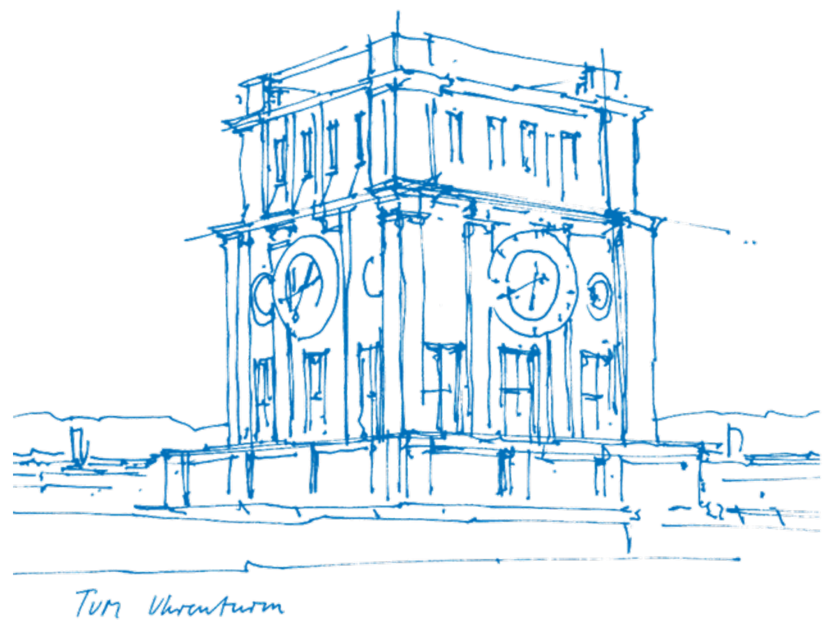
Quantum Simulation and Tensor Network Methods

Prof. Dr. Christian B. Mendl
Technische Universität München
CIT, Department of Computer Science
Chair of Scientific Computing – Quantum Computing

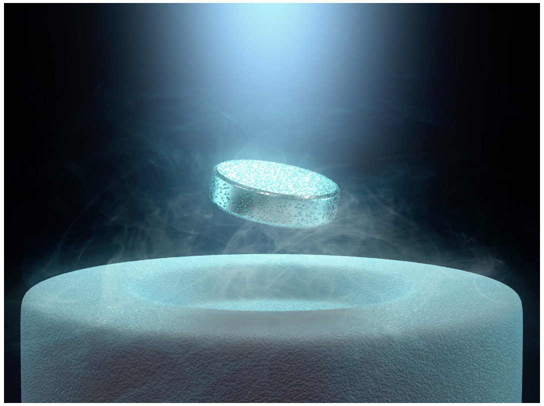
April 22, 2023

45. Edgar-Lüscher-Seminar am Gymnasium Zwiesel
Quantenphysik in der Anwendung

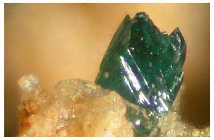


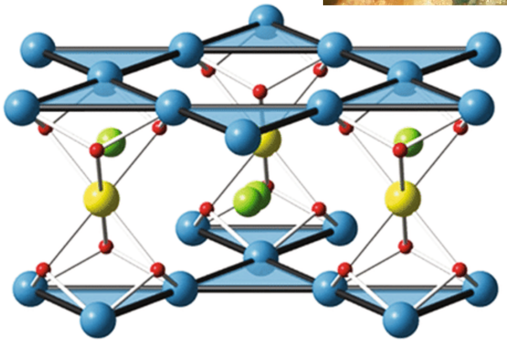
Motivation: Simulate quantum systems

Strangeness of strongly correlated quantum systems, still unsolved questions:

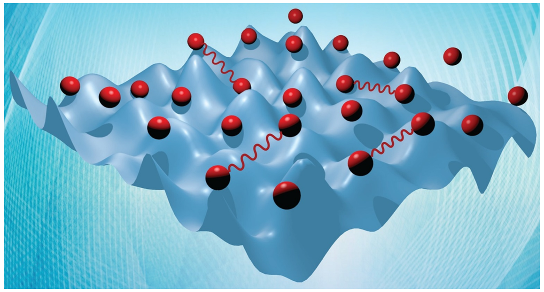


high-T_c superconductors





Novel quantum phases



Many-body localization

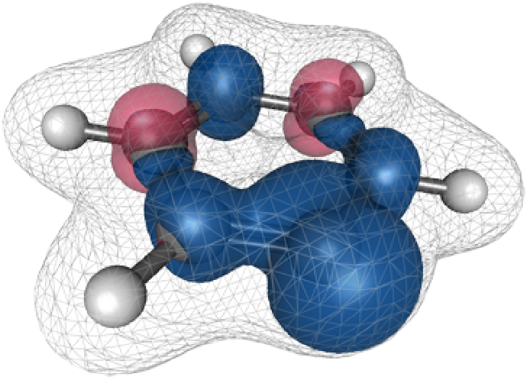
Electronic Schrödinger equation:

$$H\psi = E\psi$$

Quantum Hamiltonian H:

$$H = -\sum_{j=1}^{N} \frac{\hbar^2}{2m_e} \nabla_{r_j}^2 + \sum_{j<k}^{N} \frac{e^2}{4\pi\varepsilon_0 |r_j - r_k|} - \sum_{j=1}^{M} \sum_{k=1}^{N} \frac{Z_j e^2}{4\pi\varepsilon_0 |R_j - r_k|}$$

$\{R_j\}$: positions of atomic nuclei, $\{r_j\}$: electron positions



Source: iqmol.org

Qubitization and quantum eigenvalue transforms

$$U_{\vec{\varphi}} = \mathrm{e}^{i\varphi_0 Z} \prod_{k=1}^{d} W(a)\,\mathrm{e}^{i\varphi_k Z}$$

Quantum signal processing (QSP)

Goal: realize a function $f(a)$ using single-qubit gates

Alternating sequence of single-qubit rotation operators:

- "signal rotation operator", for $a \in [-1, 1]$:

$$W(a) = \begin{pmatrix} a & i\sqrt{1-a^2} \\ i\sqrt{1-a^2} & a \end{pmatrix}$$

- "signal-processing rotation operator", with $Z = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$:

$$S(\varphi) = \mathrm{e}^{i\varphi Z}, \quad \varphi \in \mathbb{R}$$

For phases $\vec{\varphi} = (\varphi_0, \dots, \varphi_d) \in \mathbb{R}^{d+1}$, define

$$U_{\vec{\varphi}} = \mathrm{e}^{i\varphi_0 Z} W(a) \mathrm{e}^{i\varphi_1 Z} W(a) \cdots \mathrm{e}^{i\varphi_d Z} = \mathrm{e}^{i\varphi_0 Z} \prod_{k=1}^{d} W(a) \mathrm{e}^{i\varphi_k Z}$$

Examples:

J. M. Martyn et al. "Grand unification of quantum algorithms". PRX Quantum, 040203 (2021)
G. H. Low and I. L. Chuang. "Hamiltonian simulation by qubitization". Quantum 3, 163 (2019)

Quantum signal processing theorem

Theorem (Quantum signal processing)

The QSP sequence $U_{\vec{\varphi}}$ produces a matrix that maybe be expressed as polynomial function of a:

$$U_{\vec{\varphi}} = \mathrm{e}^{i\varphi_0 Z} \prod_{k=1}^{d} W(a)\, \mathrm{e}^{i\varphi_k Z} = \begin{pmatrix} P(a) & iQ(a)\sqrt{1-a^2} \\ iQ^*(a)\sqrt{1-a^2} & P^*(a) \end{pmatrix}$$

for $a \in [-1, 1]$, and a $\vec{\varphi}$ exists for any polynomials P, Q such that:

(i) $\deg(P) \leq d$, $\deg(Q) \leq d-1$

(ii) *P has parity $d \mod 2$ and Q has parity $(d-1) \mod 2$*

(iii) $|P(a)|^2 + (1-a^2)|Q(a)|^2 = 1$

J. M. Martyn et al. “Grand unification of quantum algorithms”. PRX Quantum, 040203 (2021)
`https://github.com/ichuang/pyqsp`
`https://github.com/qsppack/QSPPACK`

