TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Tensor Networks (SS2021)

Lecture 3: Canonical form of MPS

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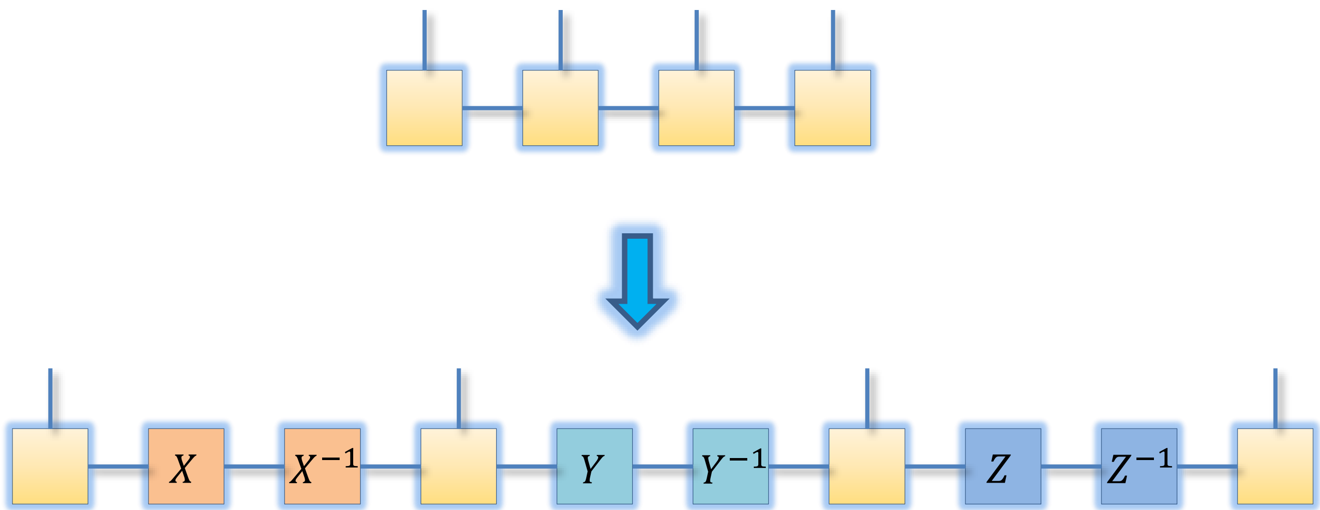
§ 1.3 Canonical forms of MPS

Gauge freedom in MPS:



- Different choices of $\{A^{s_i}_{\alpha_{i-1},\alpha_i}\}$ might give rise to the same MPS.
- We would like to define a canonical form of MPS.

§ 1.3 Canonical forms of MPS

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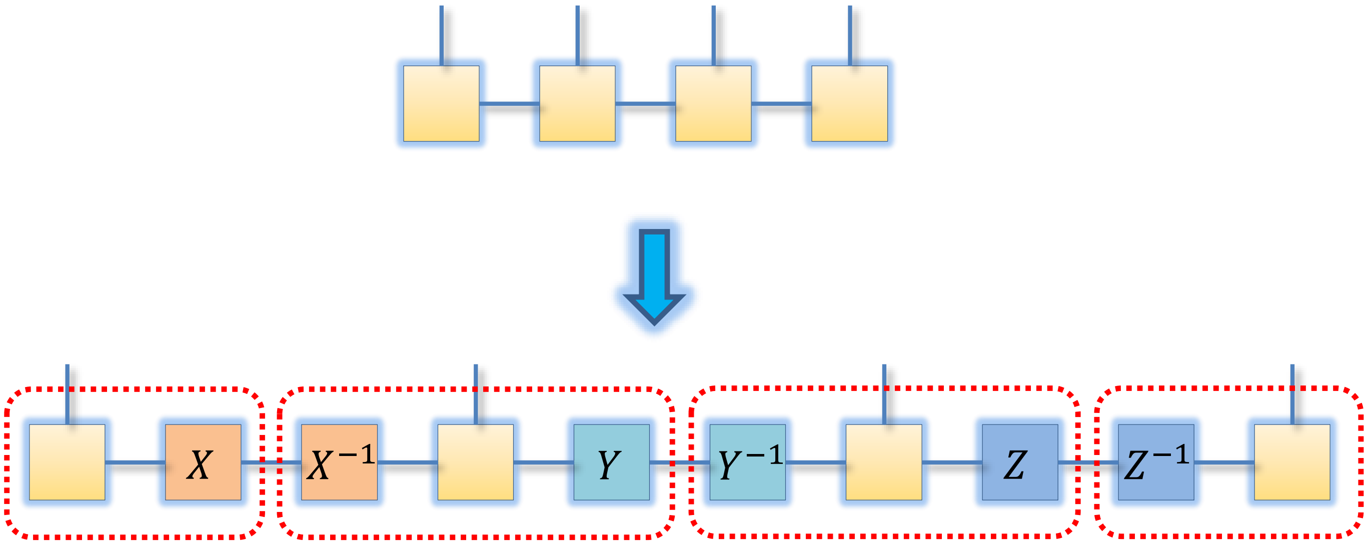

