TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Tensor Networks (SS2021)

Lecture 11: MPO-MPS evolution + Trotter-Suzuki decomposition

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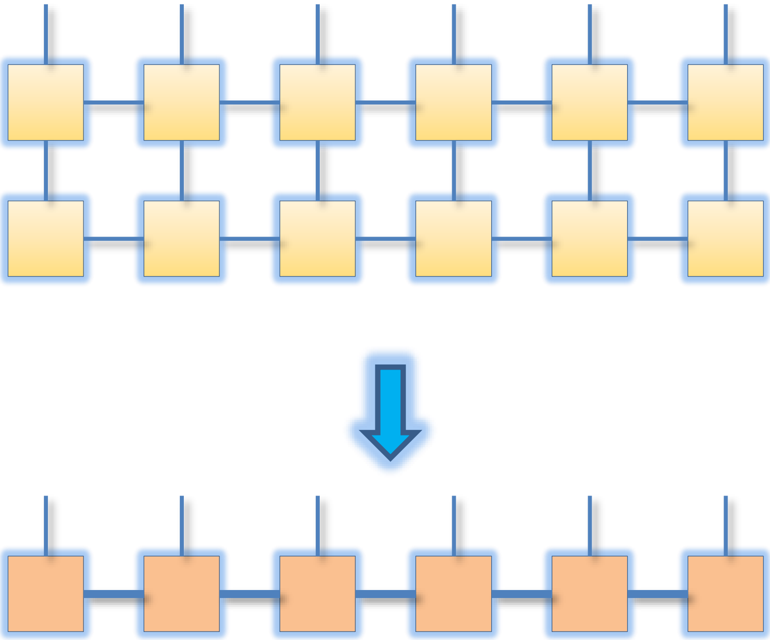
§ 3.1 MPO-MPS evolution

- In tensor network calculations, we often encounter the following MPO-MPS evolution:

