テンソルネットワーク法を用いた量子計算のシミュレーション

白川知功

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理化学研究所・数理創造プログラム

２０２３年８月３１日 HPC-Phys 勉強会

Our team https://www.r-ccs.riken.jp/labs/cms/

Computational Materials Science Research Team

Team leader: Seiji Yunoki

Numerical studies in condensed matter physics
Development of quantum algorithms

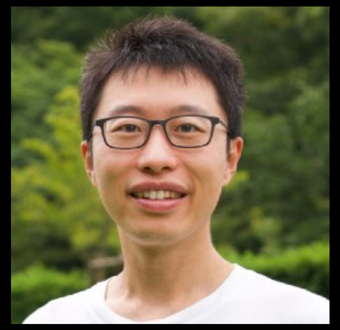
RIKEN

R-CCS

RIKEN QUANTUM COMPUTING

Tomonori Shirakawa

Numerical studies in condensed matter physics, application of quantum algorithms
Exact diagonalization, DMRG, Cluster perturbation theory, ab-initio QMC, NISQ devices, Variational Monte Carlo



Rong-Yang Sun

Numerical studies on quantum many-body problems, development of quantum algorithms
MPS, NISQ devices

Kazuma Nagao

Dynamics in quantum many-body systems
Truncated Wigner approximation

Hidehiko Koshiro

Numerical & Theoretical studies on quantum many-body systems
Tensor network methods

Libraries for tensor network methods

GraceQ

High-performance computing for the quantum world

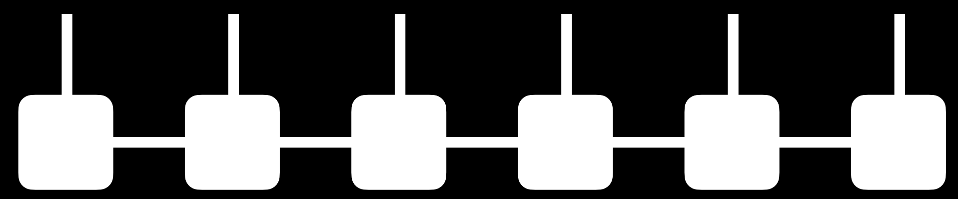
https://gracequantum.org/

Introduction

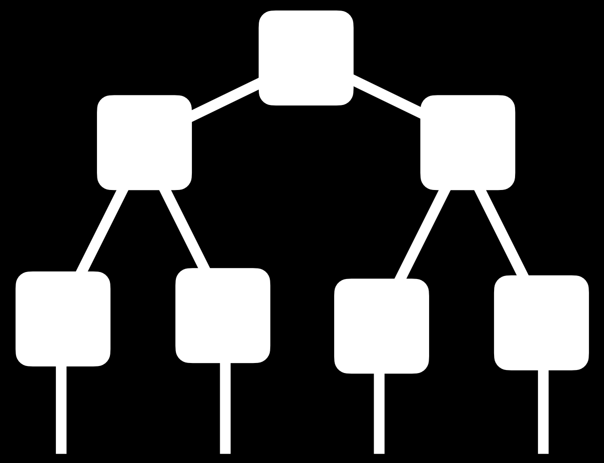
Tensor network methods

- Computational methods that have developed as a **compact** way to represent **quantum many-body states**

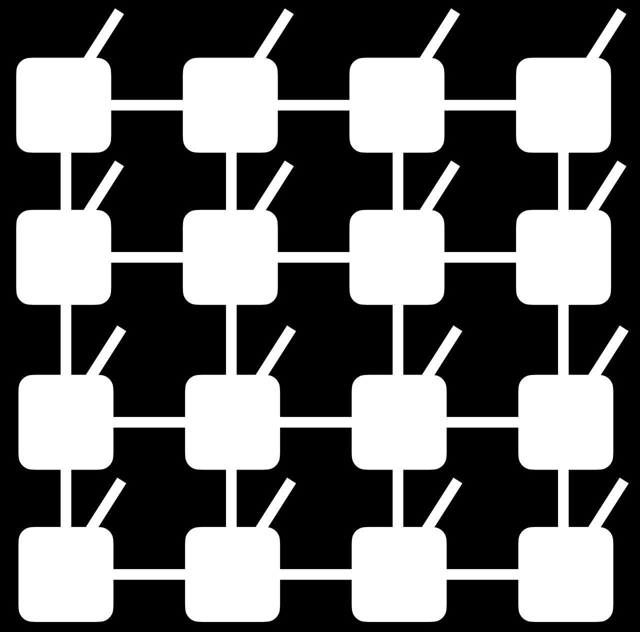
MPS



Tree tensor networks



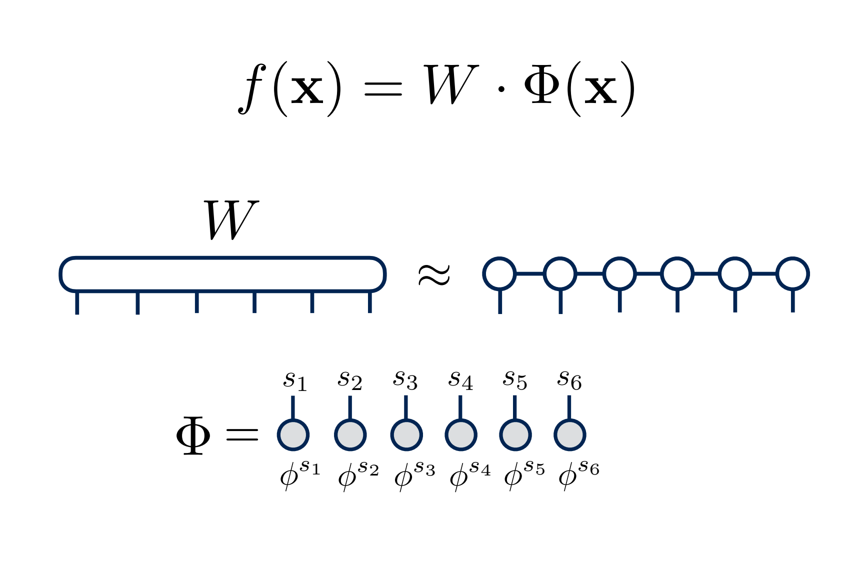
PEPS



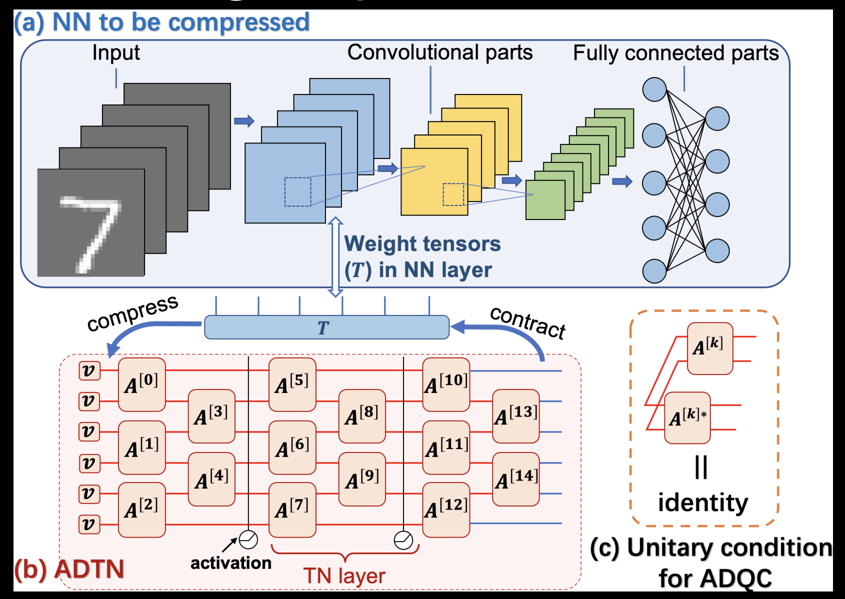
Compression of an exponentially large vector (tensor) into product of low-rank tensors

- It has recently attracted attention as an efficient representation of **machine learning** models and as a highly efficient compression method for **big data**.

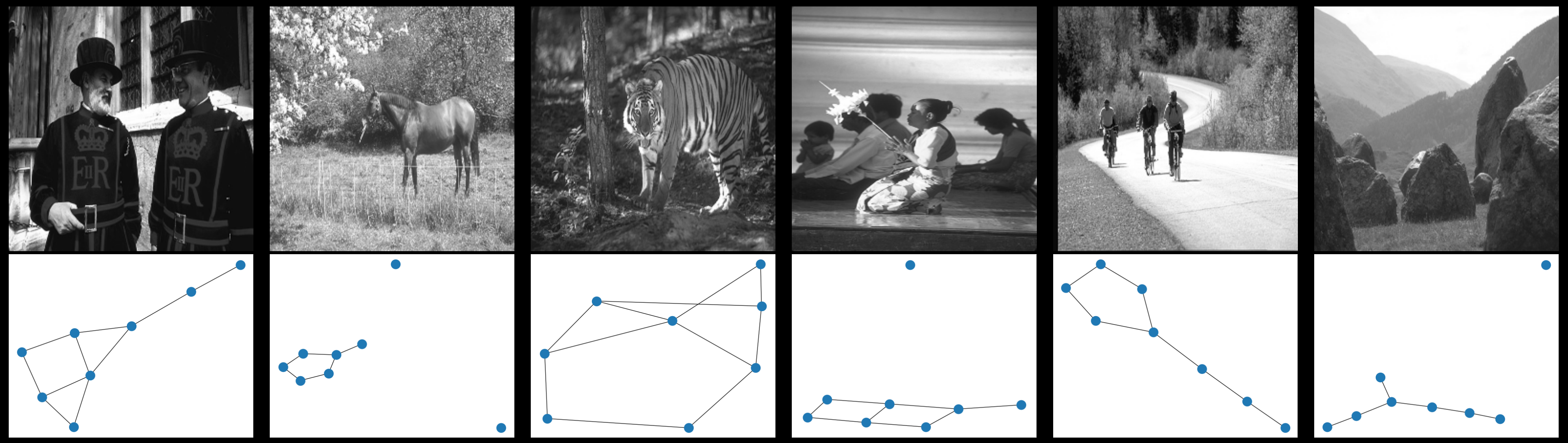
[Stoundemire&Schwab, 2017]



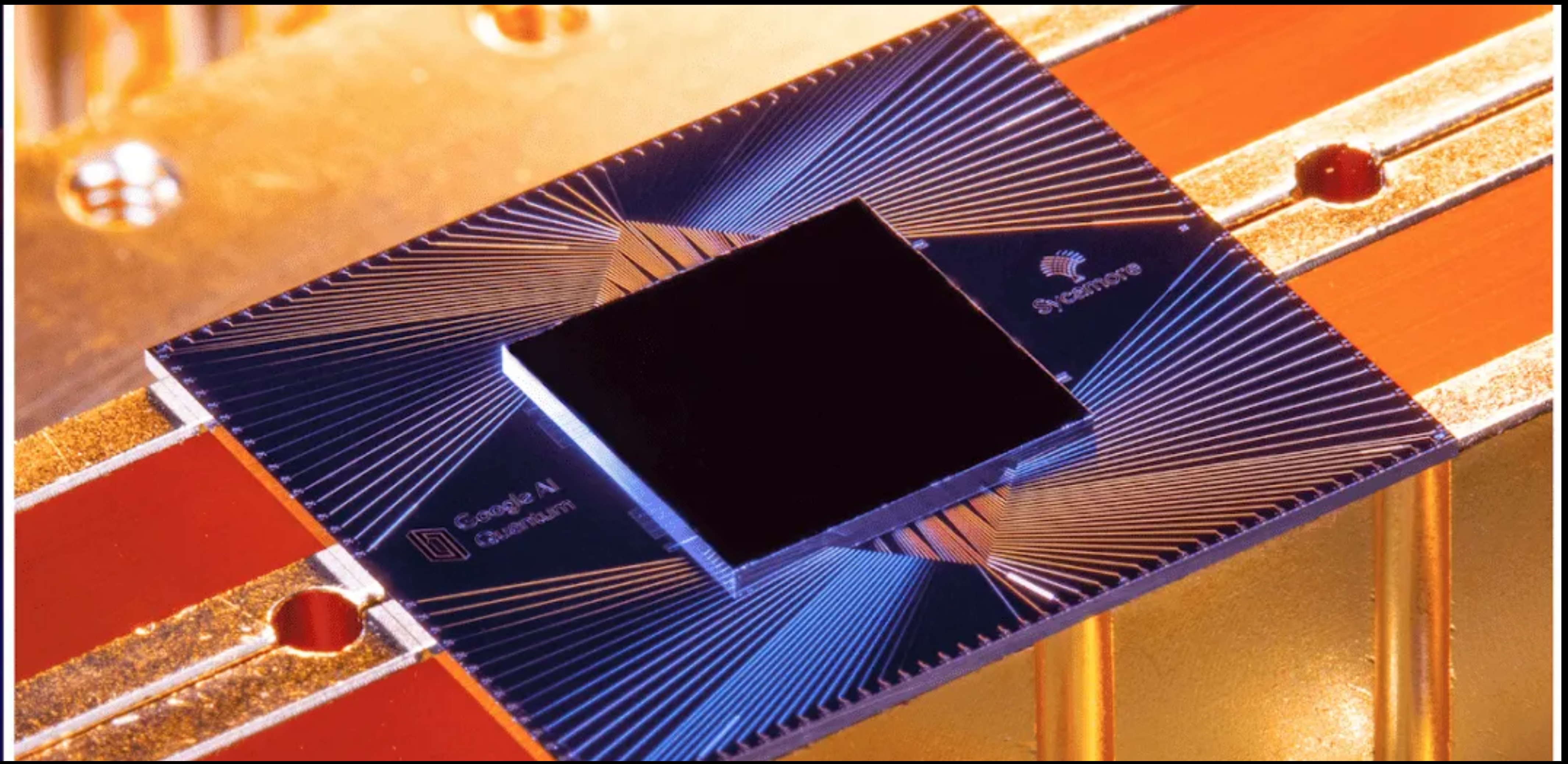
[Shi-Ju Ran group, arXiv:2305.06058]

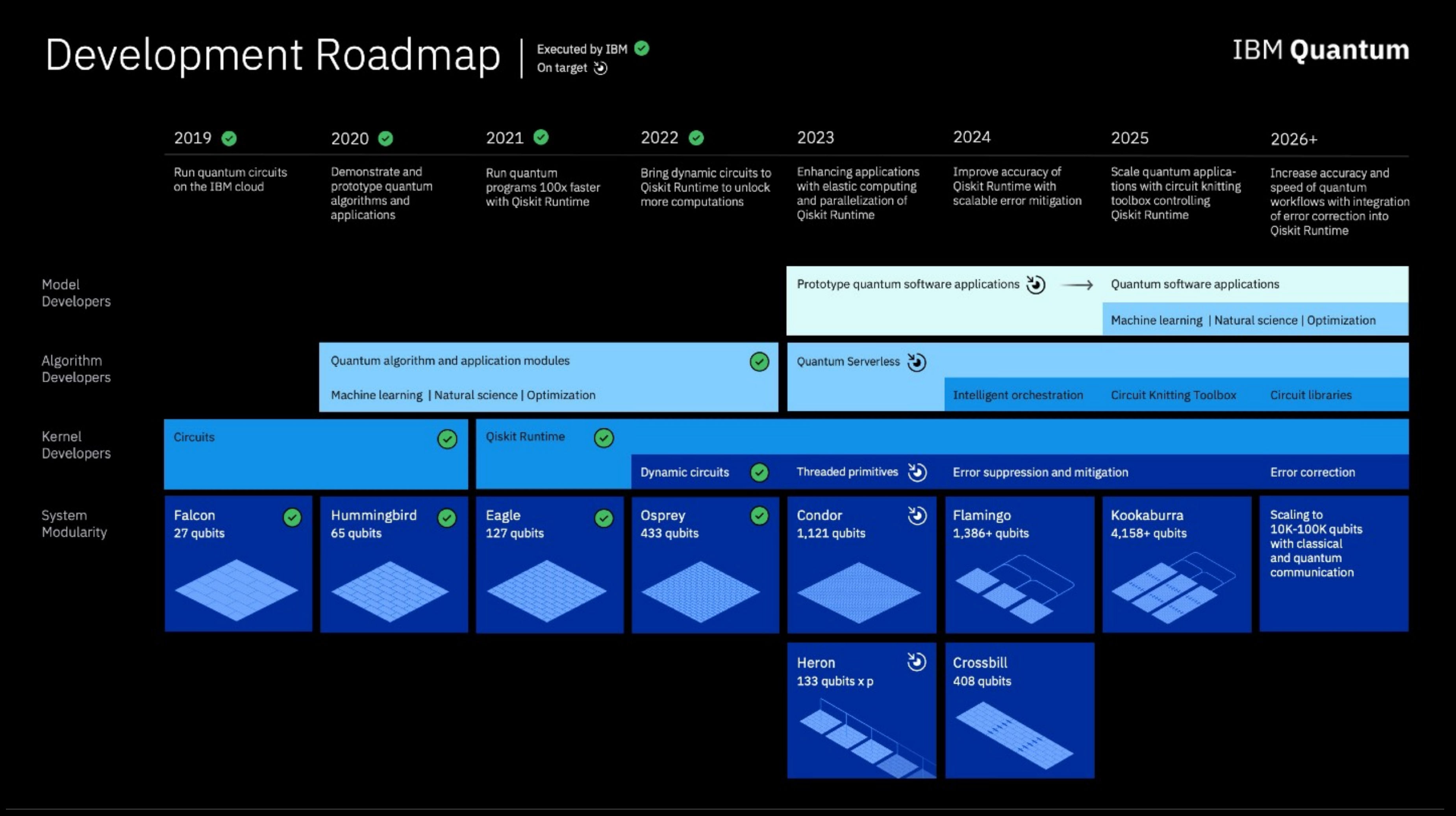


[Chao Li et al (AIP tensor learning team), 2020, 2022, 2023]



Near-term quantum devices





- Noisy intermediate-scale quantum (NISQ) era
  - A few $\mathcal{O}(10^2 \sim 10^3)$ qubits **without** error correction
  - A few $\mathcal{O}(10^1 \sim 10^2)$ depths circuit evolution

Quantum Computing in the NISQ era and beyond

John Preskill

Institute for Quantum Information and Matter and Walter Burke Institute for Theoretical Physics, California Institute of Technology, Pasadena CA 91125, USA

30 July 2018

Near-term aim: achieve useful quantum advantage on NISQ devices

Quantum computing and tensor network methods

Main uses of tensor network methods for research of quantum computing

1. Tensor network as a simulator for quantum computing

    - Exact contraction of quantum circuit (similar to the **state-vector simulator**)

      $\langle 0 | \hat{C}^\dagger \hat{O} \hat{C} | 0 \rangle = \mathrm{Tr}[\hat{U}_M \cdots \hat{U}_2 \hat{U}_1 | 0 \rangle \langle 0 | \hat{U}_1^\dagger \hat{U}_2^\dagger \cdots \hat{U}_M^\dagger \hat{O}] \longrightarrow$ Compute all contractions as products of tensors

    - Simulators using tensor network method to approximate quantum states after gate operations

      Today's topic: **tensor network simulator**

2. Development of useful algorithm based on the tensor network

    - Construct a circuit for state preparation based on the tensor network states

      Find quantum circuit $\hat{C} = \hat{U}_M \hat{U}_{M-1} \cdots \hat{U}_1 | 0 \rangle$ s.t. $| \Psi \rangle \sim \hat{U}_M \hat{U}_{M-1} \cdots \hat{U}_1 | 0 \rangle$

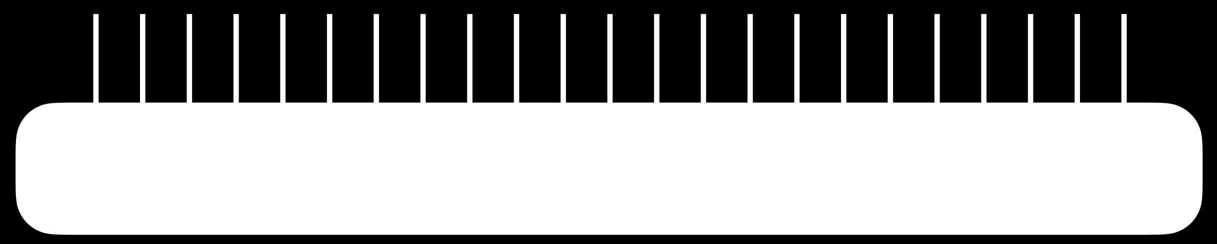
    - Circuit optimization/compilation by decomposing the large unitary operator into a product of small unitary operator

      Find optimal product of $\hat{U}_M \hat{U}_{M-1} \cdots \hat{U}_1$ s.t. $\hat{C} \sim \hat{U}_M \hat{U}_{M-1} \cdots \hat{U}_1$

    - Error mitigation utilizing the compression performance of tensor networks [Nation et al., PRX Quantum 2, 040326 (2021)]

Tensor network simulators

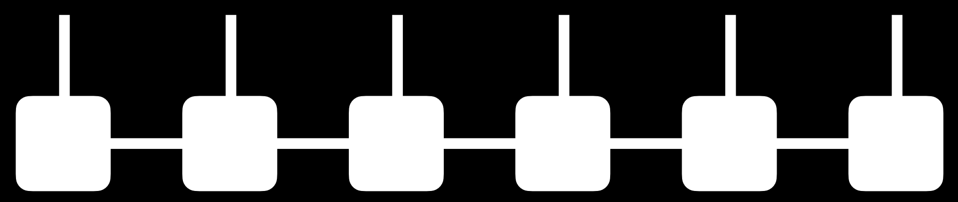
State vector simulator



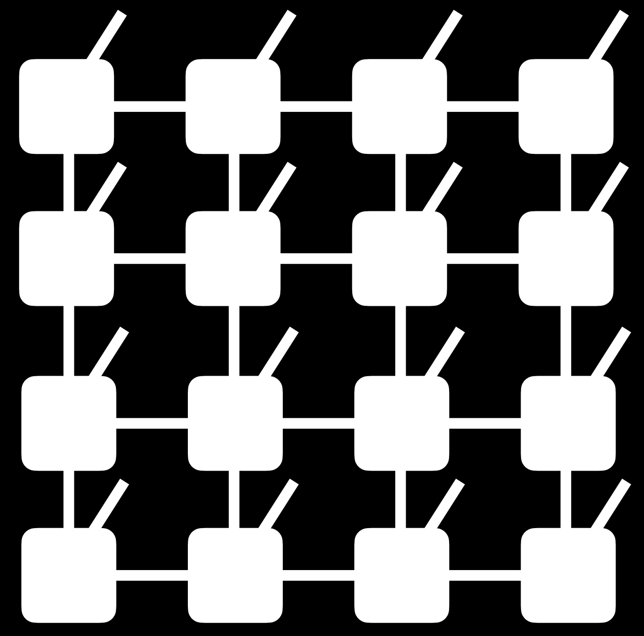
Can compute any quantum circuits
Hard limitation on number of qubits

Tensor network simulator

MPS



PEPS



Can compute quantum circuits with large qubits
Limitation on entanglements

Why we need the simulator of quantum computer?

(1) To check the validity of the quantum algorithm assuming that the quantum computer has worked correctly.

In order to explore the useful applications of quantum computers, it is necessary to check the results of quantum computers when they work properly.

(2) To verify that the quantum computer is working properly

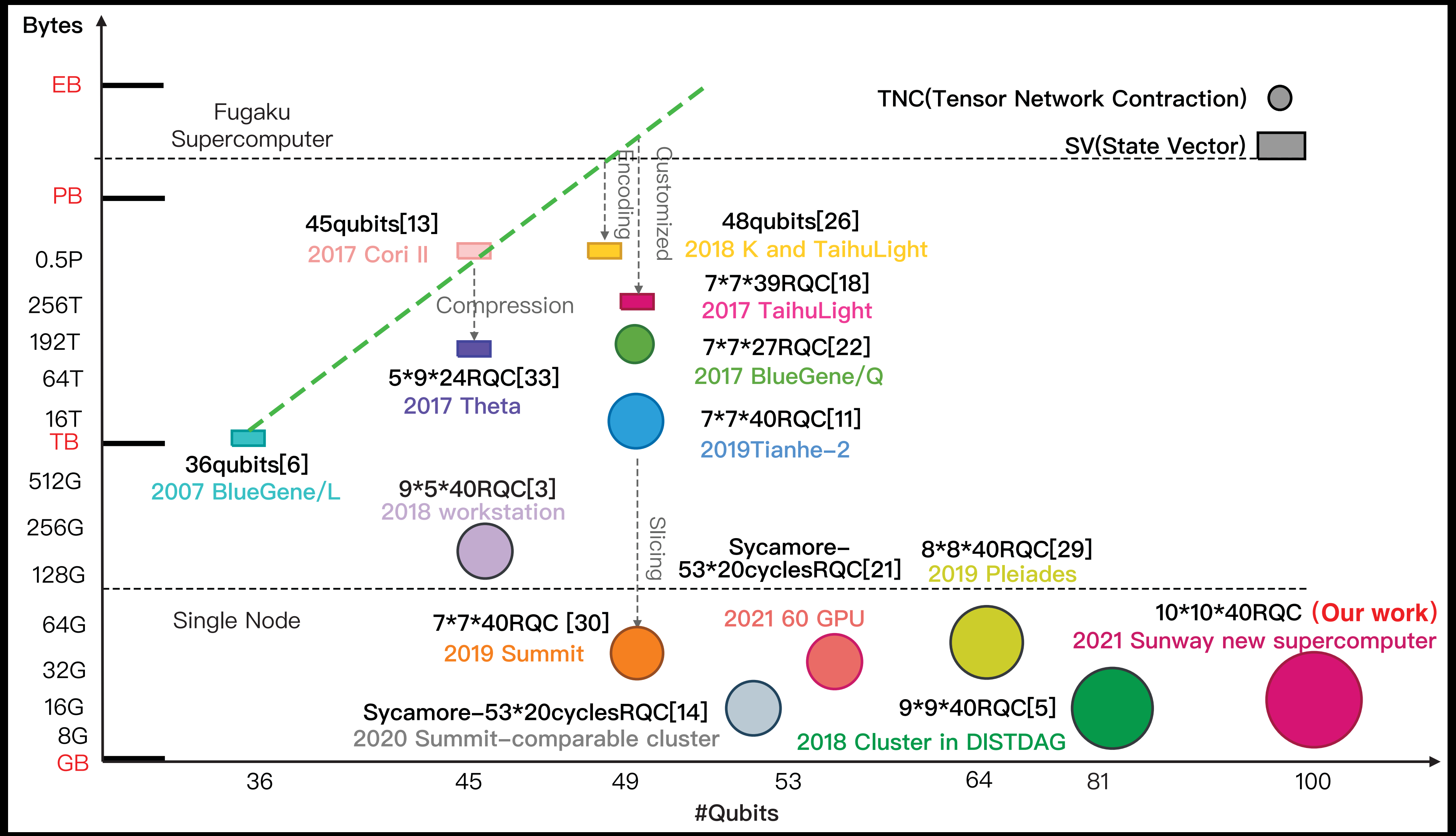
Current quantum computing devices are noisy and have no error correction, so they must be evaluated against correct operation.

(3) To bridge the classical information and quantum information

The simulator is useful in converting data for a single task in a joint effort between a quantum computer and a classical computer.

Tensor network simulators

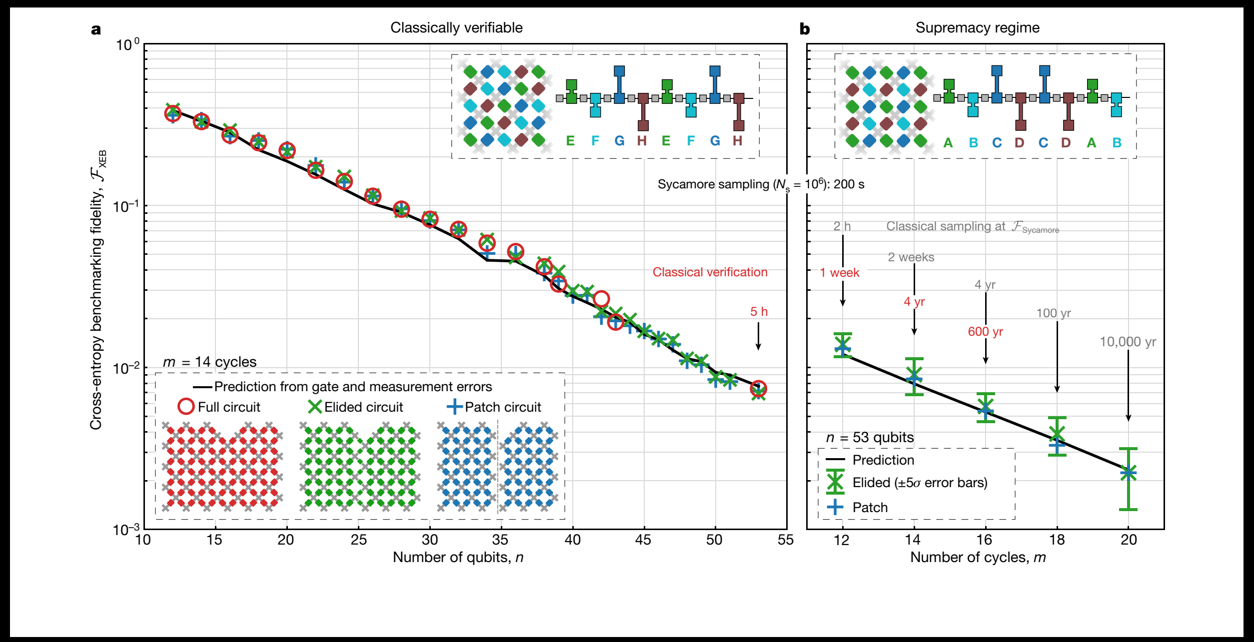
2021 ACM Gordon Bell Prize



- optimal slicing scheme
- three-level parallelization scales to about 42 million cores
- fused permutation and multiplication design for tensor contraction
- mixed-precision scheme

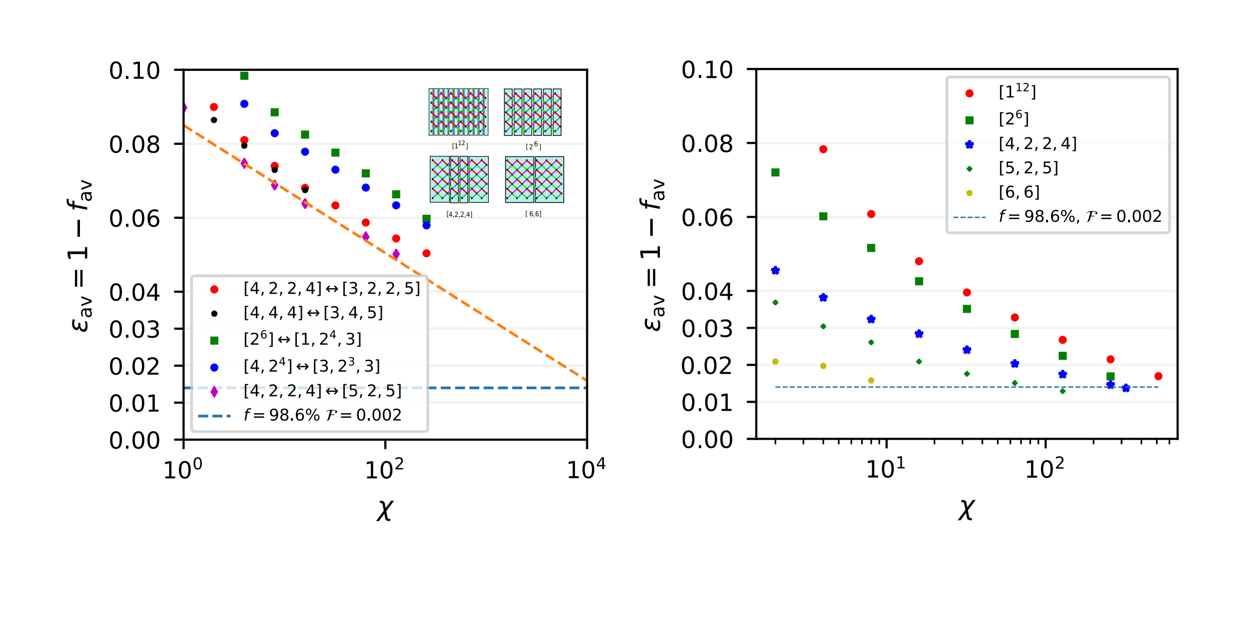
Performance comparison with real quantum devices

[Google, Nature **574**, 505-510 (2019)]



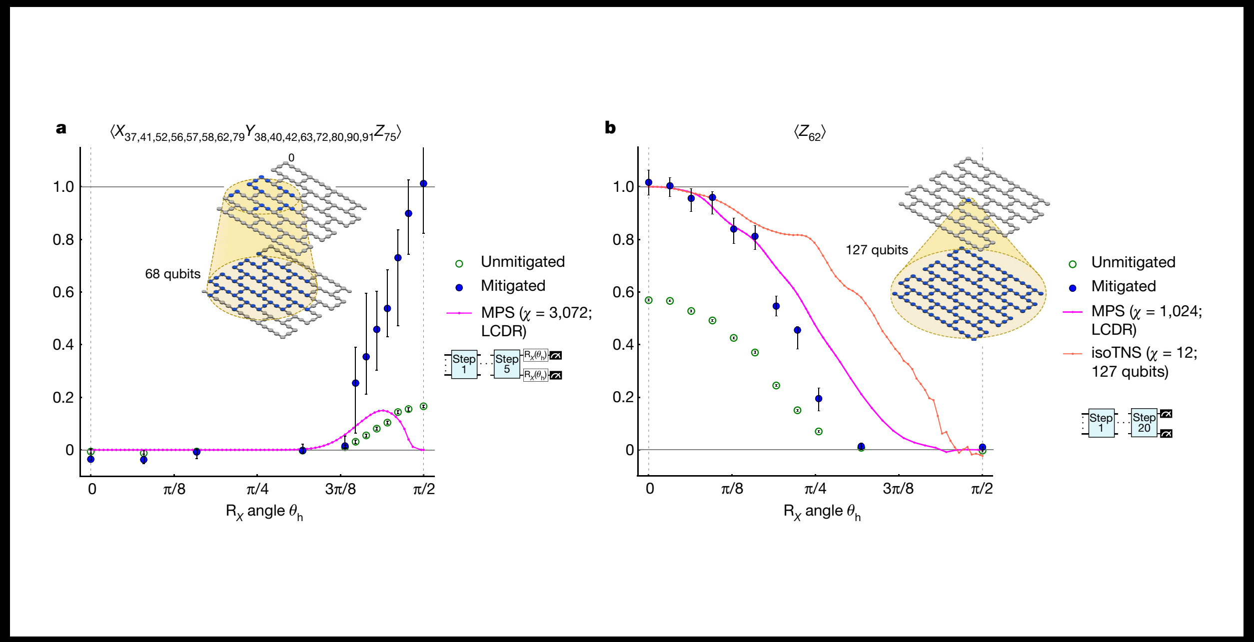
Real-device experiment
for random circuits

[Zhou et al, PRX **10**, 041038 (2020)]



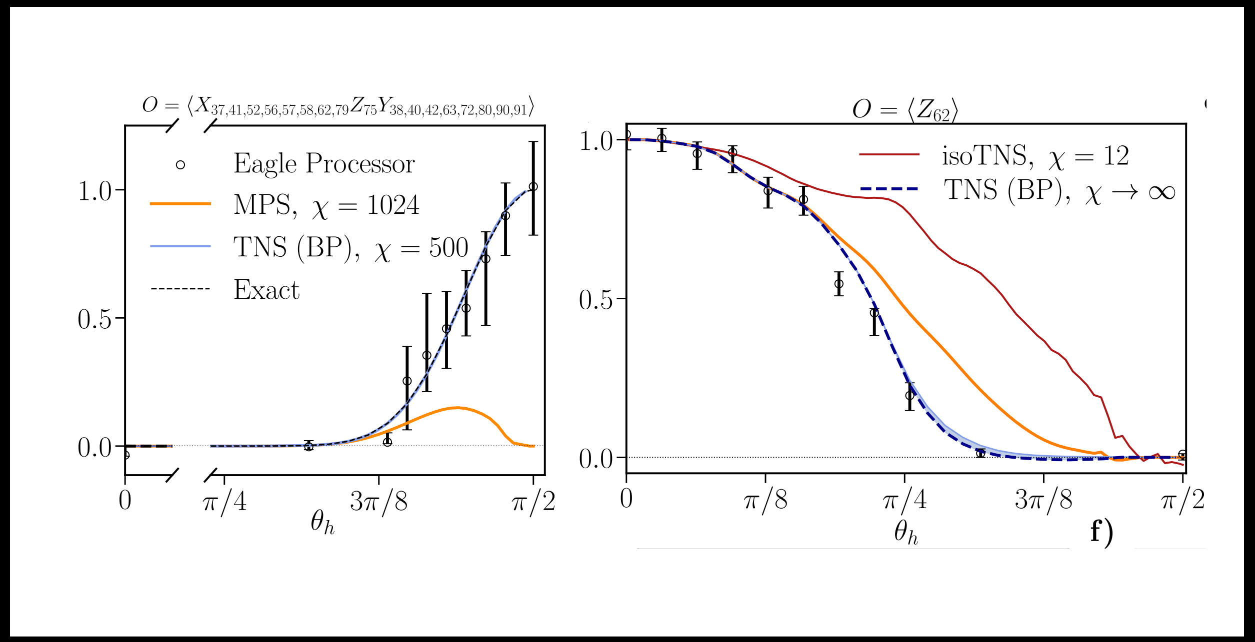
Tensor network simulation

[IBM, Nature **618**, 500 (2023)]



Real-device experiment
for quench dynamics

[Tindall et al., arXiv:2306.14887]



Tensor network simulation
(using Belief propagation technique)

No one knows the limit of performance.

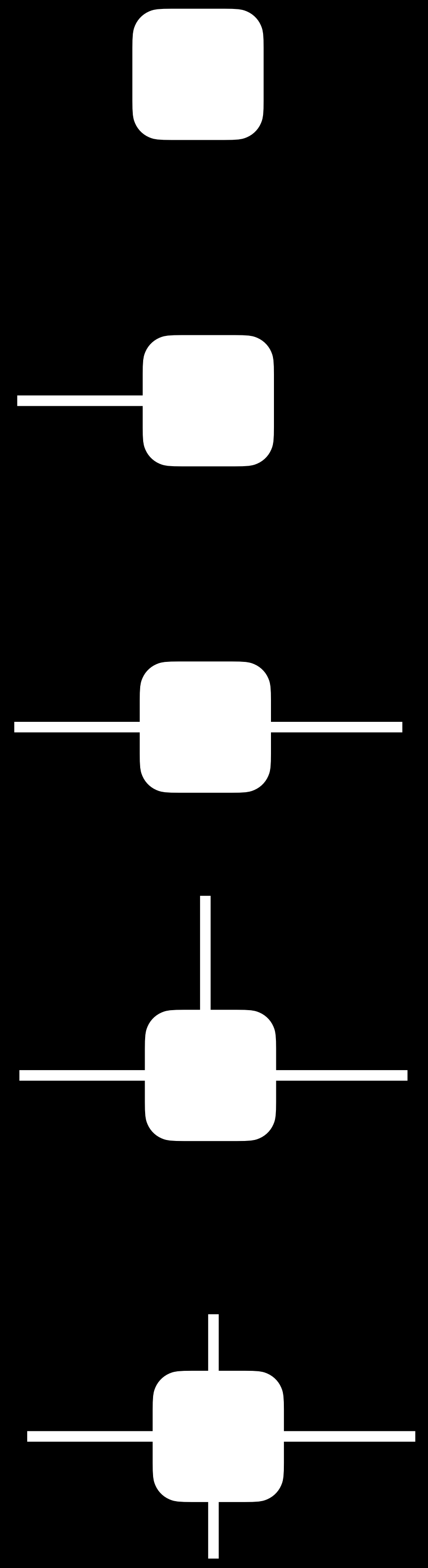
Outline

- Matrix product state
- Canonical form and gauging form
- Measurement and applying operator to state
- Time-evolving block decimation (TEBD) and its parallelization
- Extension to 2D tensor network (on-going project)
- Relation between tensor network and quantum circuit

Notations

Graphical representations of tensors

Tensors



Rank 0 tensor (scaler) c

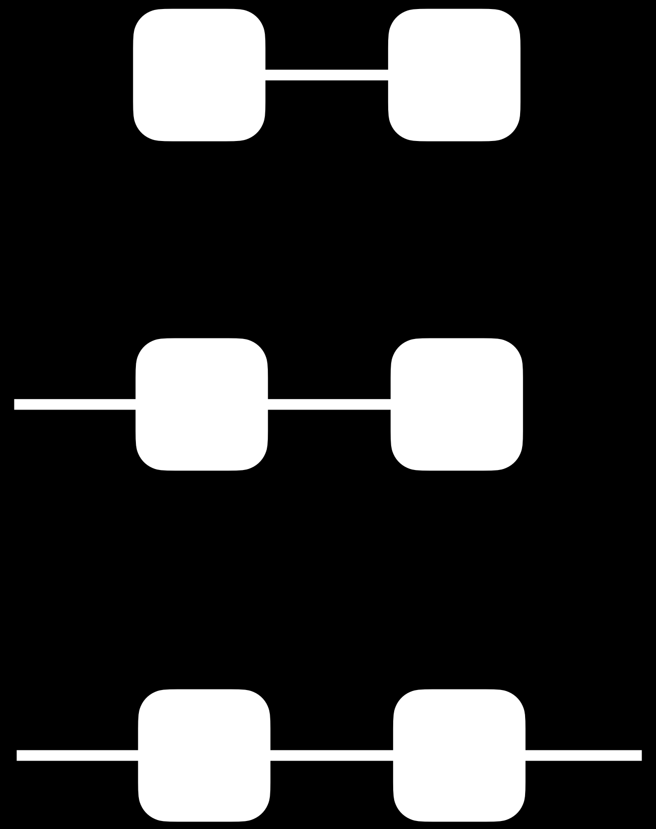
Rank 1 tensor (vector) u_i

Rank 2 tensor (matrix) A_{ij}

Rank 3 tensor T_{ijk}

Rank 4 tensor T_{ijkl}

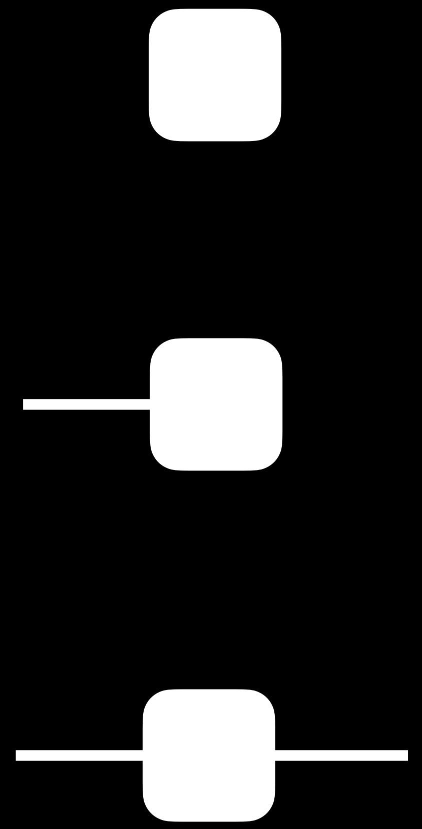
Contraction

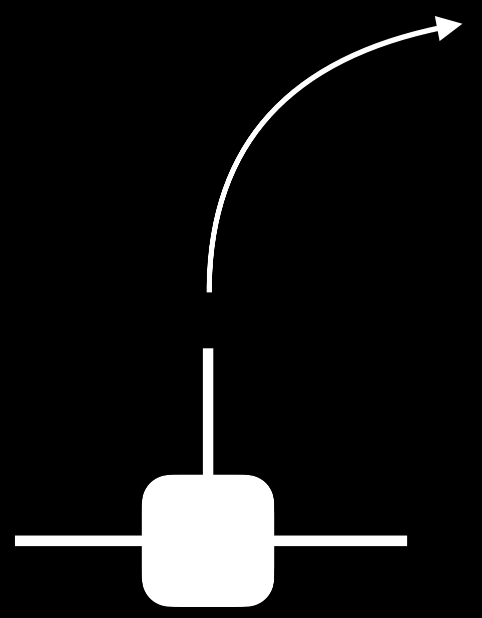


$= vu = \sum_i v_i u_i =$

$= Au = \sum_j A_{ij} u_j =$

$= AB = \sum_j A_{ij} B_{jk} =$

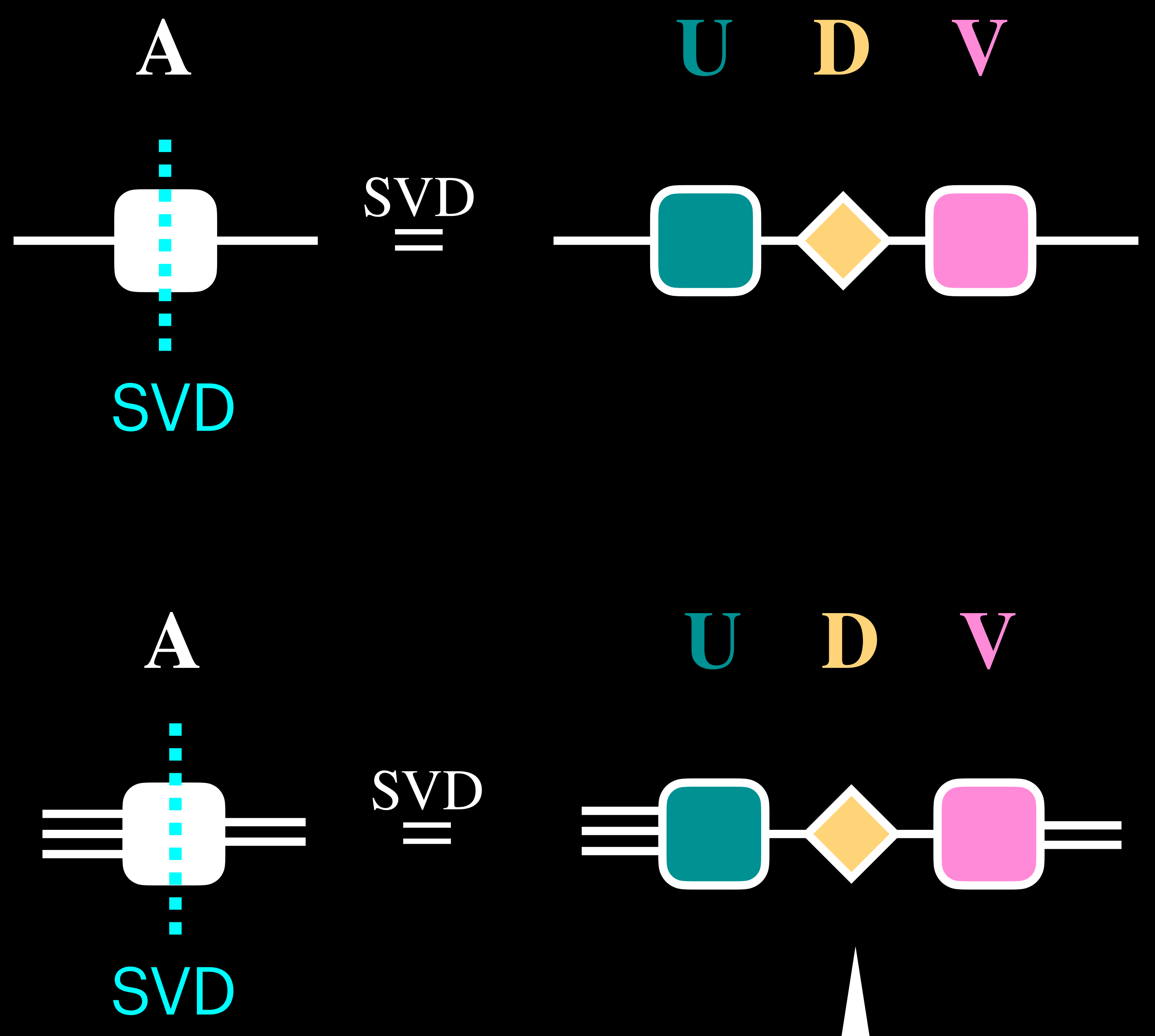




We call each line “bond”.

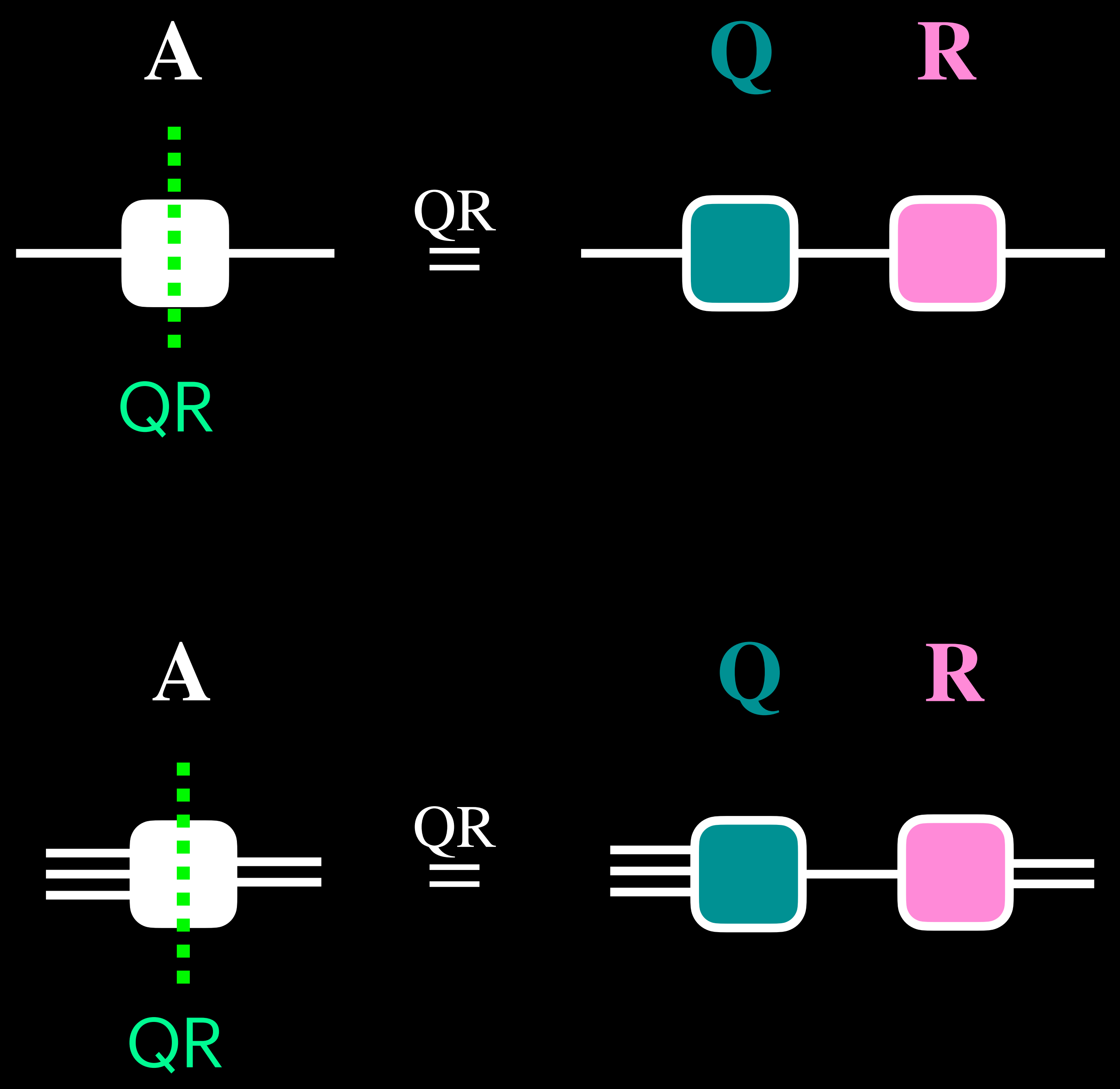
Analytical decomposition

Singular value decomposition (SVD)



Henceforth, a diagonal matrix tensor is represented using a diamond-shaped symbol.

QR decomposition



QR decomposition is not used for bond truncation, but is useful for extracting associated low-rank tensors.

1D tensor network state
(Matrix Product State, MPS)

Tensor representation of quantum states

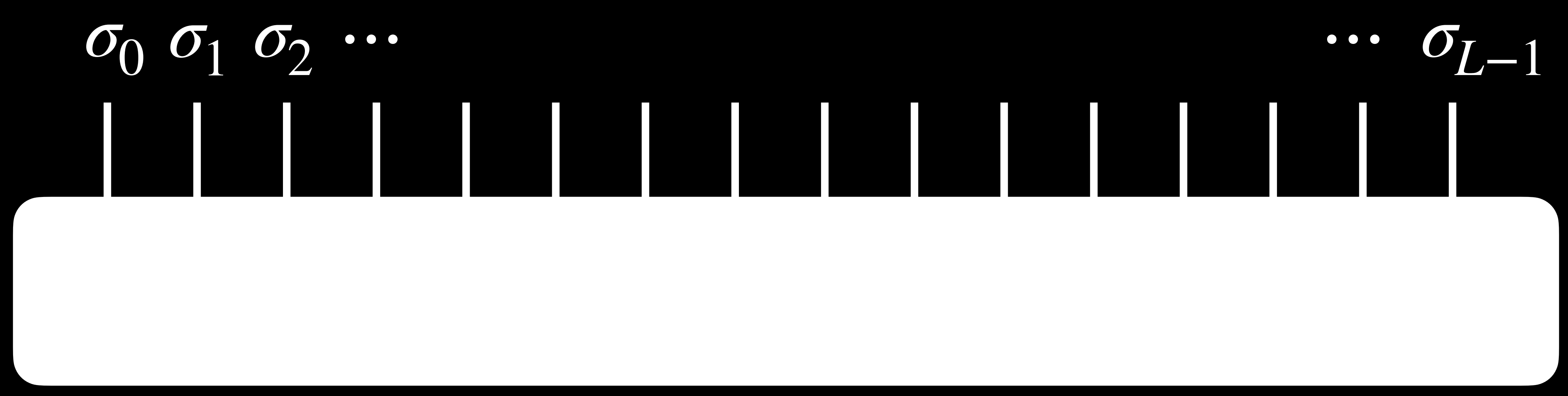
A quantum state (wave function) defined on a lattice $\mathbb{L} = \{0, 1, \cdots, L-1\}$:

$\mathbb{L}$ denotes labels of sites on a lattice.

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} \Psi_{\sigma_0\sigma_1\cdots\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$

$|\sigma_l\rangle$ ($\sigma_l = [0, d)$) denotes the local eigenstate on a site l.

The coefficients for each basis can be viewed as elements of a tensor.

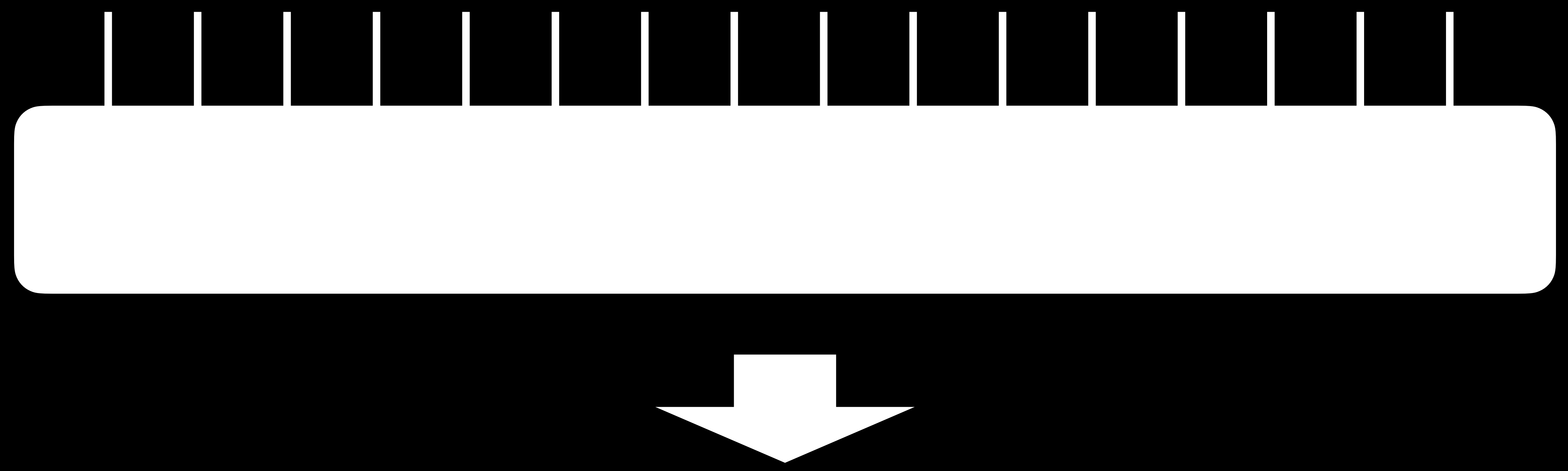


We call the subscripts corresponding to the basis of the physical system "physical bonds."

Matrix product states (MPS)

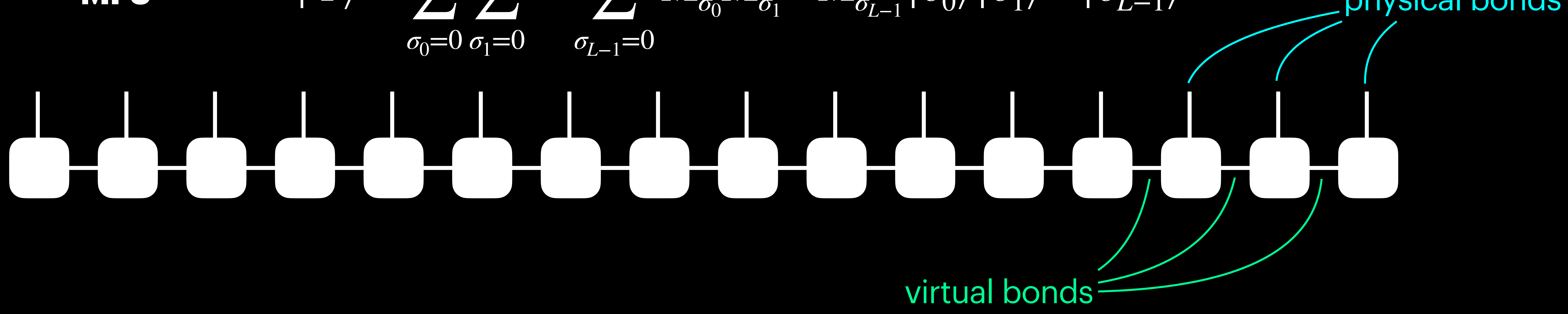
Quantum state

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1}\sum_{\sigma_1=0}^{d-1}\cdots\sum_{\sigma_{L-1}=0}^{d-1}\Psi_{\sigma_0\sigma_1\cdots\sigma_{L-1}}|\sigma_0\rangle|\sigma_1\rangle\cdots|\sigma_{L-1}\rangle$$



MPS

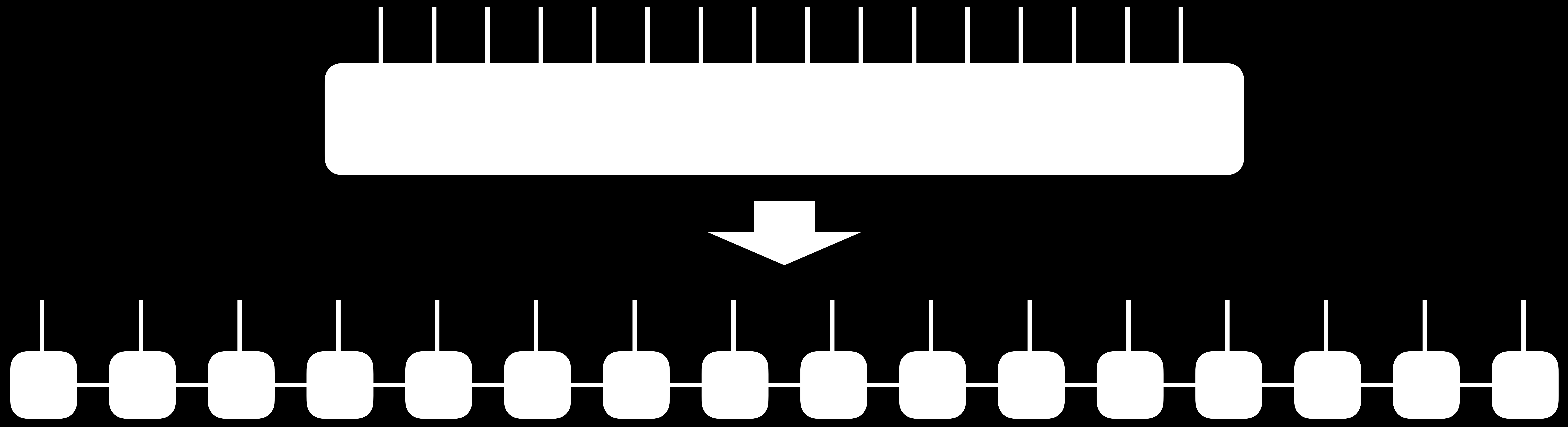
$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1}\sum_{\sigma_1=0}^{d-1}\cdots\sum_{\sigma_{L-1}=0}^{d-1}\mathbf{M}_{\sigma_0}\mathbf{M}_{\sigma_1}\cdots\mathbf{M}_{\sigma_{L-1}}|\sigma_0\rangle|\sigma_1\rangle\cdots|\sigma_{L-1}\rangle$$



Generality of MPS and “truncation”

Generality of MPS: Any quantum state can be expressed as a MPS form.