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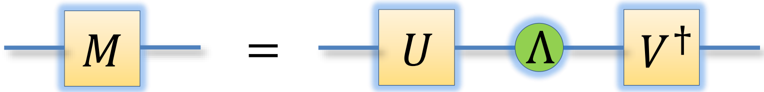
§ 1.3 Canonical forms of MPS

Singular value decomposition (SVD) of matrices:

$$M = U\Lambda V^\dagger$$



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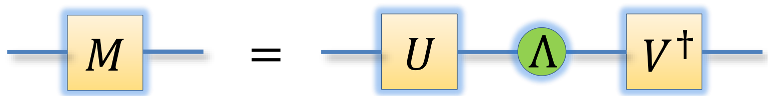
$m \times n$



Case 1: $m \leq n$

- U: $m \times m$ unitary matrix
- $V^\dagger$: $m \times n$ matrix satisfying $V^\dagger V = I_{m\times m}$ (isometry)
- Λ: diagonal matrix with non-negative diagonal entries (singular values)

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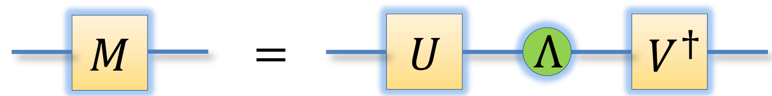

Case 2: $m > n$

- U: $m \times n$ matrix satisfying $U^\dagger U = I_{n\times n}$ (isometry)
- $V^\dagger$: $n \times n$ unitary matrix
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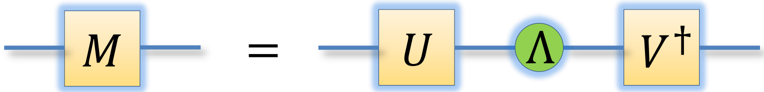

Example (from Wikipedia):

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} 3 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{5} & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & -1 & 0 & 0 \\ -\sqrt{0.2} & 0 & 0 & 0 & -\sqrt{0.8} \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -\sqrt{0.8} & 0 & 0 & 0 & \sqrt{0.2} \end{bmatrix}$$

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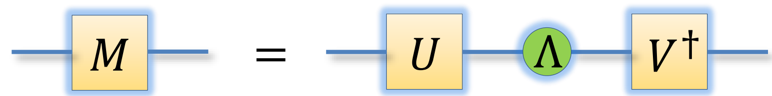

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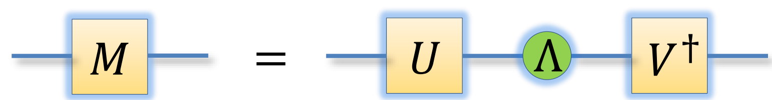


Remark:

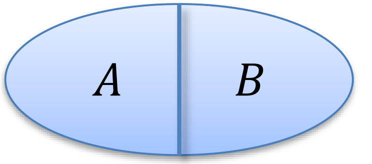
- It's often more convenient to delete zero singular values (U and $V^{\dagger}$ are then both isometries).