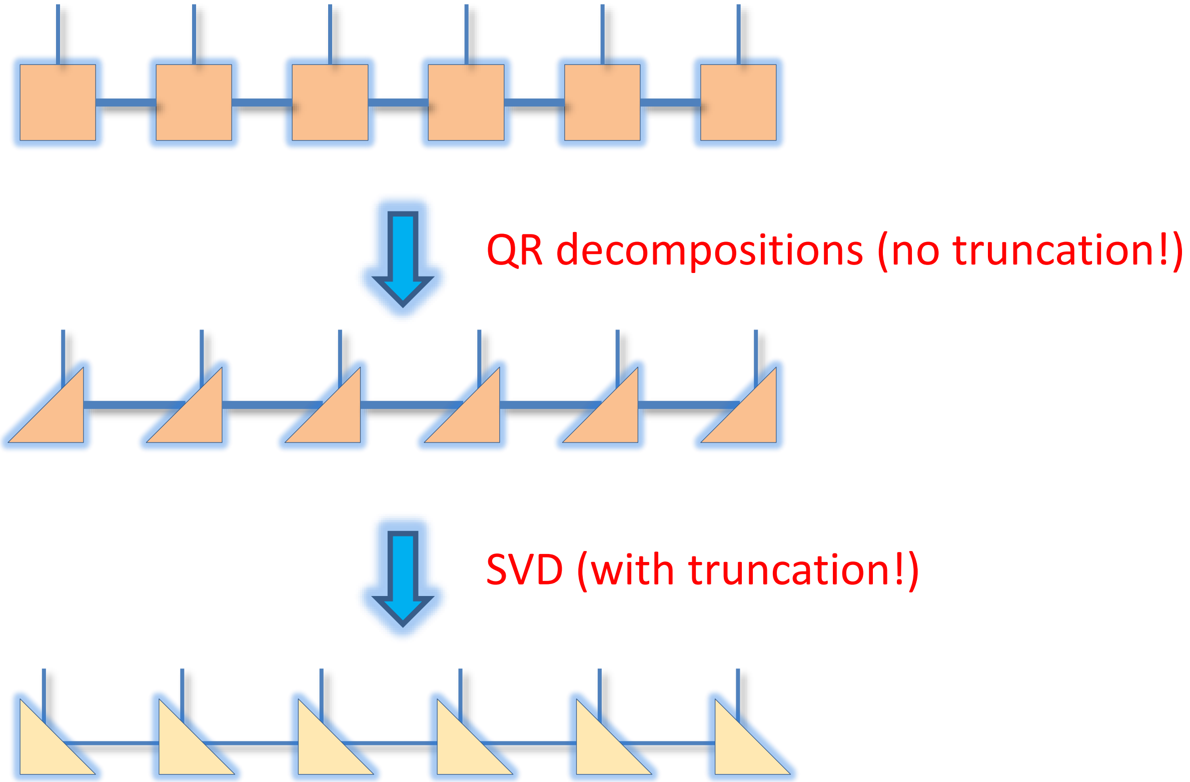
$$|\psi'\rangle = W|\psi\rangle$$



Bond dimension increases!
How to truncate?

§ 3.1 MPO-MPS evolution

- Use bond canonical form (truncating reduced density matrices)

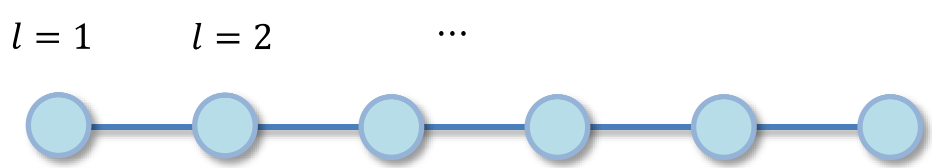


§ 3.1 MPO-MPS evolution

Example: Convert a Fermi sea into MPS

$$|\psi\rangle = \prod_{m=1}^{M} d_m^\dagger \, |0\rangle$$

$$d_m^\dagger = \sum_{l=1}^{N} A_{ml} c_l^\dagger$$



Y.-H. Wu, L. Wang & HHT, Phys. Rev. Lett. 124, 246401 (2020).

§ 3.1 MPO-MPS evolution

$$d_m^\dagger = \sum_{l=1}^{N} A_{ml} c_l^\dagger$$

$$= \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ A_{m1} c_1^\dagger & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ A_{m2} c_2^\dagger & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ A_{m,N} c_N^\dagger & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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$$= \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} I & 0 \\ A_{m1} \sigma_1^+ & -\sigma_1^z \end{pmatrix} \begin{pmatrix} I & 0 \\ A_{m2} \sigma_2^+ & -\sigma_2^z \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ A_{m,N} \sigma_N^+ & -\sigma_N^z \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Jordan-Wigner transformation: $c_l^\dagger = (-\sigma_1^z) \cdots (-\sigma_{l-1}^z) \sigma_l^+$

§ 3.1 MPO-MPS evolution

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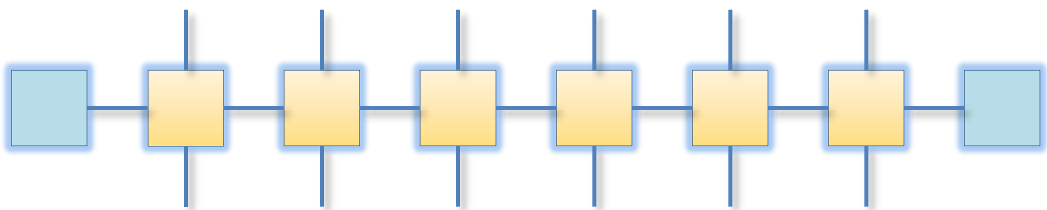
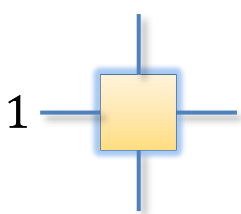
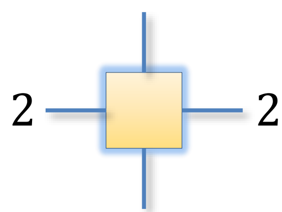
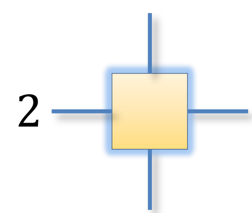
$=$ 