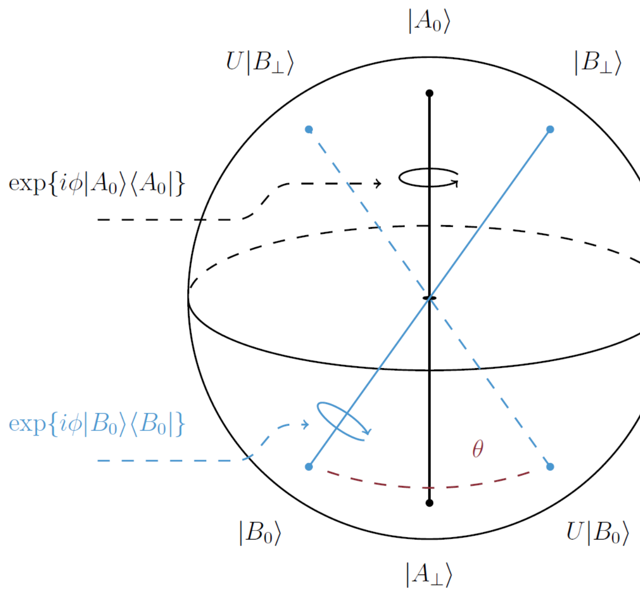
Qubitization illustrated by amplitude amplification

Given:

- (black box) unitary operator U
- quantum state $|A_0\rangle$, $|B_0\rangle$ with $a := \langle A_0|U|B_0\rangle \neq 0$ (w.l.o.g. $a \in \mathbb{R}$)
- corresponding phase rotation gates

$$A_\varphi = e^{i\varphi|A_0\rangle\langle A_0|}, \quad B_\varphi = e^{i\varphi|B_0\rangle\langle B_0|}$$

Goal: construct quantum circuit C from U, $U^\dagger$, A_φ, B_φ such that $|\langle A_0|C|B_0\rangle| \to 1$

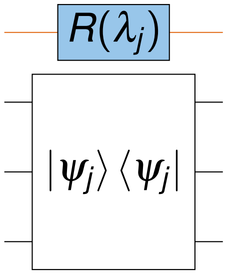


Quantum eigenvalue transforms

So far: QSP with parameter $a \in [-1, 1]$

It turns out: can apply QSP to all eigenvalues $\{\lambda_j\}$ of a Hermitian matrix H simultaneously, with "$a = \lambda_j$"

Strategy: block-encode H into a larger unitary matrix V:

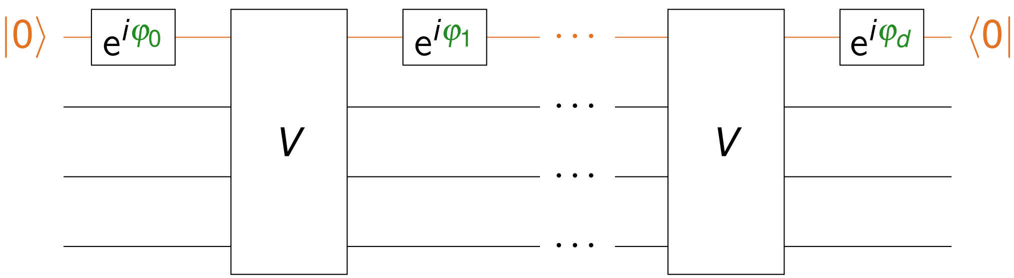
$V = \sum_j$ 

J. M. Martyn et al. "Grand unification of quantum algorithms". PRX Quantum, 040203 (2021)
G. H. Low and I. L. Chuang. "Hamiltonian simulation by qubitization". Quantum 3, 163 (2019)
A. Gilyén et al. "Quantum singular value transformation and beyond: exponential improvements for quantum matrix arithmetics". STOC 2019

Quantum eigenvalue transforms (cont.)