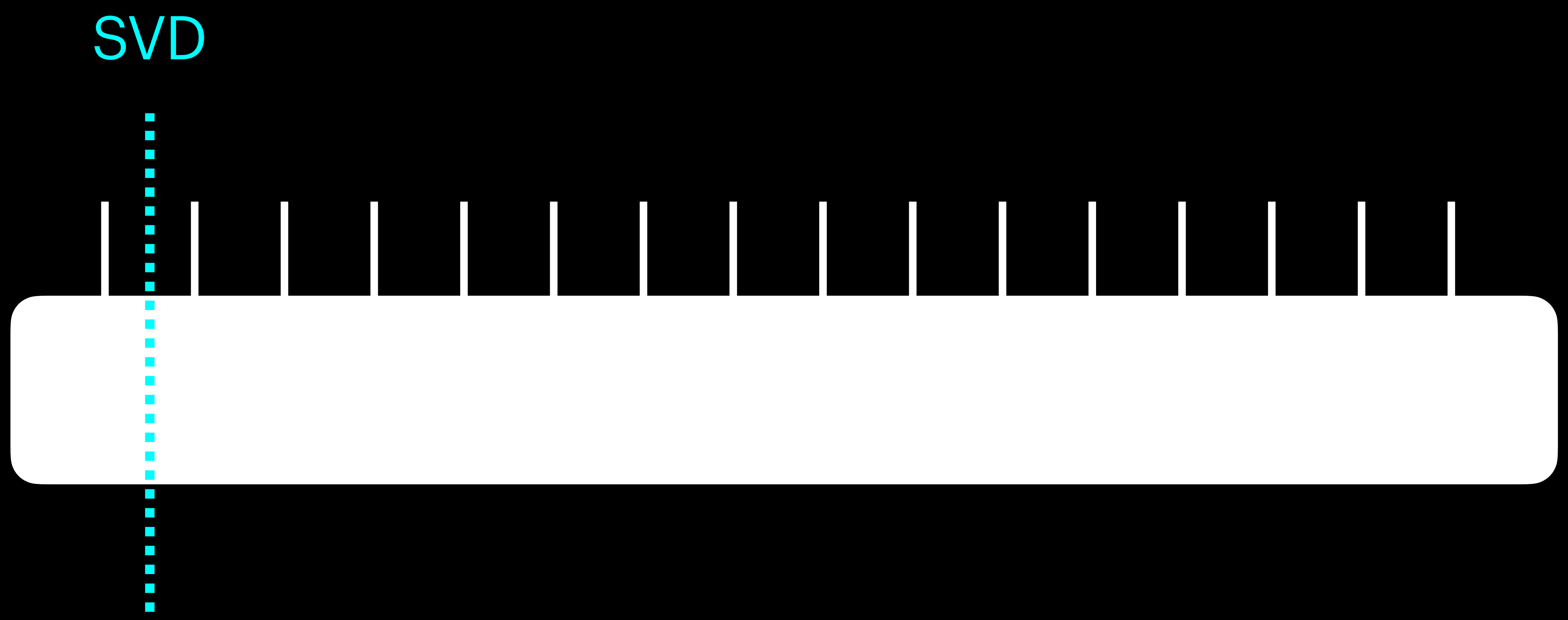
$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} \Psi_{\sigma_0\sigma_1\cdots\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$



Generality of MPS

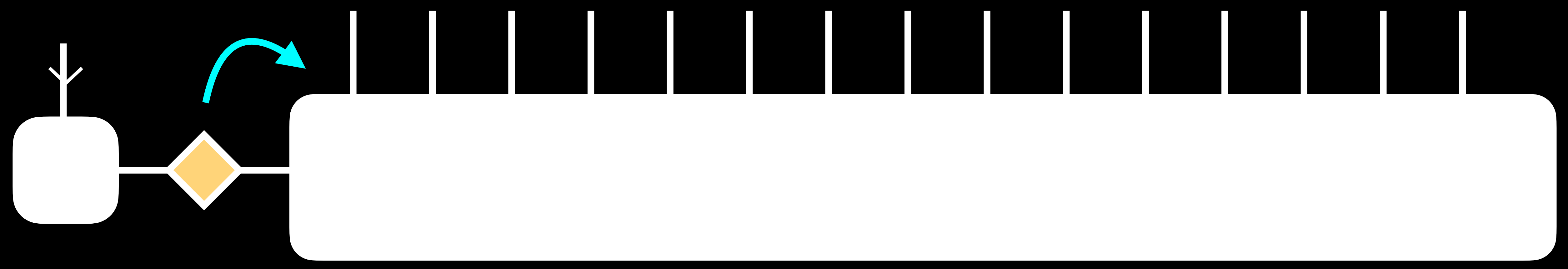
$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} \Psi_{(\sigma_0)(\sigma_1 \cdots \sigma_{L-1})} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$

row column



Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\alpha_0} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0} D^{(0)}_{\alpha_0\alpha_0} V^{(0)}_{\alpha_0(\sigma_1\cdots\sigma_{L-1})} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$



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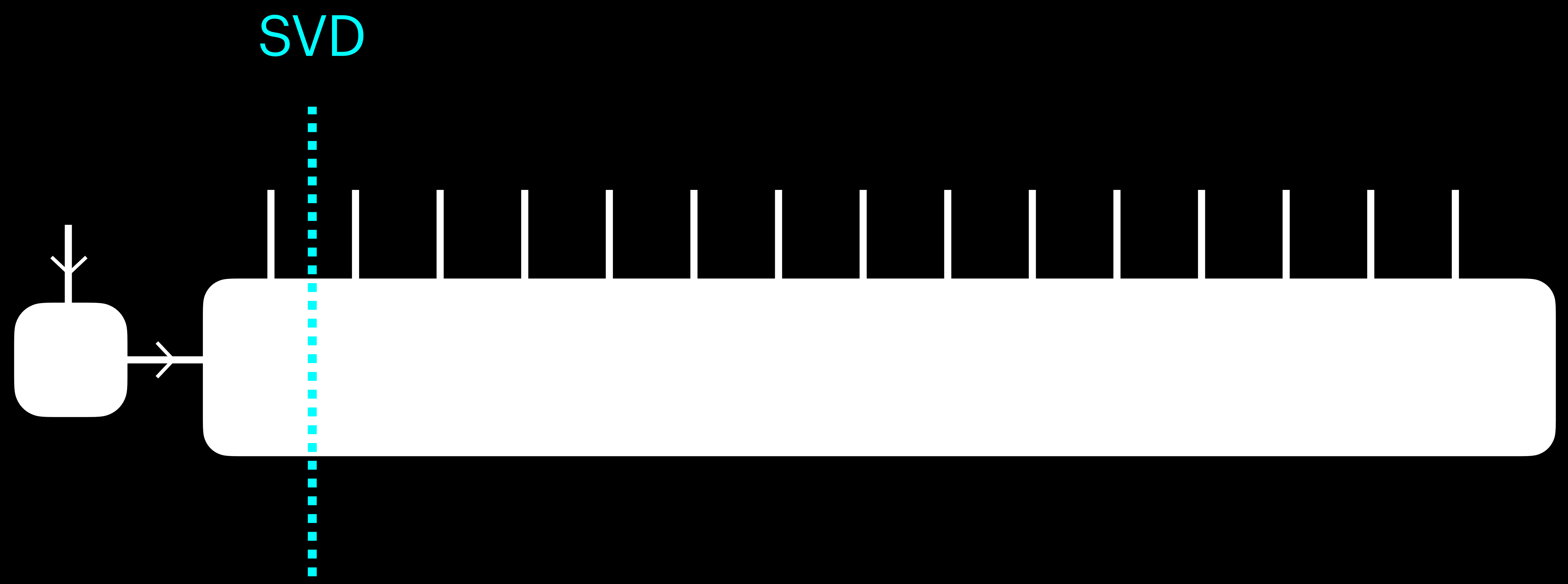
row

column



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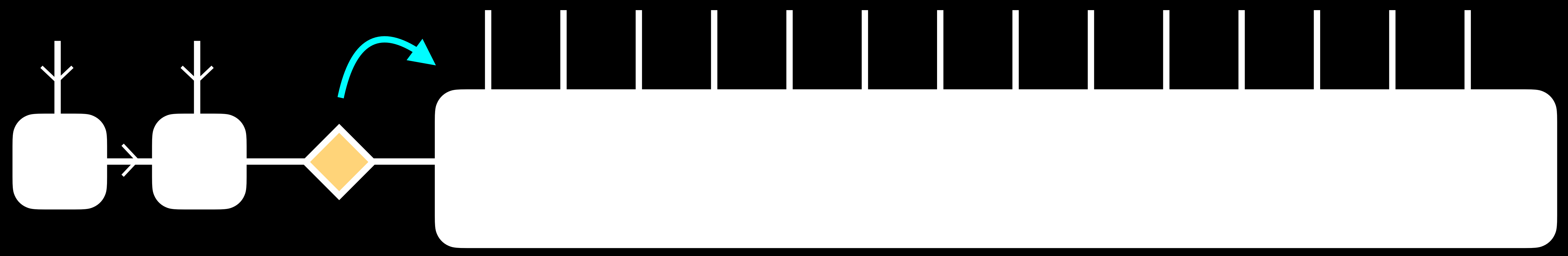

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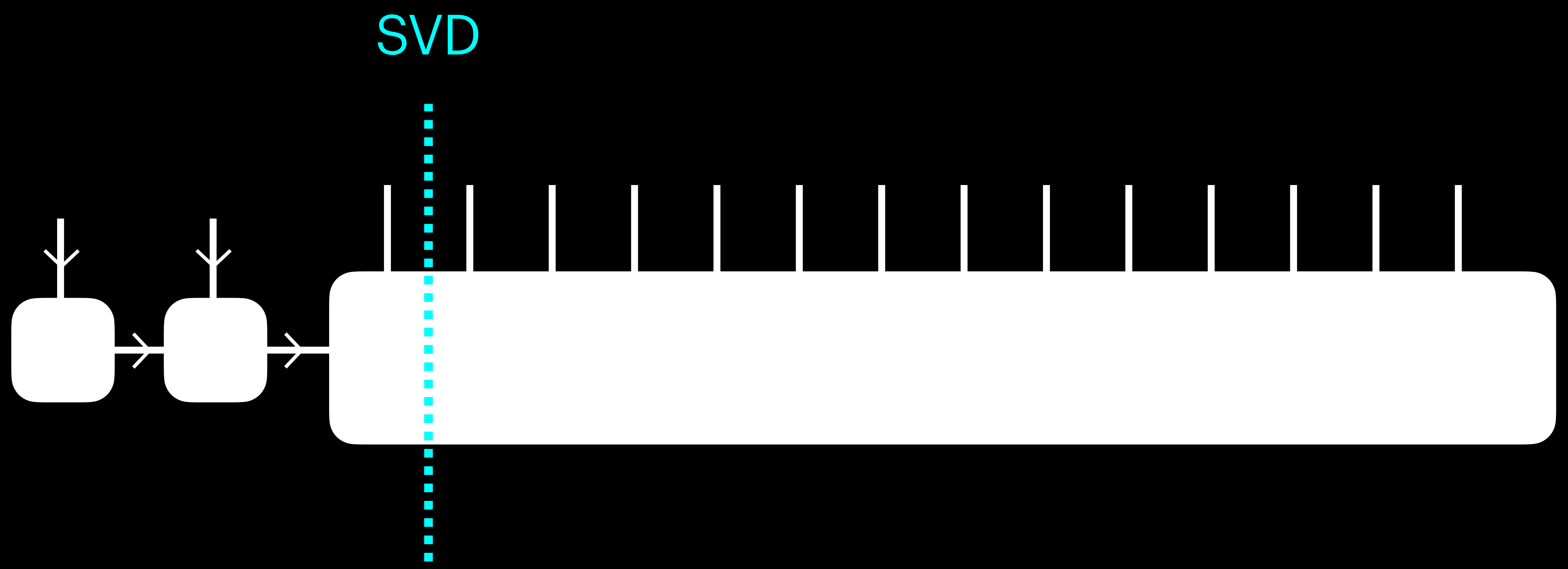
row

column



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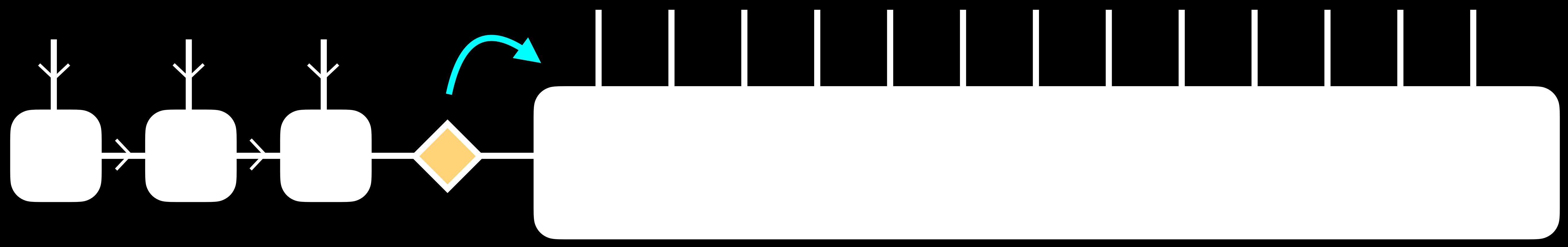

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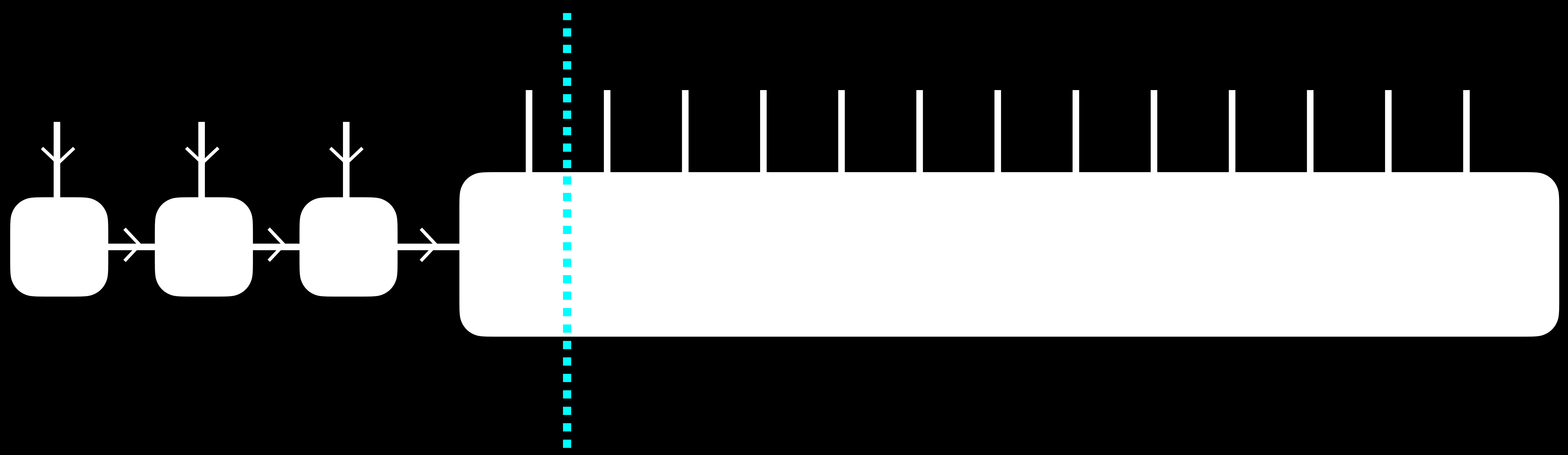
row column

SVD



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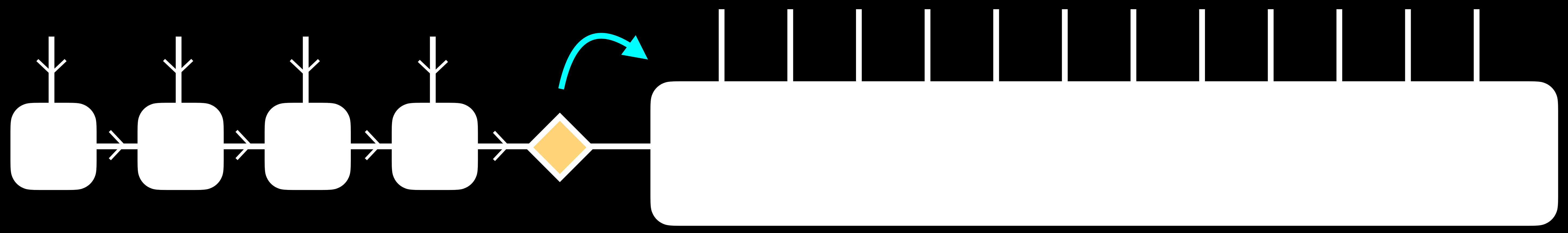

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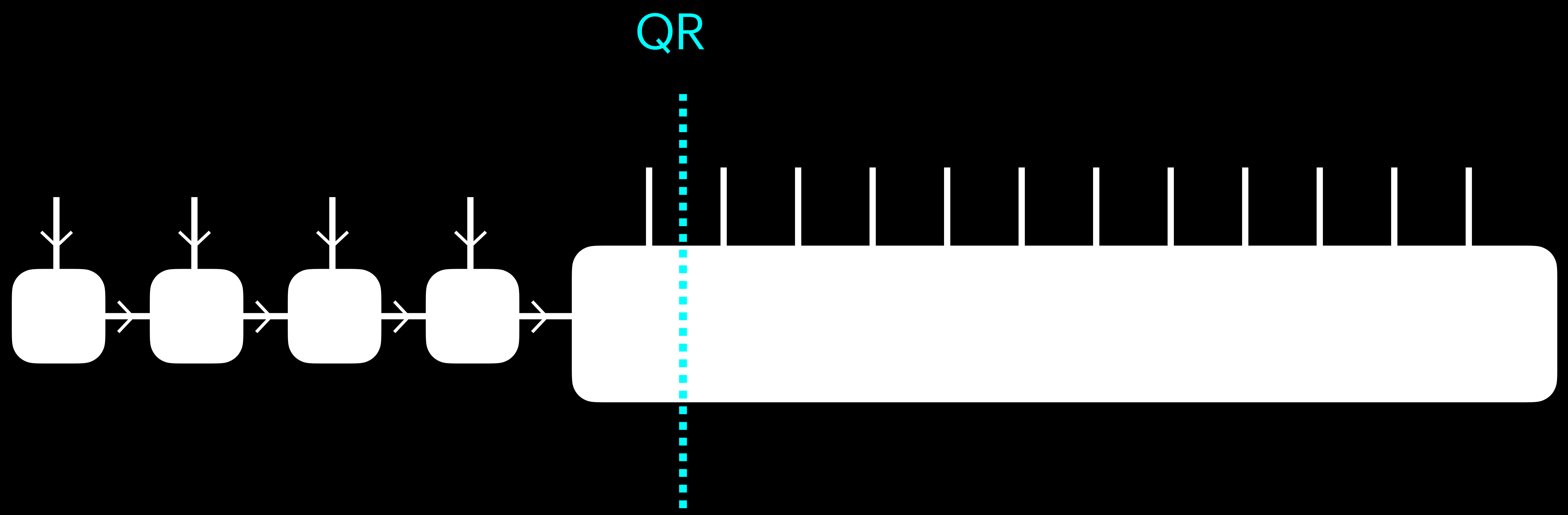
row column



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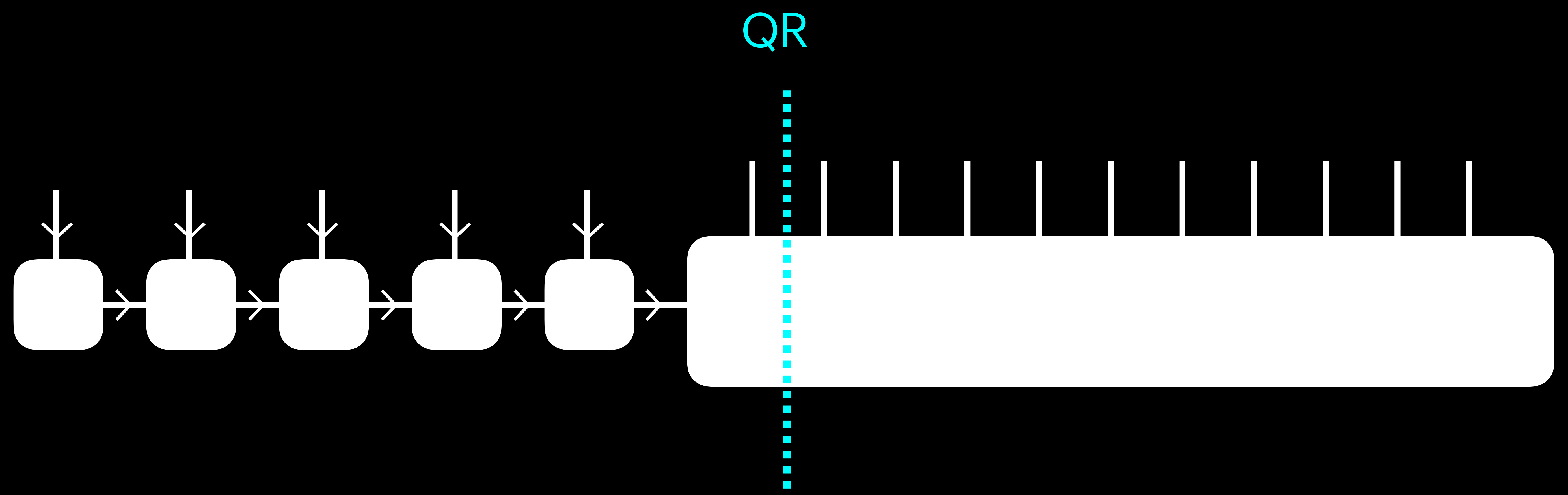

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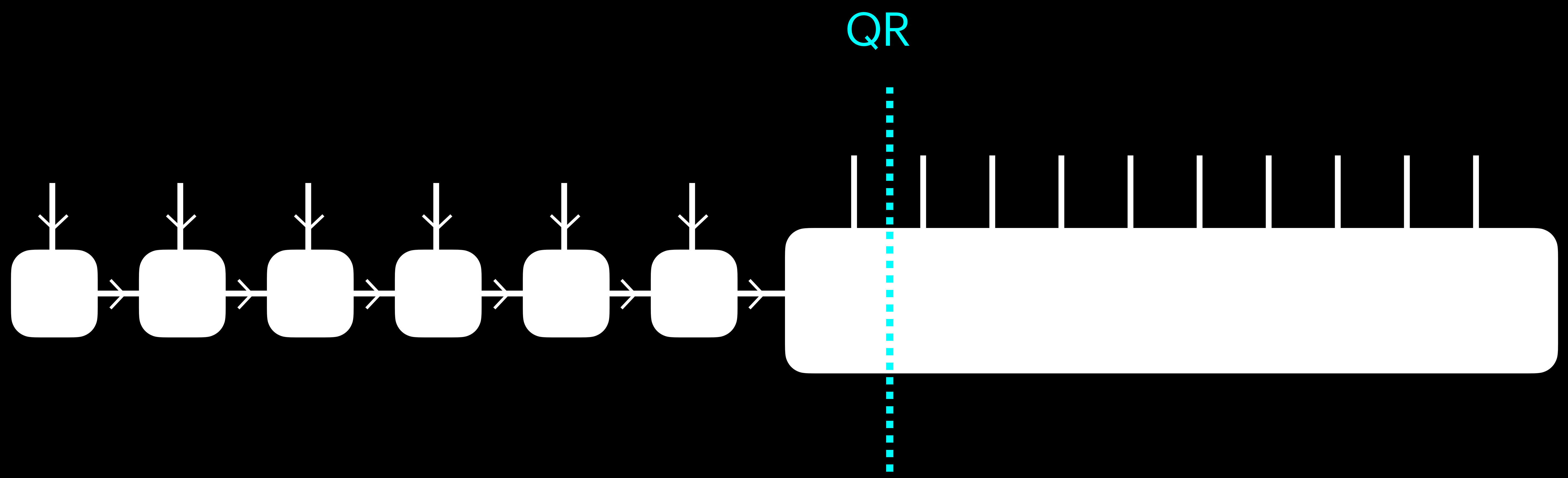
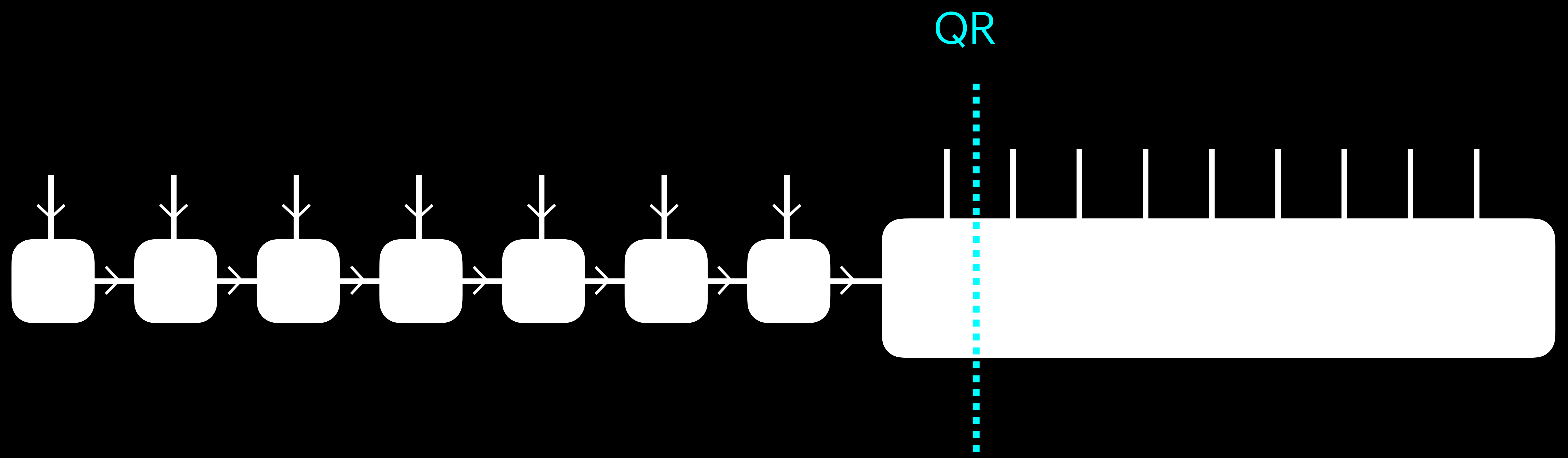


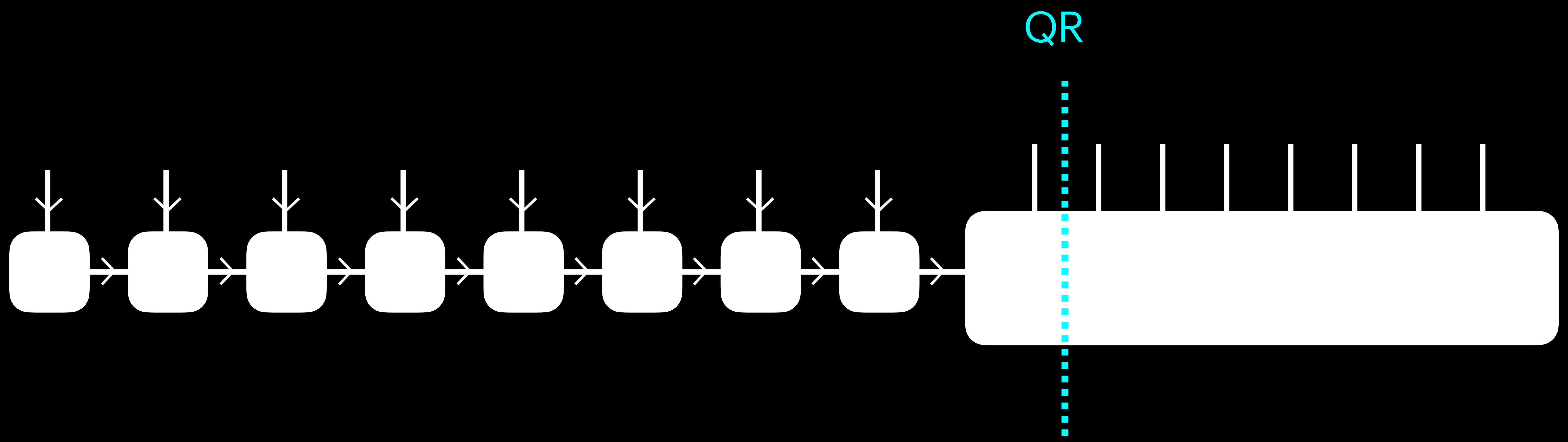
Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\alpha_0} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0} U^{(1)}_{\alpha_0\sigma_1\alpha_1} \cdots U^{(6)}_{\alpha_5\sigma_6\alpha_6} \Psi^{(7)}_{\alpha_6\sigma_7\sigma_8\cdots\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$



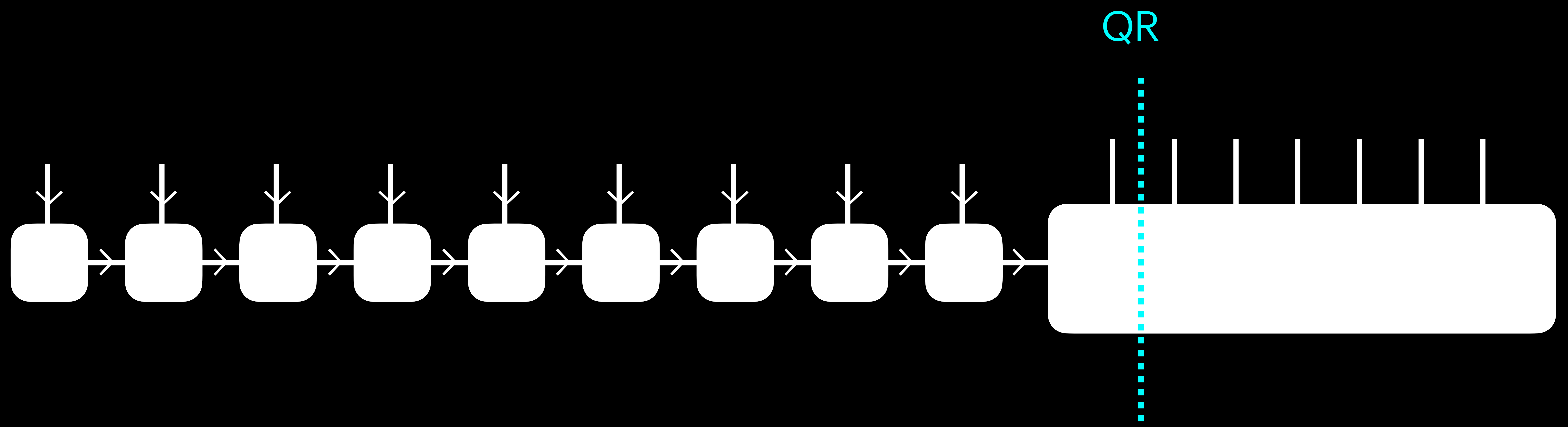
Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\alpha_0} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0} U^{(1)}_{\alpha_0\sigma_1\alpha_1} \cdots U^{(7)}_{\alpha_6\sigma_7\alpha_7} \Psi^{(8)}_{\alpha_7\sigma_8\sigma_9\cdots\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$



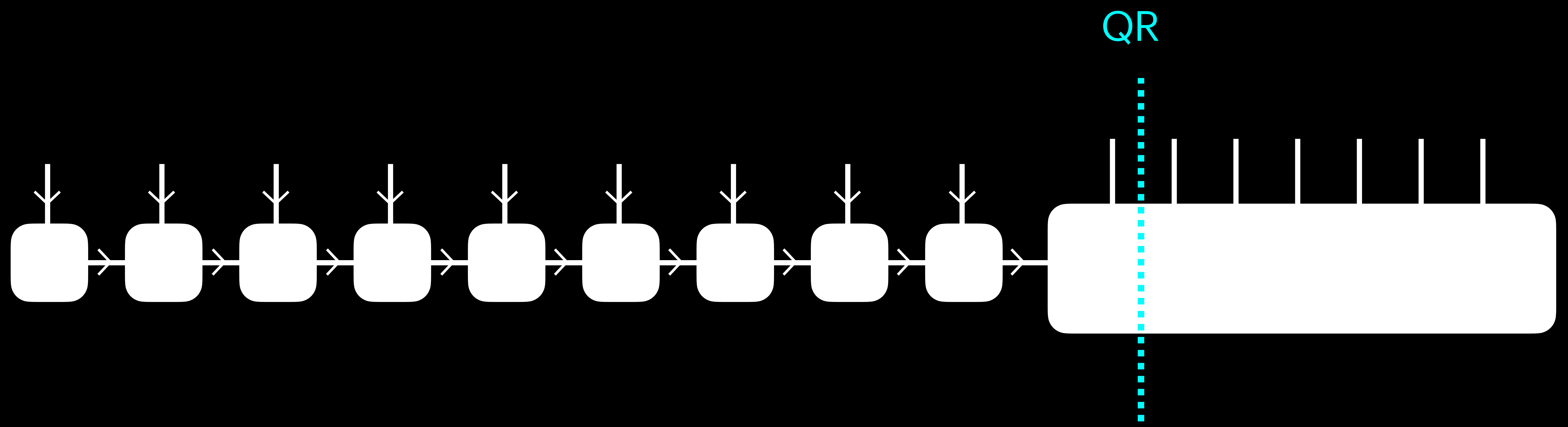
Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1}\sum_{\alpha_0}\sum_{\sigma_1=0}^{d-1}\cdots\sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0}U^{(1)}_{\alpha_0\sigma_1\alpha_1}\cdots U^{(l-1)}_{\alpha_{l-2}\sigma_{l-1}\alpha_{l-1}}\Psi^{(l)}_{\alpha_{l-1}\sigma_l\sigma_{l+1}\cdots\sigma_{L-1}}|\sigma_0\rangle|\sigma_1\rangle\cdots|\sigma_{L-1}\rangle$$



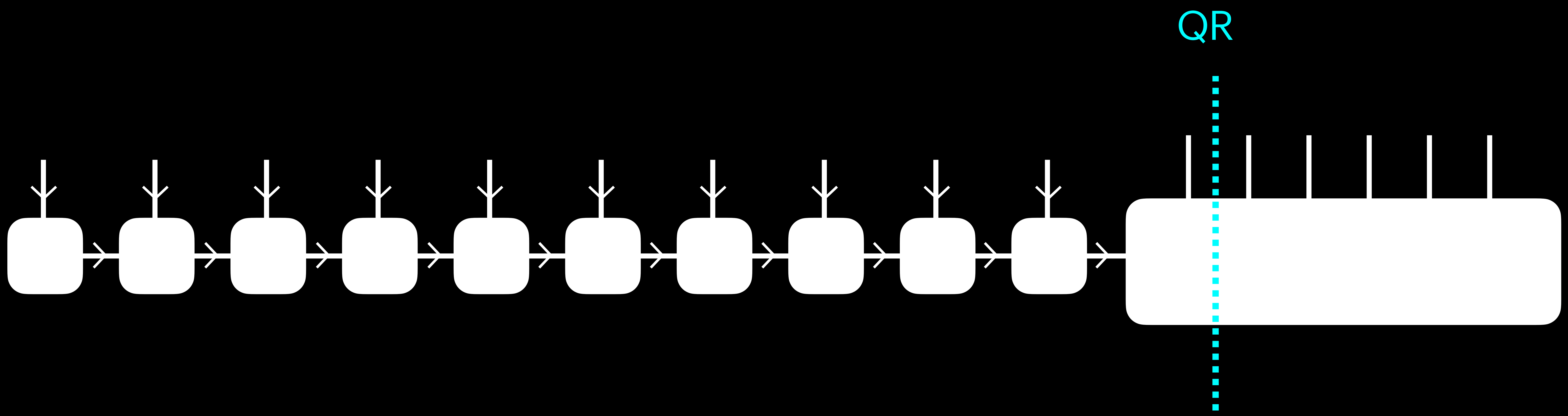
Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\alpha_0} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0} U^{(1)}_{\alpha_0\sigma_1\alpha_1} \cdots U^{(l-1)}_{\alpha_{l-2}\sigma_{l-1}\alpha_{l-1}} \Psi^{(l)}_{\alpha_{l-1}\sigma_l\sigma_{l+1}\cdots\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$



Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1}\sum_{\alpha_0}\sum_{\sigma_1=0}^{d-1}\cdots\sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0}U^{(1)}_{\alpha_0\sigma_1\alpha_1}\cdots U^{(l-1)}_{\alpha_{l-2}\sigma_{l-1}\alpha_{l-1}}\Psi^{(l)}_{\alpha_{l-1}\sigma_l\sigma_{l+1}\cdots\sigma_{L-1}}|\sigma_0\rangle|\sigma_1\rangle\cdots|\sigma_{L-1}\rangle$$



Generality of MPS

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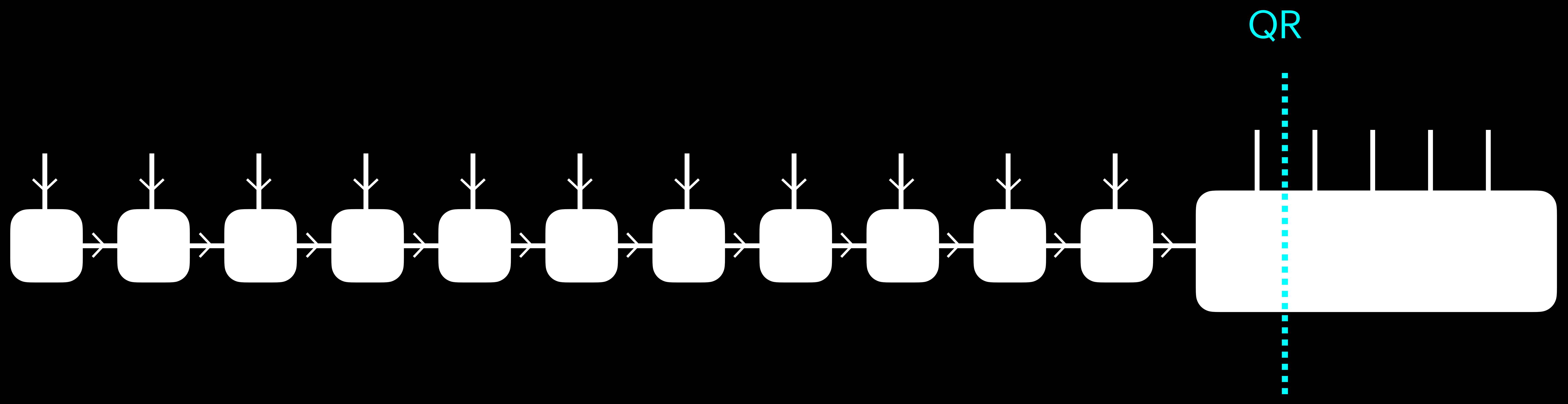
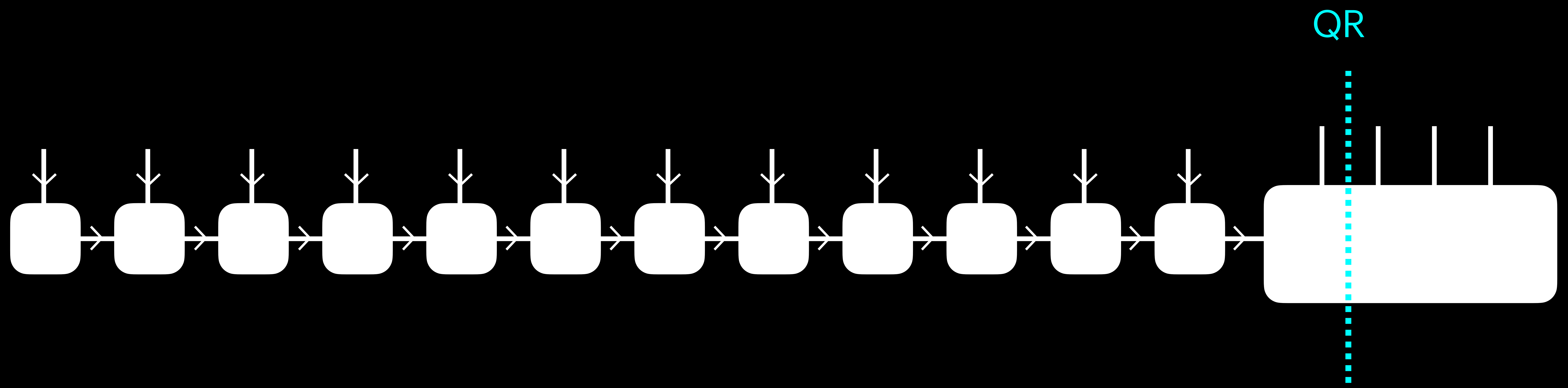


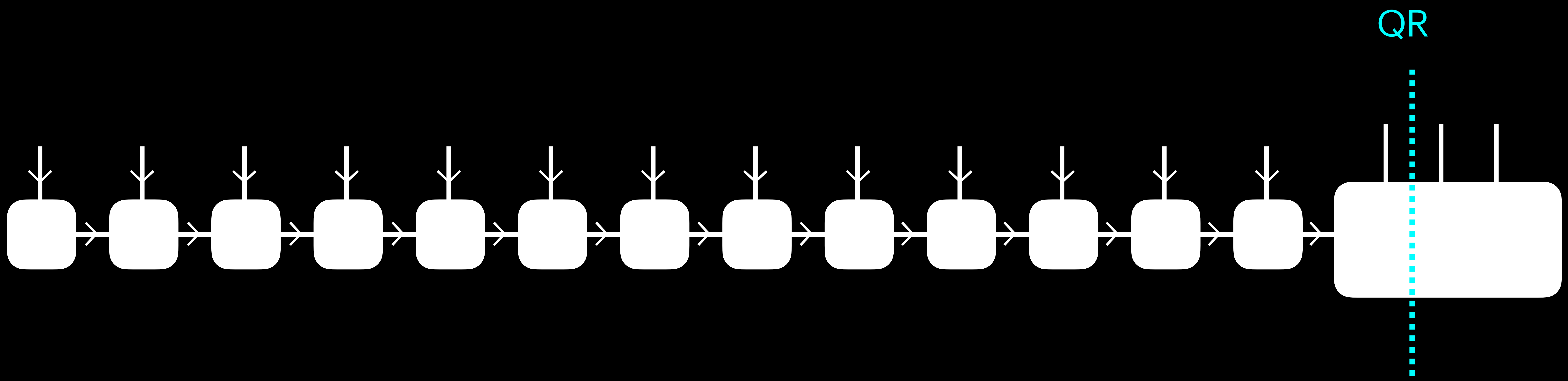
Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1}\sum_{\alpha_0}\sum_{\sigma_1=0}^{d-1}\cdots\sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0}U^{(1)}_{\alpha_0\sigma_1\alpha_1}\cdots U^{(l-1)}_{\alpha_{l-2}\sigma_{l-1}\alpha_{l-1}}\Psi^{(l)}_{\alpha_{l-1}\sigma_l\sigma_{l+1}\cdots\sigma_{L-1}}|\sigma_0\rangle|\sigma_1\rangle\cdots|\sigma_{L-1}\rangle$$



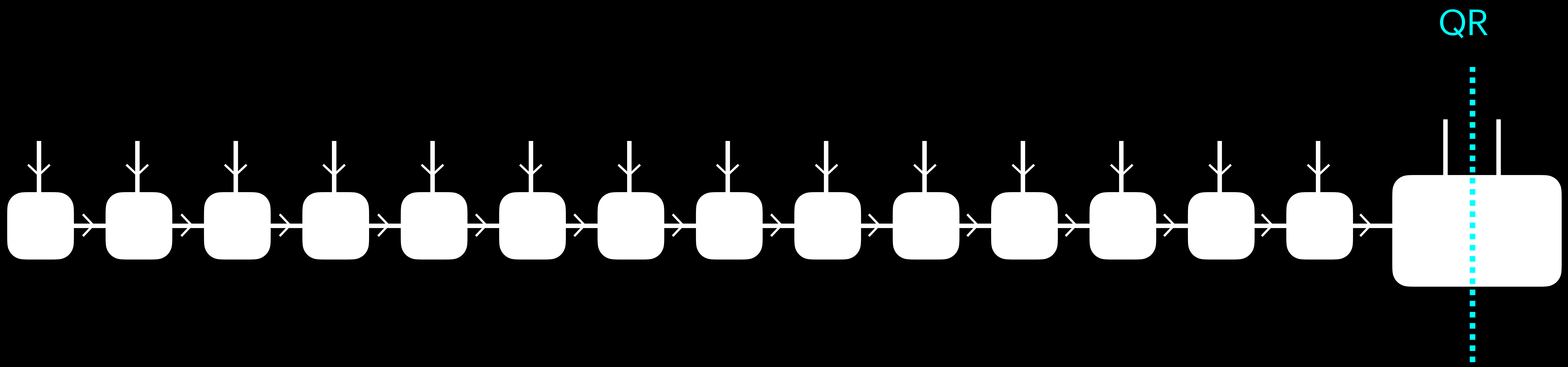
Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\alpha_0} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0} U^{(1)}_{\alpha_0\sigma_1\alpha_1} \cdots U^{(l-1)}_{\alpha_{l-2}\sigma_{l-1}\alpha_{l-1}} \Psi^{(l)}_{\alpha_{l-1}\sigma_l\sigma_{l+1}\cdots\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$



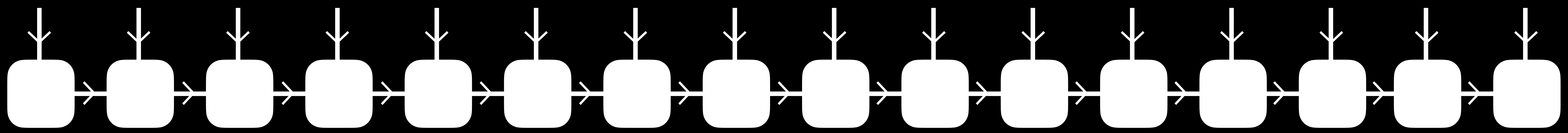
Generality of MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1}\sum_{\alpha_0}\sum_{\sigma_1=0}^{d-1}\cdots\sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0}U^{(1)}_{\alpha_0\sigma_1\alpha_1}\cdots U^{(L-3)}_{\alpha_{L-4}\sigma_{L-3}\alpha_{L-3}}\Psi^{(L-2)}_{\alpha_{L-3}\sigma_{L-2}\sigma_{L-1}}|\sigma_0\rangle|\sigma_1\rangle\cdots|\sigma_{L-1}\rangle$$



Generality of MPS

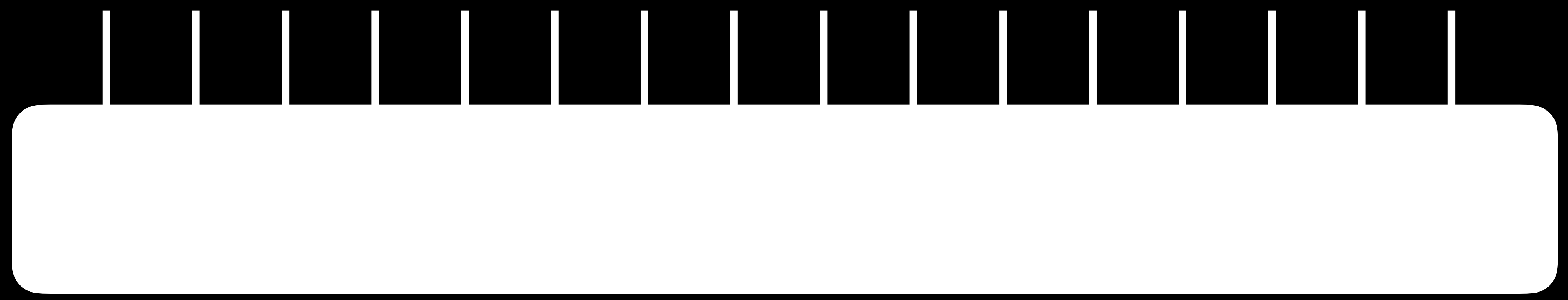
$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\alpha_0} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0} U^{(1)}_{\alpha_0\sigma_1\alpha_1} \cdots U^{(L-3)}_{\alpha_{L-4}\sigma_{L-3}\alpha_{L-3}} \Psi^{(L-2)}_{\alpha_{L-3}\sigma_{L-2}\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$



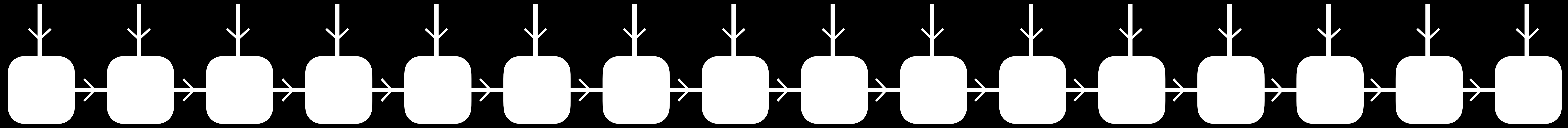
Generality of MPS

Corollary 1: Any quantum state $|\Psi\rangle$ can be transformed into a MPS form.

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} \Psi_{\sigma_0\sigma_1\cdots\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$

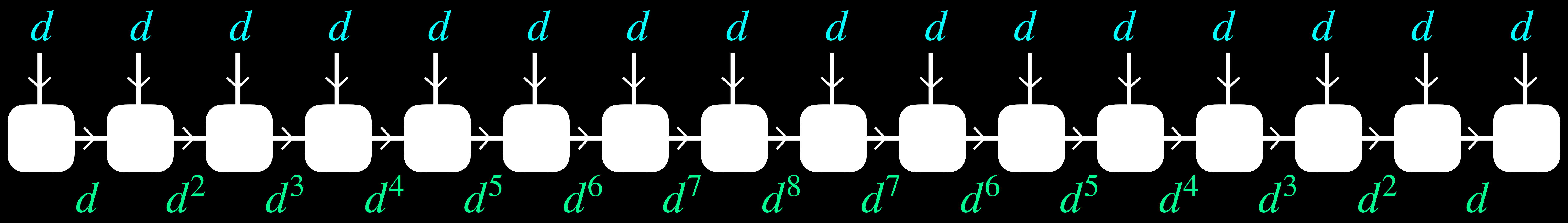


$$= \sum_{\sigma_0=0}^{d-1} \sum_{\alpha_0} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0} U^{(1)}_{\alpha_0\sigma_1\alpha_1} \cdots U^{(L-3)}_{\alpha_{L-4}\sigma_{L-3}\alpha_{L-3}} U^{(L-2)}_{\alpha_{L-3}\sigma_{L-2}\alpha_{L-2}} \Psi^{(L-1)}_{\alpha_{L-2}\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$

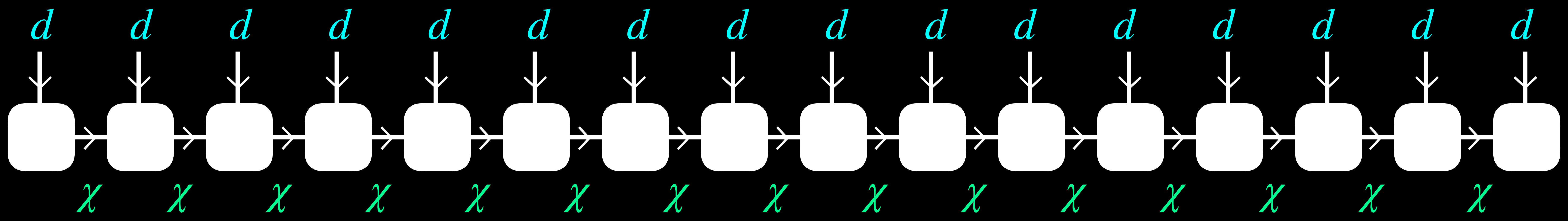


Approximation in MPS

$$|\Psi\rangle = \sum_{\sigma_0=0}^{d-1} \sum_{\alpha_0} \sum_{\sigma_1=0}^{d-1} \cdots \sum_{\sigma_{L-1}=0}^{d-1} U^{(0)}_{\sigma_0\alpha_0} U^{(1)}_{\alpha_0\sigma_1\alpha_1} \cdots U^{(L-3)}_{\alpha_{L-4}\sigma_{L-3}\alpha_{L-3}} U^{(L-2)}_{\alpha_{L-3}\sigma_{L-2}\alpha_{L-2}} \Psi^{(L-1)}_{\alpha_{L-2}\sigma_{L-1}} |\sigma_0\rangle |\sigma_1\rangle \cdots |\sigma_{L-1}\rangle$$



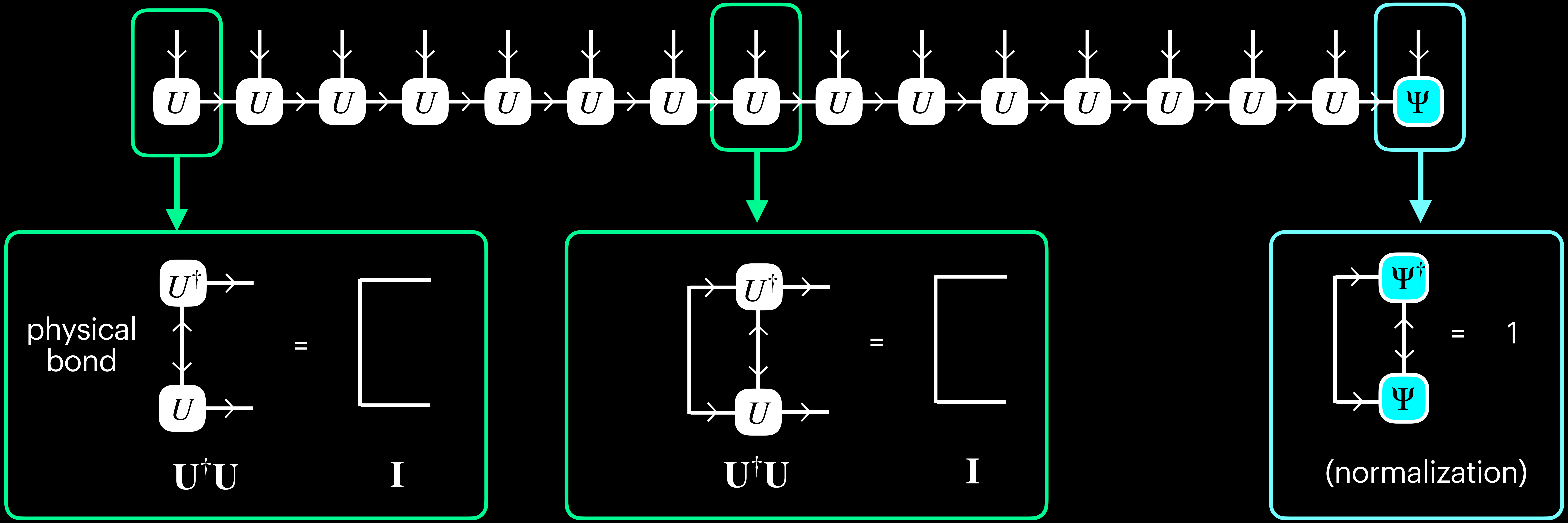
Without any approximation, the dimensions of virtual bonds grow exponentially toward the middle as above.



So, as a way to avoid this, we approximate by setting the maximum value χ that can be calculated for the bond dimension of each virtual bond. → **Truncation**

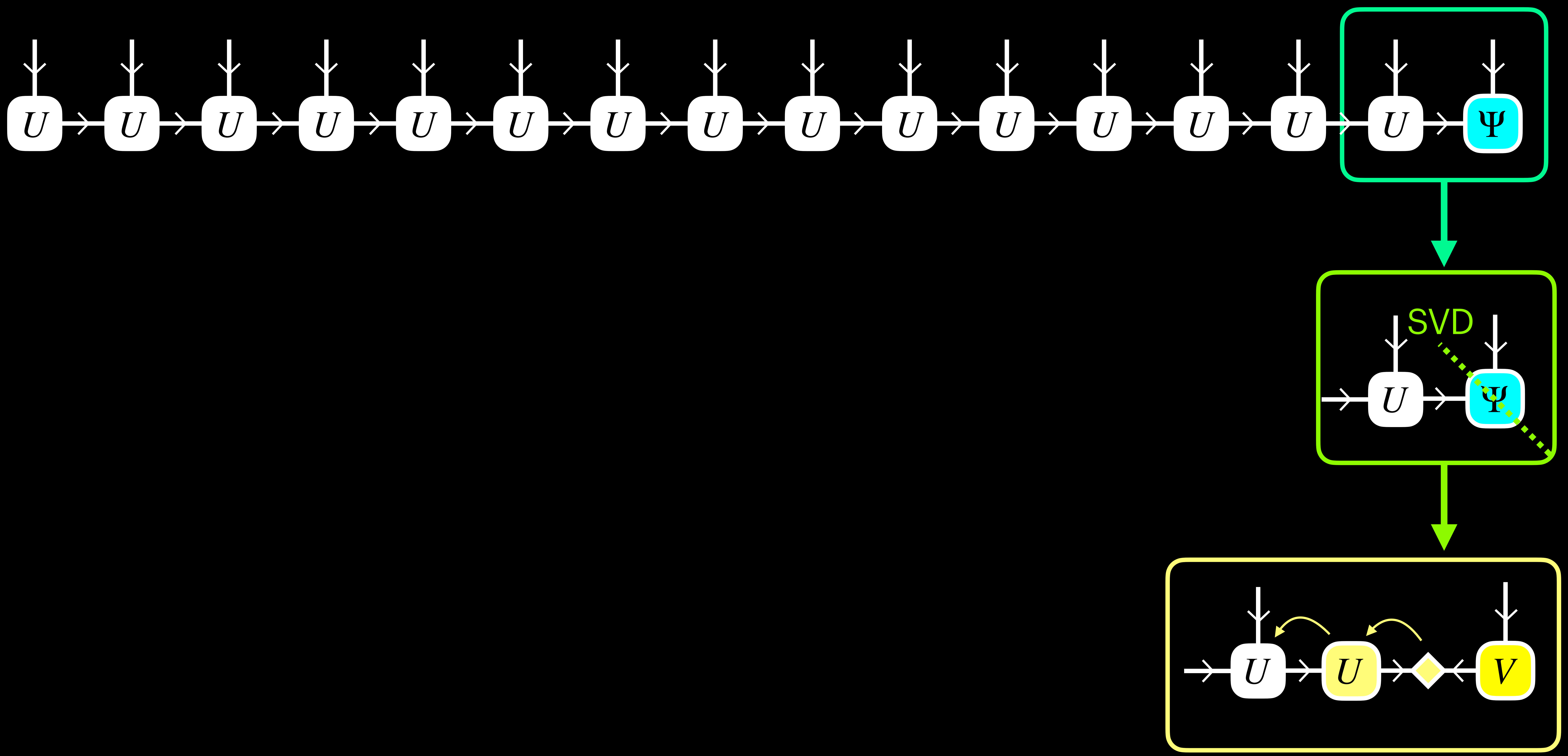
How to Choose Bond Dimensions Appropriately?

Canonical forms of MPS

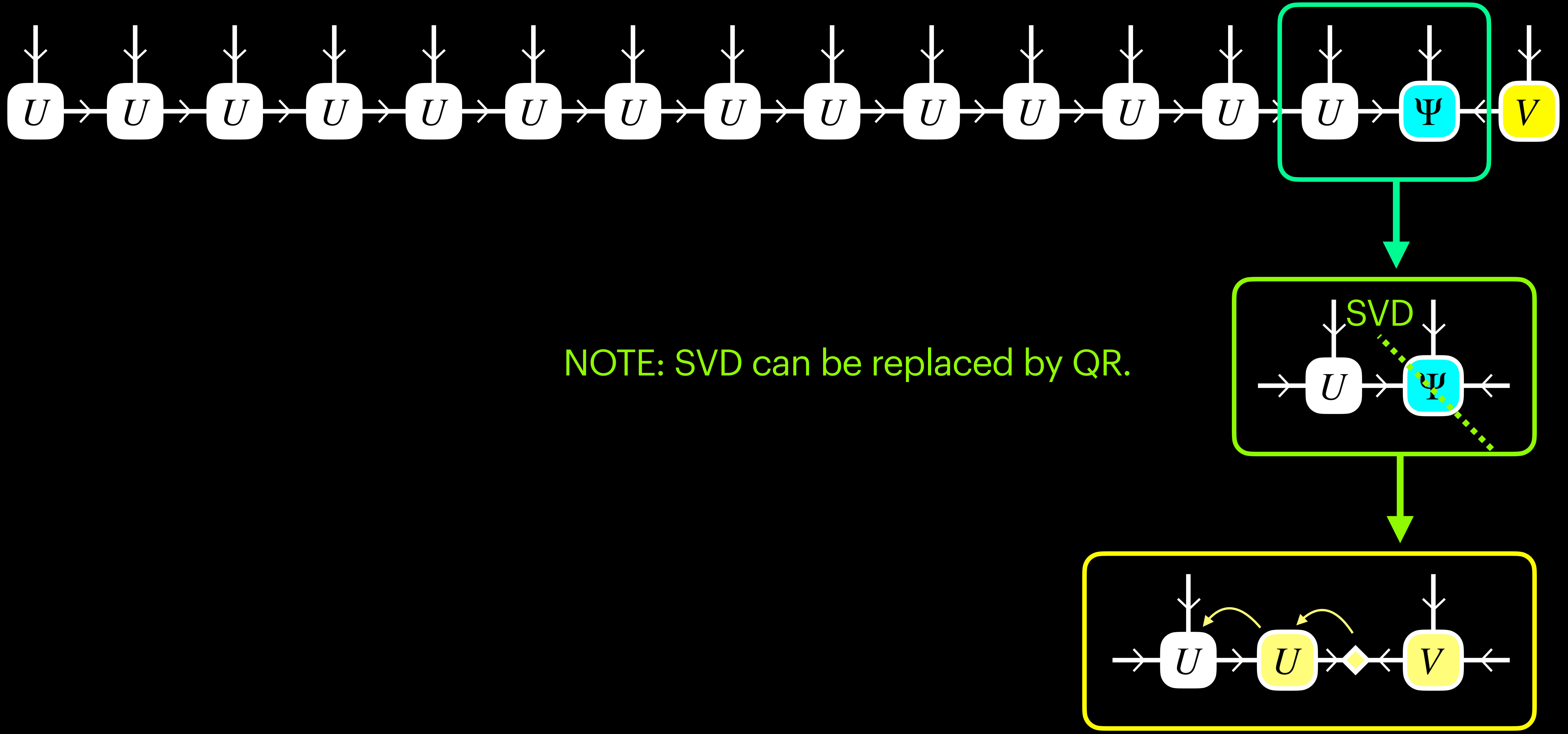


In the previous method, the structure is as described above. This situation is called **left canonical form**.

Canonical forms of MPS

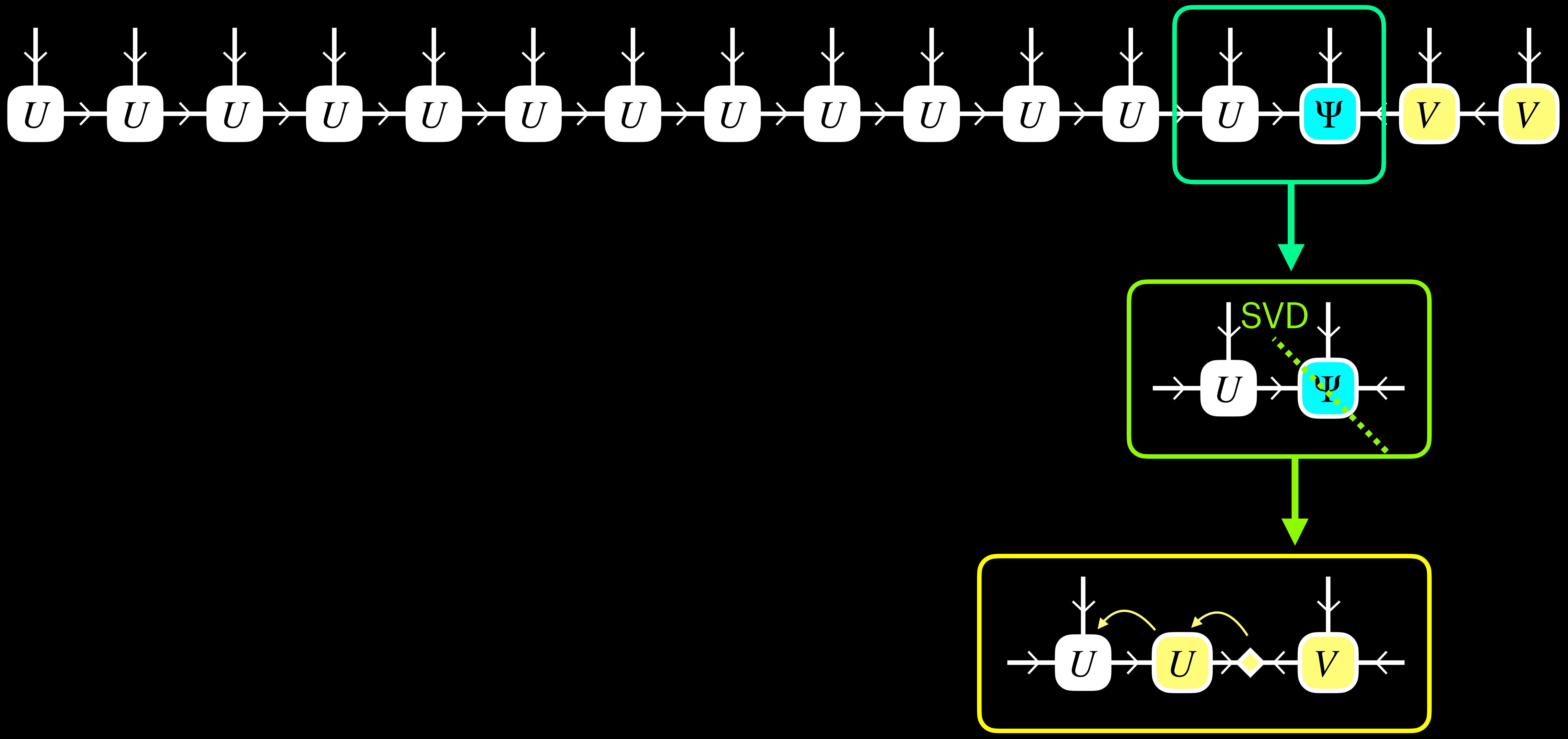


Canonical forms of MPS

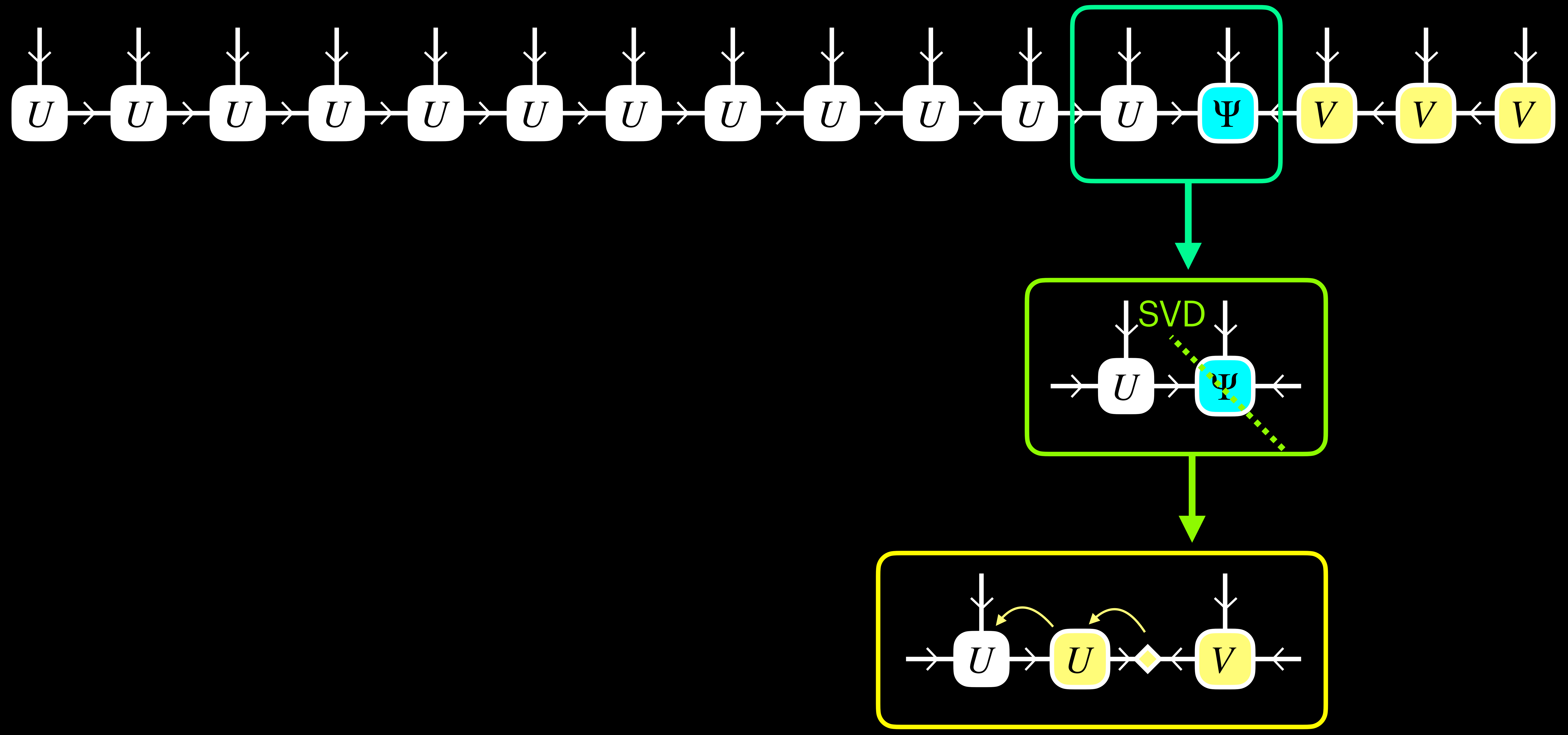


NOTE: SVD can be replaced by QR.

