Russian Quantum Center
MISIS National University of Science and Technology

TENSOR NETWORKS: FROM NUMERICAL METHODS TO UNDERSTANDING QUANTUM SYSTEMS

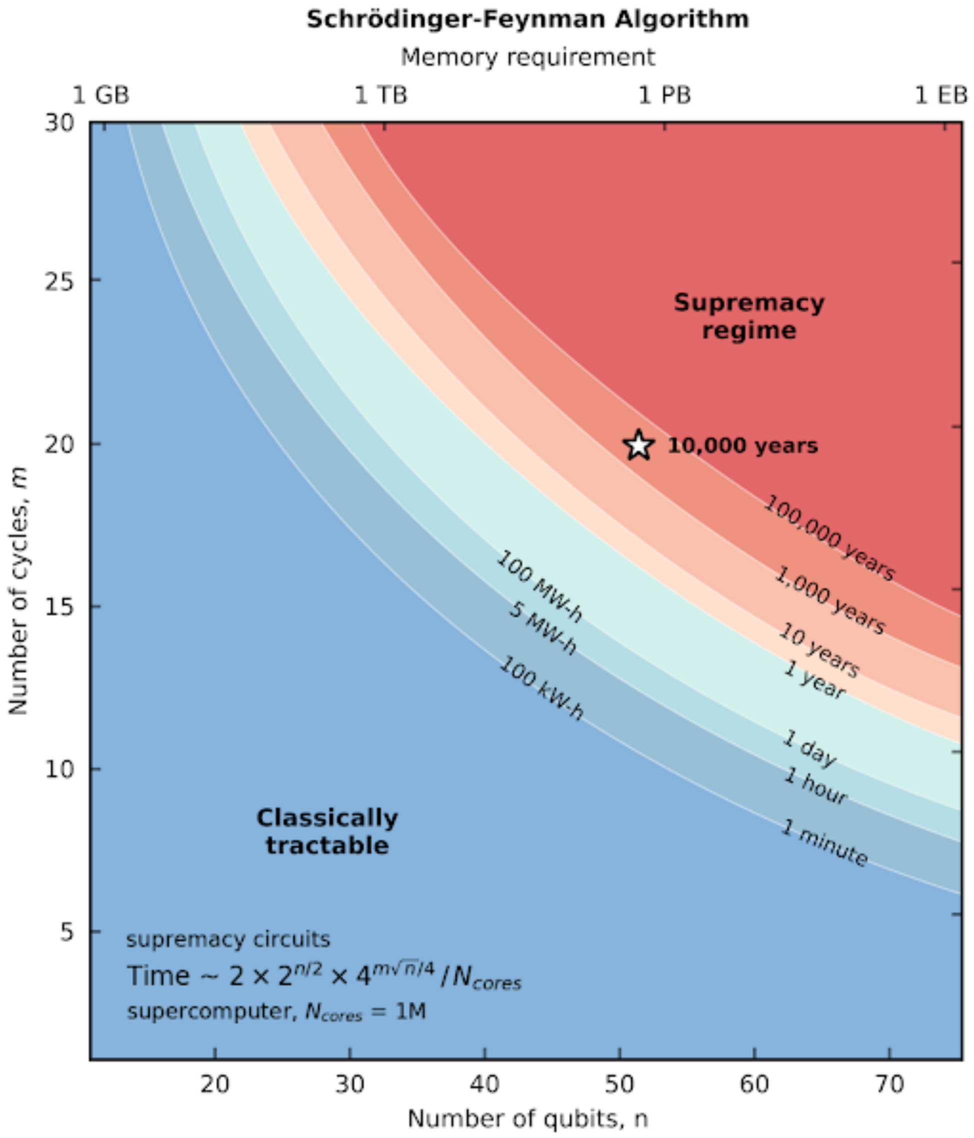
Gavreev Maxim Alexandrovich
m.gavreev@rqc.ru

Introduction

➢ **Tensor Networks** (TN's) are **emerging interdisciplinary** field. It provide an elegant and efficient way to represent and compute properties of complex quantum systems.

➢ By expressing large quantum states as **interconnected** networks of **smaller** tensors, they allow us to overcome the exponential complexity inherent to many-body problems.

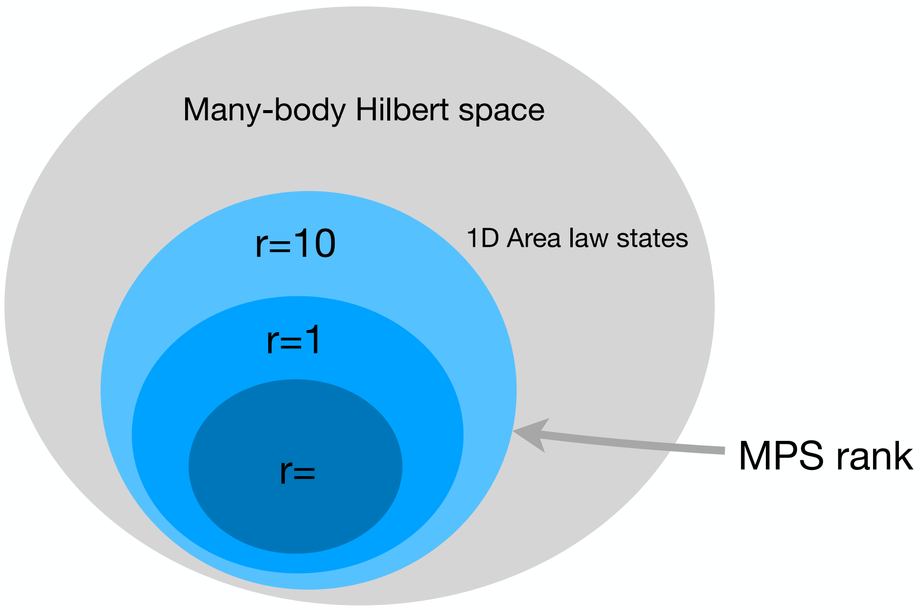
➢ In quantum physics and quantum optics, tensor networks serve as a bridge between abstract theory and computational practice — enabling **simulations** of entangled systems, optimization of quantum circuits, and exploration of novel quantum phases of matter.

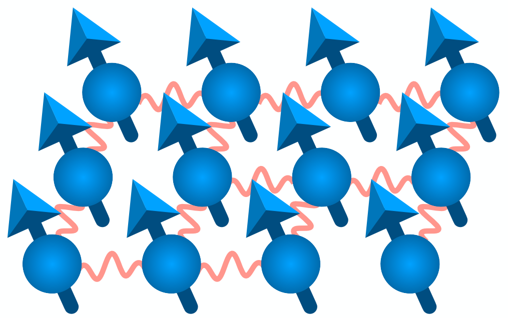


Motivation

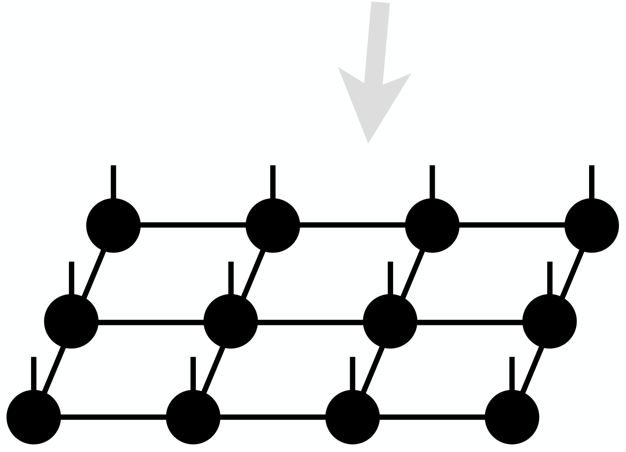
➢ **Simulation** of many-body quantum systems requires **enormous computational** resources.

➢ Finding the **ground states** of many-body quantum systems are of particular interest but **intractable** at scale.





Quantum many-body system



Model (Tensor Network)

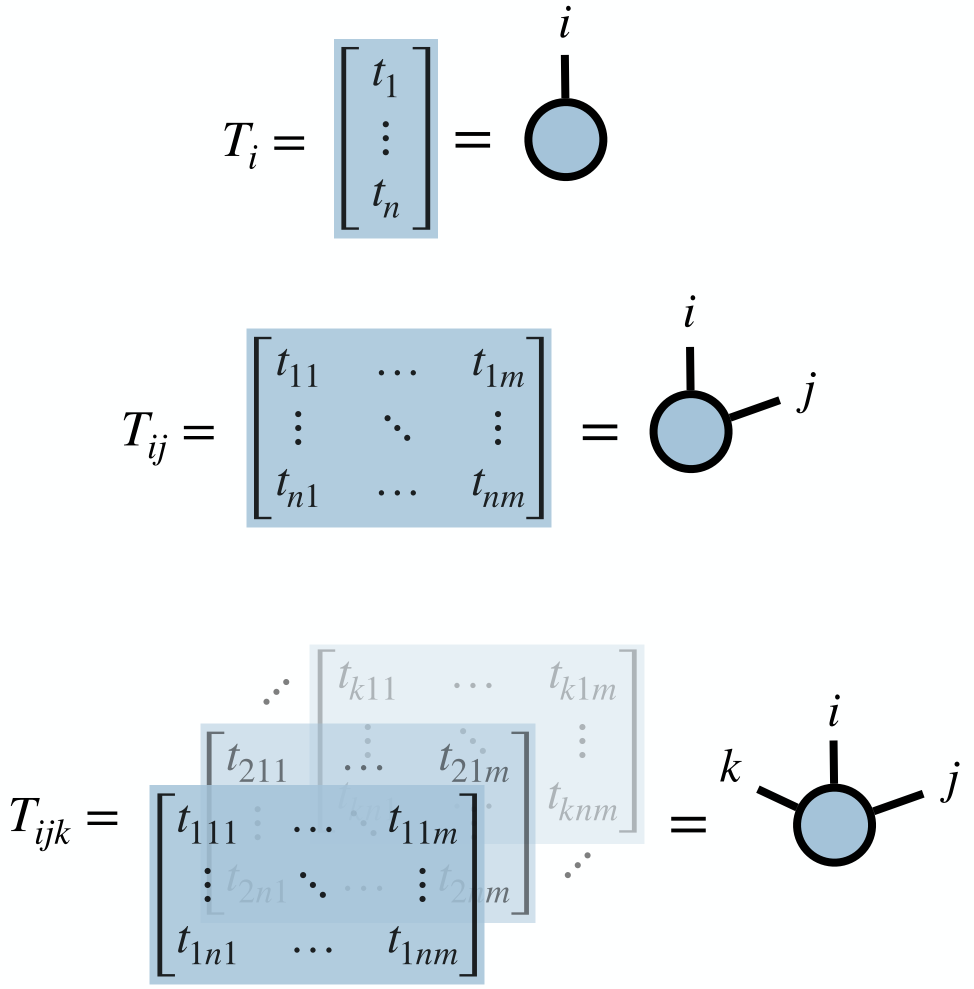
Introduction to tensor networks

➢There are two primary rules of tensor diagrams:

- **Tensors** are notated by **shapes**, and tensor **indices** are notated by **lines**.
- **Connecting** two index lines implies a **contraction**, or summation over the connected indices.

➢ Despite its graphical and intuitive nature, tensor diagram notation is completely **rigorous** and well defined.

➢ Inspired by the **Einstein summation** convention for notating tensor contractions.



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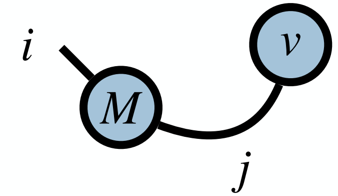
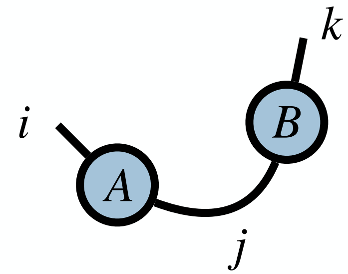
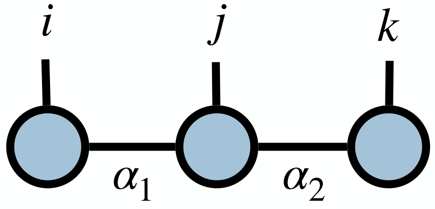


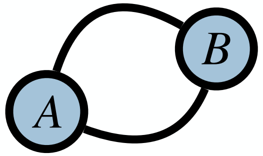
$$= \sum_j M_{ij} v_j$$



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

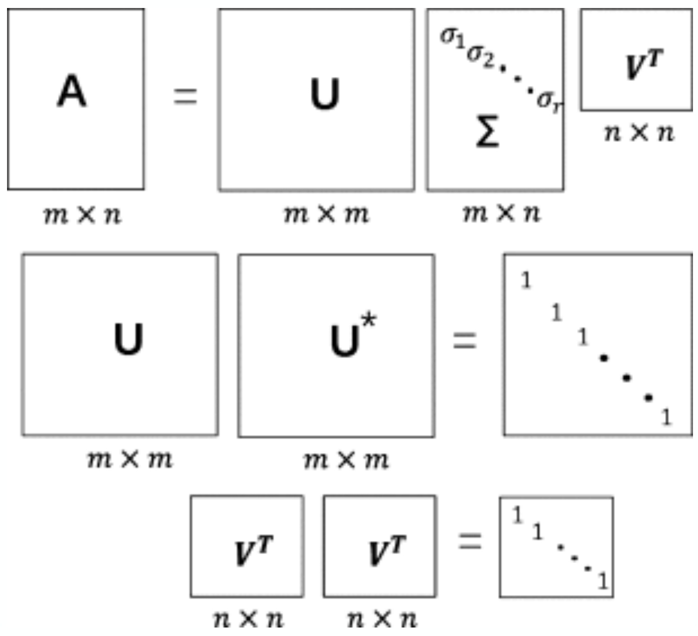


$$= \sum_{\alpha_1,\alpha_2} A^i_{\alpha_1} B^j_{\alpha_1,\alpha_2} C^k_{\alpha_2}$$

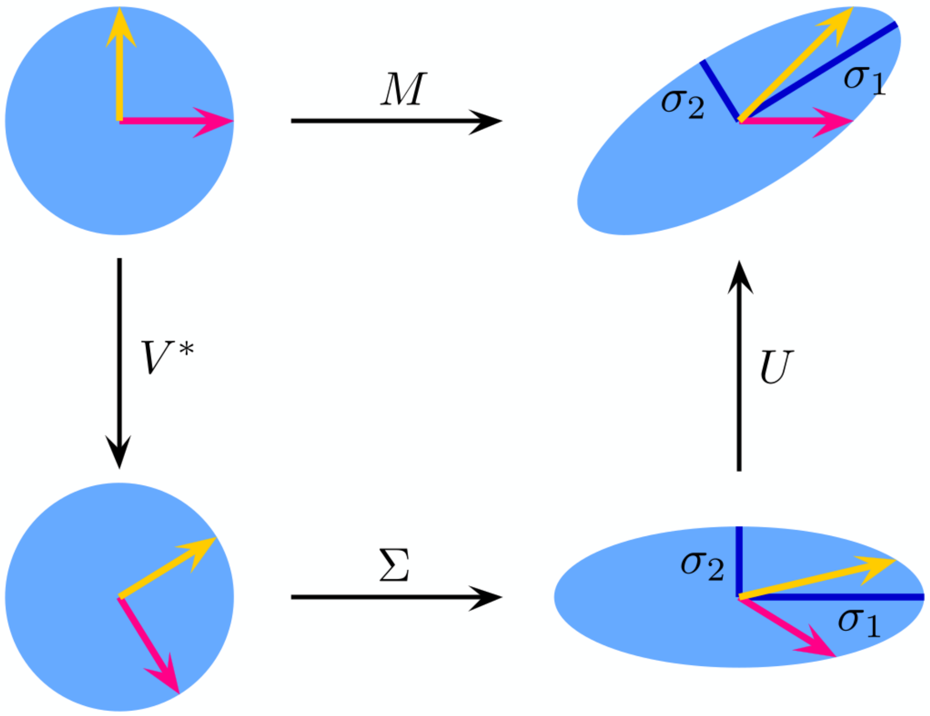


$$= \sum_{ij} A_{ij} B_{ji} = Tr[AB]$$

Singular value decomposition



Singular value decomposition (SVD)



$$M = U \cdot \Sigma \cdot V^*$$

Schmidt decomposition

➢ Suppose we are given a bipartite quantum state

$\{|i\rangle_A\} \in \mathscr{H}_A, \{|j\rangle_A\} \in \mathscr{H}_B$

$$|\psi\rangle_{AB} = \sum_{ij} C_{ij}|i\rangle_A|j\rangle_B$$

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$$|\psi\rangle_{AB} = \sum_{ij} C_{ij} |i\rangle_A |j\rangle_B$$

➢ Represent state vector as a matrix with each index (dimension) being a physical dimension of a subsystem.

➢ Apply singular value decomposition (SVD)

$$\sum_{ij} C_{ij} |i\rangle_A |j\rangle_B = \sum_{ij} \sum_{\alpha=1}^{\min(N_A,N_B)} U_{i\alpha} \Lambda_{\alpha\alpha} V^*_{j\alpha} |i\rangle_A |j\rangle_B =$$

$$= \sum_{\alpha=1}^{\min(N_A,N_B)} \lambda_\alpha |\alpha\rangle_A |\alpha\rangle_B$$

Schmidt decomposition

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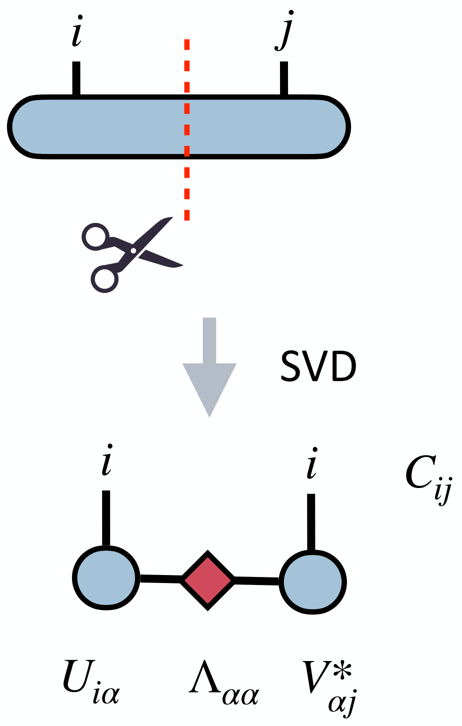
➢ **Schmidt decomposition**



von Neumann entropy $S = -\sum_\alpha \lambda_\alpha \log(\lambda_\alpha)$

MPS construction

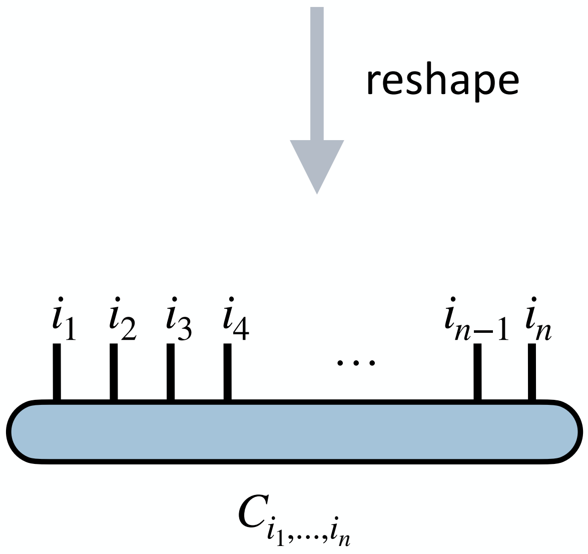
➢ Suppose we are given a multi-qubit quantum state vector $|\psi\rangle \in \mathscr{H}^{\otimes n}$:

$$|\psi\rangle = \sum_{i_1,\ldots,i_n} C_{i_1,\ldots,i_n} |i_1, \ldots, i_n\rangle, \quad i_k \in \{0,1\}$$

➢ Exponential number of complex amplitudes $C_{i_1,\ldots,i_n}$ are hard to process.