Apply QSP sequence to auxiliary qubit $\rightsquigarrow$ transforms all eigenvalues simultaneously!

$$U_{\vec{\varphi},\mathrm{eig}} = \mathrm{e}^{i\varphi_0 Z} \prod_{k=1}^{d} V \,\mathrm{e}^{i\varphi_k Z} = \begin{pmatrix} \mathrm{Poly}(H) & \cdot \\ \cdot & \cdot \end{pmatrix}$$



$$= \mathrm{Poly}(H)$$

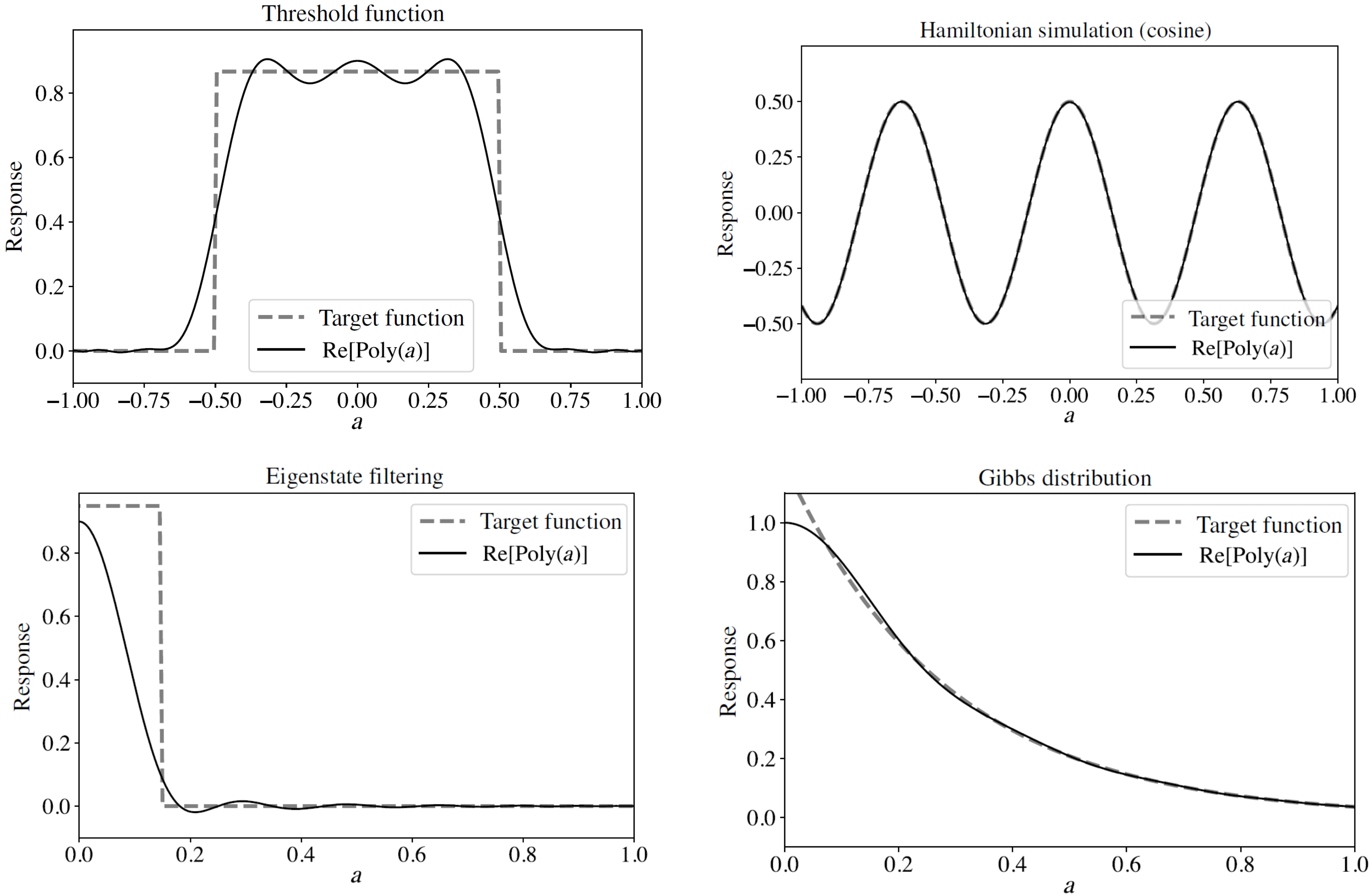
$\rightsquigarrow$ broad usefulness for designing matrix functions:

- time evolution e^{-iHt}
- thermal Gibbs ensemble $\rho(\beta) = \frac{1}{Z(\beta)} \mathrm{e}^{-\beta H}$
- spectral filtering (selecting subspaces of certain eigenvalues)
- ...

J. M. Martyn et al. “Grand unification of quantum algorithms”. PRX Quantum, 040203 (2021)

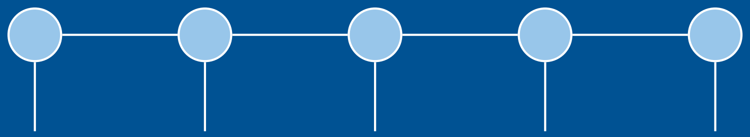
Applications of quantum eigenvalue transforms

Demo: github.com/cmendl/edgar-luescher-seminar-2023/blob/master/notebooks/qsp_eigenstate_filtering.ipynb



J. M. Martyn et al. “Grand unification of quantum algorithms”. PRX Quantum, 040203 (2021)

Tensor network methods



Linear algebra: singular value decomposition

Theorem (Singular value decomposition (SVD))

*Let $A \in \mathbb{C}^{n\times n}$ be a square matrix. Then there exist unitary matrices $U, V \in \mathbb{C}^{n\times n}$ and real numbers $\sigma_1, \dots, \sigma_n$ with $\sigma_1 \geq \dots \geq \sigma_n \geq 0$ called **singular values**, such that*

$$A = U \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} V^\dagger.$$

Can be used to "compress" a matrix by discarding small singular values ($k \leq n$):

$$A \approx U \begin{pmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_k & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix} V^\dagger = U_{:,:k} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{pmatrix} V^\dagger_{:,:k}.$$

Demo: github.com/cmendl/edgar-luescher-seminar-2023/blob/master/notebooks/svd_compression.ipynb

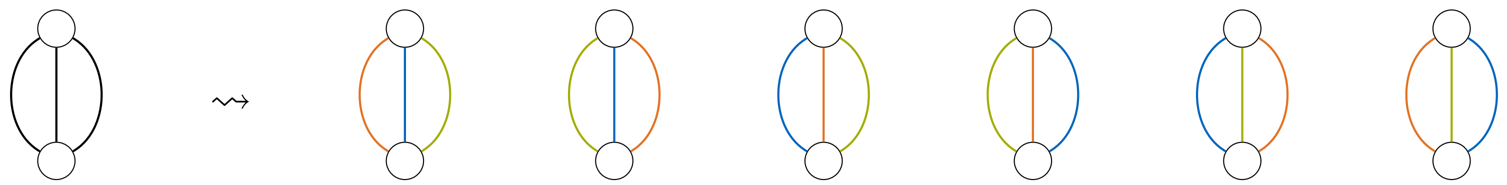
Tensors and graphical tensor diagrams

Example: matrix-matrix multiplication

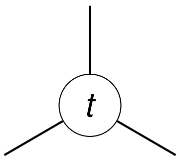
J. C. Bridgeman and C. T. Chubb "Hand-waving and interpretive dance: An introductory course on tensor networks". J. Phys. A: Math. Theor. 50, 223001 (2017)

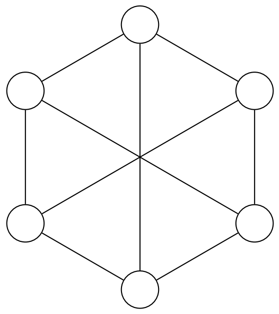
Example: counting graph colorings

Given a 3-regular graph, how many edge colorings using three colors exist, such that the edges at each vertex have distinct colors?



