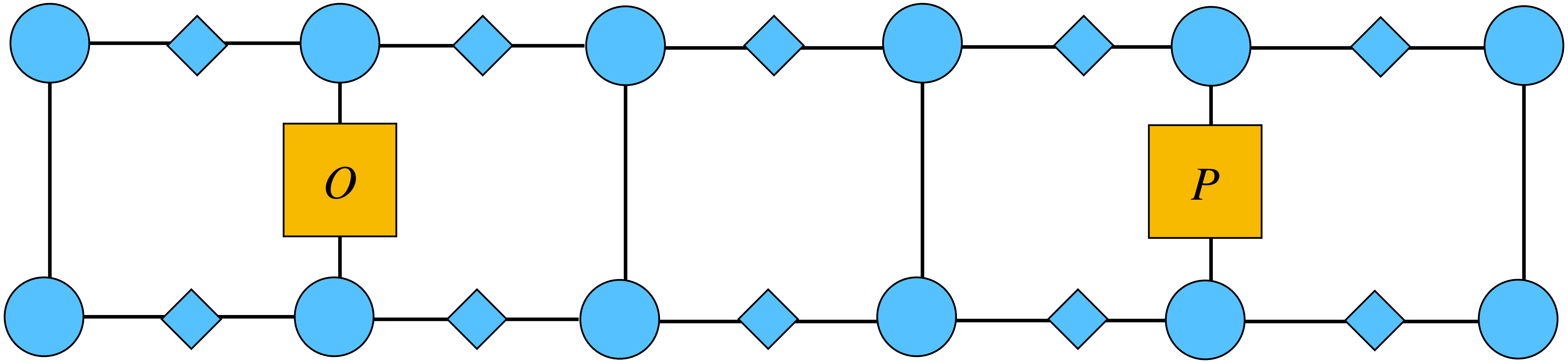
$\langle \psi | O | \psi \rangle =$



MPS contraction

Correlator

$$\langle \psi | O_i P_j | \psi \rangle =$$



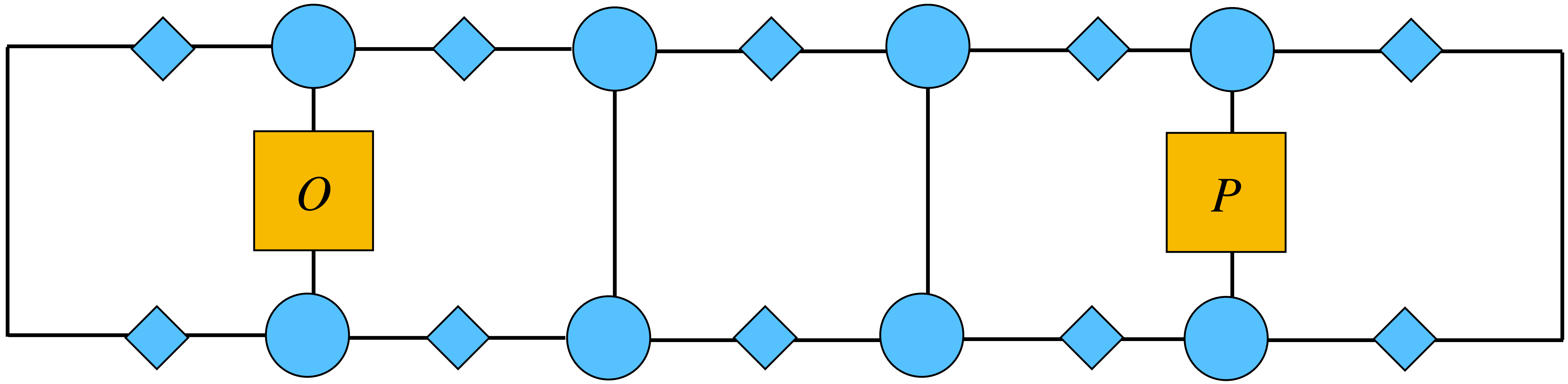
Left canonical

Right canonical

MPS contraction

Correlator

$$\langle \psi | O_i P_j | \psi \rangle =$$

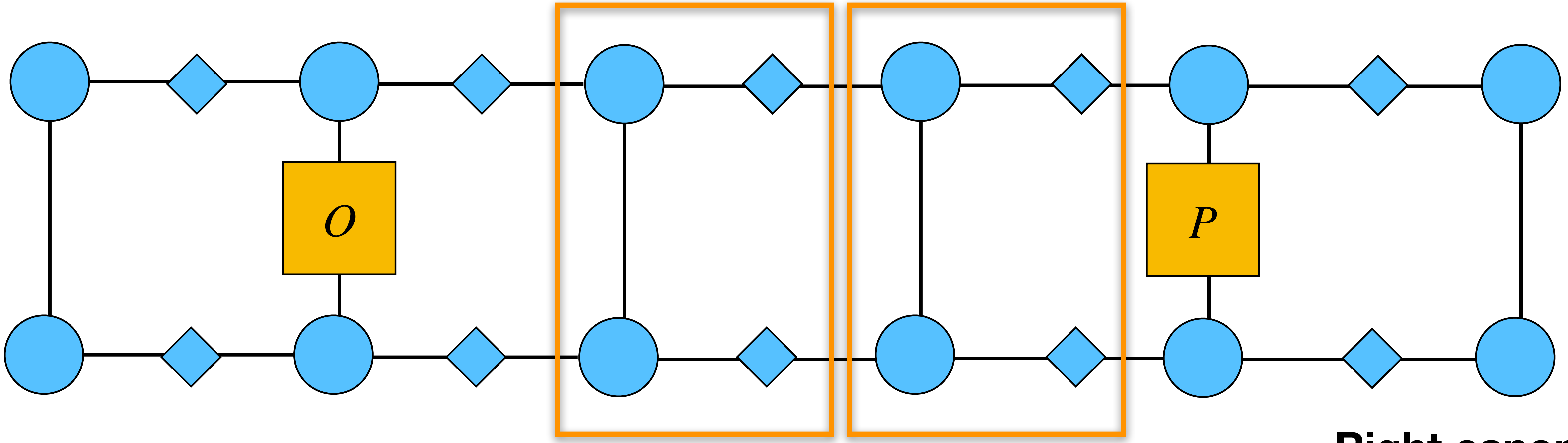


MPS contraction

Correlator

$\langle \psi | O_i P_j | \psi \rangle =$

Right ransfer matrix: T^R



Left canonical

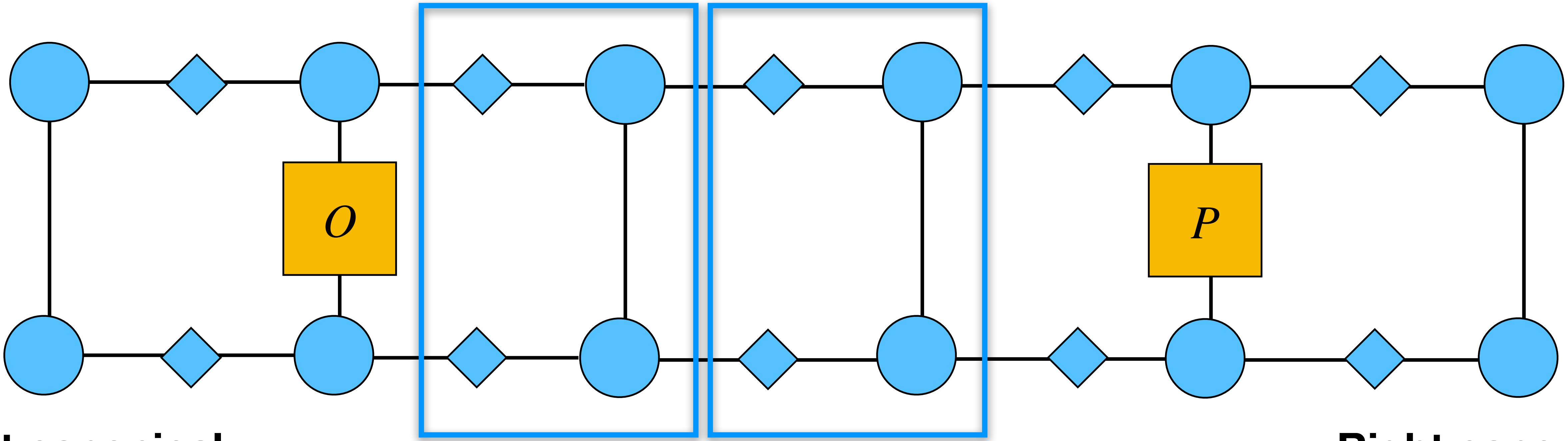
Right canonical

MPS contraction

Correlator

$\langle\psi|O_iP_j|\psi\rangle =$

Left transfer matrix: T^L



Left canonical

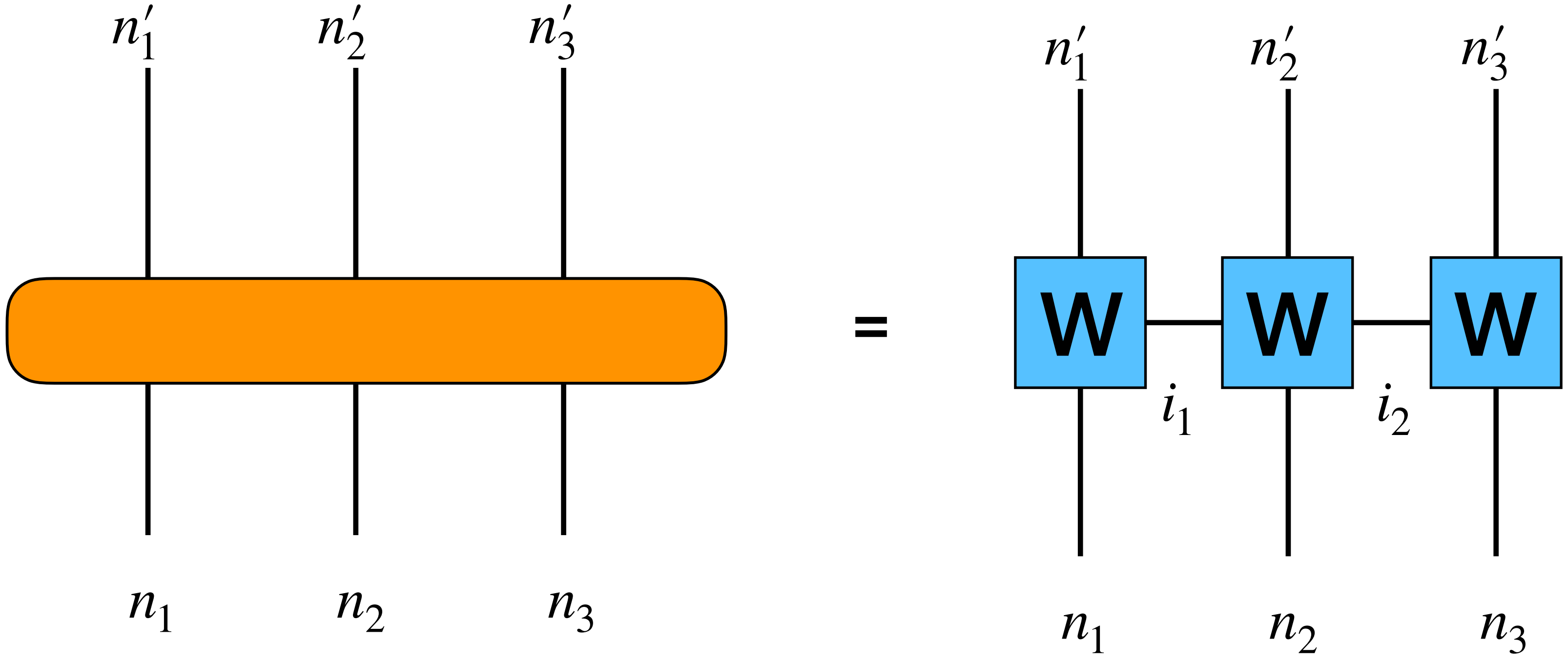
Right canonical

Matrix Product Operators

- Operator can also be represented as a matrix product form

$$O^{n_1'n_2'n_3'\dots n_l'}_{n_1n_2n_3\dots n_l} = \sum W^{i_1}_{n_1,n_1'} W^{i_1i_2}_{n_2,n_2'} W^{i_2i_3}_{n_3n_3'} \dots W^{i_l}_{n_ln_l'}$$

$$\hat{O} = \sum_i \left(\hat{A}_i \hat{B}_{i+1} + \hat{B}_i \hat{A}_{i+1} \right)$$