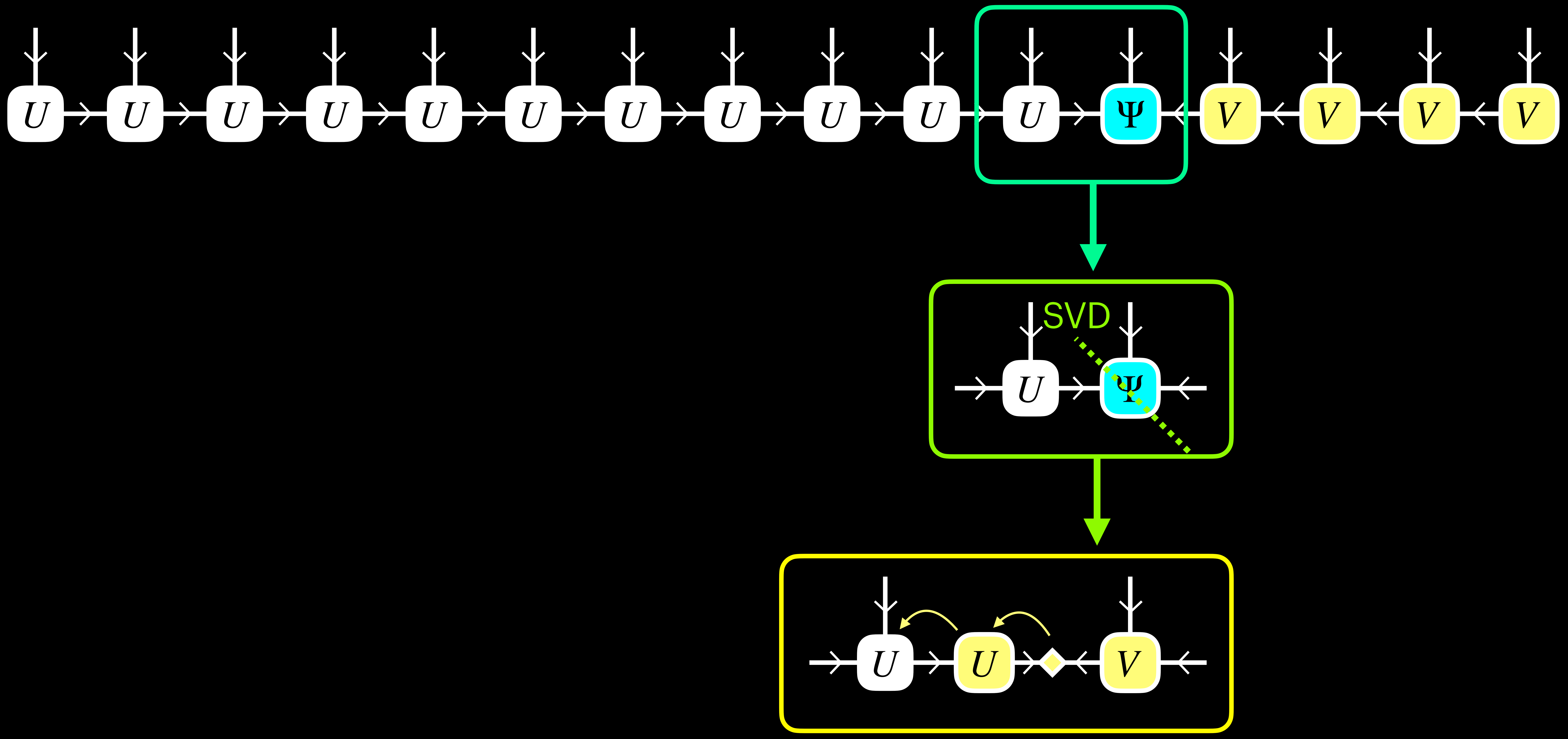
Canonical forms of MPS



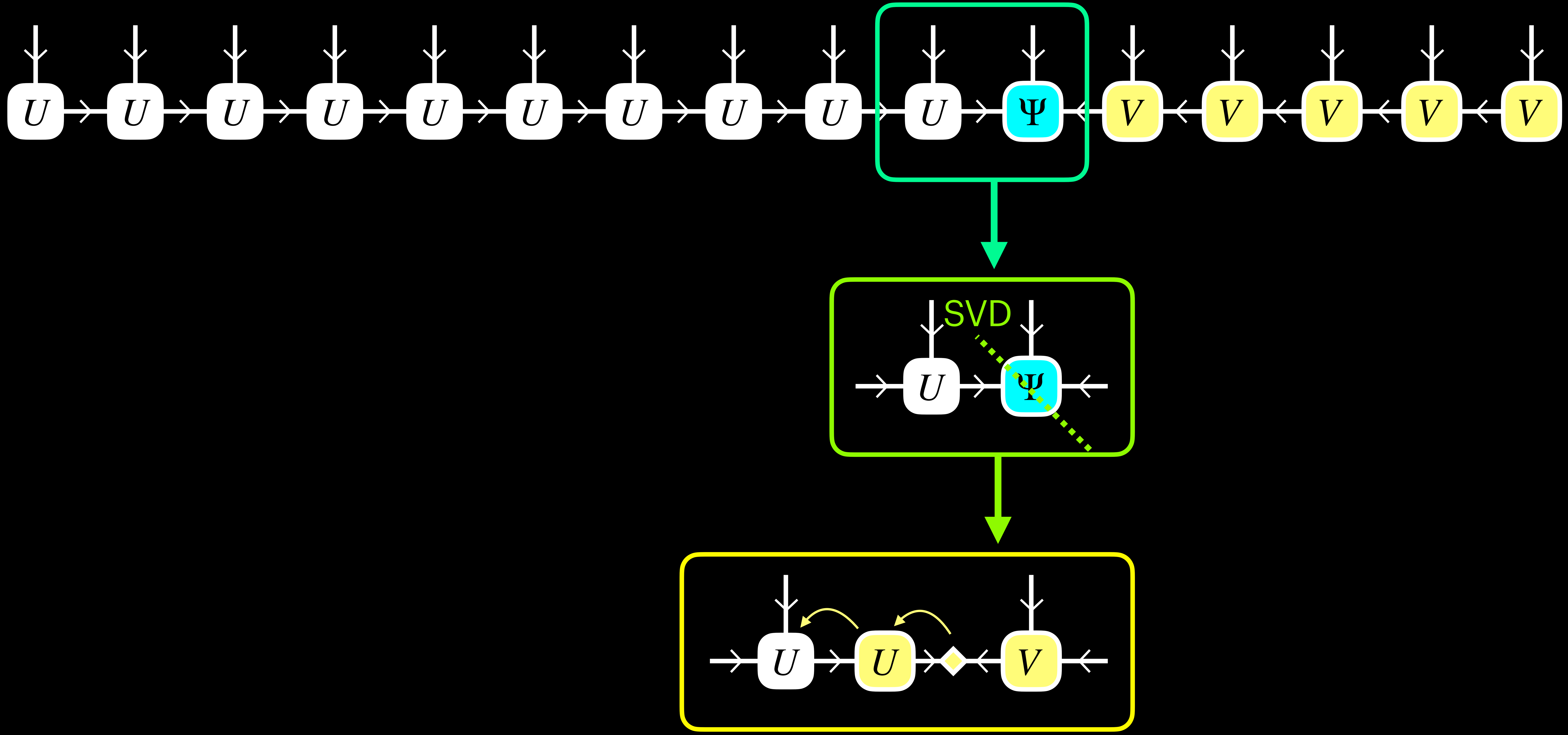
Canonical forms of MPS



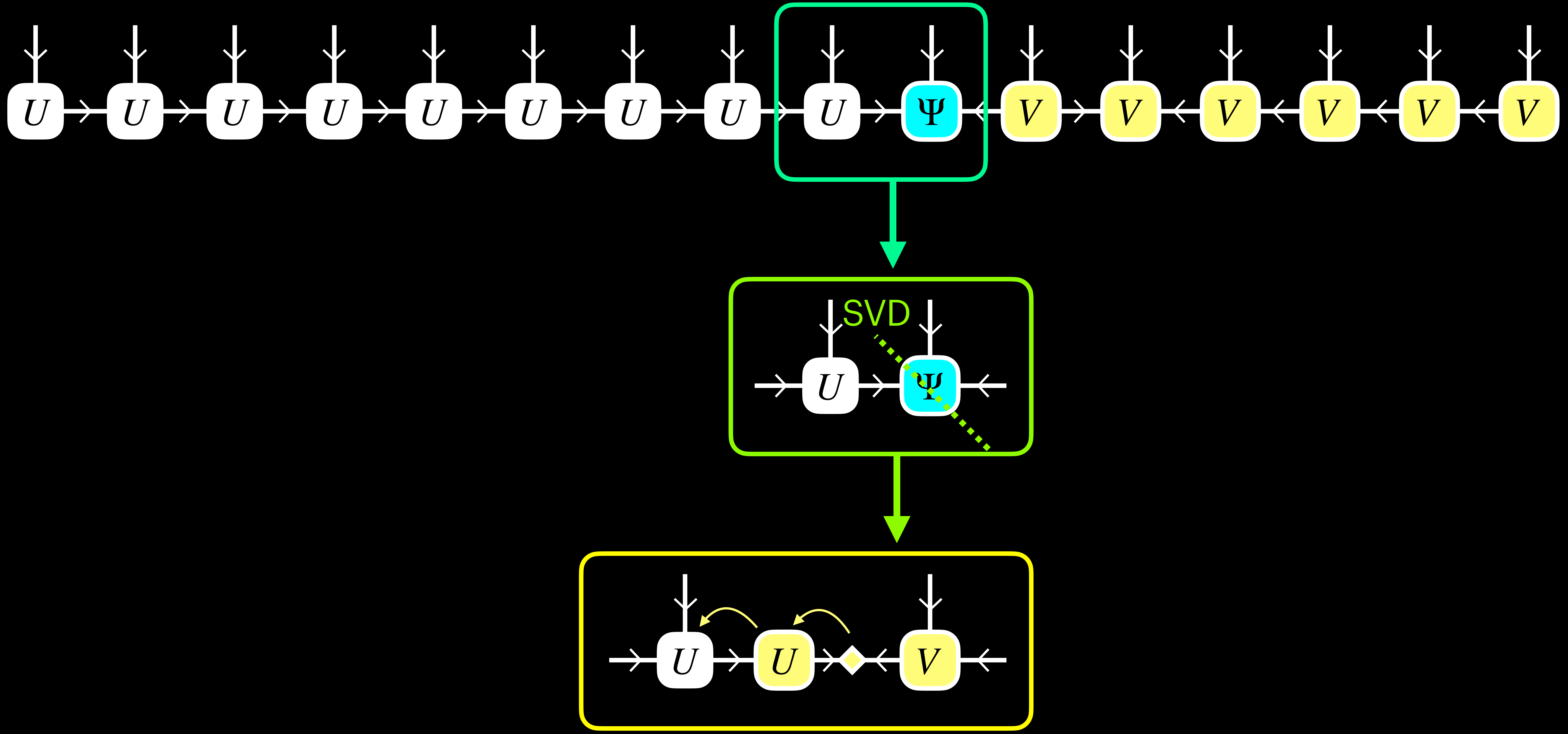
Canonical forms of MPS



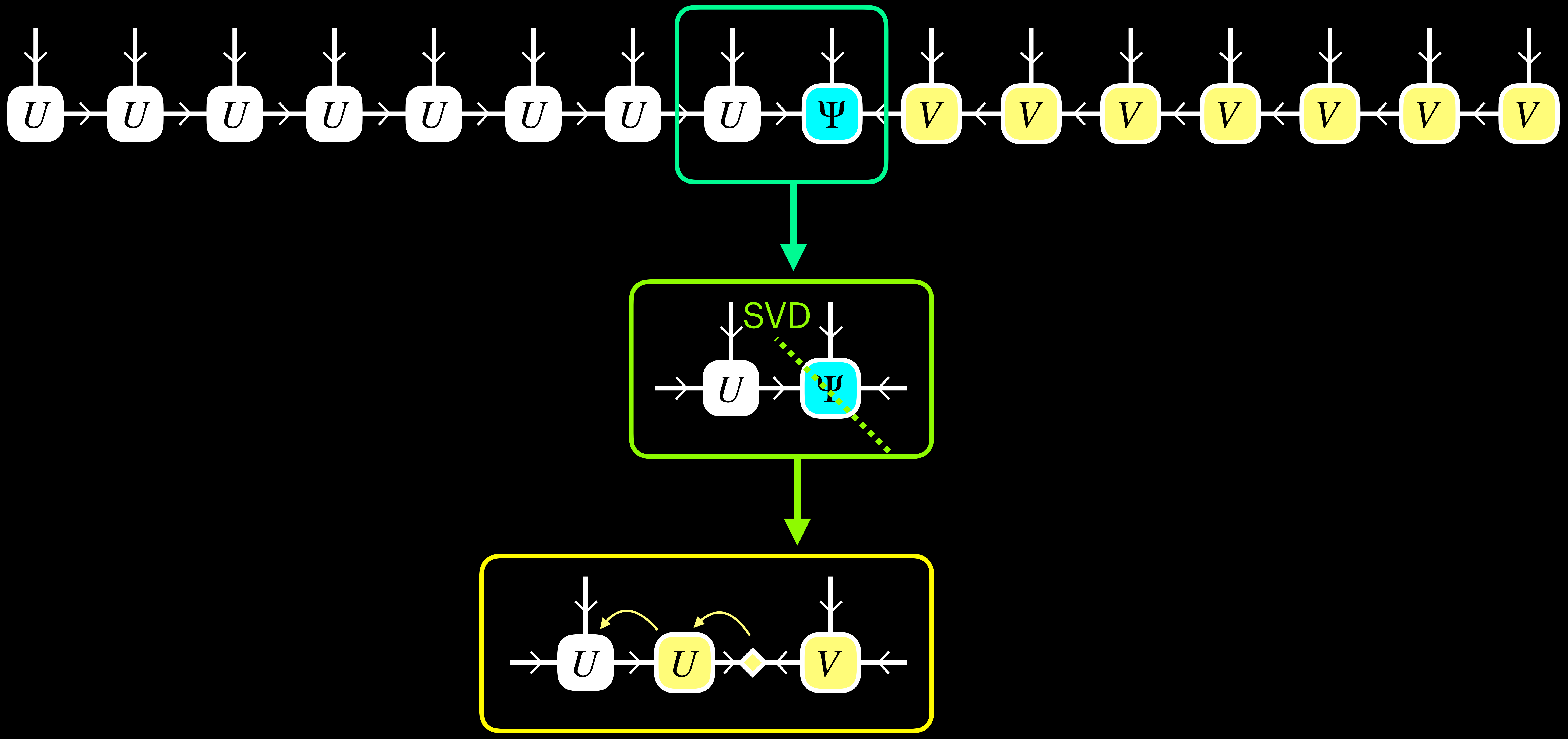
Canonical forms of MPS



Canonical forms of MPS

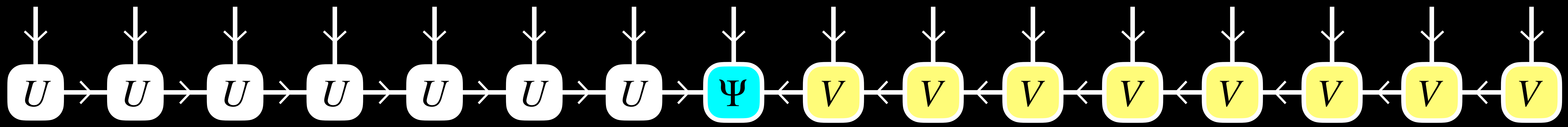


Canonical forms of MPS

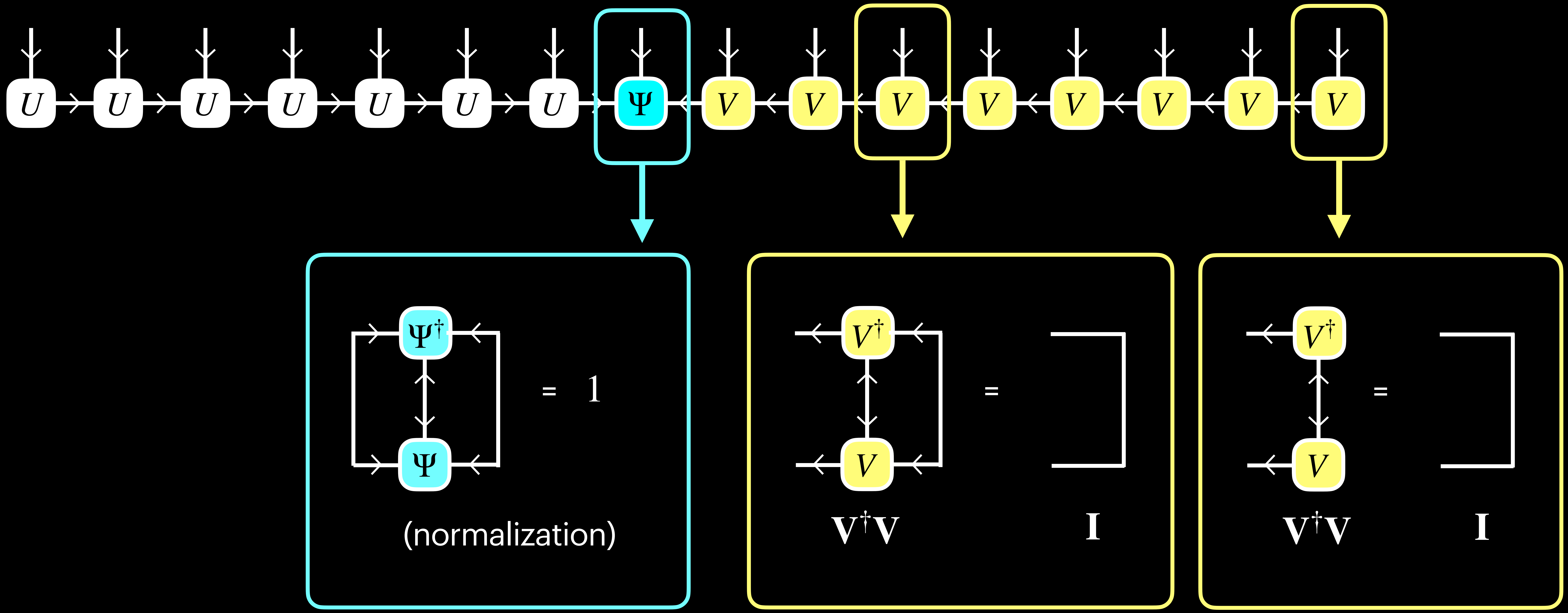


Canonical forms of MPS

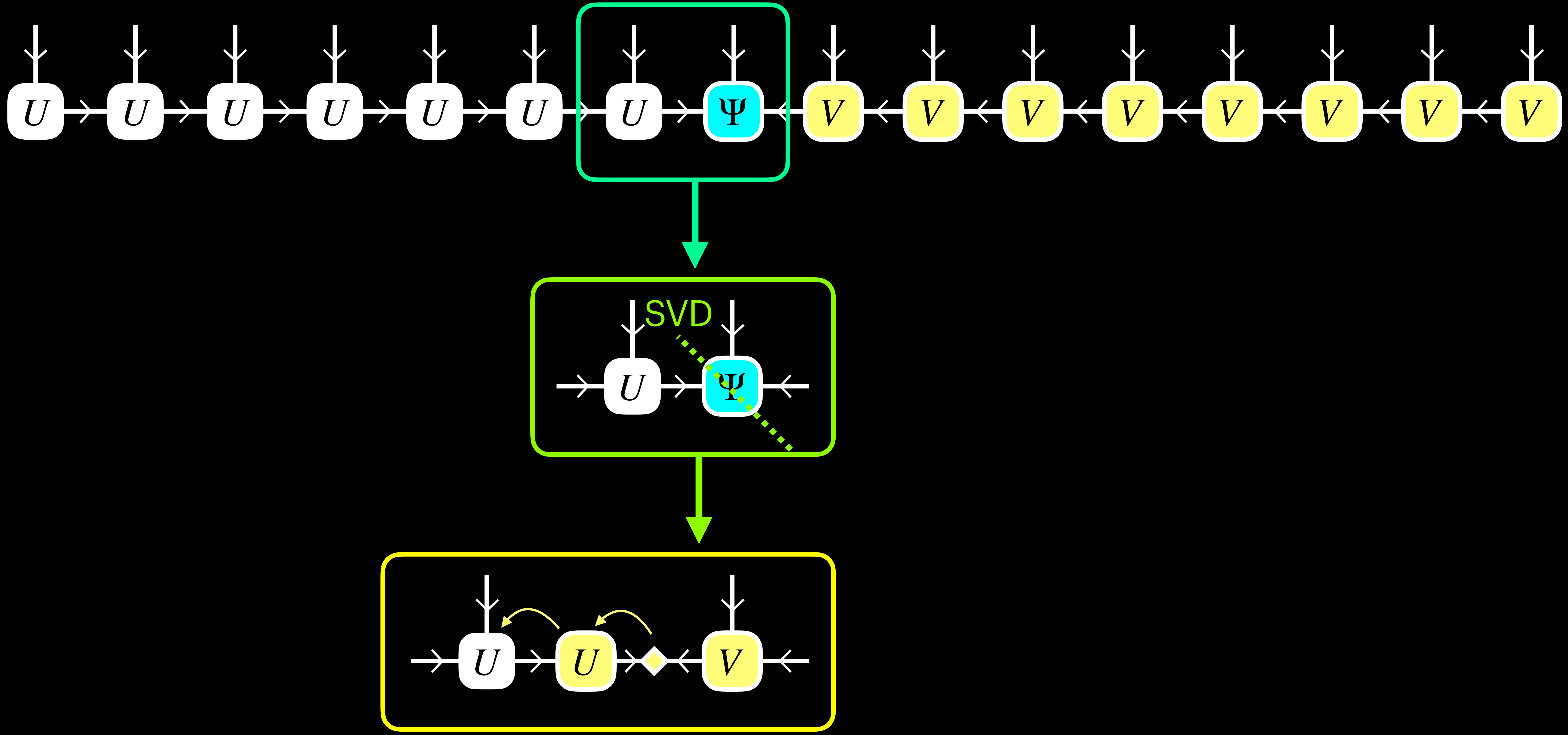
This situation is called **mixed canonical form**.



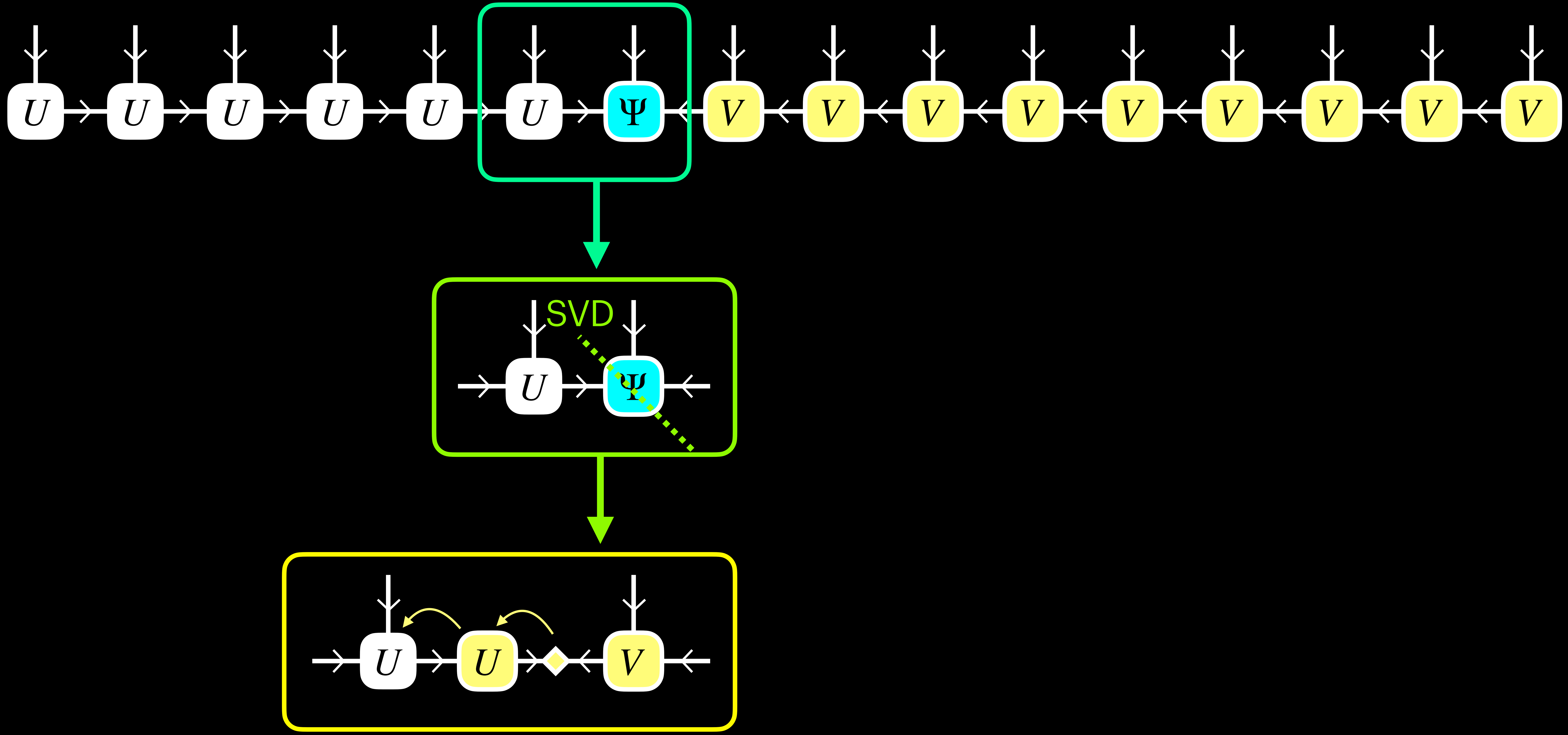
Canonical forms of MPS



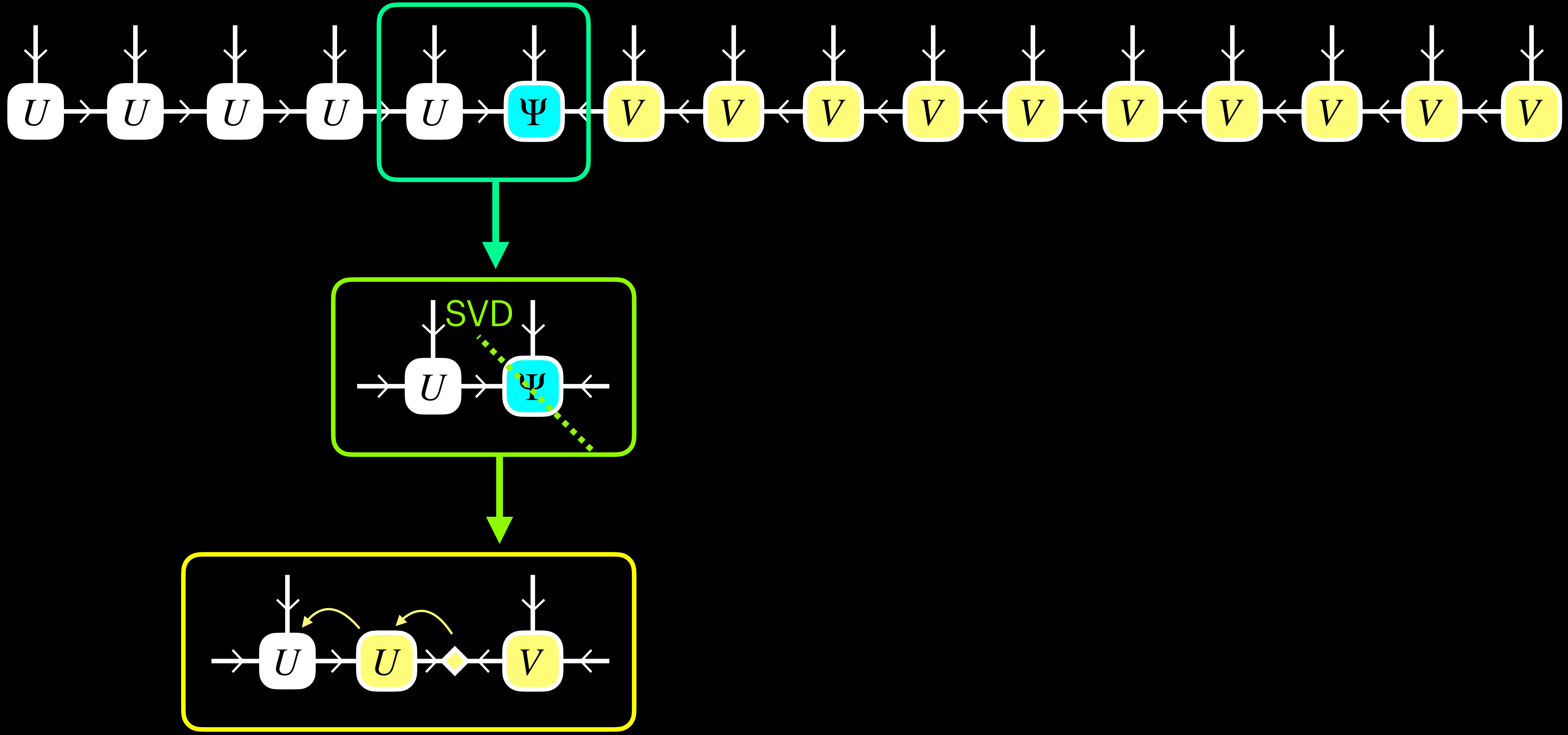
Canonical forms of MPS



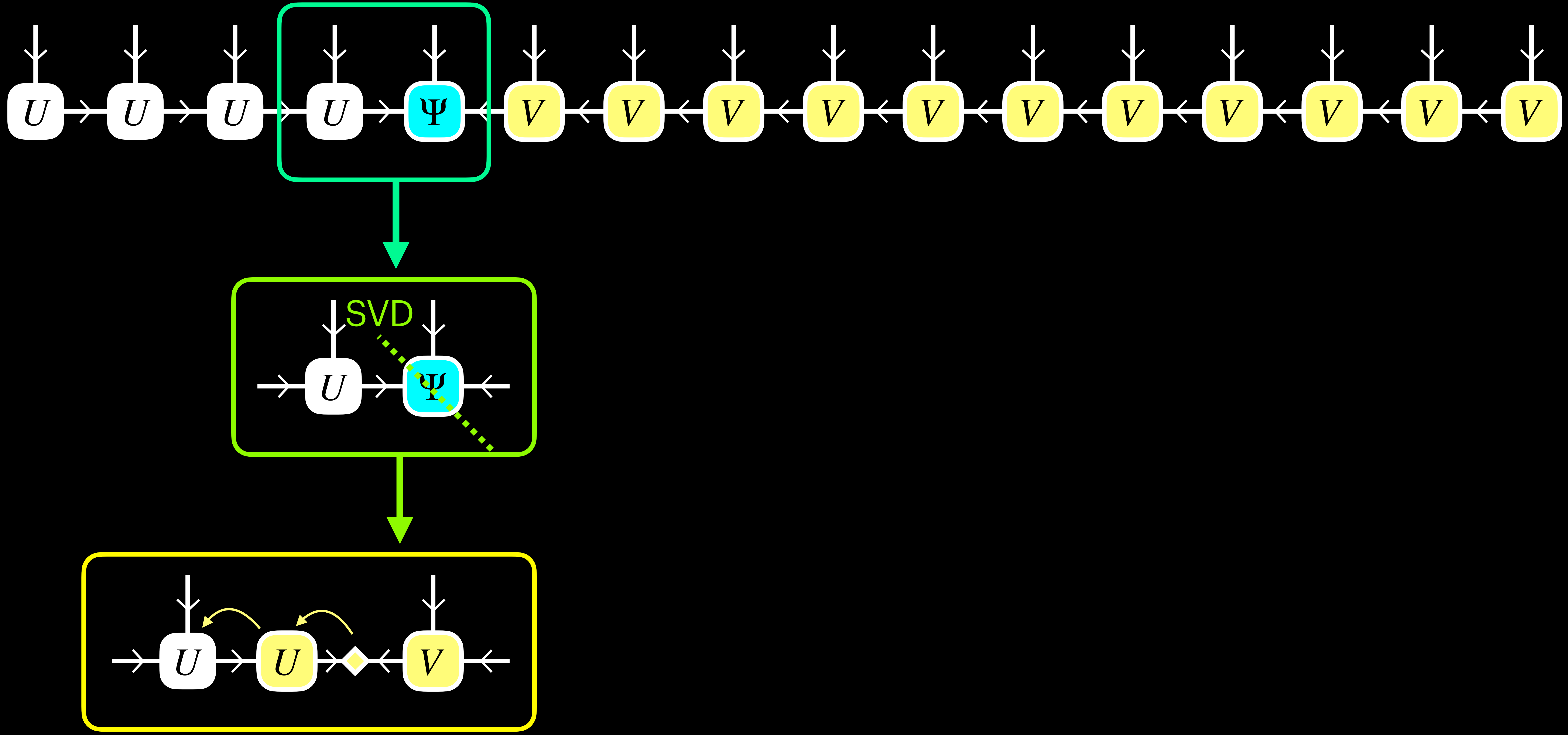
Canonical forms of MPS



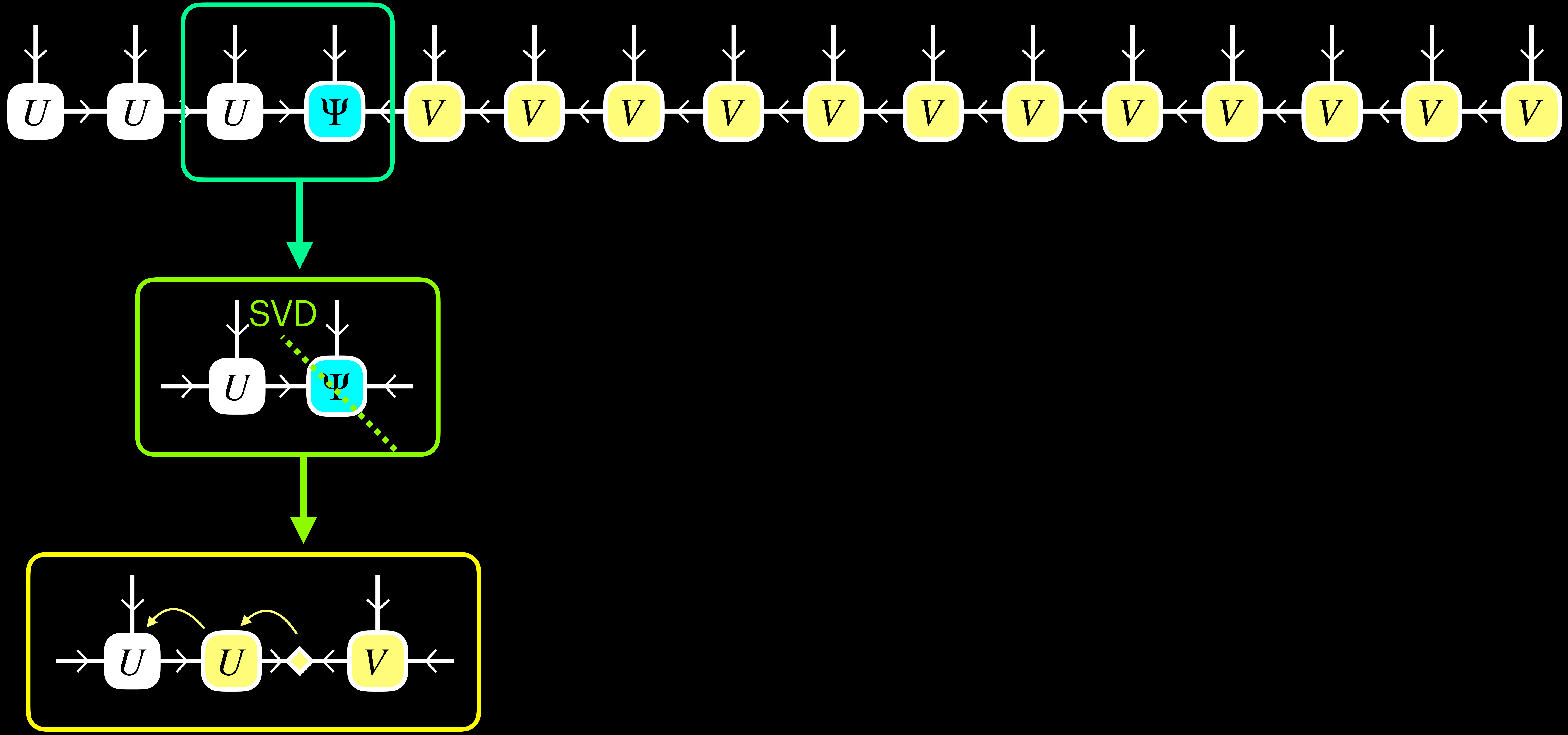
Canonical forms of MPS



Canonical forms of MPS



Canonical forms of MPS



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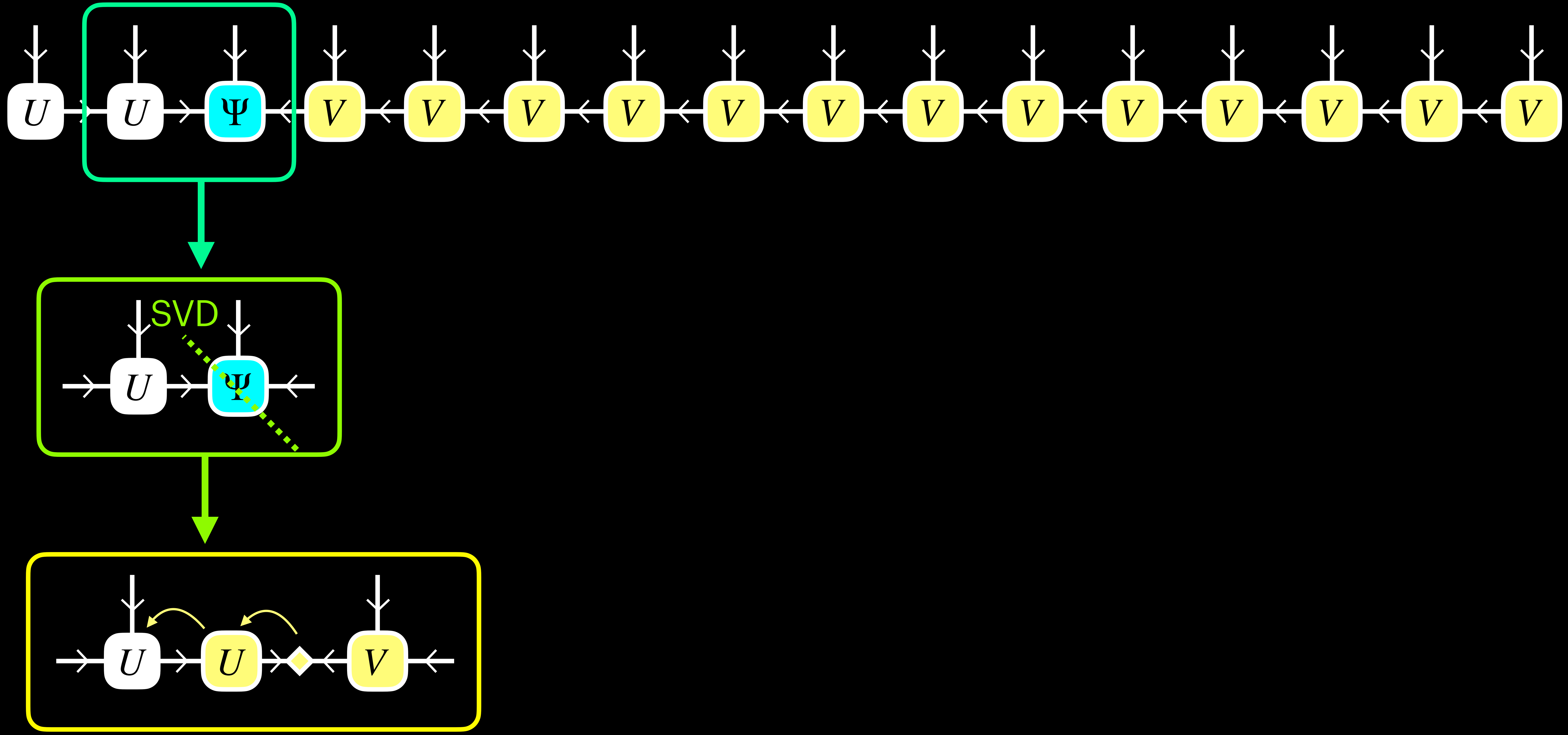

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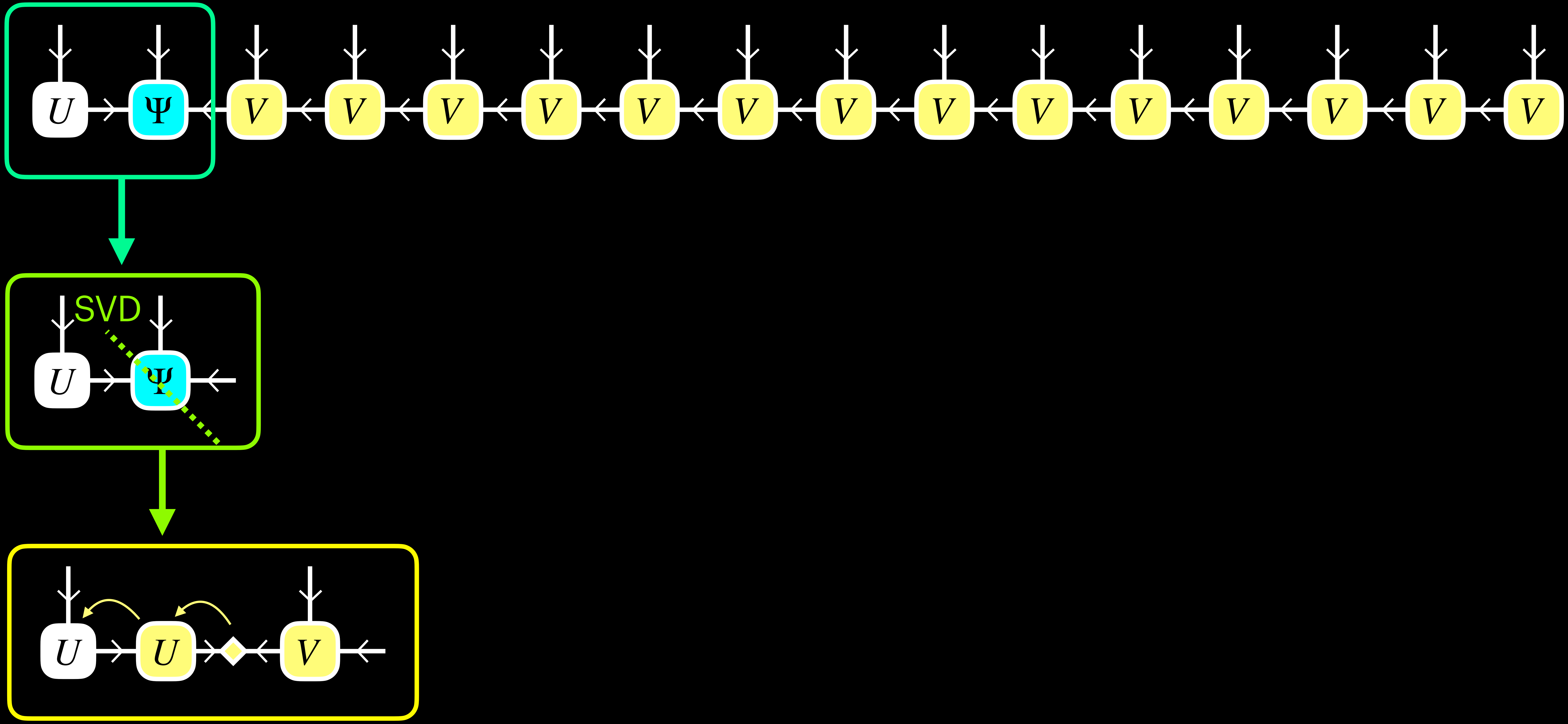

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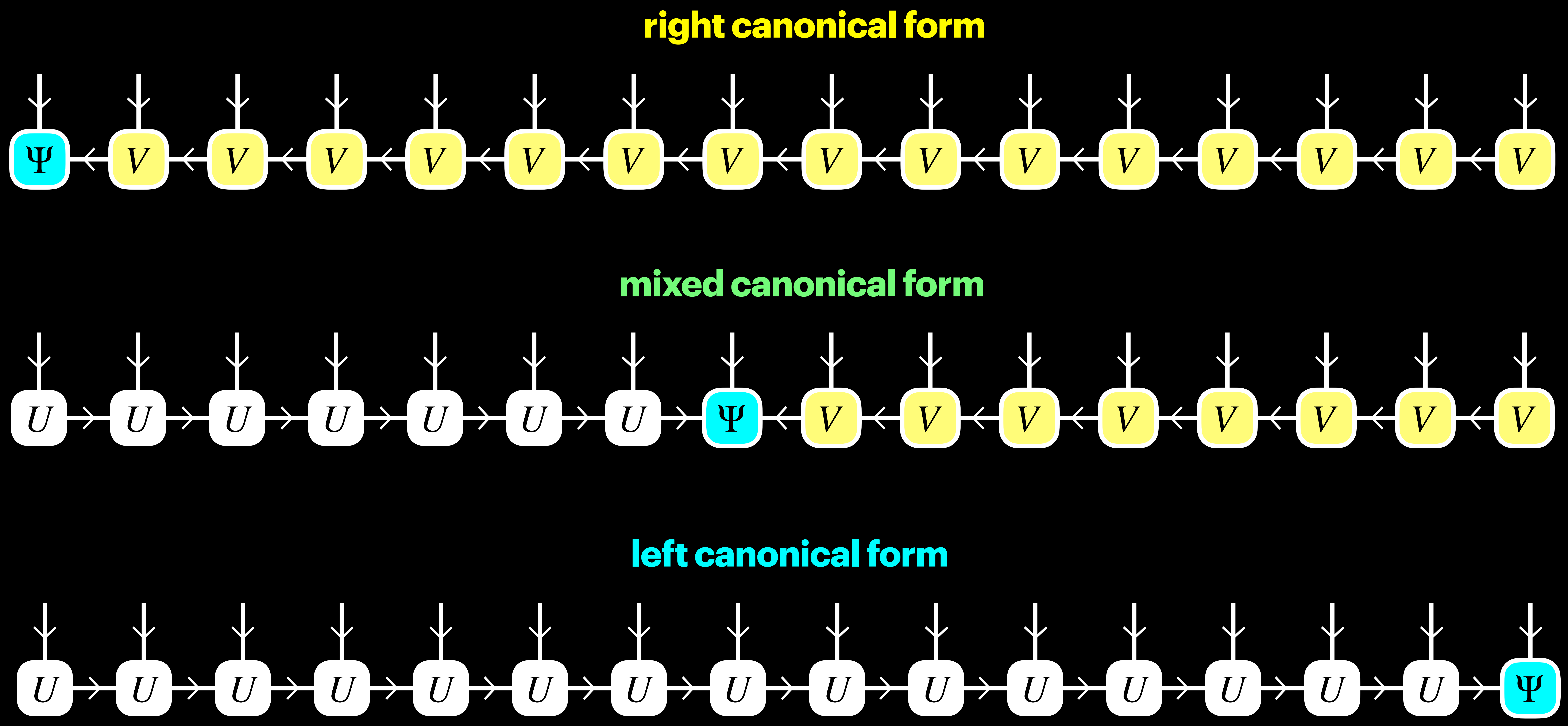

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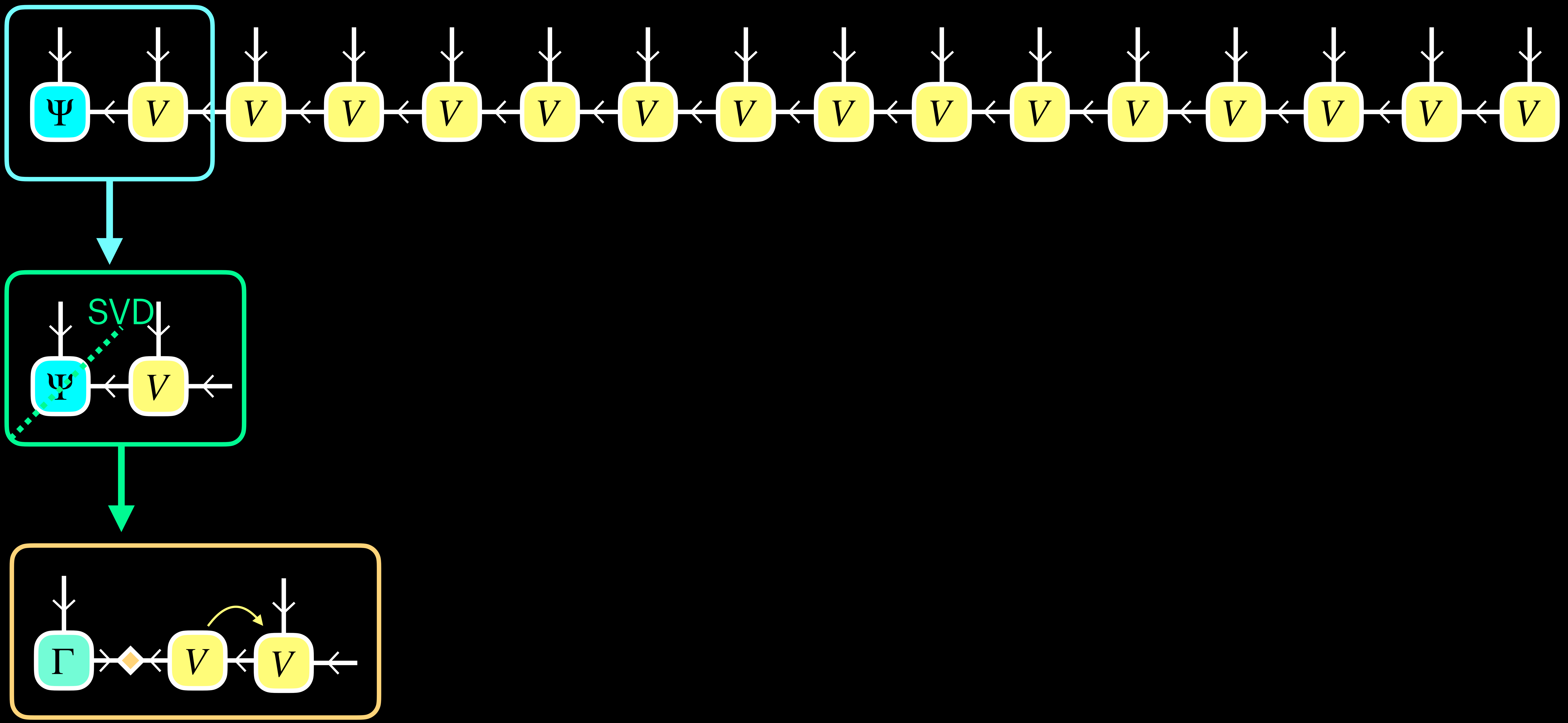

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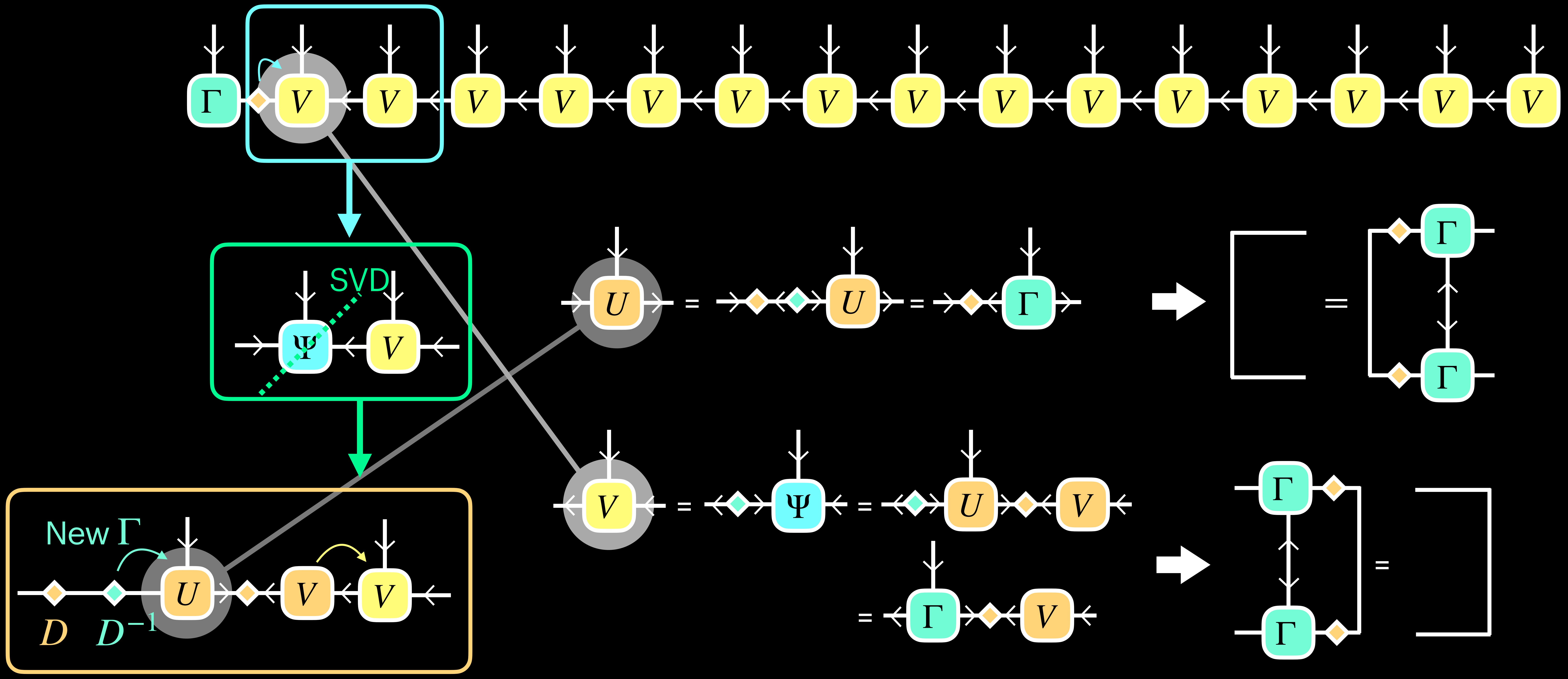

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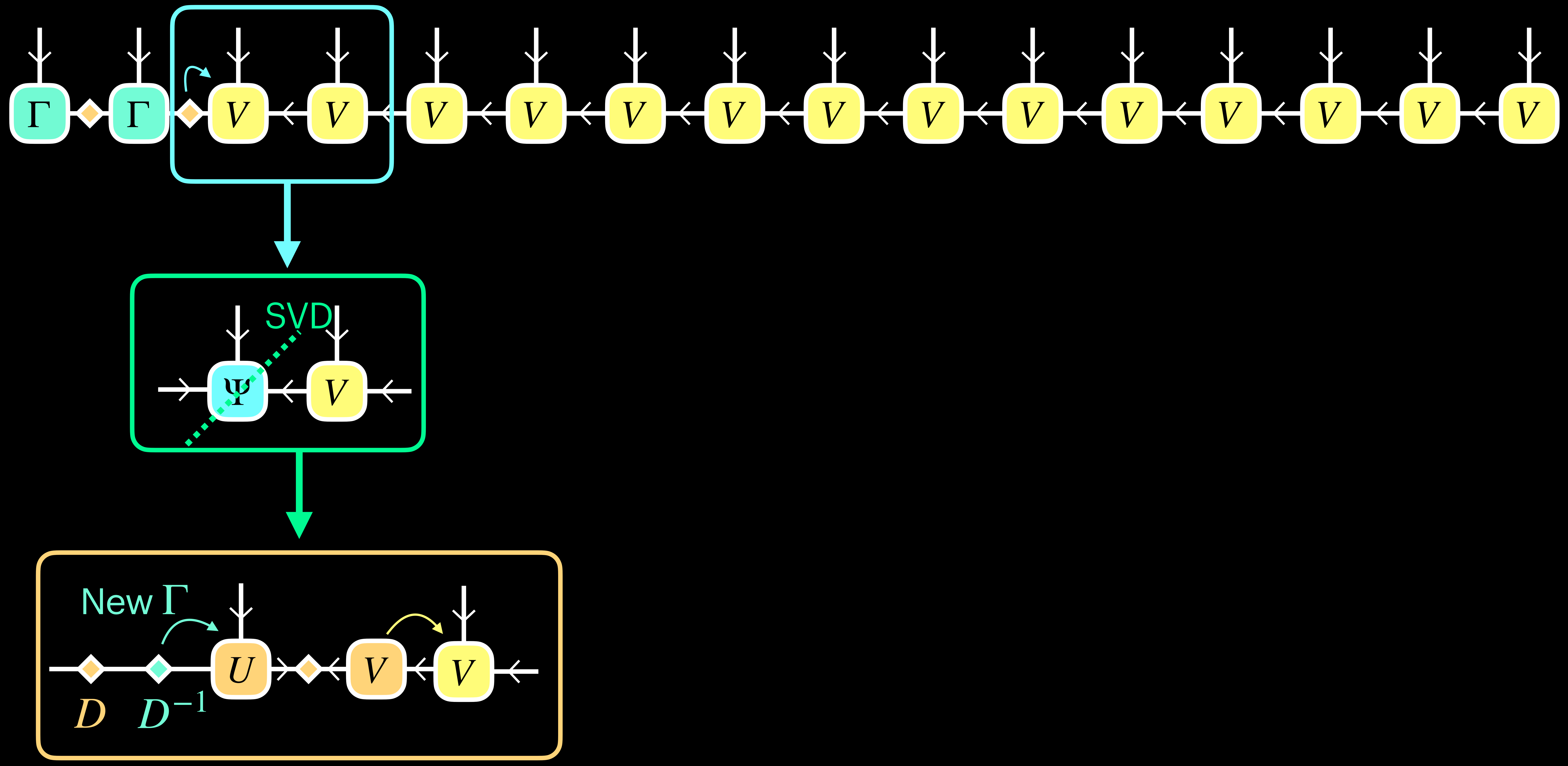

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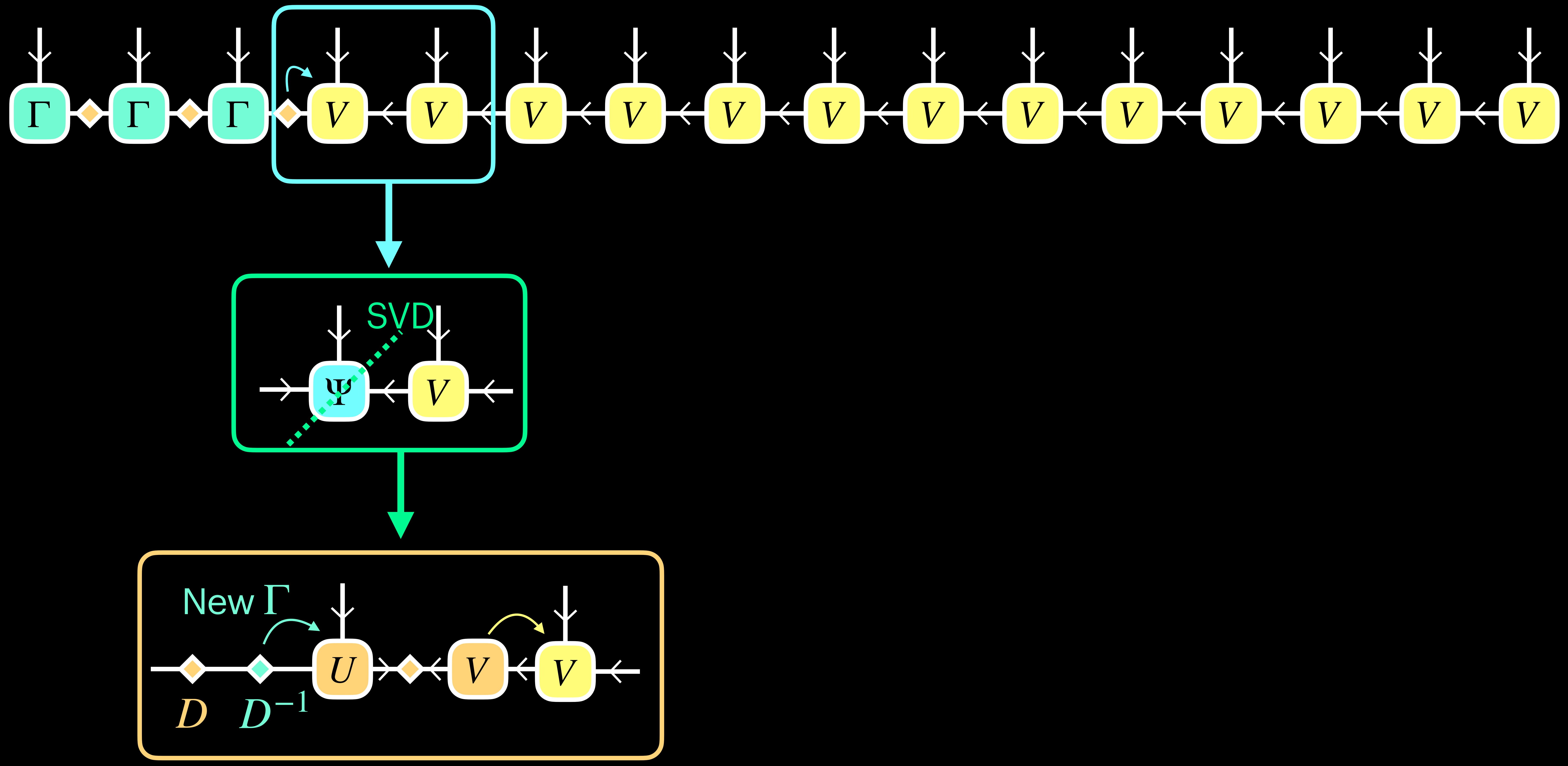

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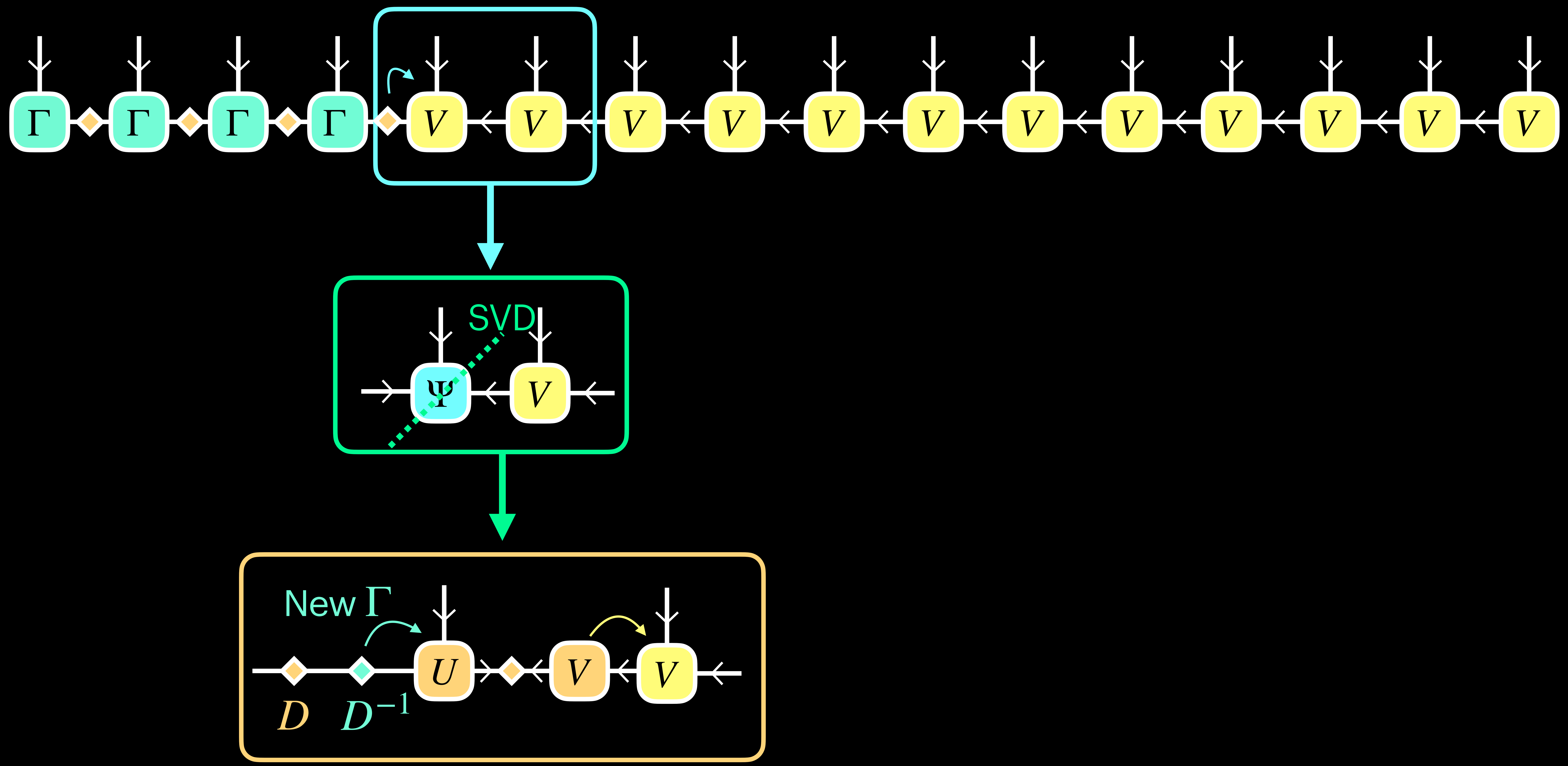

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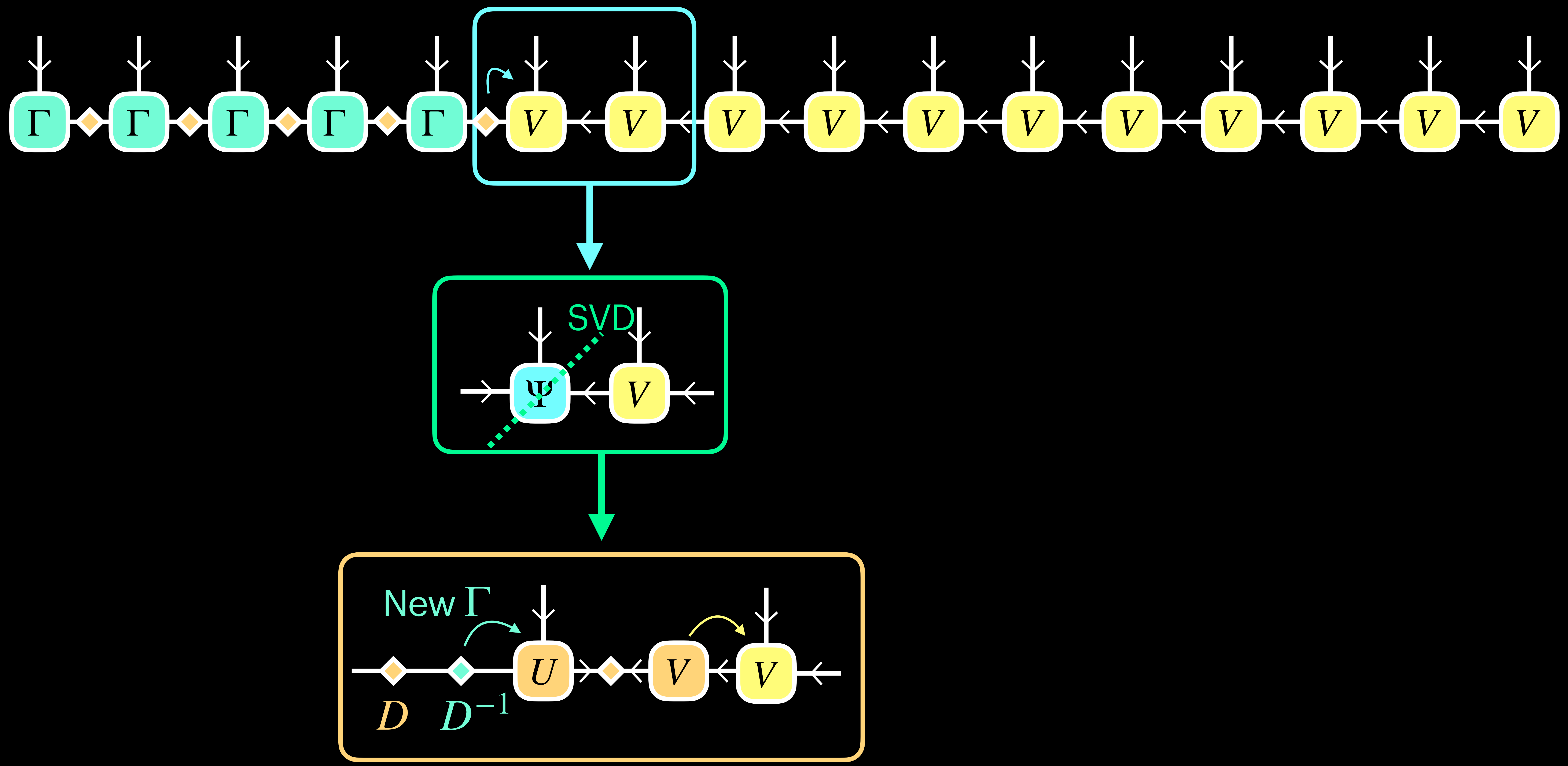

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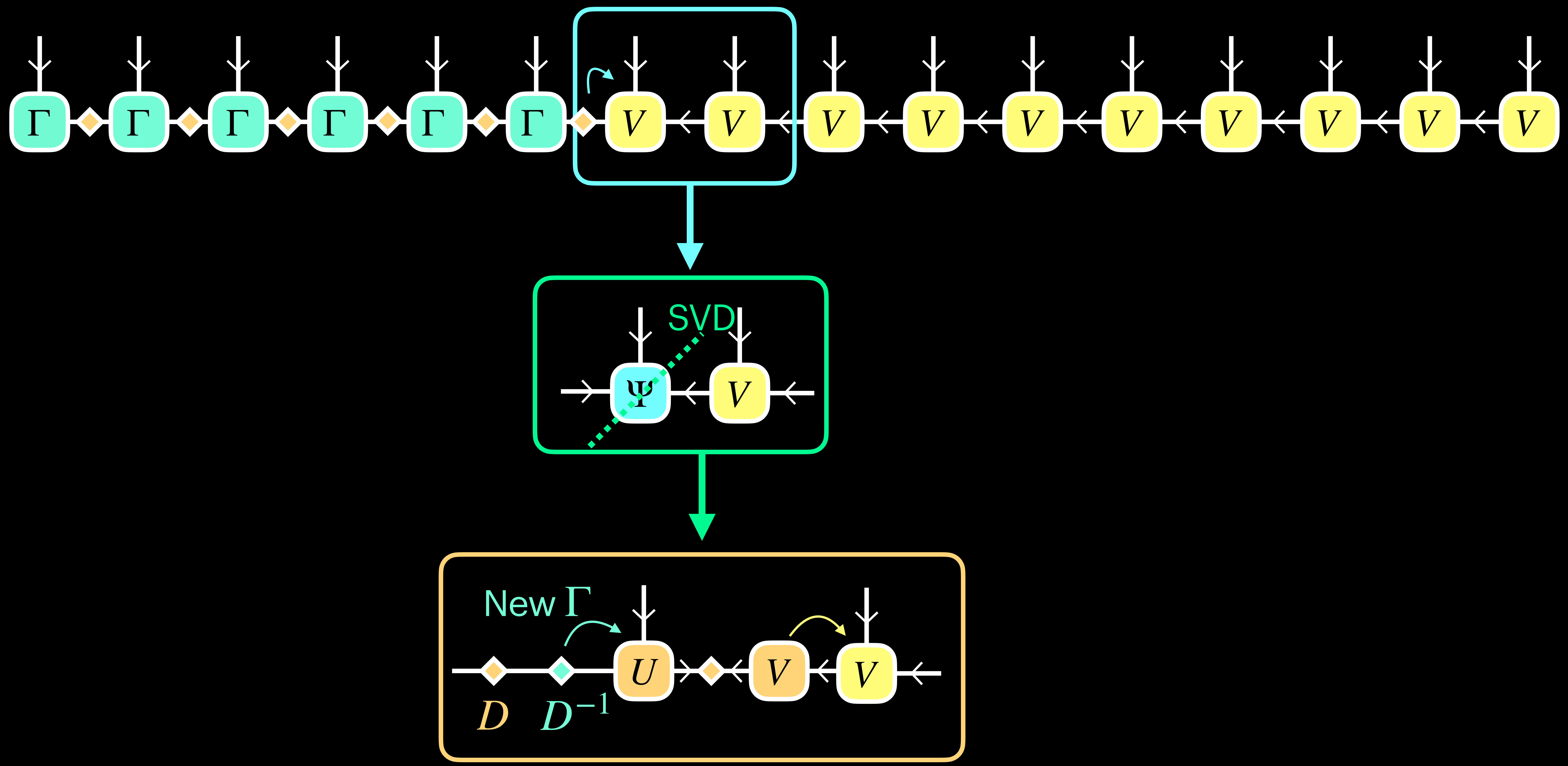