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 & \cancel{0} \\ -1 & 0 & 0 & \cancel{0} \\ 0 & 0 & 0 & \cancel{-1} \\ 0 & 0 & -1 & \cancel{0} \end{bmatrix} \begin{bmatrix} 3 & 0 & 0 & \cancel{0} & \cancel{0} \\ 0 & \sqrt{5} & 0 & \cancel{0} & \cancel{0} \\ 0 & 0 & 2 & \cancel{0} & \cancel{0} \\ \cancel{0} & \cancel{0} & \cancel{0} & \cancel{0} & \cancel{0} \end{bmatrix} \begin{bmatrix} 0 & 0 & -1 & 0 & 0 \\ -\sqrt{0.2} & 0 & 0 & 0 & -\sqrt{0.8} \\ 0 & -1 & 0 & 0 & 0 \\ \cancel{0} & \cancel{0} & \cancel{0} & \cancel{1} & \cancel{0} \\ \cancel{-\sqrt{0.8}} & \cancel{0} & \cancel{0} & \cancel{0} & \cancel{\sqrt{0.2}} \end{bmatrix}$$

§ 1.3 Canonical forms of MPS

Schmidt decomposition of a quantum state:

$$|\psi\rangle = \sum_{\alpha=1}^{m} \sum_{\beta=1}^{n} \psi_{\alpha\beta} |\alpha\rangle_A \otimes |\beta\rangle_B$$



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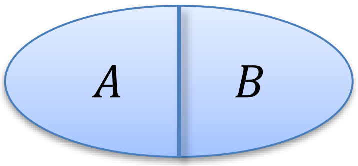

SVD: $$\psi_{\alpha\beta} = \sum_{\gamma=1}^{\chi} U_{\alpha\gamma}\, \lambda_\gamma V^\dagger_{\gamma\beta}$$

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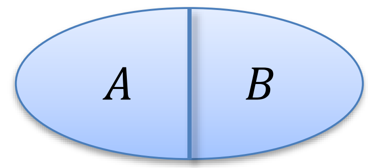

$$= \sum_{\gamma=1}^{\chi} \lambda_\gamma \left|\phi_\gamma^A\right\rangle \otimes \left|\phi_\gamma^B\right\rangle$$

Schmidt coefficients Schmidt vectors

$$\left|\phi_\gamma^A\right\rangle = \sum_{\alpha=1}^{m} U_{\alpha\gamma} |\alpha\rangle_A$$

χ: Schmidt rank

$$\left|\phi_\gamma^B\right\rangle = \sum_{\beta=1}^{n} V_{\gamma\beta}^\dagger |\beta\rangle_B$$

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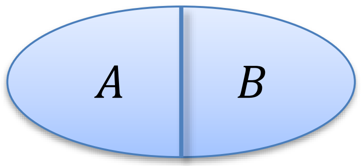
Reduced density matrix:

$$|\psi\rangle = \sum_{\gamma=1}^{\chi} \lambda_\gamma |\phi_\gamma^A\rangle \otimes |\phi_\gamma^B\rangle$$



$$\rho_A = \mathrm{tr}_B(|\psi\rangle\langle\psi|)$$

$$= \sum_{\gamma=1}^{\chi} \lambda_\gamma^2 |\phi_\gamma^A\rangle\langle\phi_\gamma^A|$$

Entanglement entropy: $S = -\mathrm{tr}_A(\rho_A \ln \rho_A) \leq \ln \chi$

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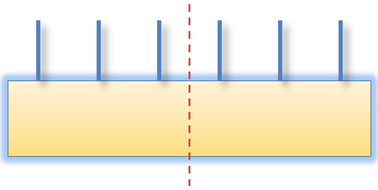
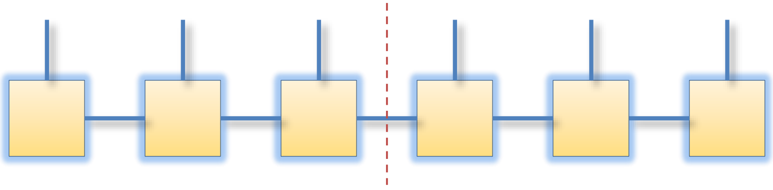
- Computing the Schmidt decomposition of a general many-body state is difficult.