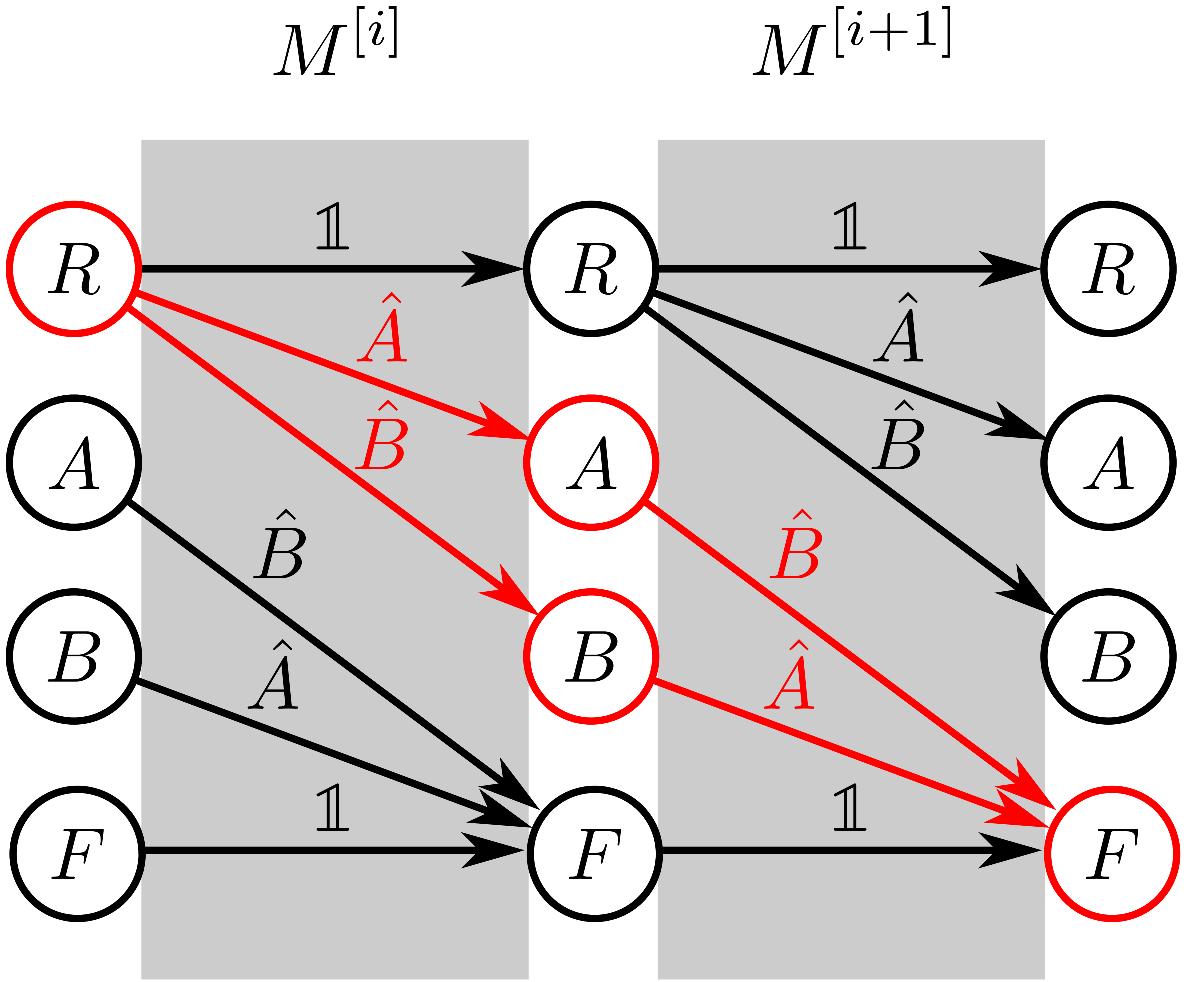
Matrix Product Operators

- MPO representation of $\hat{O} = \sum_i \left(\hat{A}_i \hat{B}_{i+1} + \hat{B}_i \hat{A}_{i+1} \right)$

$$
\begin{aligned}
&= \hat{A} \otimes \hat{B} \otimes I \otimes \cdots \otimes I \\
&\quad + I \otimes \hat{A} \otimes \hat{B} \otimes I \otimes \cdots \otimes I + \cdots \\
&\quad + \hat{B} \otimes \hat{A} \otimes I \otimes \cdots \otimes I \\
&\quad + I \otimes \hat{B} \otimes \hat{A} \otimes I \otimes \cdots \otimes I + \cdots
\end{aligned}
$$

Matrix Product Operators

- MPO representation of $\hat{O} = \sum_i \left(\hat{A}_i \hat{B}_{i+1} + \hat{B}_i \hat{A}_{i+1} \right)$

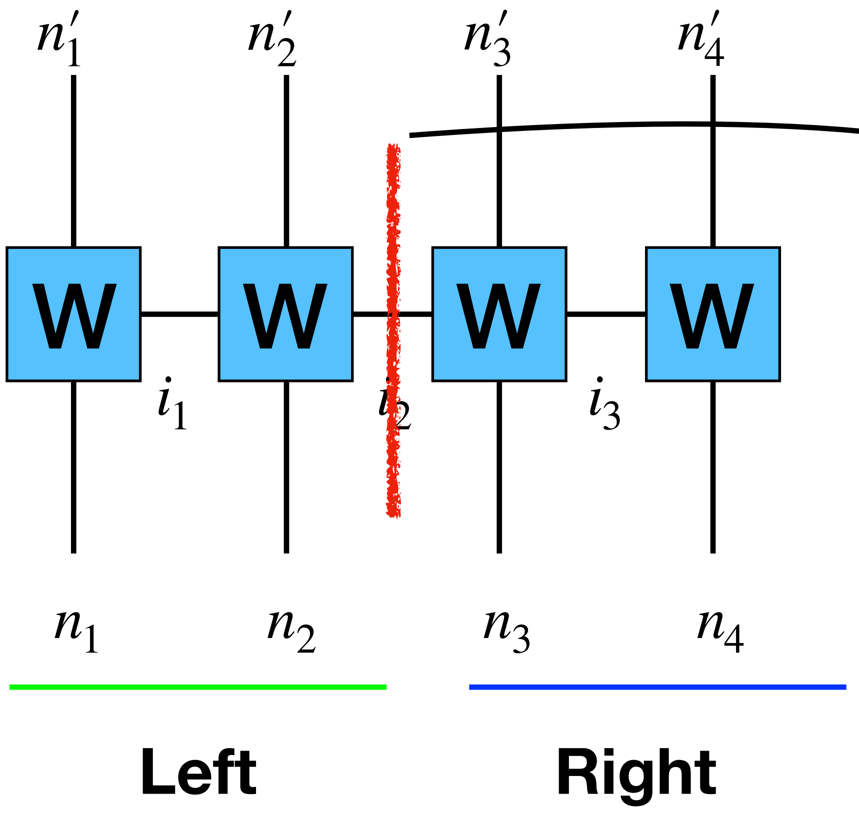


$$M = \begin{array}{c} \\ \\ \end{array} \begin{array}{cccc|c} R & A & B & F & \\ I & 0 & 0 & 0 & R \\ \hat{A} & 0 & 0 & 0 & A \\ \hat{B} & 0 & 0 & 0 & B \\ 0 & \hat{B} & \hat{A} & I & F \end{array}$$

Matrix Product Operators

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

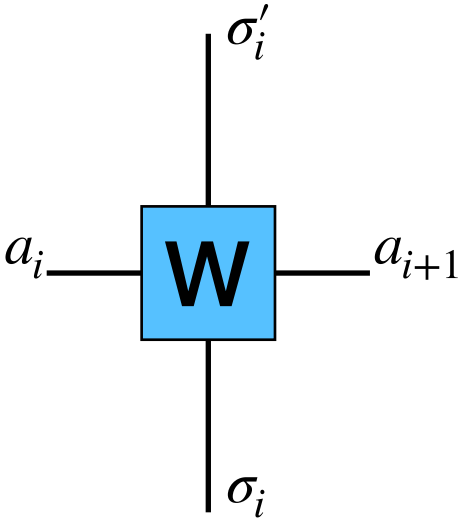
- Bond dimension of the MPO?



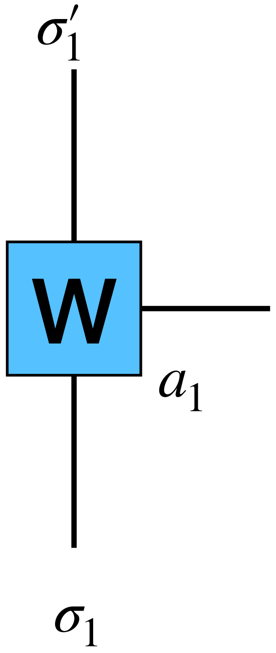
$$H_L \otimes \mathbf{1}_R + \mathbf{1}_L \otimes H_R + \sum_{\alpha=x,y,z} S_2^\alpha \cdot S_3^\alpha$$

Matrix Product Operators

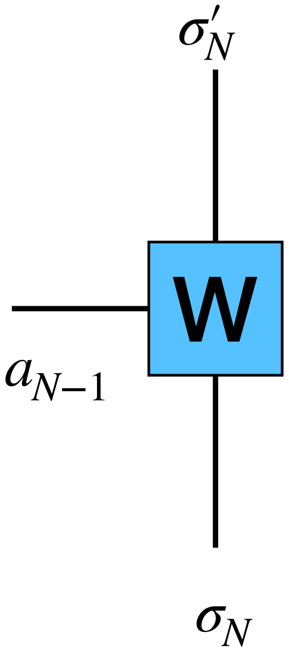
$$H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$



$$W^{\sigma_i'\sigma_i}_{a_i a_{i+1}} = \begin{bmatrix} I & 0 & 0 & 0 & 0 \\ S_i^+ & 0 & 0 & 0 & 0 \\ S_i^- & 0 & 0 & 0 & 0 \\ S_i^z & 0 & 0 & 0 & 0 \\ 0 & \frac{J}{2}S_i^- & \frac{J}{2}S_i^+ & JS_i^z & I \end{bmatrix}$$

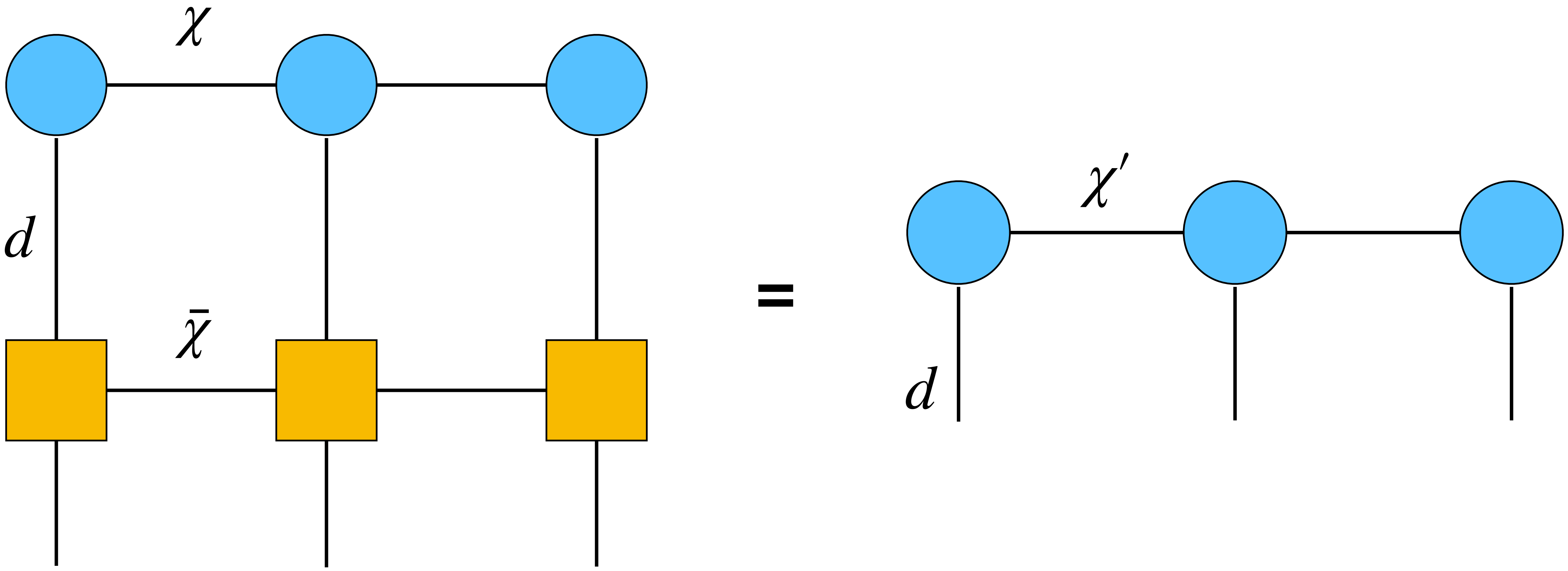


$$W^{\sigma_1'\sigma_1}_{a_1} = \begin{bmatrix} 0 & \frac{J}{2}S_1^- & \frac{J}{2}S_1^+ & JS_1^z & I \end{bmatrix}$$



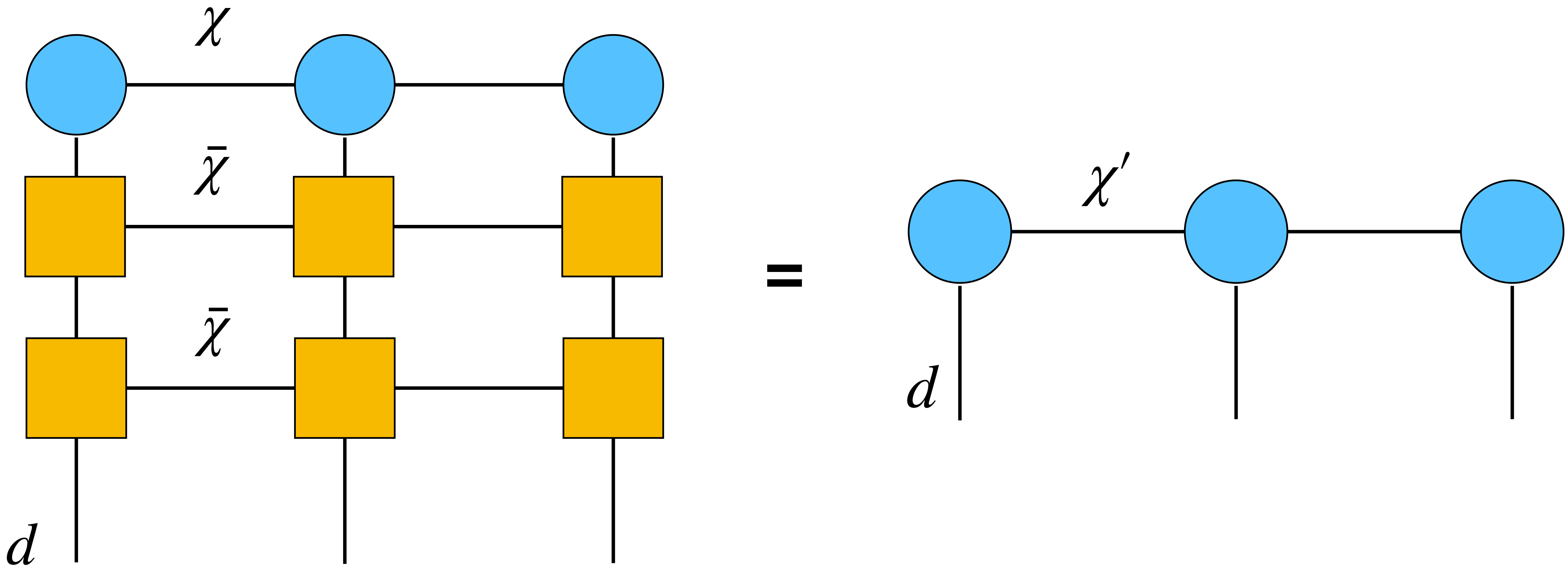
$$W^{\sigma_N'\sigma_N}_{a_{N-1}} = \begin{bmatrix} I \\ S_N^+ \\ S_N^- \\ S_N^- \\ S_N^Z \\ 0 \end{bmatrix}$$

MPO acting on MPS



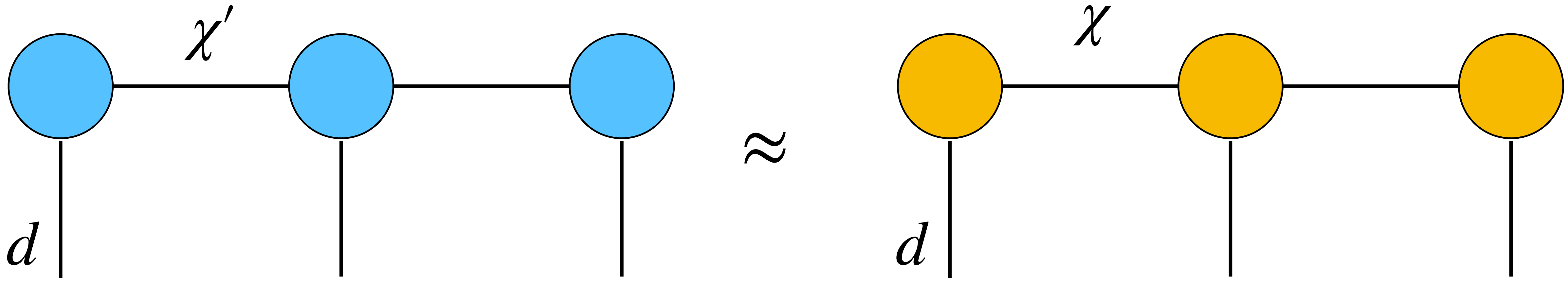
- What is χ' ?