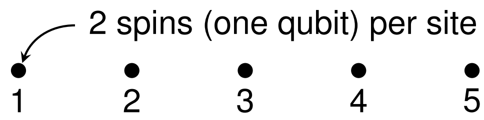
Interpreted as tensor network, how to define tensors such that contracting the network gives the number of edge colorings?





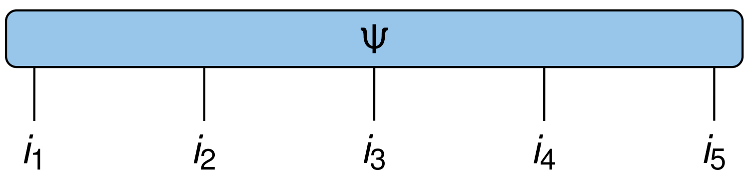
Matrix product states (MPS)

Lattice (1D):

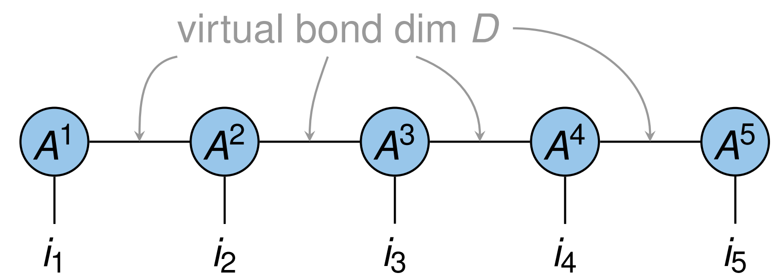


Wavefunction: $\Psi = \sum_{i \in \{0,1\}^N} \Psi_{i_1,\dots,i_N} |i_1,\dots,i_N\rangle$

Exact representation:



MPS approximation:



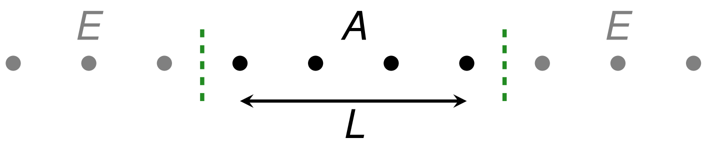
$$\Psi_{i_1,\dots,i_N} \approx A^{(1)}_{i_1} \cdot A^{(2)}_{i_2} \cdots A^{(N)}_{i_N}$$

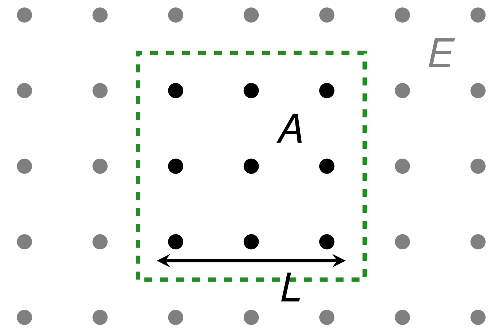
exp(N) many numbers

poly(D, N) numbers

Why a good approximation?
D bounded for typical Ψ

Area law of the entanglement entropy





Entanglement entropy:

$$S(L) = -\operatorname{tr}[\rho_A \log(\rho_A)] \quad \text{with} \quad \rho_A = \operatorname{tr}_E[|\psi\rangle\langle\psi|]$$

Required bond dimension: $D \sim e^{S(L)}$

General random $\lvert\psi\rangle$ on a d-dim lattice	$S(L) \sim L^d$	(volume)
Critical ground state on a 1D lattice	$S(L) \sim \log(L)$	
Ground state for local H on a d-dim lattice	$S(L) \sim L^{d-1}$	(area law)

Thus $S(L) = \text{const}$, $D = \text{const}$ for local H on a 1D lattice!