➢ Lets «reshape» it into tensor to separate physical degrees of freedom.

$$\sum_{i_1,\ldots,i_n} C_{i_1,\ldots,i_n} |i_1, \ldots, i_n\rangle = \begin{pmatrix} C_{00\ldots0} \\ C_{00\ldots1} \\ \vdots \\ C_{11\ldots0} \\ C_{11\ldots1} \end{pmatrix}$$



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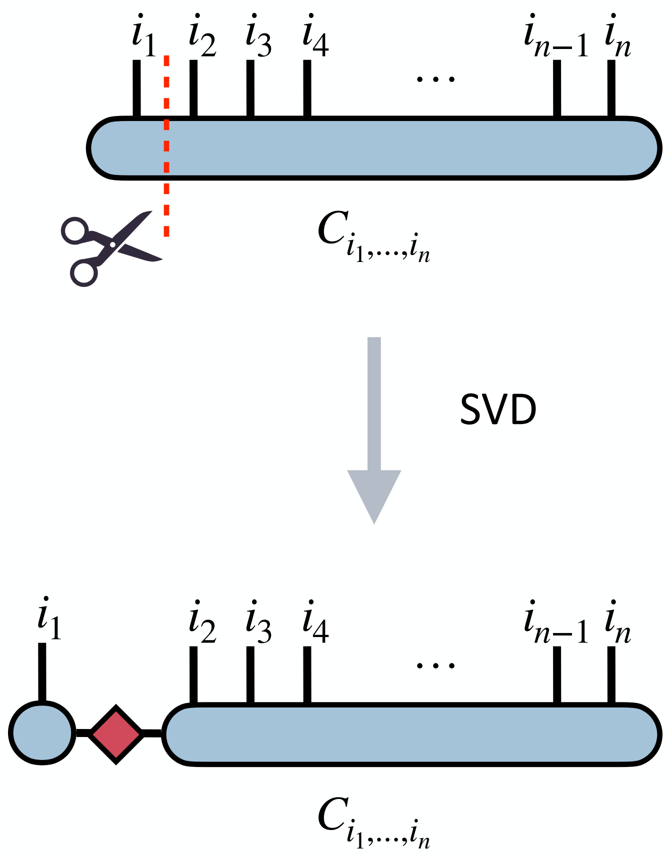
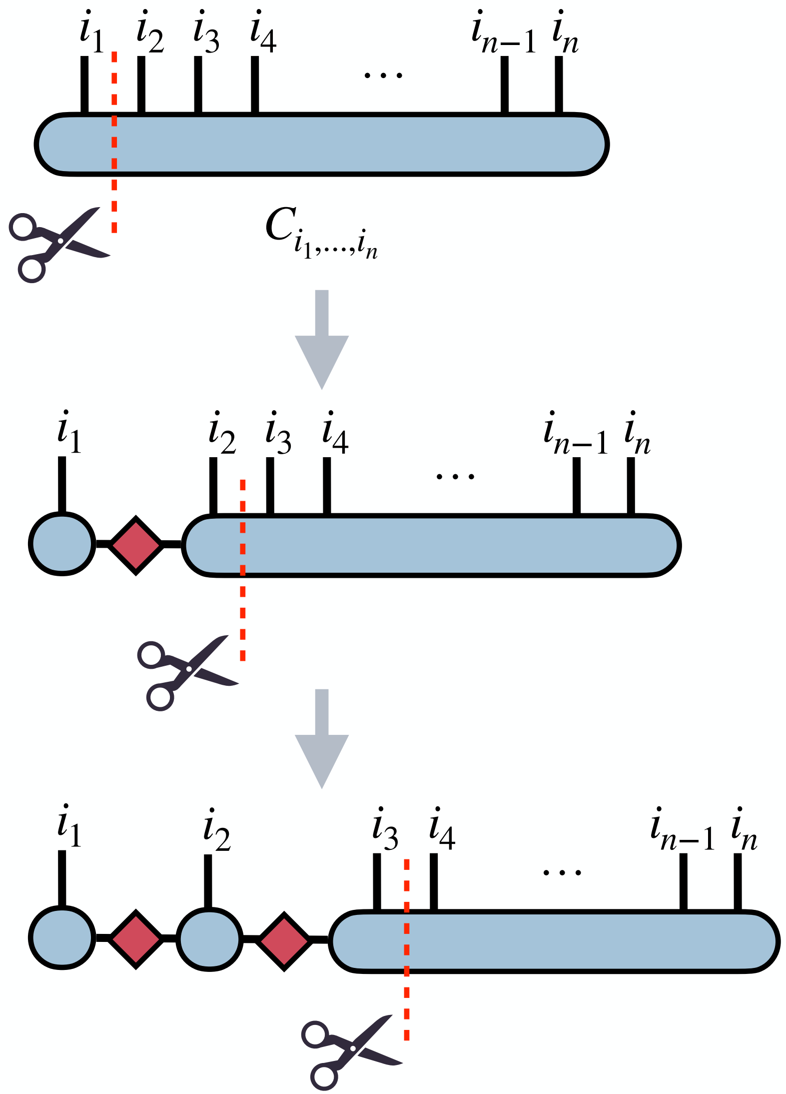
➢ Exponential number of complex amplitudes $C_{i_1,\ldots,i_n}$ are hard to process.

➢ Lets «reshape» it into tensor to separate physical degrees of freedom.

➢ Following the idea of Schmidt decomposition physical degrees of freedom can be factored using SVD.



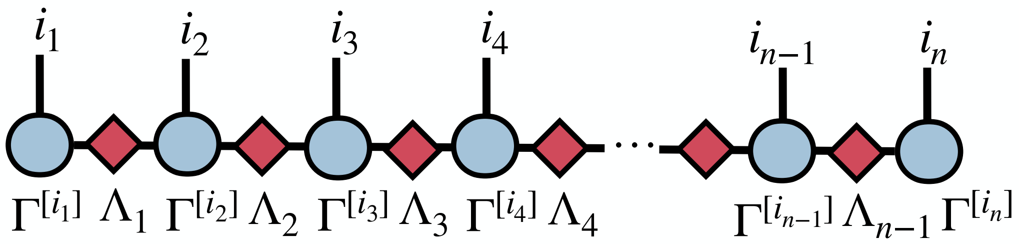
MPS construction



➢ An iterative process of factorization of physical degrees of freedom using SVD yields a tensor network.

➢ This tensor network is called Matrix Product State (MPS).

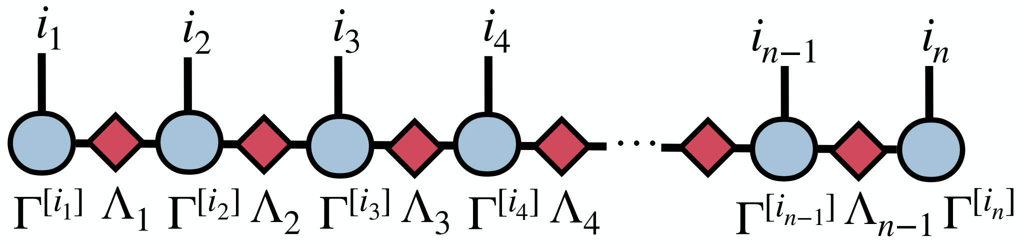
➢ In this network we have two types of indices: physical (free) and internal (bonds).



MPS
(Vidal's form)

$$|\psi\rangle = \sum_{\{i\}} \Gamma^{[i_1]}\Lambda_1\Gamma^{[i_2]}\Lambda_1\ldots\Lambda_{n-1}\Gamma^{[i_n]}|i_1,\ldots,i_n\rangle, \quad i_k \in \{0,1\}$$

MPS canonical forms



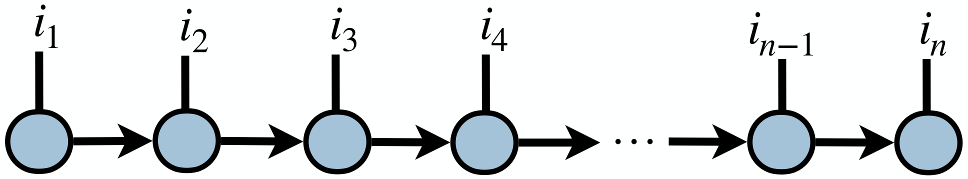
MPS
(Vidal's form)

➢ There are three main forms of MPS:

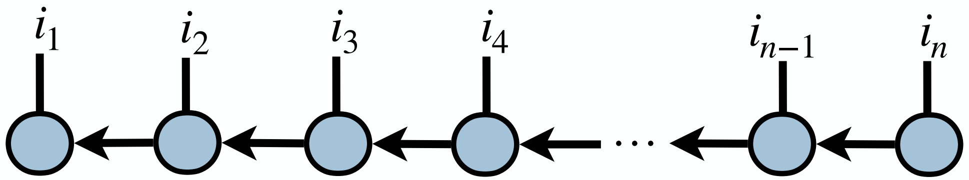
- Mixed canonical (or Vidal's form)
- Left canonical
- Right canonical

$$|\psi\rangle = \sum_{\{i\}} \Gamma^{[i_1]}\Lambda_1\Gamma^{[i_2]}\Lambda_1 \ldots \Lambda_{n-1}\Gamma^{[i_n]}|i_1, \ldots, i_n\rangle, \quad i_k \in \{0,1\}$$