MPO acting on MPS



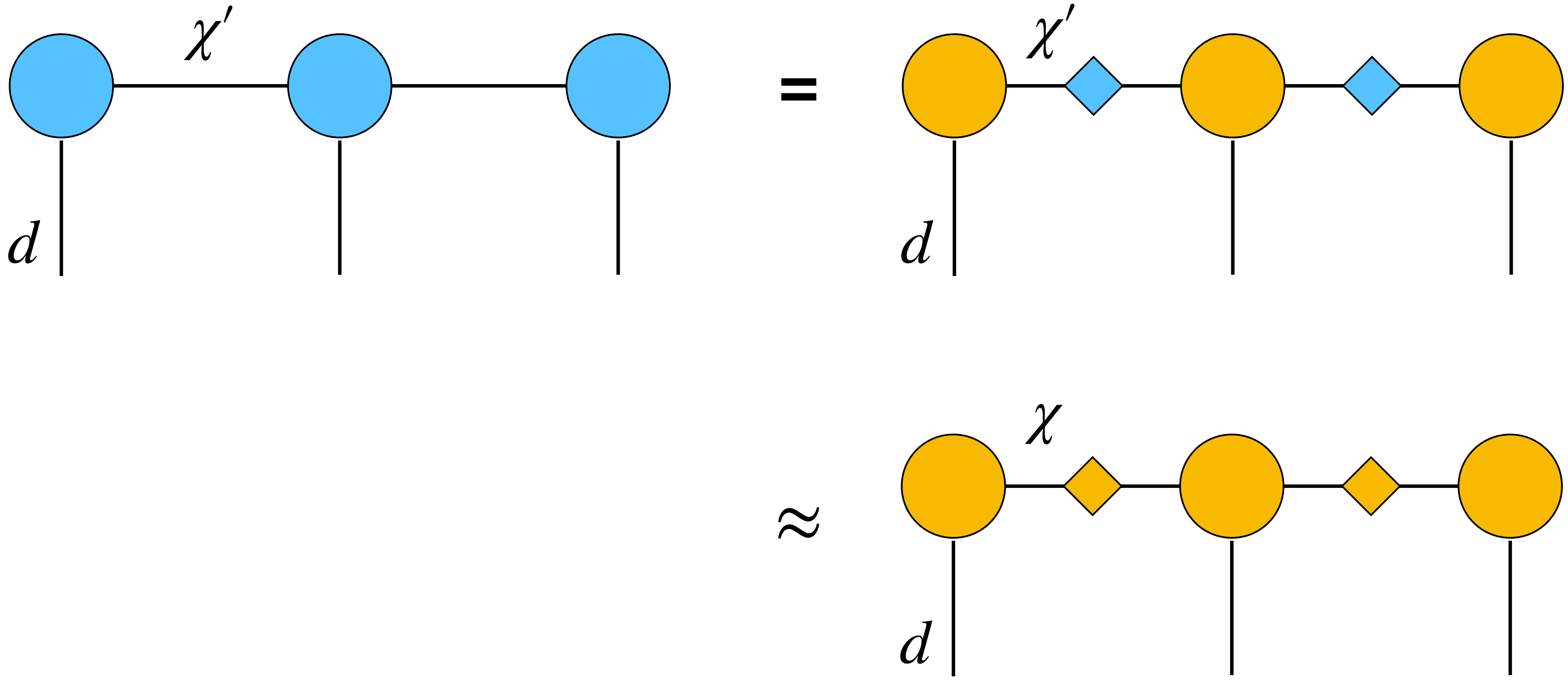
- What is χ' ?

MPO acting on MPS



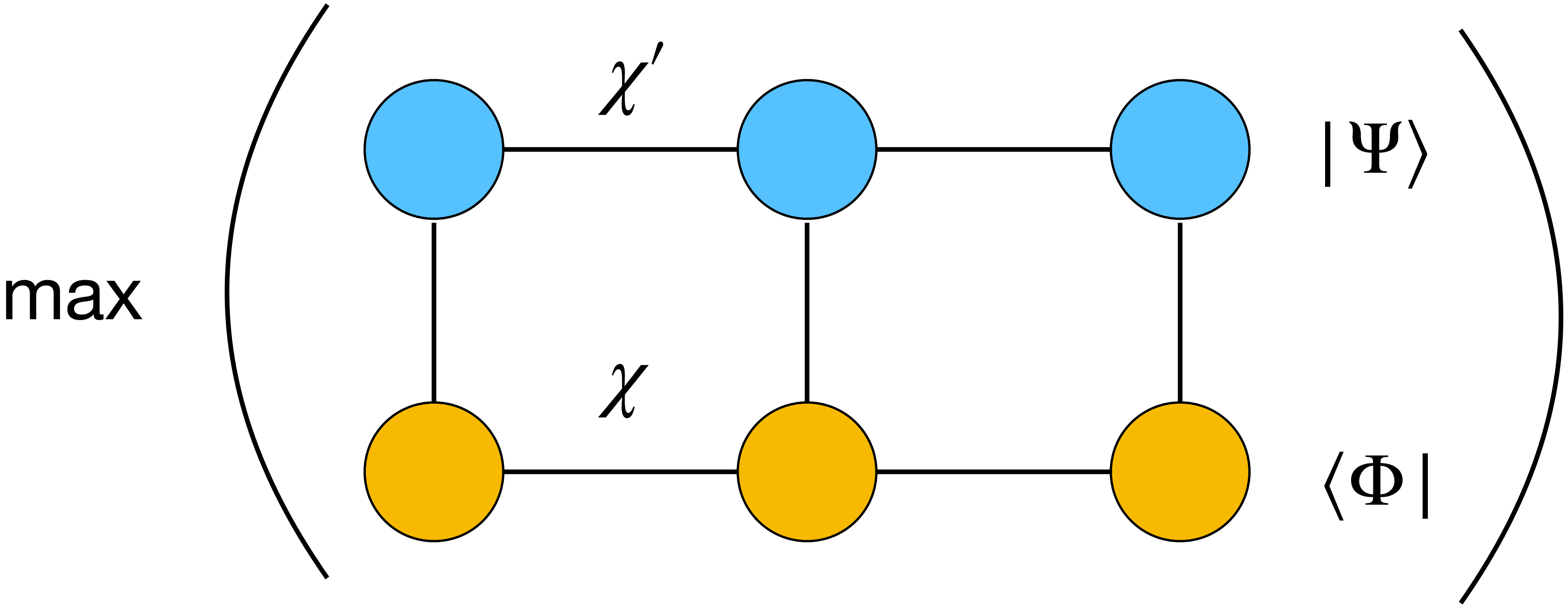
- Need to truncate back to bond dimension χ

Compression



- Transform into canonical form and truncate the singular matrix

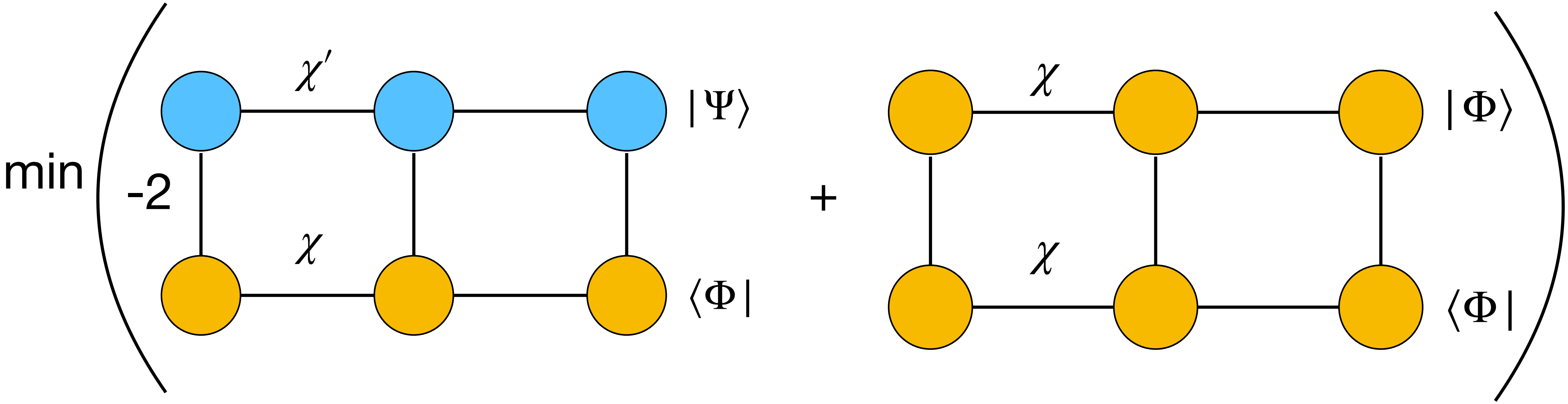
Variational Method



- Find a bond dimension χ MPS such that the overlap between two MPS's is maximal.

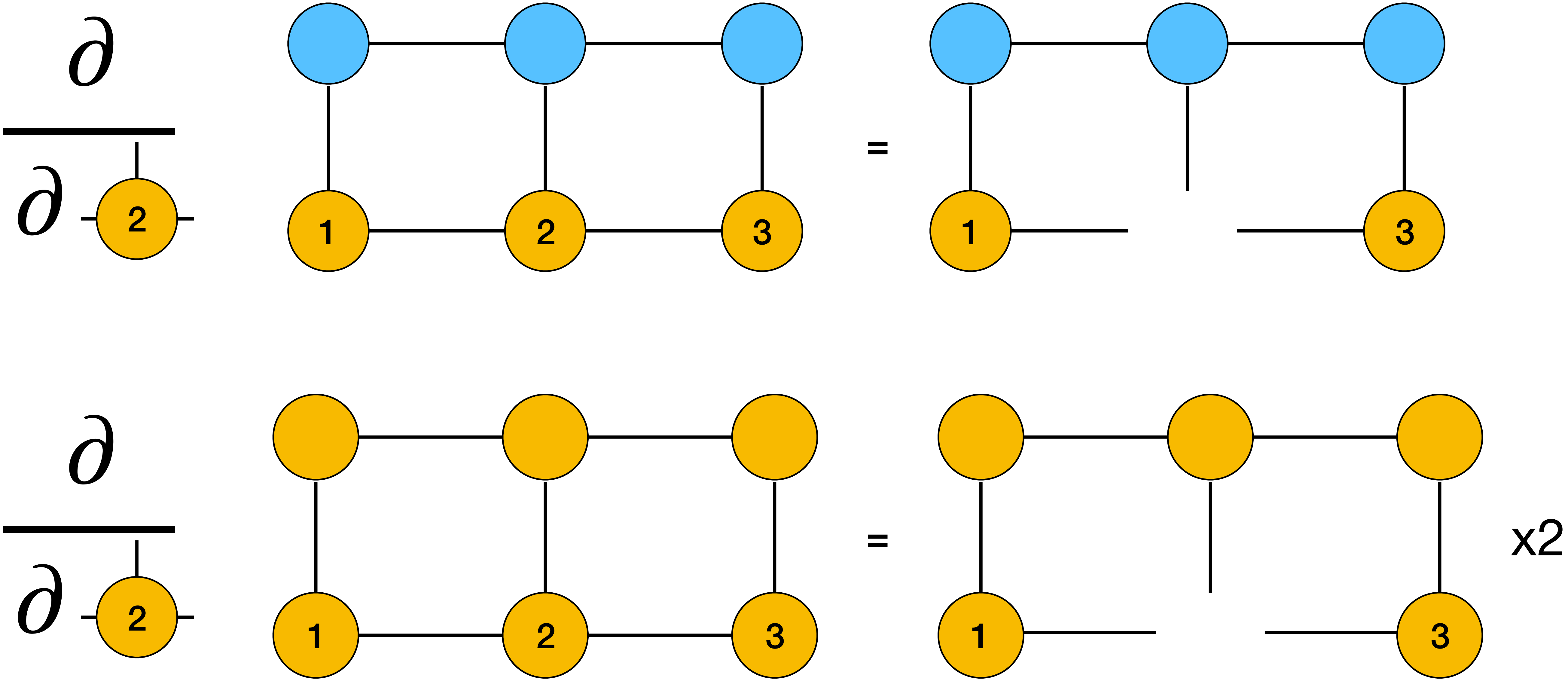
Variational Method

$$\min_{\Phi}\langle\Psi-\Phi|\Psi-\Phi\rangle=\min_{\Phi}[-2\langle\Phi|\Psi\rangle+\langle\Phi|\Phi\rangle],\quad\langle\Psi|\Psi\rangle=1$$



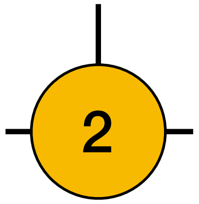
- Find a bond dimension χ MPS $|\Phi\rangle$ such that the distance between $|\Phi\rangle$ and $|\Psi\rangle$ is minimal.

