" The $\chi \times \chi$ matrix Q encodes boundary conditions at sites $j = 0, n$, with $Q = \mathbb{1}$ corresponding to a translation invariant state with periodic boundary conditions

$\rightsquigarrow$ $\boxed{\text{DMRG produces MPS of bond dimension } \chi}$

- Basic idea of general MPS algorithms: Directly perform variational optimization in the space of MPS rather than following the specific DMRG algorithm.

- For an overview of MPS methods, see U. Schollwoeck, arXiv: 1008.3477.

- Basic example: tMPS for real (and imaginary) time evolution

- Key assumption: Local Hamiltonian, e.g. $H = \sum_i h_i$, where h_i acts on sites i and $i+1$ (nearest neighbors).

↳ Trotter decomposition: $e^{-iH\delta t} = e^{-ih_1\delta t} \cdots e^{-ih_{N-1}\delta t} + O(\delta t^2)$ (naive)

⇝ Better: $e^{-i\delta t H} = e^{-i\delta t H_{odd}}\, e^{-i\delta t H_{even}} + O(\delta t^2)$ with

$$H_{even} = \sum_i h_{2i}, \quad H_{odd} = \sum_i h_{2i-1}, \quad [h_i, h_{i+2}] = 0.$$

⇝ Even better: $e^{-iH\delta t} = e^{-iH_{odd}\frac{\delta t}{2}}\, e^{-iH_{even}\delta t}\, e^{-iH_{odd}\frac{\delta t}{2}} + O(\delta t^3)$.

higher order Trotter expansions improve scaling in δt.

- Problem: Applying 2-site operators such as $e^{-ih_1\delta t}$ to an MPS destroys the MPS form

Solution: Bring 2-body operator

$$e^{-ih_1\delta t} = \sum_{\substack{\sigma_1 \sigma_2 \\ \sigma_1' \sigma_2'}} O^{\sigma_1 \sigma_2}_{\sigma_1' \sigma_2'} |\sigma_1 \sigma_2\rangle\langle\sigma_1' \sigma_2'|$$

into so called MPO-form by SVD:

$$O^{\sigma_1 \sigma_2}_{\sigma_1' \sigma_2'} = \sum_k \tilde{U}_{\sigma_1 \sigma_1', k} S_{kk} V^{\dagger}_{k, \sigma_2 \sigma_2'} = \sum_k U_k^{\sigma_1 \sigma_1'} \bar{U}_k^{\sigma_2 \sigma_2'}$$

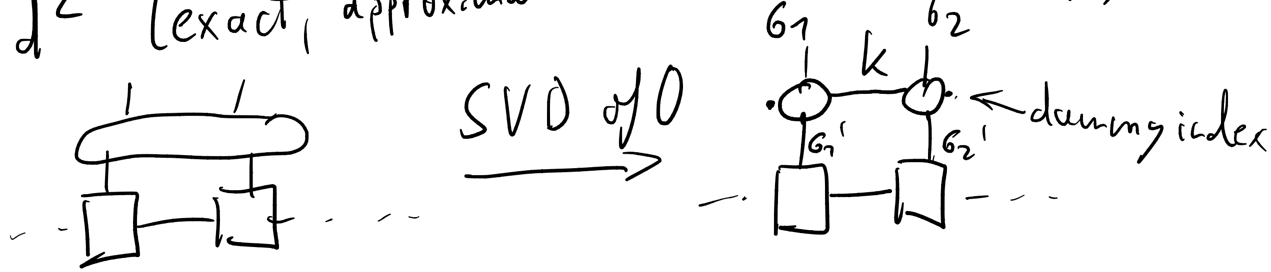
$$=: \sum_k U_{1,k}^{\sigma_1 \sigma_1'} \bar{U}_{k,1}^{\sigma_2 \sigma_2'}$$

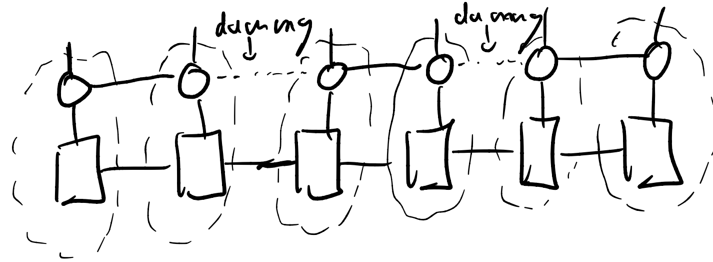
trivial dummy indices 1 for boundary sites of MPO

with $U_{1,k}^{\sigma_1 \sigma_1'} = \tilde{U}_{\sigma_1 \sigma_1', k} \sqrt{S_{kk}}$ and $\bar{U}_{k,1}^{\sigma_2 \sigma_2'} = \sqrt{S_{kk}} V^{\dagger}_{k, \sigma_2 \sigma_2'}$,

$k = 1, \dots, d^2$ (exact, approximate when not all S_{kk} are kept)

Graphical representation



i.e. $|\tilde{\psi}\rangle = e^{-iH_{odd}\delta t}|\psi\rangle =$ 

- $|\tilde{\psi}\rangle$ is an MPS of bond dimension $\chi \cdot d^2$, which needs to be compressed to an MPS of dimension χ (or χ_{max}) at every Trotter step (e.g. by SVD).