DMRG algorithm

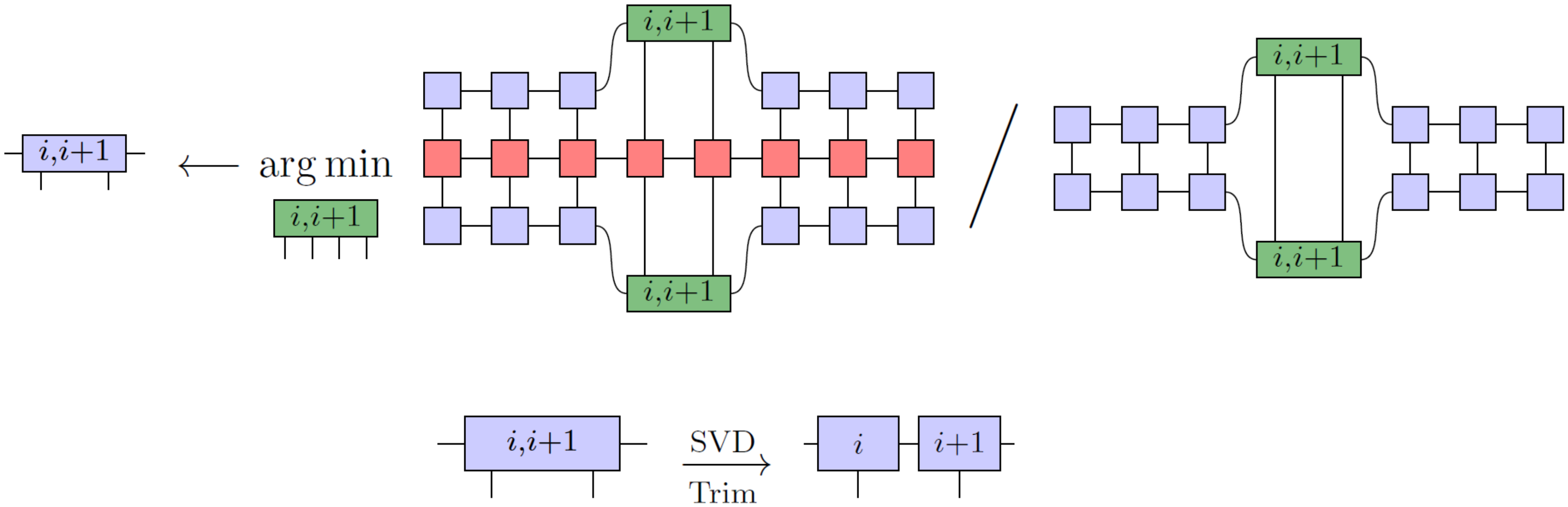


Image source: Bridgeman and Chubb (2017)

Demo: github.com/cmendl/edgar-luescher-seminar-2023/blob/master/notebooks/mps_ground_state.ipynb

J. C. Bridgeman and C. T. Chubb “Hand-waving and interpretive dance: An introductory course on tensor networks”. J. Phys. A: Math. Theor. 50, 223001 (2017)

U. Schollwöck “The density-matrix renormalization group in the age of matrix product states”. Ann. Physics 326, 96–192 (2011)

References

- Bridgeman, J. C. and Chubb, C. T. (2017). “Hand-waving and interpretive dance: An introductory course on tensor networks”. In: *J. Phys. A: Math. Theor.* 50, p. 223001. DOI: 10.1088/1751-8121/aa6dc3.
- Gilyén, A. et al. (2019). “Quantum singular value transformation and beyond: exponential improvements for quantum matrix arithmetics”. In: *Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of Computing*. STOC 2019. Association for Computing Machinery, pp. 193–204. DOI: 10.1145/3313276.3316366.
- Low, G. H. and Chuang, I. L. (2019). “Hamiltonian simulation by qubitization”. In: *Quantum* 3, p. 163. DOI: 10.22331/q-2019-07-12-163.
- Martyn, J. M. et al. (2021). “Grand unification of quantum algorithms”. In: *PRX Quantum* 2, p. 040203. DOI: 10.1103/PRXQuantum.2.040203.
- Schollwöck, U. (2011). “The density-matrix renormalization group in the age of matrix product states”. In: *Ann. Physics* 326, pp. 96–192. DOI: 10.1016/j.aop.2010.09.012.