$= I$



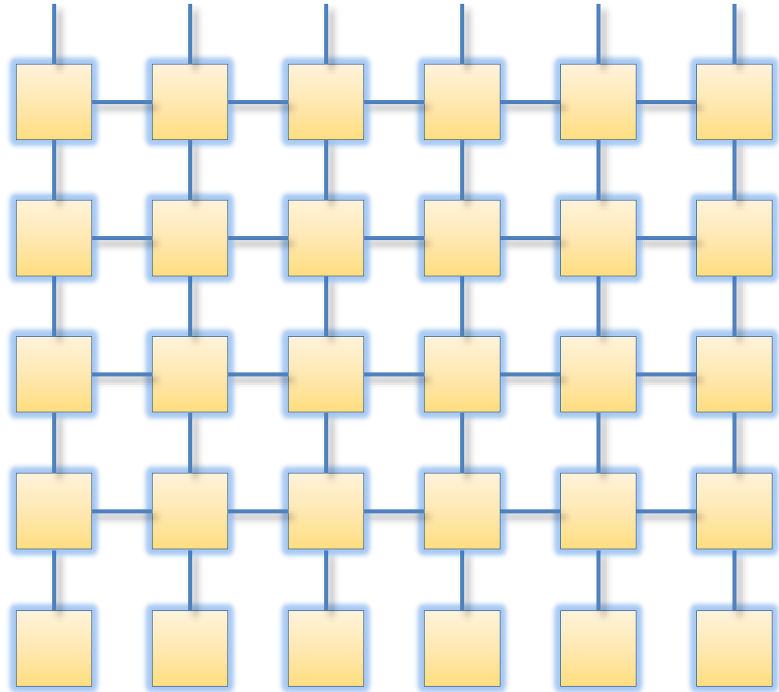
$= -\sigma^z$



$= A_{ml}\sigma^+$

§ 3.1 MPO-MPS evolution

$$\prod_{m=1}^{M} d_m^\dagger |0\rangle \sim$$



$d_M^\dagger$

$\vdots$

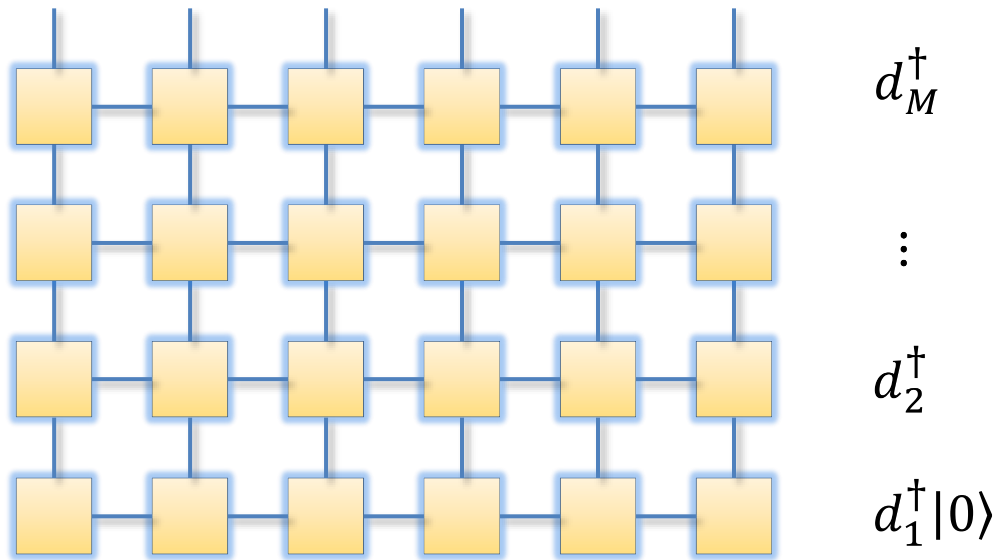
$d_2^\dagger$

$d_1^\dagger$

$|0\rangle$

§ 3.1 MPO-MPS evolution

$$\prod_{m=1}^{M} d_m^\dagger \, |0\rangle \sim$$



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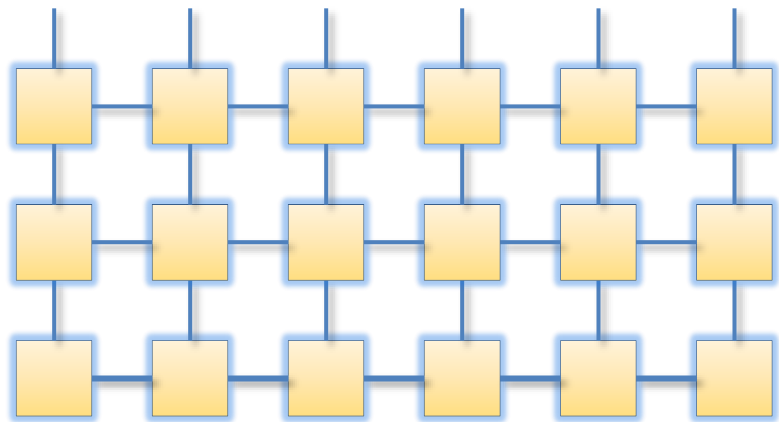
$$\prod_{m=1}^{M} d_m^\dagger \, |0\rangle \sim$$