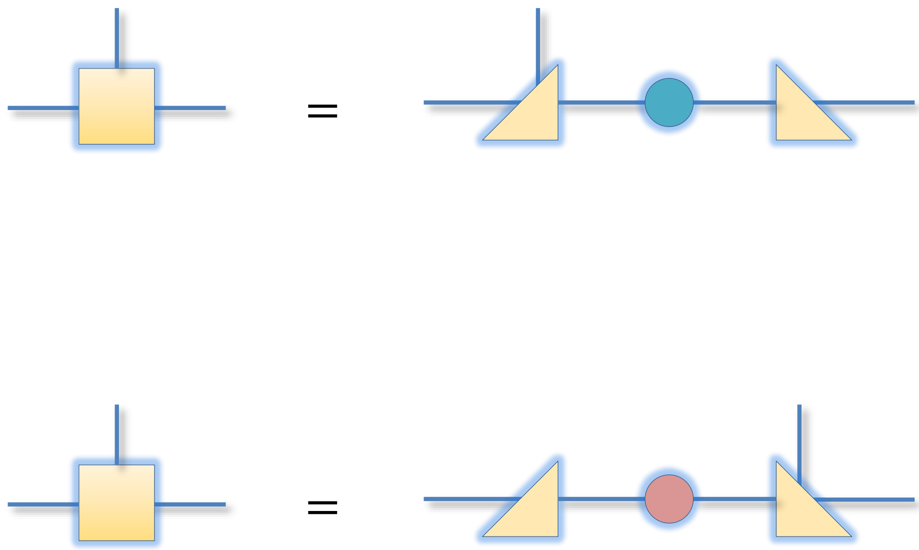


- Computing the Schmidt decomposition of an MPS is easy.



§ 1.3 Canonical forms of MPS

Use SVD:



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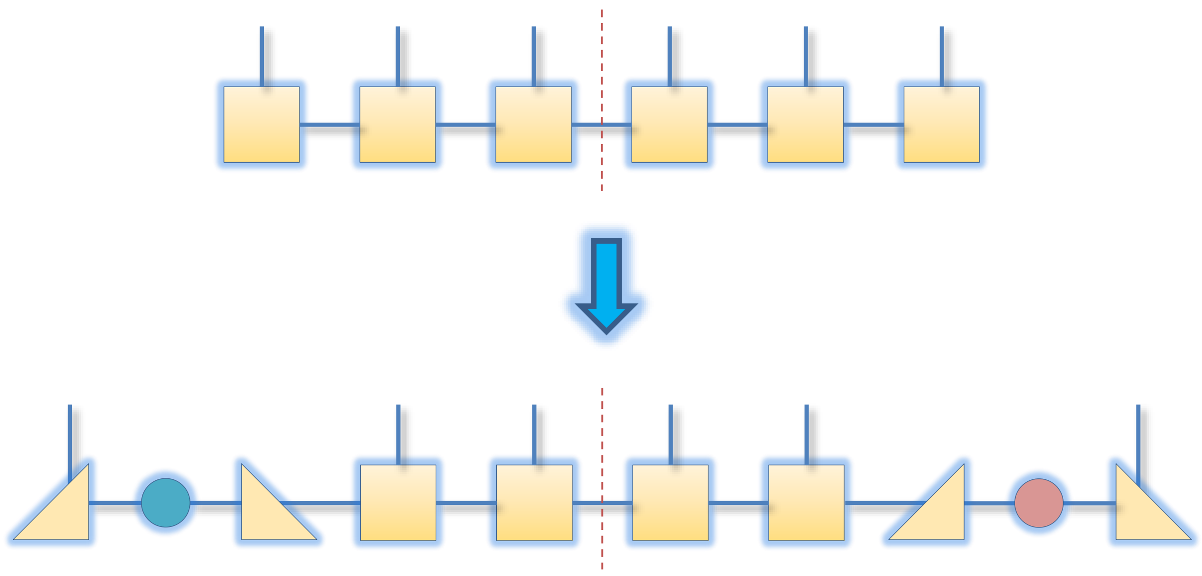