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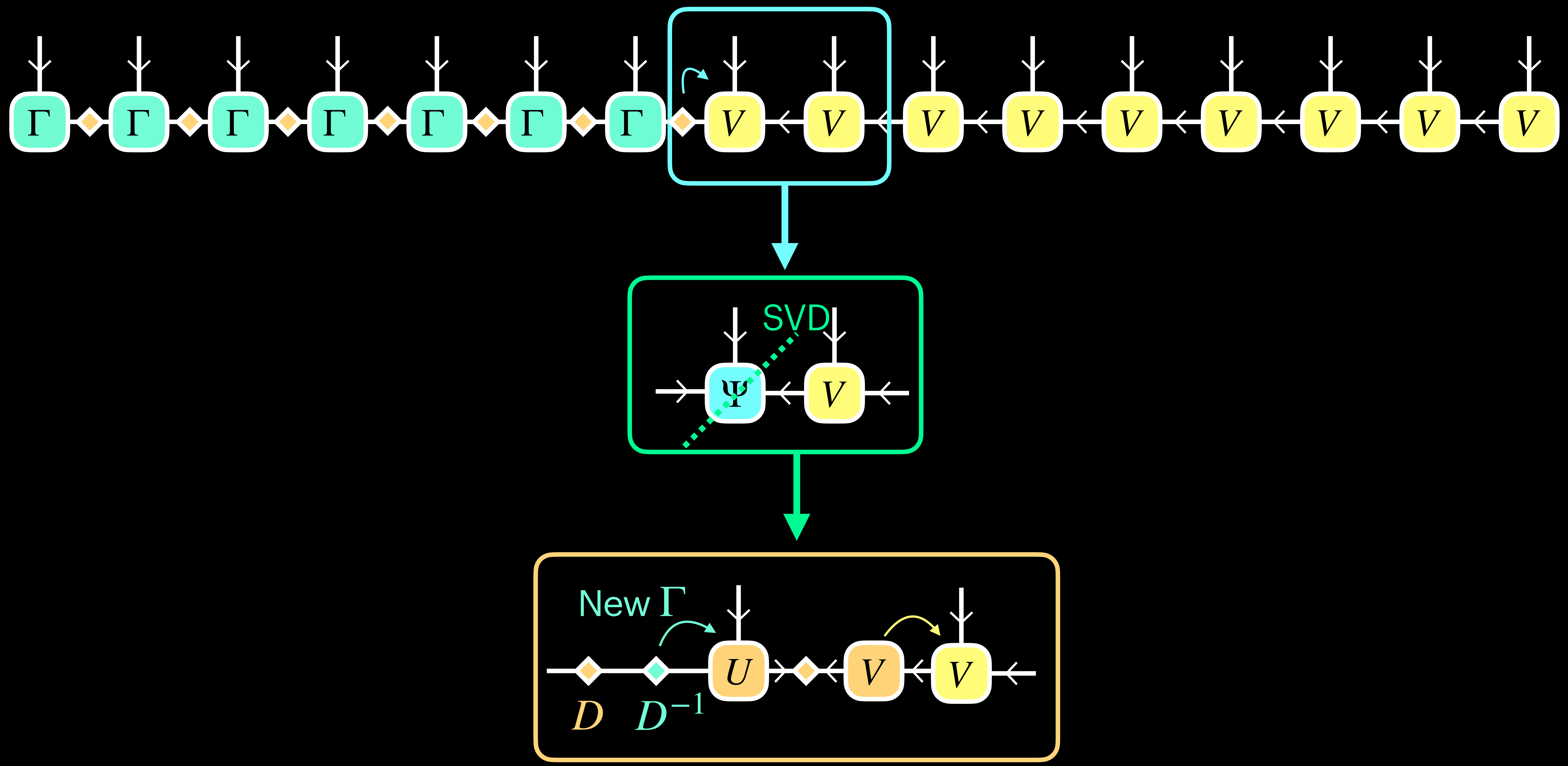

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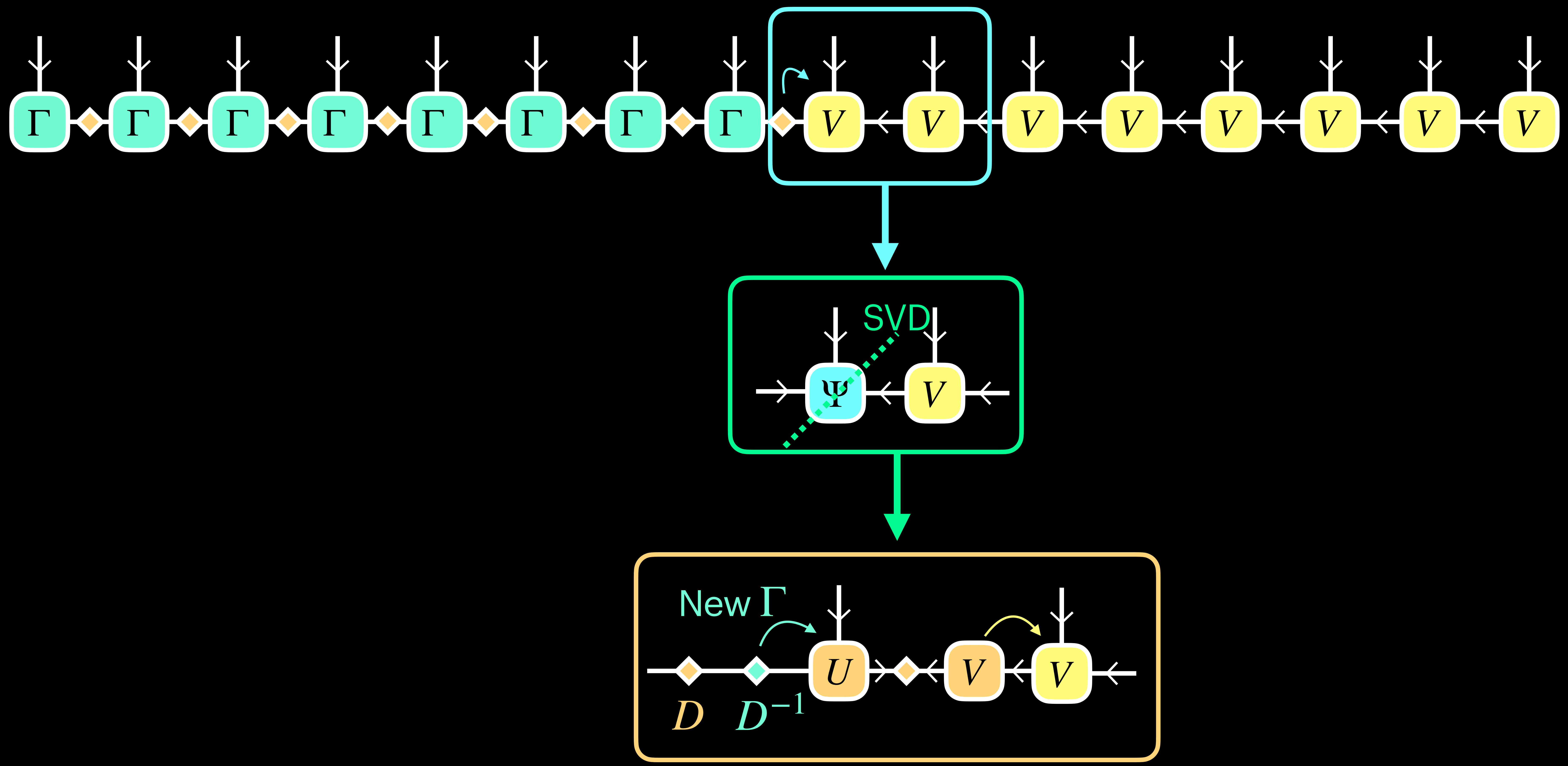

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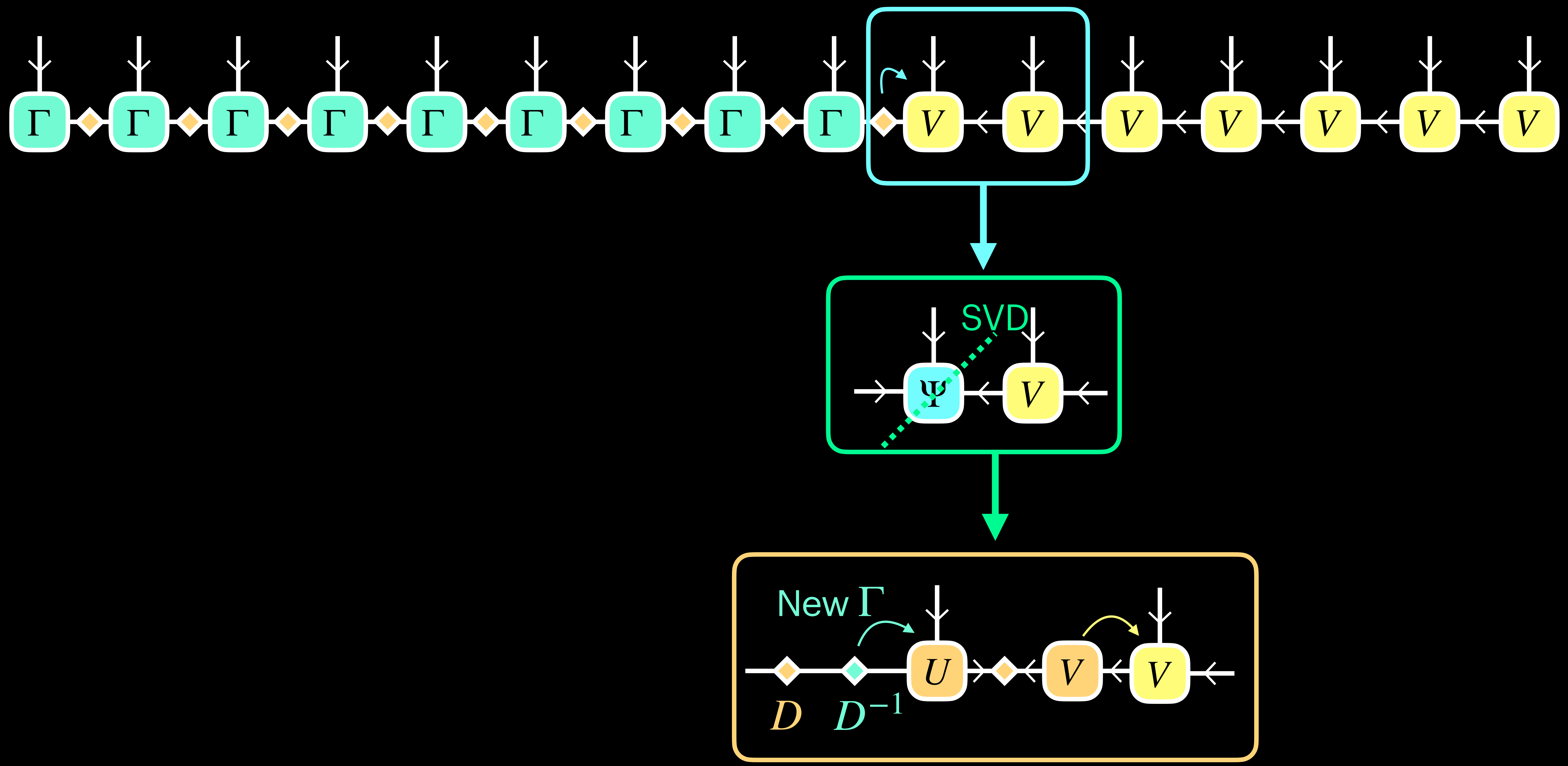

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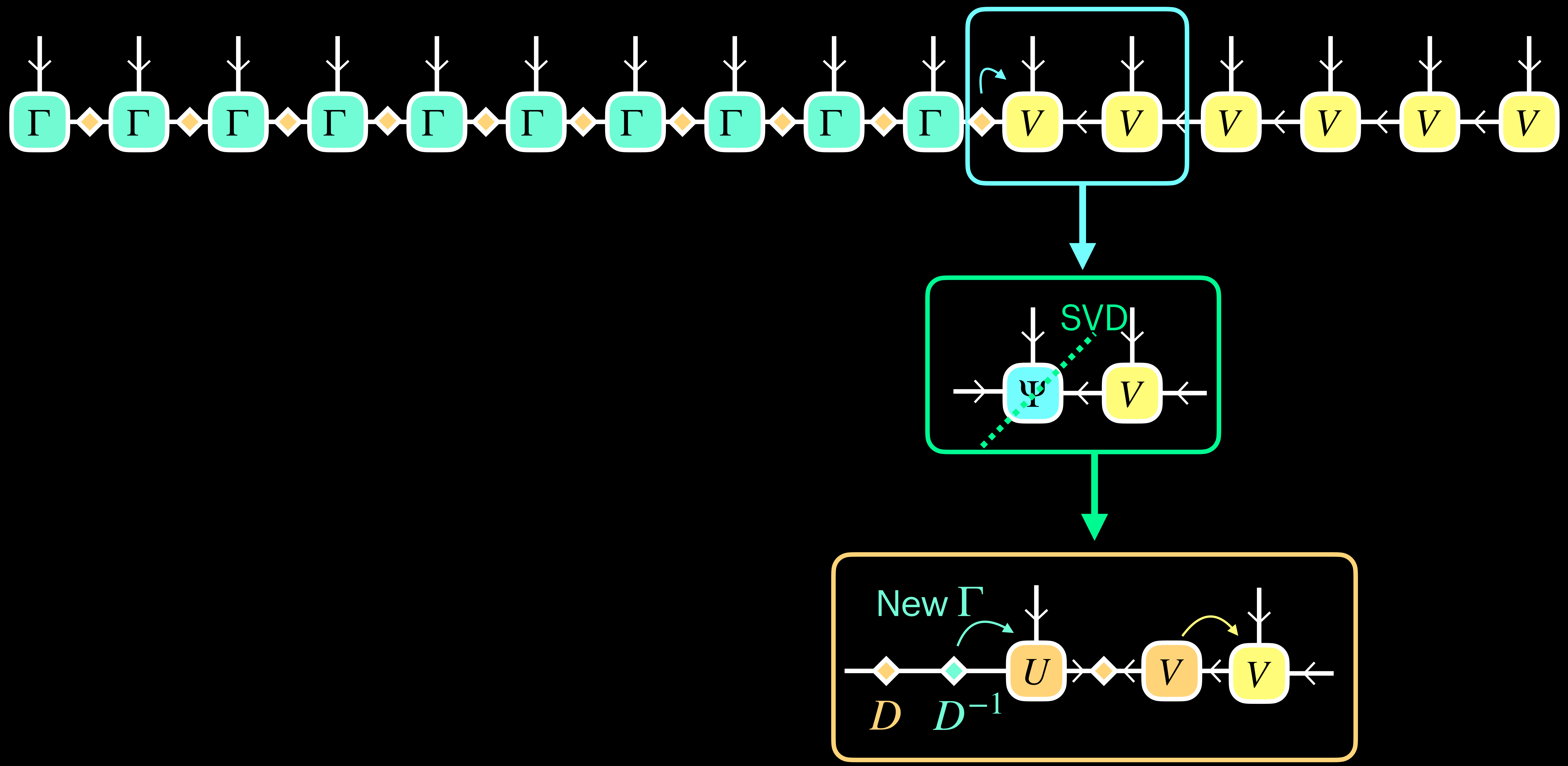

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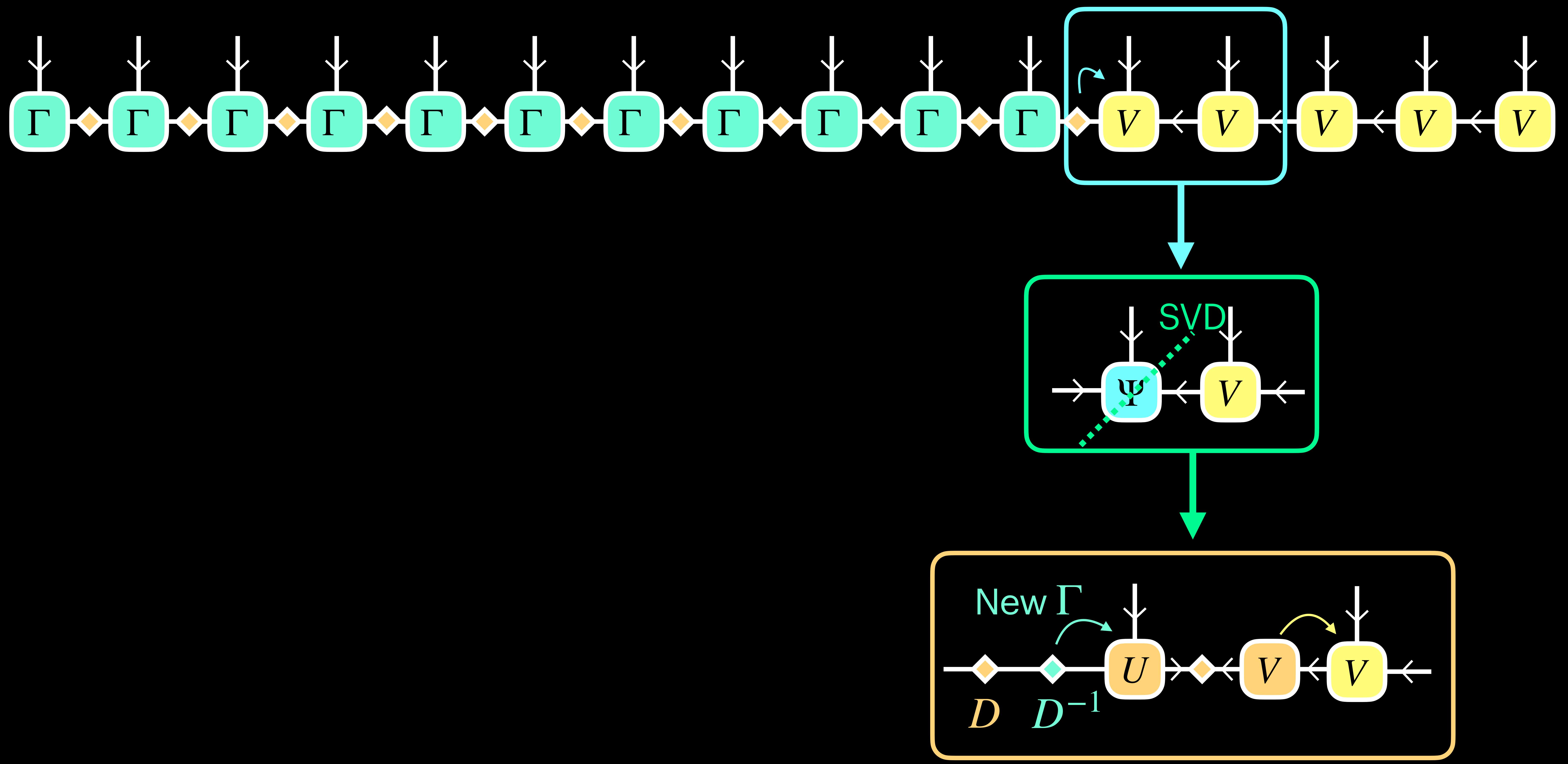

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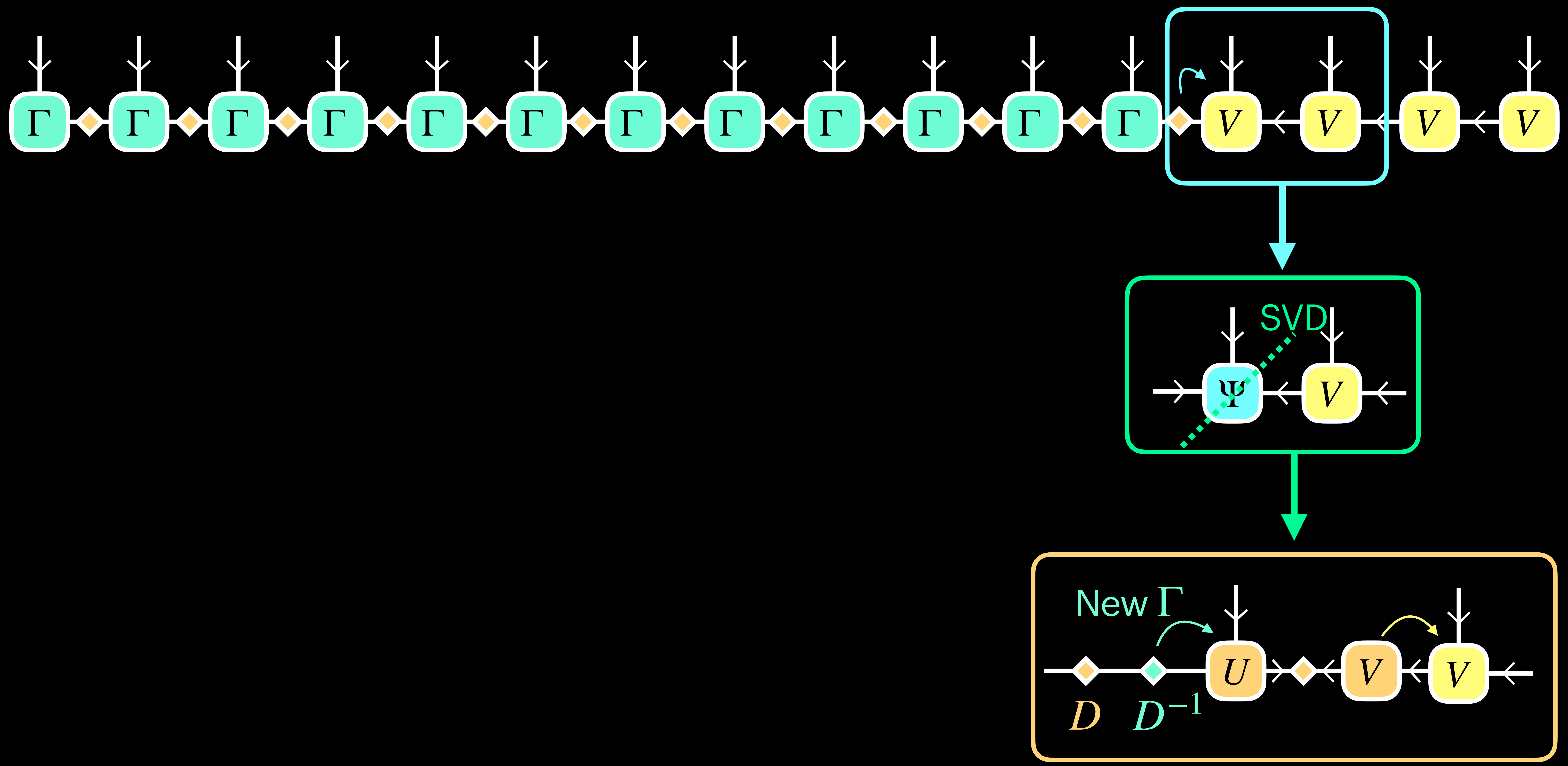
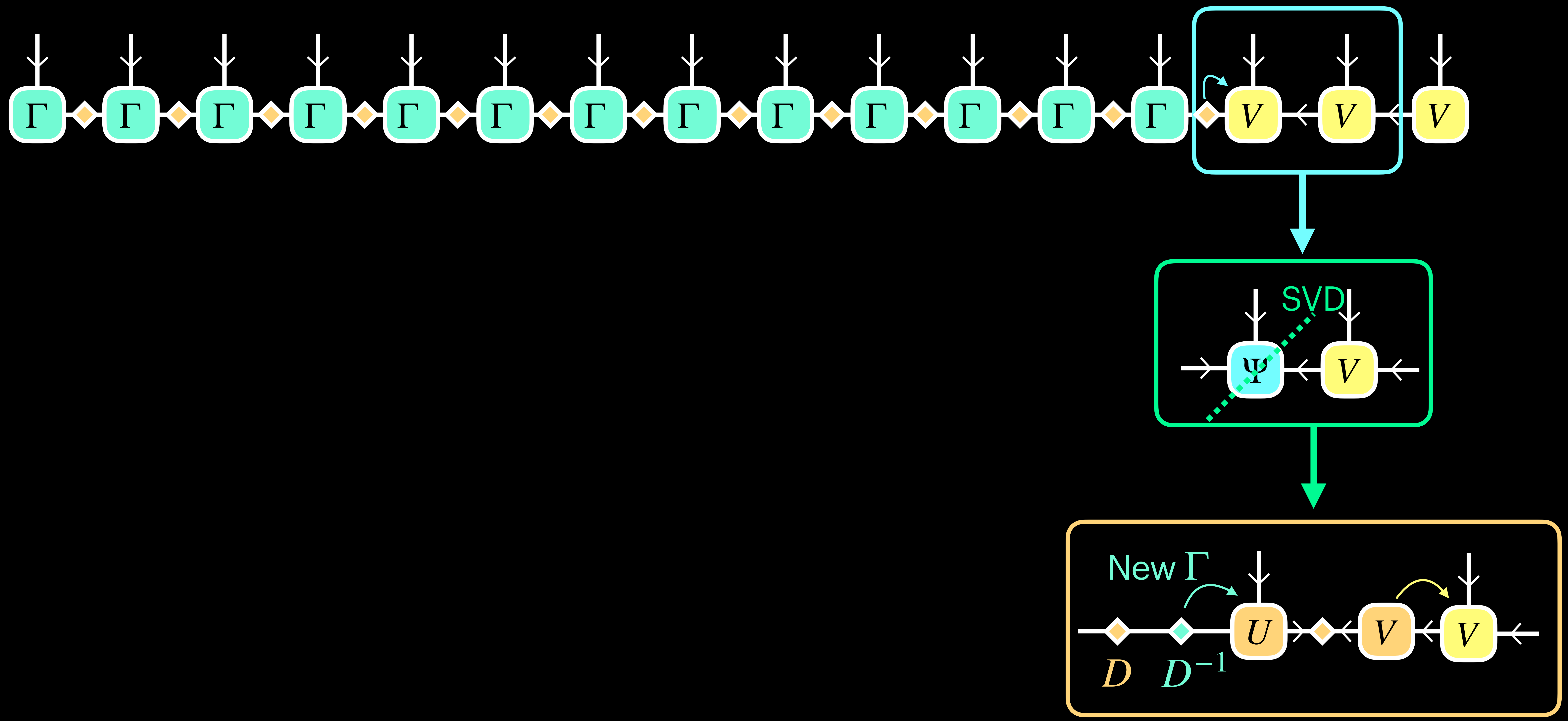
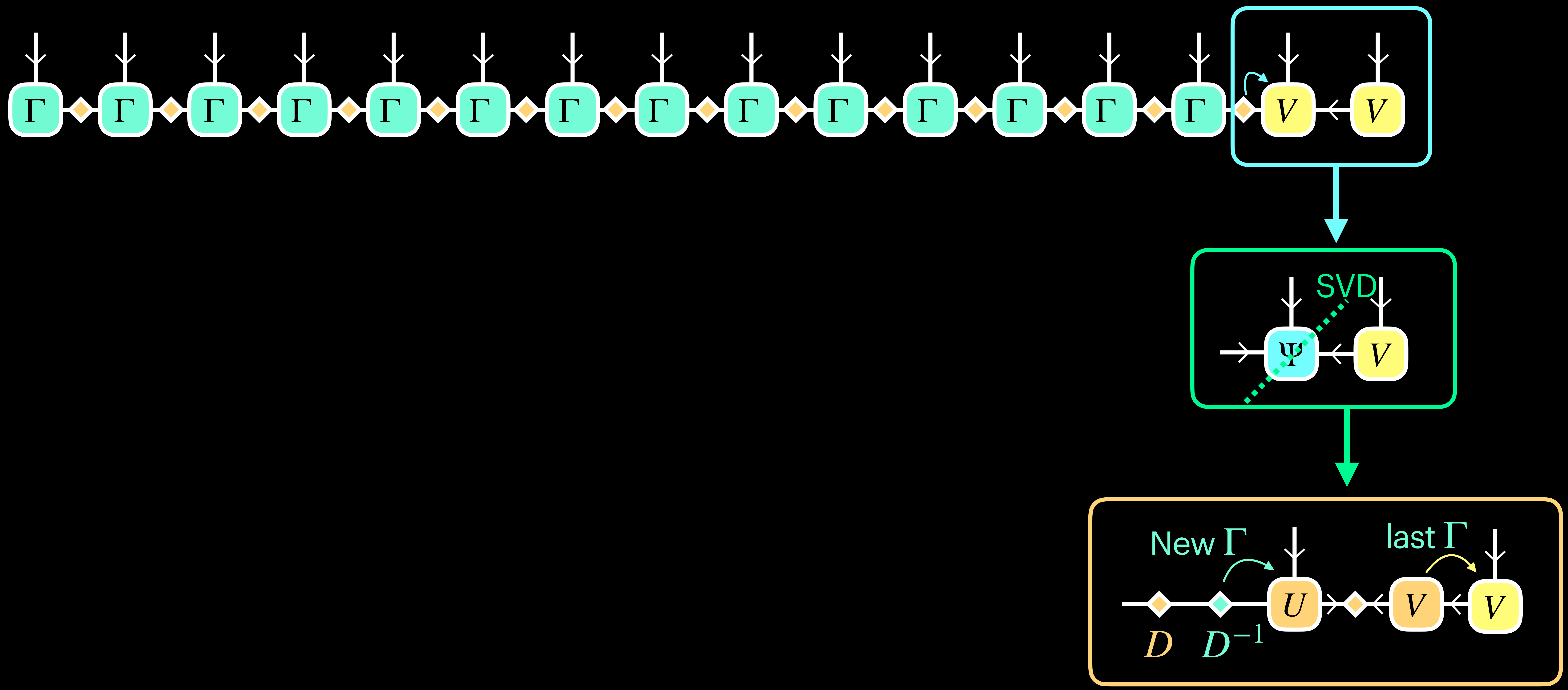


Canonical forms of MPS

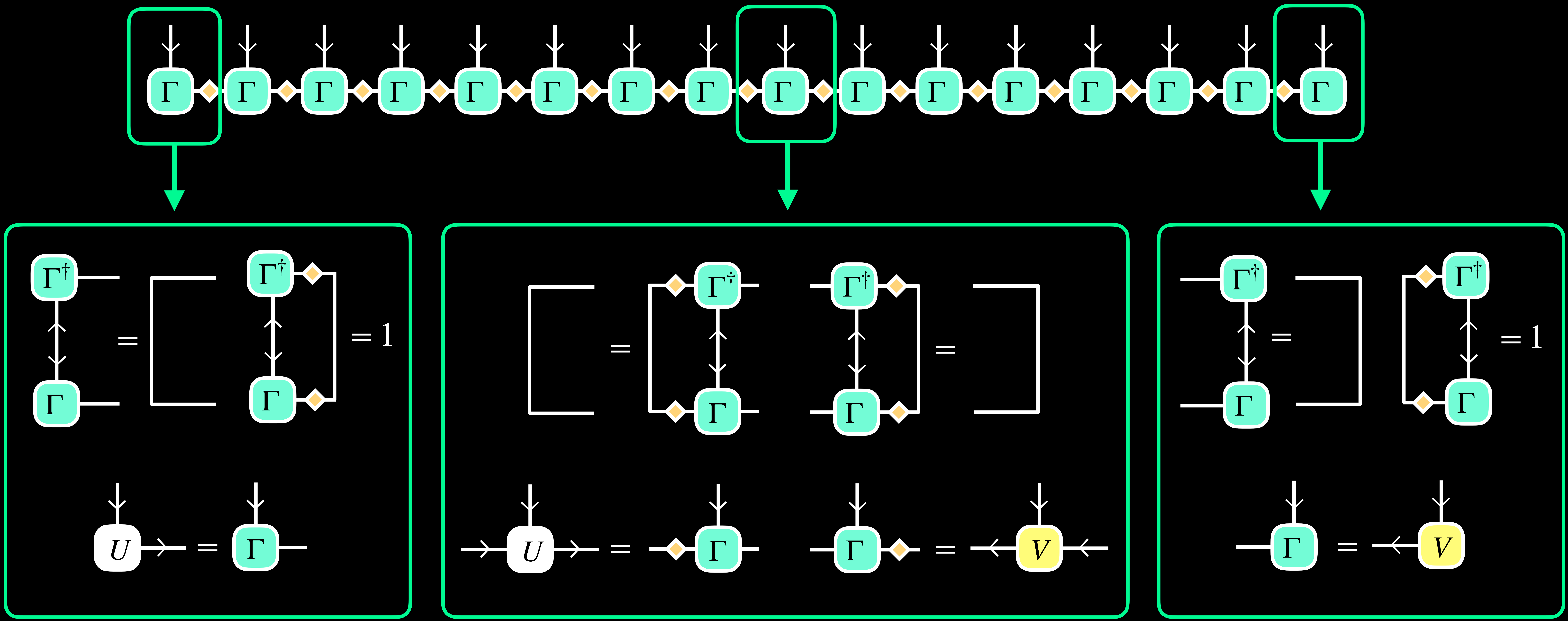


Canonical forms of MPS



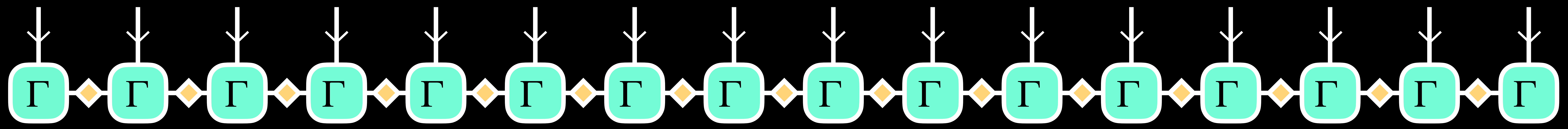
Canonical forms of MPS

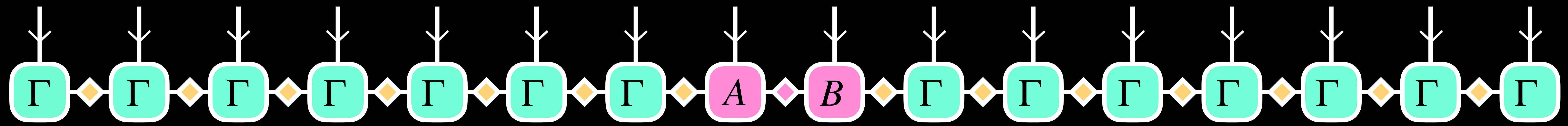
Vidal gauge



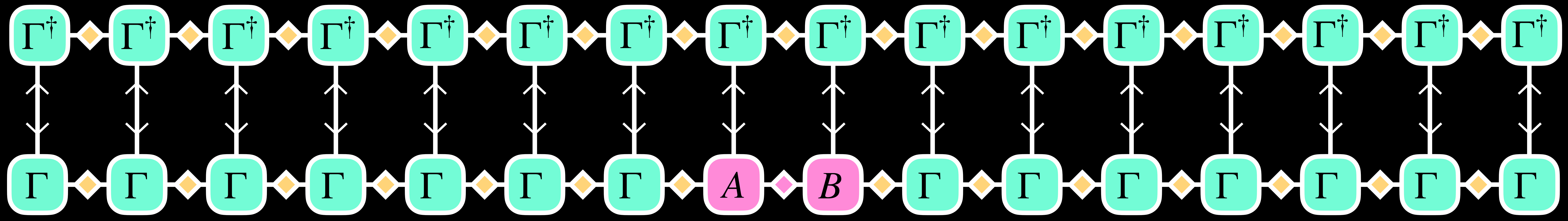
Truncation in mixed canonical form

Problem: For a given MPS $|\Psi\rangle$, we want to change some two tensors and determine a new MPS $|\Phi\rangle$ that best approximates the original MPS $|\Psi\rangle$, i.e., $|\Phi\rangle \sim |\Psi\rangle$ for

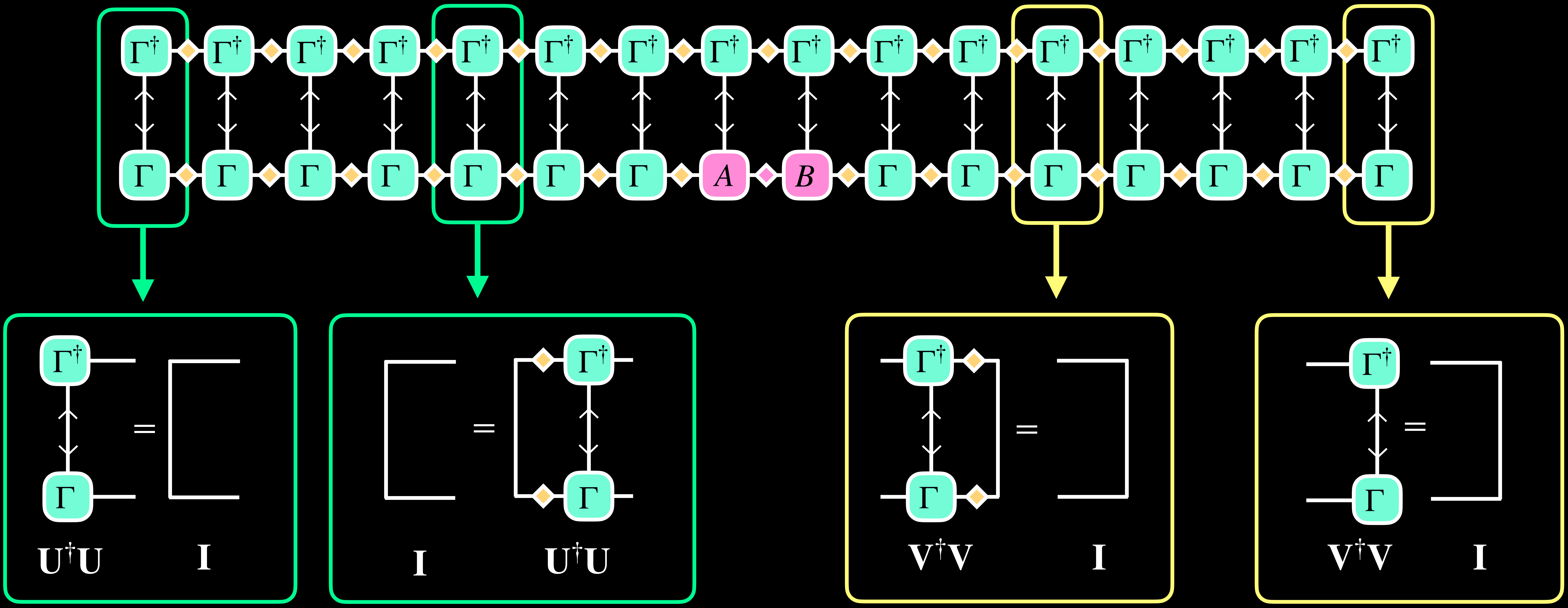
$|\Psi\rangle =$ 

$|\Phi\rangle =$ 

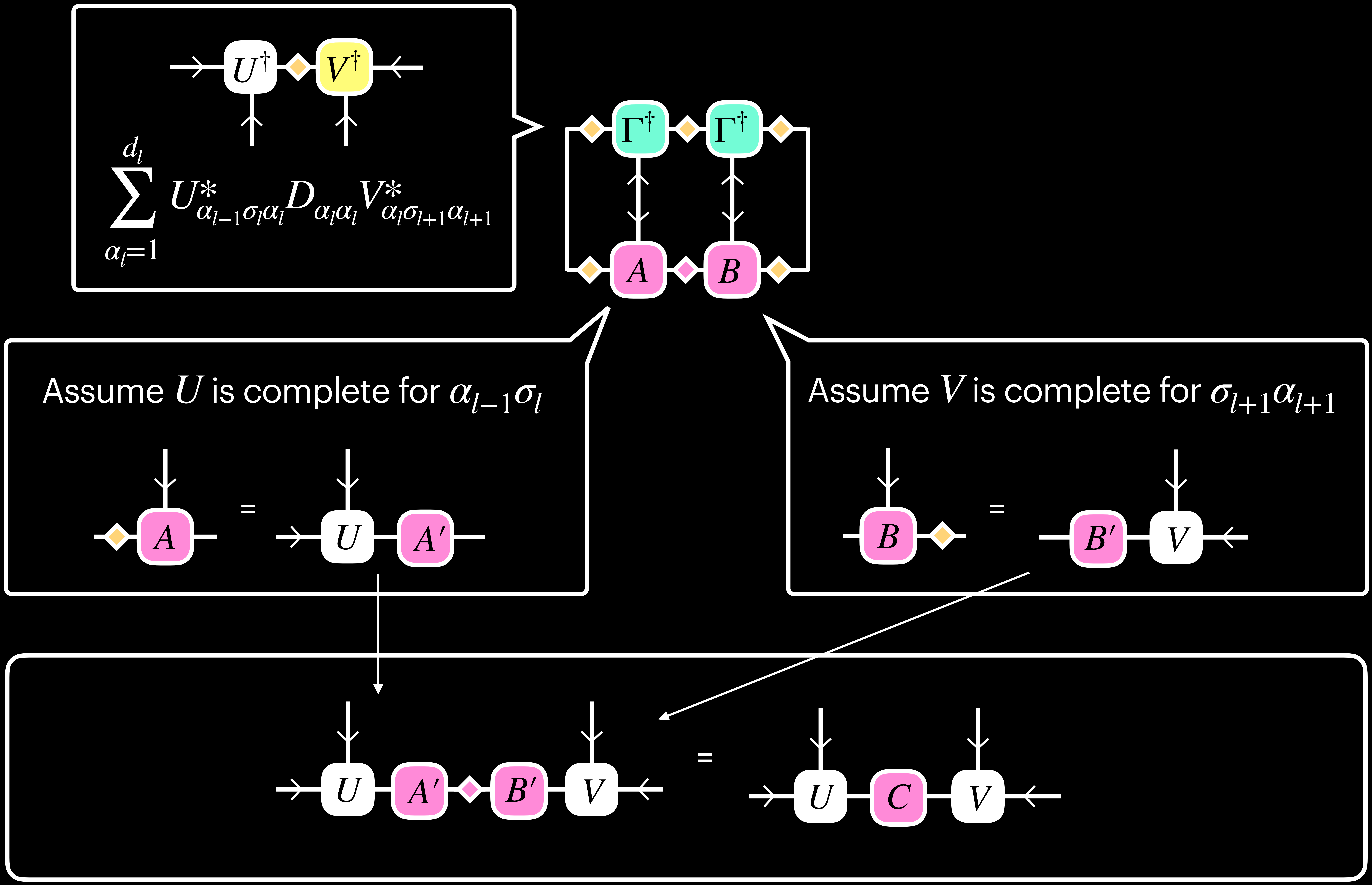
Strategy: Choose two tensor A and B so as to maximize the overlap $\langle\Psi|\Phi\rangle$.



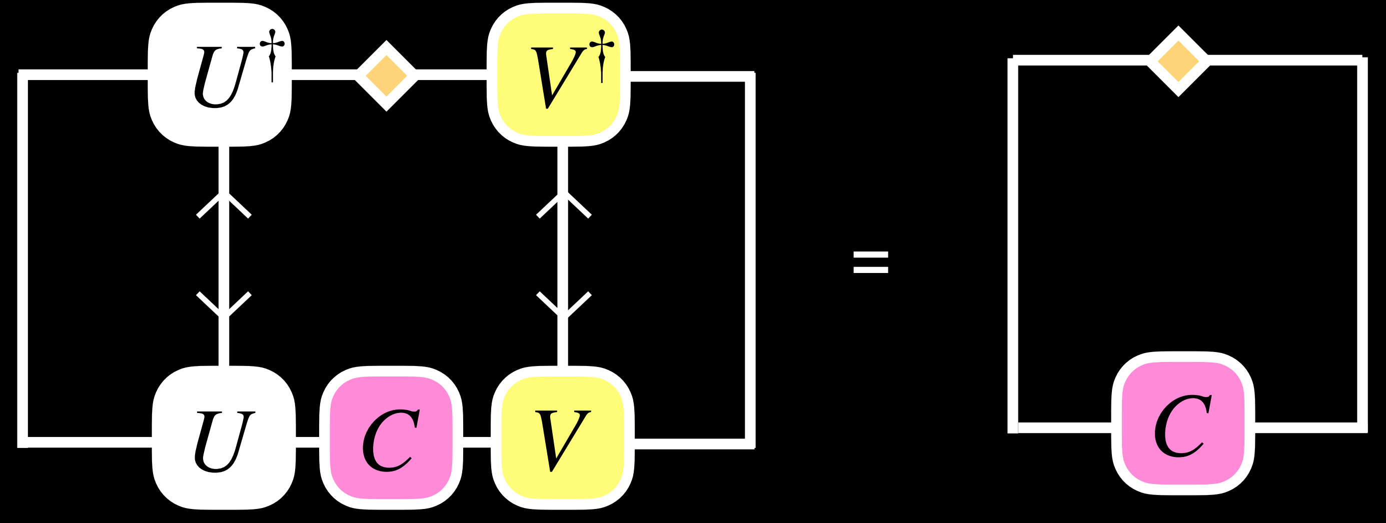
Truncation in mixed canonical form



Truncation in mixed canonical form

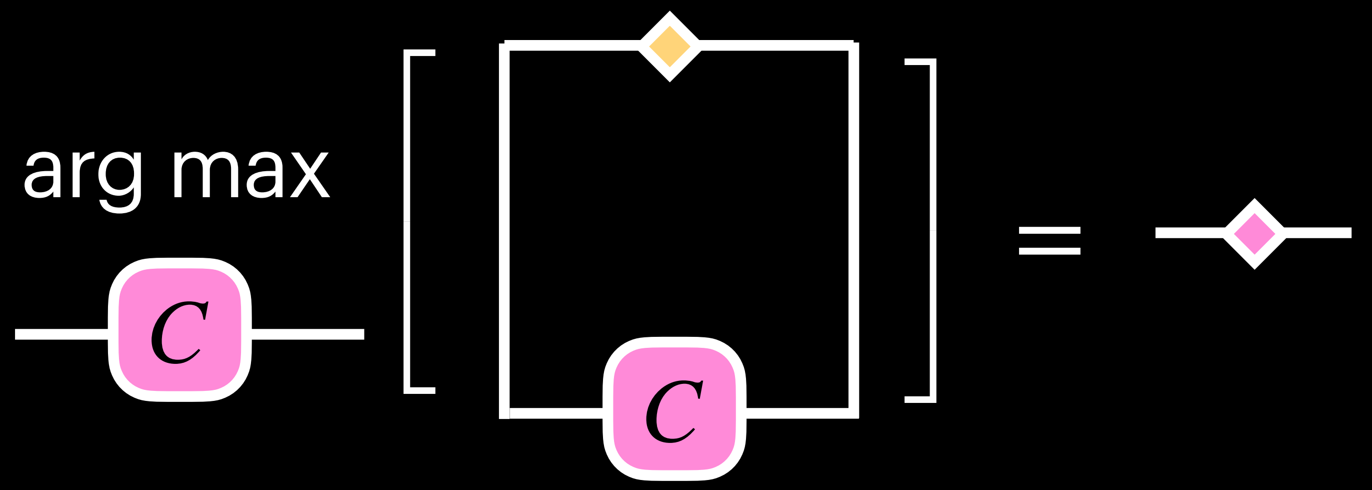


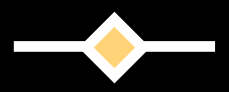
Truncation in mixed canonical form



$= \sum_{\alpha_l=1}^{\dim[D]} D_{\alpha_l\alpha_l} C_{\alpha_l\alpha_l}$

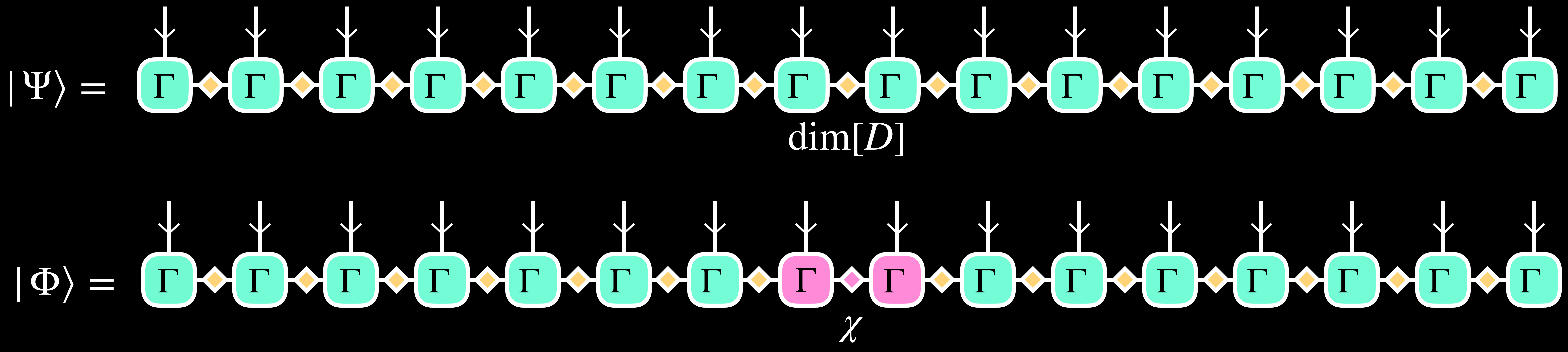
- Off-diagonal elements of C are not relevant.
- We assume that the rank of C is $\chi < \dim[D]$
- Normalization condition yields $\sum_{\alpha_l=1}^{\chi} C_{\alpha_l\alpha_l}^2 = 1.$
- Then, $C_{\alpha_l\alpha_l} \propto D_{\alpha_l\alpha_l}$ gives maximum of overlap because of Cauchy-Schwarz inequality.



: Same as  but the rank is truncated.

Truncation in mixed canonical form

Problem: For a given MPS $|\Psi\rangle$, we want to change some two tensors and determine a new MPS $|\Phi\rangle$ that best approximates the original MPS $|\Psi\rangle$, i.e., $|\Phi\rangle \sim |\Psi\rangle$ for

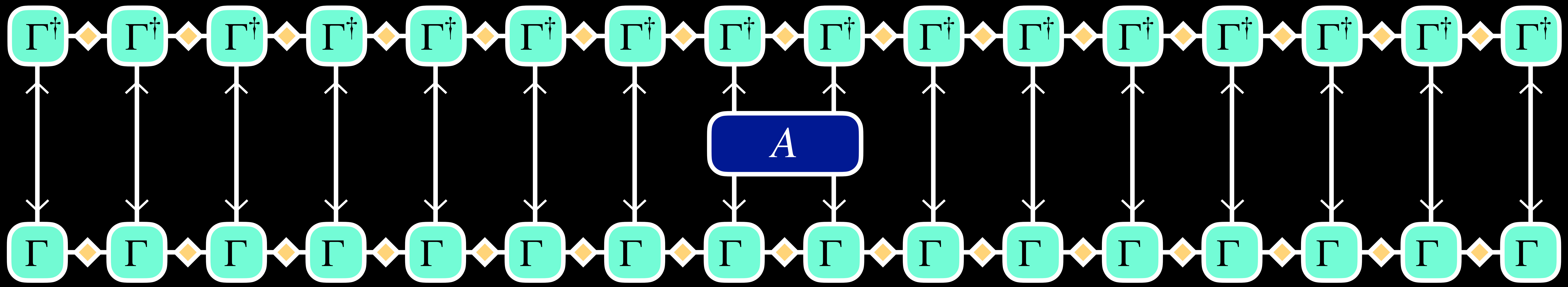


Solution: Select the same tensor with reduced rank. ⟶ **truncation**

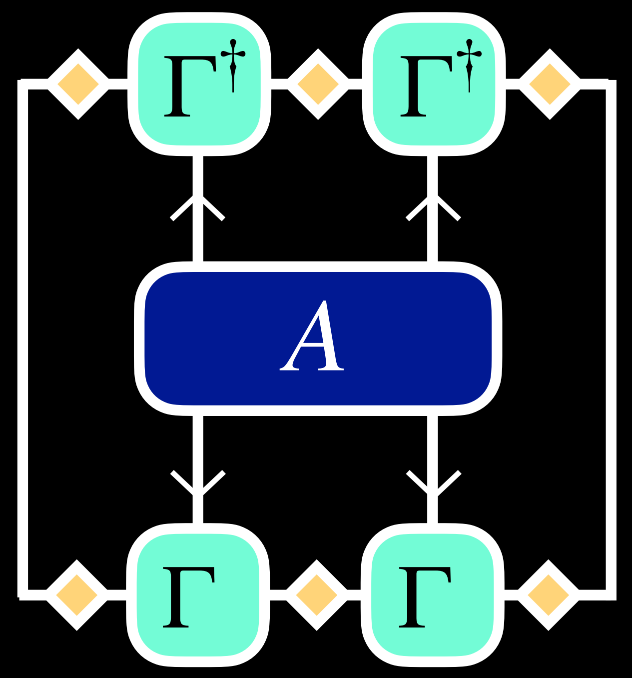
Note: Usually, truncation is performed at the same time that the canonical form is obtained.

Measurement of local operator

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



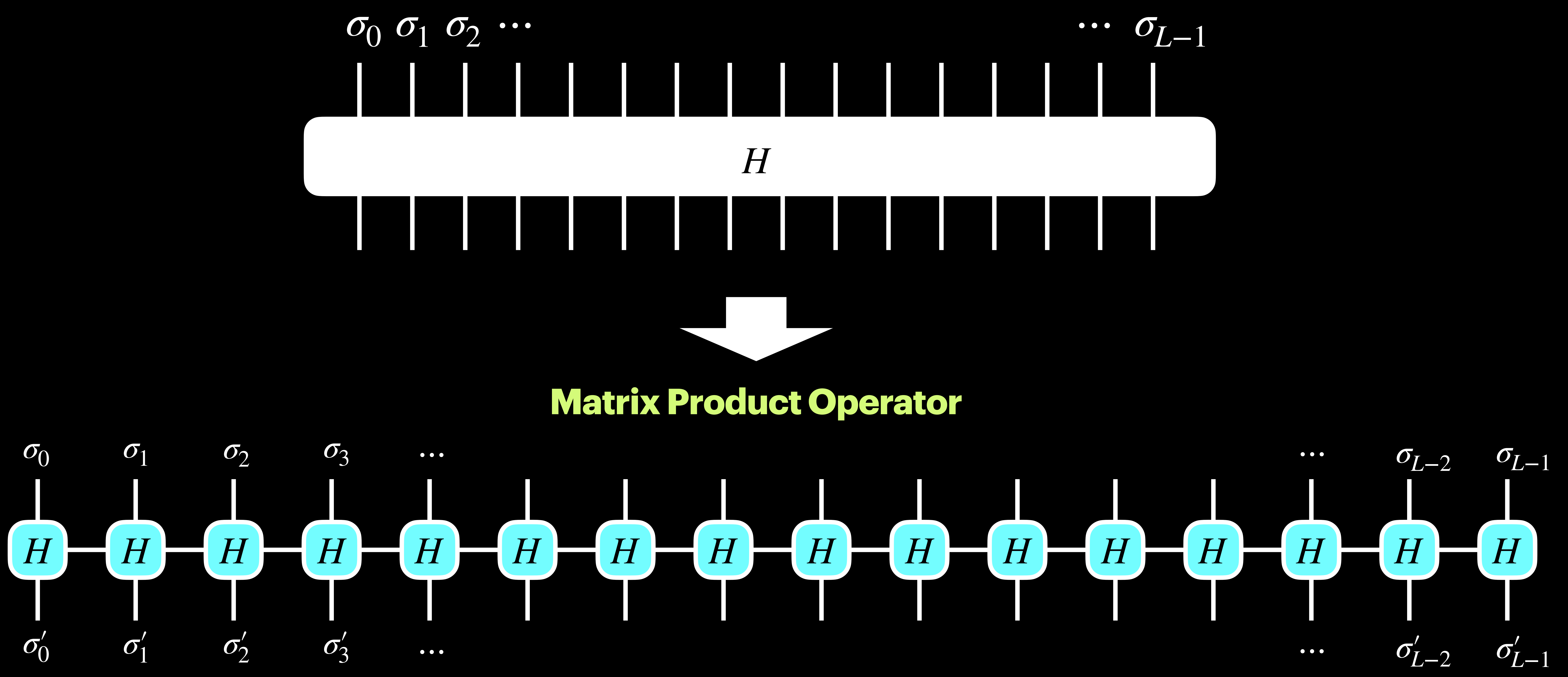
$=$



A big advantage of representations satisfying the isometric condition is that computation of expectation value of an local operator $\hat{A}$ can be replaced by local tensor contraction computation.

Matrix product operator (MPO)

$$\text{Operator } H = \sum_{\sigma_0\sigma_1\cdots\sigma_{L-1}} \sum_{\sigma'_0\sigma'_1\cdots\sigma'_{L-1}} H_{(\sigma_0\sigma_1\cdots\sigma_{L-1})(\sigma'_0\sigma'_1\cdots\sigma'_{L-1})} |\sigma_0\sigma_1\cdots\sigma_{L-1}\rangle\langle\sigma'_0\sigma'_1\cdots\sigma'_{L-1}|$$

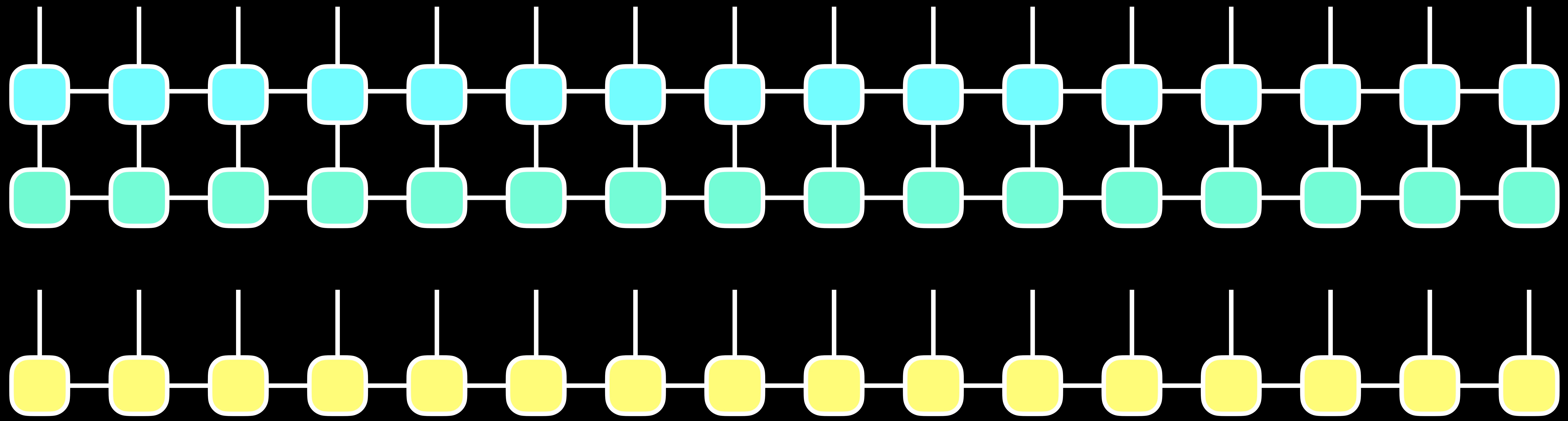


Apply MPO to MPS

Applying MPO to MPS increases the bond dimension. Therefore, an approximation is required to suppress the bond dimension.