MPS (**Left** canonical from)

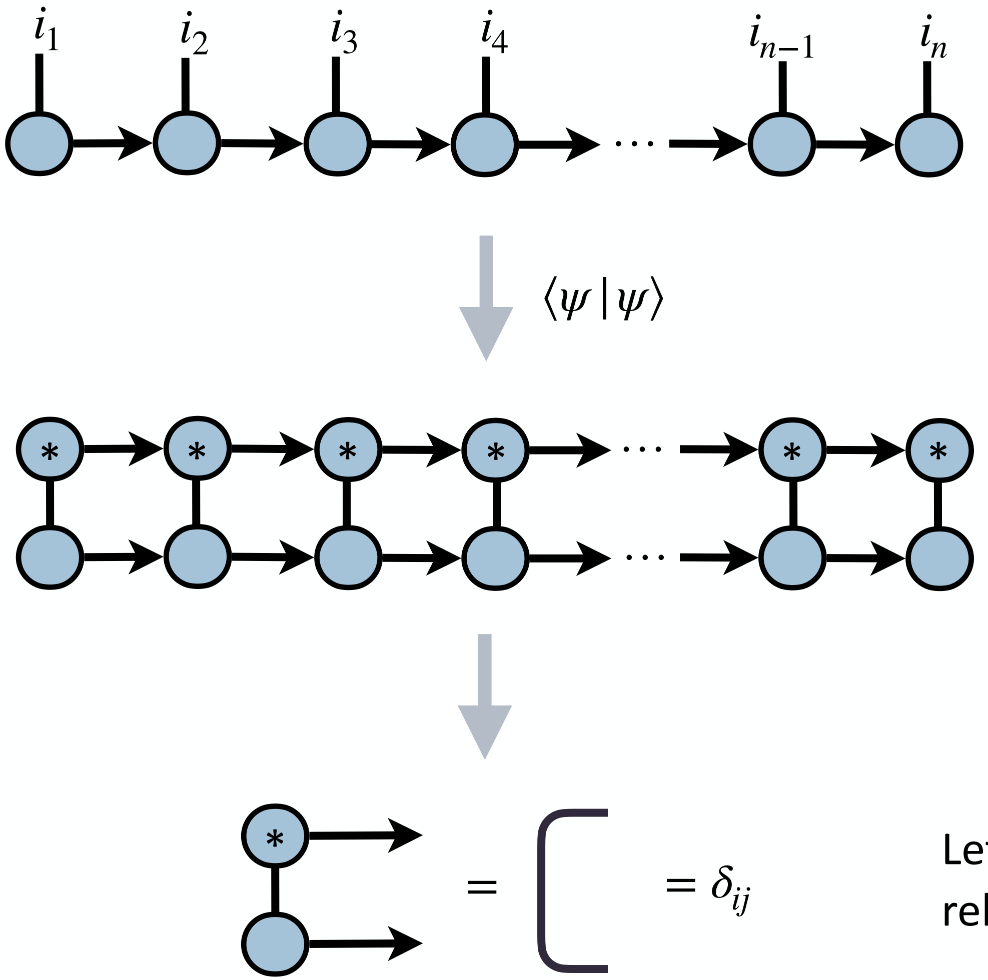


MPS (**Right** canonical from)

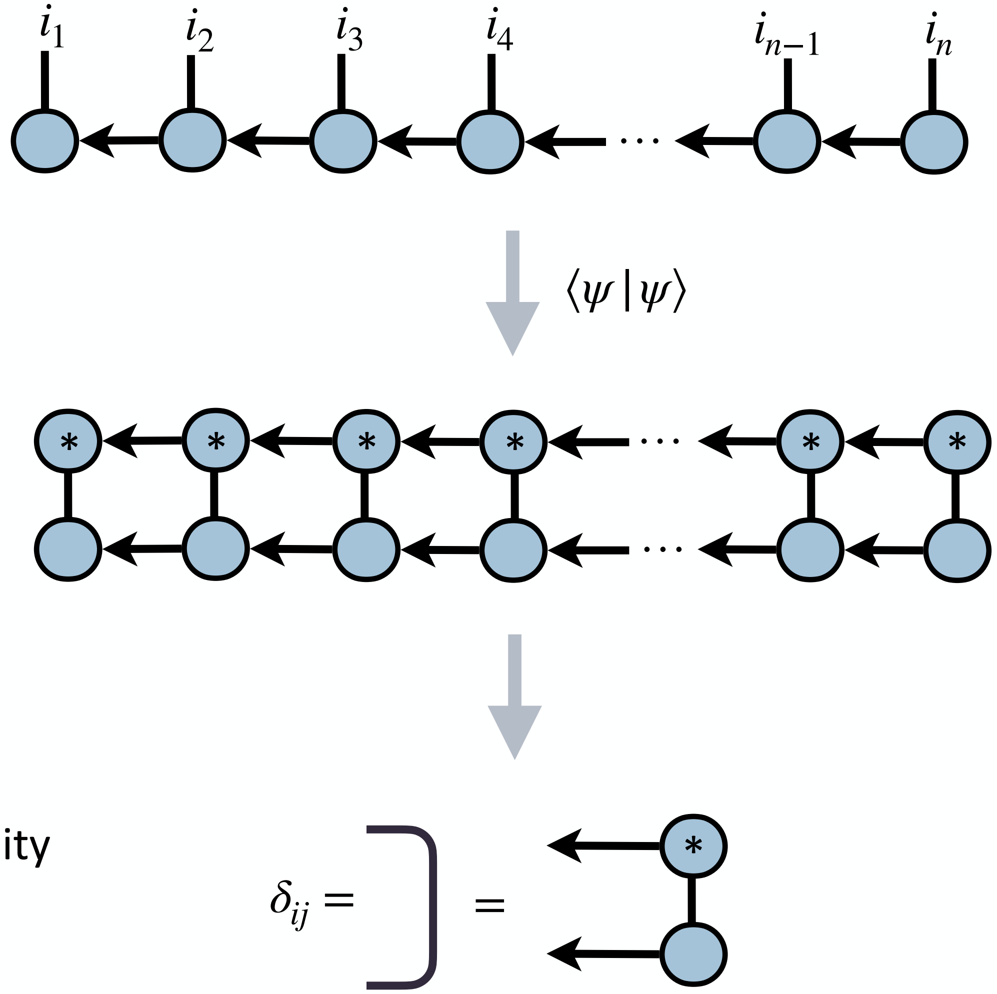


MPS canonical forms

MPS (**Left** canonical from)



MPS (**Right** canonical from)



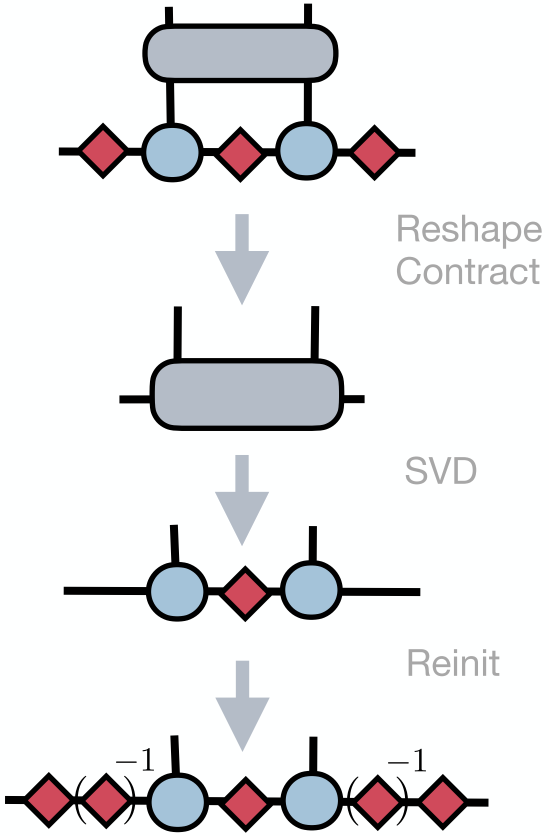
Left/Right orthogonality relations

Time-Evolving Block Decimation (TEBD)

➢ At its heart, this method relies on a Trotter-Suzuki decomposition and subsequent approximation of the time-evolution operator.