Optimization



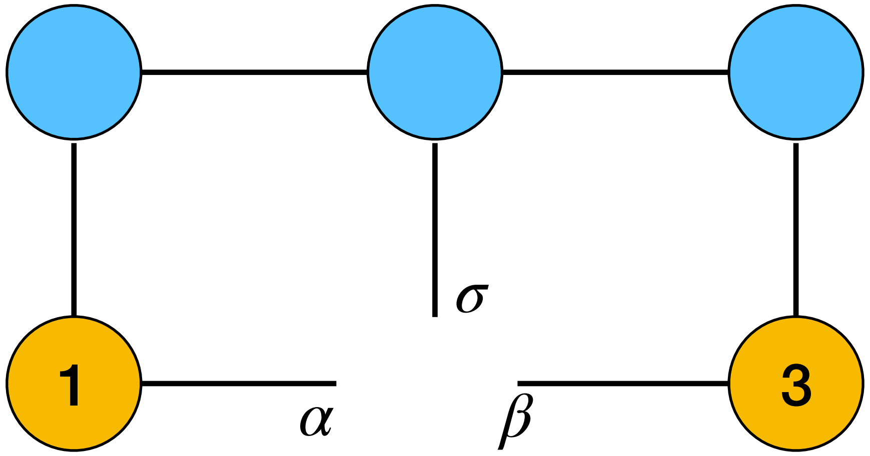
Linear Equations

- Treat tensor as a vector

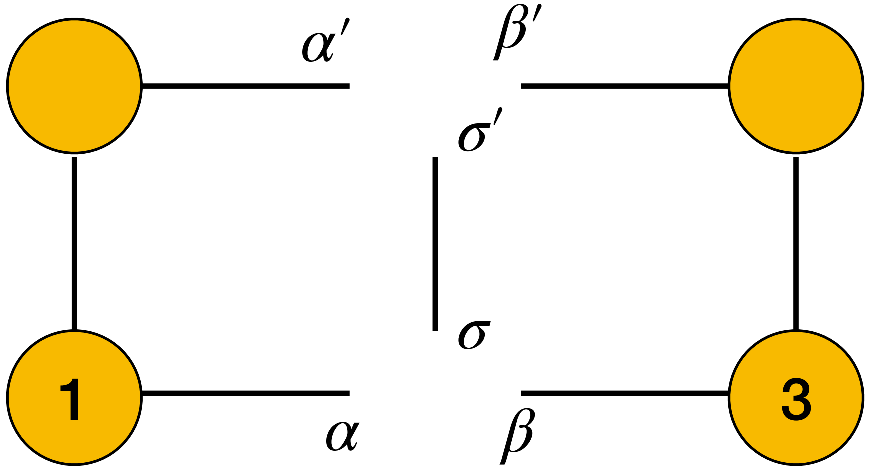


$= A_2[\sigma]_{\alpha\beta} = V_n^\sigma, \quad n = [\alpha\beta]$

B_n^σ =



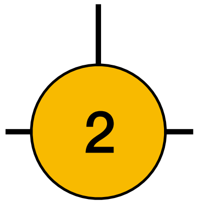
$M_{mn}^{\sigma\sigma'}$ =



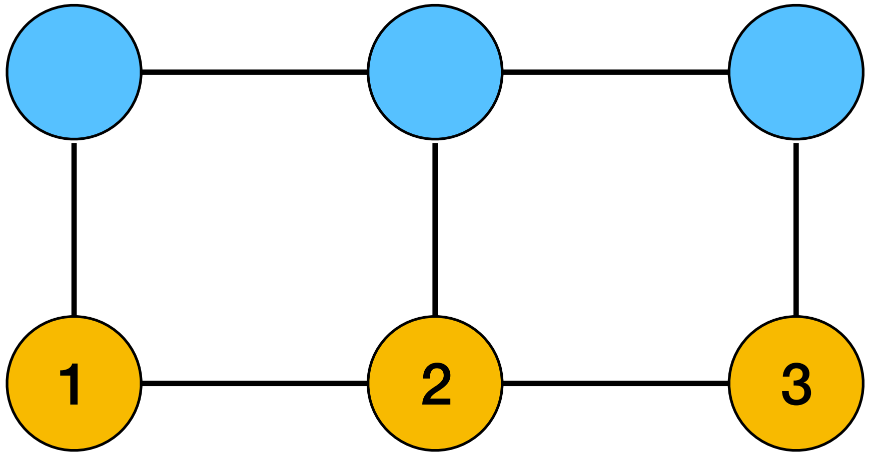
$m = [\alpha'\beta']$

Linear Equations

- Treat tensor as a vector

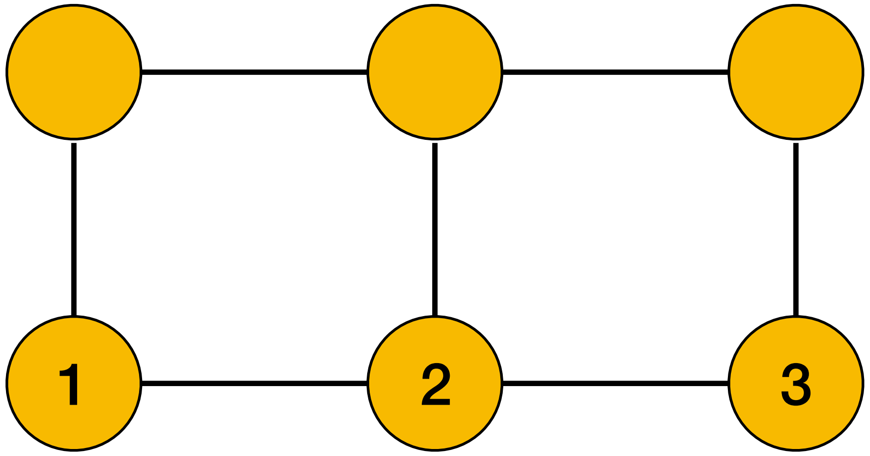


$= A_2[\sigma]_{\alpha\beta} = V_n^{\sigma}, \quad n = [\alpha\beta]$



= $B_n^{\sigma} V_n^{\sigma}$

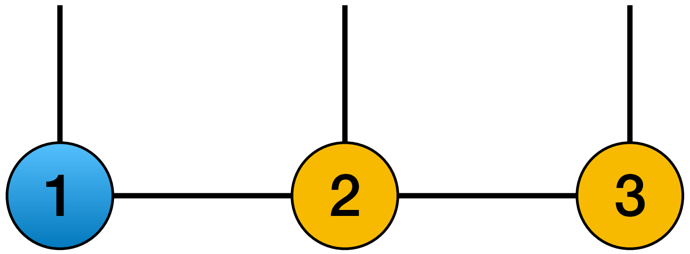
$$\min_{V} \left(V^{\dagger} M V - B V \right) \Rightarrow M = B V$$



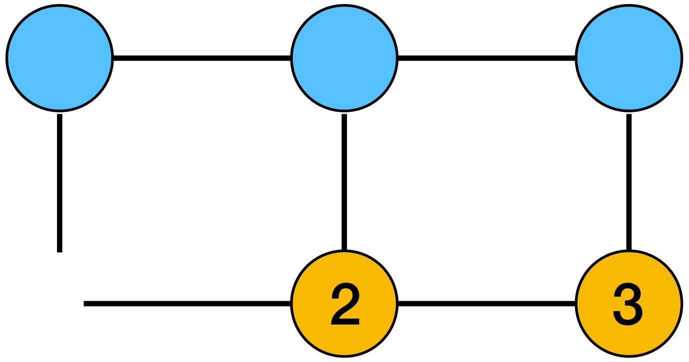
= $V_m^{\sigma' *} M_{mn}^{\sigma' \sigma} V_n^{\sigma}$