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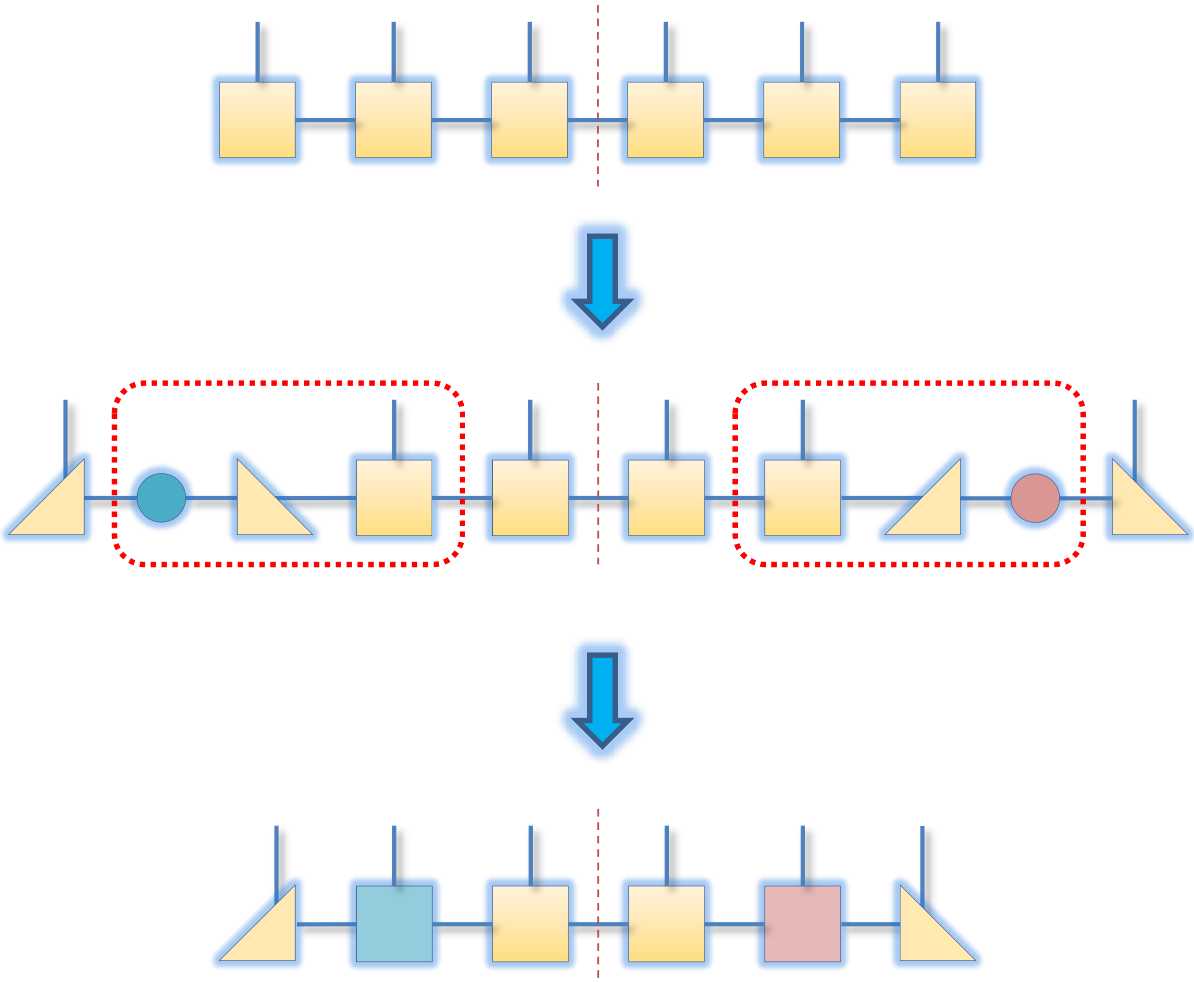