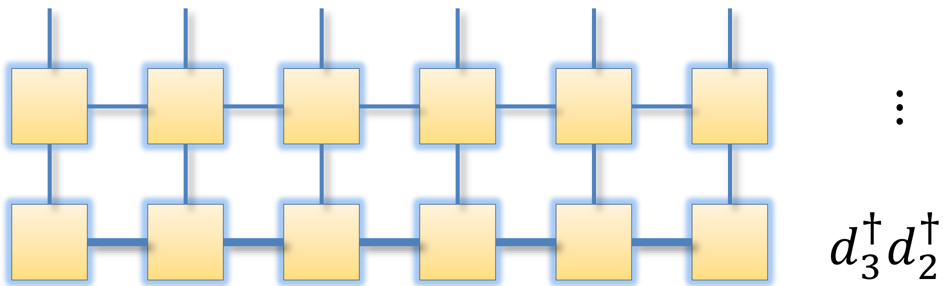
$d_M^\dagger$

$\vdots$

$d_2^\dagger d_1^\dagger |0\rangle$

§ 3.1 MPO-MPS evolution

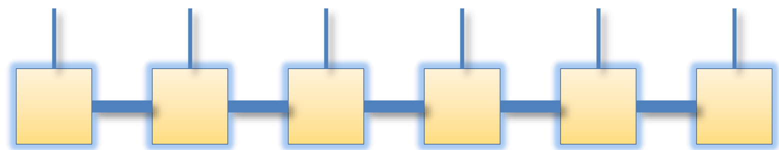
$$\prod_{m=1}^{M} d_m^\dagger |0\rangle \sim$$



$$d_3^\dagger d_2^\dagger d_1^\dagger |0\rangle$$

§ 3.1 MPO-MPS evolution

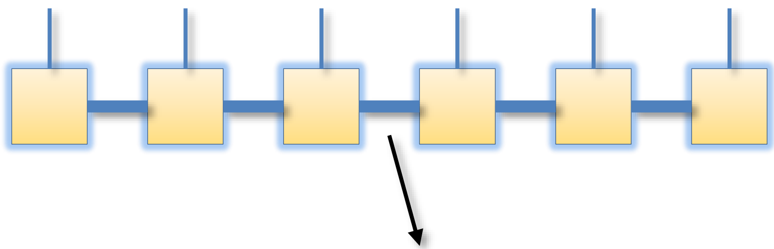
$$\prod_{m=1}^{M} d_m^\dagger |0\rangle \sim$$



$$\prod_{m=M}^{1} d_m^\dagger |0\rangle$$

§ 3.1 MPO-MPS evolution

$$\prod_{m=1}^{M} d_m^\dagger |0\rangle \sim$$



$$\prod_{m=M}^{1} d_m^\dagger |0\rangle$$

$D = 2^M$

- If M is large, truncations are needed in intermediate steps.

High fidelity compression requires low-entanglement "intermediate" states!

§ 3.1 MPO-MPS evolution

$$\prod_{m=1}^{M} d_m^\dagger |0\rangle \propto \prod_{r=1}^{M} f_r^\dagger |0\rangle$$

$$f_r^\dagger = \sum_{m=1}^{M} U_{rm} d_m^\dagger$$

U: unitary matrix
(single-particle basis change)

Proof:

$$f_1^\dagger f_2^\dagger \cdots f_M^\dagger |0\rangle = \sum_{m_1 \ldots m_M = 1}^{M} U_{1m_1} U_{2m_2} \cdots U_{Mm_M} d_{m_1}^\dagger \cdots d_{m_M}^\dagger |0\rangle$$

$$= \sum_{\sigma \in S_M} U_{1,\sigma(1)} U_{2,\sigma(2)} \cdots U_{M,\sigma(M)} \operatorname{sgn}(\sigma)\, d_1^\dagger \cdots d_M^\dagger |0\rangle$$

