TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Tensor Networks (SS2021)

Lecture 8: single-site vs. two-site DMRG

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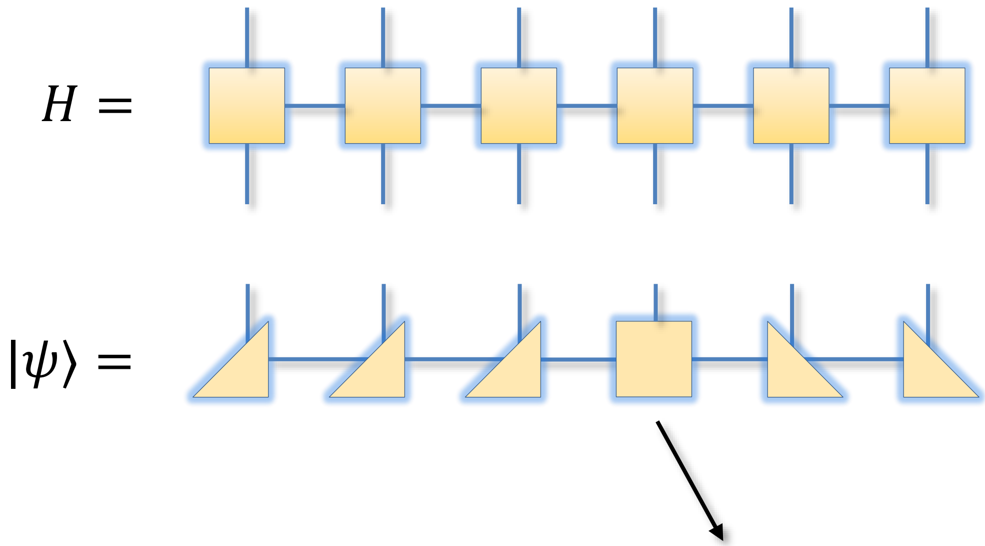
May 17th, 2021

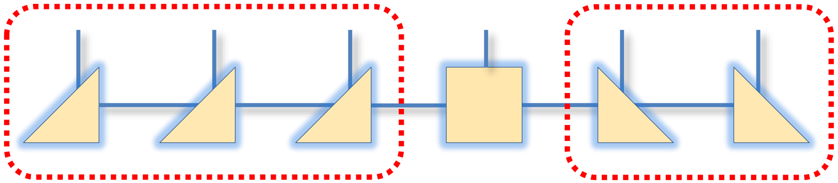
§ 2.2 Single-site DMRG

- Key step of the single-site DMRG:

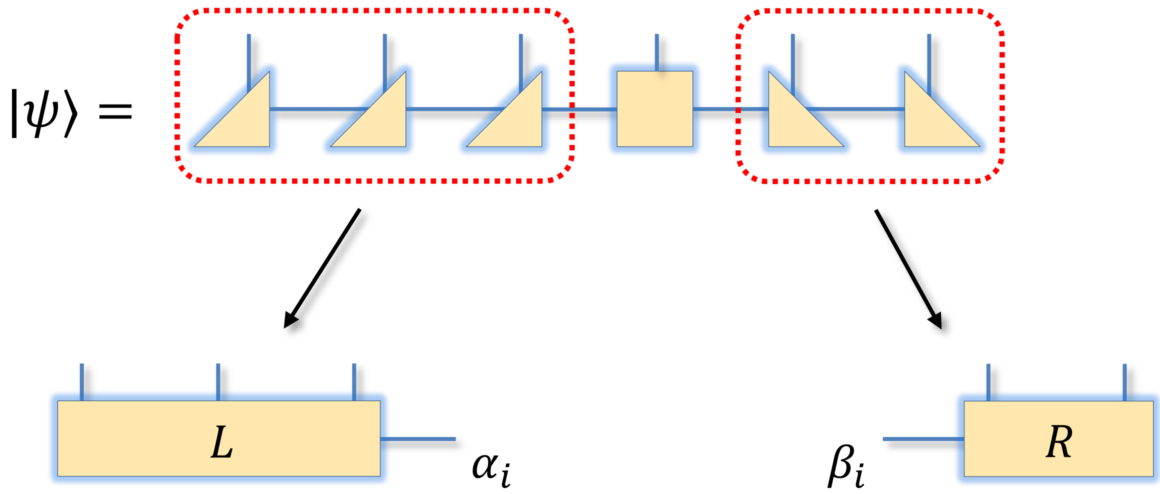


Optimize $A^{s_i}_{\alpha_i \beta_i}$ with respect to H

§ 2.2 Single-site DMRG

$|\psi\rangle =$ 

§ 2.2 Single-site DMRG



Orthonormal basis: $\langle L_{\alpha_i'} | L_{\alpha_i} \rangle = \delta_{\alpha_i' \alpha_i}$ $\langle R_{\beta_i'} | R_{\beta_i} \rangle = \delta_{\beta_i' \beta_i}$

They define the "kept subspace" for left/right environments!