$H|\Psi\rangle =$

$\sim |\Phi\rangle =$



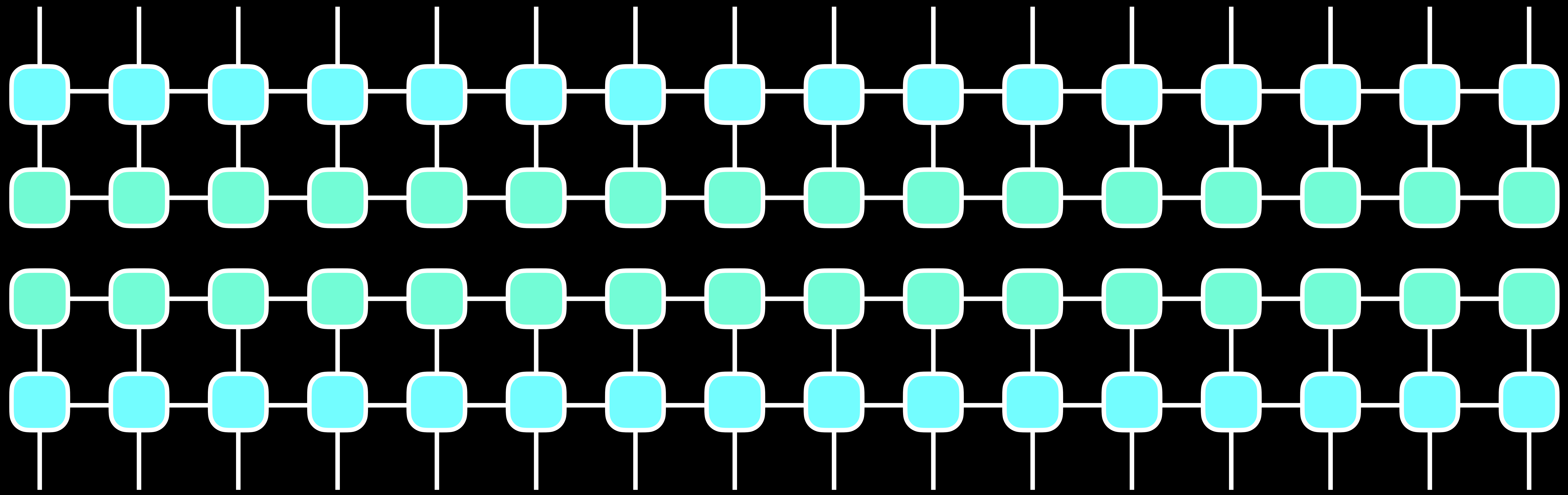
There is two major methods : 1. Method utilizing the density matrices. ⟶ This time, I will explain this.
[https://tensornetwork.org/mps/algorithms/denmat_mpo_mps/]

2. Fitting algorithm Need sweeps and good initialization

Apply MPO to MPS

Density matrix for all system

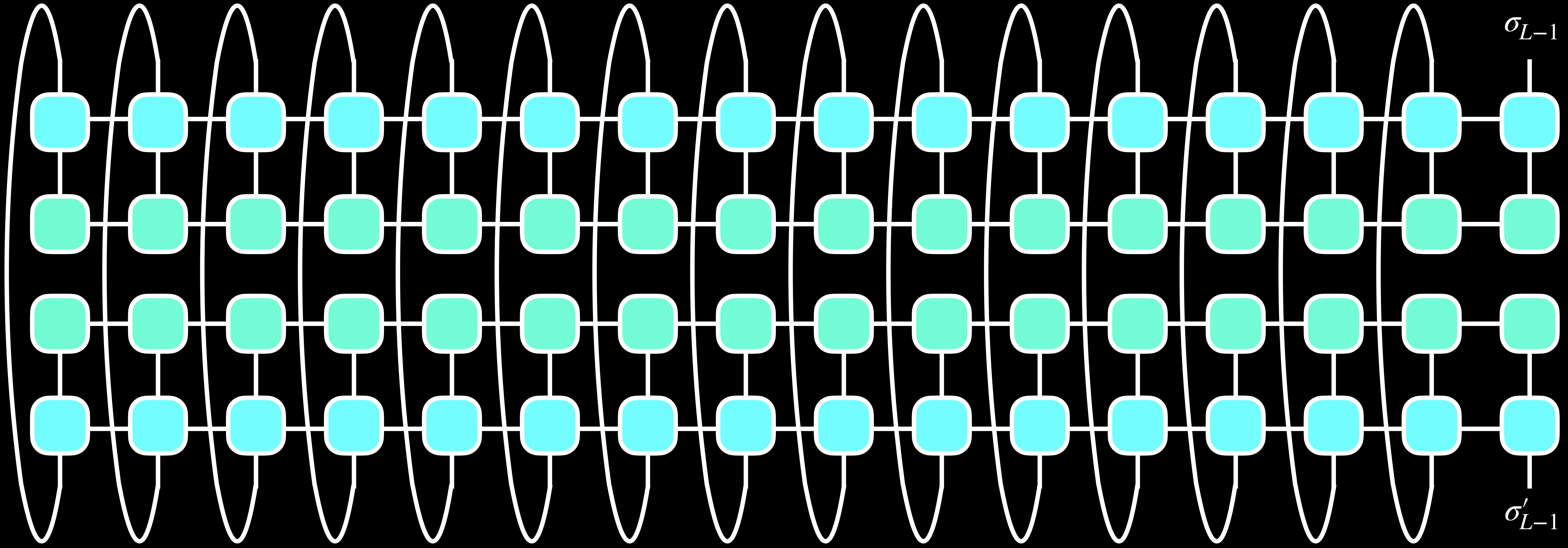
$\rho =$



Apply MPO to MPS

Reduced density matrix for the right-edge site

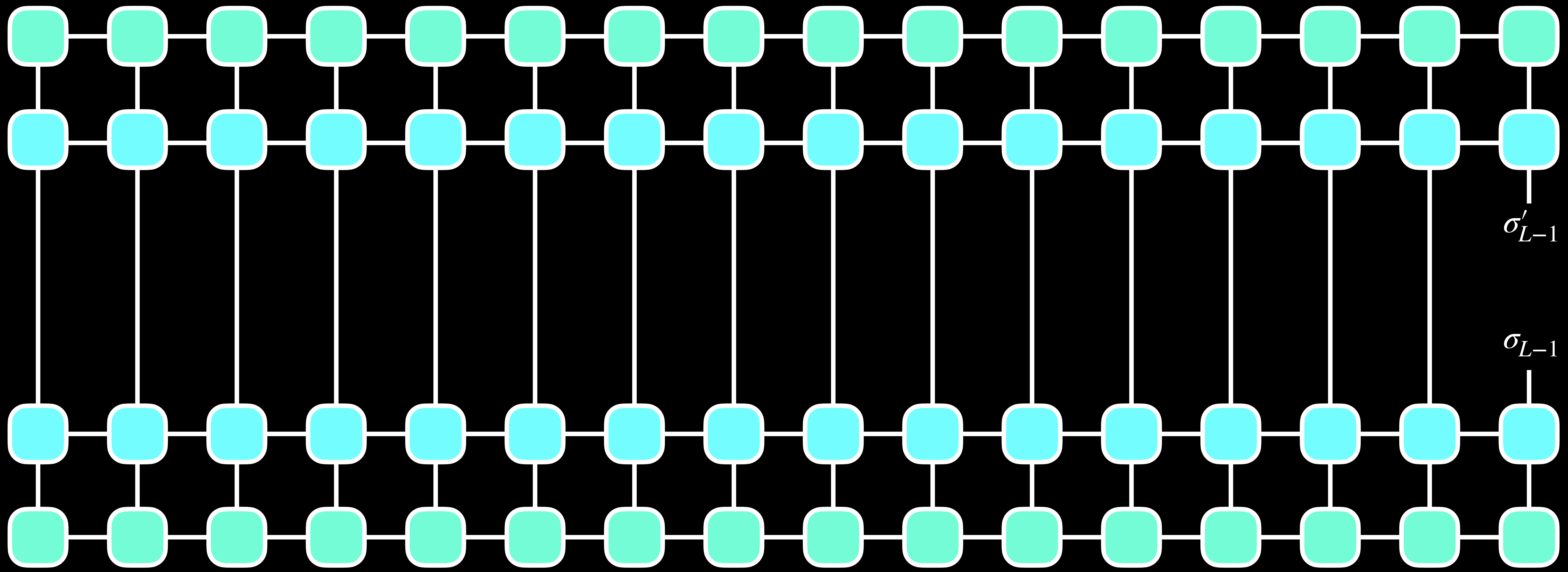
$\rho_{L-1} =$



Apply MPO to MPS

Reduced density matrix for the right-edge site

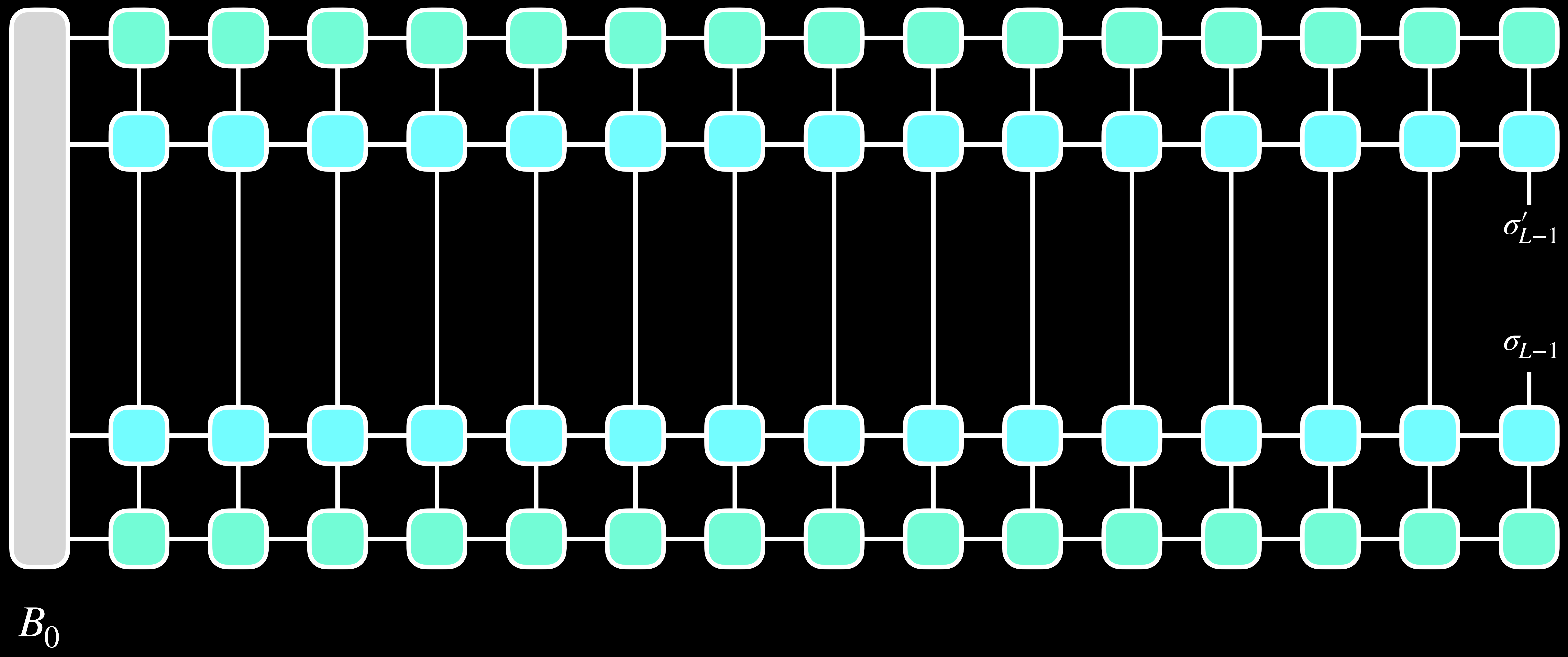
$$\rho_{L-1} =$$



Apply MPO to MPS

Reduced density matrix for the right-edge site

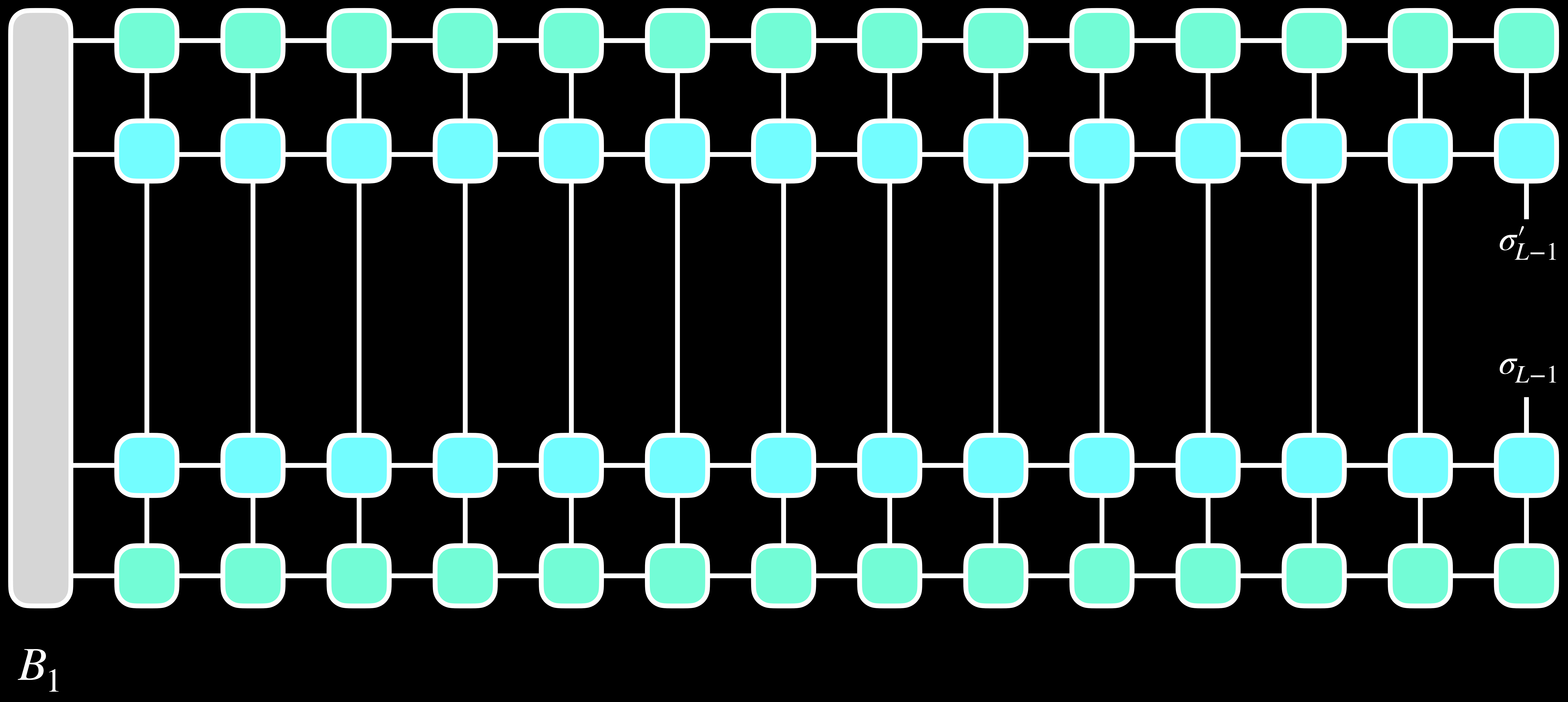
$\rho_{L-1} =$



Apply MPO to MPS

Reduced density matrix for the right-edge site

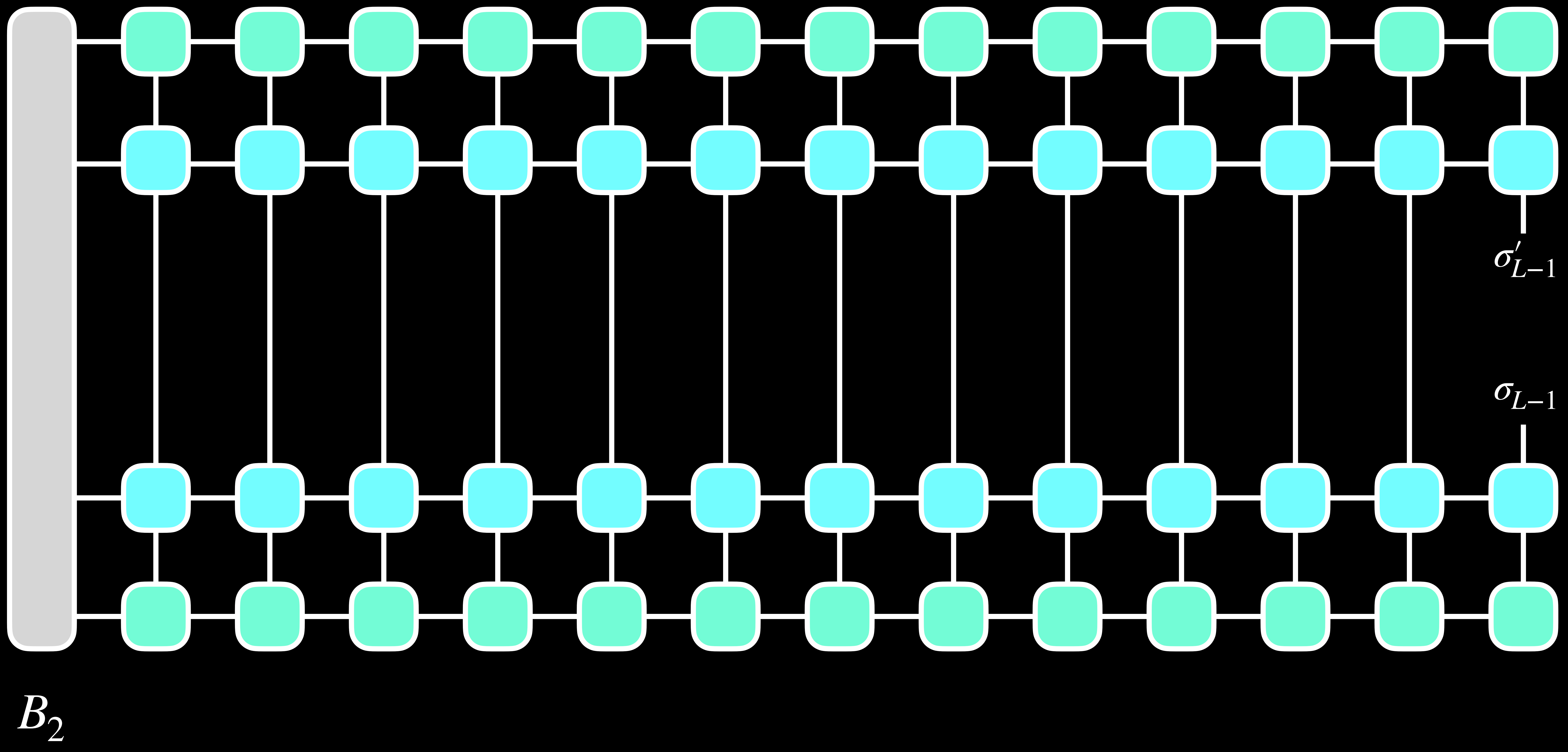
$\rho_{L-1} =$



Apply MPO to MPS

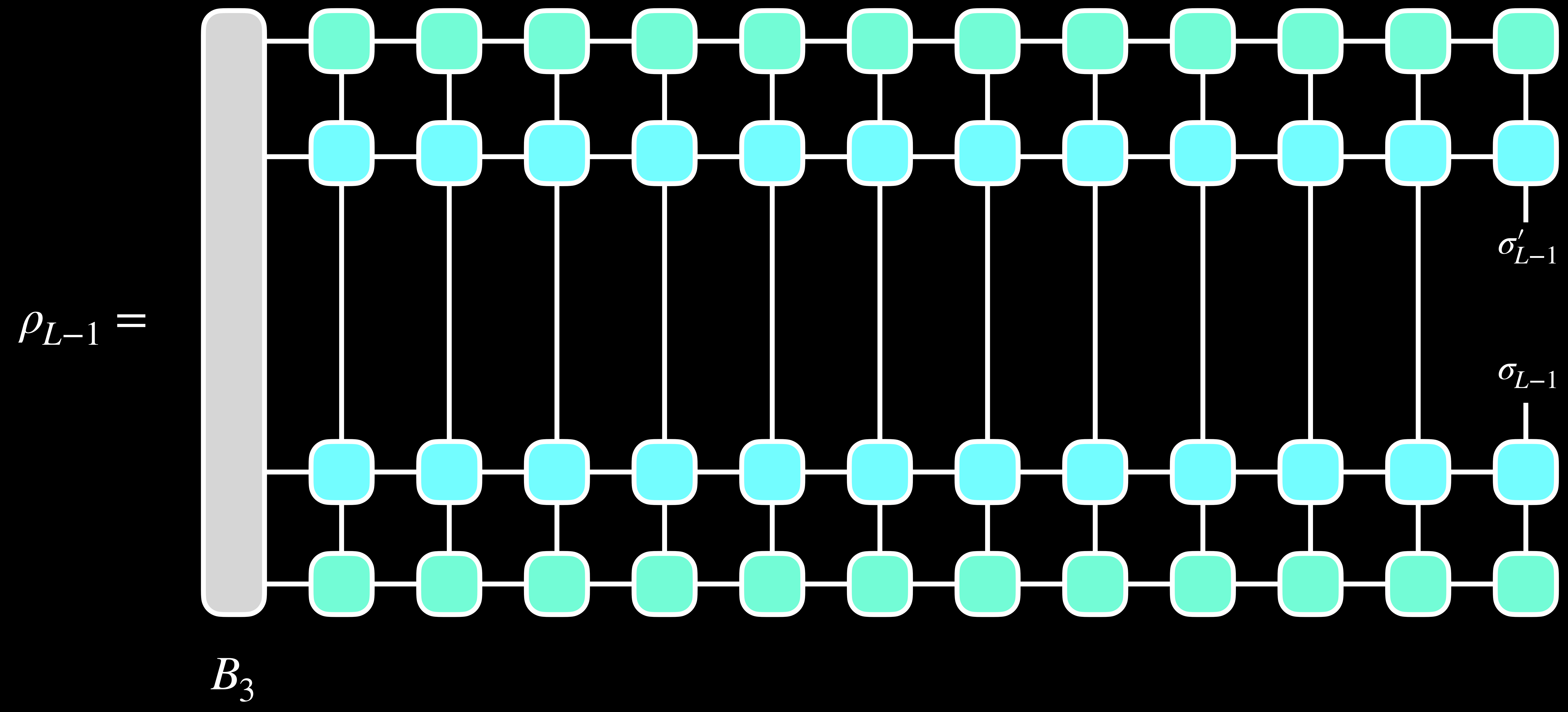
Reduced density matrix for the right-edge site

$\rho_{L-1} =$



Apply MPO to MPS

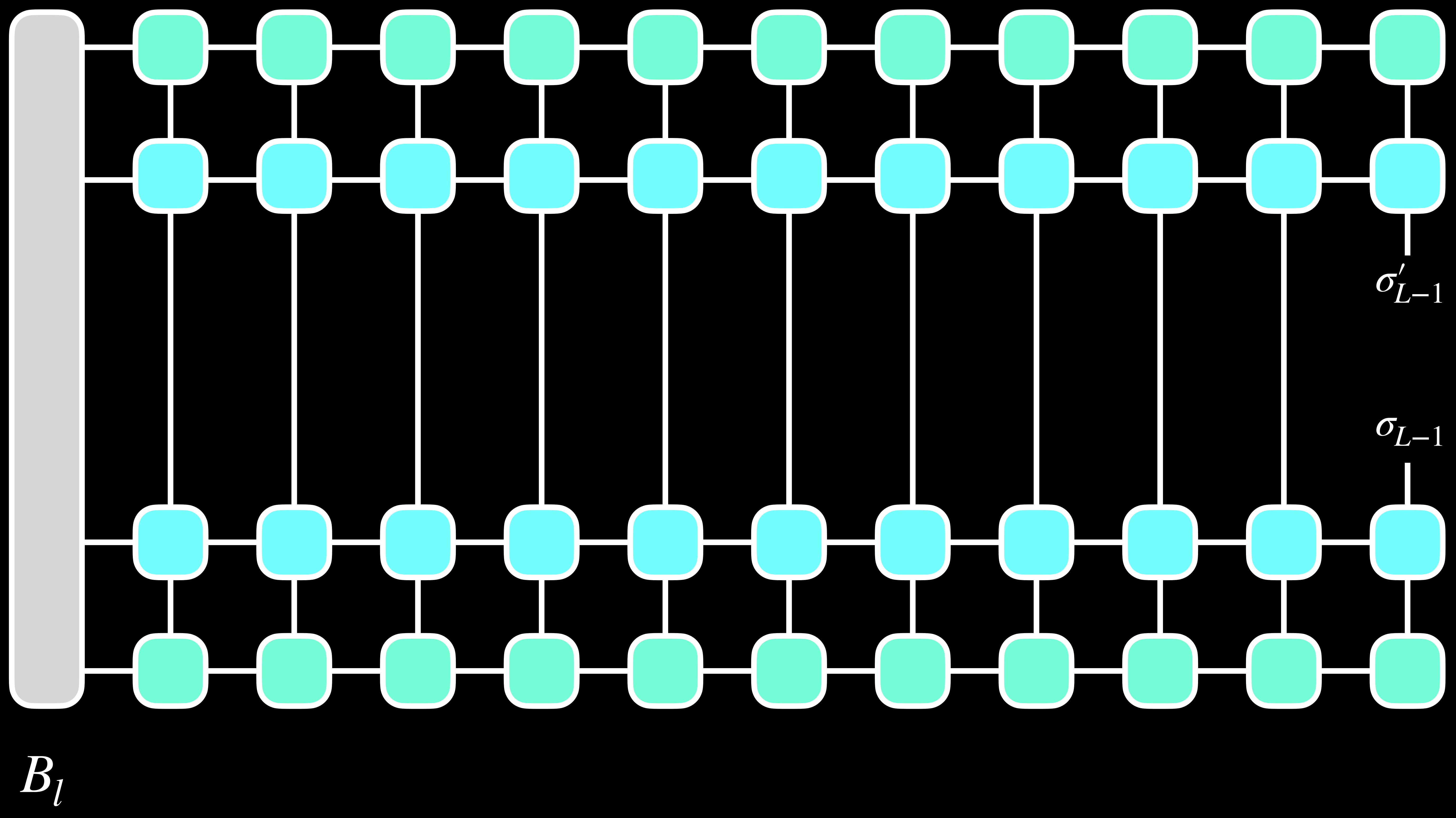
Reduced density matrix for the right-edge site



Apply MPO to MPS

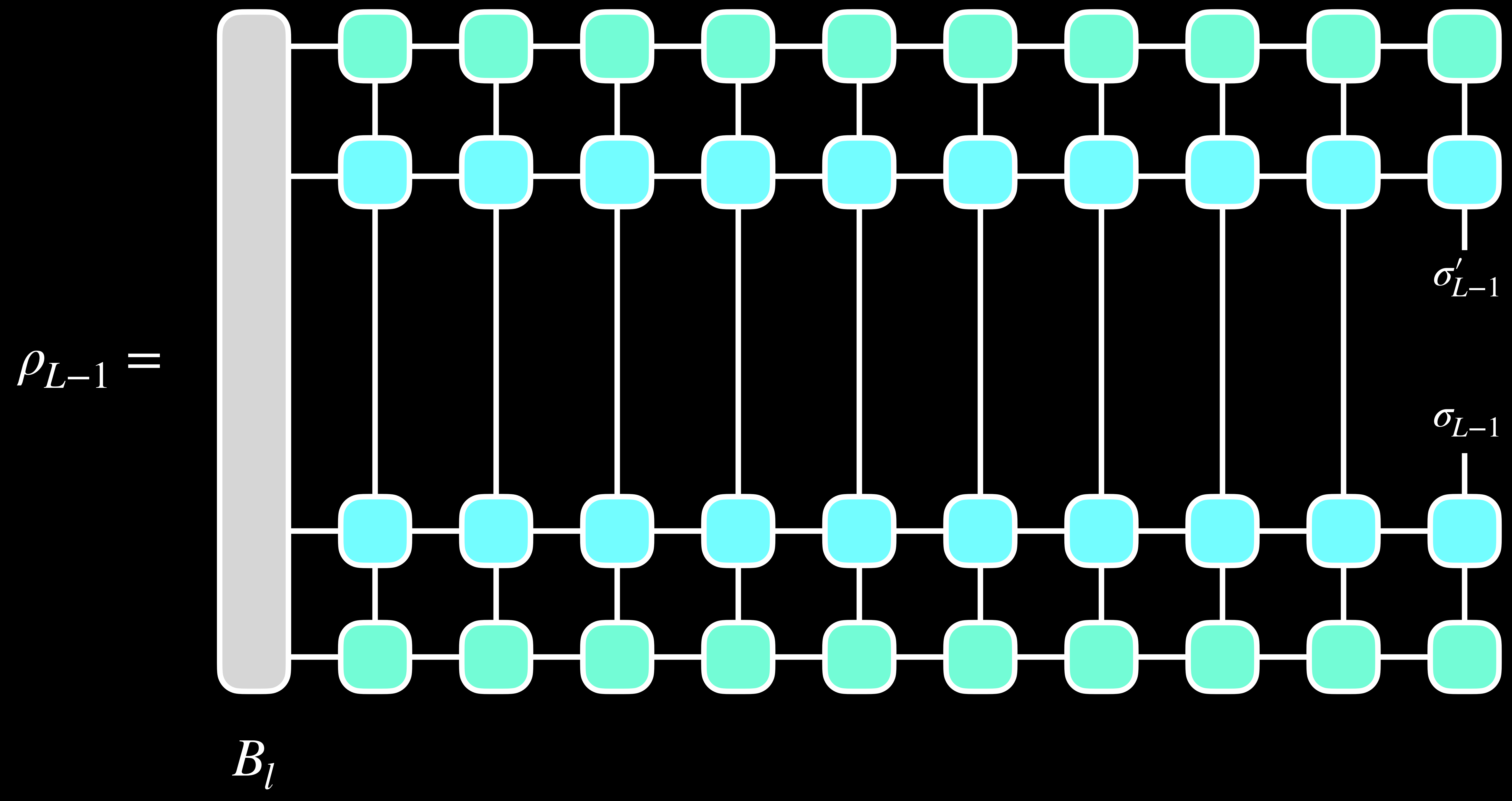
Reduced density matrix for the right-edge site

$\rho_{L-1} =$



Apply MPO to MPS

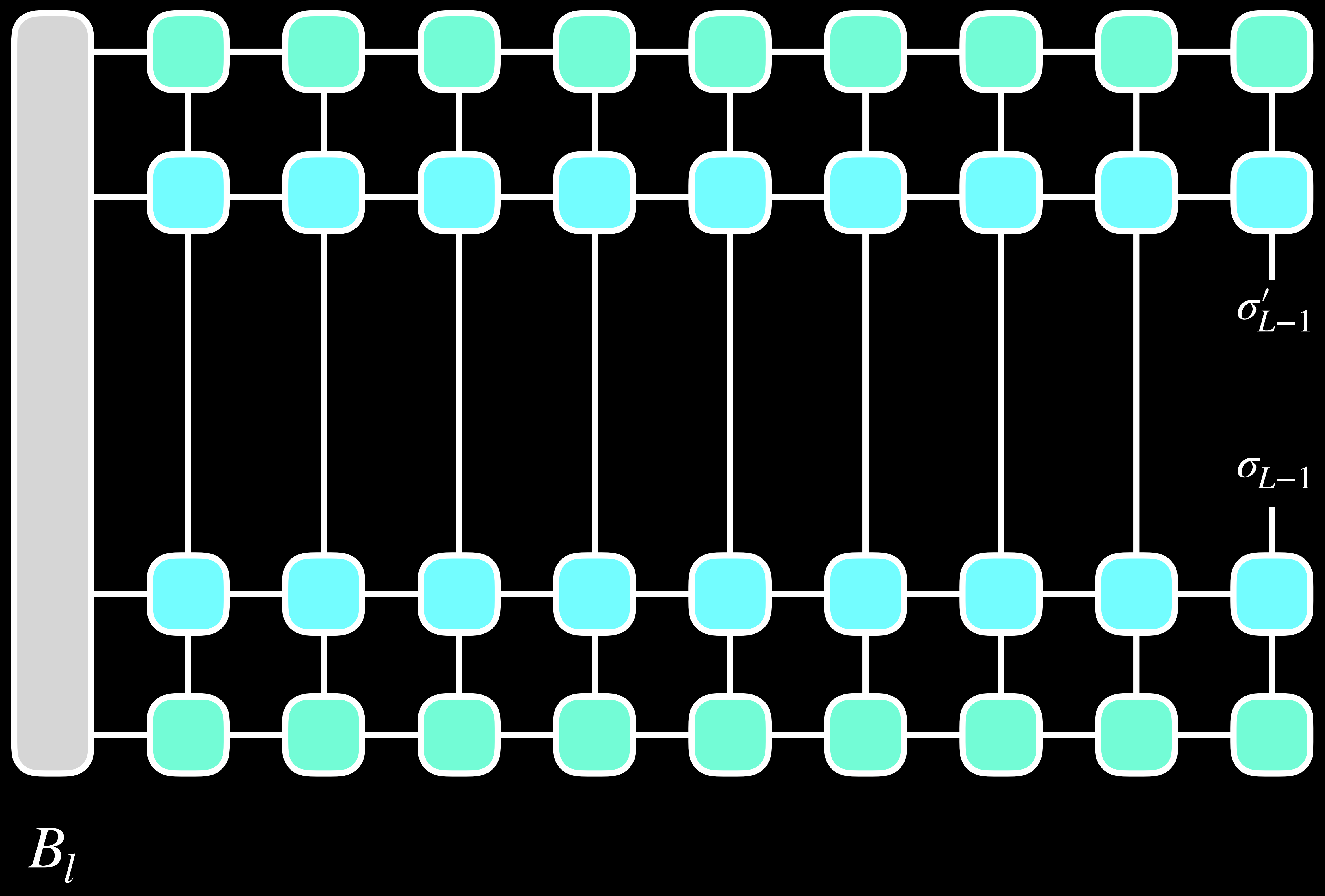
Reduced density matrix for the right-edge site



Apply MPO to MPS

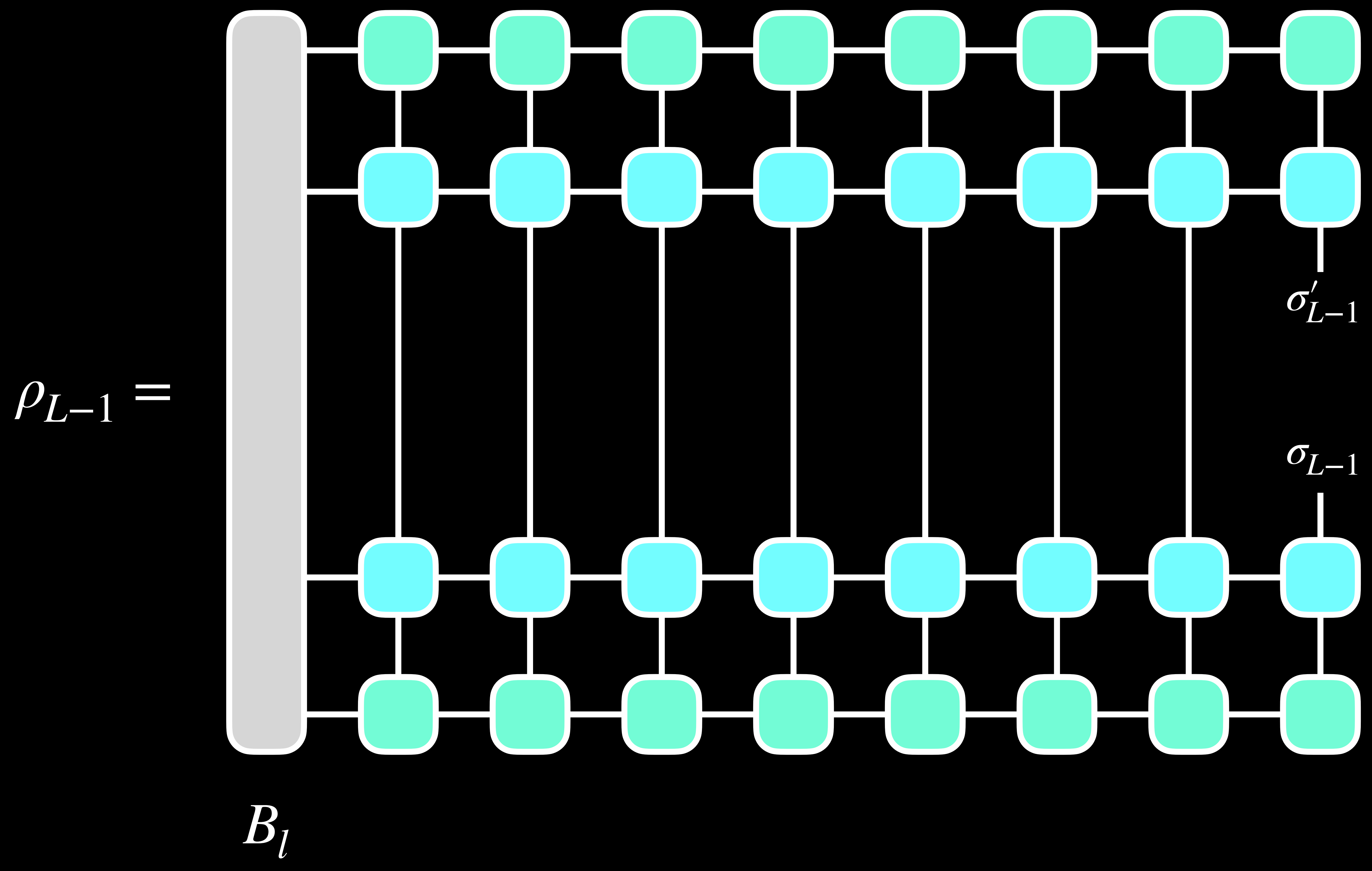
Reduced density matrix for the right-edge site

$\rho_{L-1} =$



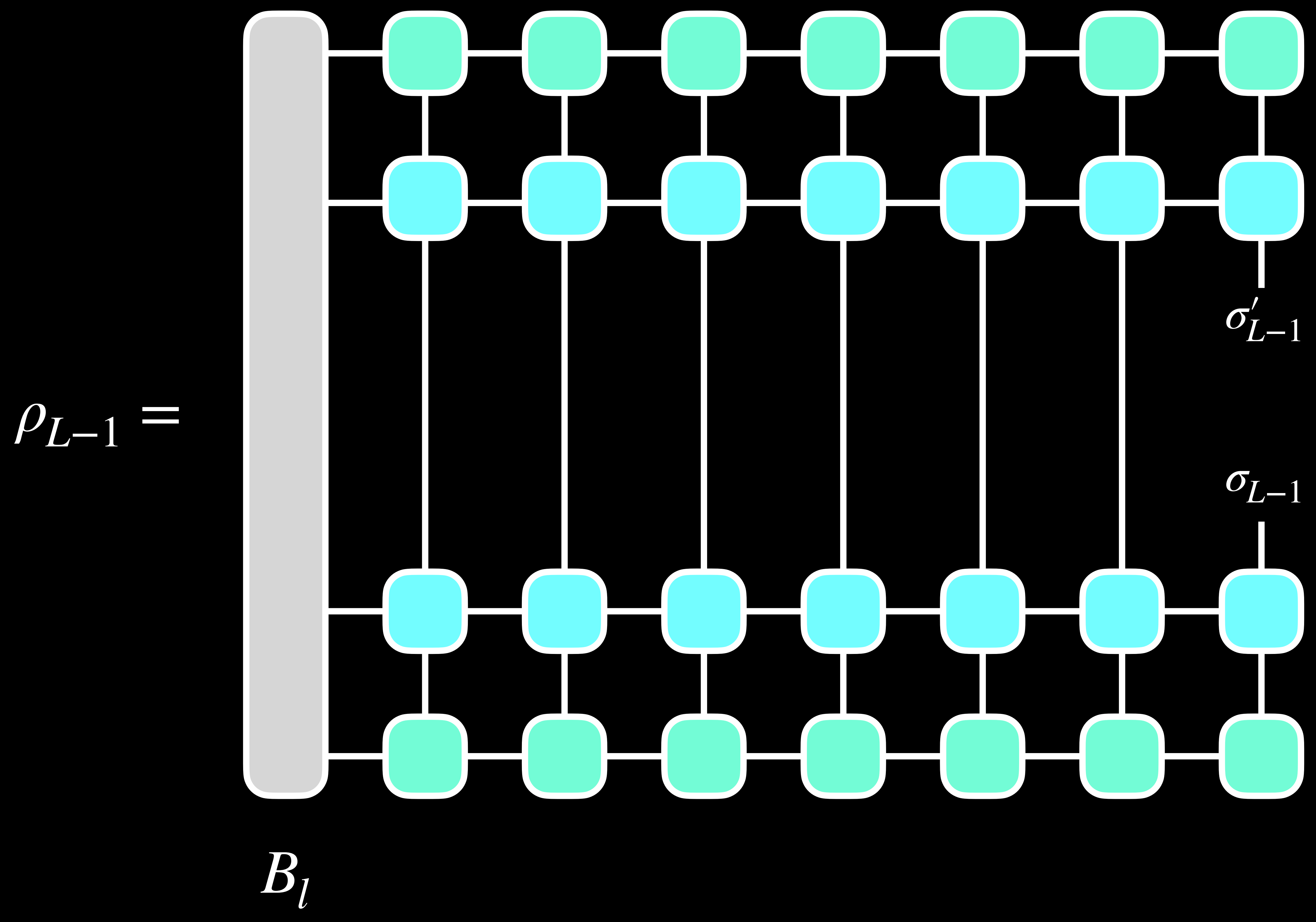
Apply MPO to MPS

Reduced density matrix for the right-edge site



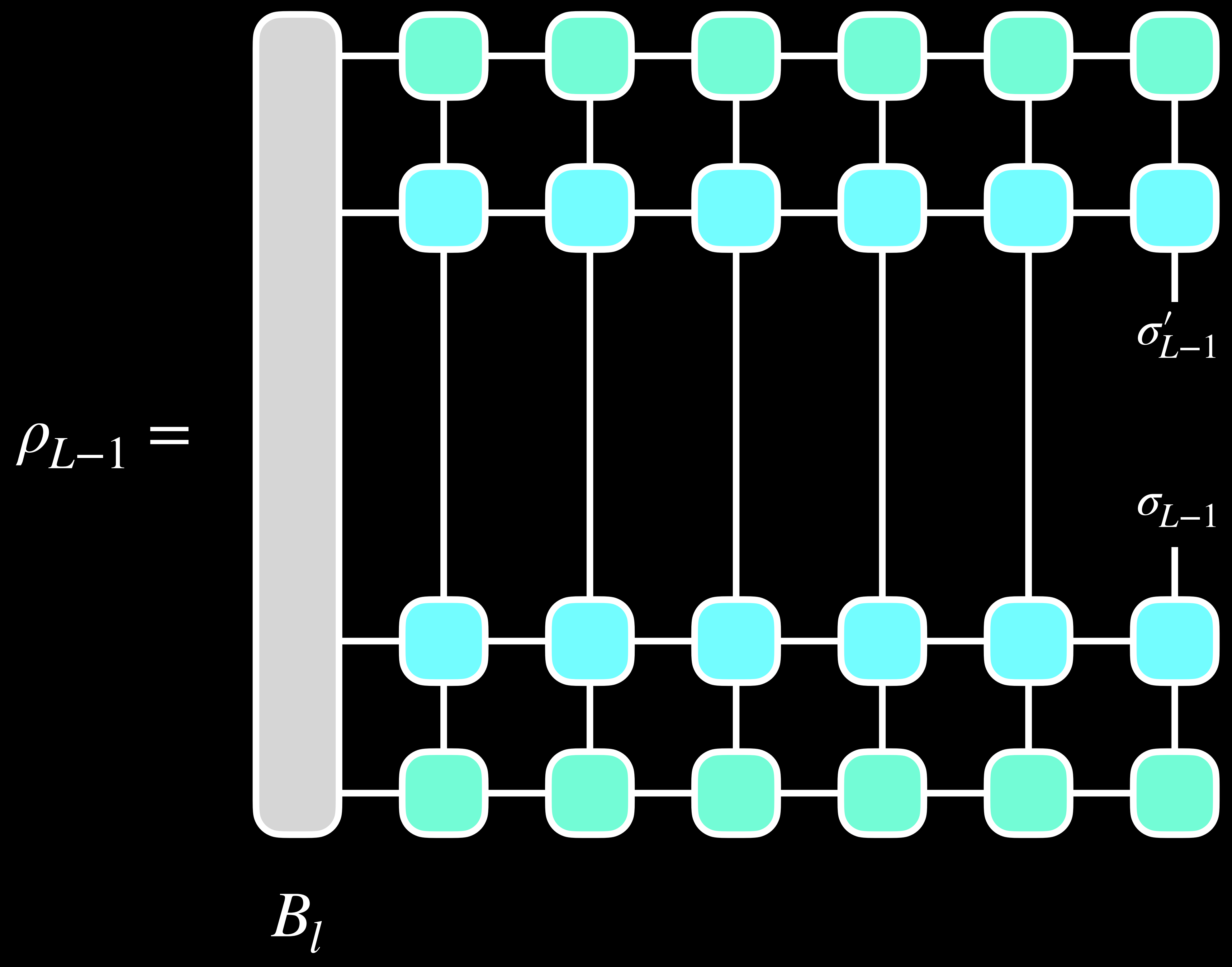
Apply MPO to MPS

Reduced density matrix for the right-edge site



Apply MPO to MPS

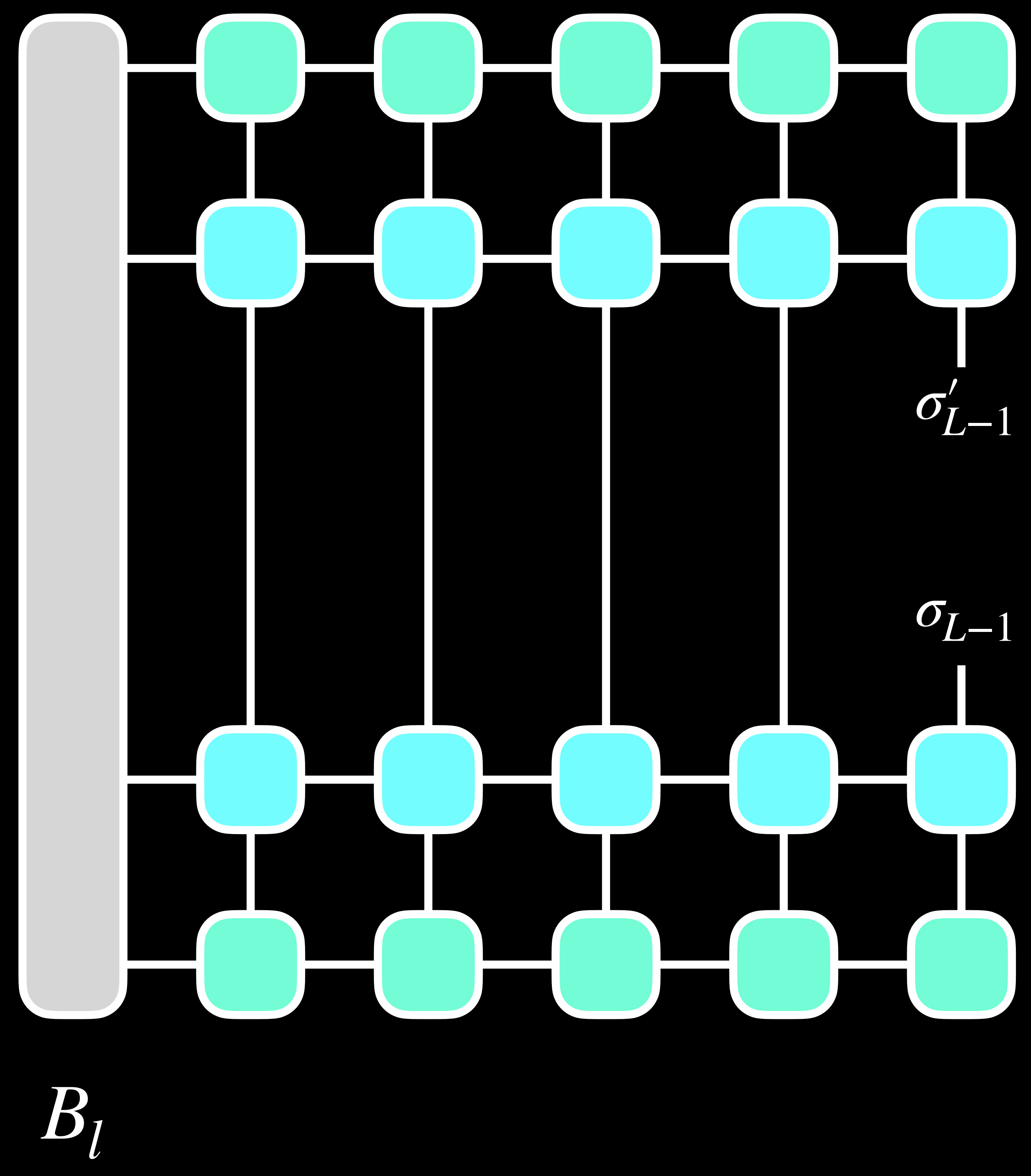
Reduced density matrix for the right-edge site



Apply MPO to MPS

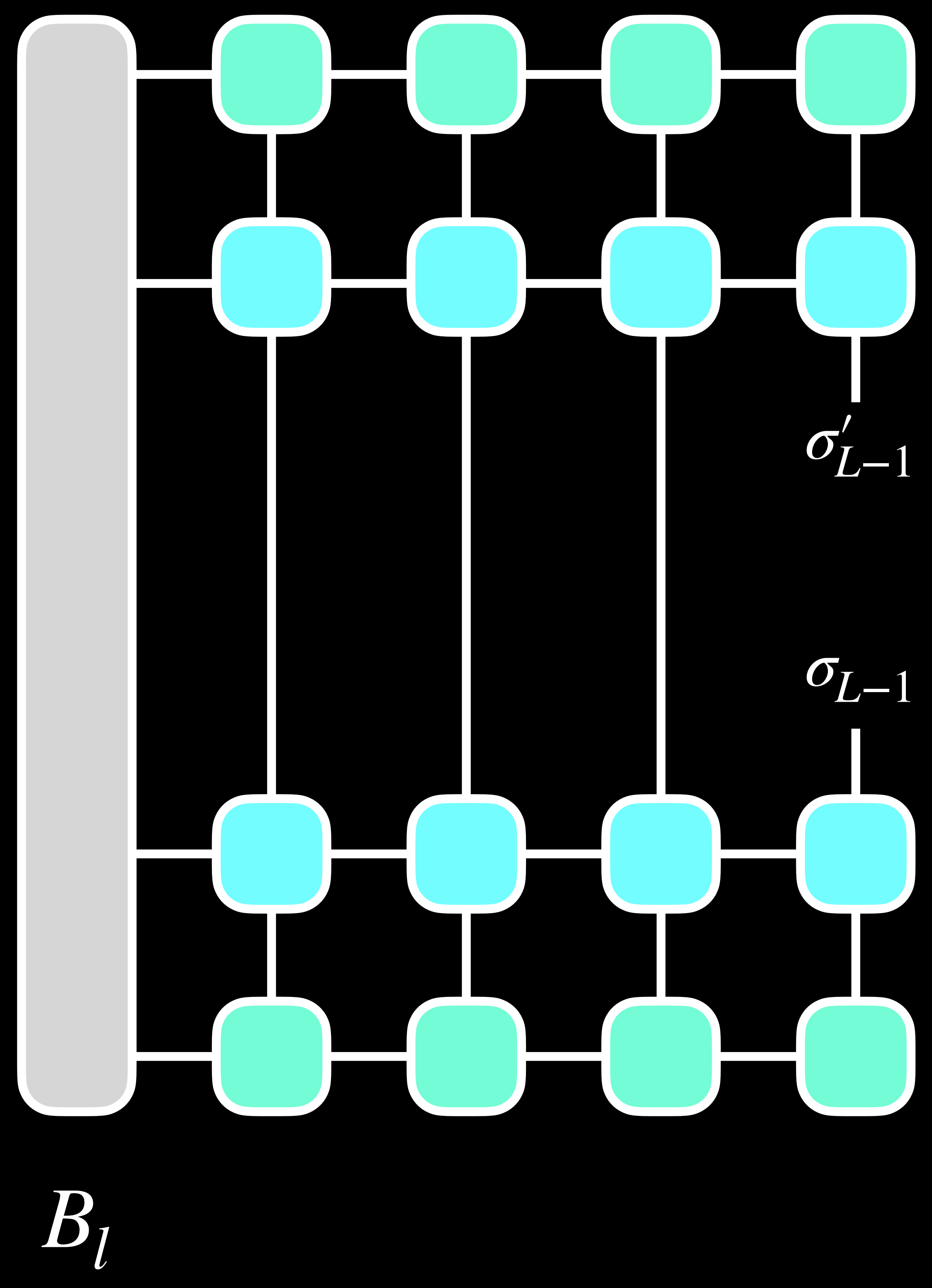
Reduced density matrix for the right-edge site

$\rho_{L-1} =$



Apply MPO to MPS

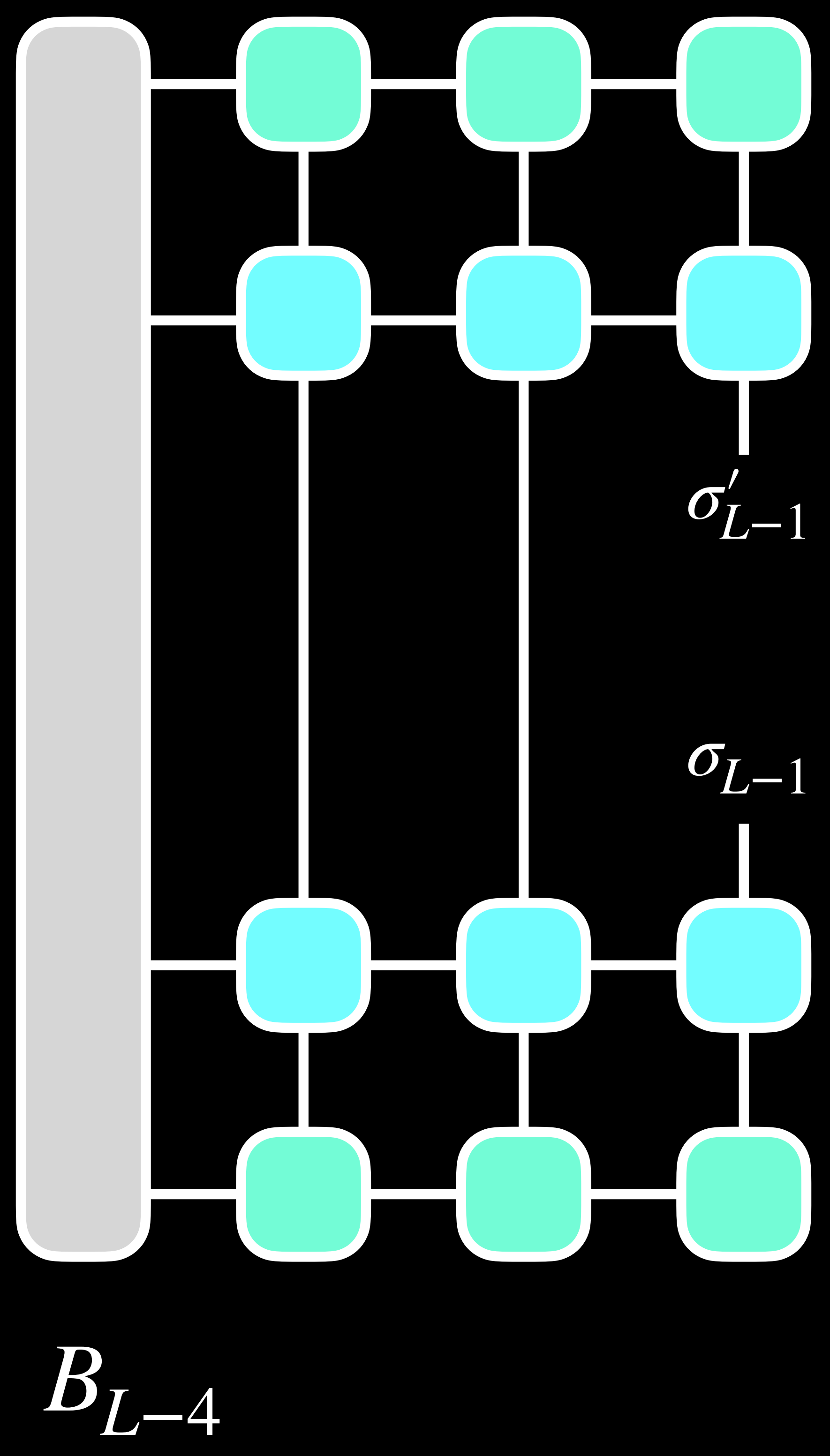
Reduced density matrix for the right-edge site

$\rho_{L-1} =$ 

Apply MPO to MPS

Reduced density matrix for the right-edge site

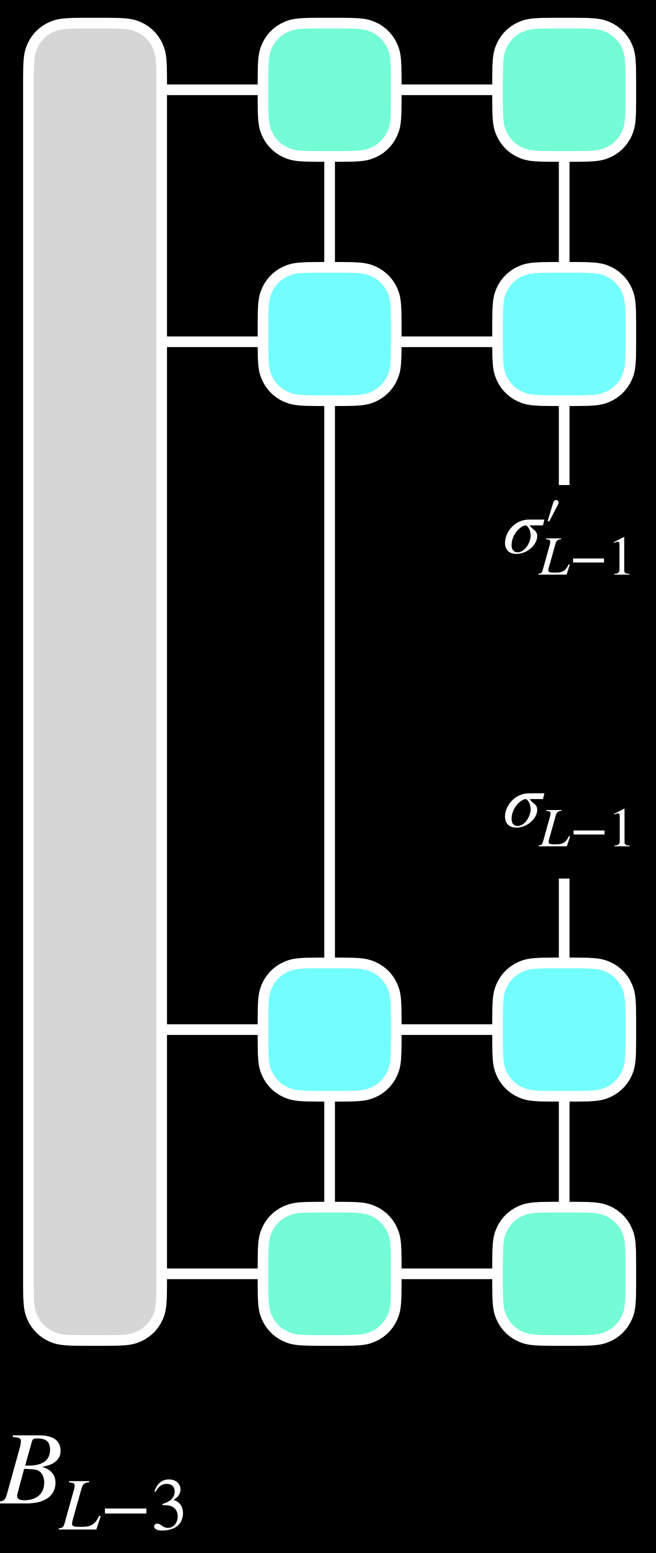
$$\rho_{L-1} =$$



Apply MPO to MPS

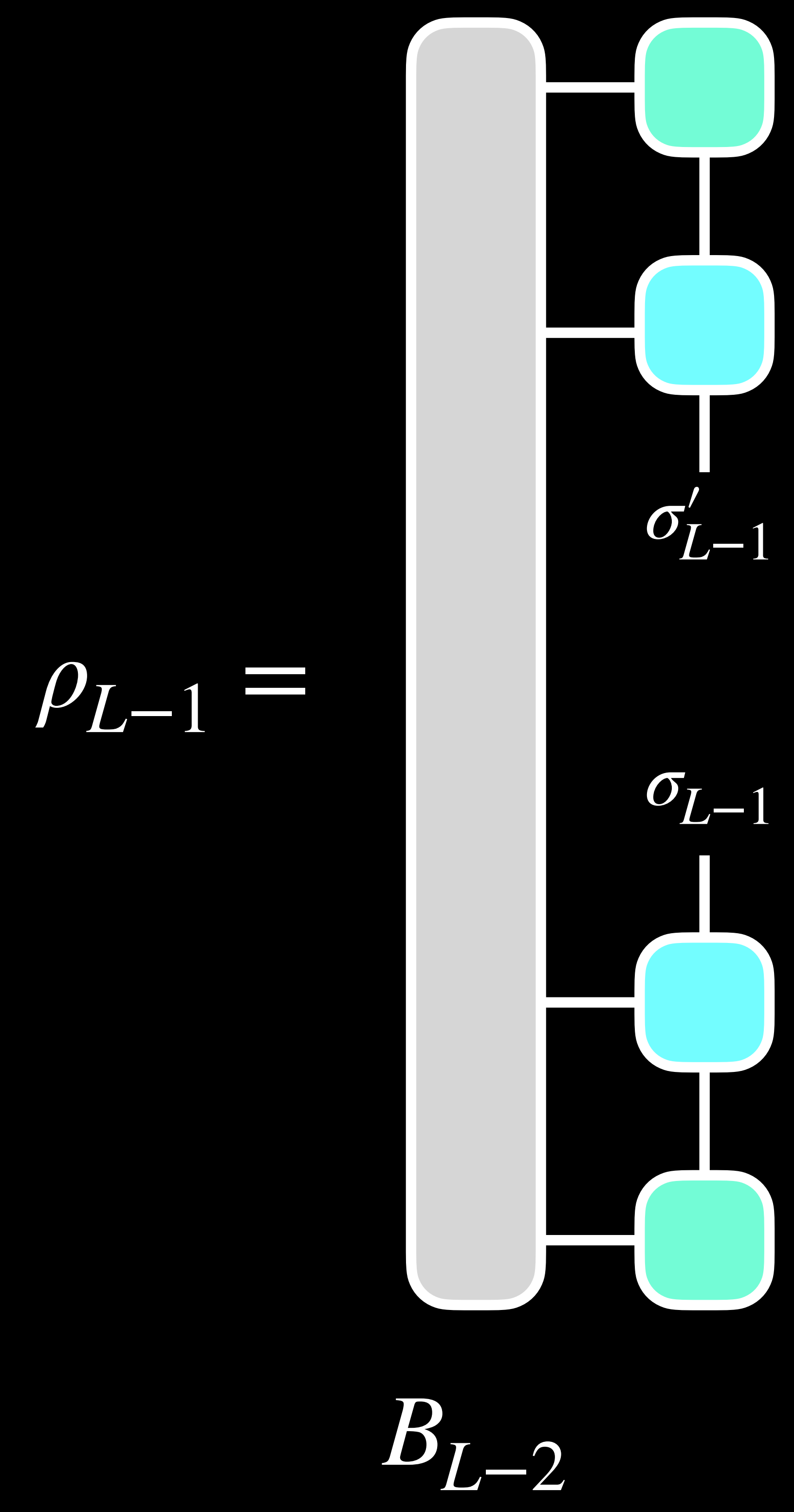
Reduced density matrix for the right-edge site

$$\rho_{L-1} =$$



Apply MPO to MPS

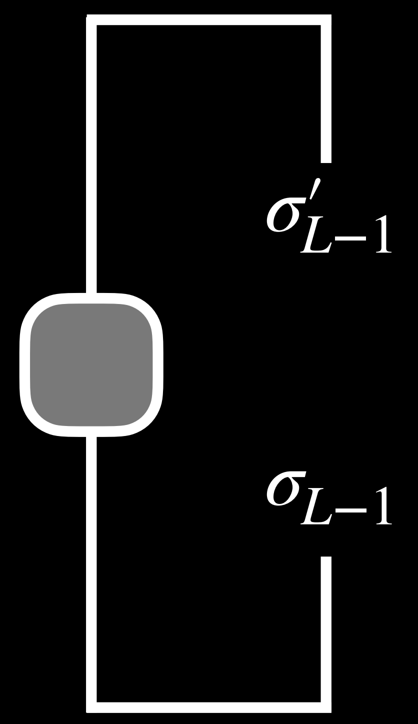
Reduced density matrix for the right-edge site



Apply MPO to MPS

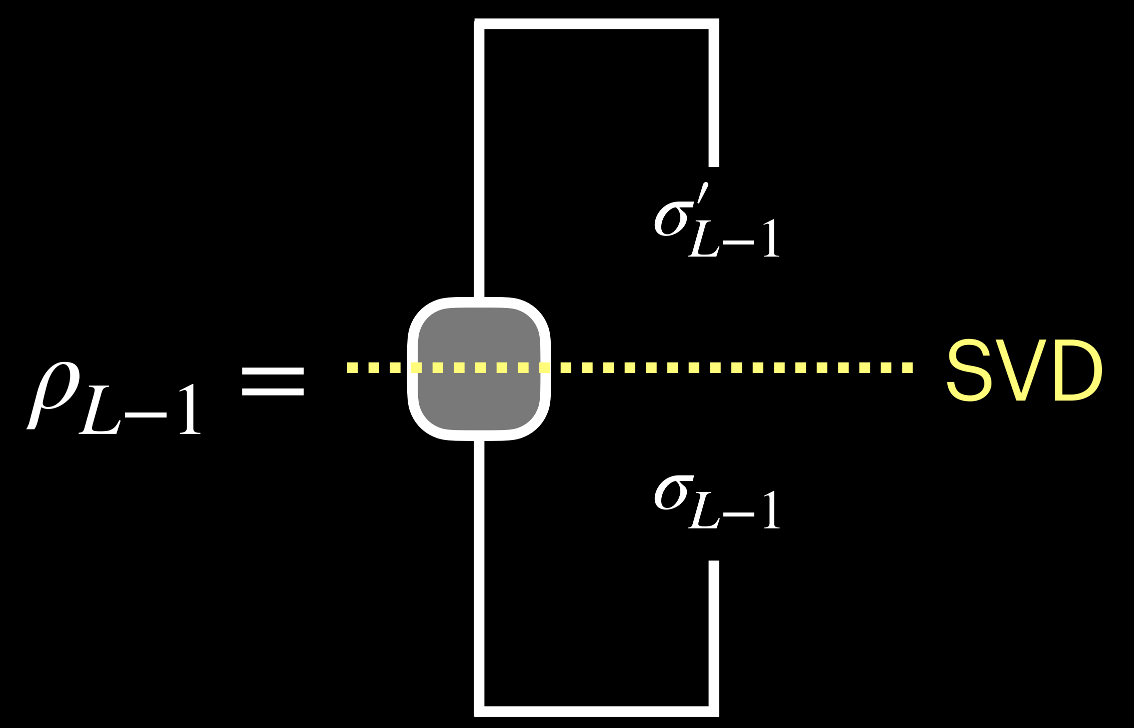
Reduced density matrix for the right-edge site

$\rho_{L-1} =$



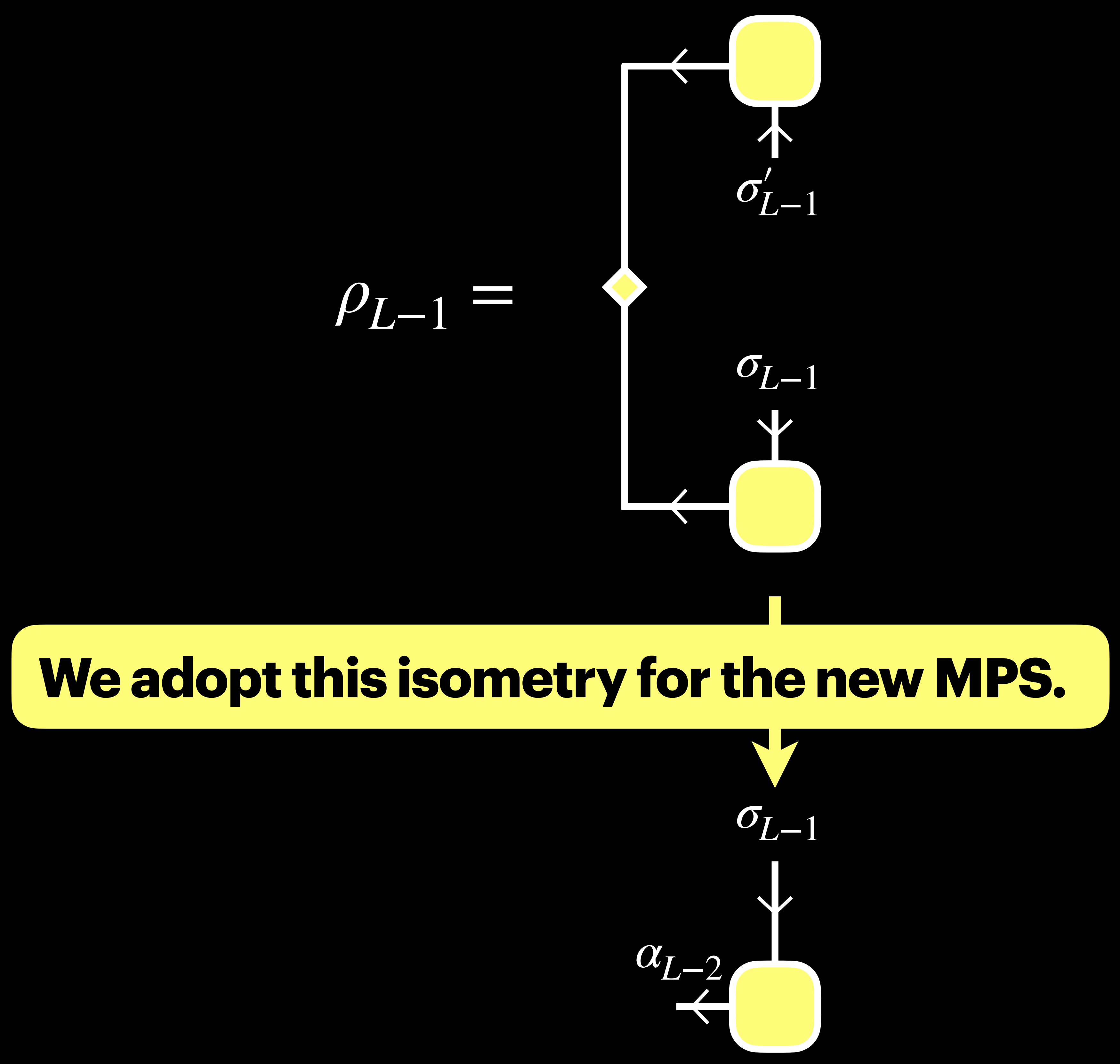
Apply MPO to MPS

Reduced density matrix for the right-edge site



Apply MPO to MPS

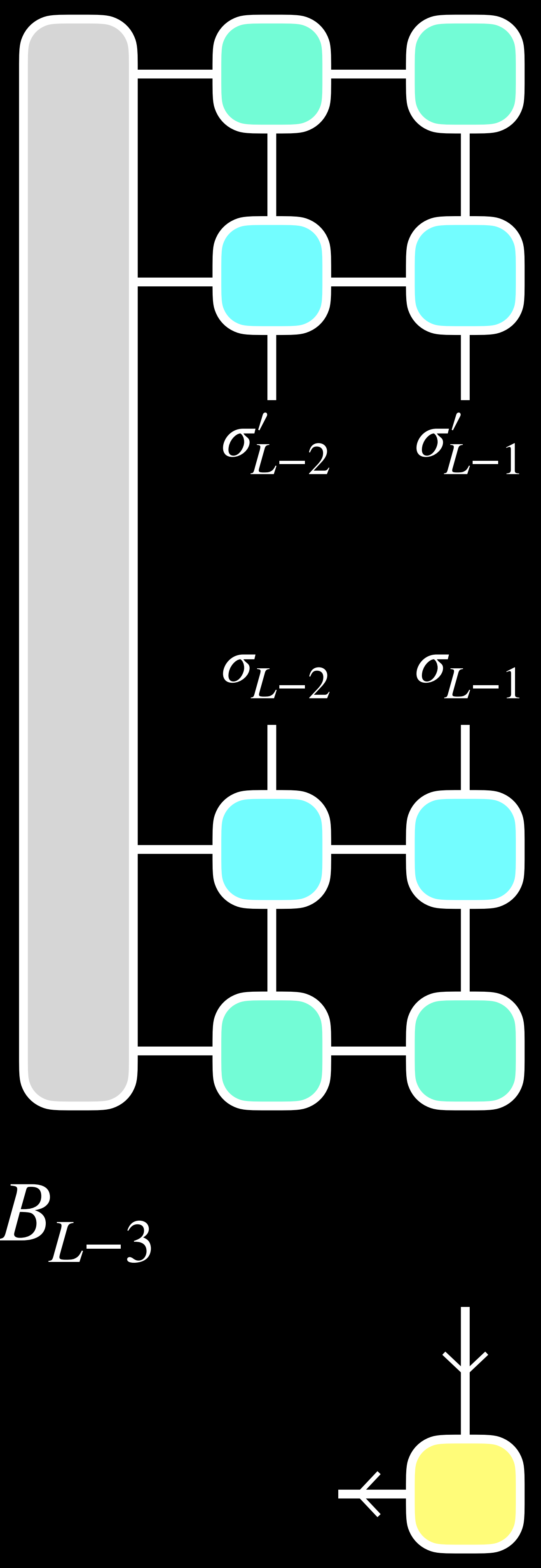
Reduced density matrix for the right-edge site