S_M: permutation of $\{1,2,\ldots,M\}$

$$= \det U \; d_1^\dagger \cdots d_M^\dagger |0\rangle \propto d_1^\dagger \cdots d_M^\dagger |0\rangle$$

§ 3.1 MPO-MPS evolution

$$\prod_{m=1}^{M} d_m^\dagger |0\rangle \propto \prod_{r=1}^{M} f_r^\dagger |0\rangle$$

$$f_r^\dagger = \sum_{m=1}^{M} U_{rm} d_m^\dagger = \sum_{l=1}^{N} (UA)_{rl} c_l^\dagger$$

Construct Wannier orbitals:

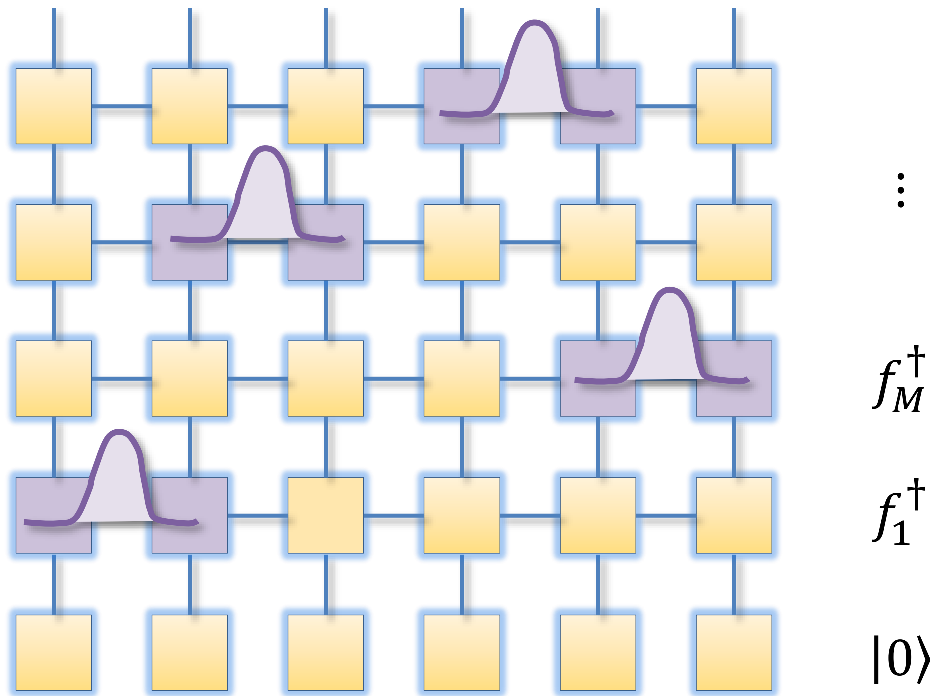
Position operator: $X = \sum_{l=1}^{N} l c_l^\dagger c_l$ $\tilde{X}_{nm} = \langle 0 | d_m X d_n^\dagger | 0 \rangle$

Diagonalize "projected" position operator: $U \tilde{X} U^\dagger = \mathrm{diag}(x_1, \dots, x_M)$