➢ Consider the nearest-neighbor Heisenberg chain. Its Hamiltonian is given by

$$\hat{H} = \sum_j \hat{h}_{j,j+1} \quad \hat{h}_{j,j+1} = \hat{s}^x_j \hat{s}^x_{j+1} + \hat{s}^y_j \hat{s}^y_{j+1} + \hat{s}^z_j \hat{s}^z_{j+1}$$

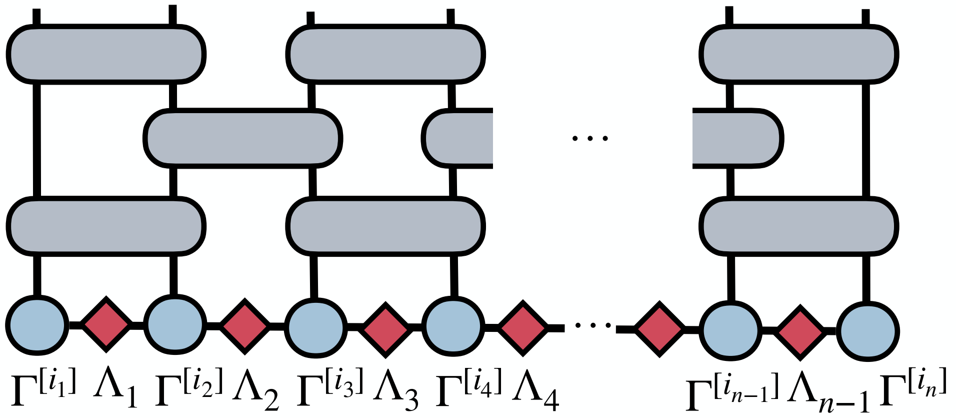


➢ Split the summands

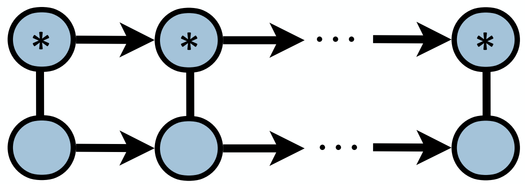
$$\hat{H}_{\text{even}} = \sum_{j \text{ even}} \hat{h}_{j,j+1} \quad \hat{H}_{\text{odd}} = \sum_{j \text{ odd}} \hat{h}_{j,j+1} \quad \hat{\boldsymbol{H}} = \hat{H}_{\text{even}} + \hat{H}_{\text{odd}} \ ,$$

➢ We can use the Baker-Campbell-Hausdorff formula to approximate

$$\hat{U}^{\text{exact}}(\delta) = e^{-\mathrm{i}\delta\hat{H}} = e^{-\mathrm{i}\delta\hat{H}_{\text{even}}} e^{-\mathrm{i}\delta\hat{H}_{\text{odd}}} e^{-\mathrm{i}\delta^2\left[\hat{H}_{\text{even}}, \hat{H}_{\text{odd}}\right]} \approx e^{-\mathrm{i}\delta\hat{H}_{\text{even}}} e^{-\mathrm{i}\delta\hat{H}_{\text{odd}}} \equiv \hat{U}^{\text{TEBD1}}(\delta) \ .$$



Autoregressive sampling from MPS

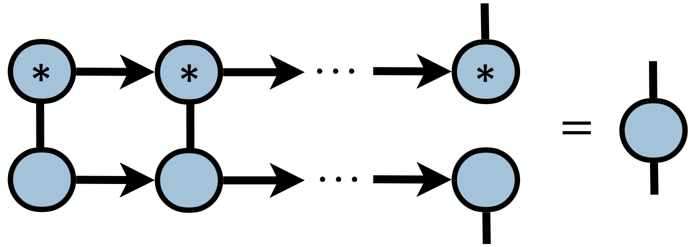


➢ Bitstring probability

$$p(i_1, \ldots, i_n) = |C_{i_1,\ldots,i_n}|^2, \quad \sum_{i_1,\ldots,i_n} |C_{i_1,\ldots,i_n}|^2 = 1$$

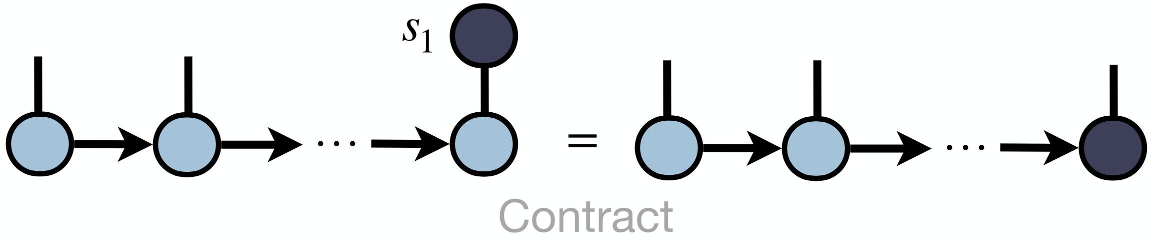
➢ Chain-rule for probabilities (Byes rule):

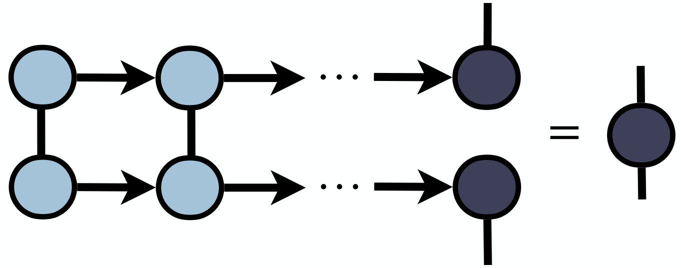
$$p(i_1, \ldots, i_n) = p(i_1)p(i_2 | i_1)\ldots p(i_n | i_1, \ldots, i_{n-1})$$



$= p(i_1)$

Random uniform
$r \in [0,1] \to s_1$
$p(0) + p(1) = 1$





$= p(i_2 | i_1)$

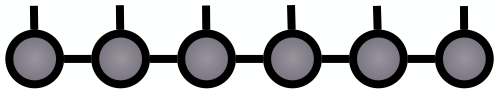
Iterate →

➢ Sample from probability distribution defined by MPS:

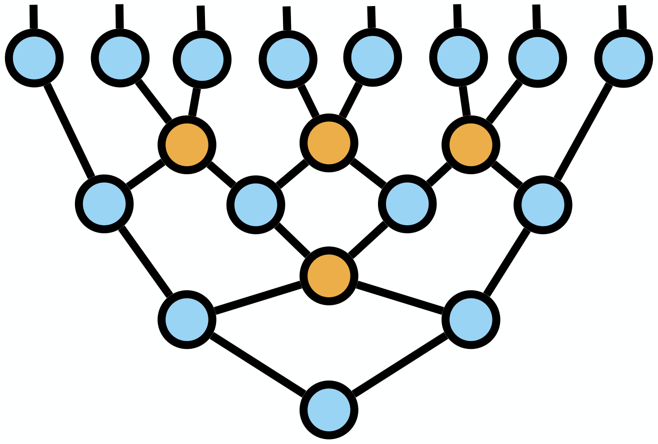
$$s_1, s_2, \ldots, s_n$$

Tensor network architectures

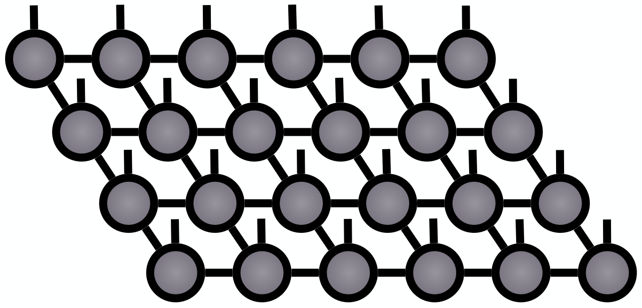
Matrix Product State (MPS)



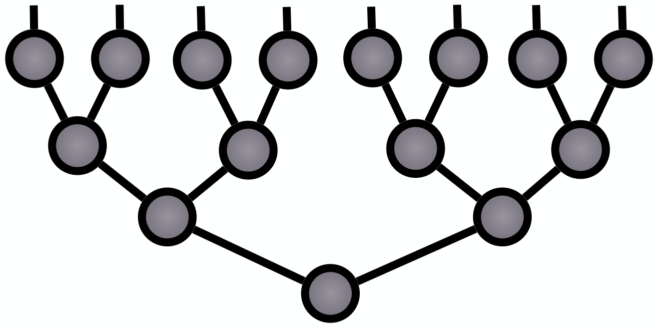
Multiscale Entanglement Renormalization Ansätze (MERA)



Projected Entangled Pair States (PEPS)

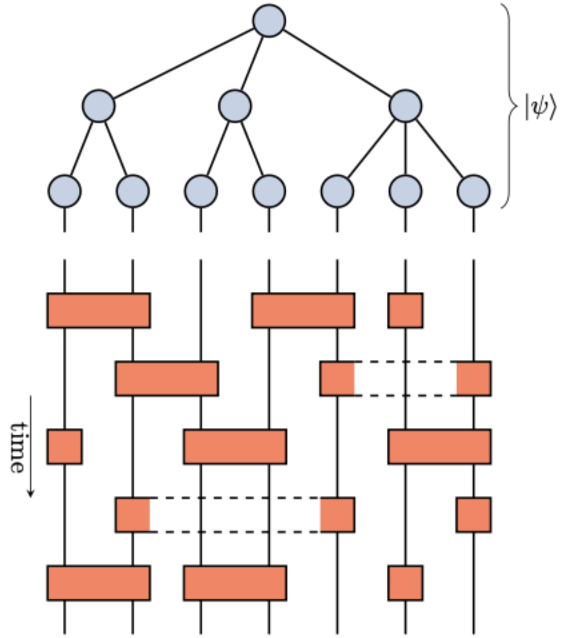


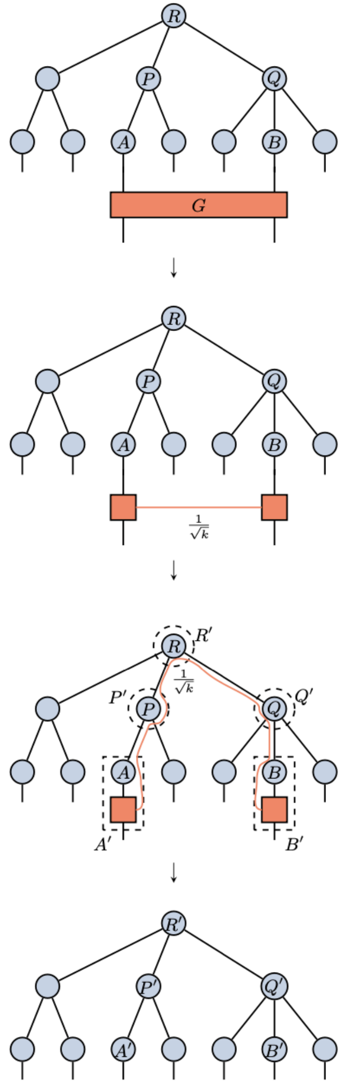
Tree Tensor Network (TTN)