Similar operations in full updates in TNS

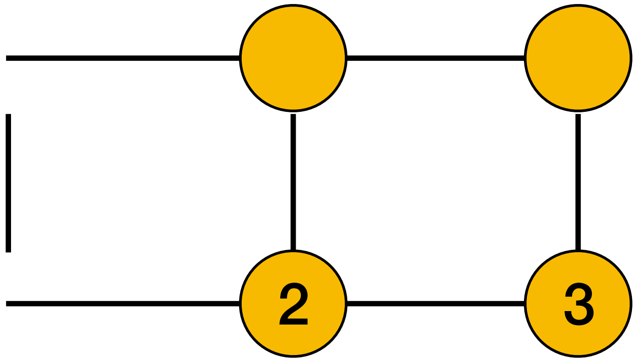
Sweeping



$B =$

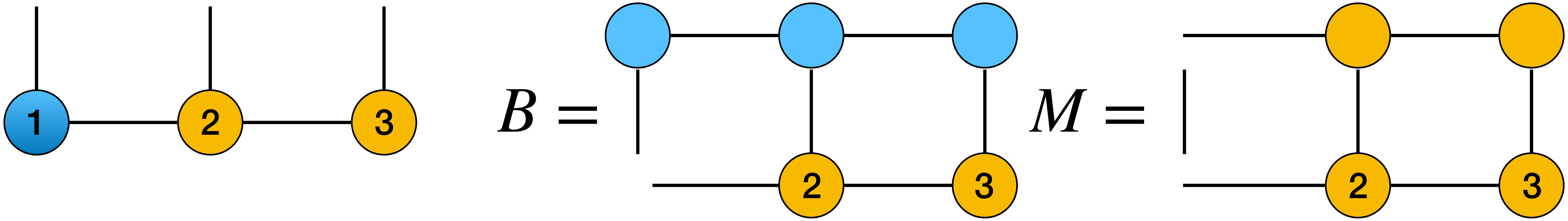


$M =$

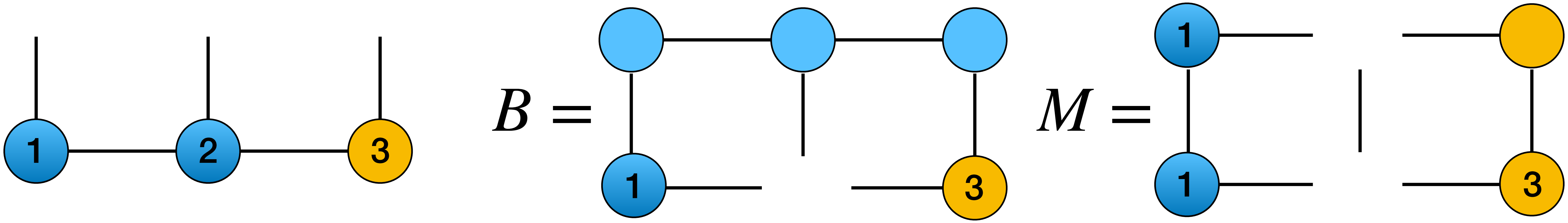


Solve $M = BV$ for A_1

Sweeping

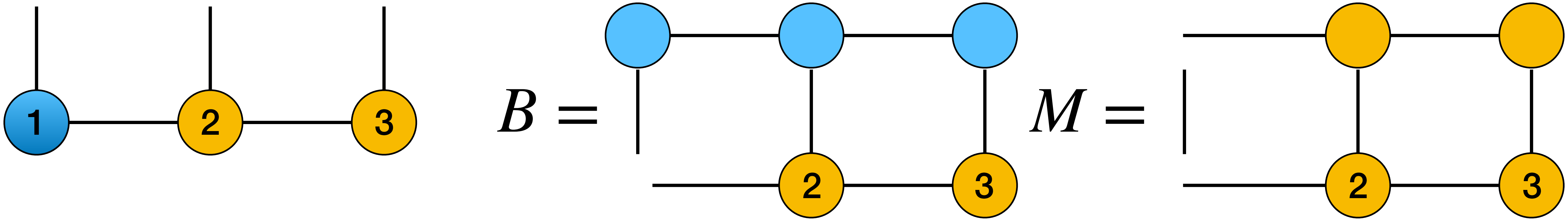


Solve $M = BV$ for A_1

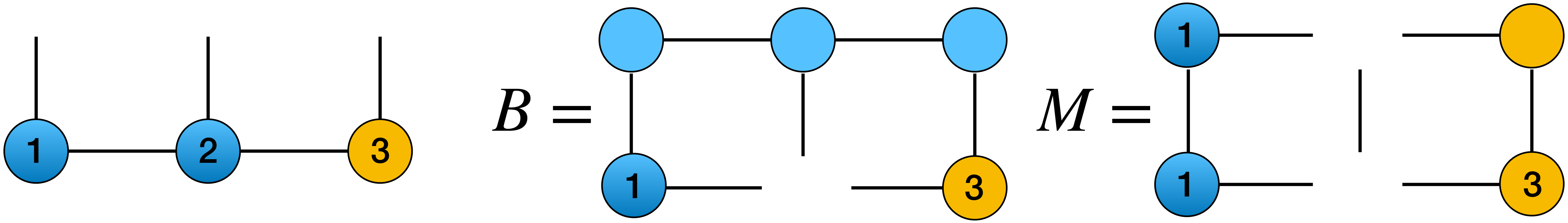


Solve $M = BV$ for A_2

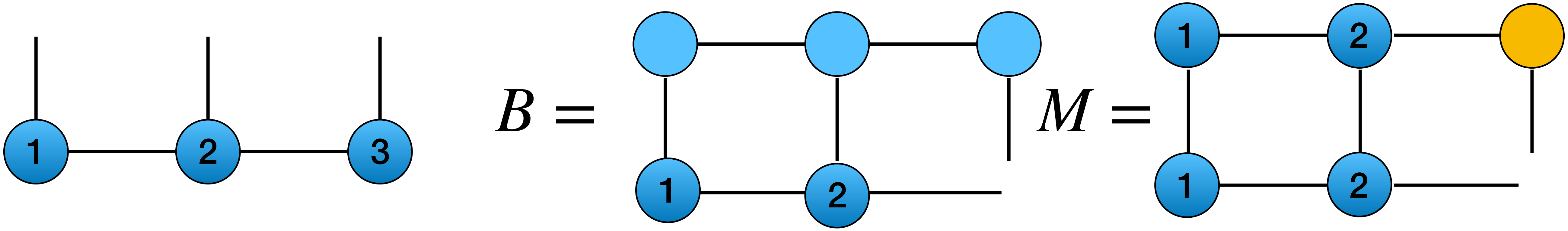
Sweeping



Solve $M = BV$ for A_1



Solve $M = BV$ for A_2



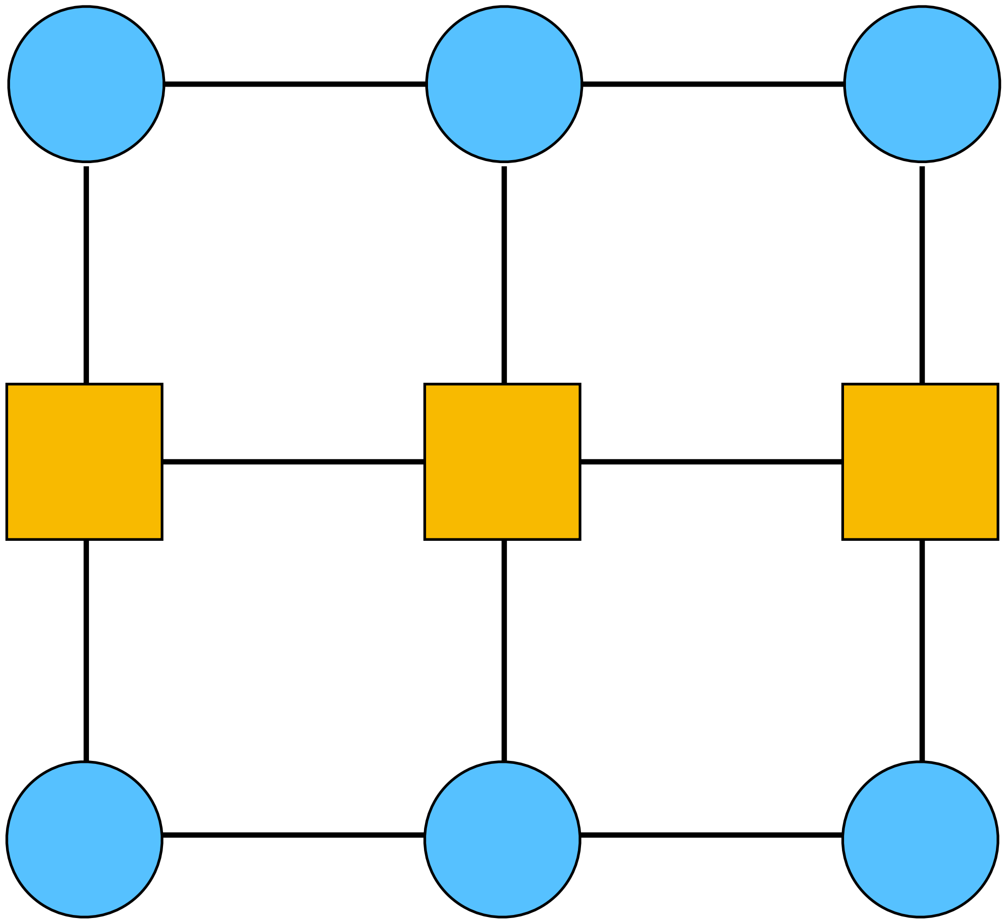
Solve $M = BV$ for A_3

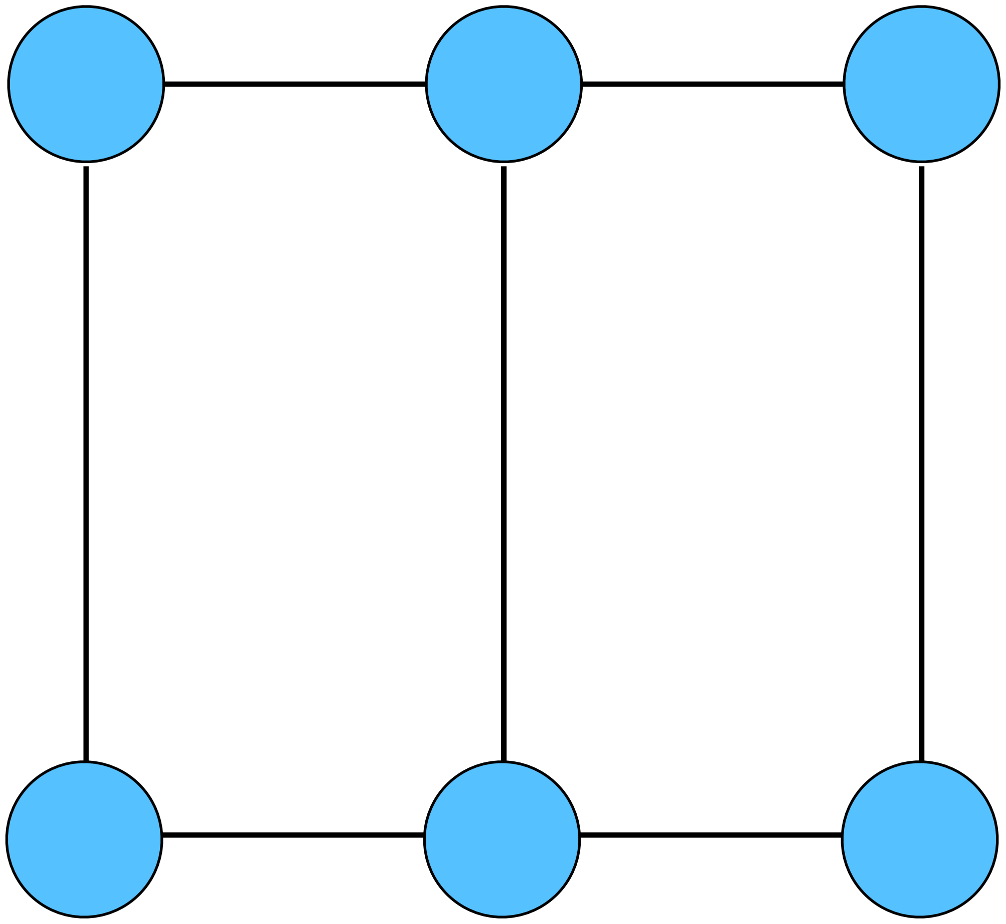
Energy optimization

$$\min_{\psi} \left(\langle \psi | H | \psi \rangle - \lambda(\langle \psi | \psi \rangle - 1) \right)$$

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

$\langle \psi | \psi \rangle$

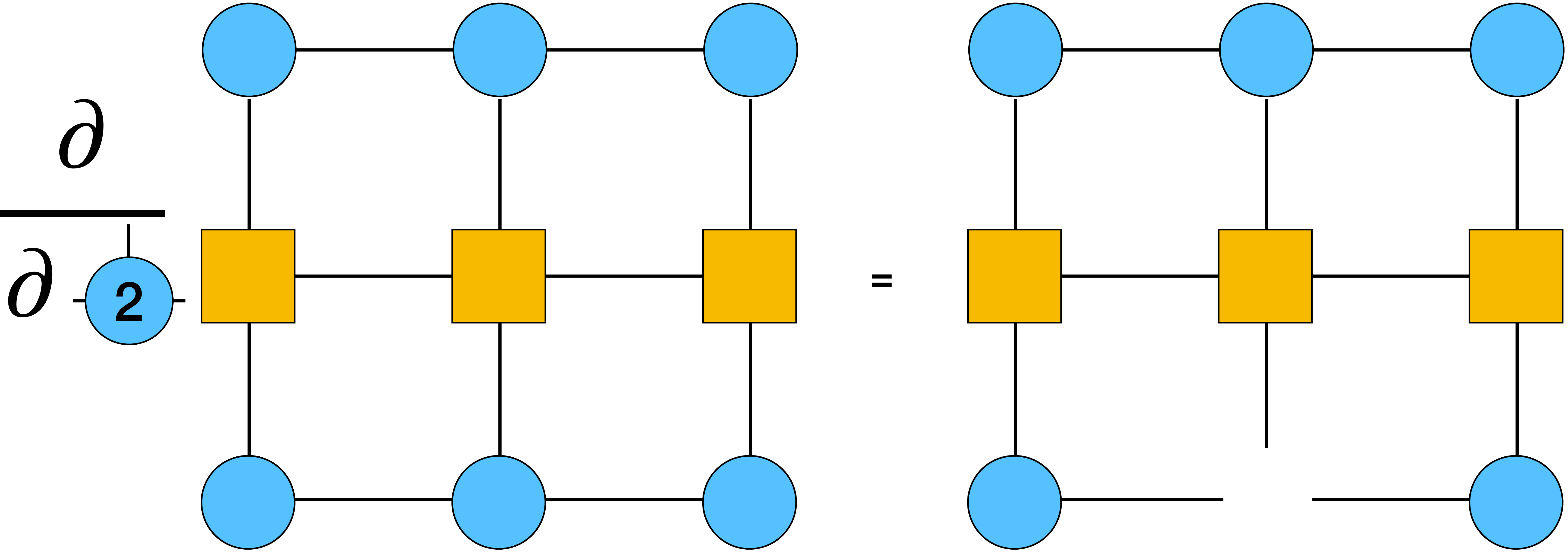




Energy optimization

$$\min\Big(\langle\psi|H|\psi\rangle - \lambda(\langle\psi|\psi\rangle - 1)\Big)$$

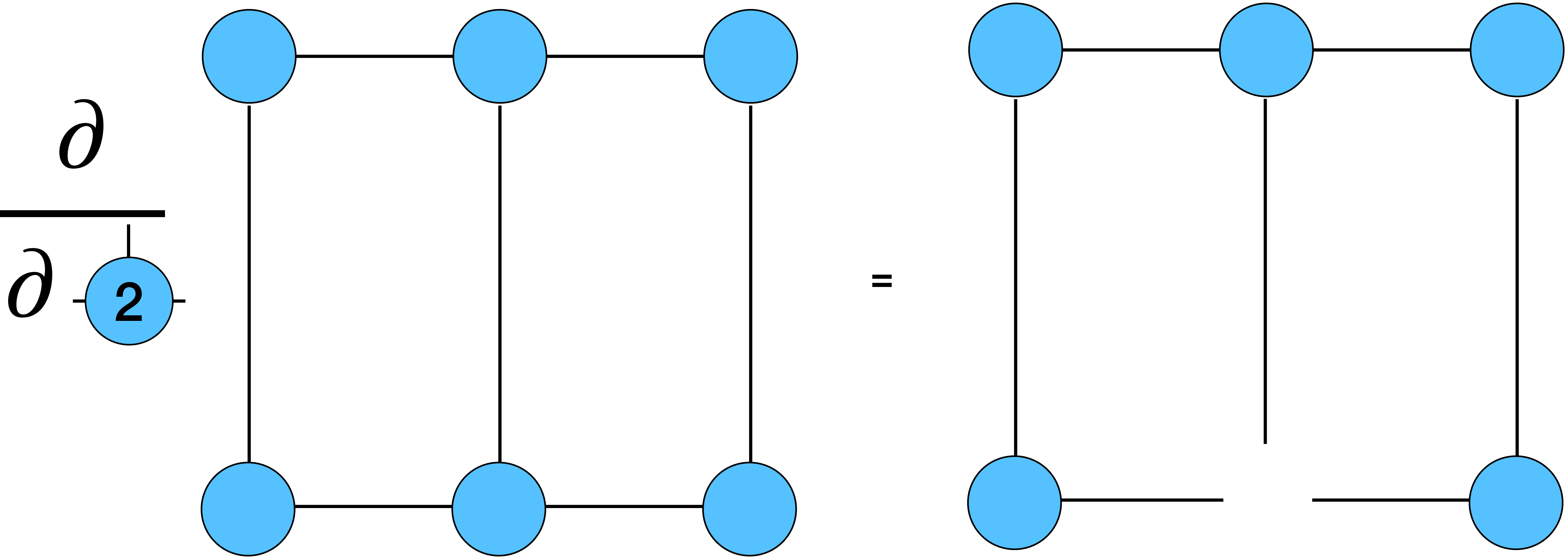
$\langle\psi|H|\psi\rangle$



Energy optimization

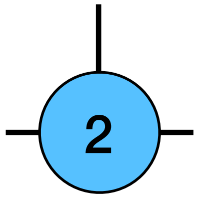
$$\min\left(\langle\psi|H|\psi\rangle - \lambda(\langle\psi|\psi\rangle - 1)\right)$$