S. Kivelson, Phys. Rev. B 26, 4269 (1982).

§ 3.1 MPO-MPS evolution

$$\prod_{r=1}^{M} f_r^\dagger \left|0\right\rangle \sim$$

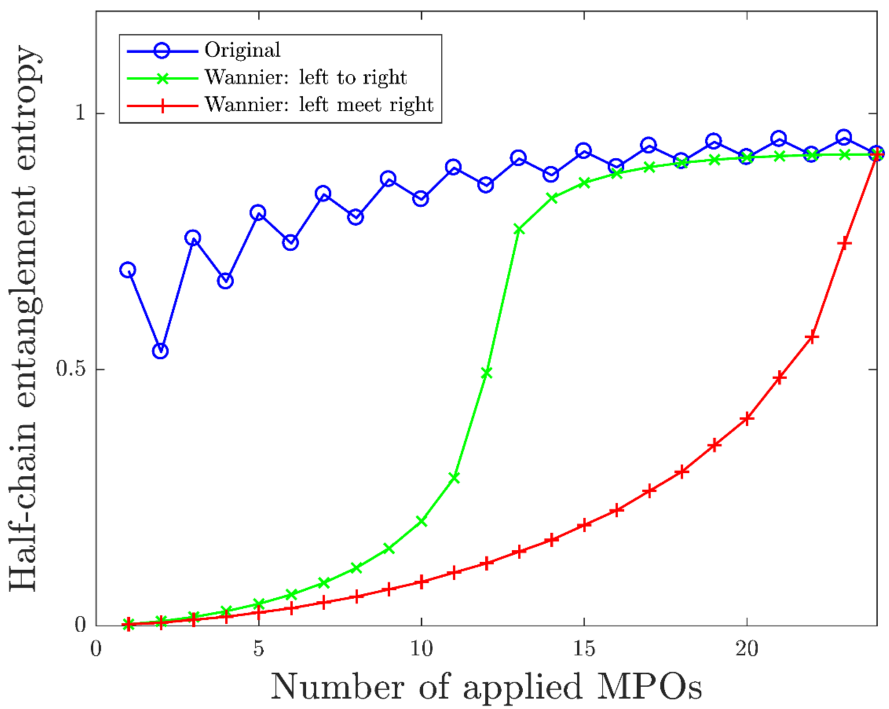


- Slow entanglement growth substantially suppresses truncation error!

§ 3.1 MPO-MPS evolution

$$H = -\sum_{j=1}^{N-1} (c_j^\dagger c_{j+1} + \mathrm{h.c.})$$

$N = 48$, half filling ($M = 24$)



§ 3.2 Time evolution

- We also encounter MPO-MPS contractions when dealing with time evolutions:

$$|\psi(t)\rangle = e^{-iHt}|\psi\rangle$$ Real-time evolution

$$|\psi(\tau)\rangle = e^{-\tau H}|\psi\rangle$$ Imaginary-time evolution

$\tau \to \infty$: projection onto the ground state

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$\tau \to \infty$: projection onto the ground state

Q: Can we represent $e^{-\tau H}$ as an MPO (or a sequence of MPOs)?

§ 3.2 Time evolution

- Consider 1D spin Hamiltonians with nearest-neighbor interactions:

$$H = \sum_{j=1}^{N-1} h_{j,j+1}$$

$$= \underbrace{(h_{12} + h_{34} + \cdots)}_{H_{\mathrm{odd}}} + \underbrace{(h_{23} + h_{45} + \cdots)}_{H_{\mathrm{even}}}$$

$\Rightarrow$ $$e^{-\tau H} = e^{-\tau(H_{\mathrm{even}} + H_{\mathrm{odd}})}$$

§ 3.2 Time evolution

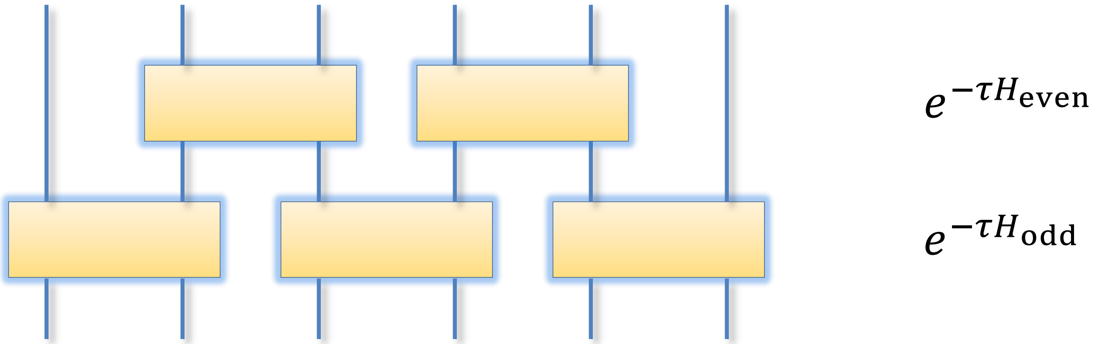
- Simple case: commuting Hamiltonian with $[H_{\text{odd}}, H_{\text{even}}] = 0$