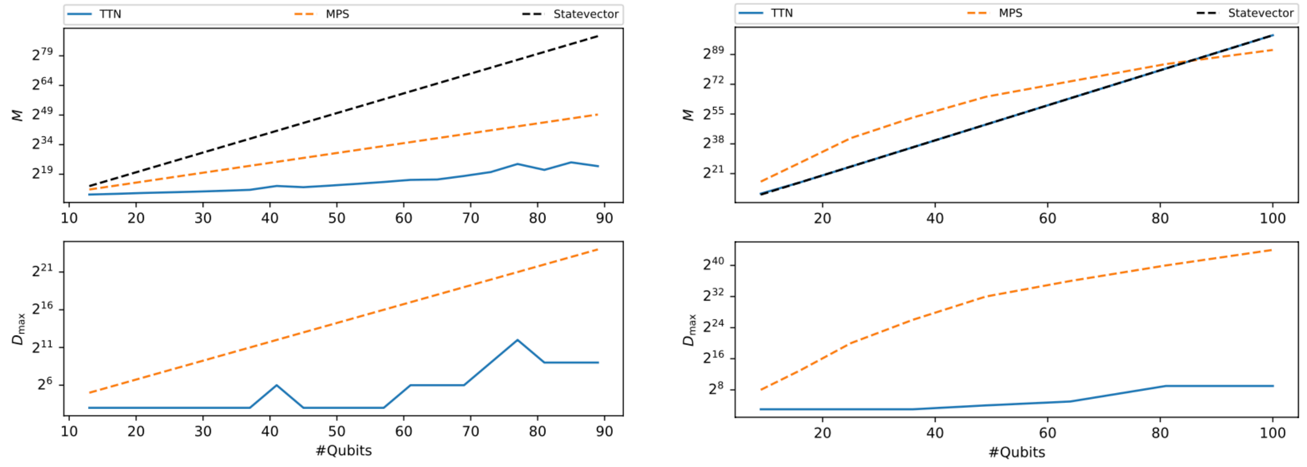


Overview (TTN simulation of quantum computation)

TTN-Tree Tensor Network







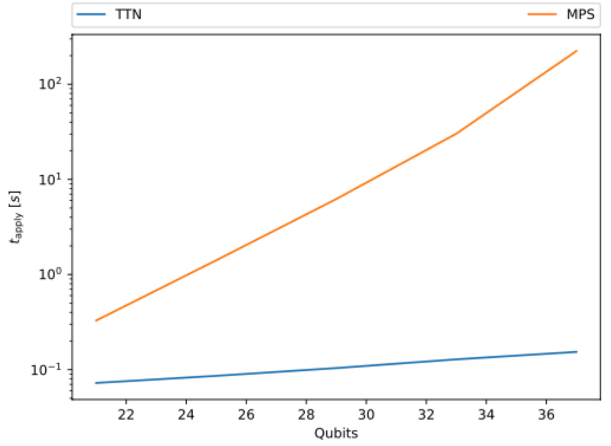


Figure 13: Wall-clock time of applying gates and re-orthonormalization, comparing a MPS with a TTN representation of the quantum state for the *tree-like* circuit.

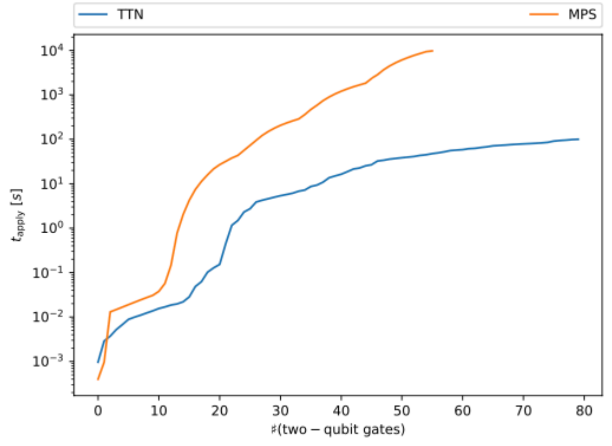
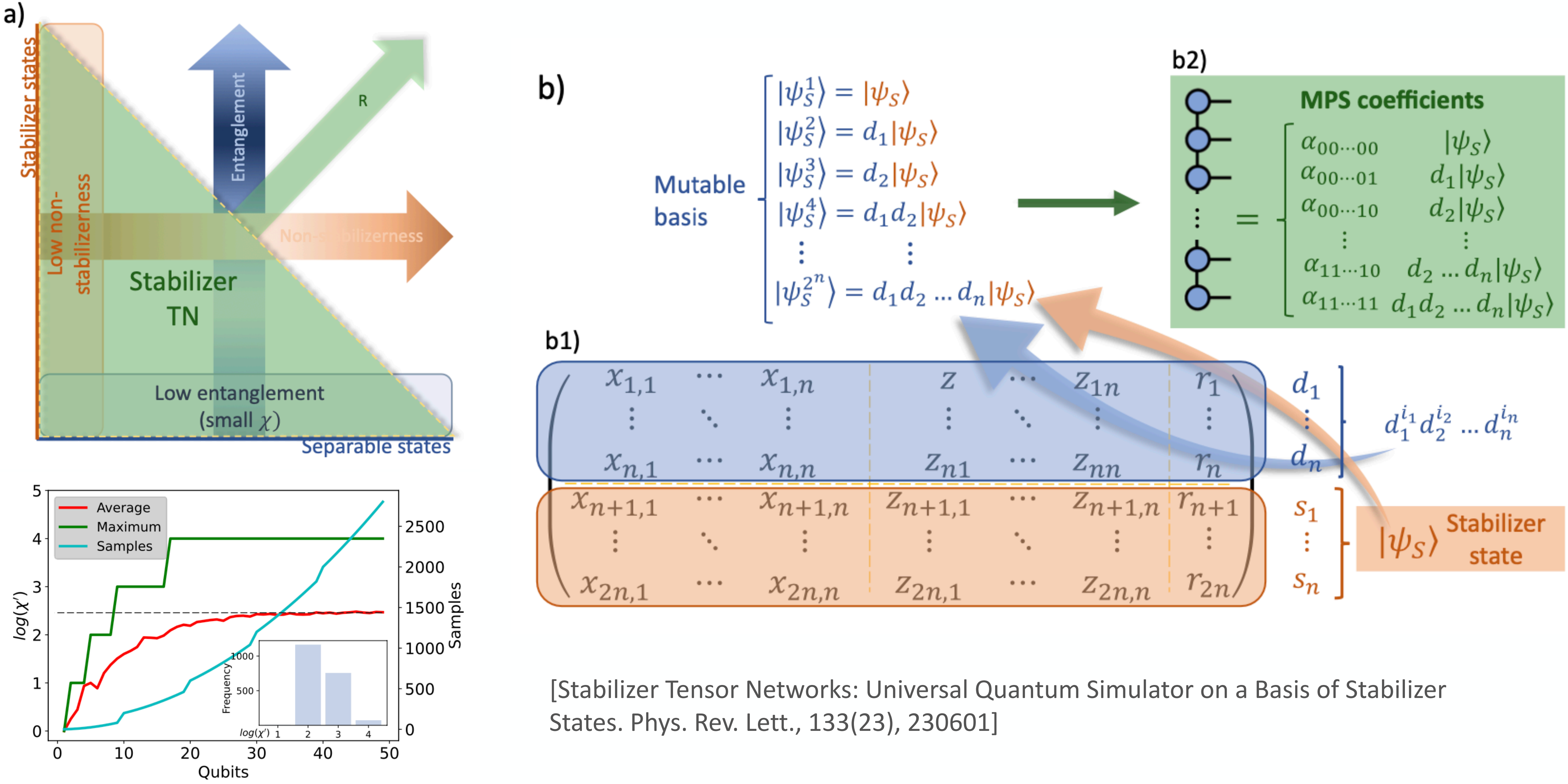


Figure 14: Accumulated wall-clock time of applying gates and re-orthonormalization, on the *lattice* circuit (for 25 qubits). For gate 57 the MPS fails to normalize.

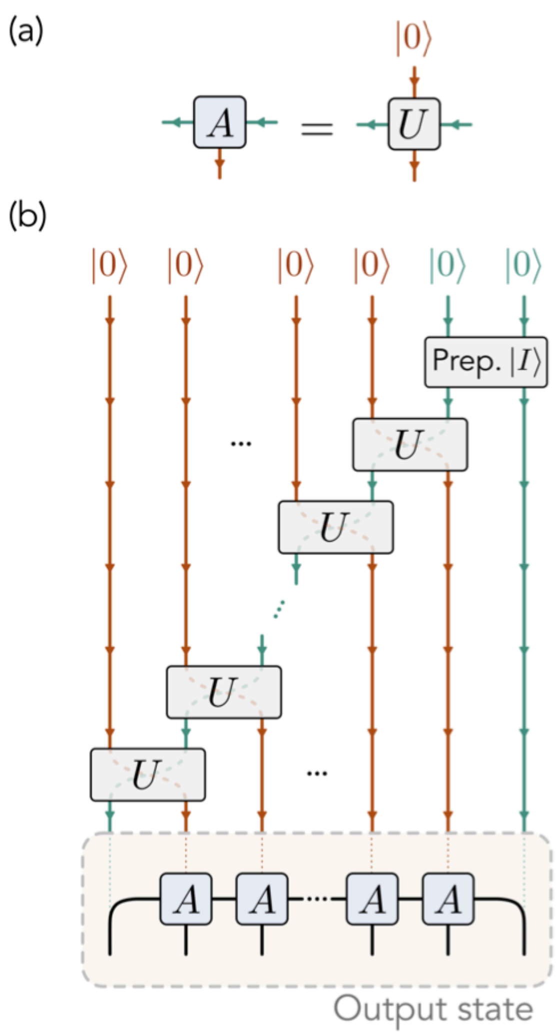
[Simulating quantum circuits using tree tensor networks, Quantum 7, 964 (2023).]