§ 2.2 Single-site DMRG

- The (local) optimization looks for the best variational ansatz formed by the orthonormal basis $|L_{\alpha_i}\rangle \otimes |s_i\rangle \otimes |R_{\beta_i}\rangle$:

$$|\psi\rangle = \sum_{\alpha_i \beta_i s_i} A_{\alpha_i \beta_i s_i} |L_{\alpha_i}\rangle \otimes |s_i\rangle \otimes |R_{\beta_i}\rangle$$

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- The "projected" Hamiltonian within this truncated basis is just the effective Hamiltonian:

$$(H_{\text{eff}})_{(\alpha_i \beta_i s_i);(\alpha_i' \beta_i' s_i')} = \left\langle L_{\alpha_i}, s_i, R_{\beta_i} \middle| H \middle| L_{\alpha_i'}, s_i', R_{\beta_i'} \right\rangle$$

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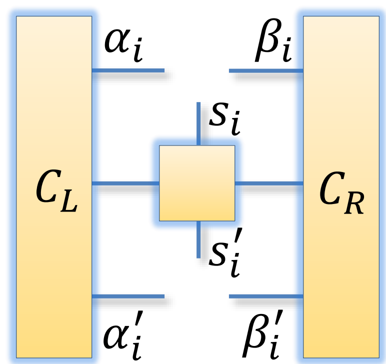
$$\Rightarrow \quad H_{\text{eff}} A = \lambda_{\min} A$$

§ 2.3 Lanczos algorithm

- Technically, it's not a good idea to explicitly write down H_{eff} and diagonalize it.

$$(H_{\text{eff}})_{(\alpha_i \beta_i s_i);(\alpha_i' \beta_i' s_i')} =$$



Dimension $\sim dD^2 \times dD^2$

§ 2.3 Lanczos algorithm

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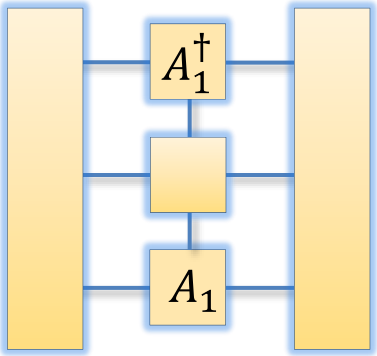
Lanczos method:

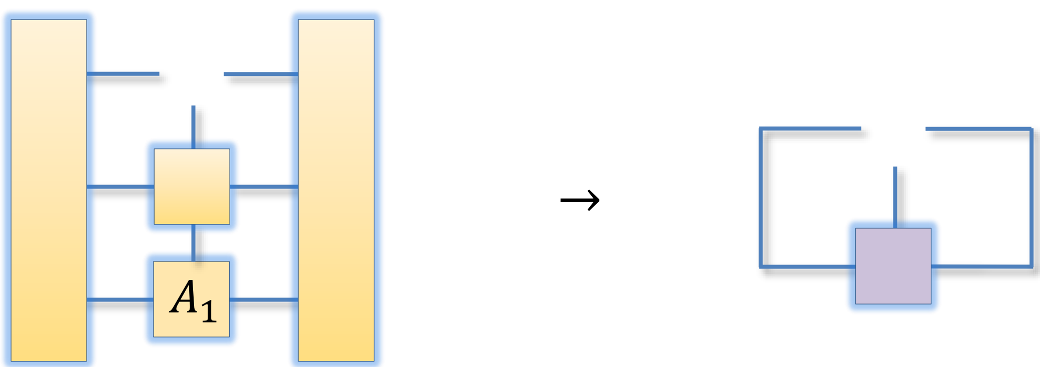
➢ Start with a normalized initial vector: A_1

$$\mu_1 \equiv A_1^\dagger H_{\mathrm{eff}} A_1 \quad =$$



§ 2.3 Lanczos algorithm

- Apply H_{eff} to A_1 and extract a new normalized vector A_2:



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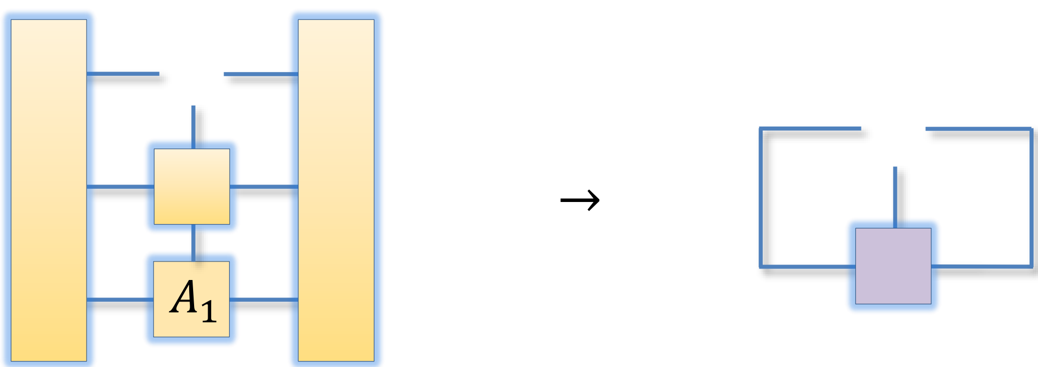


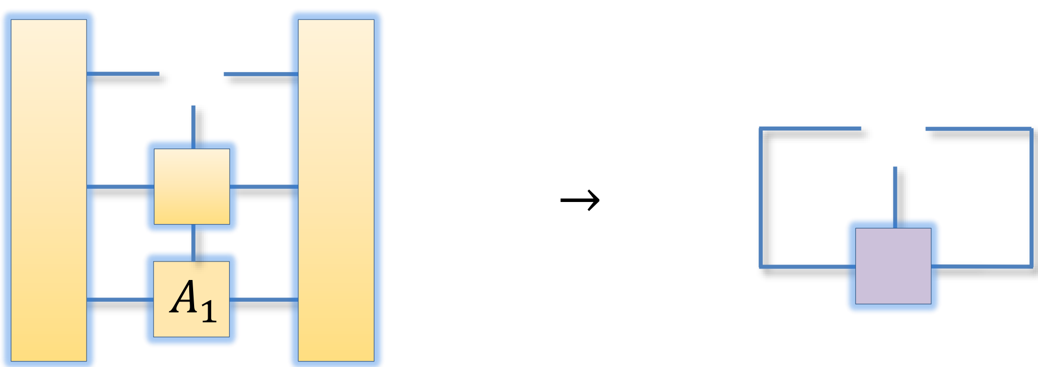
$$H_{\text{eff}} A_1 = \mu_1 A_1 + \nu_1 A_2$$

$$v_1 = \|(H_{\text{eff}} - \mu_1) A_1\|_2$$

$$A_2 = \frac{1}{v_1} (H_{\text{eff}} - \mu_1) A_1$$

§ 2.3 Lanczos algorithm

- Apply H_{eff} to A_1 and extract a new normalized vector A_2:



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$$A_2 = \frac{1}{\nu_1} (H_{\text{eff}} - \mu_1) A_1$$

$$\mu_2 \equiv A_2^{\dagger} H_{\text{eff}} A_2$$

§ 2.3 Lanczos algorithm

- Apply H_{eff} to A_2 and extract a new normalized vector A_3:

$$H_{\mathrm{eff}} A_2 = \mu_2 A_2 + \nu_1 A_1 + \nu_2 A_3$$

§ 2.3 Lanczos algorithm

- Apply H_{eff} to A_2 and extract a new normalized vector A_3:

$$H_{\text{eff}} A_2 = \mu_2 A_2 + \nu_1 A_1 + \nu_2 A_3$$

$$\nu_2 = \|(H_{\text{eff}} - \mu_2) A_2 - \nu_1 A_1\|_2$$

$$A_3 = \frac{1}{\nu_2}[(H_{\text{eff}} - \mu_2) A_2 - \nu_1 A_1]$$

$$\mu_3 \equiv A_3^\dagger H_{\text{eff}} A_3$$

§ 2.3 Lanczos algorithm

- Repeat the Lanczos step:

$$H_{\mathrm{eff}} A_3 = \mu_3 A_3 + \nu_2 A_2 + \nu_3 A_4$$

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$$H_{\text{eff}}A_3 = \underline{\mu_3 A_3 + \nu_2 A_2 + \nu_3 A_4}$$

No A_1 contribution!