$$\langle\psi|\psi\rangle$$



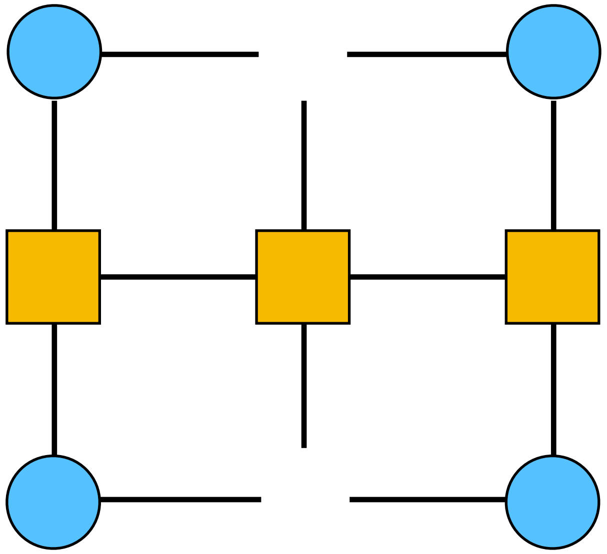
Energy optimization

- Treat tensor as a vector

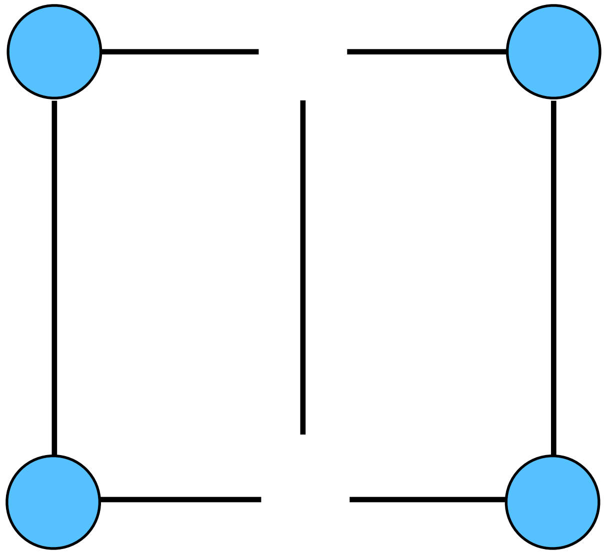


$= A_2[\sigma]_{\alpha\beta} = V_n^{\sigma}, \quad n = [\alpha\beta]$

$H_{eff} =$

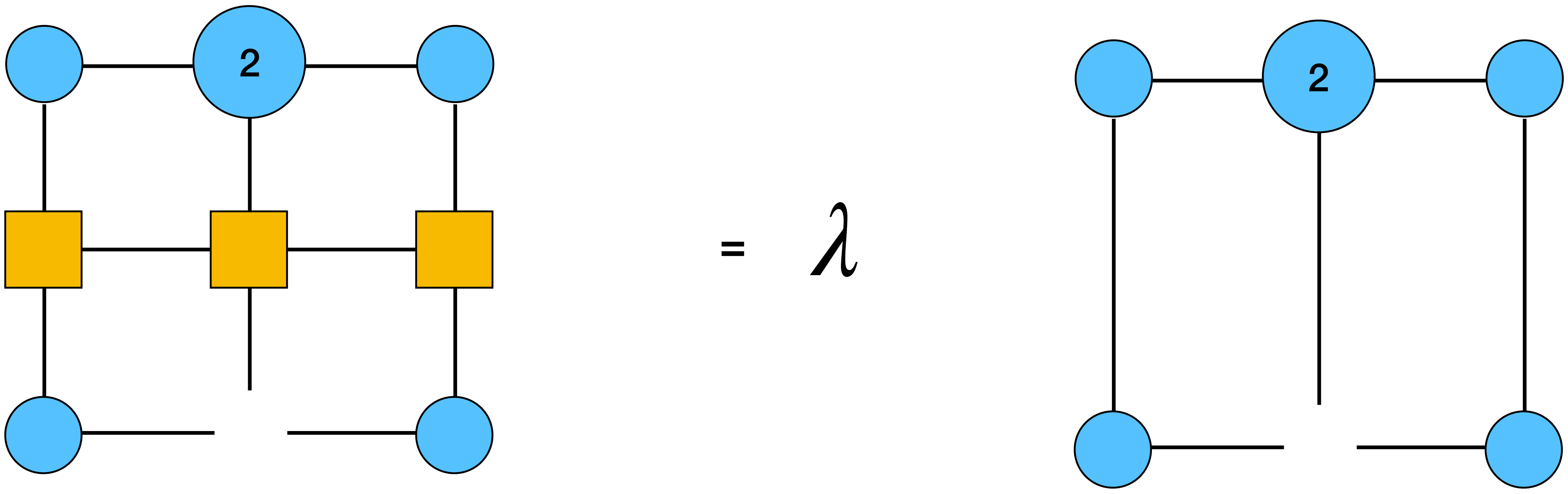


$N =$



Energy optimization

$$\min_{\psi}\left(\langle\psi|H|\psi\rangle-\lambda(\langle\psi|\psi\rangle-1)\right)\Rightarrow\frac{\partial}{\partial A}\left(\langle\psi|H|\psi\rangle-\lambda(\langle\psi|\psi\rangle)\right)=0$$

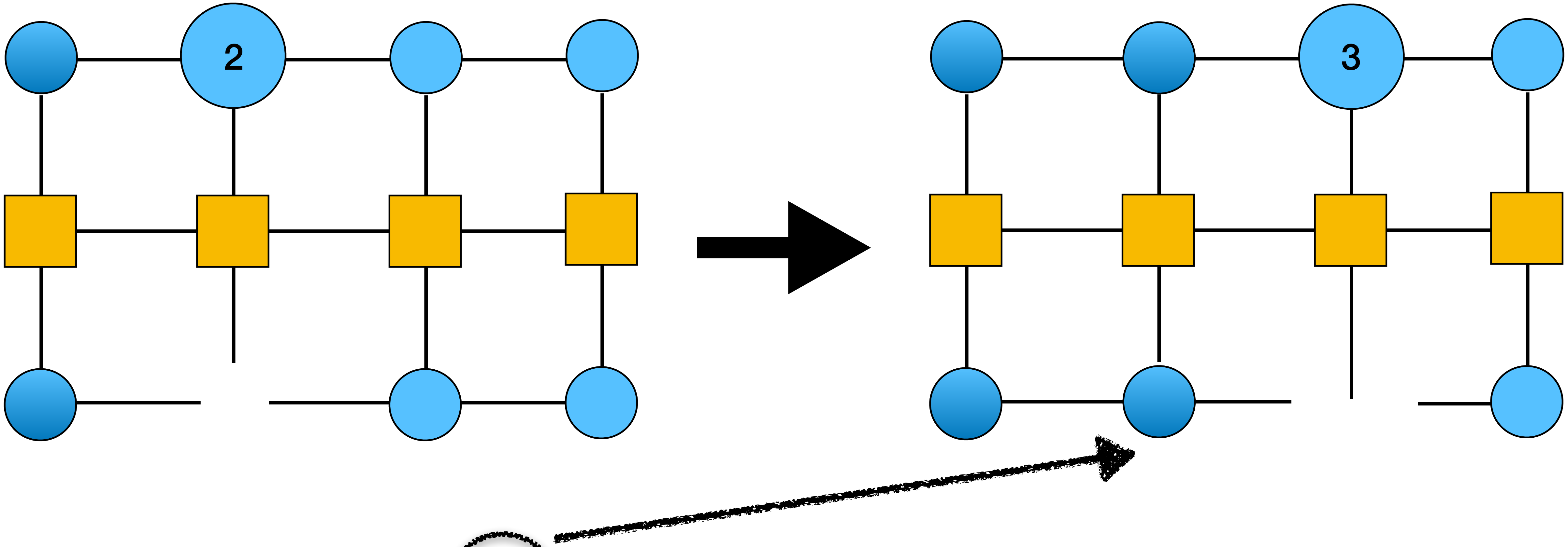


$$H_{eff}V=\lambda NV$$

Mixed Canonical Form: $N=I$

- Updating A becomes a generalized eigenvalue problem
- Find the ground state of H_{eff}

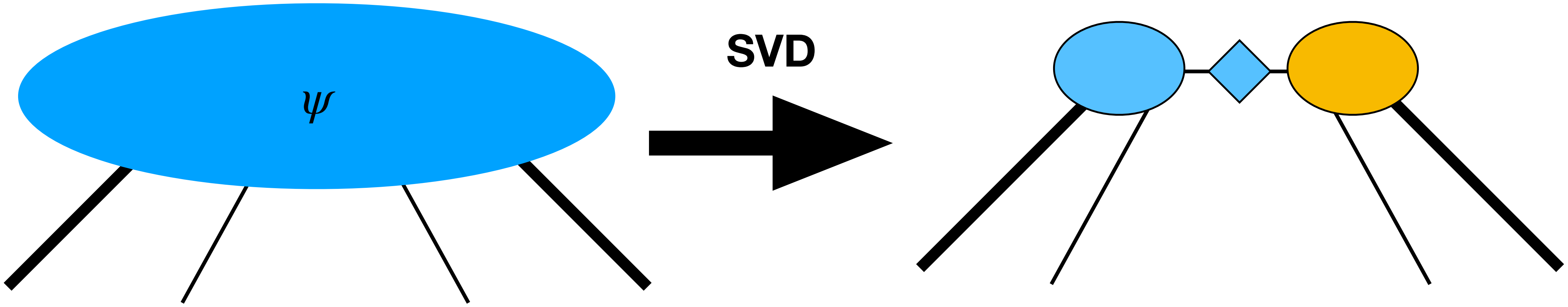
Sweeping



$$H_{eff}V_2 = \lambda \boxed{V_2}$$

$$H_{eff}V_3 = \lambda V_3$$

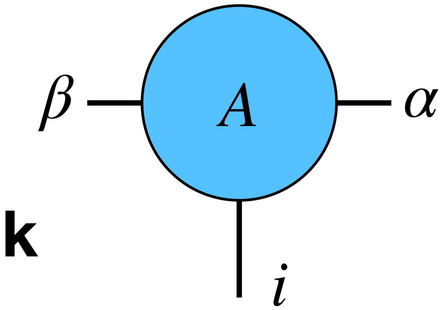
Connection between DMRG and MPS



block site site **block**

System Environment System Environment

$$|\psi\rangle = \sum_{\alpha} \lambda_{\alpha} |\psi^{S}_{\alpha}\rangle |\psi^{E}_{\alpha}\rangle$$



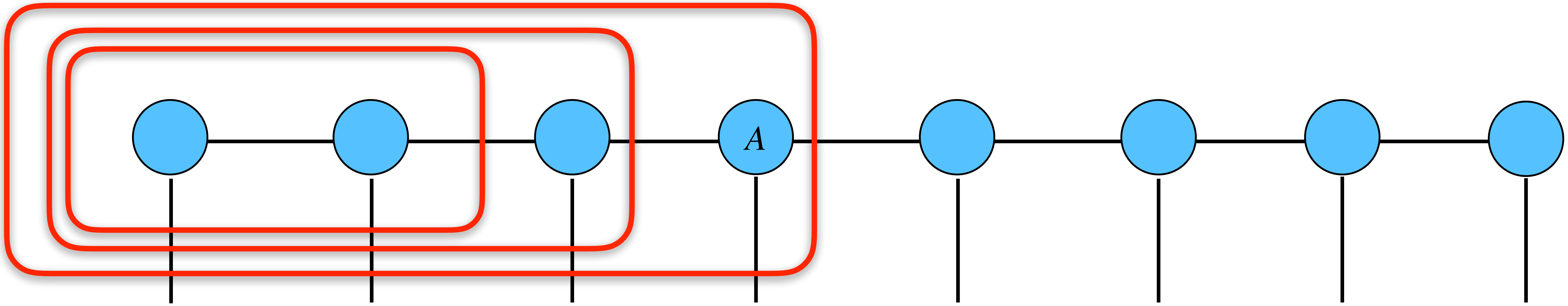
block

site

$$\left|\psi^{S}_{\alpha}\right\rangle = \sum_{\beta i} A^{i}_{\alpha\beta} \left|\psi_{\beta}\right\rangle |i\rangle$$

change of basis

Connection between DMRG and MPS



MPS tensors = sequence of change of basis

Time Evolution

- Real time evolution

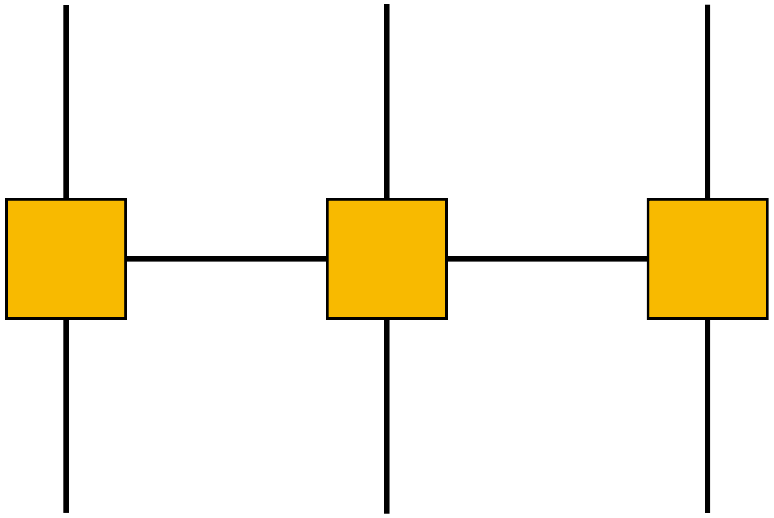
$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$$

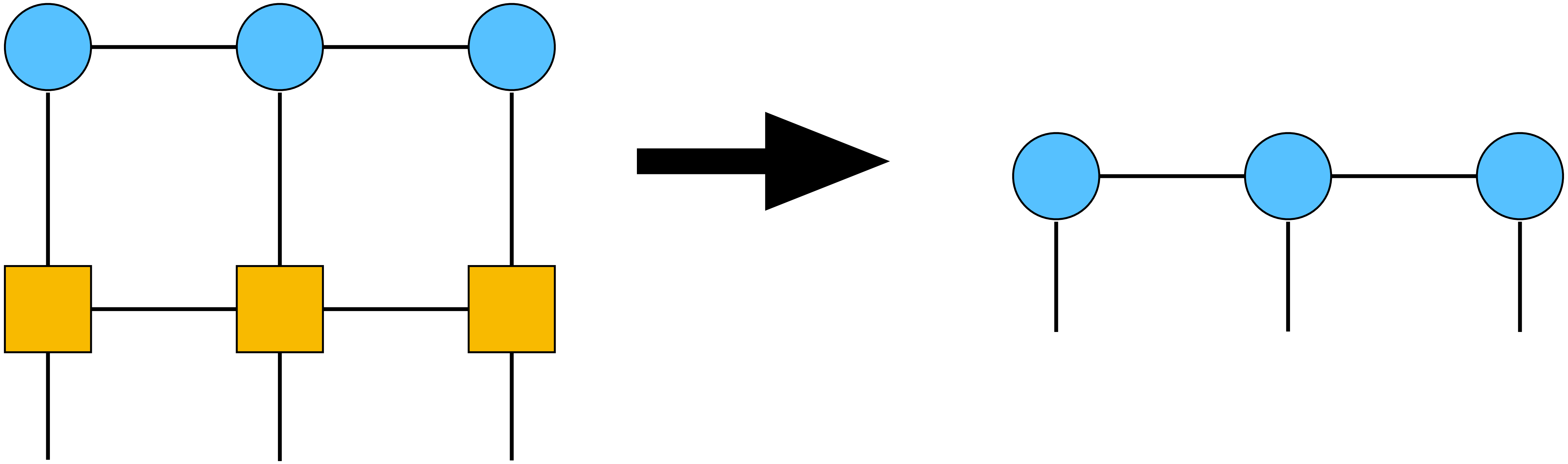
- Imaginary time evolution

$$|\psi_g\rangle = \lim_{\tau\to\infty}\frac{e^{-H\tau}|\psi\rangle}{|e^{-H\tau}|\psi\rangle|}$$