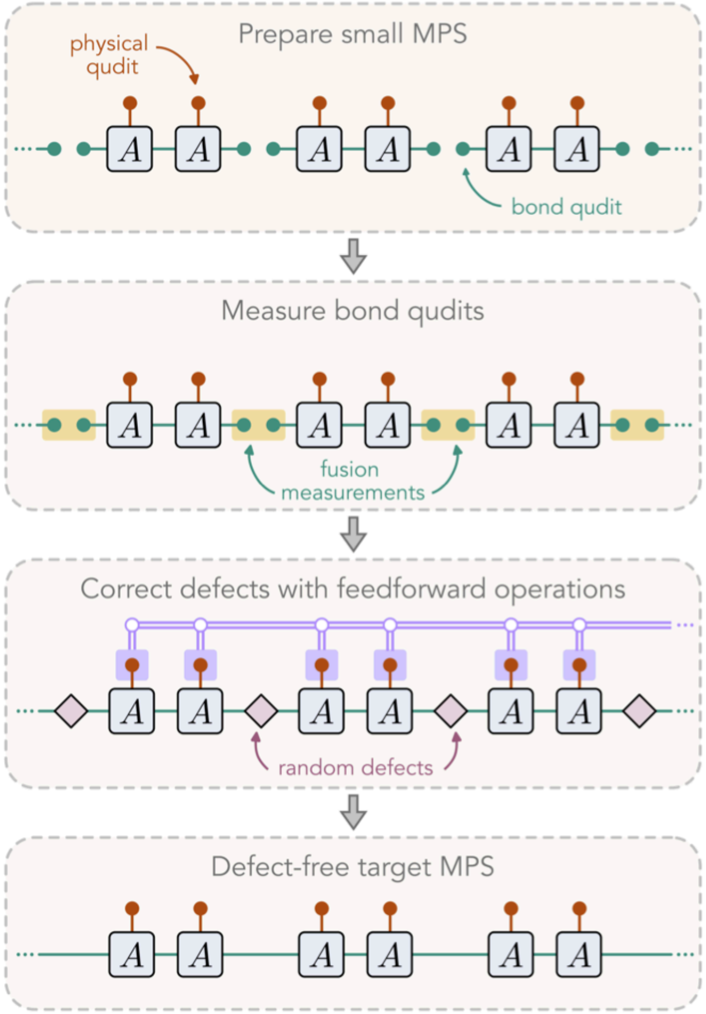
Overview (Tensor Networks in Stabilizer basis)



[Stabilizer Tensor Networks: Universal Quantum Simulator on a Basis of Stabilizer States. Phys. Rev. Lett., 133(23), 230601]

Overview (Quantum State Preparation using MPS)





- **Linear depth**

  [Encoding of matrix product states into quantum circuits of one- and two-qubit gates. Phys. Rev. A, 101(3), 032310]

- **Log depth**

  [Preparation of matrix product states with log-depth quantum circuits Phys. Rev. Lett. 132, 040404 (2024)]

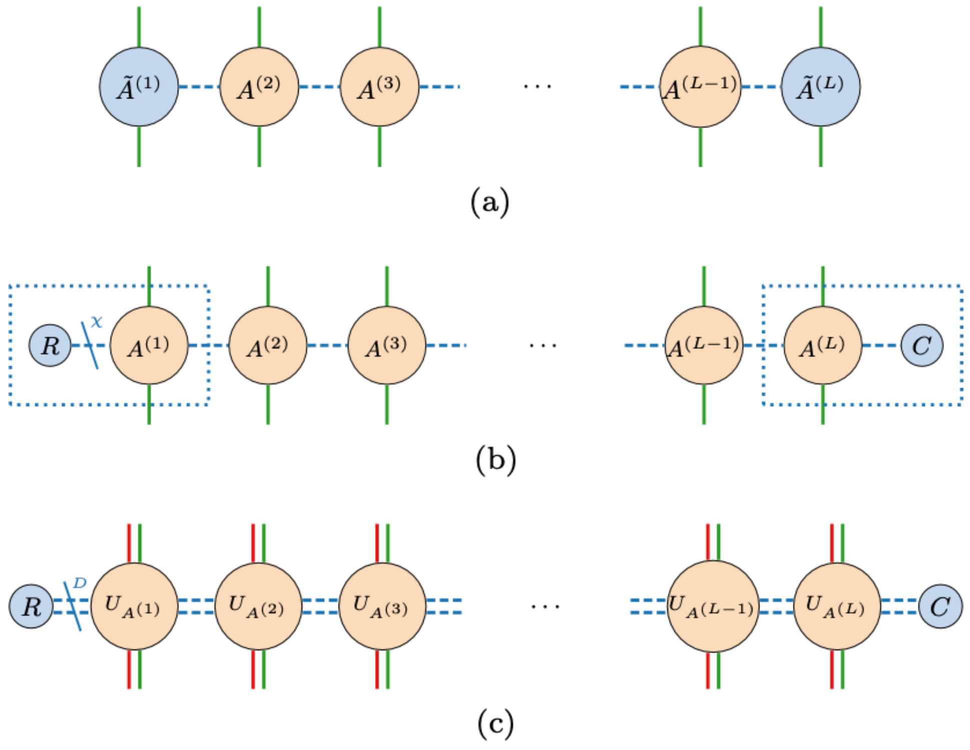
- **Constant depth**

  [Preparing matrix product states via fusion: constraints and extensions arXiv:2404.16360]

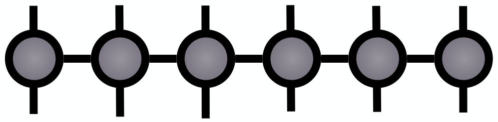
  [Constant-depth preparation of matrix product states with adaptive quantum circuits arXiv:2404.16083]

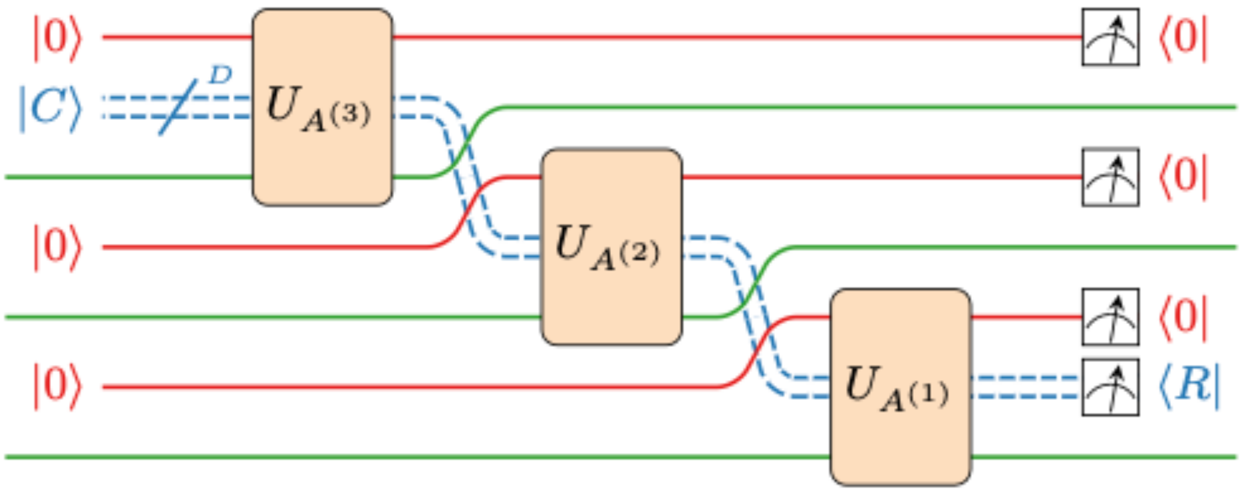
Overview (Block Encodings using MPO)