(since $H_{\text{eff}}A_1 = \mu_1 A_1 + \nu_1 A_2$)

§ 2.3 Lanczos algorithm

- The Lanczos steps generate the Krylov subspace $\{A_1, A_2, \ldots\}$.
  In the Krylov subspace, H_{eff} is a tridiagonal matrix:

$$H_{\mathrm{eff}} = \begin{pmatrix} \mu_1 & \nu_1 & & & \\ \nu_1 & \mu_2 & \nu_2 & & \\ & \nu_2 & \mu_3 & \nu_3 & \\ & & \nu_3 & \ddots & \\ & & & & \ddots \end{pmatrix}$$

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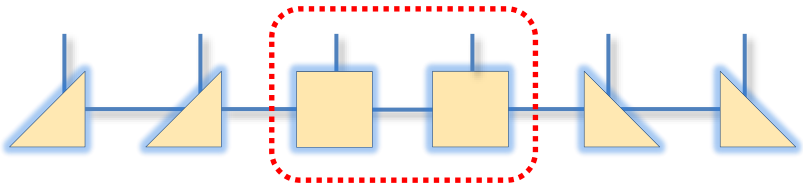
- Diagonalize H_{eff} in this (small) Krylov subspace to obtain $\lambda_{\min}$ and $A_{\alpha_i \beta_i s_i}$.

§ 2.4 Two-site DMRG

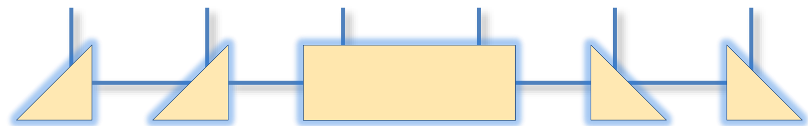
- Optimize two sites at the same time?

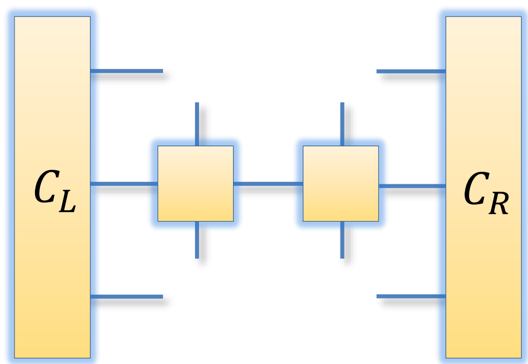
$|\psi\rangle =$



§ 2.4 Two-site DMRG

- Formalism is similar to one-site DMRG:

$|\psi\rangle =$ 

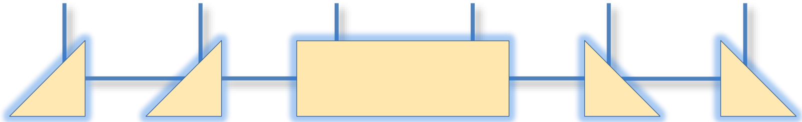
$H_{\text{eff}} =$ 

Dimension $\sim d^2 D^2 \times d^2 D^2$

§ 2.4 Two-site DMRG

- Once the optimized tensor $B_{\alpha\beta}^{s_i s_{i+1}}$ is obtained, it's necessary to perform an SVD to restore the MPS form.