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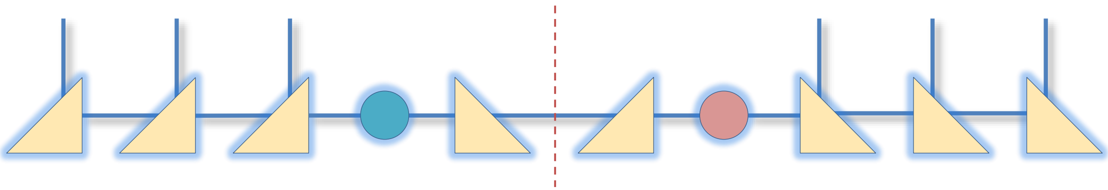
Use SVD successively, until



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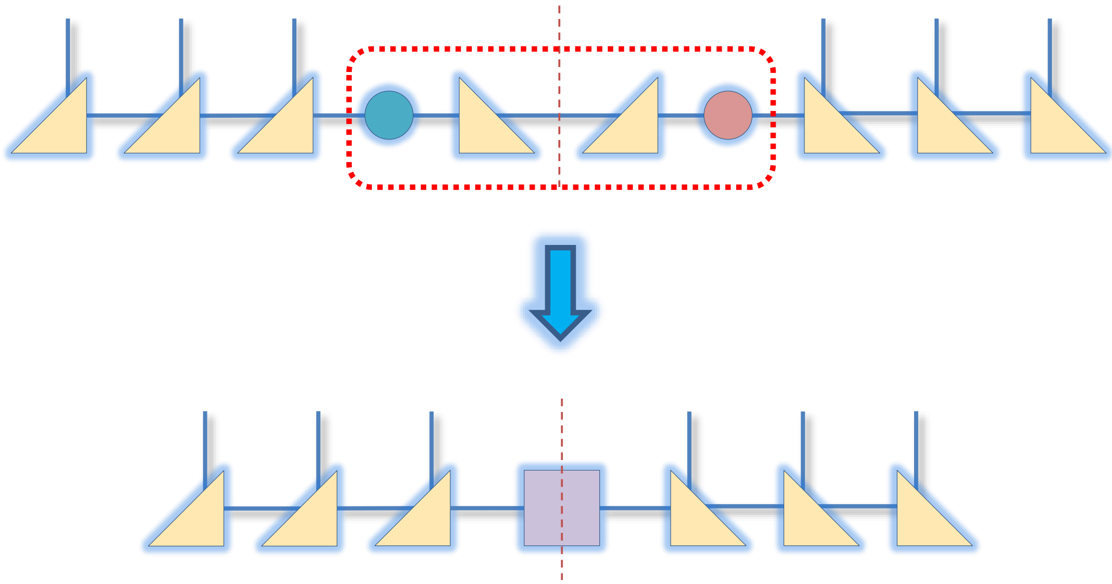