Apply MPO to MPS

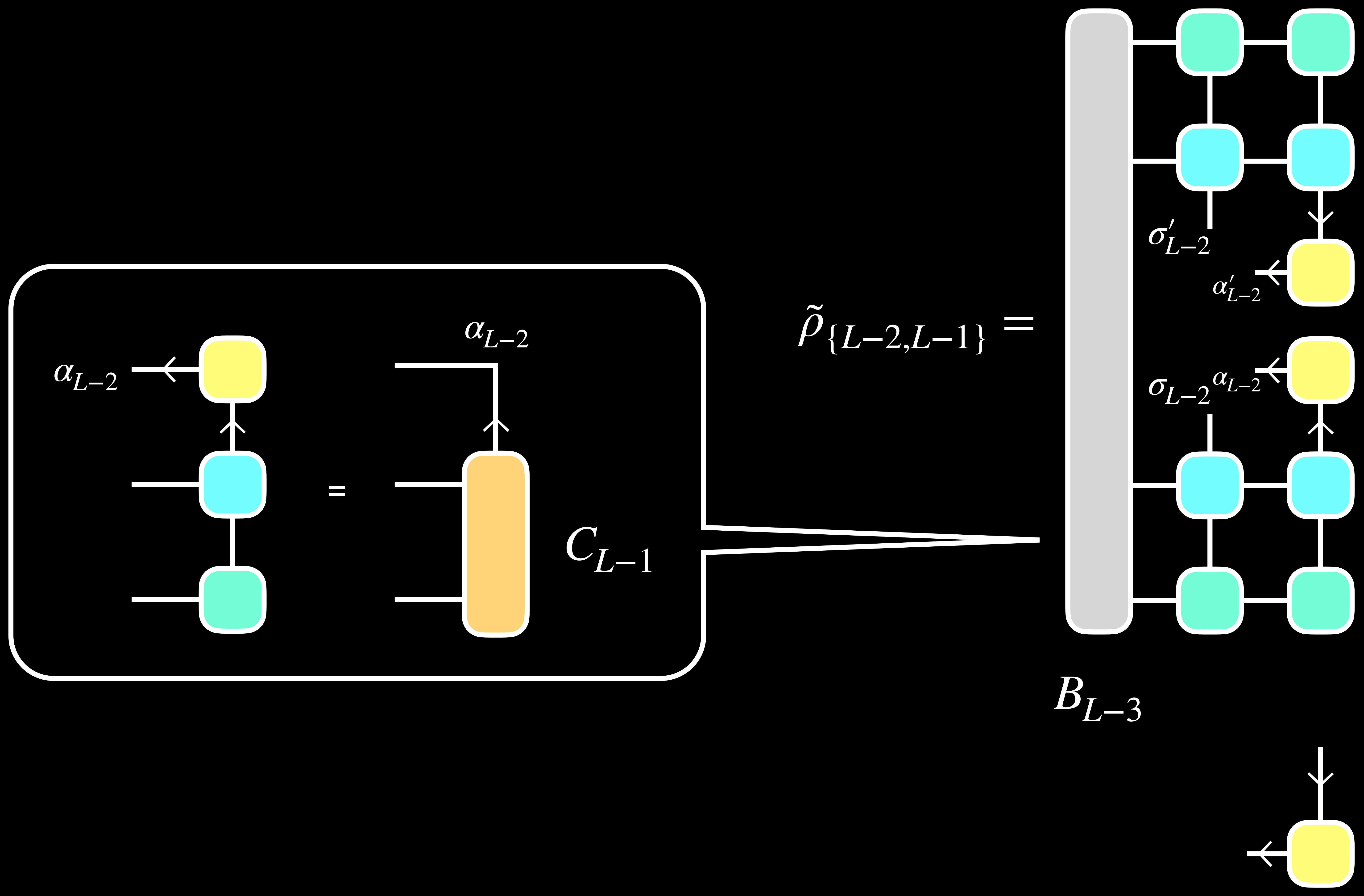
Reduced density matrix for the $\{L-2, L-1\}$ sites

$$\rho_{\{L-2,L-1\}} =$$



Apply MPO to MPS

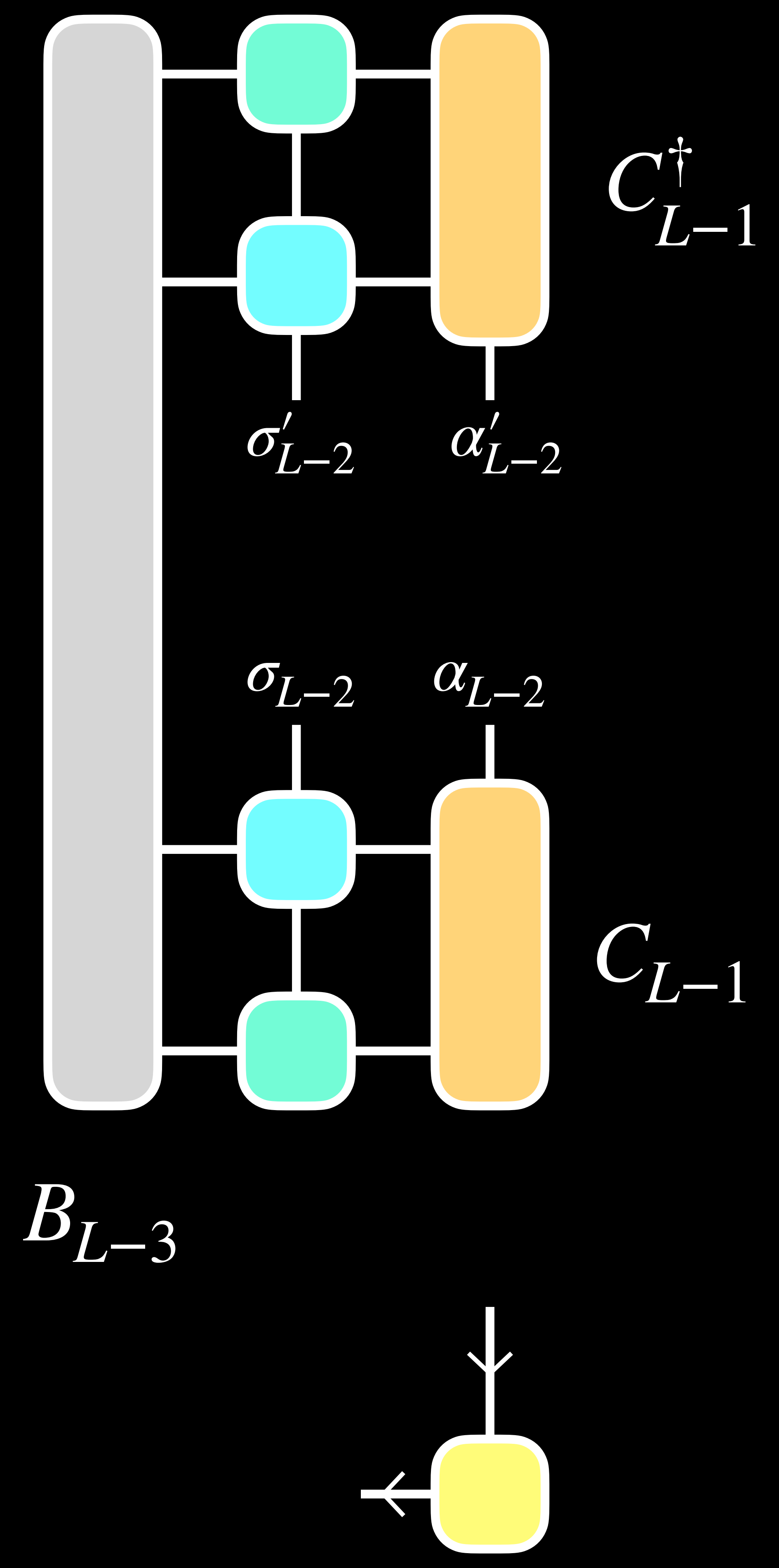
Approximated reduced density matrix for the $\{L-2, L-1\}$ sites



Apply MPO to MPS

Approximated reduced density matrix for the $\{L-2, L-1\}$ sites

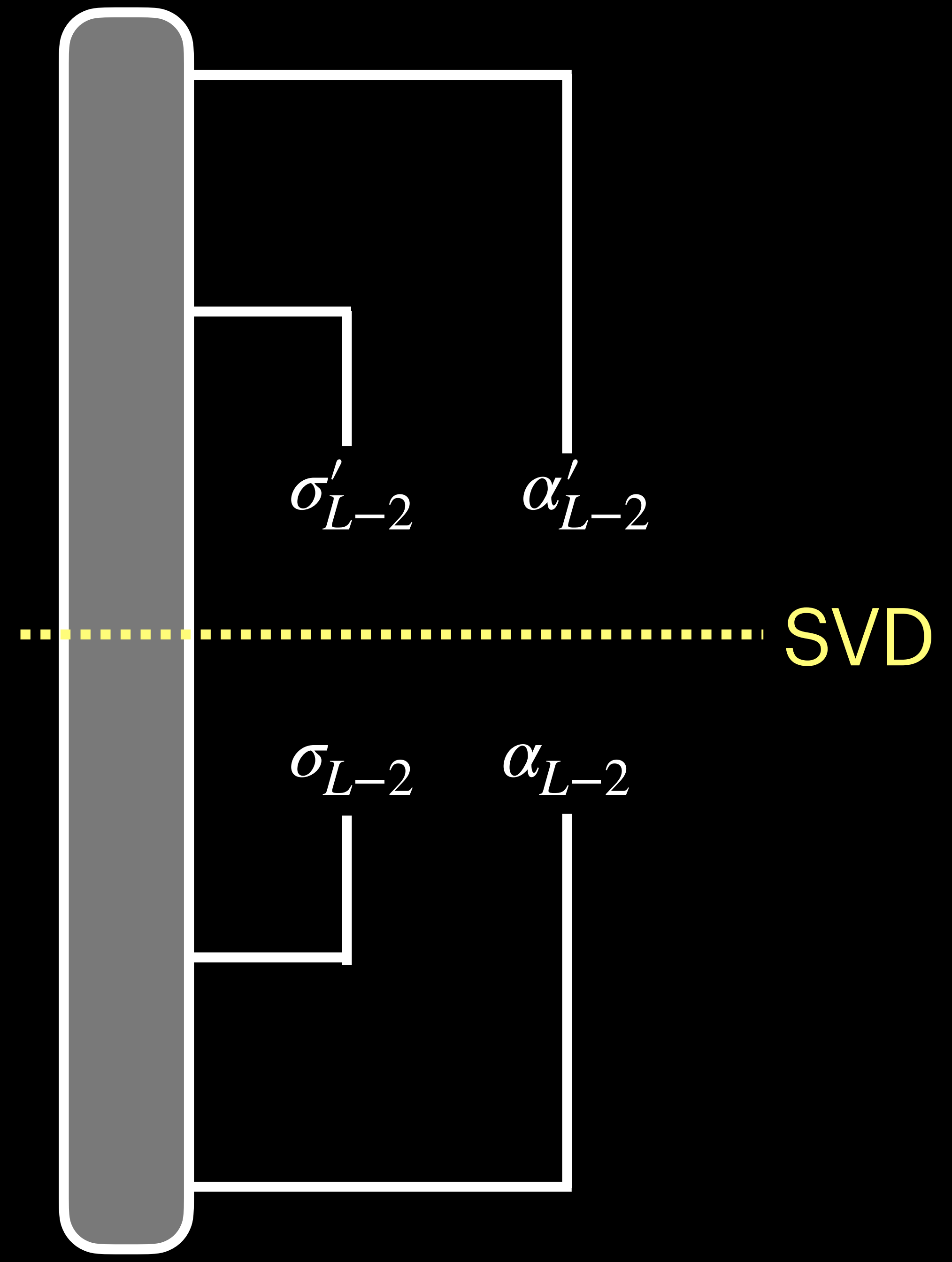
$\tilde{\rho}_{\{L-2,L-1\}} =$

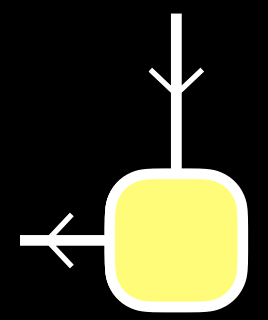


Apply MPO to MPS

Approximated reduced density matrix for the $\{L-2, L-1\}$ sites

$\tilde{\rho}_{\{L-2,L-1\}} =$

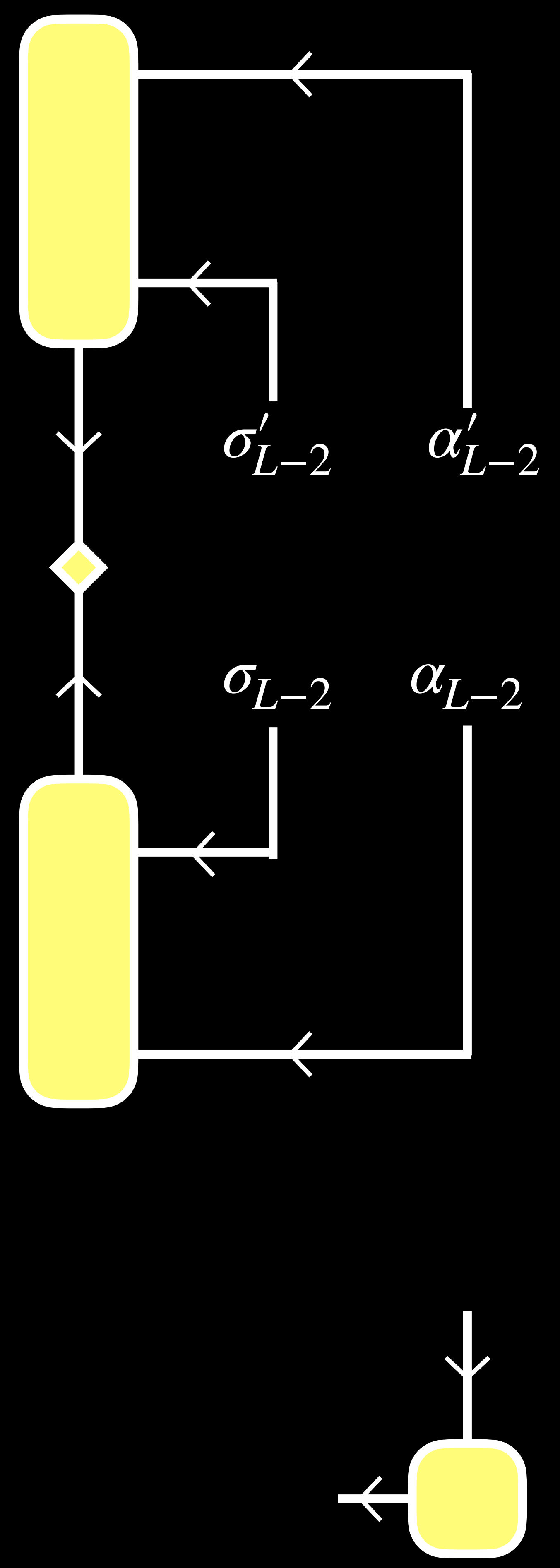




Apply MPO to MPS

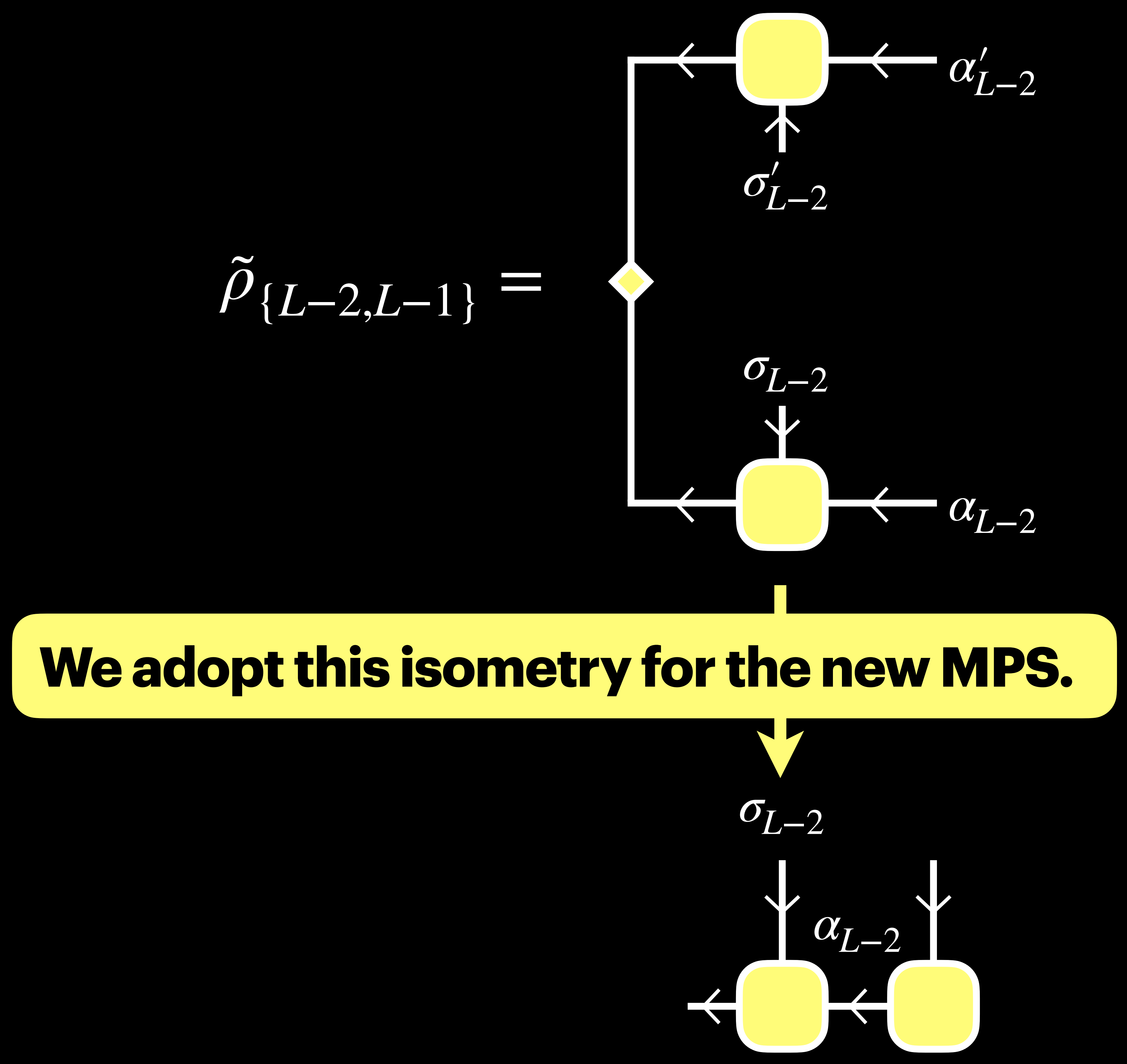
Approximated reduced density matrix for the $\{L-2, L-1\}$ sites

$\tilde{\rho}_{\{L-2,L-1\}} =$



Apply MPO to MPS

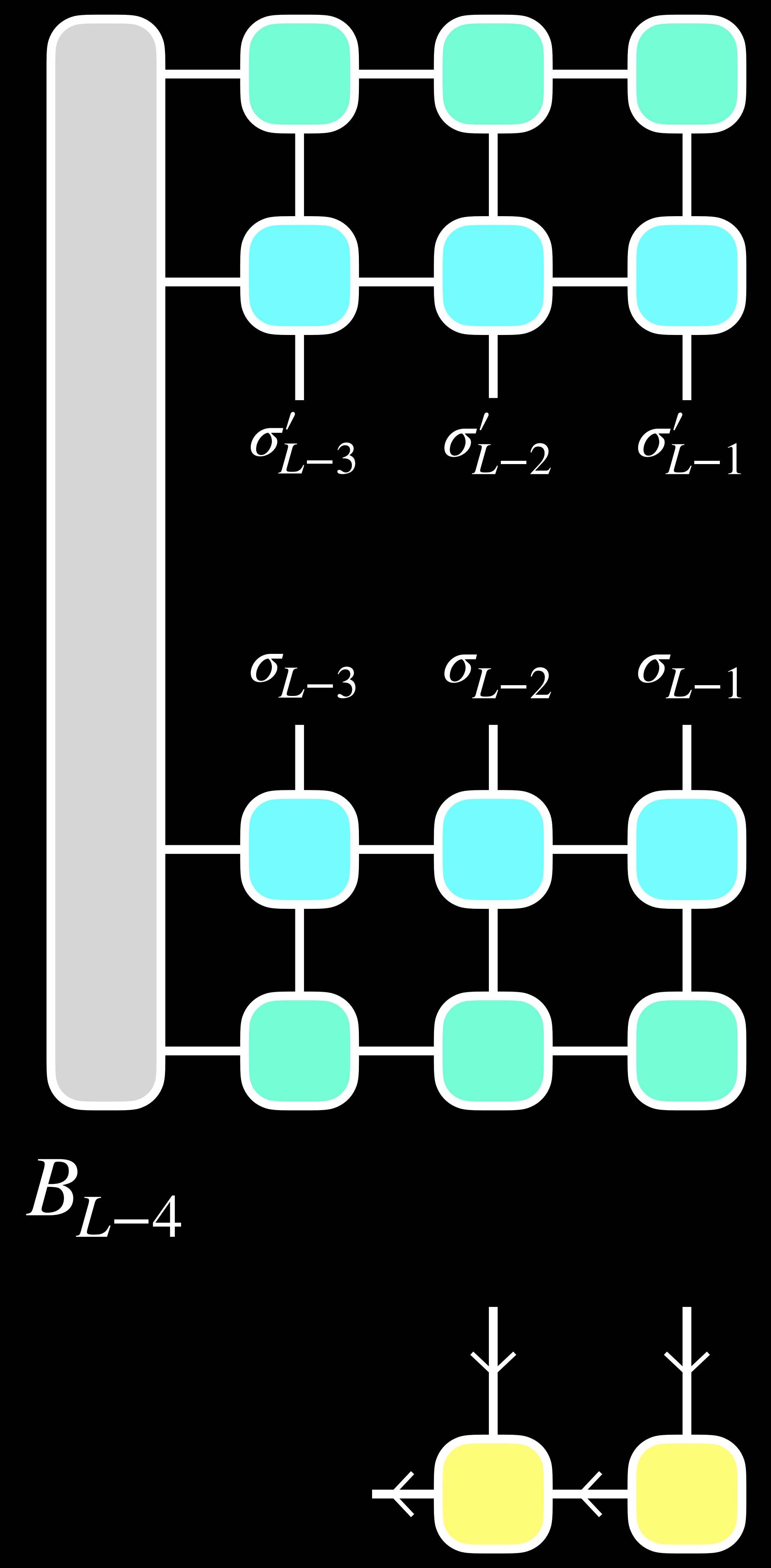
Approximated reduced density matrix for the $\{L-2, L-1\}$ sites



Apply MPO to MPS

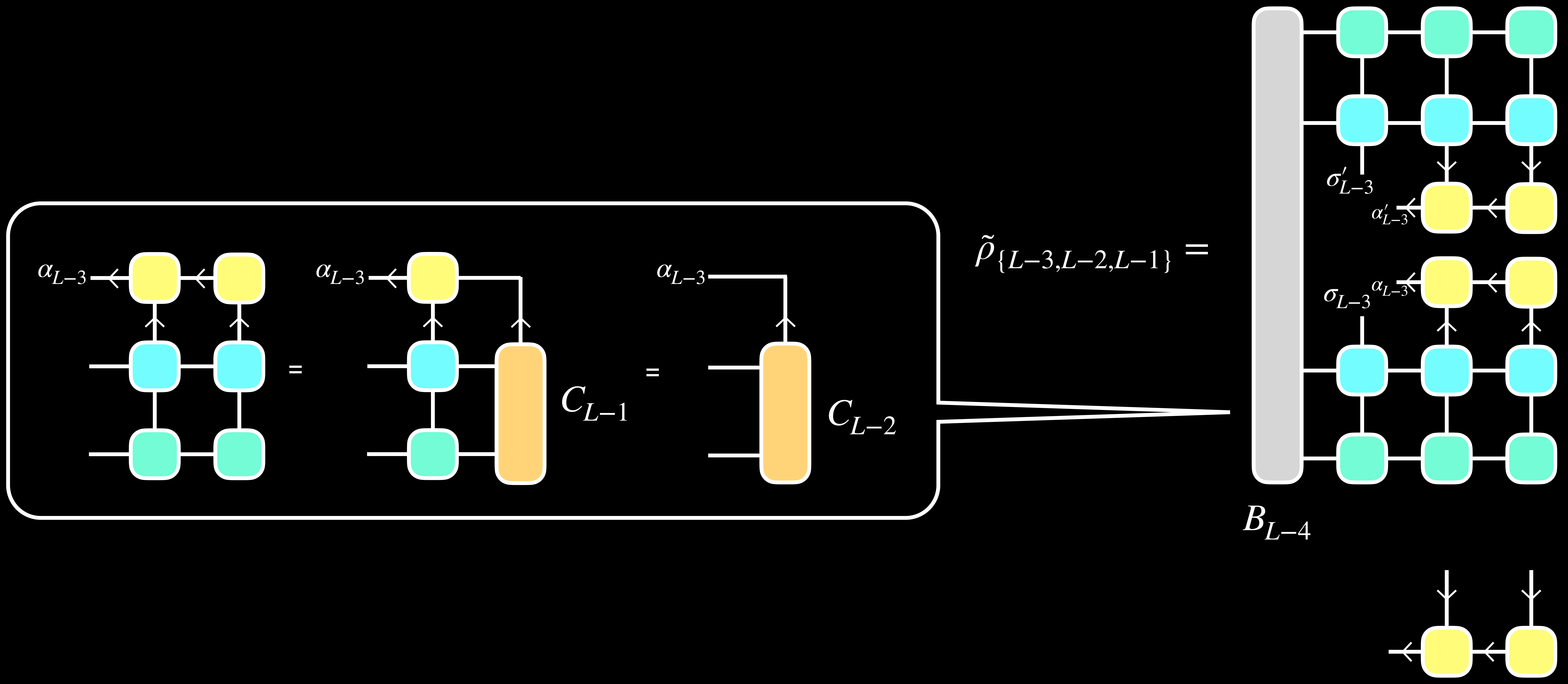
Reduced density matrix for the $\{L-3,\ L-2,\ L-1\}$ sites

$$\rho_{\{L-3,L-2,L-1\}} =$$



Apply MPO to MPS

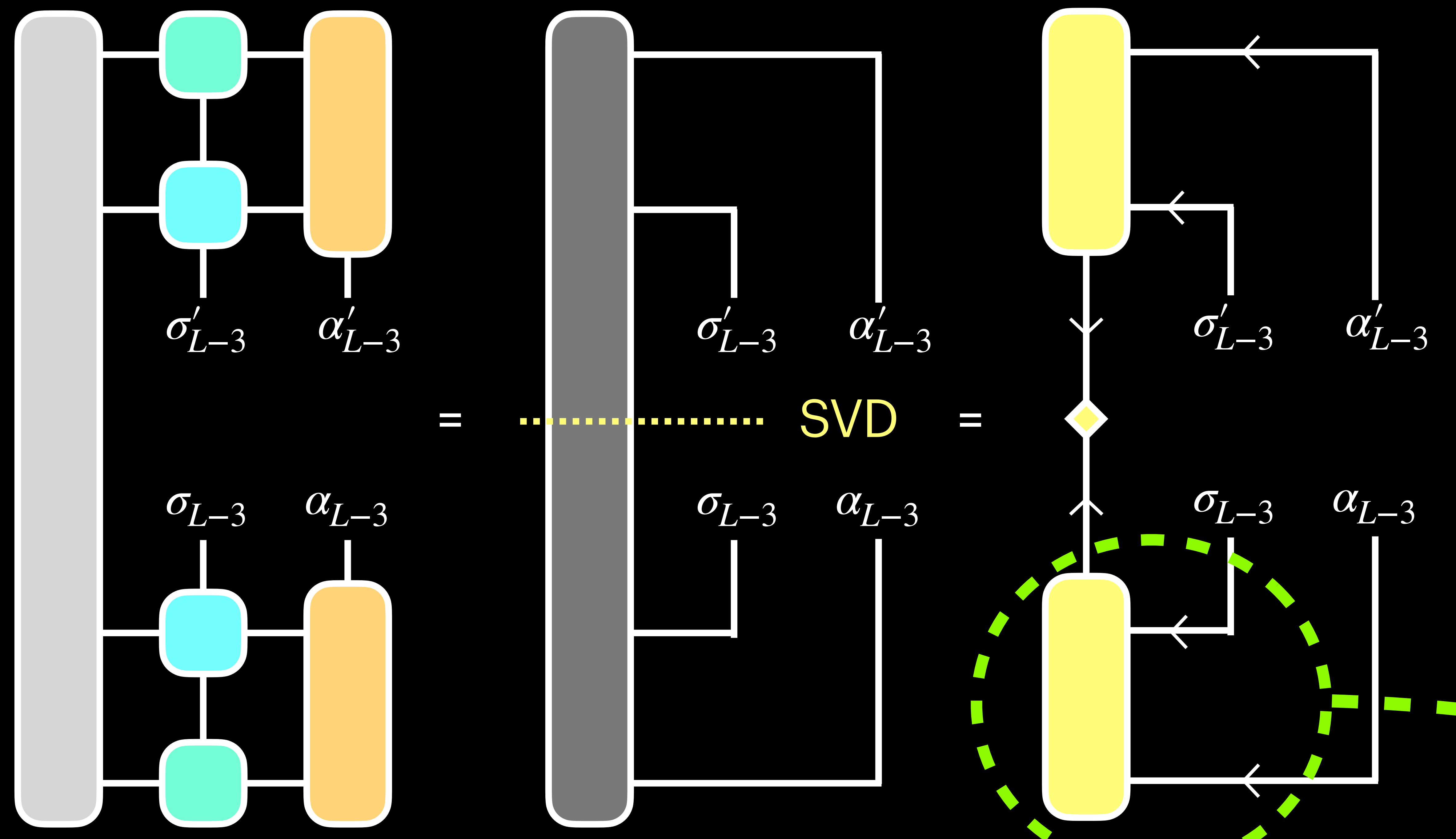
Approximated reduced density matrix for the $\{L-3,\ L-2,\ L-1\}$ sites

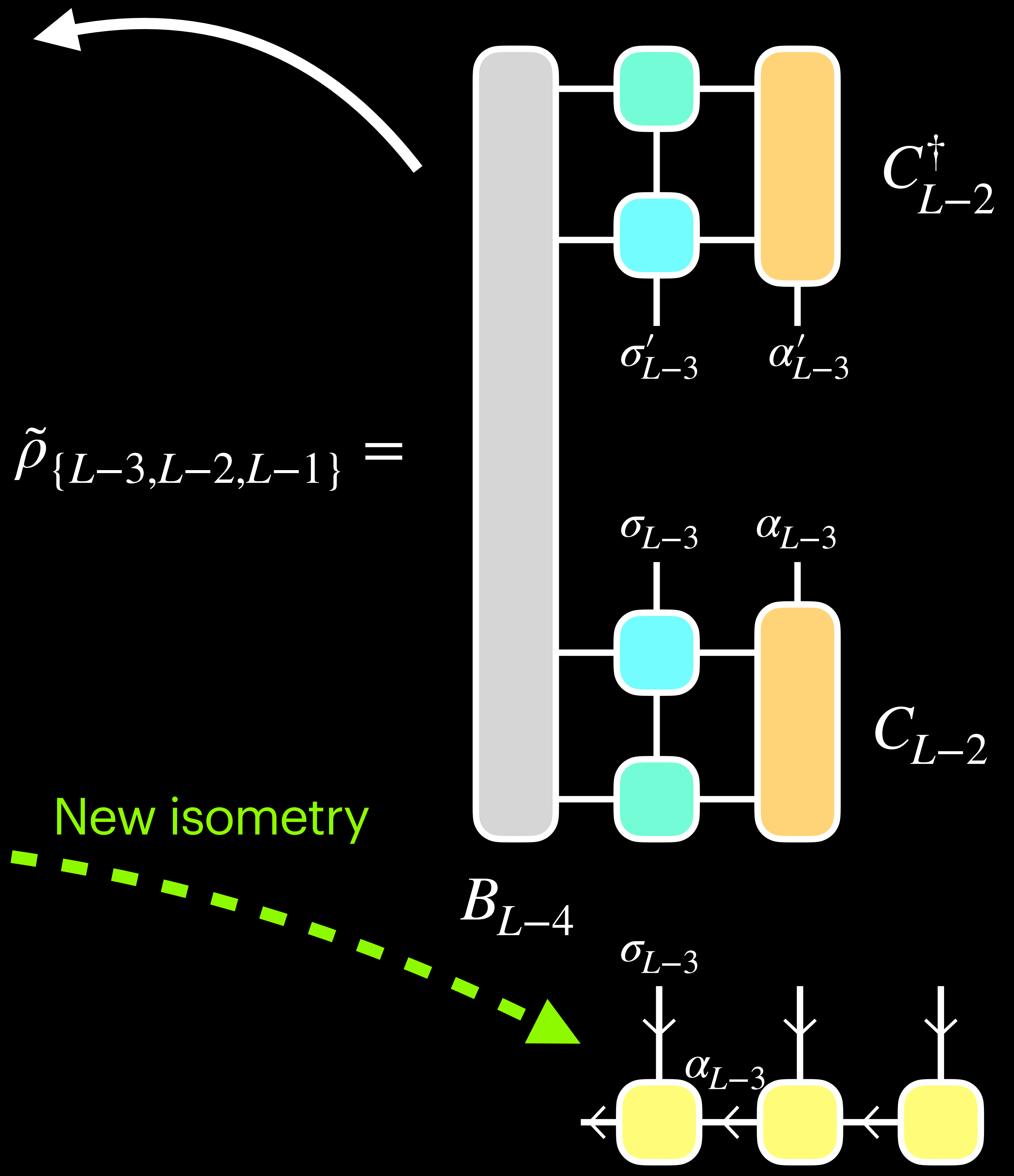


Apply MPO to MPS

Approximated reduced density matrix for the $\{L-3,\ L-2,\ L-1\}$ sites

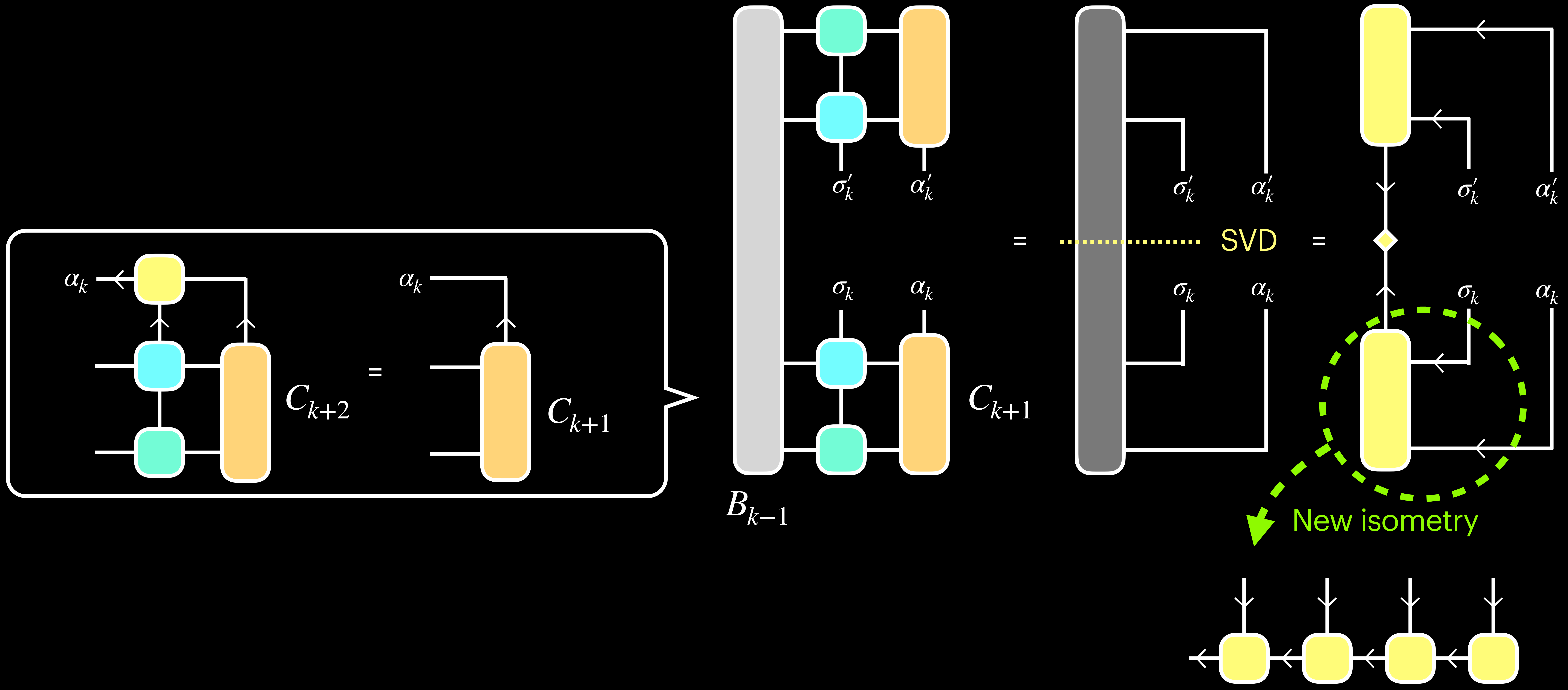
Structure of tensor network is same with previous one.
Therefore, one can obtain isometry using same technique.





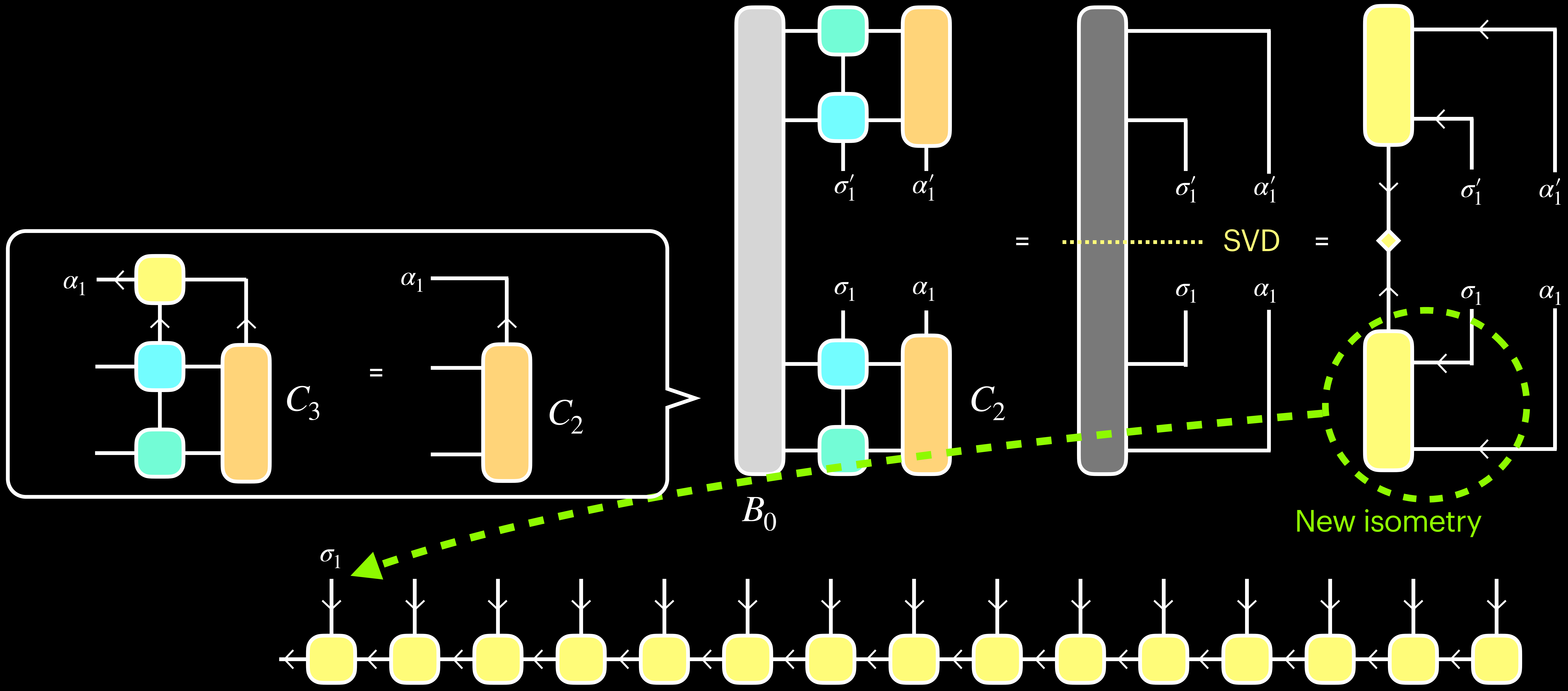
Apply MPO to MPS

Approximated reduced density matrix for the $\{k,\ k+1,\cdots,L-1\}$ sites



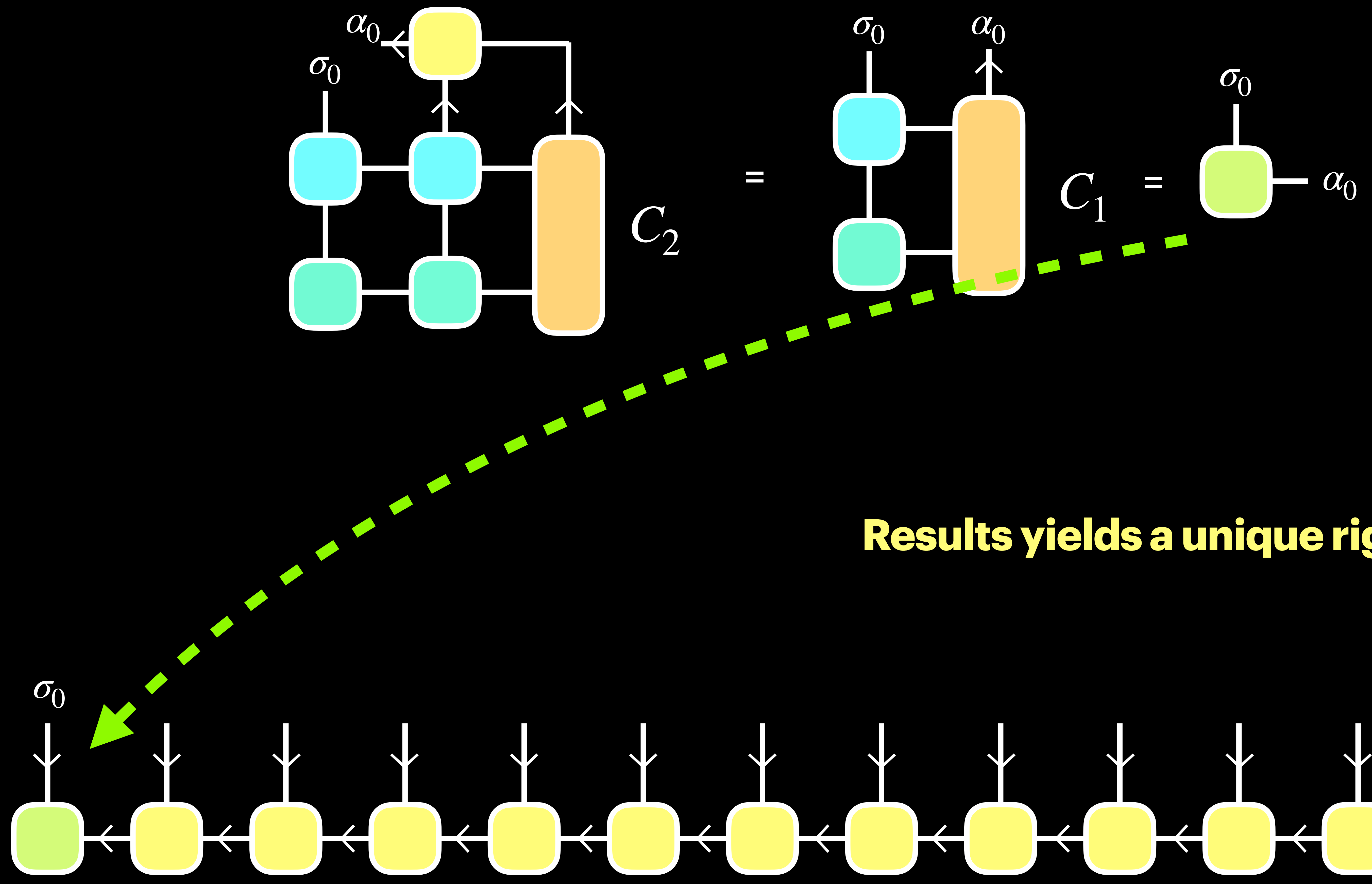
Apply MPO to MPS

Approximated reduced density matrix for the $\{1, 2, \cdots, L-1\}$ sites



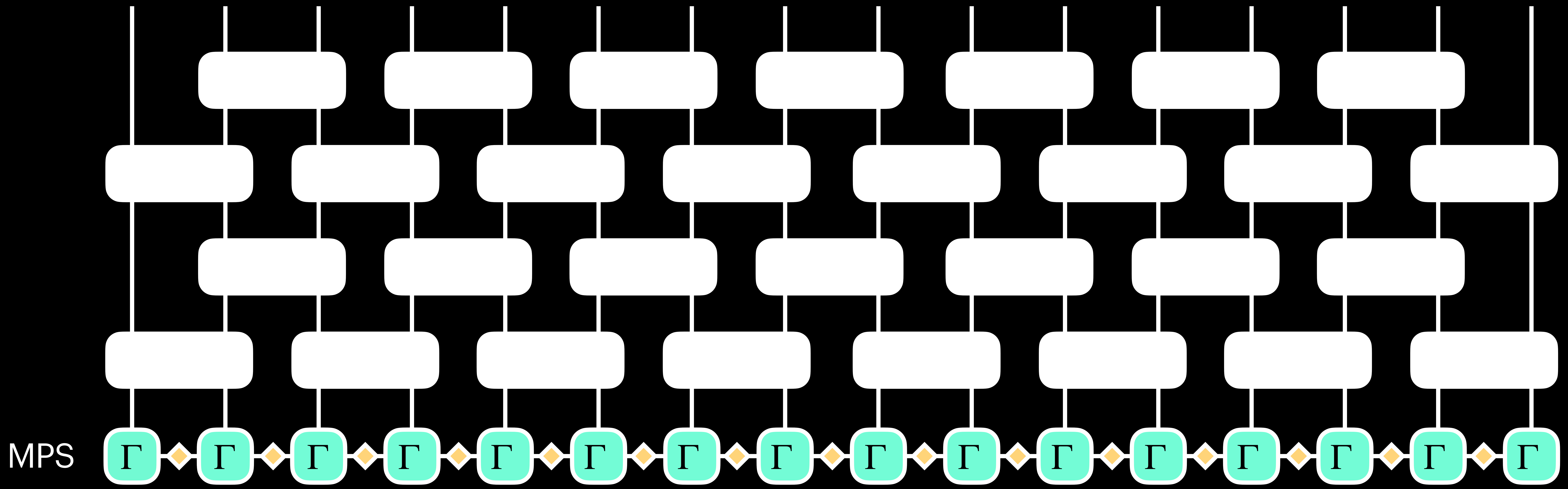
Apply MPO to MPS

Left-edge tensor



Results yields a unique right canonical form automatically.

Time-evolving block decimation (TEBD)

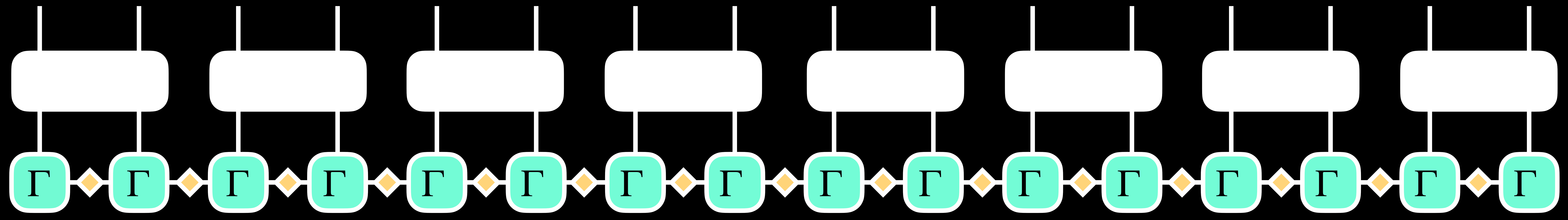


When performing time evolution calculations on MPS, the simplest method is to calculate Trotter slices called **time-evolving block decimation**.

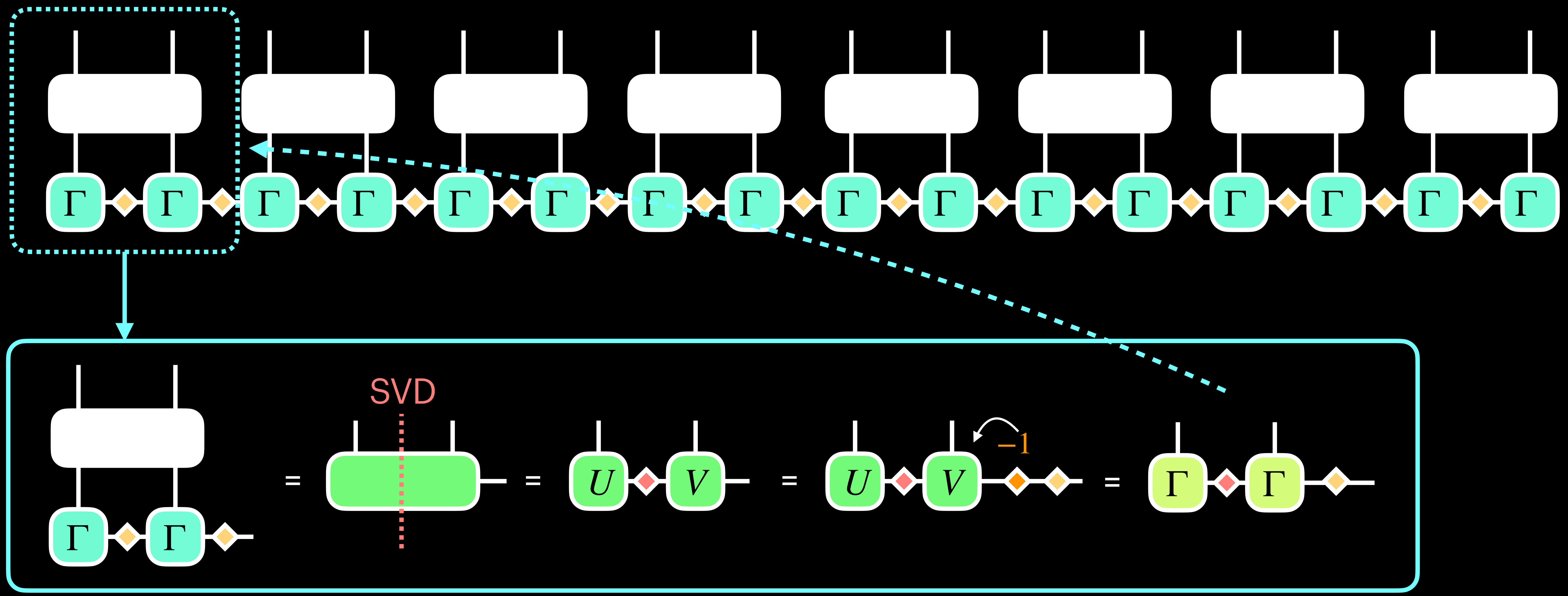
Quantum computing is a time-evolution starting from a trivial initial state (a **direct product state**).

A direct product state is a matrix product state with bond dimension 1.

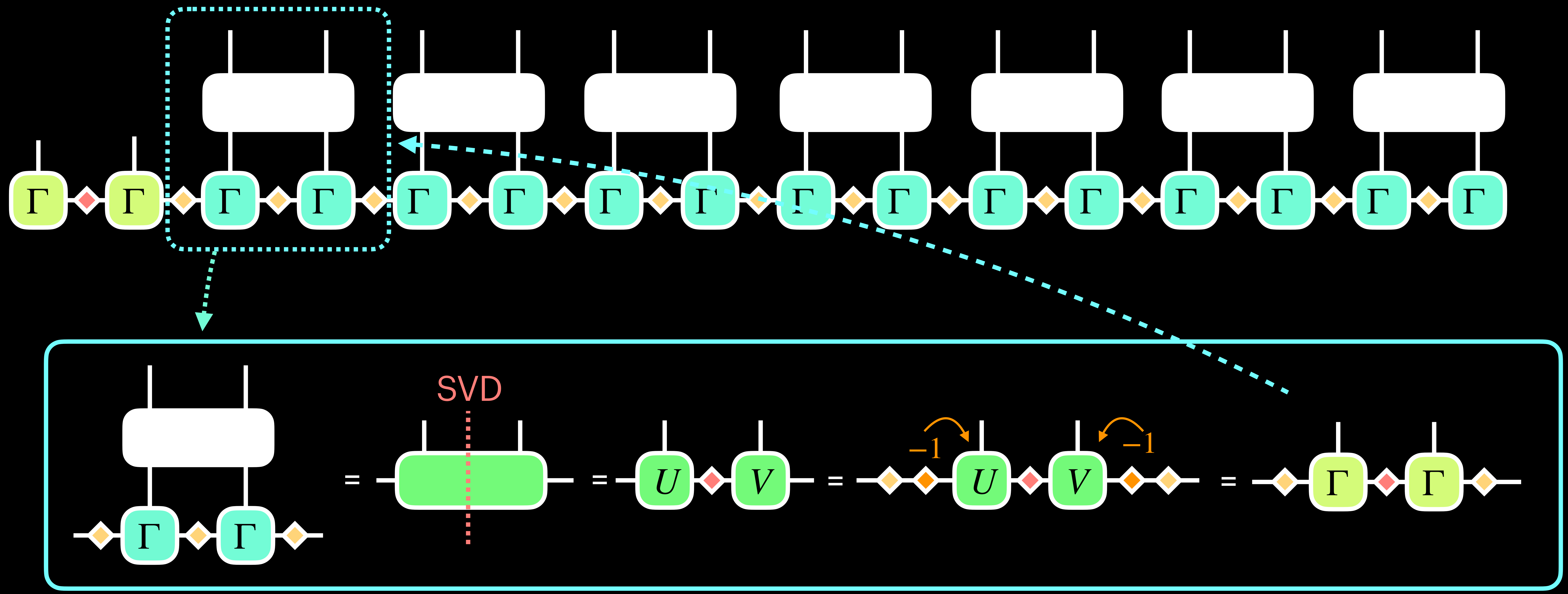
Time-evolving block decimation (TEBD)



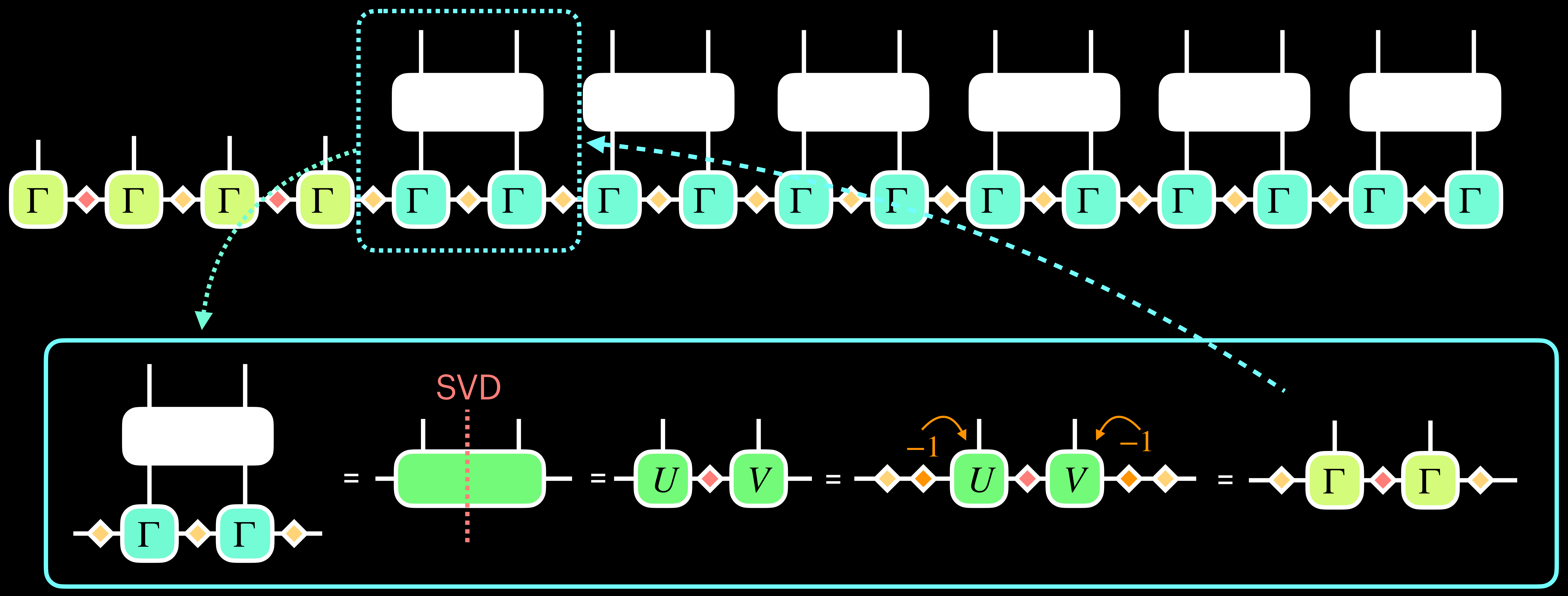
Time-evolving block decimation (TEBD)



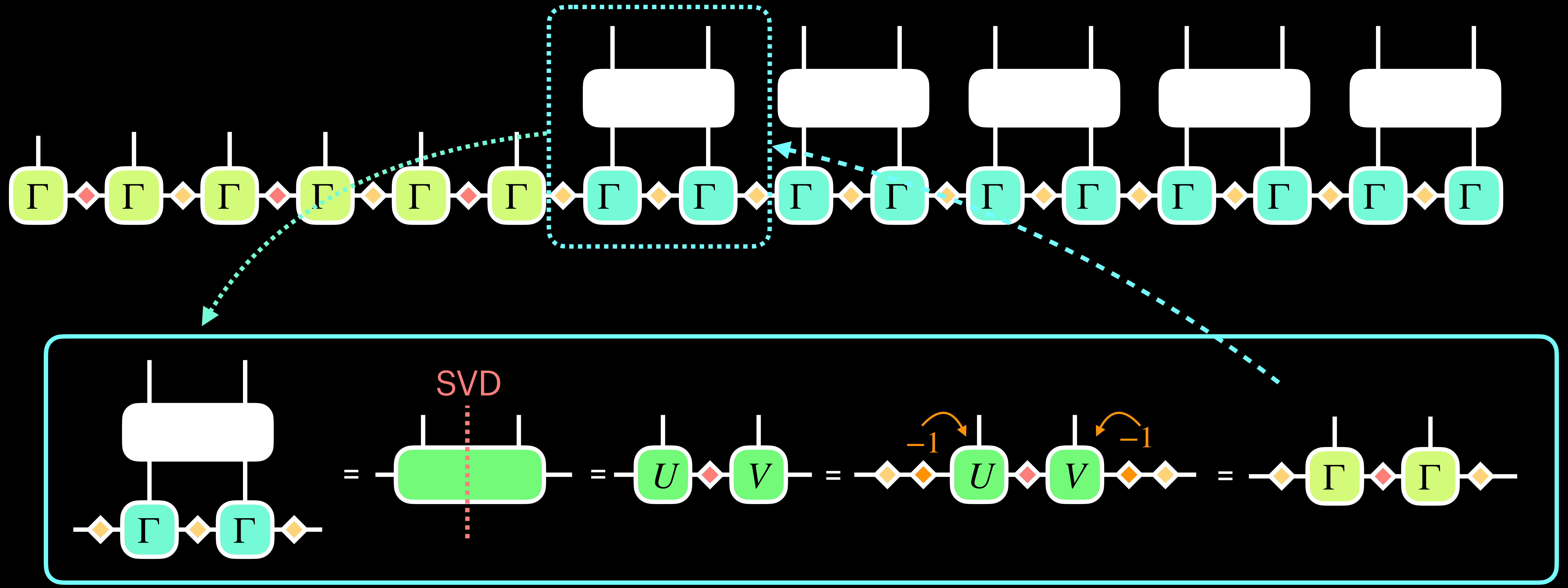
Time-evolving block decimation (TEBD)



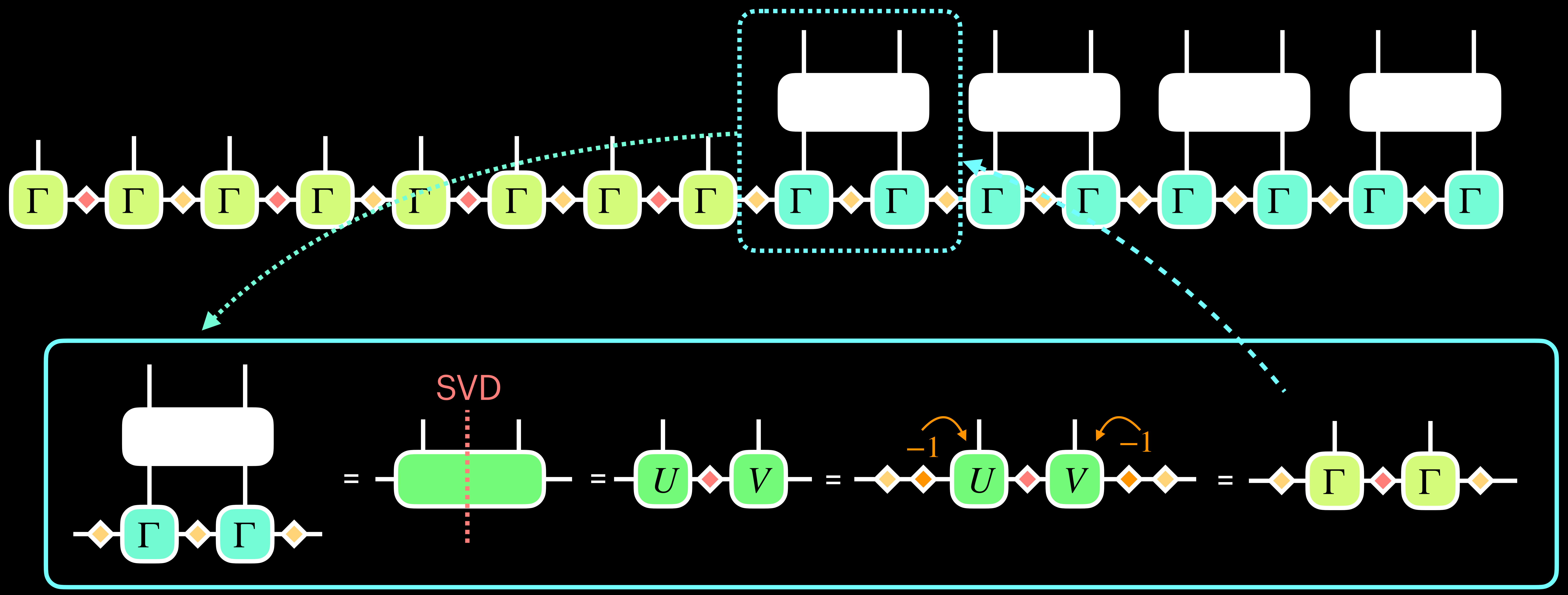
Time-evolving block decimation (TEBD)



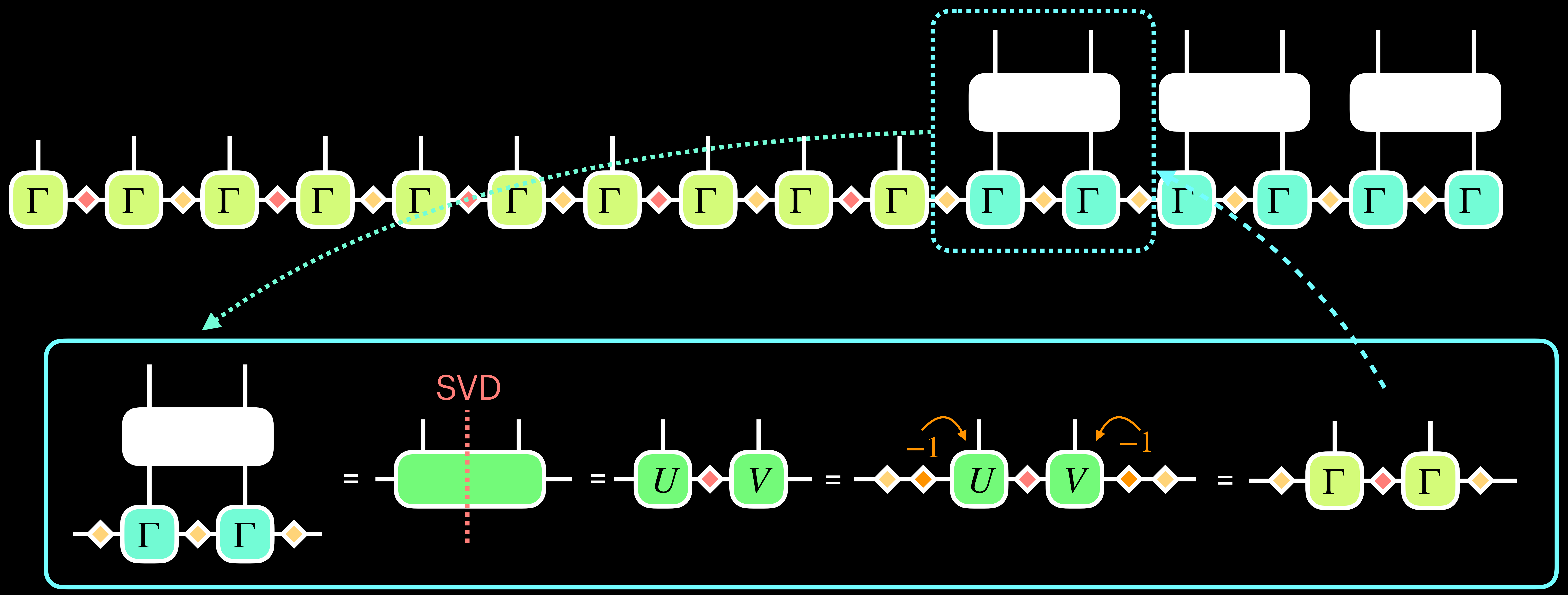
Time-evolving block decimation (TEBD)



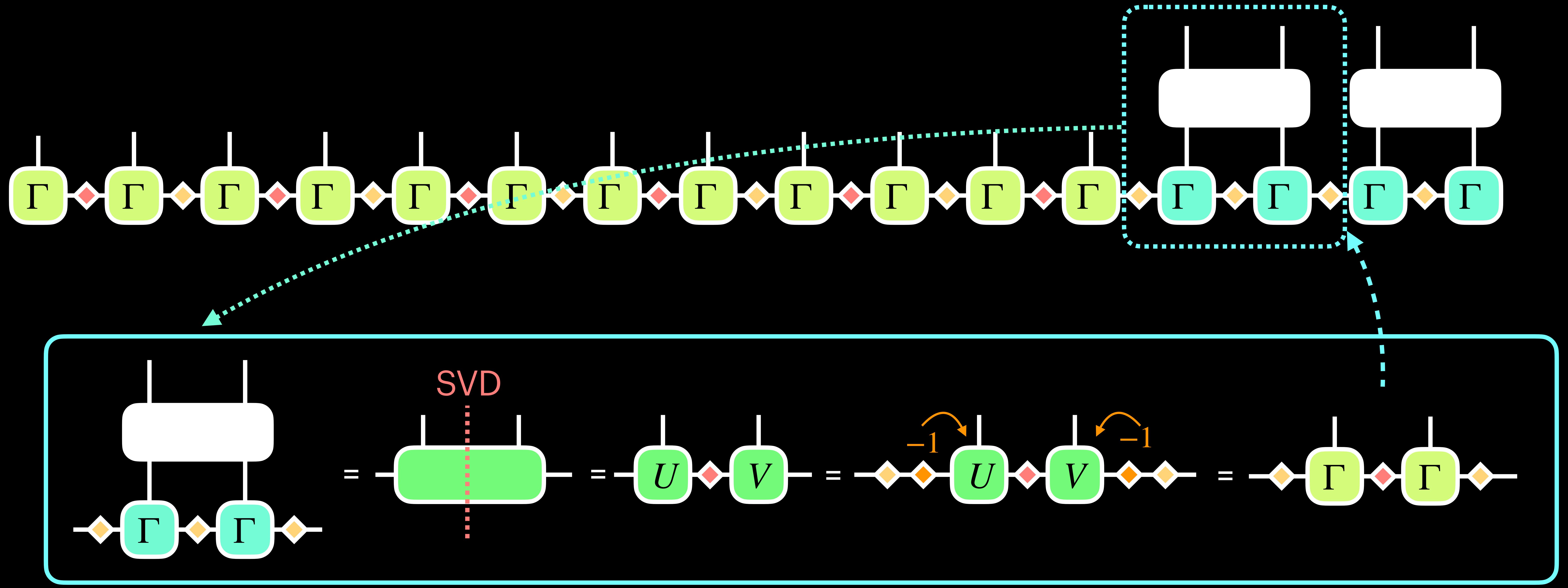
Time-evolving block decimation (TEBD)