$|\psi\rangle =$



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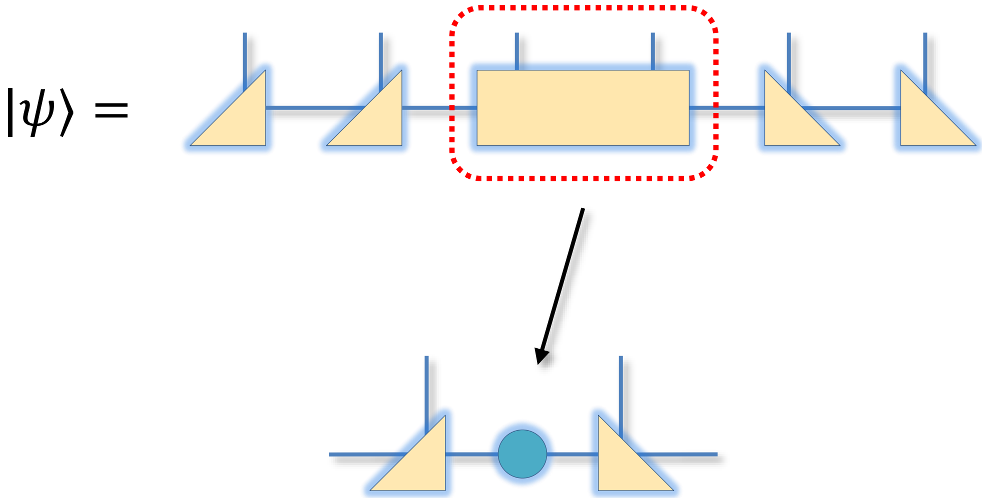
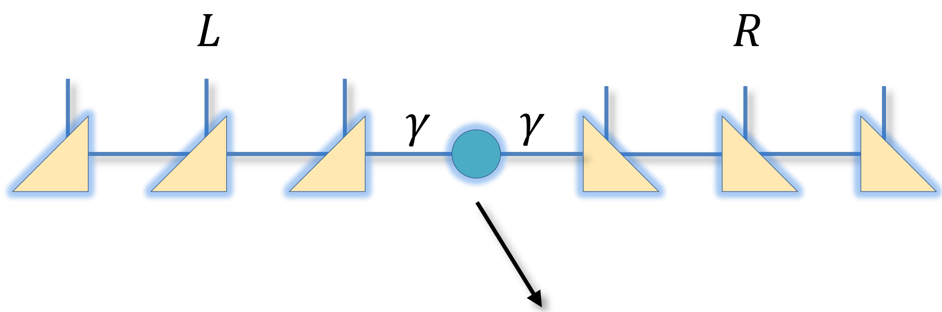


§ 2.4 Two-site DMRG

- For the SVD step, it's necessary to perform truncations!



$\lambda_\gamma > 0$ and $\sum_{\gamma=1}^{dD} \lambda_\gamma^2 = 1$

$$|\psi\rangle = \sum_{\gamma=1}^{dD} \lambda_\gamma |L_\gamma\rangle \otimes |R_\gamma\rangle \quad \Rightarrow \quad |\psi'\rangle = \sum_{\gamma=1}^{D_{\max}} \lambda_\gamma |L_\gamma\rangle \otimes |R_\gamma\rangle$$

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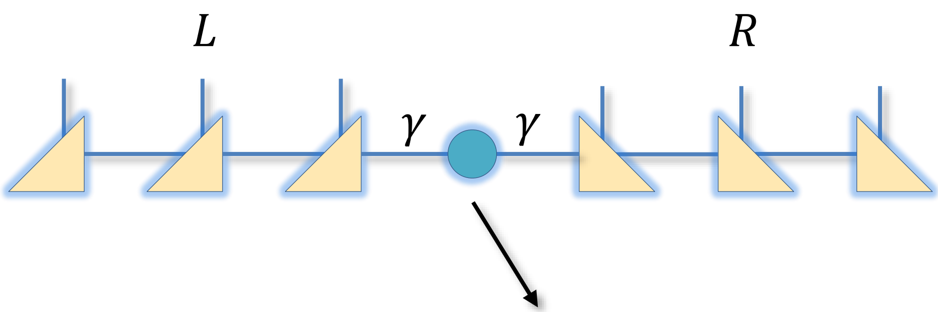

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Truncation error: $\delta \equiv \| |\psi\rangle - |\psi'\rangle \|_2^2 = \sum_{\gamma=D_{\max}+1}^{dD} \lambda_\gamma^2$

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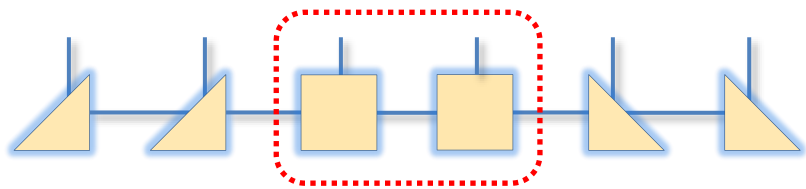
$|\psi\rangle =$ 

Advantage:
- Bond dimensions adjusted on the fly
- Better chance to escape local minima
- Convergence quantified by truncation error

Disadvantage: larger computational cost