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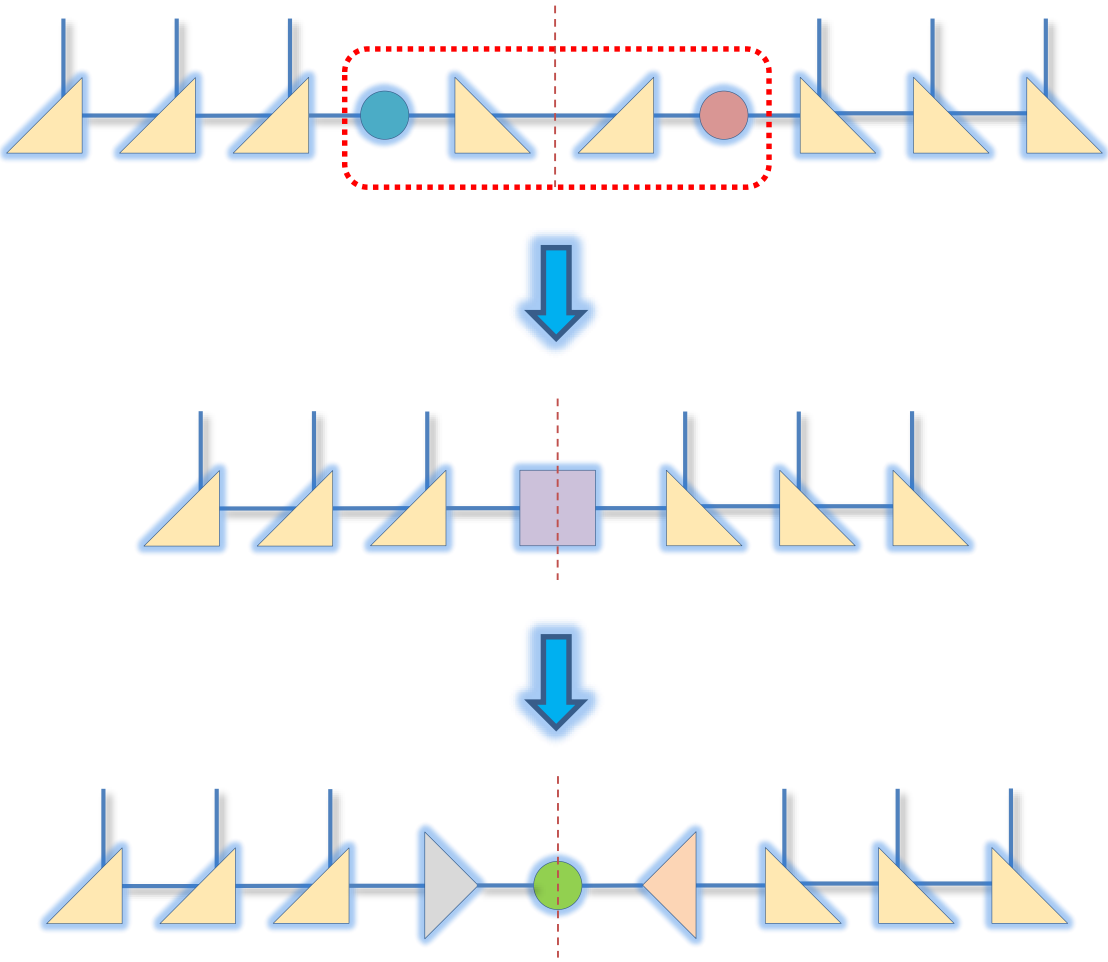