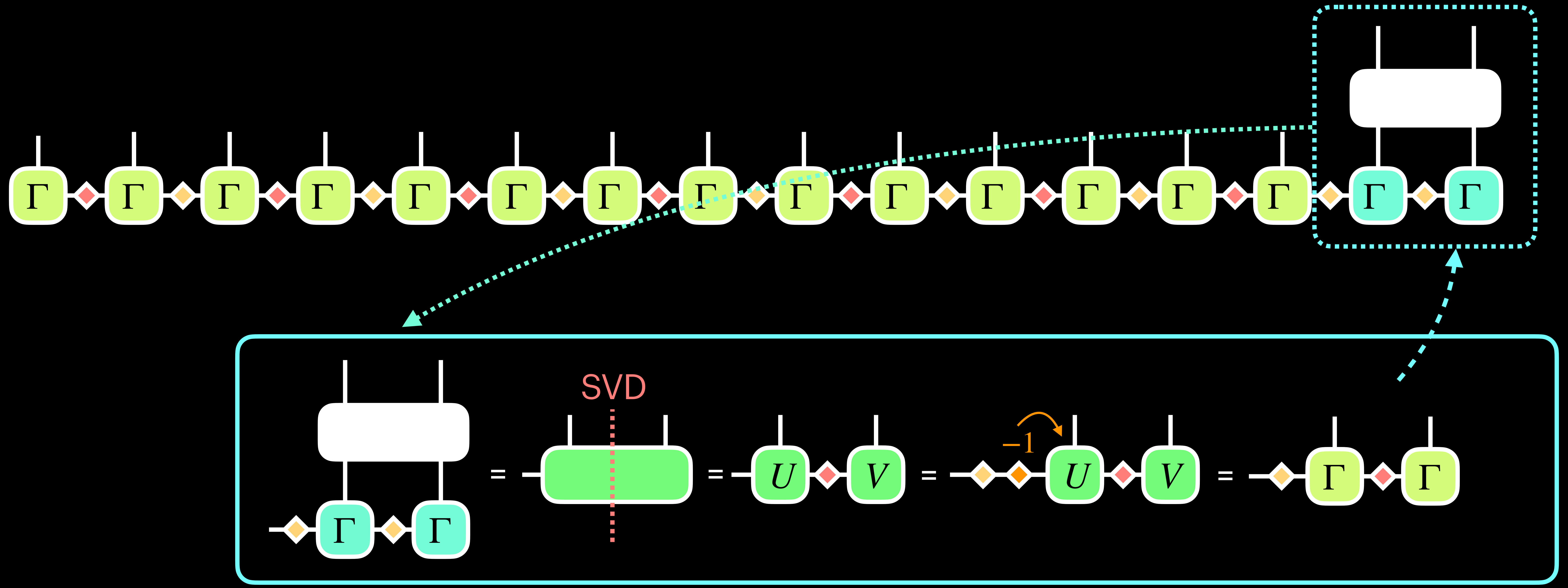
Time-evolving block decimation (TEBD)



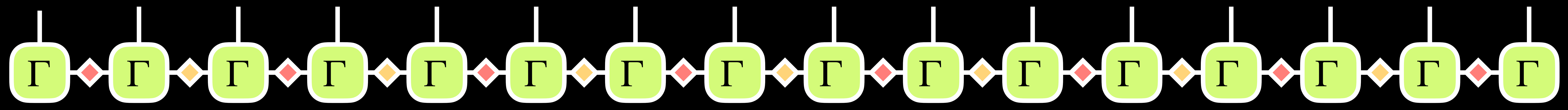
Time-evolving block decimation (TEBD)



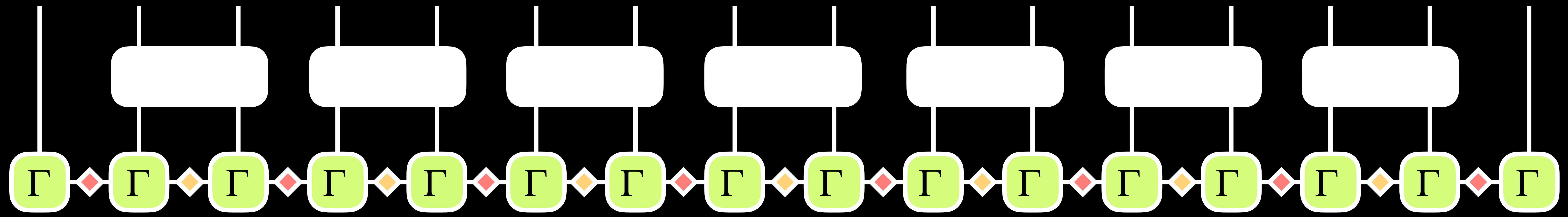
Time-evolving block decimation (TEBD)



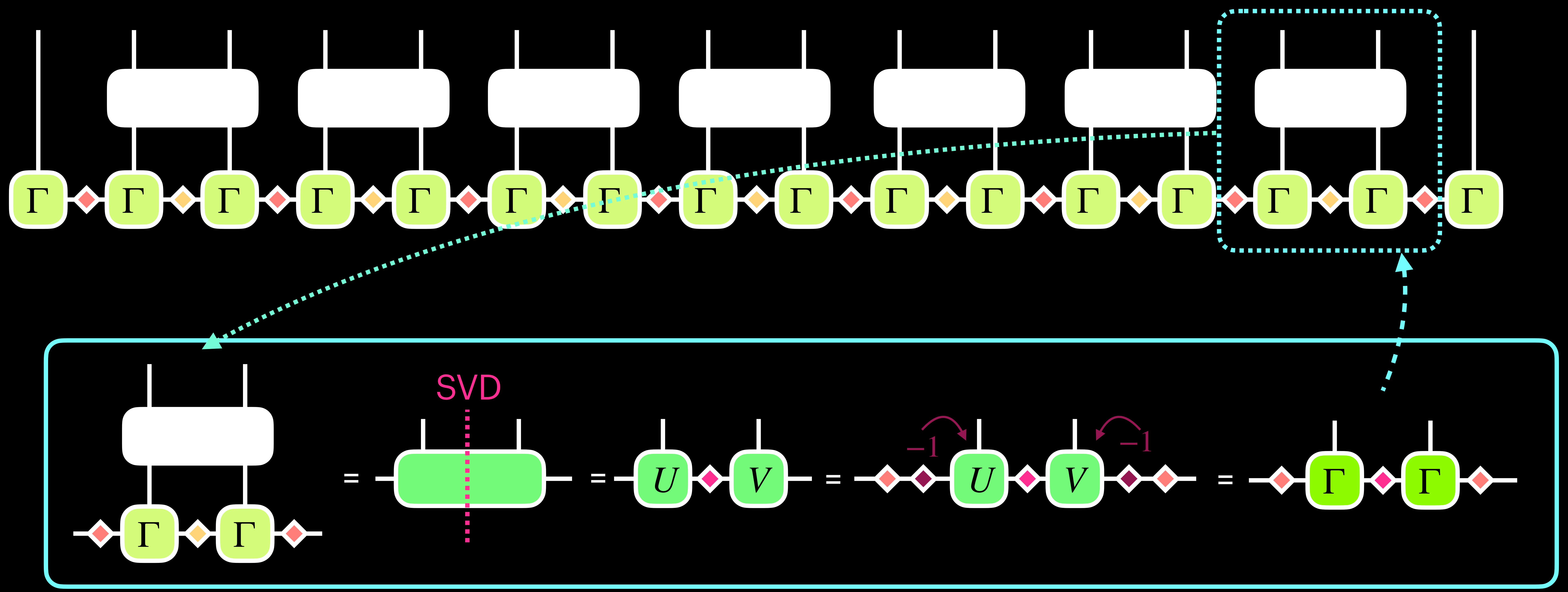
Time-evolving block decimation (TEBD)



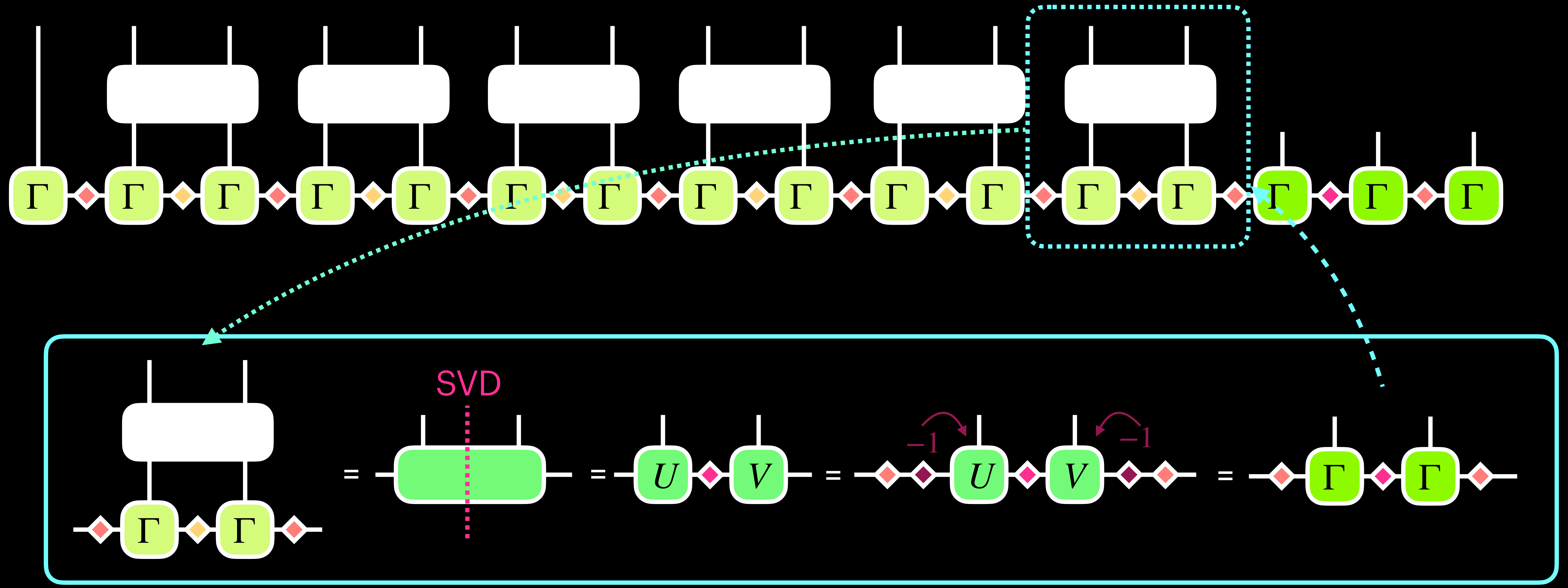
Time-evolving block decimation (TEBD)



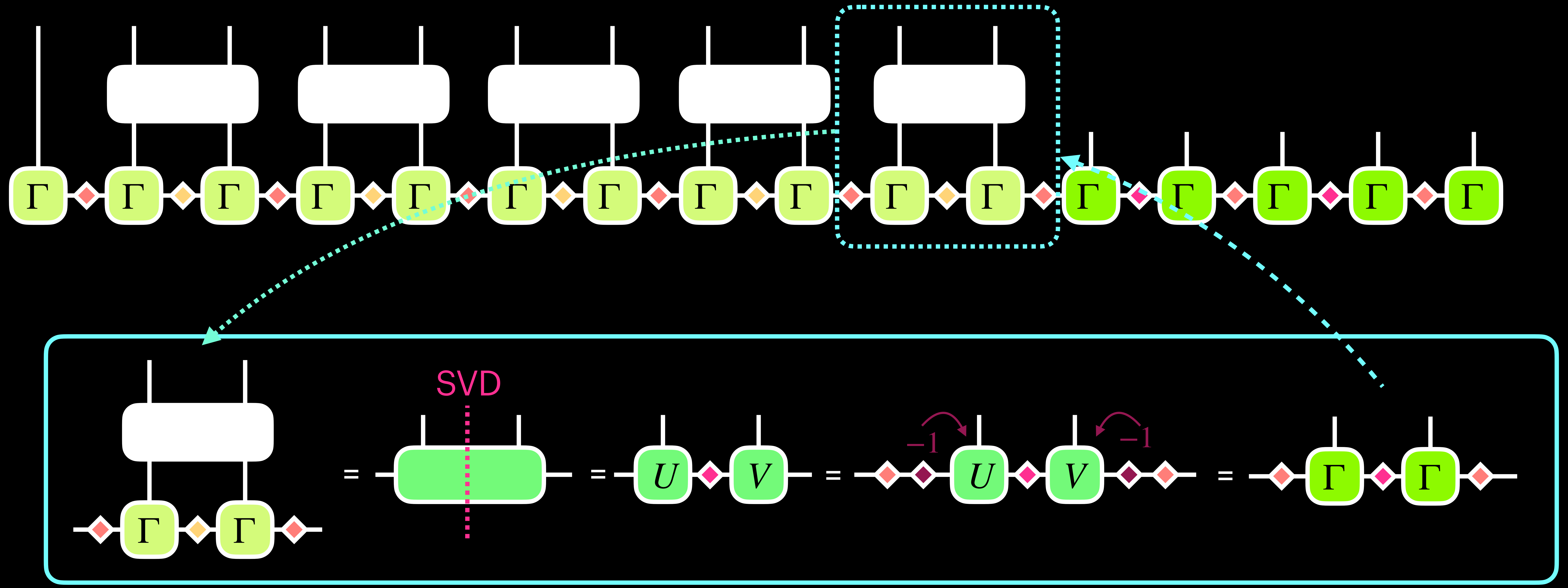
Time-evolving block decimation (TEBD)



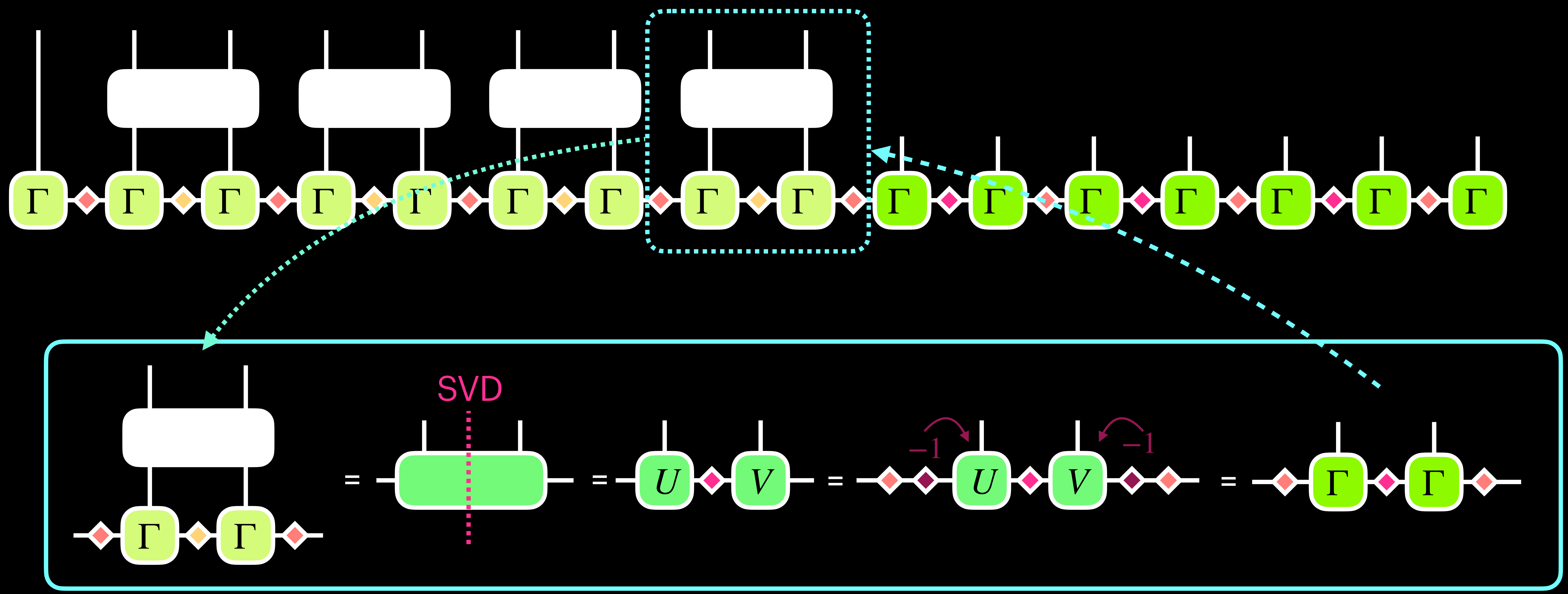
Time-evolving block decimation (TEBD)



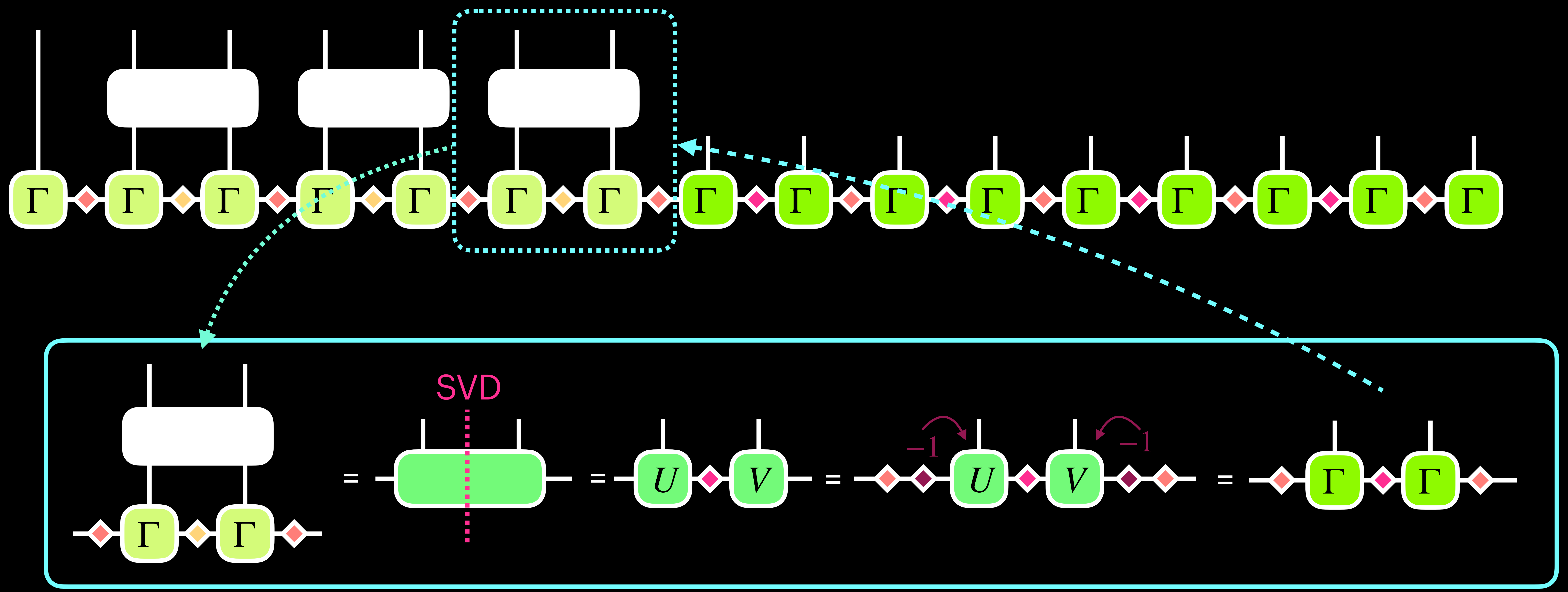
Time-evolving block decimation (TEBD)



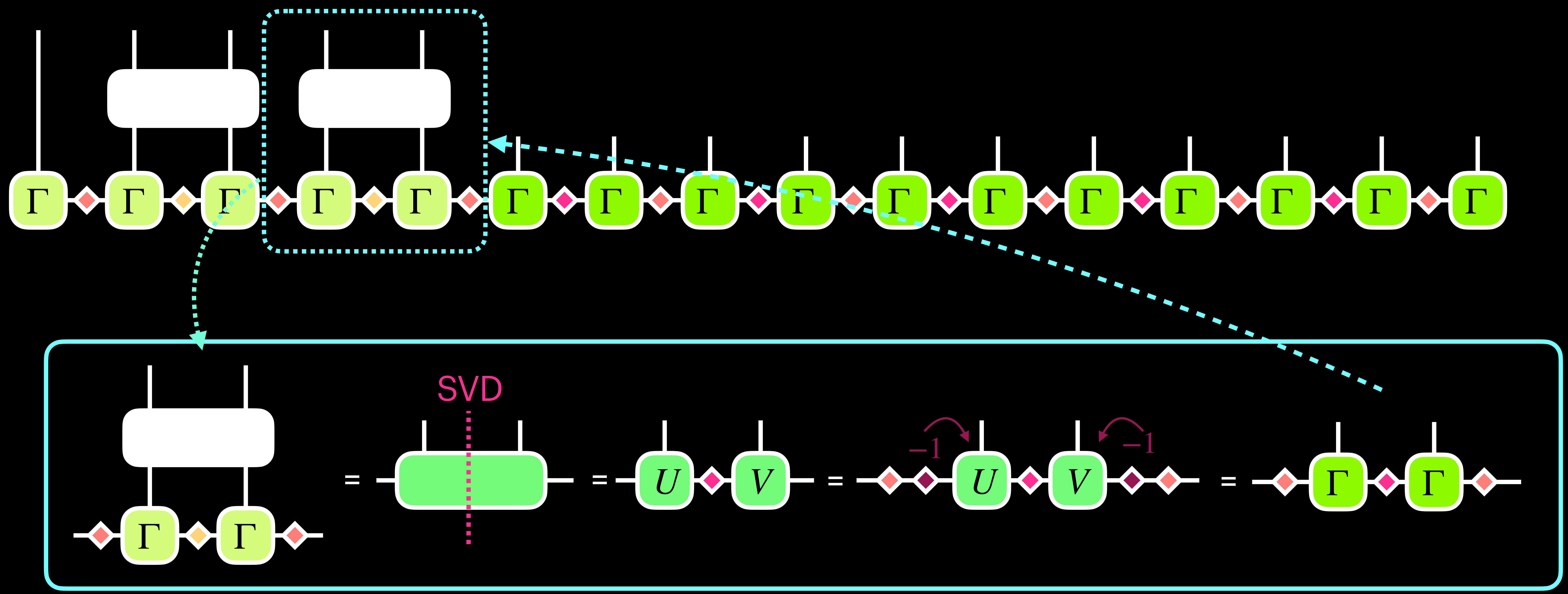
Time-evolving block decimation (TEBD)



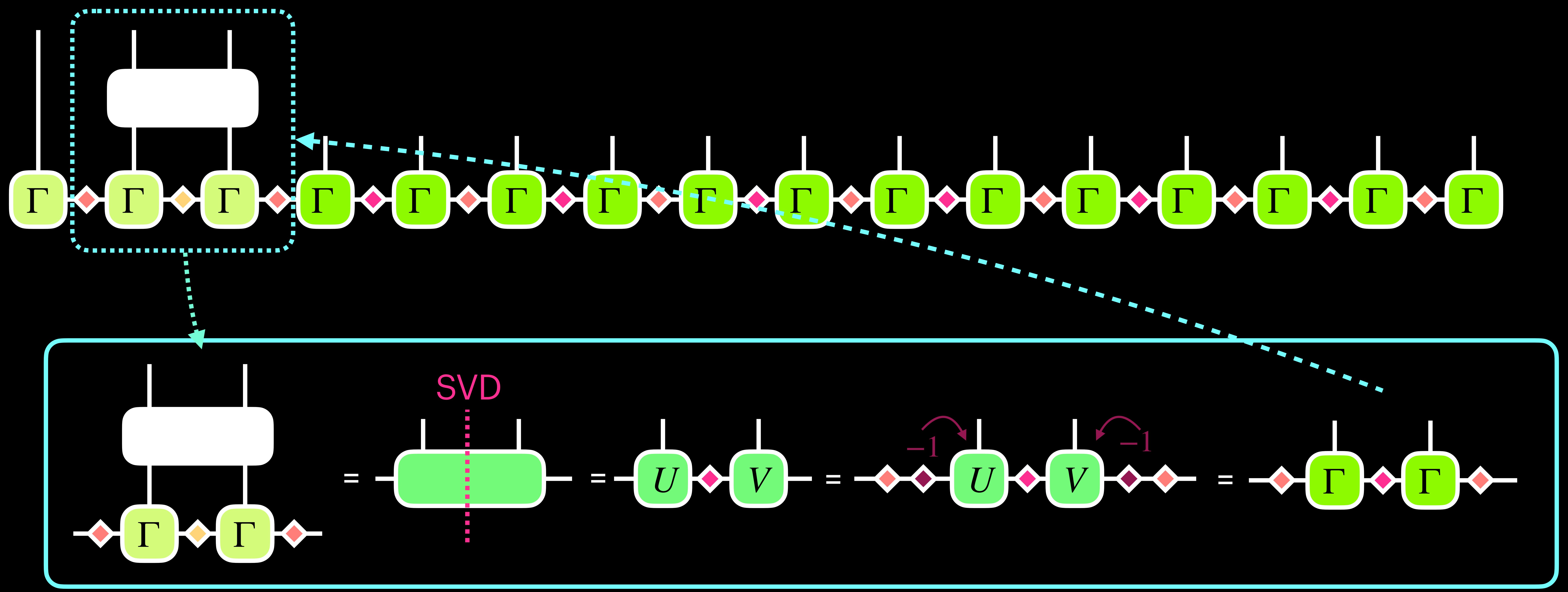
Time-evolving block decimation (TEBD)



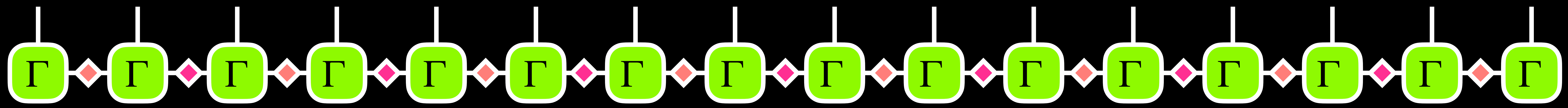
Time-evolving block decimation (TEBD)



Time-evolving block decimation (TEBD)

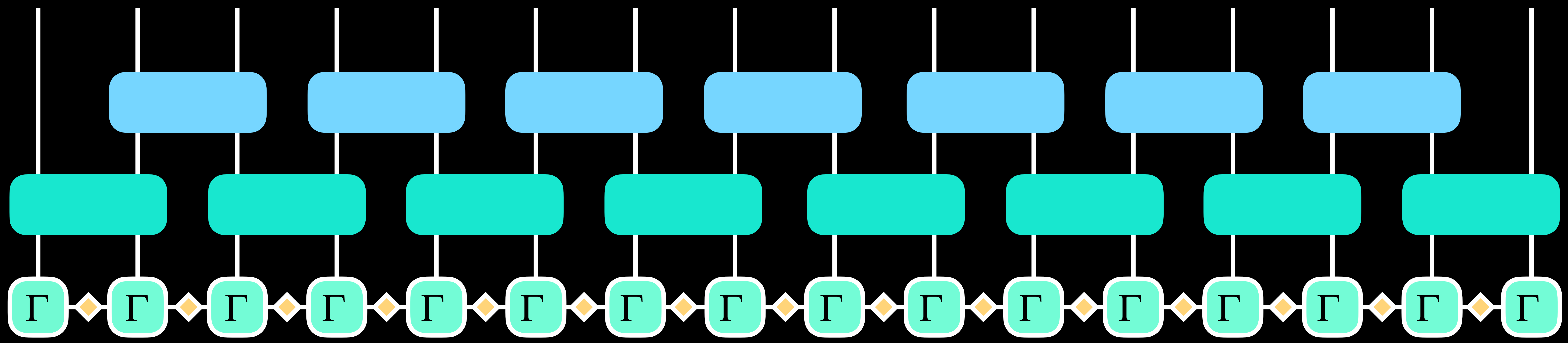


Time-evolving block decimation (TEBD)



Parallelization of TEBD (pTEBD)

R.-Y. Sun, T. Shirakawa & S. Yunoki, in preparation



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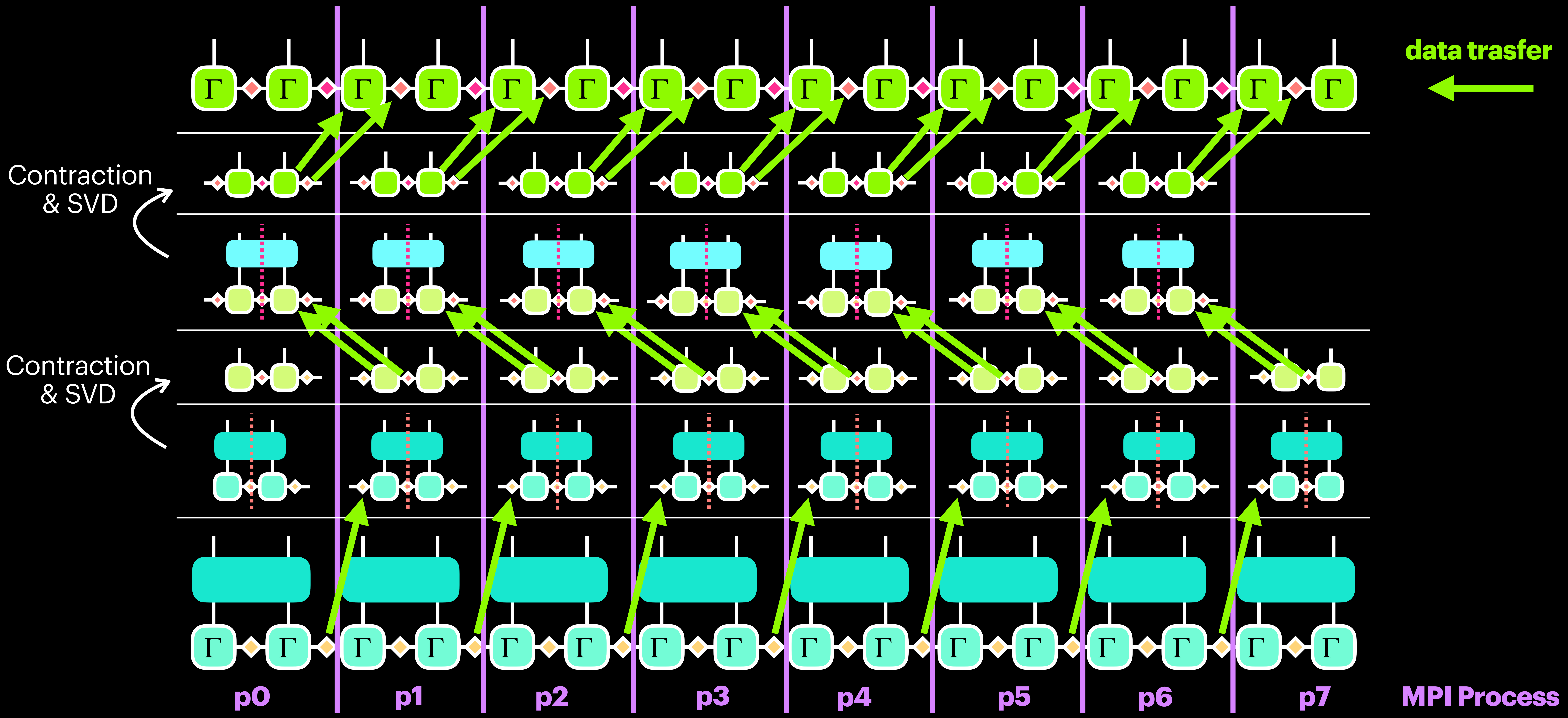
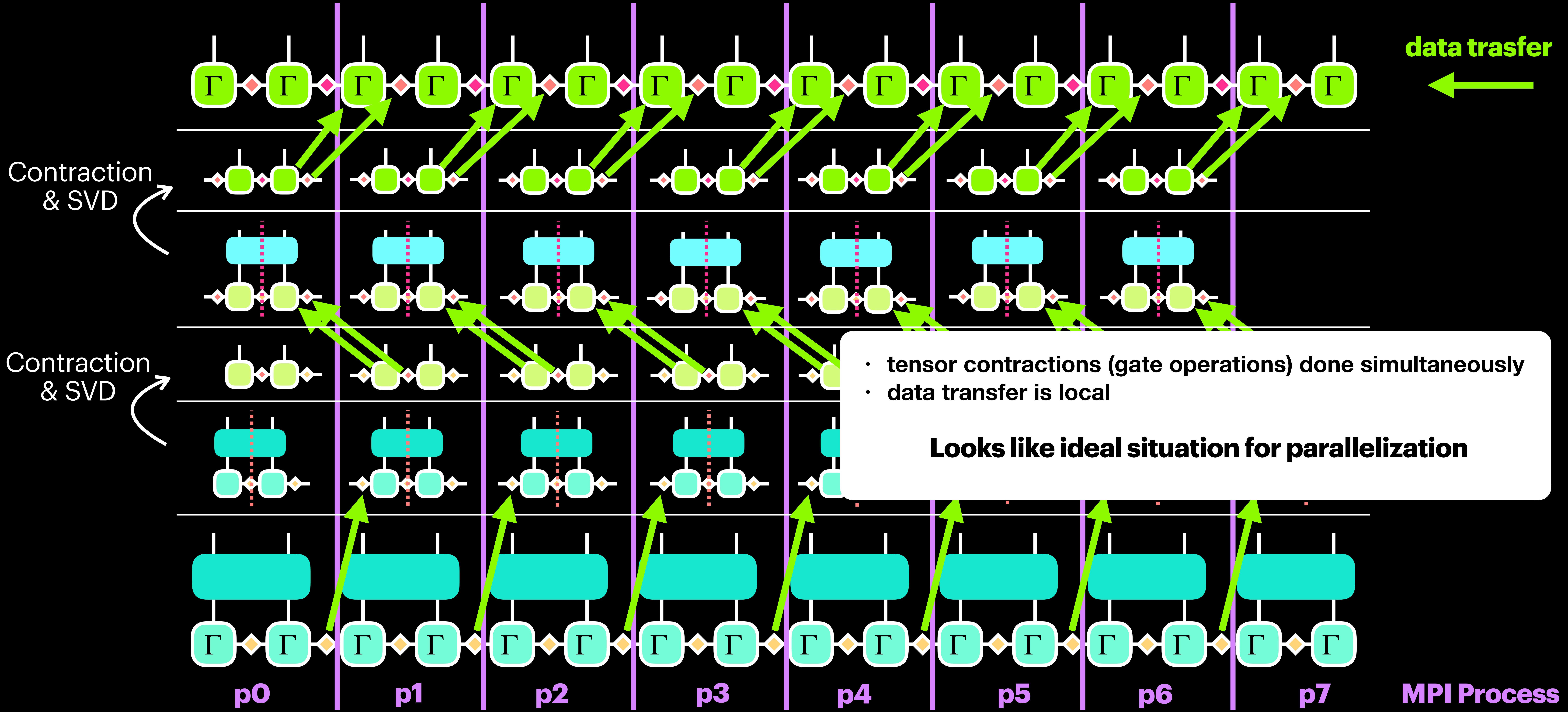


Parallelization of TEBD (pTEBD)

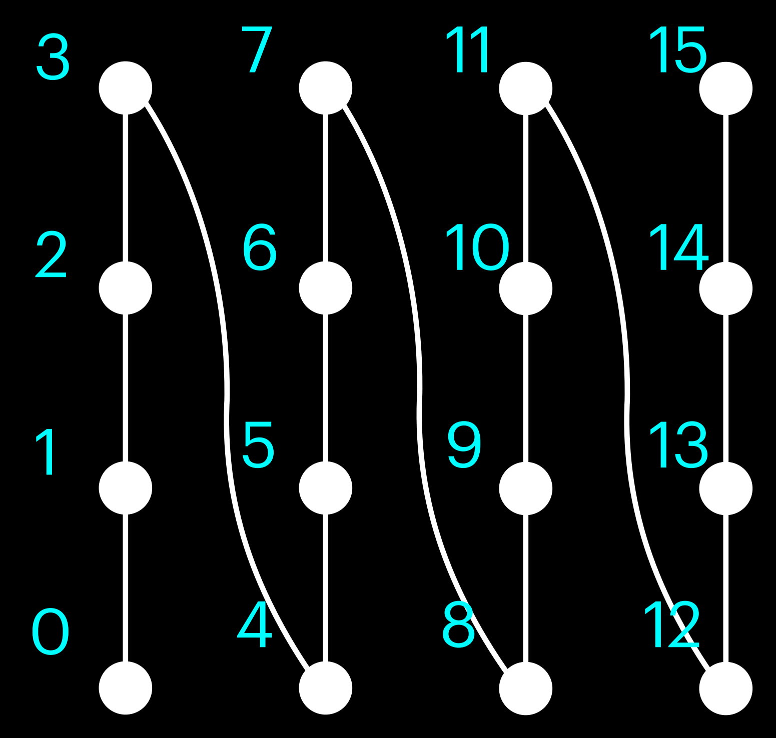
R.-Y. Sun, T. Shirakawa & S. Yunoki, in preparation

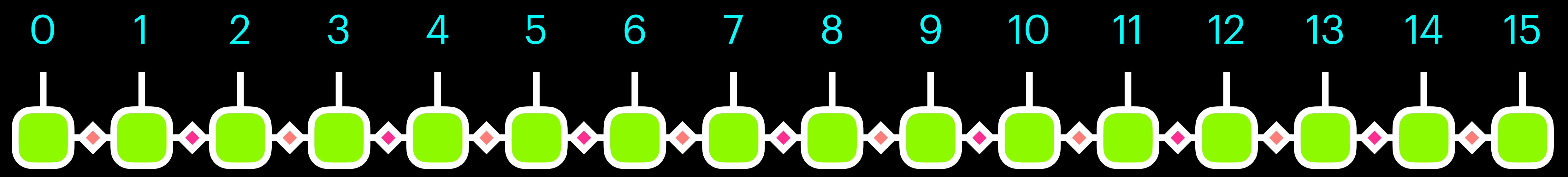


- tensor contractions (gate operations) done simultaneously
- data transfer is local

Looks like ideal situation for parallelization

Simulation for 2D quantum circuit





In order to calculate a 2D system using MPS, the 2D system is forcibly regarded as a 1D system.

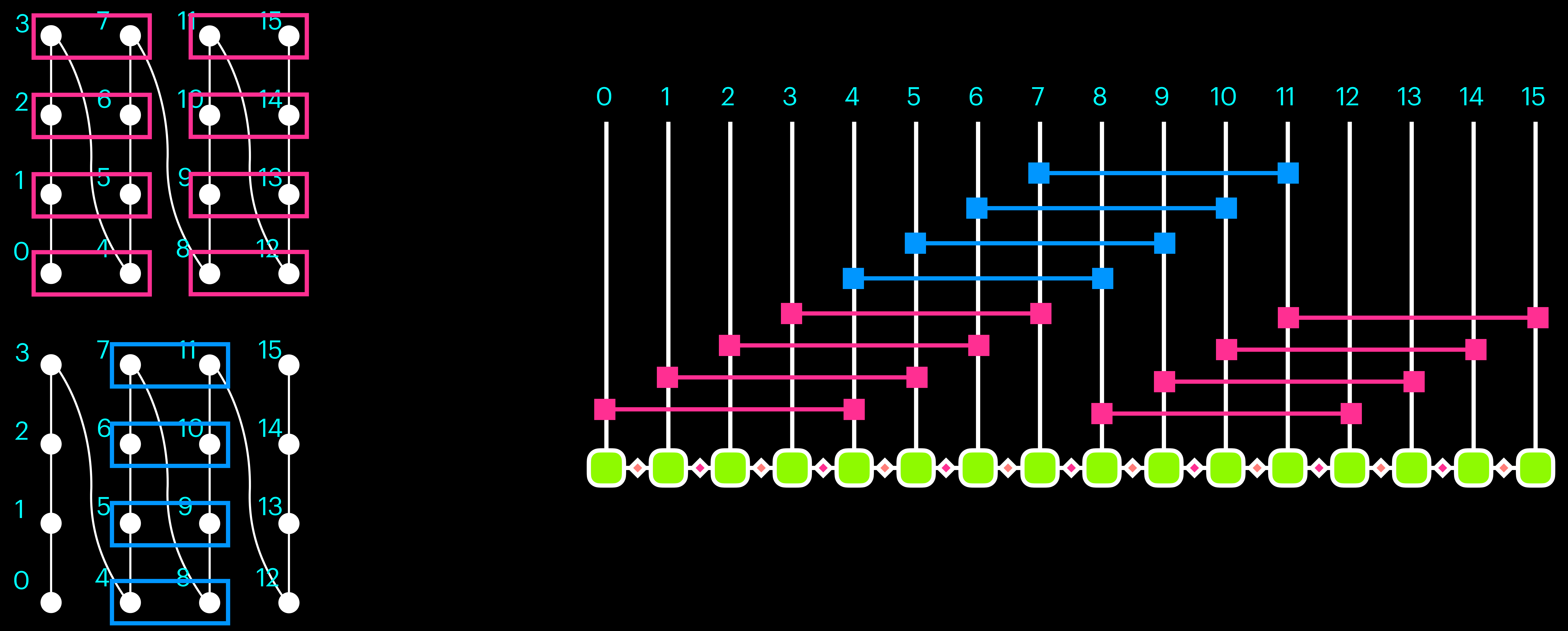
Simulation for 2D quantum circuit

Position of 1st layer operators

Position of 2nd layer operators

1st layer operators

2nd layer operators



Then, the nearest-neighbor operators in the 2D system become distant operators in the virtual 1D system.

Simulation for 2D quantum circuit

Position of 1st layer operators

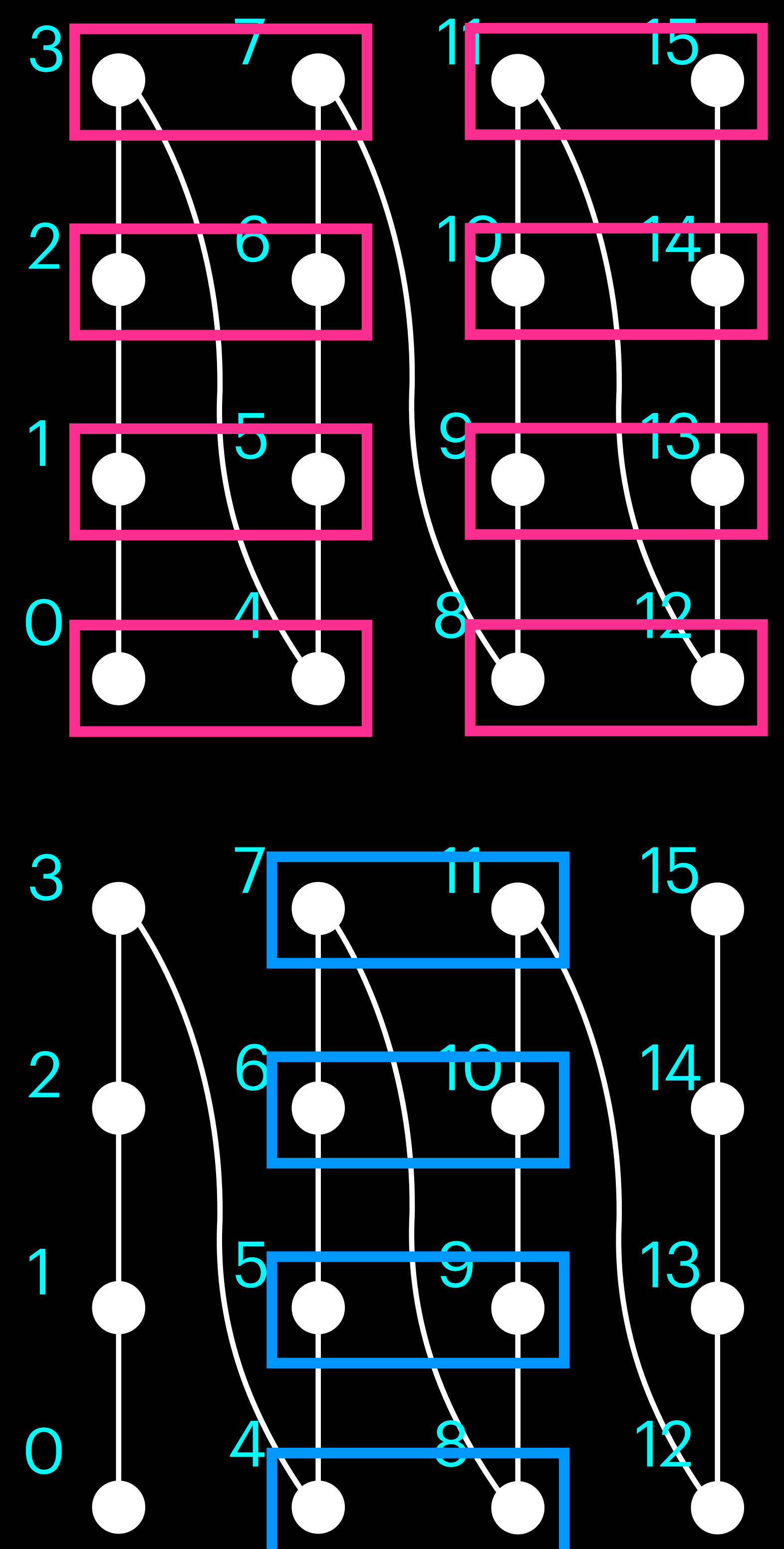
Position of 2nd layer operators

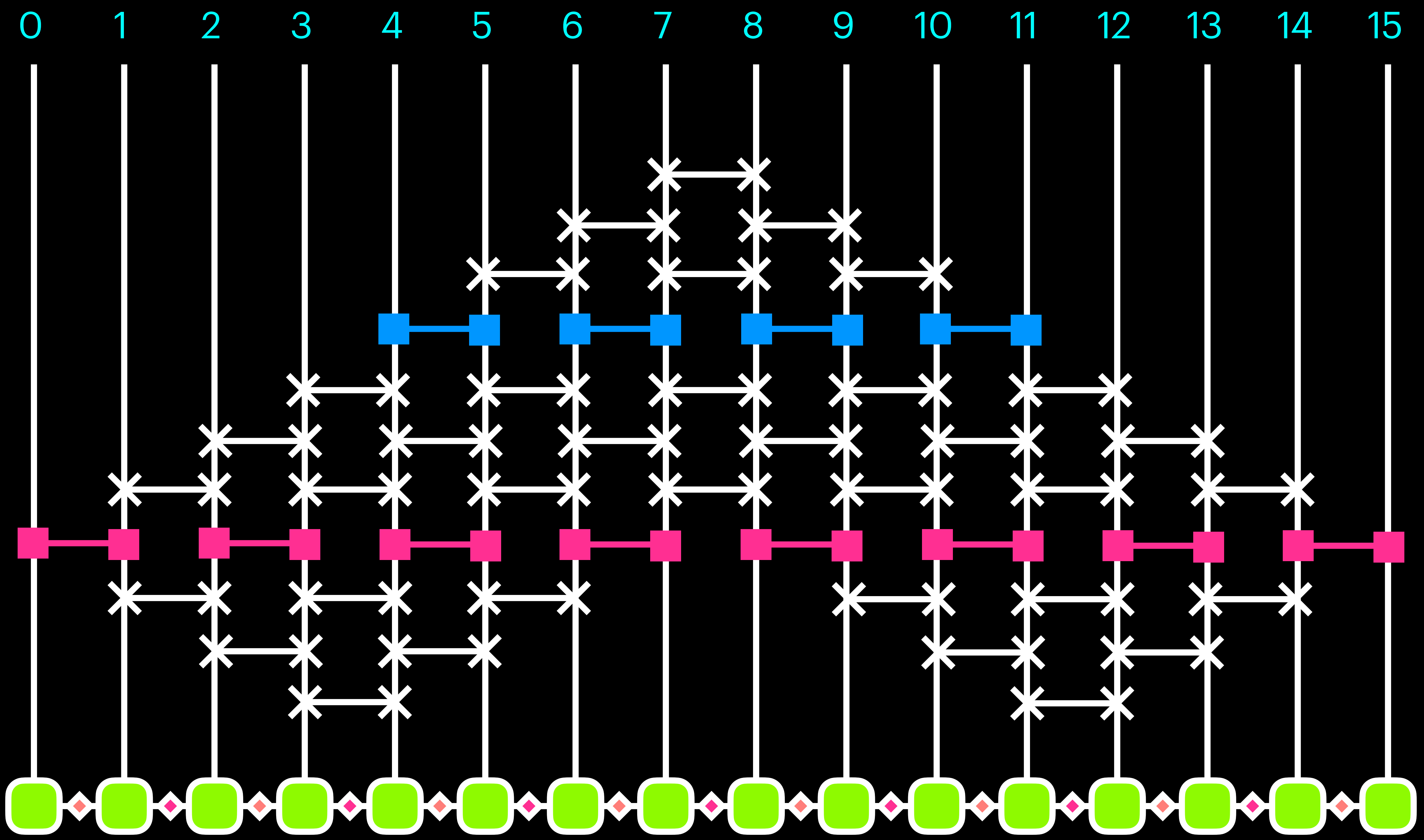
1st layer operators

2nd layer operators

SWAP operator S_{ij}

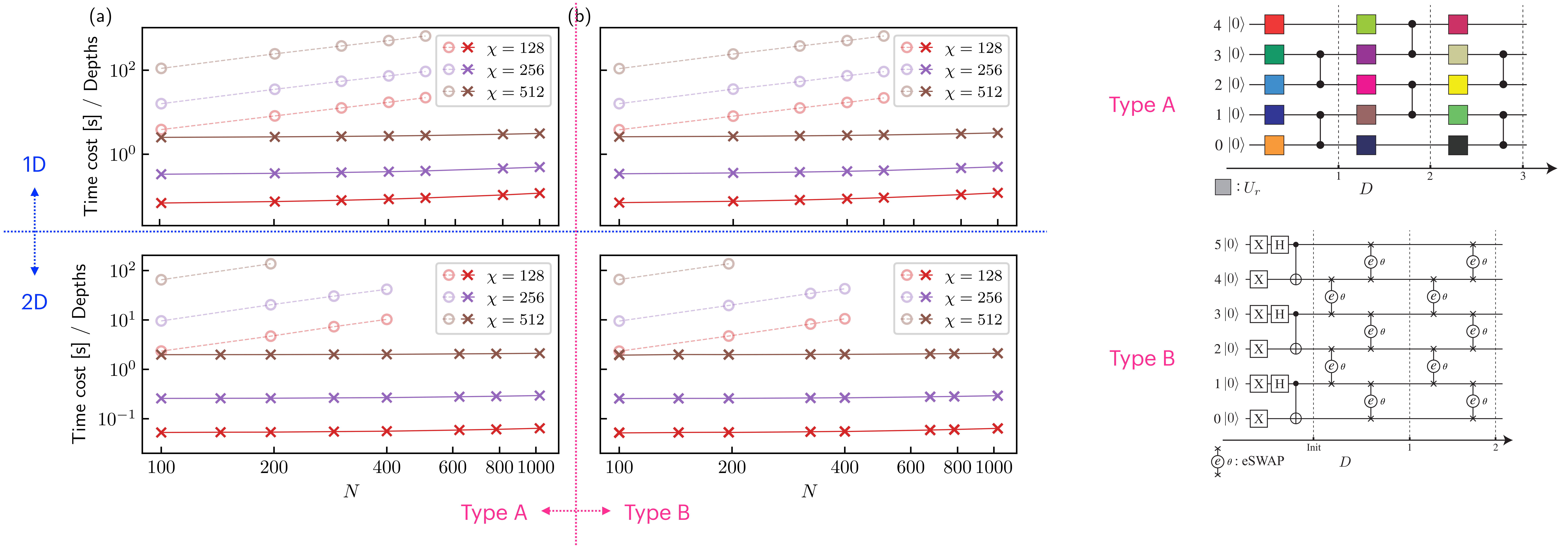
$$S_{ij}\,|\,\sigma_i\sigma_j\rangle = |\,\sigma_j\sigma_i\rangle$$





The simplest and most efficient way to handle these bonds in TEBD is by sandwiching the swap operator.

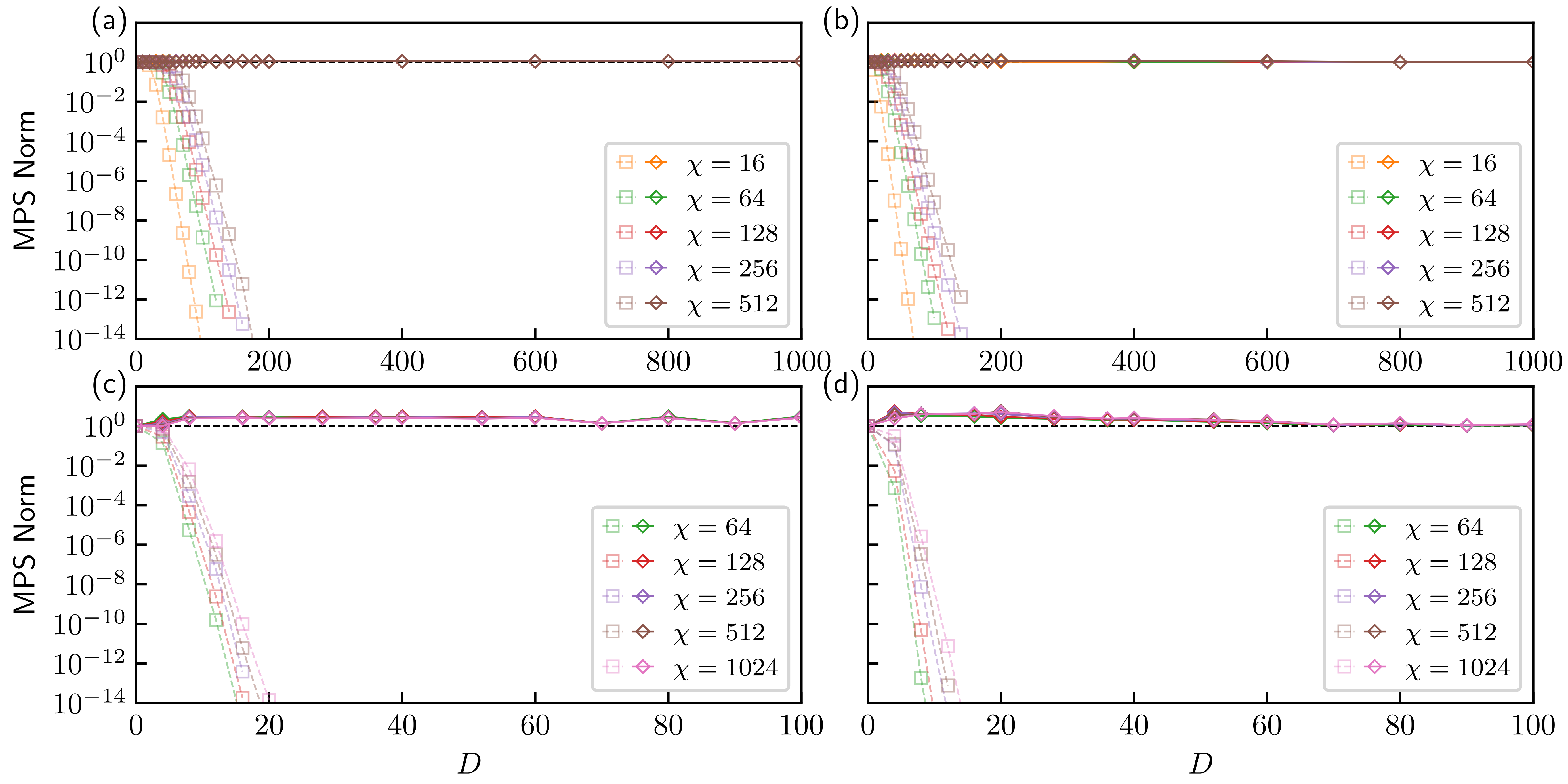
Benchmark



Random circuit benchmarks on Fugaku show weak scaling.

Wavefunction norm stabilization

- Although the norm of the wavefunction is an unphysical quantity which means it does not have an impact on the calculation of physical observables, it turns out strongly influencing the stability when performing numerical simulations in practice, hence we need be elaborative to the norm deviation induced by the parallel MPS compression.

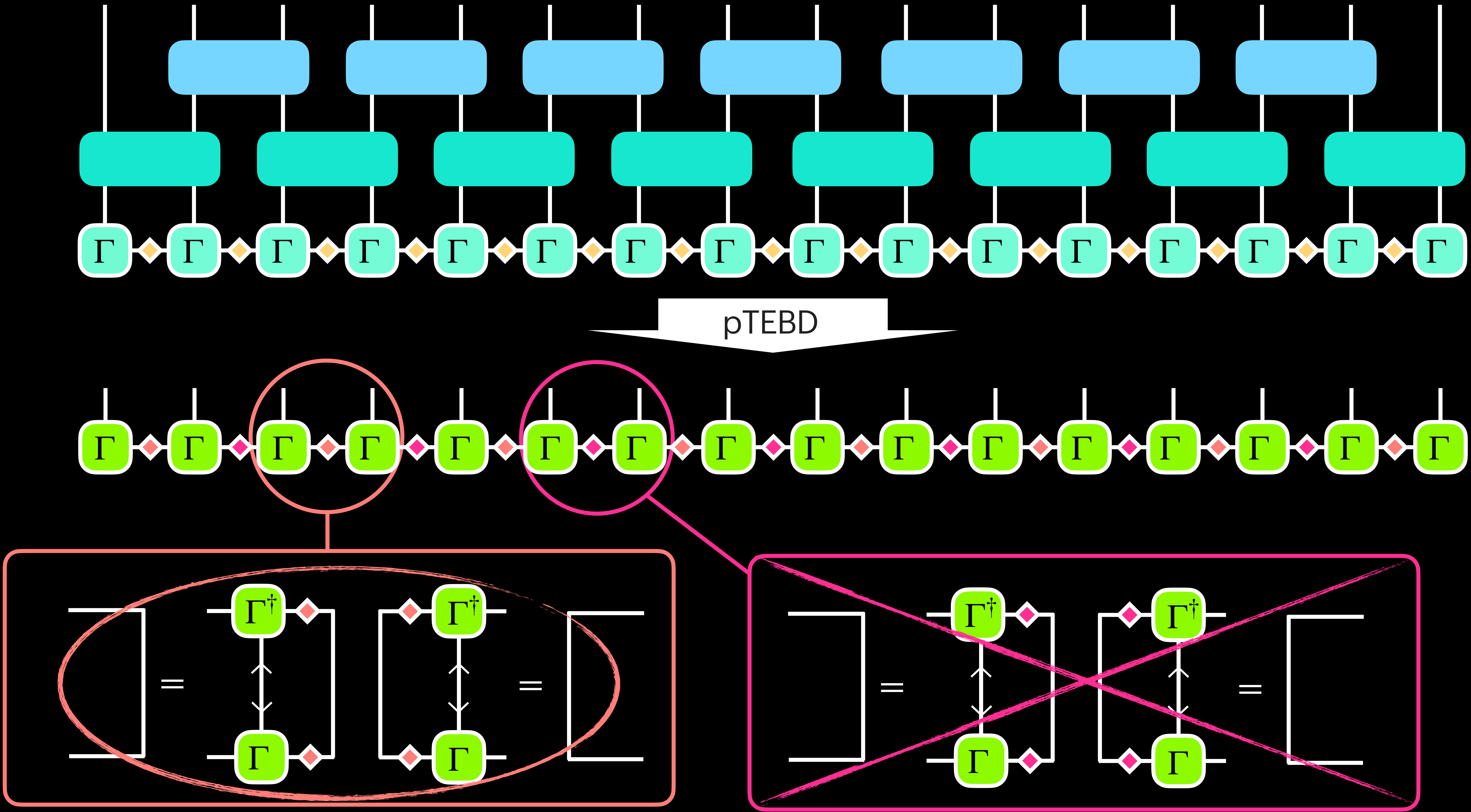


D: Number of layers

We find that local rescaling of the diagonal singular value tensor stabilize the norm of MPS wavefunction.

Problem

Simple TEBD/pTEBD algorithm breaks the isometric condition.



Problem

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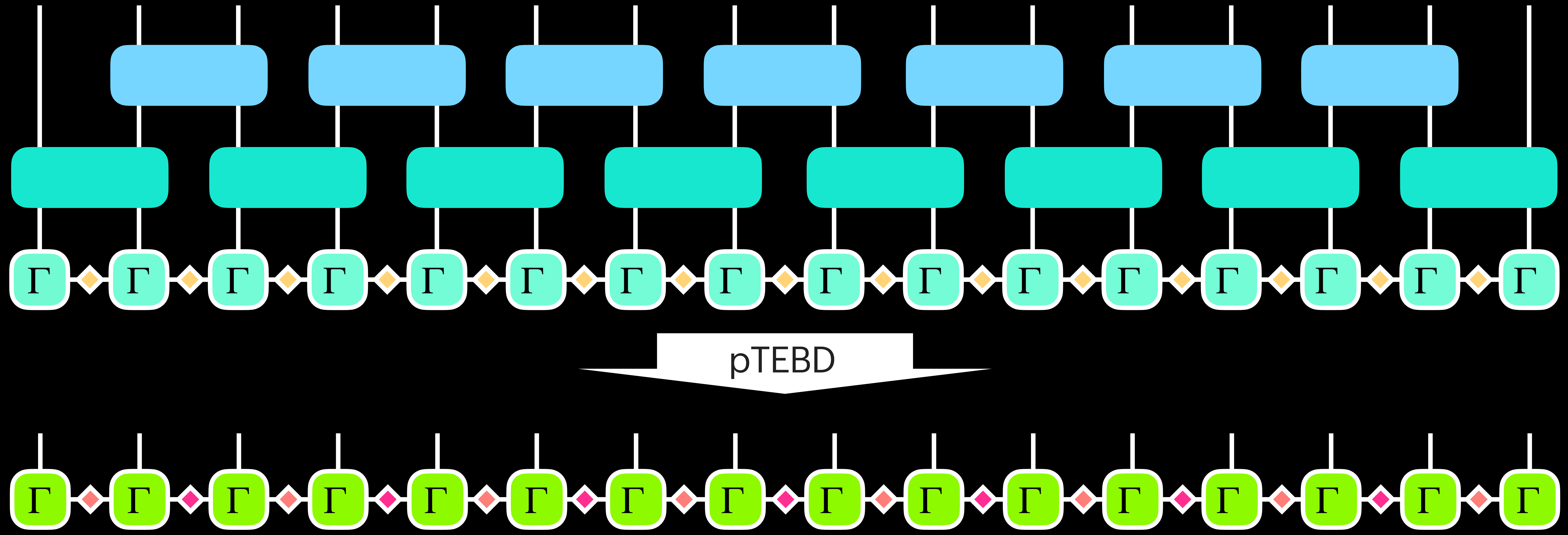


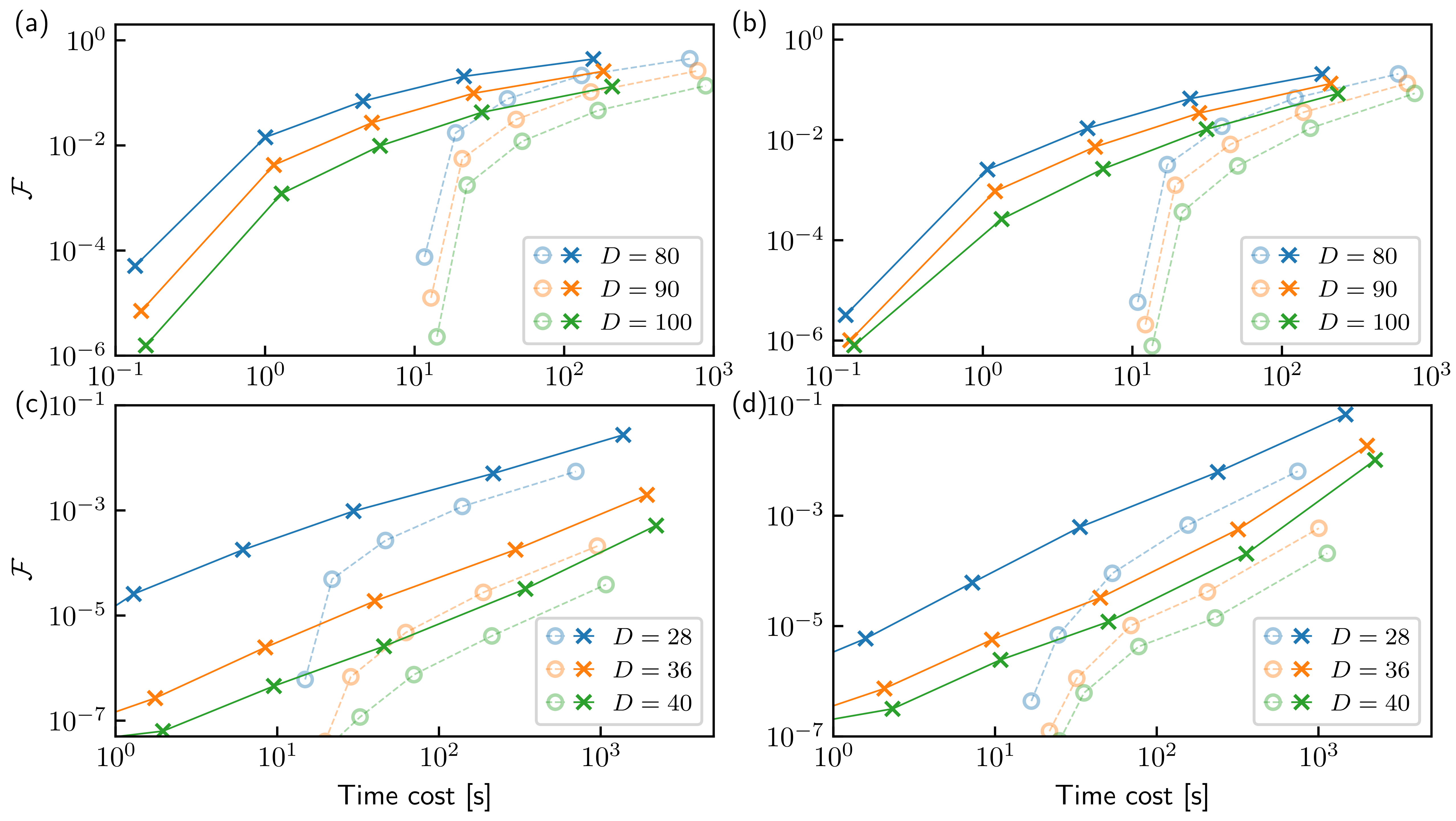
No simplification is possible in the calculation of expected values for local physical quantities

Possibly less accurate than sequential methods

To recover the isometric condition, end-to-end sweeps that cannot be parallelized are required.

Problem

Simple TEBD/pTEBD algorithm breaks the isometric condition.



However, even after taking accuracy into account, the gain over computation time is superior to the sequential method.