General Time Evolution

$$e^{-iH\delta t} \approx 1 - iH\delta t$$





Time evolving block decimation

- Consider a Hamiltonian of the form (short range)

$$H = \sum_j h^{[j,j+1]}$$

- Decompose the Hamiltonian into $H = F + G$

$$F = \sum_{j \in \text{even}} F^{[j]} = \sum_{j \in \text{even}} h^{[j,j+1]}$$

$$G = \sum_{j \in \text{odd}} G^{[j]} = \sum_{j \in \text{odd}} h^{[j,j+1]}$$

- $[F^{[r]}, F^{[r']}] = [G^{[r]}, G^{[r']}] = 0$, but $[F, G] \neq 0$

Time evolving block decimation

- Trotter-Suzuki approximation

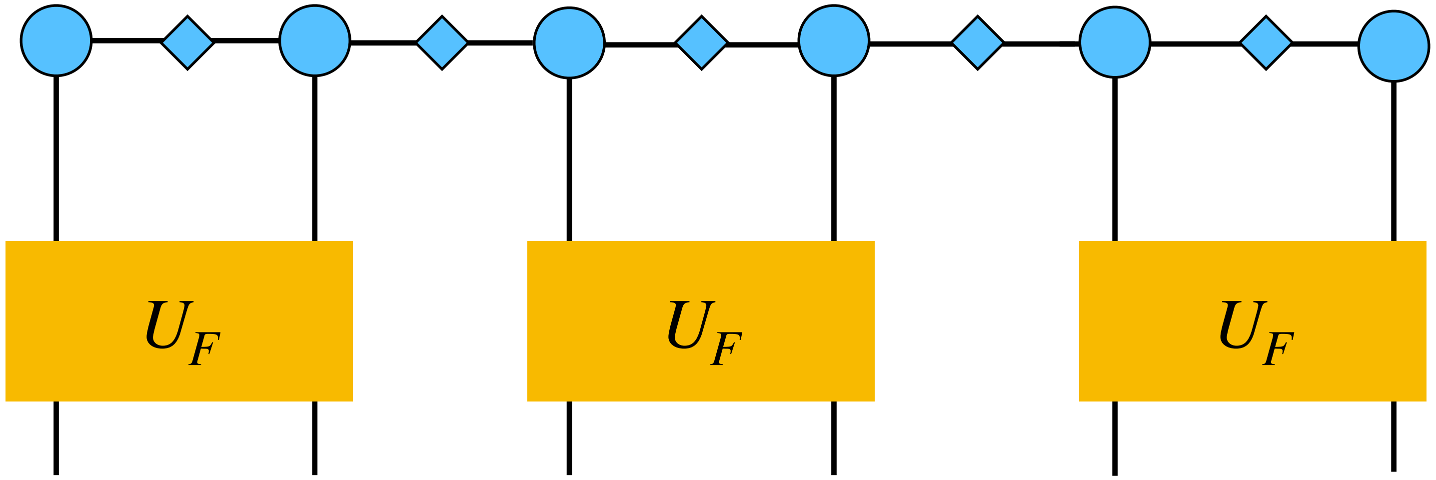
$$e^{-i(F+G)\delta t} = e^{-iF\delta t}e^{-iG\delta t} + O(\delta t^2)$$

- Time evolution operators

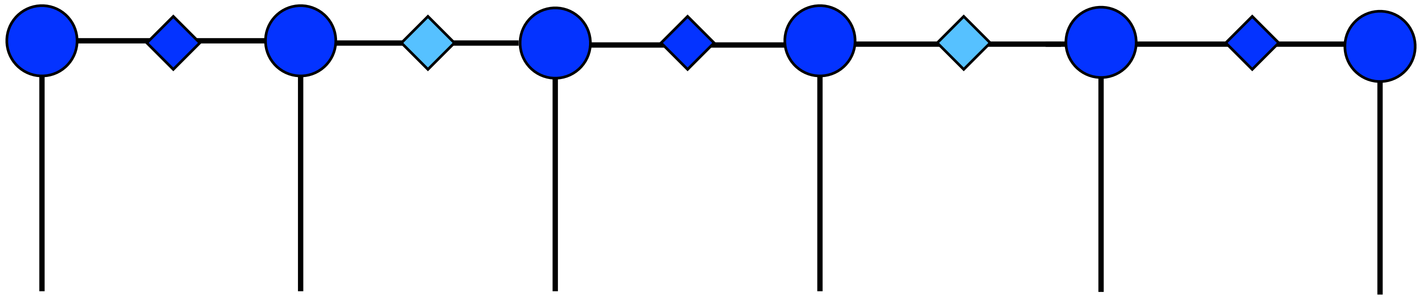
$$U_F = \prod_{r \in \text{ even}} e^{-iF^{[r]}\delta t}, \quad U_G = \prod_{r \in \text{ odd}} e^{-iG^{[r]}\delta t}$$