Block Encoding (BE) $U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix}$



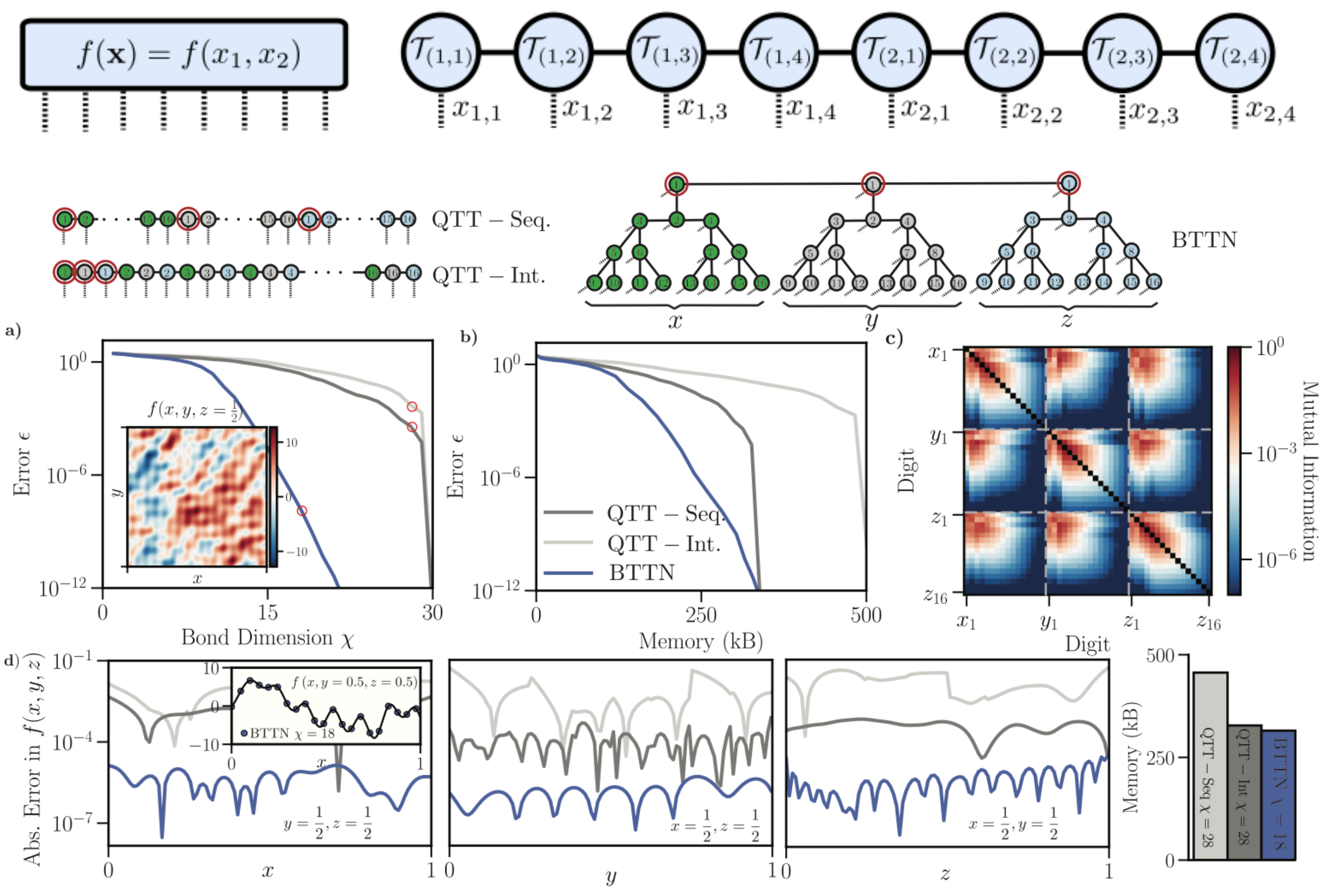
Matrix Product Operator (MPO)

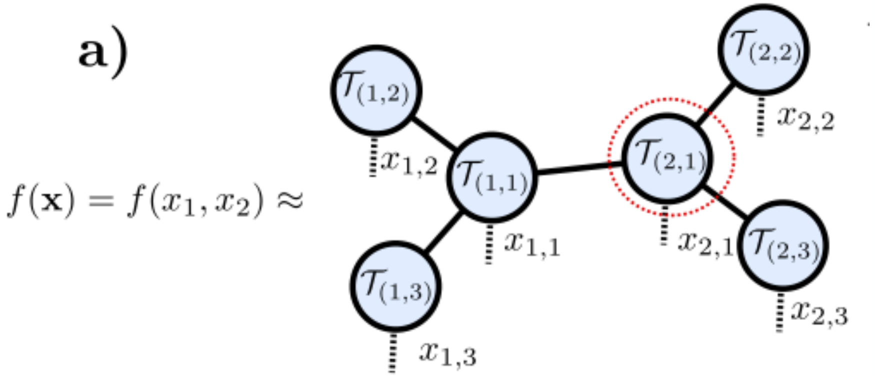




[Block encoding of matrix product operators Phys. Rev. A 110, 042427 (2024)]

Overview (Compressing Multivariate Functions)





b)

α_1	$x_{1,1}, x_{1,2}, x_{1,3}$		
0	1	1	0
1	0	0	0
2	0	1	1

[Compressing multivariate functions with tree tensor networks arXiv:2410.03572 (2024)]

Conclusion

➢ Tensor Networks, especially MPS, provide compact and scalable representations of quantum many-body states, efficiently capturing entanglement structure.

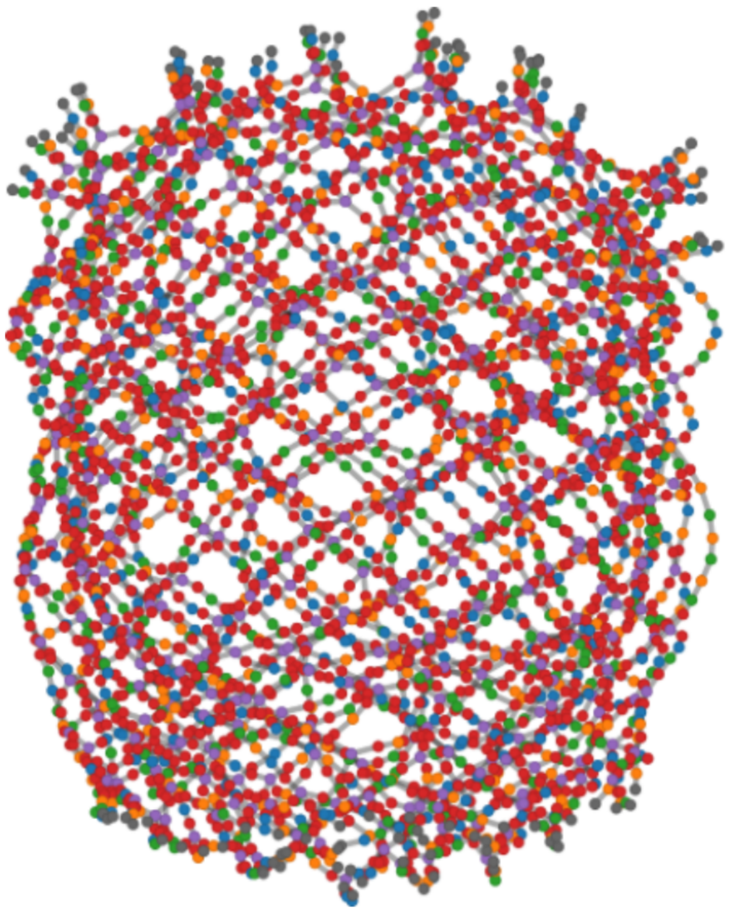
➢Canonical forms and TEBD enable stable time evolution and analysis of complex quantum dynamics.

➢ Autoregressive sampling and function representation extend tensor networks beyond simulation — linking quantum physics with machine learning and data modeling.

➢ Applications in quantum state preparation and quantum optics demonstrate their growing experimental relevance.

➢ Ongoing research targets higher-dimensional networks, hybrid classical–quantum schemes, and noise-resilient methods for near-term quantum devices.

➢ Overall, tensor networks bridge theory, computation, and experiment — forming a versatile framework for advancing quantum technologies.



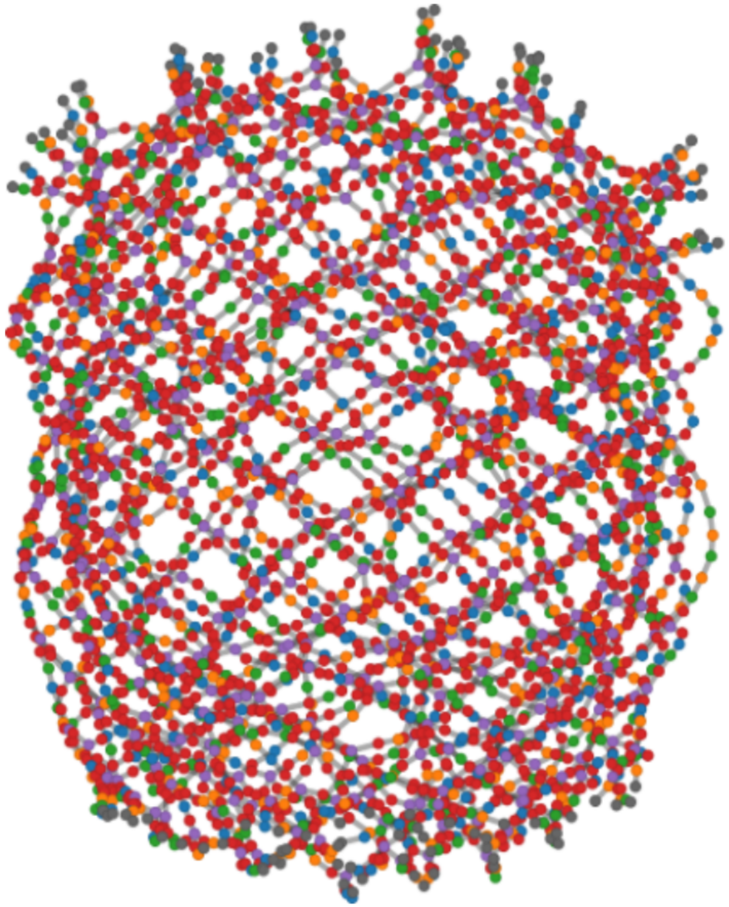
Literature

➢ A Practical Introduction to Tensor Networks: Matrix Product States and Projected Entangled Pair States, Roman Orus, Annals of Physics 349 (2014) 117-158

➢ The density-matrix renormalization group in the age of matrix product states, Ulrich Schollwoeck, Annals of Physics 326, 96 (2011)

➢ Tensor-Train Decomposition, Ivan Oseledets, SIAM J. Sci. Comput., 33(5), 2295 (2011)

➢ A Practical Guide to the Numerical Implementation of Tensor Networks I: Contractions, Decompositions and Gauge Freedom, Glen Evenbly, arXiv: 2202.02138



Thank you for your attention!