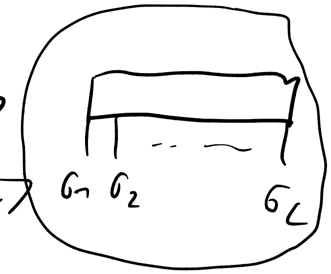
  b.d. of $|\psi\rangle$

For algebraic details on MPS and MPO calculus, see supplementary material of this section.

Supplement: MPS and MPO algebra

- Decomposition of an arbitrary QMB state into MPS:

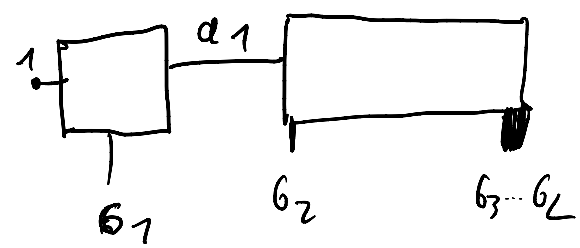
↳ Starting point: $|\Psi\rangle = \sum_{\{\sigma\}} c_{\sigma_1, \ldots, \sigma_L} |\sigma_1, \ldots, \sigma_L\rangle$



↳ Interpret $\Psi_{\sigma_1, (\sigma_2 \ldots \sigma_L)} := c_{\sigma_1, \ldots, \sigma_L}$ as a matrix with two indices:

↳ SVD of matrix Ψ gives $\Psi_{\sigma_1, (\sigma_2 \ldots \sigma_L)} = \sum_{a_1} U_{\sigma_1 a_1} S_{a_1 a_1} V^{\dagger}_{a_1, (\sigma_2 \ldots \sigma_L)}$

$$= \sum_{a_1} A^{\sigma_1}_{1, a_1} \Psi_{(a_1 \sigma_2), (\sigma_3 \ldots \sigma_L)}$$

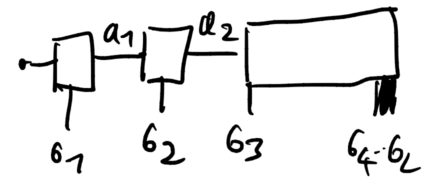


$A^{\sigma_1}_{1, a_1} = U_{\sigma_1, a_1}$

$\Psi_{(a_1 \sigma_2), (\sigma_3 \ldots \sigma_L)} : S_{a_1 a_1} V^{\dagger}_{a_1, (\sigma_2 \ldots \sigma_L)}$

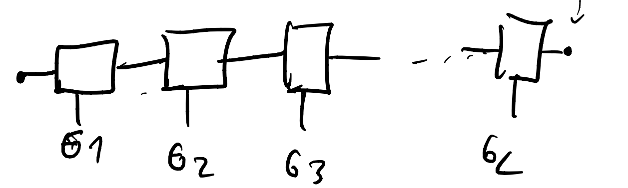
$$= \sum_{a_1,a_2} A^{\sigma_1}_{1,a_1} \underbrace{U_{a_1\sigma_2,a_2}}_{=:A^{\sigma_2}_{a_1a_2}} \underbrace{S_{a_2a_2} V^\dagger_{a_2,(\sigma_3\cdots\sigma_L)}}_{=:\Psi_{a_2\sigma_3,(\sigma_4\cdots\sigma_L)}}$$

SVD of $\Psi_{(a_1a_2),(\sigma_3\cdots\sigma_L)}$



$$= \cdots = \sum_{a_1,\dots,a_{L-1}} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} \underbrace{S_{a_{L-1}a_{L-1}} V^\dagger_{a_{L-1},\sigma_L}}_{=:A^{\sigma_L}_{a_{L-1},1}}$$

i.e. $|\Psi\rangle = \sum_{\sigma_1,\dots,\sigma_L} A^{\sigma_1}\cdots A^{\sigma_L}|\sigma_1,\dots,\sigma_L\rangle$



Since $U^\dagger U = \mathbb{1}$ in SVD, we have $\sum_{\sigma_l} A^{\sigma_l\dagger} A^{\sigma_l} = \mathbb{1}$ for $l = 1,\dots,L-1$ (left-canonical form)

$\sum_{\sigma_L} A^{\sigma_L\dagger} A^{\sigma_L} = 1$ only if $|\Psi\rangle$ is normalized, i.e. $\langle\Psi|\Psi\rangle = 1$.

- Warning: Scope of indices in general increases exponentially in system size:

$$d_1 = 1 \ldots d$$
$$d_2 = 1 \ldots d^2$$
$$d_L = 1, \ldots, d^{L/2}$$