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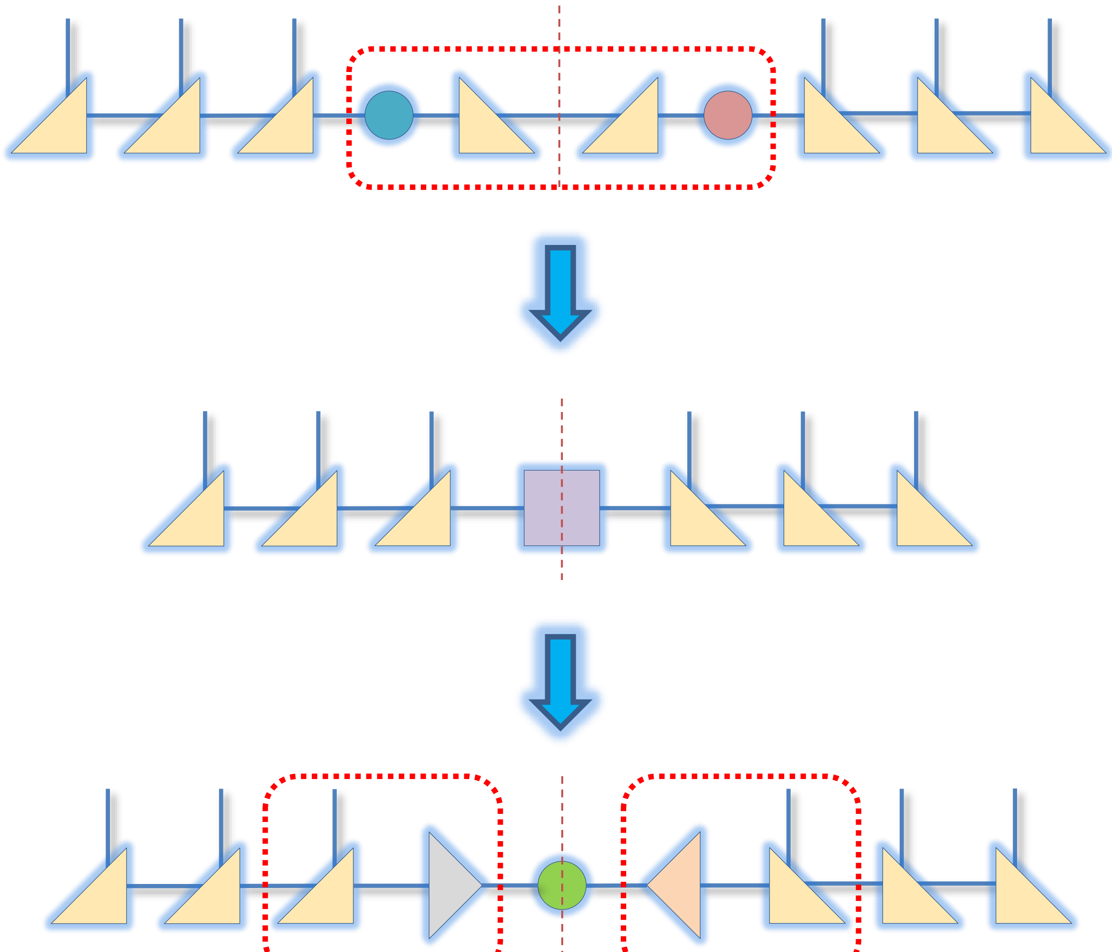

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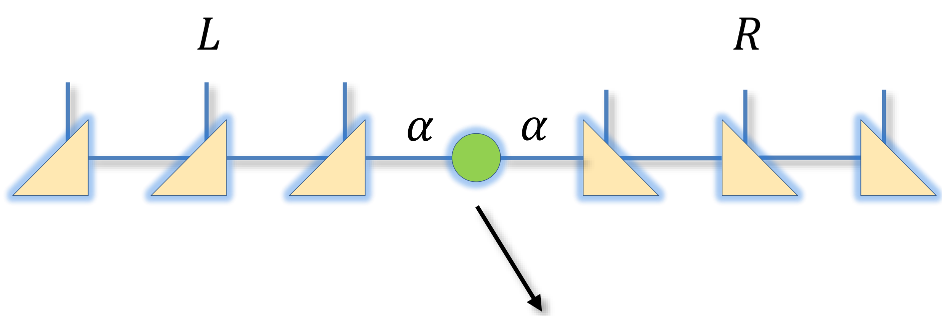
Mixed (bond) canonical form:



Diagonal matrix: $\lambda_\alpha > 0$ and $\sum_{\alpha=1}^{D} \lambda_\alpha^2 = 1$

- MPS in mixed canonical form is normalized.

- The mixed canonical form gives the Schmidt decomposition of the bipartite partition:

$$|\psi\rangle = \sum_{\alpha=1}^{D} \lambda_\alpha |\phi_\alpha^L\rangle \otimes |\phi_\alpha^R\rangle$$