Therefore, in the case of the MPS simulator, the benefit of parallelization is tremendous.

open circles: sequential method
cross: pTEBD

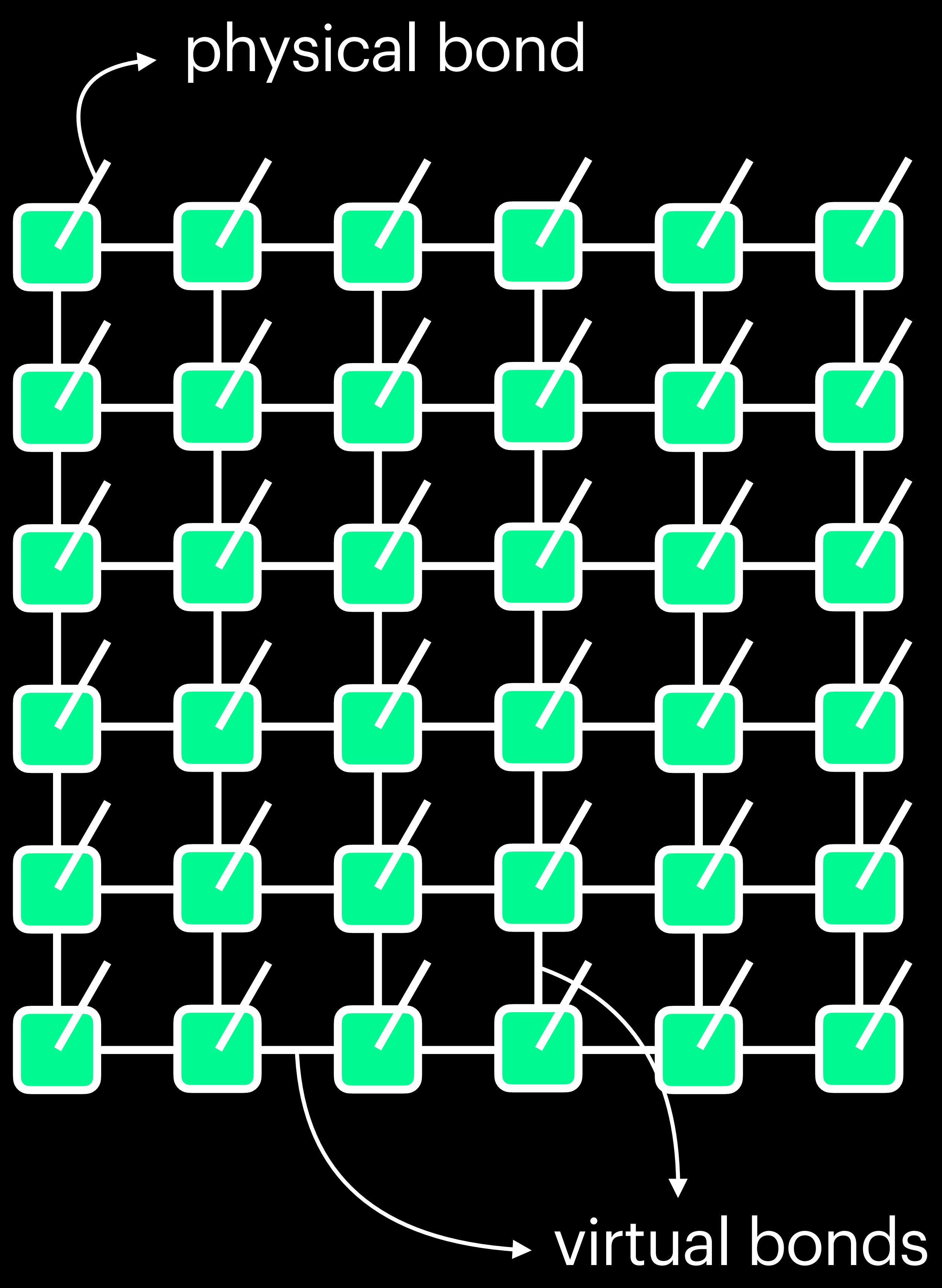
No simplification is possible in the calculation of expected values for local physical quantities

Possibly less accurate than sequential methods

To recover the isometric condition, end-to-end sweeps that cannot be parallelized are required.

2D tensor network state
(Projective Entanglement-Pair States, PEPS)

Projected Entangled Pair States (PEPS)



- PEPS is a 2D tensor network version of MPS

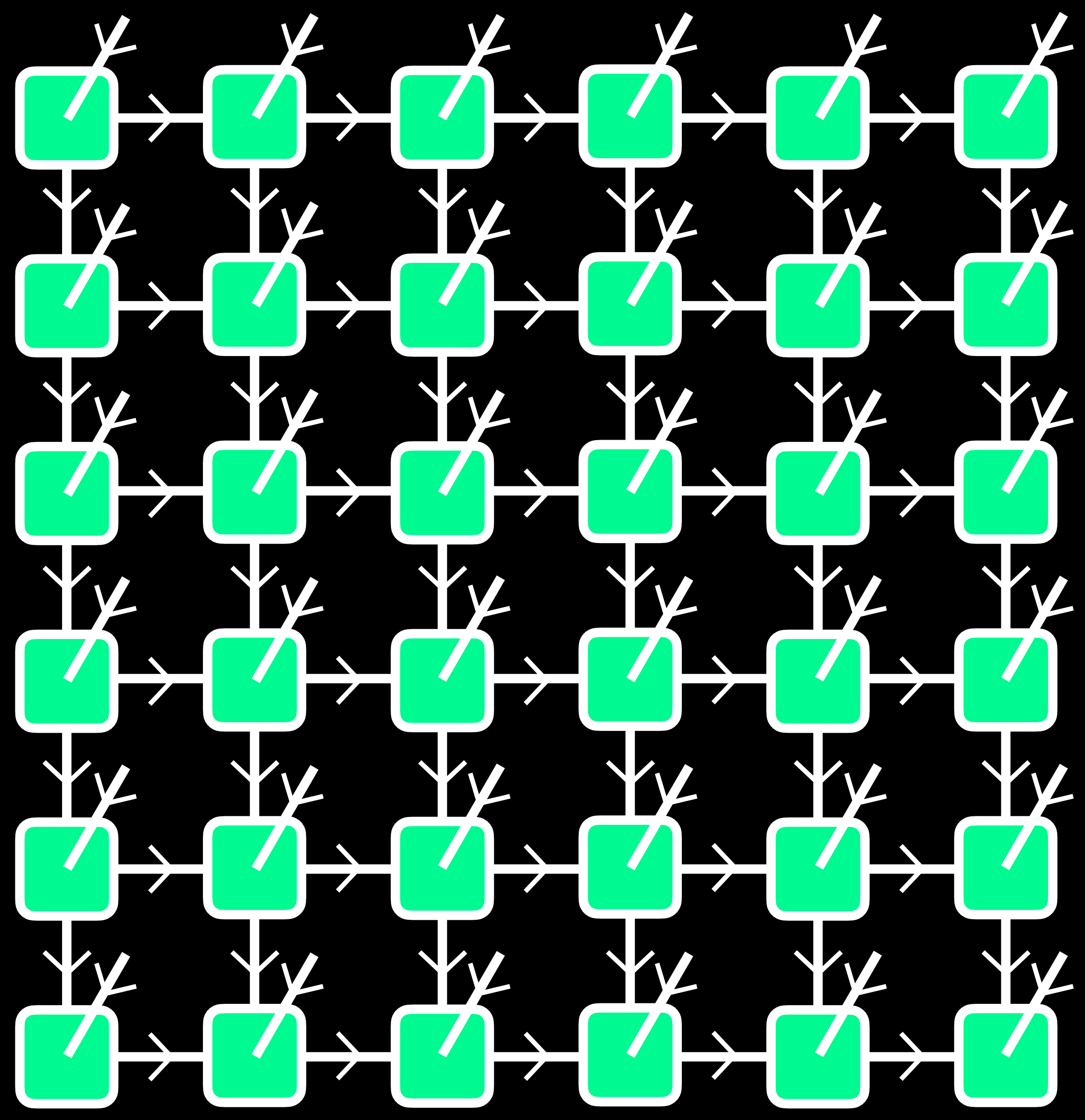
- Each tensor has virtual bonds on 2D lattice and one physical bond.

- Any state can be transformed into PEPS form
(if we do not limit the bond dimension.)

- Approximation sets the maximum bond dimension χ

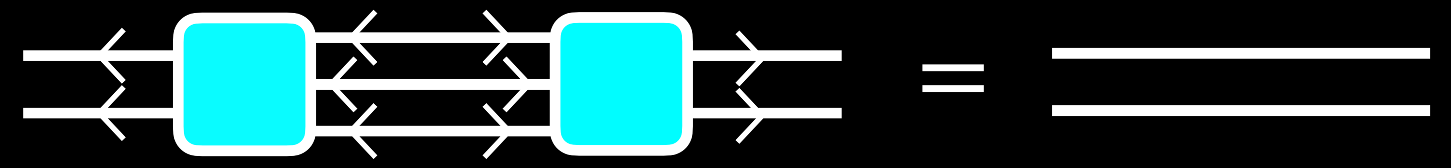
Isometric tensor network state (IsoTNS)

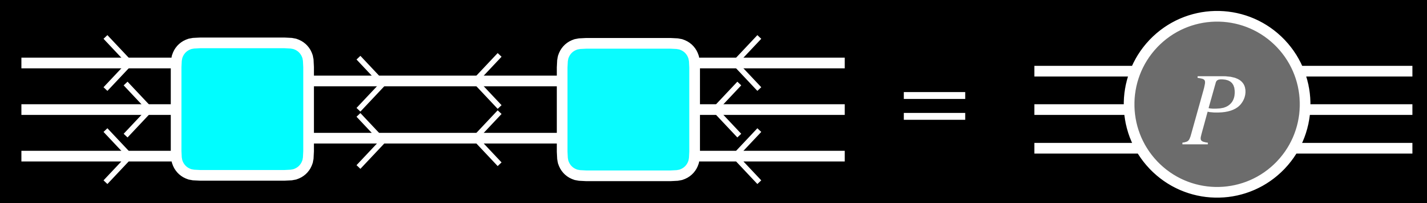
[Zeletel&Pollmann, PRL **124**, 037201 (2020)]



- Tensor network composed of isometric tensors

- To clarify the direction of isometry, we use arrows.





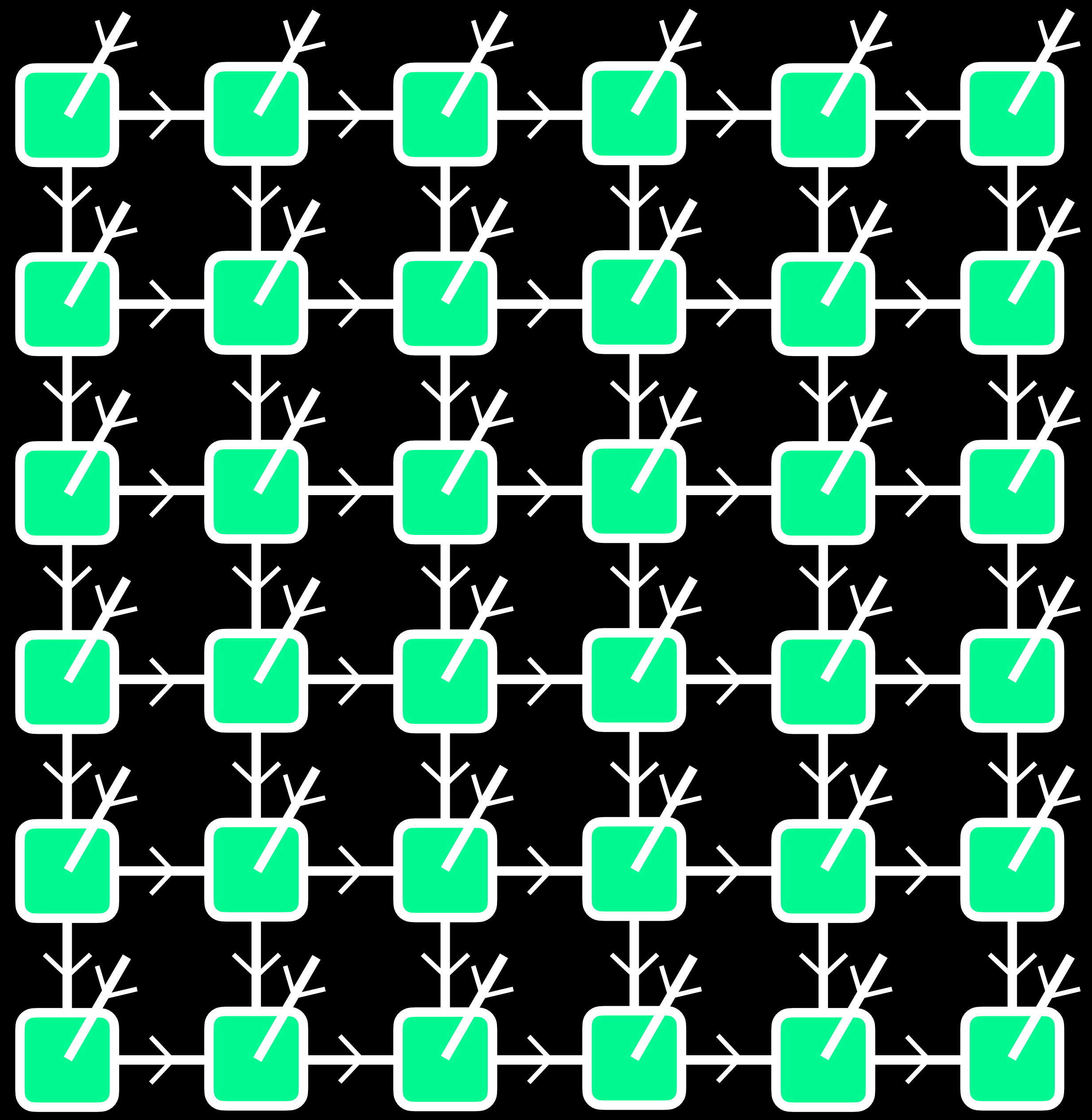
For isometry, opposite contraction yields projector.

- Assume that the arrows of physical bonds always point into the tensor.

- For 1D system, MPS's with canonical form are IsoTNS.

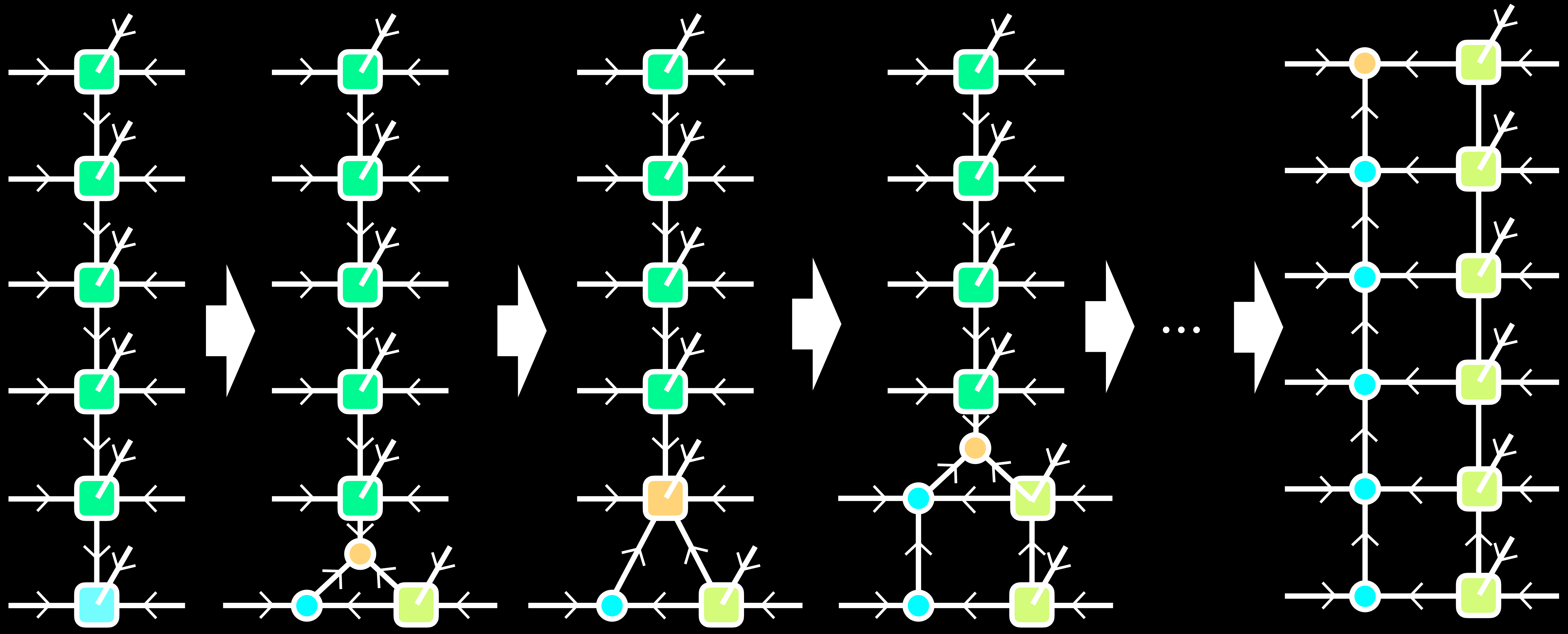
- For 2D system, IsoTNS is a PEPS with Isometric condition.

Isometric tensor network state (IsoTNS)



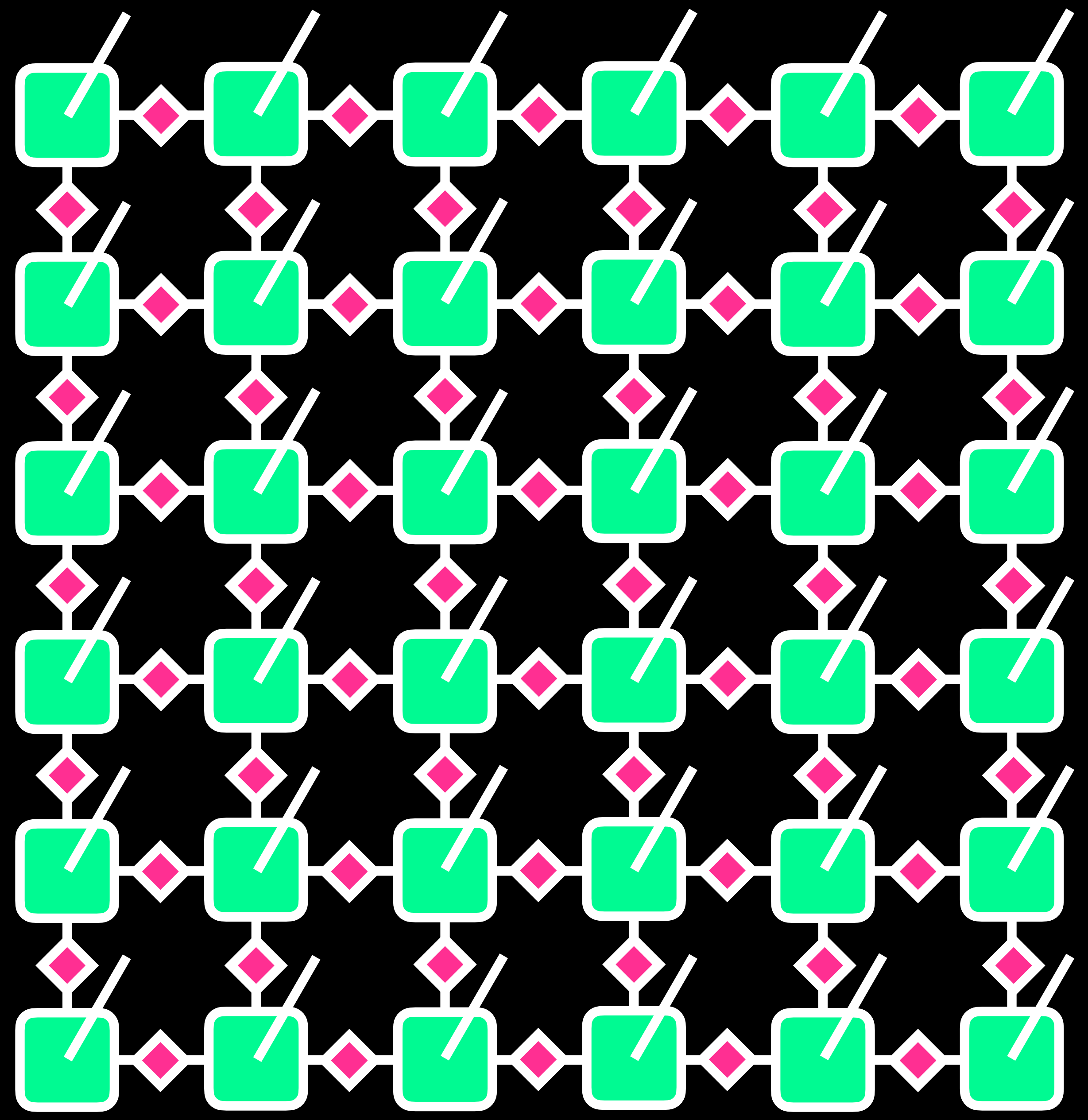
Unlike in MPS, reversing the direction of Isometry is non-trivial.

Moses move method [Zeletel&Pollmann, PRL **124**, 037201 (2020)]



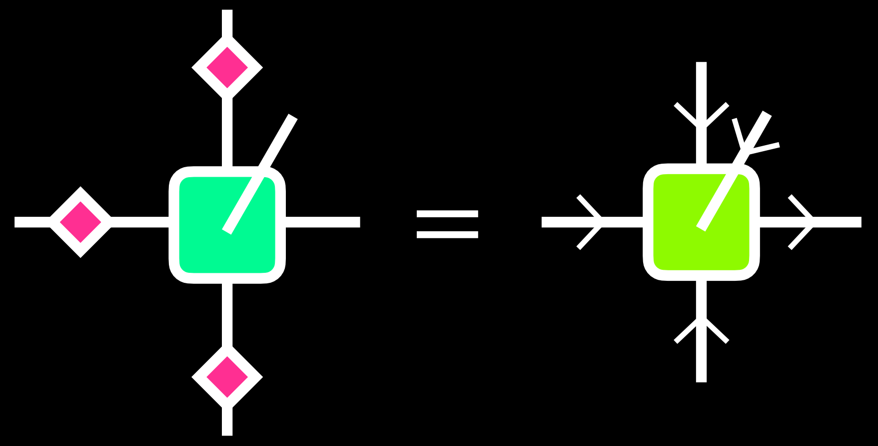
Unlike QR/SVD, Moses move is an approximation method.

Isometric tensor network state (IsoTNS)



Gauging Tensor Network [Tindall&FIshman, arXiv:2306.1783]

- Vidal gauge

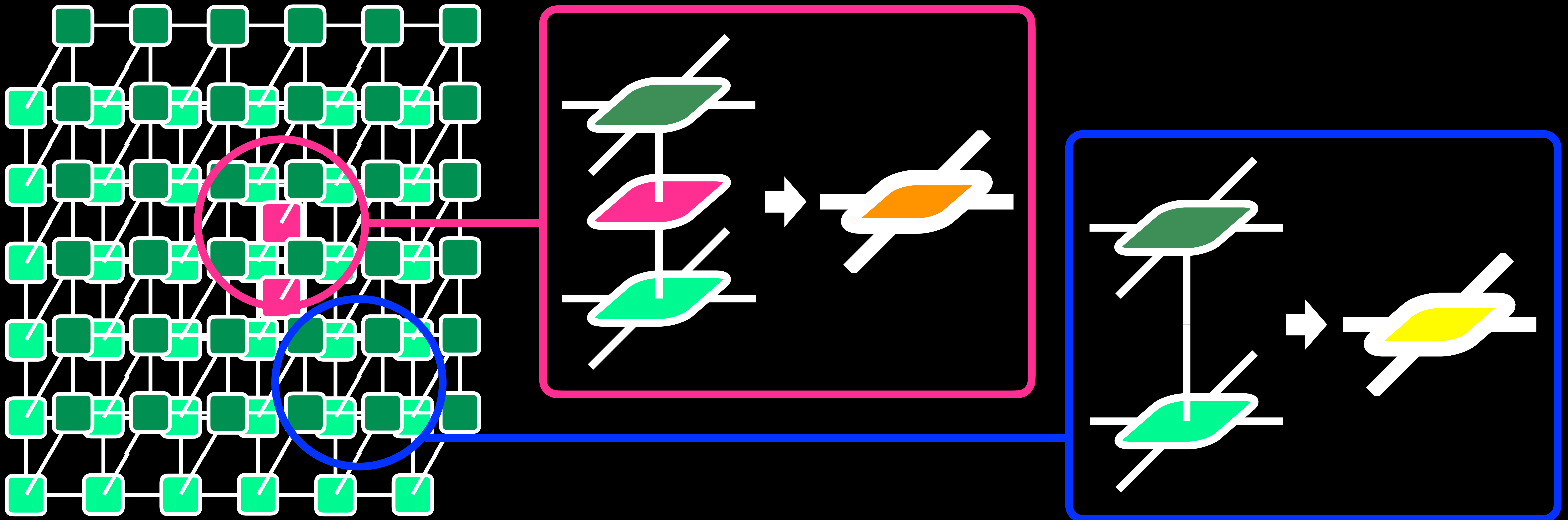


- A approximate **iterative** method to obtain this gauge using belief propagation has been proposed. [Tindall&Fishman, arXiv:2306.17837]

- Evenbly gauge [Evenbly, Phys. Rev. B **98**, 085155 (2018)]

Calculation of expectation value

When taking expectation value of local quantity for PEPS, the computation time is exponential if we try to take all contractions.



Calculation of expectation value

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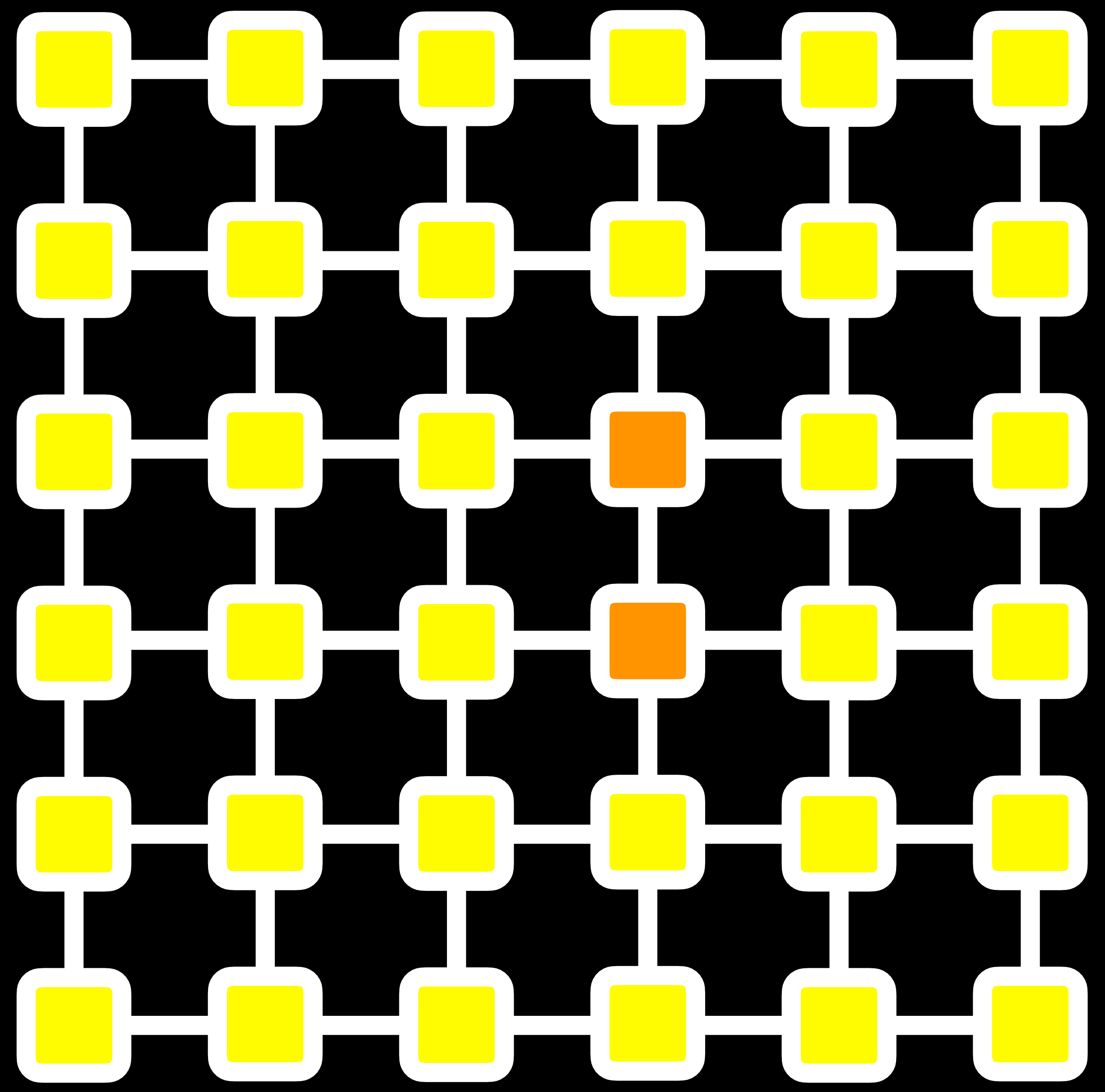
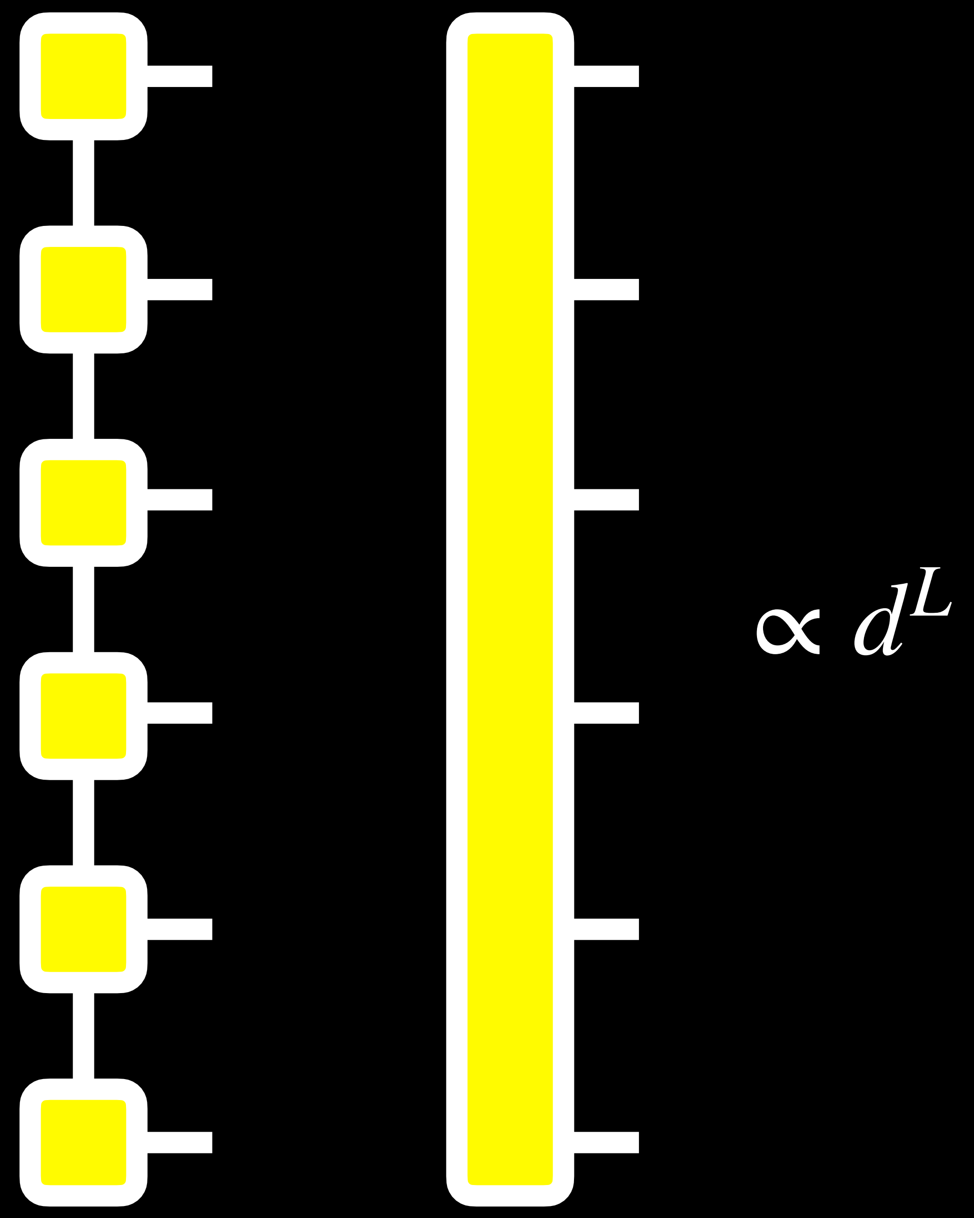
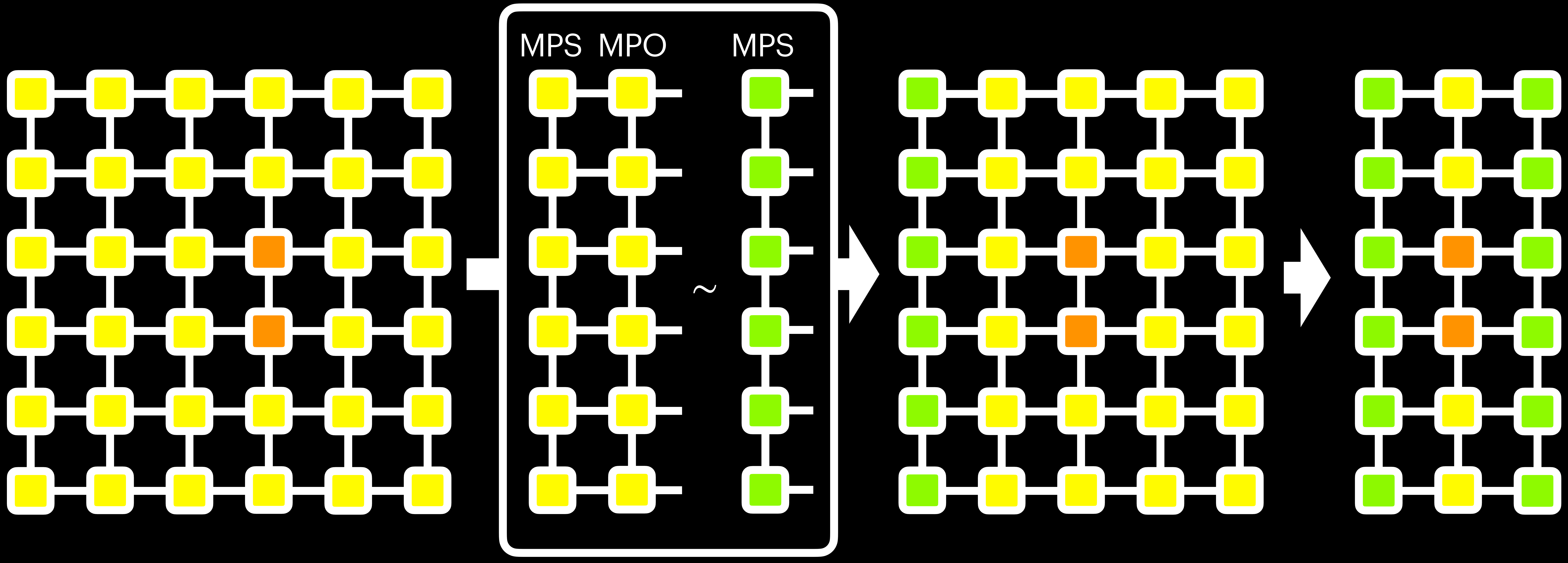




Calculation of expectation value

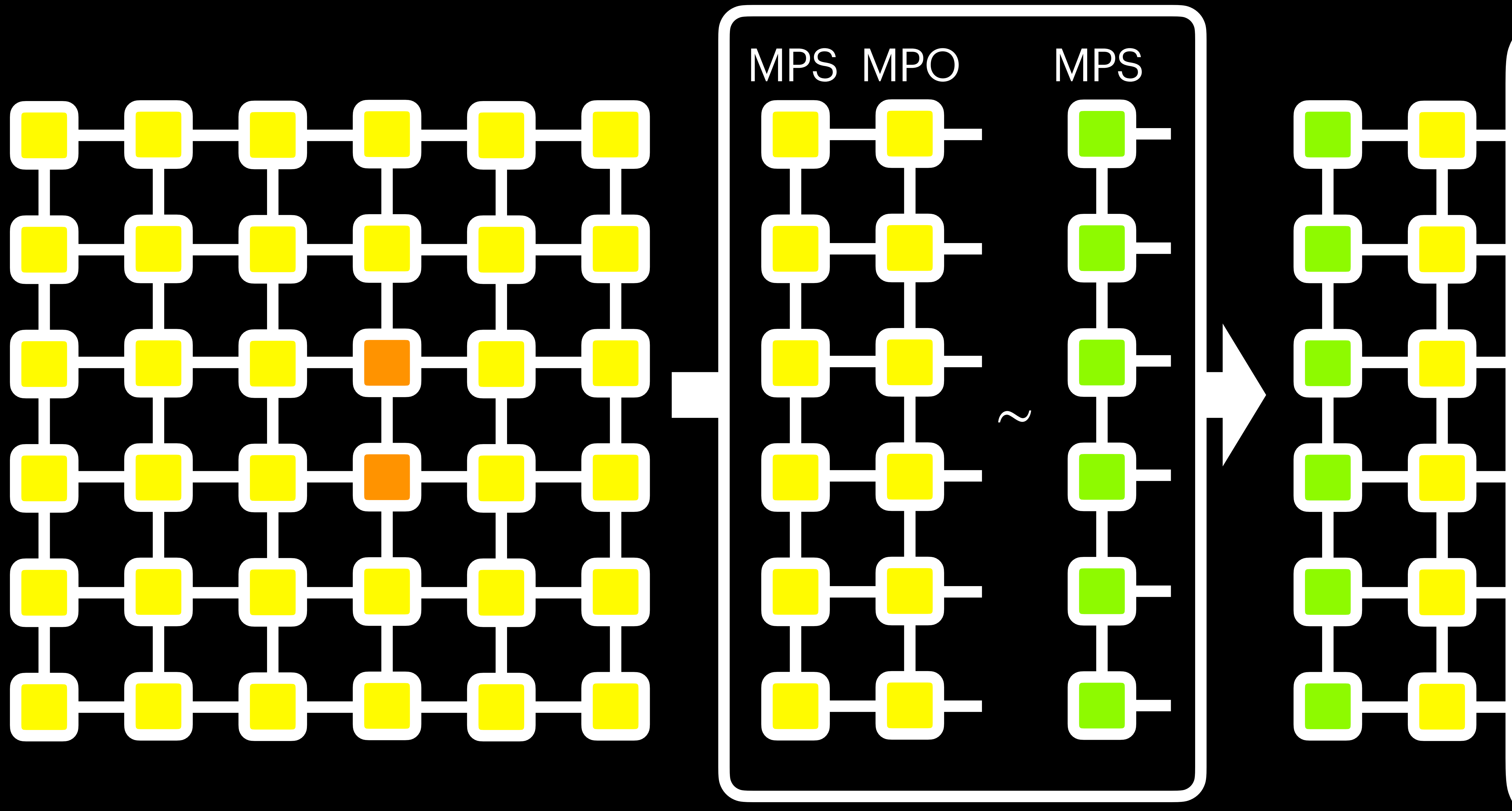
A possible way of the contraction is “boundary-MPS” method



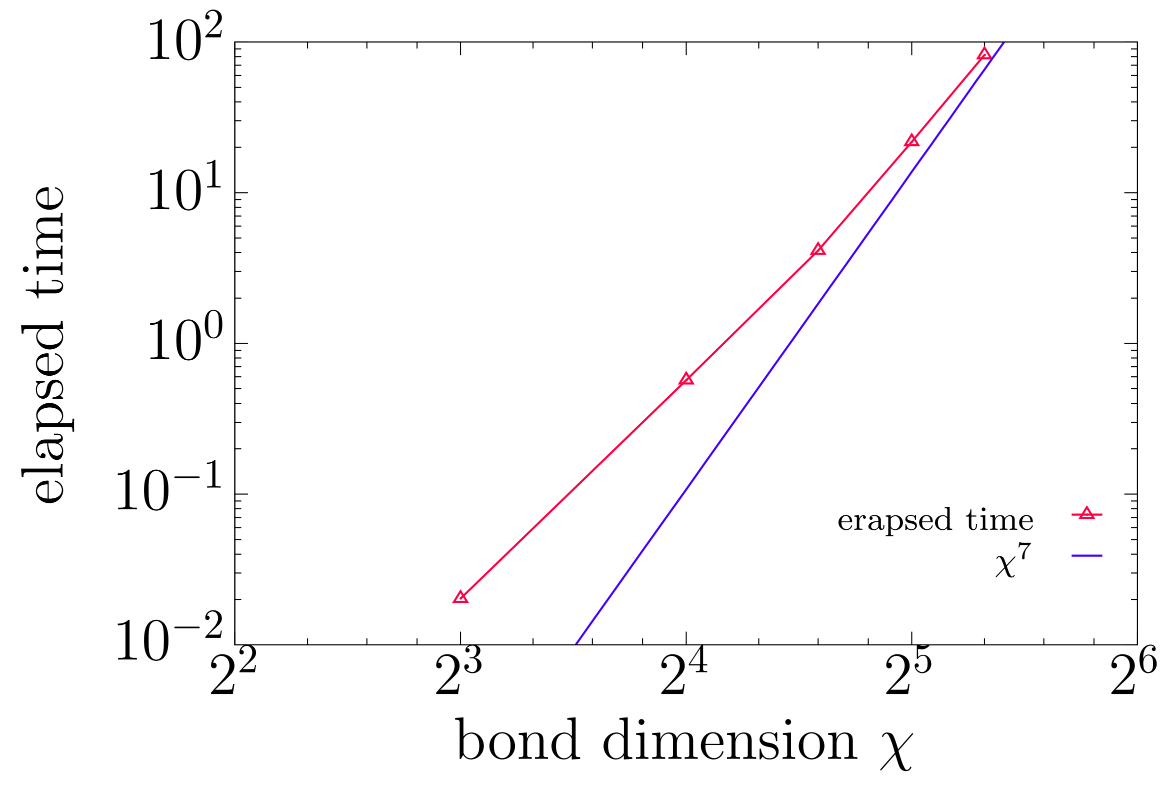
However, computational cost becomes large.

Calculation of expectation value

A possible way of the contraction is “boundary-MPS” method



By using the Monte Carlo method, the computational cost can be reduced.

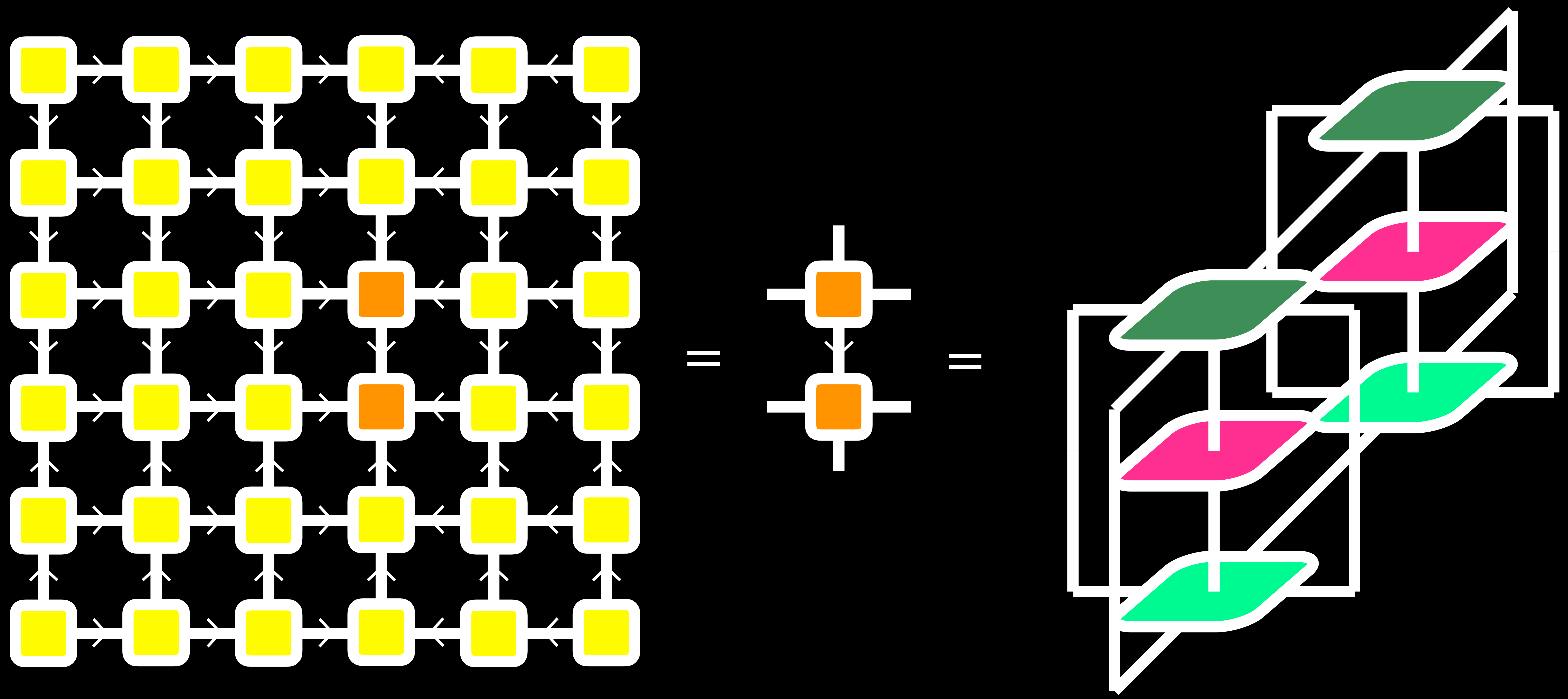


Calculation cost for MPO-MPS part scales as $O(\chi^7)$

However, computational cost becomes large.

Calculation of expectation value

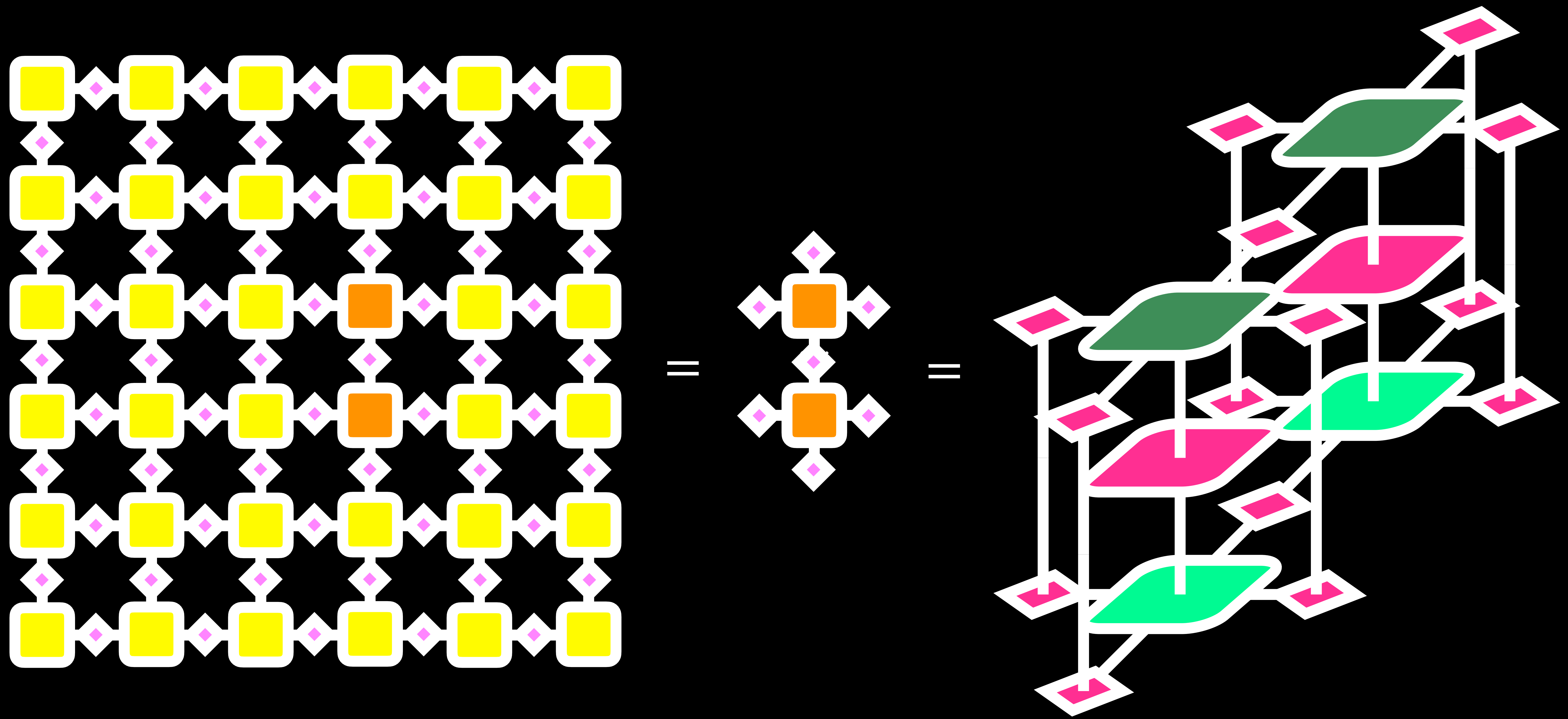
However, in IsoTNS, it is drastically easy.



Problem is that we need “**sequential transformation using Moses move.**”

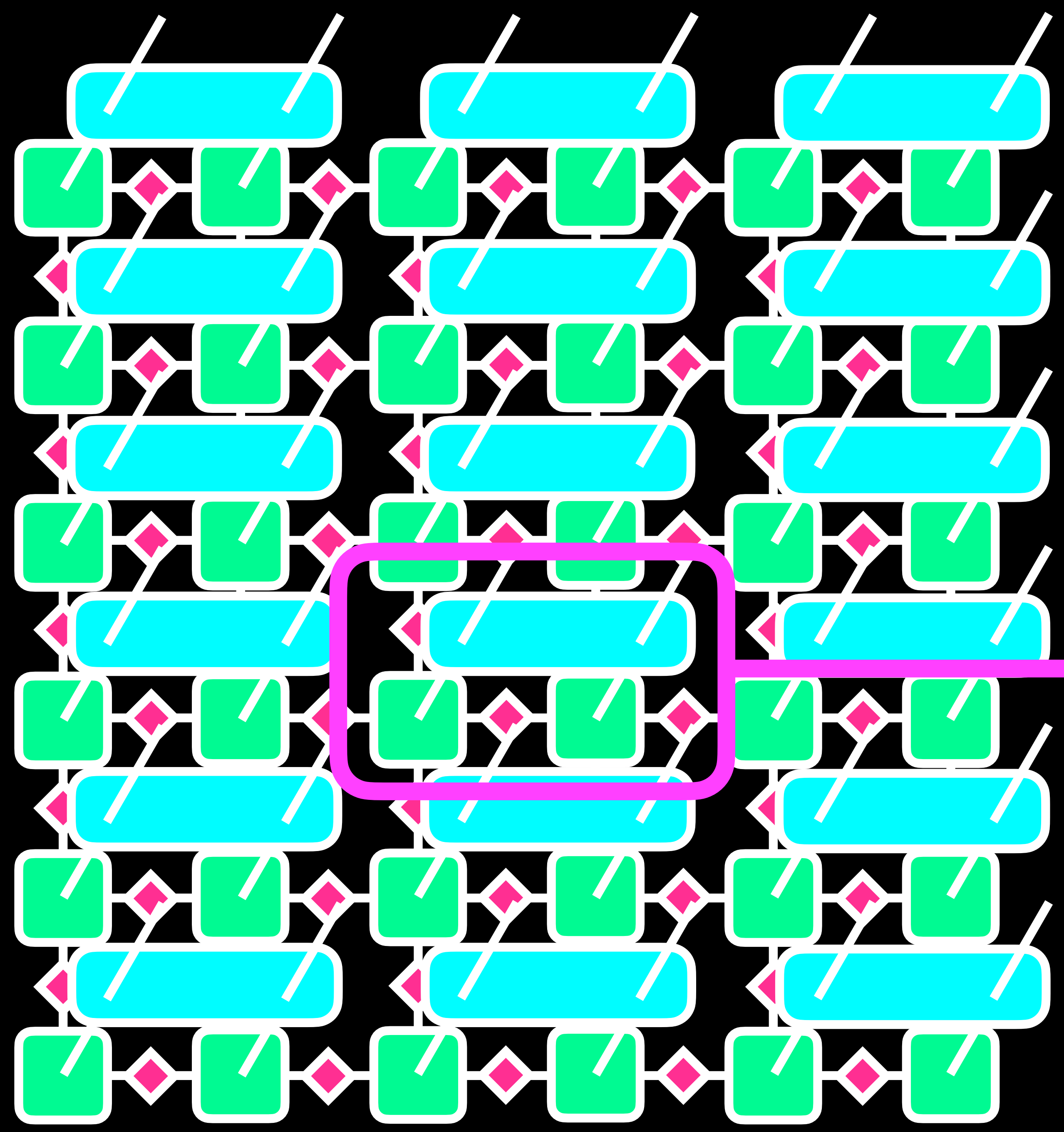
Calculation of expectation value

GaugingTNS also becomes same to IsoTNS.

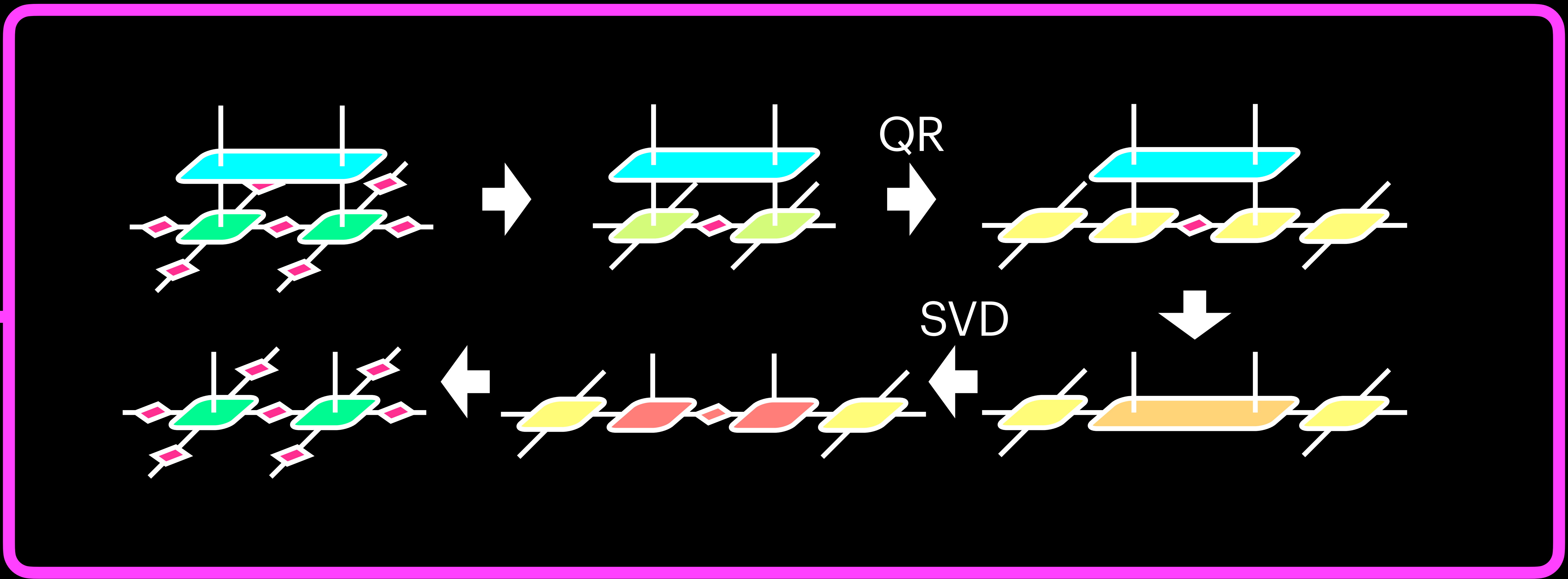


Problem is that belief propagation needs **sequential optimization**.

Parallel TEBD²



Like pTEBD, local unitary operation can be parallelized

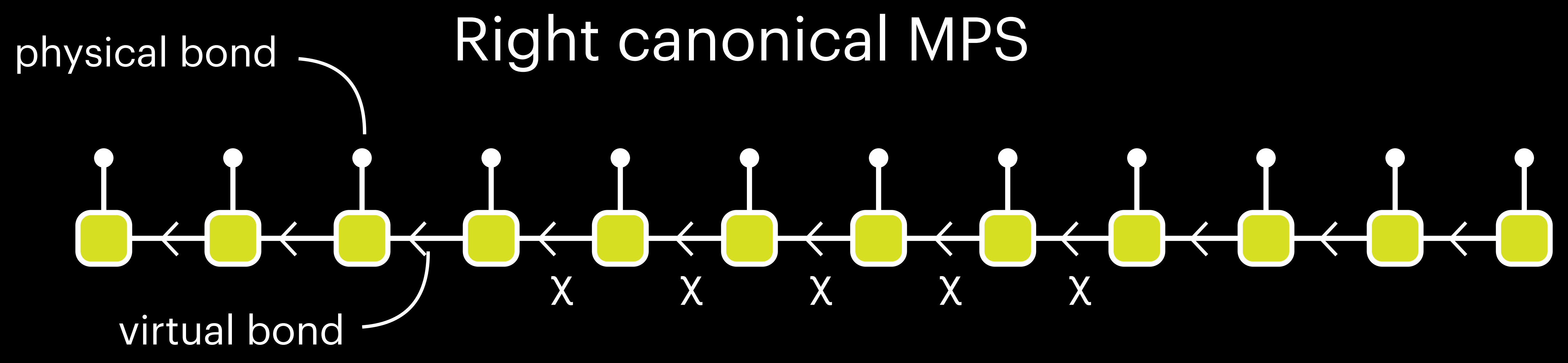


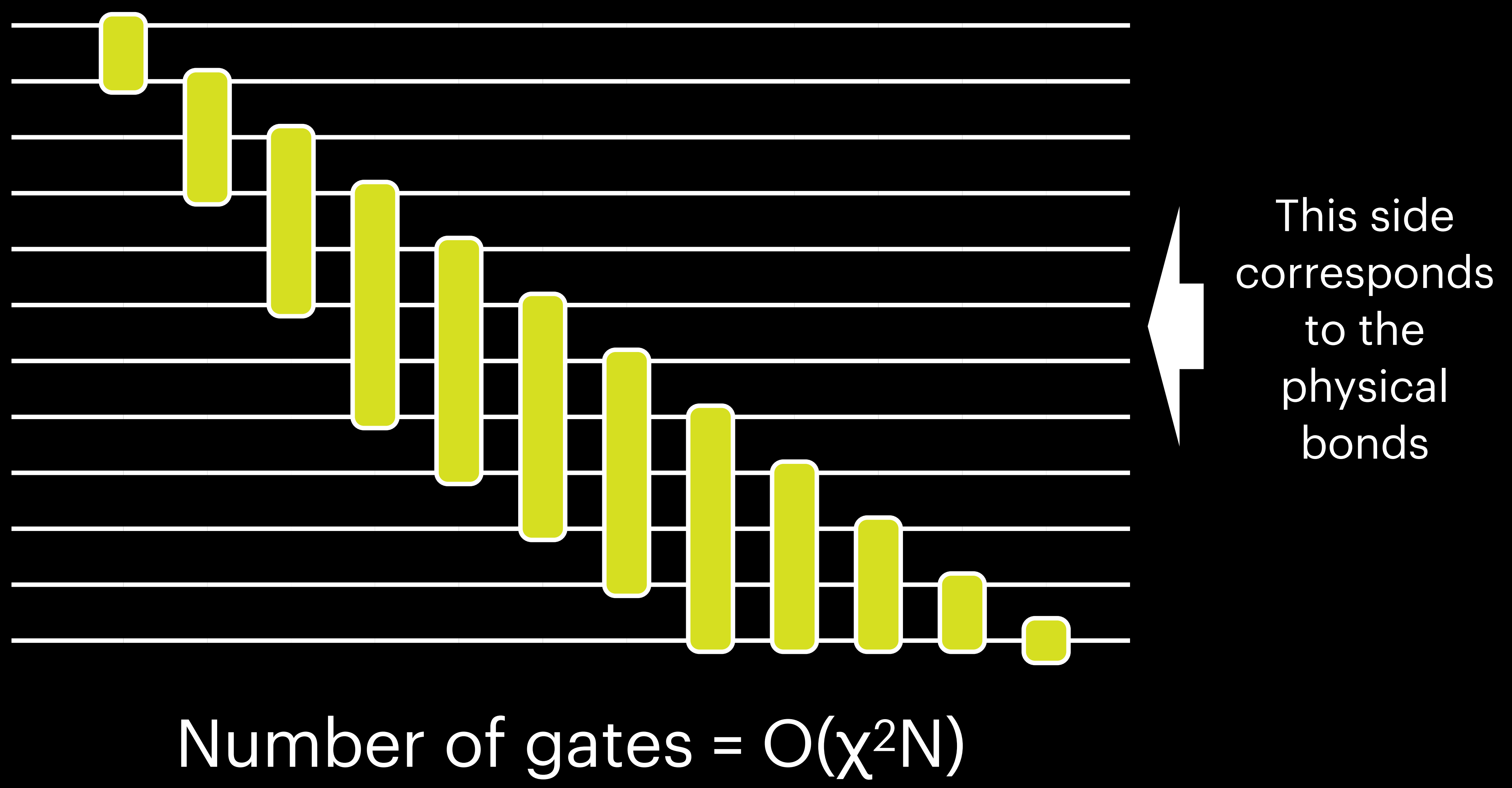
We are now exploring the way to recover the Vidal gauge efficiently.

Relation to Quantum Computing

Tensor network and Quantum Circuit

MPS and Quantum Circuit





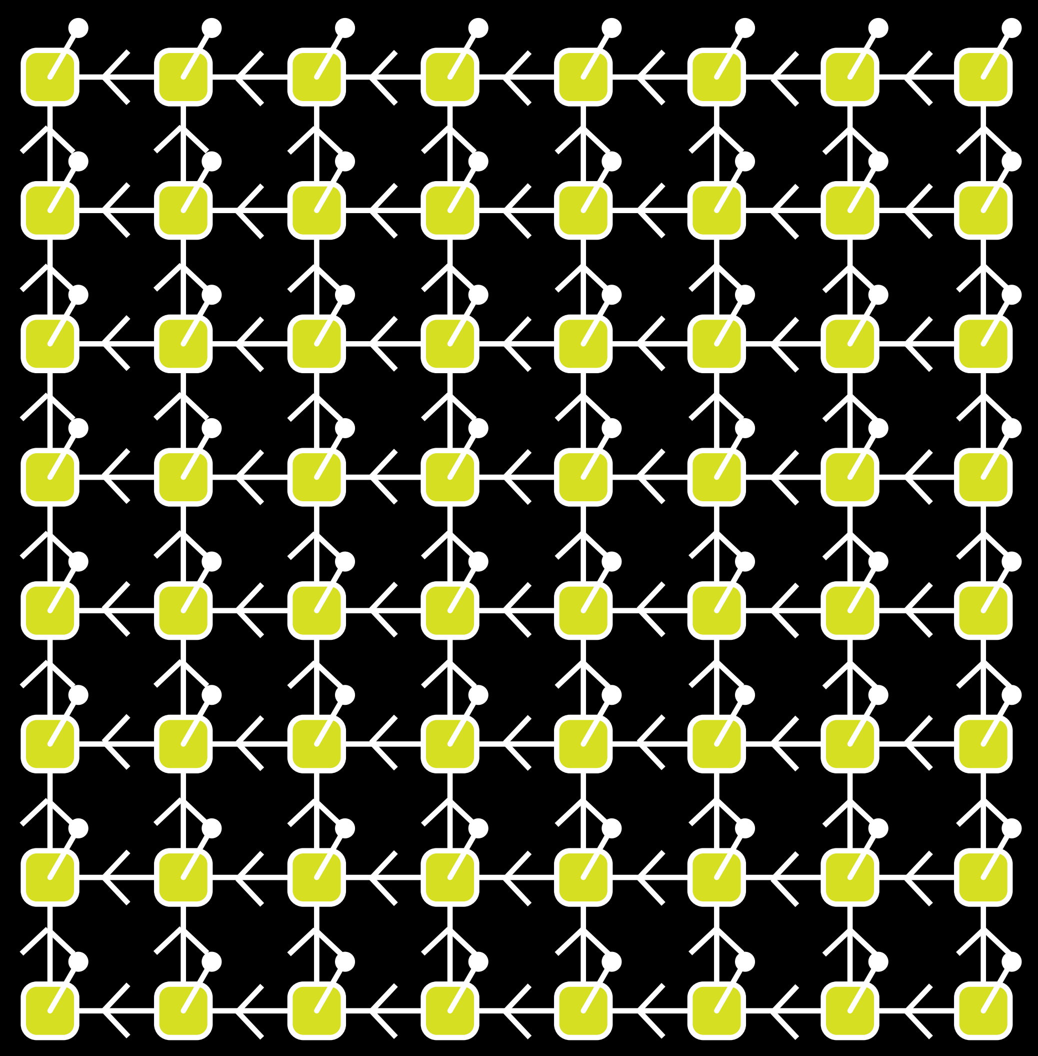
MPS-based circuits can be simulated efficiently in classical computer.

This means the simulator is useful for preparing the input states by MPS-based circuit

Tensor network and Quantum Circuit

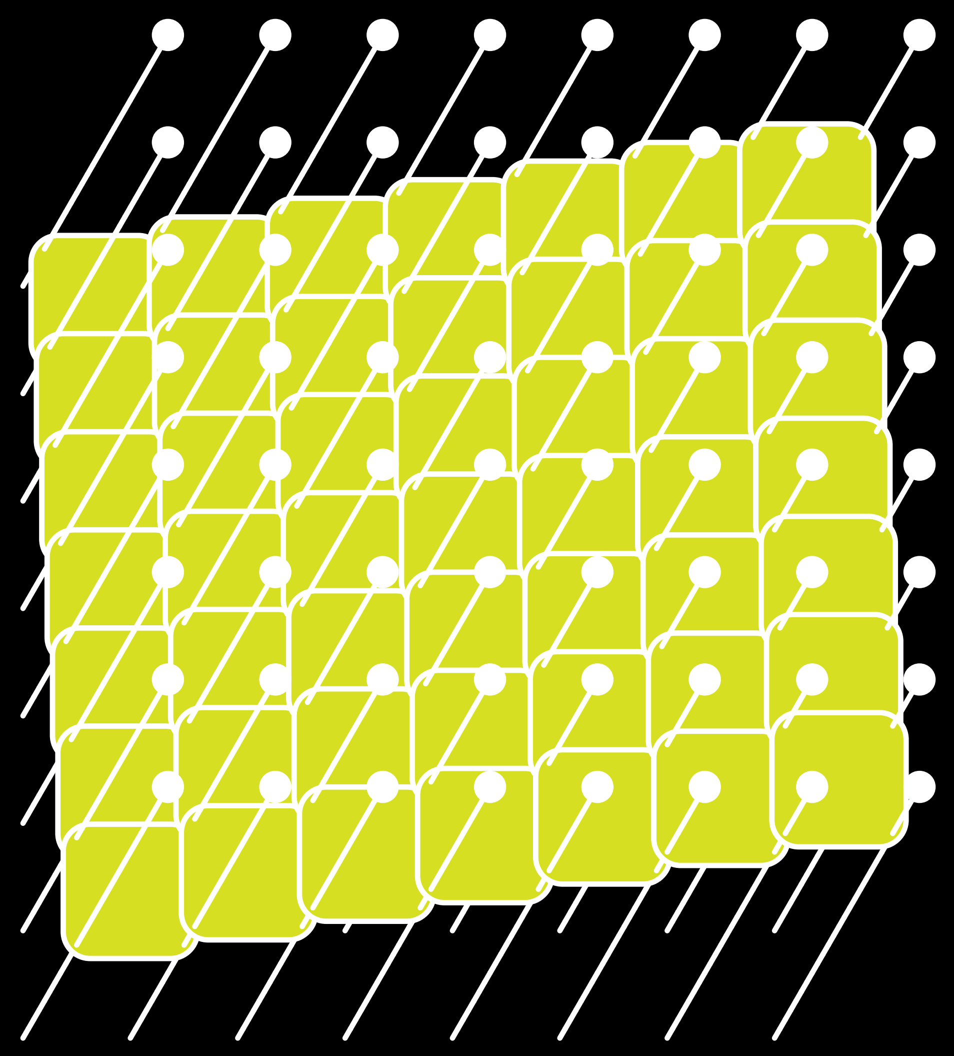
MPS and Quantum Circuit

2D IsoTNS



Absence of barren plateau in 2D IsoTNS circuit [Slattery&Clark, arXiv:2108.02792]

A circuit representation of PEPS



Number of gates = $O(\chi^4 N)$

PEPS-based circuits require exponential computational cost on classical computers but $O(\chi^4 N)$ on a quantum computer.

Summary

Isometric tensor network (**IsoTN**) and **gauging tensor network** (**GaugingTN**) have big advantages for

- evaluating expectation value of local quantity
- sometime accuracy
- **converting the classical information to the quantum circuit**

However, **converting to isometric form requires sequential operations,** so it is **difficult to parallelize that part.**