$$[h_{j-1,j}, h_{j,j+1}] = 0 \ \forall j$$

$$e^{-\tau H} = e^{-\tau(H_{\text{even}}+H_{\text{odd}})}$$

$$= e^{-\tau H_{\text{even}}} e^{-\tau H_{\text{odd}}}$$

$=$

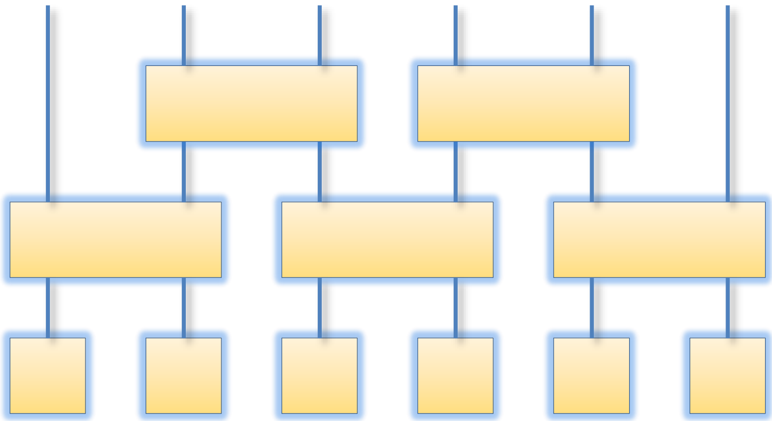


§ 3.2 Time evolution

- Simple case: commuting Hamiltonian with $[H_{\mathrm{odd}}, H_{\mathrm{even}}] = 0$

MPS ground state: $\tau \to \infty$

$$e^{-\tau H}|\phi\rangle =$$



$e^{-\tau H_{\mathrm{even}}}$

$e^{-\tau H_{\mathrm{odd}}}$

$|\phi\rangle$

§ 3.2 Time evolution

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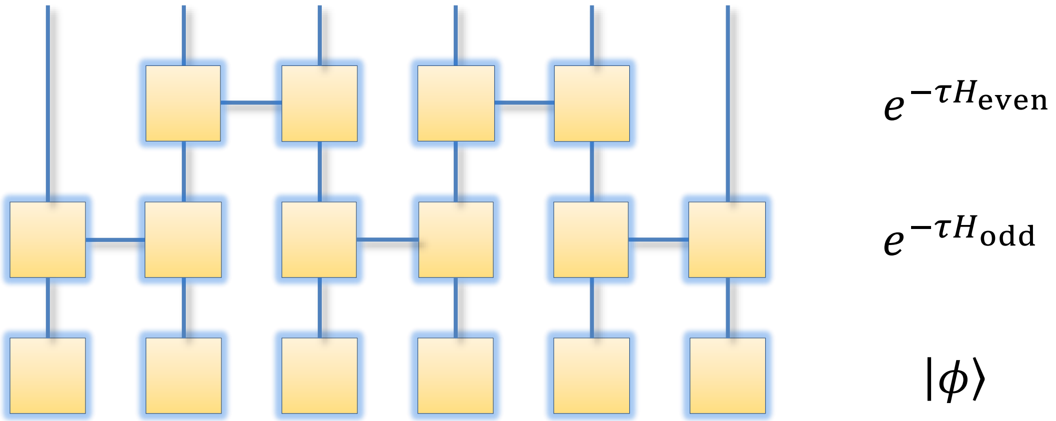

§ 3.2 Time evolution

- General case: non-commuting, $[H_{\mathrm{odd}}, H_{\mathrm{even}}] \neq 0$

Trotter-Suzuki decomposition:

$$e^{-\tau H} = e^{-\tau(H_{\mathrm{even}}+H_{\mathrm{odd}})}$$

$$= \left[e^{-\delta\tau(H_{\mathrm{even}}+H_{\mathrm{odd}})}\right]^M$$

Dividing into tiny time intervals: $\delta\tau = \tau/M$

$$e^{-\delta\tau(H_{\mathrm{even}}+H_{\mathrm{odd}})} = e^{-\delta\tau H_{\mathrm{even}}} e^{-\delta\tau H_{\mathrm{odd}}} + O(\delta\tau^2)$$

§ 3.2 Time evolution

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Dividing into tiny time intervals: $\delta\tau = \tau/M$

$$= \left[e^{-\delta\tau(H_{\mathrm{even}}+H_{\mathrm{odd}})}\right]^M$$

$$= \lim_{M\to\infty}\left[e^{-\delta\tau H_{\mathrm{even}}} e^{-\delta\tau H_{\mathrm{odd}}}\right]^M$$

G. Vidal, Phys. Rev. Lett. 91, 147902 (2003); Phys. Rev. Lett. 93, 040502 (2004).