Time evolving block decimation

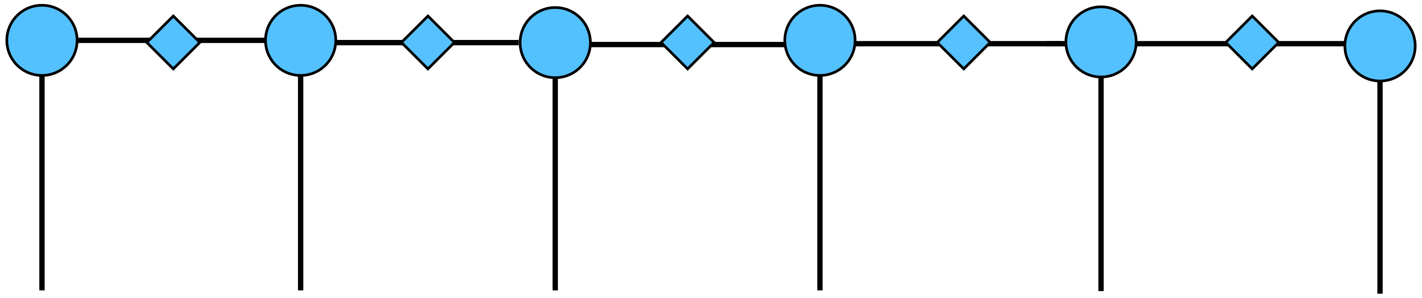
Time Evolution



Tensor Contraction

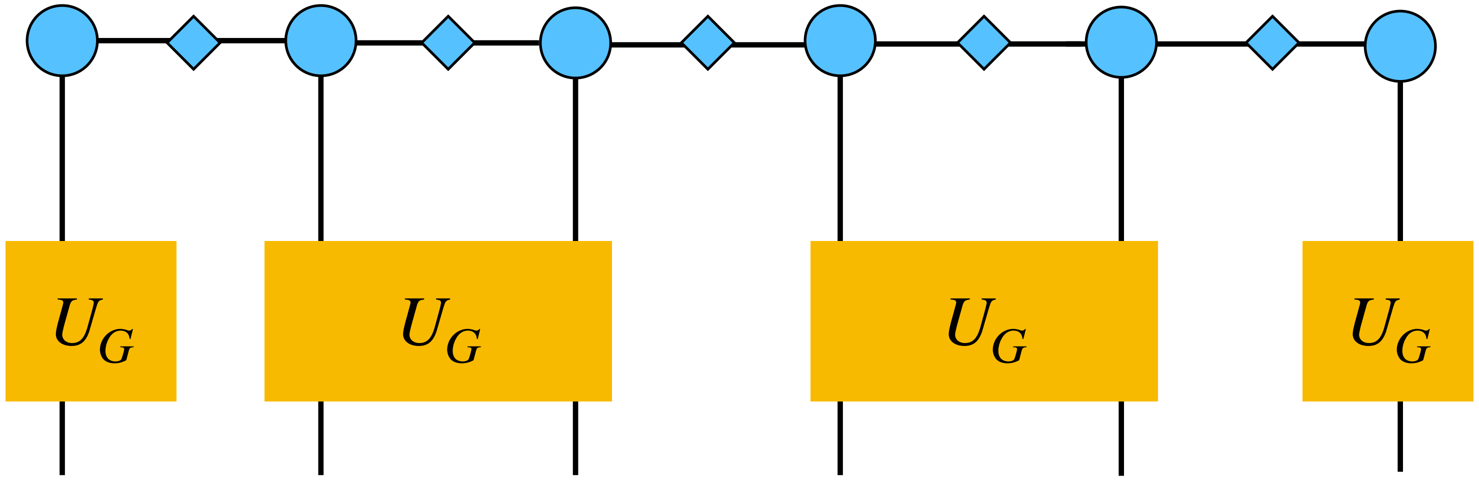


Truncation

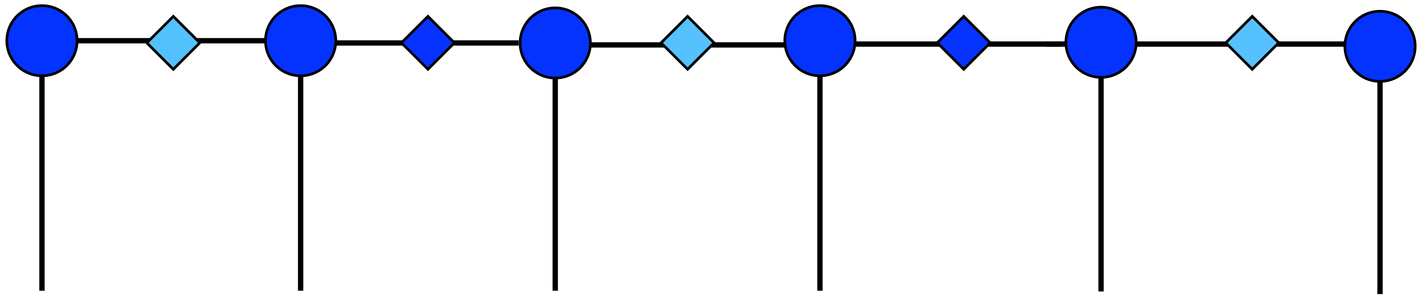


Time evolving block decimation

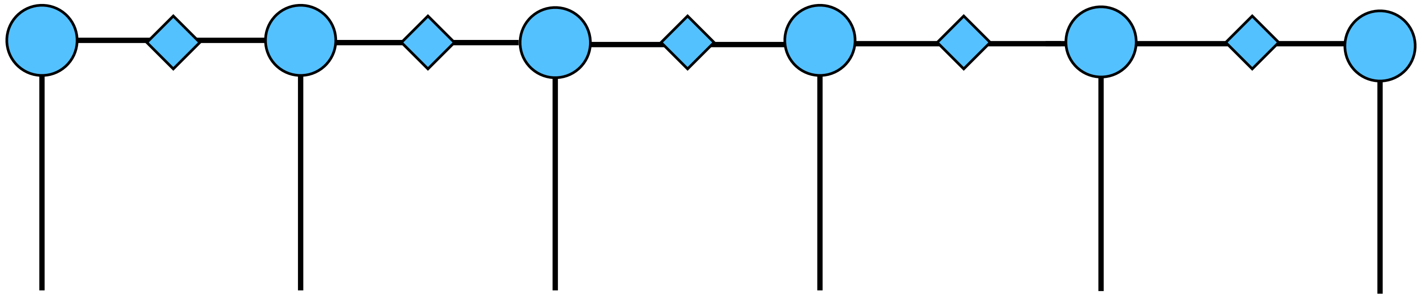
Time Evolution



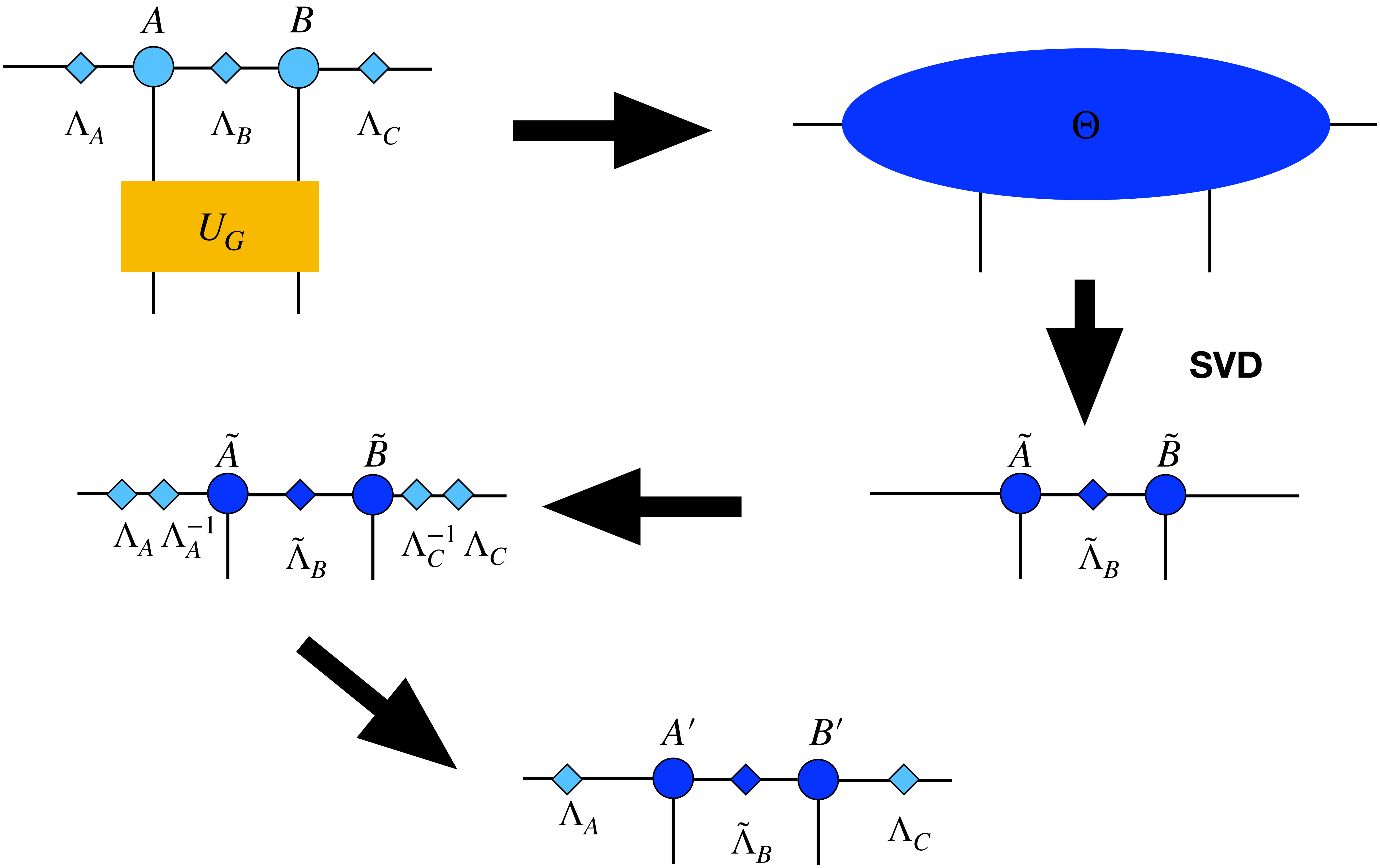
Tensor Contraction



Truncation

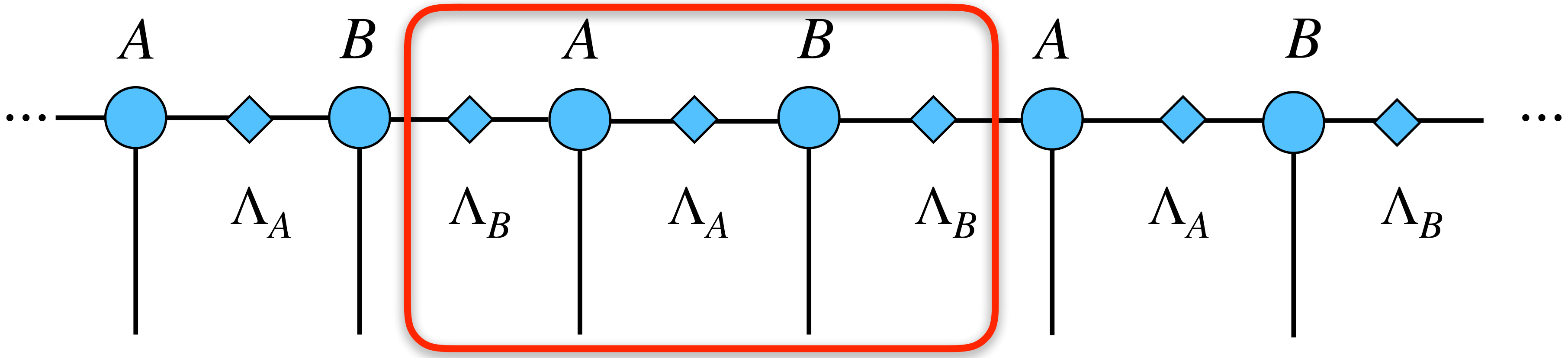


Time evolving block decimation



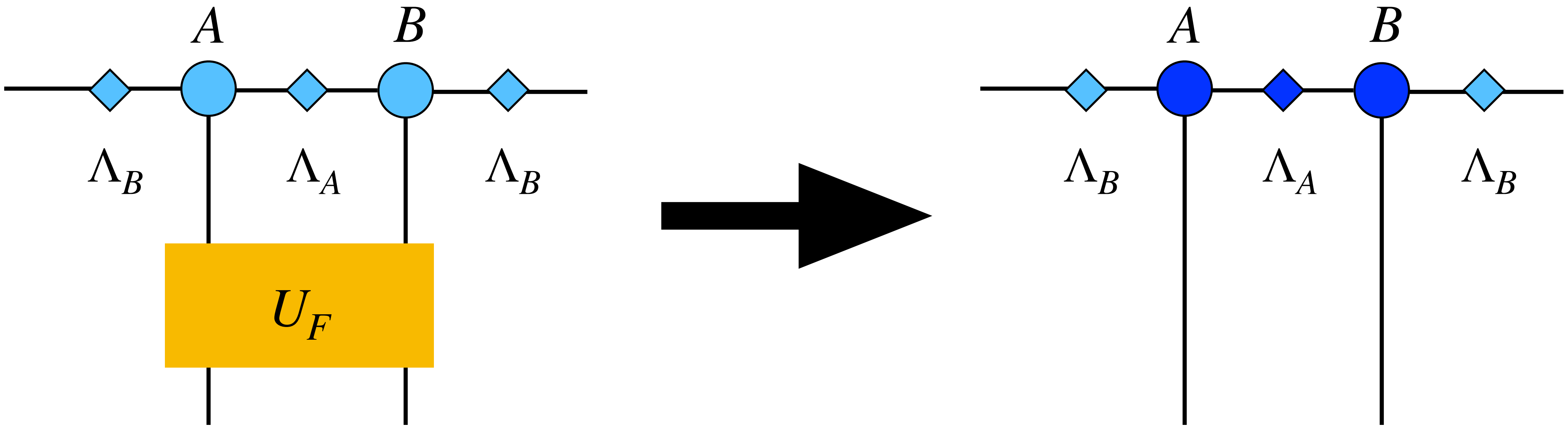
Infinite TEBD

- Assume translational invariant wave function, and $N \to \infty$.
- Partially breaks the translational invariance to perform time evolution
- Two-site unit cell

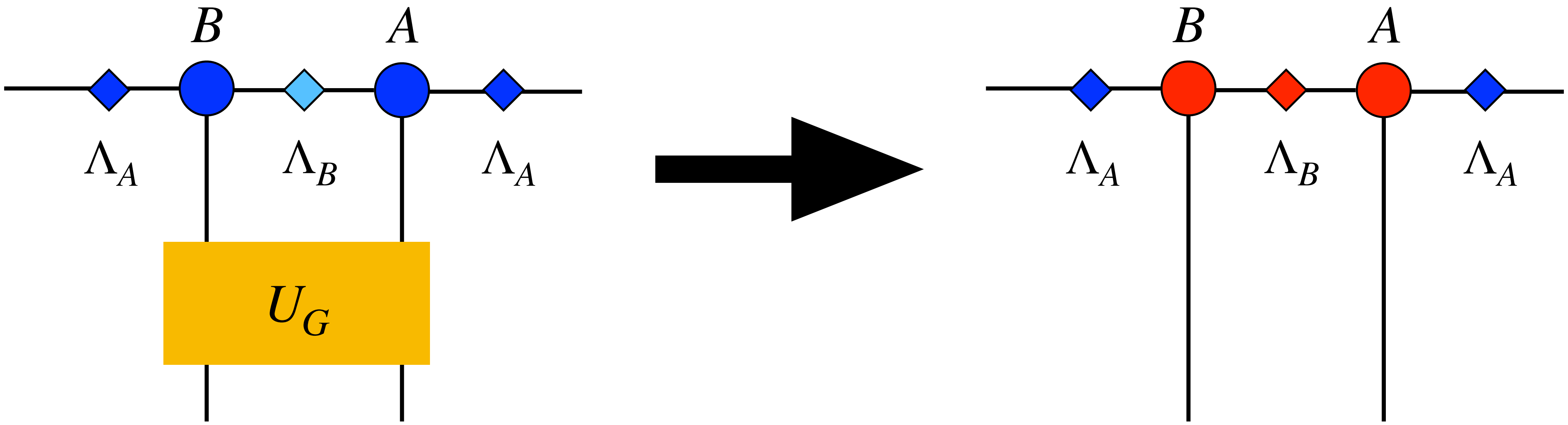


Infinite TEBD

Step 1

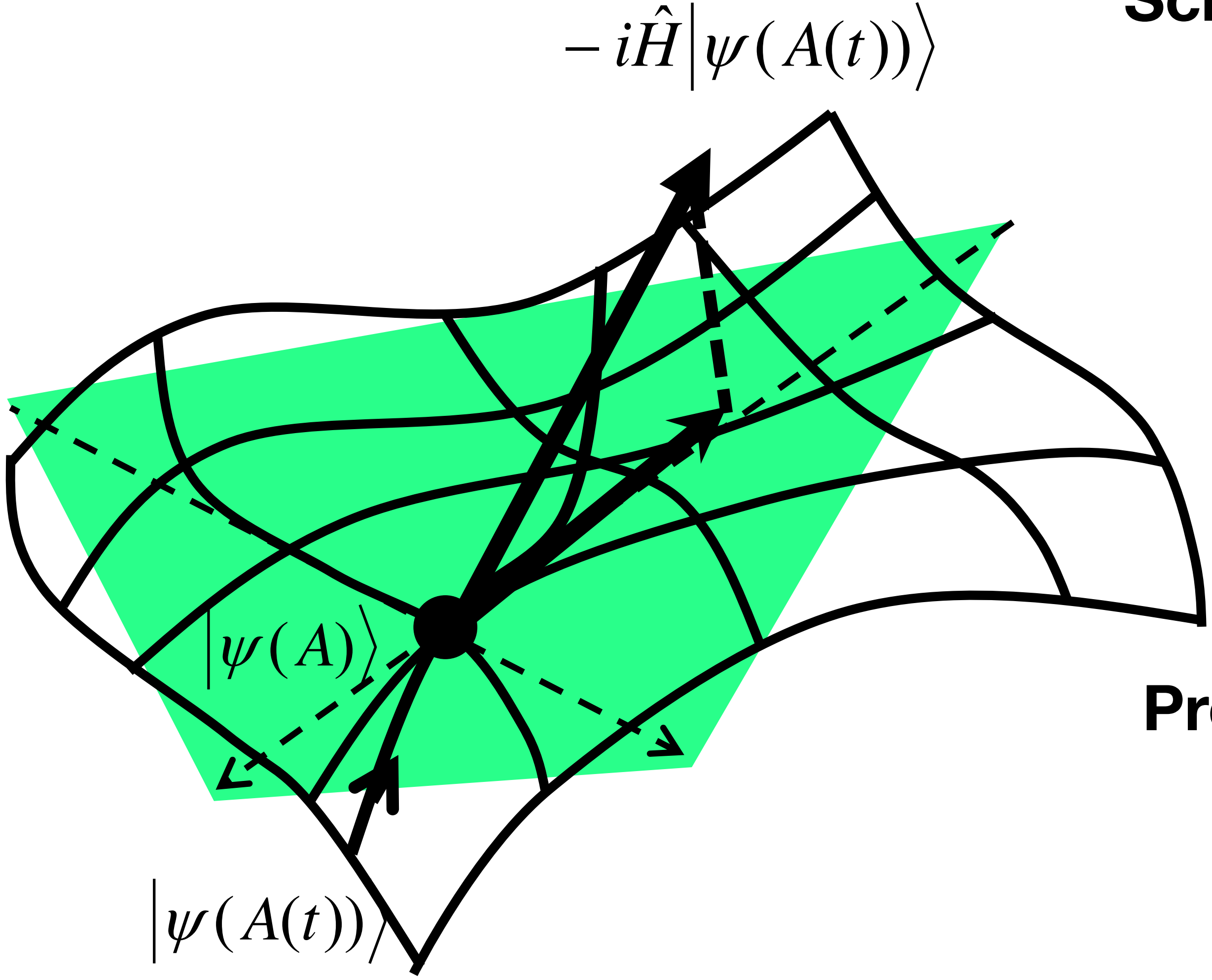


Step 2



Repeat

Time-dependent Variational Principle



Schrödinger Equation

$$i\frac{d}{dt}|\psi(A(t))\rangle = \hat{H}|\psi(A(t))\rangle$$

Projected Schrödinger Equation

$$i\frac{d}{dt}|\psi(A(t))\rangle = \boxed{P_{|\psi(A)\rangle}}\hat{H}|\psi(A(t))\rangle$$

Quantum numbers

- Given global symmetry group, local site basis can be labeled by irreducible representations of group – **quantum numbers**

- U(1): site basis labelled by integer *n* (particle number)
  $|n\rangle, \quad n = 0,1,\ldots$

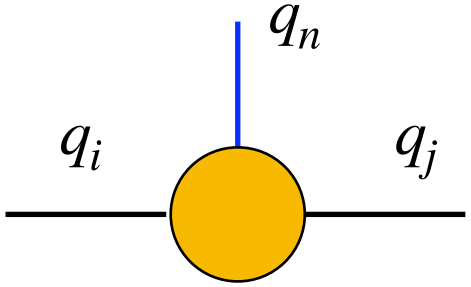
- SU(2): site basis labelled by *j*, *m* (spin) $|j, m\rangle$

Total state associated with good quantum numbers

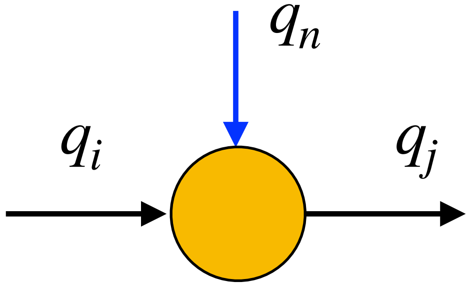
$$|\Psi\rangle = |\Psi(n, j, m\ldots)\rangle$$

Symmetry in MPS

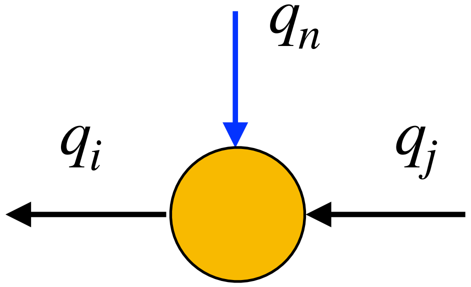
- Bond indices can be labelled by same symmetry labels as physical sites
- U(1) symmetry



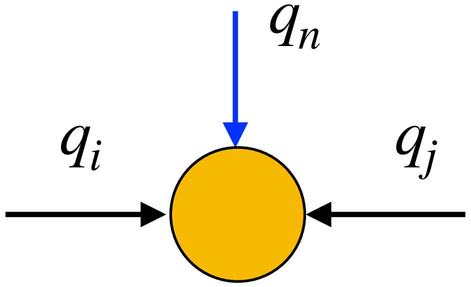
$$\sum q_{in} = \sum q_{out}$$



$q_i + q_n = q_j$



$q_j + q_n = q_i$



$q_j + q_n + q_i = Q$

Perform computation in different *q* sectors