TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Tensor Networks (SS2021)

Lecture 7: MPO and single-site DMRG

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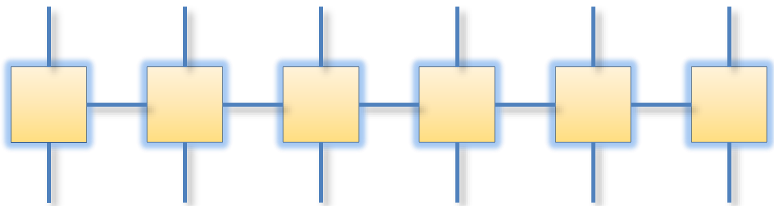
§ 2.1 Matrix Product Operator

Matrix Product Operator:

$$W = \sum_{s_1', s_1, \ldots, s_N', s_N} \sum_{\alpha_1, \ldots, \alpha_{N-1}} B_{\alpha_1}^{s_1', s_1} B_{\alpha_1 \alpha_2}^{s_2', s_2} \cdots B_{\alpha_{N-1}}^{s_N', s_N} \, |s_1', \ldots, s_N'\rangle\langle s_1, \ldots, s_N|$$



§ 2.1 Matrix Product Operator

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$$W = \sum_{s'_1,s_1,\ldots,s'_N,s_N} \sum_{\alpha_1,\ldots,\alpha_{N-1}} B_{\alpha_1}^{s'_1,s_1} B_{\alpha_1\alpha_2}^{s'_2,s_2} \cdots B_{\alpha_{N-1}}^{s'_N,s_N} |s'_1,\ldots,s'_N\rangle\langle s_1,\ldots,s_N|$$

$$= \sum_{\alpha_1,\ldots,\alpha_{N-1}} O_{\alpha_1} O_{\alpha_1,\alpha_2} \cdots O_{\alpha_{N-1}}$$

$$O_{\alpha_{i-1},\alpha_i} = \sum_{s'_i,s_i} B_{\alpha_{i-1}\alpha_i}^{s'_i,s_i} |s'_i\rangle\langle s_i|$$

- Product of matrices whose matrix entries are local operators.

§ 2.1 Matrix Product Operator

Example:

$$\sum_{j=1}^{N} S_j^z = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} I & 0 \\ S_1^z & I \end{pmatrix} \begin{pmatrix} I & 0 \\ S_2^z & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ S_{N-1}^z & I \end{pmatrix} \begin{pmatrix} I & 0 \\ S_N^z & I \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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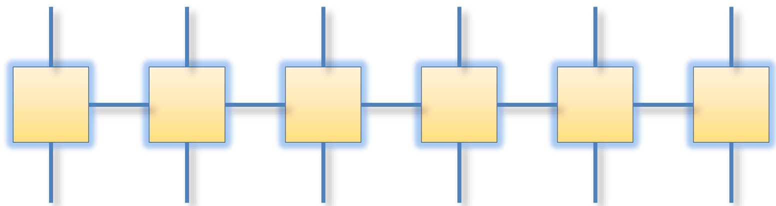
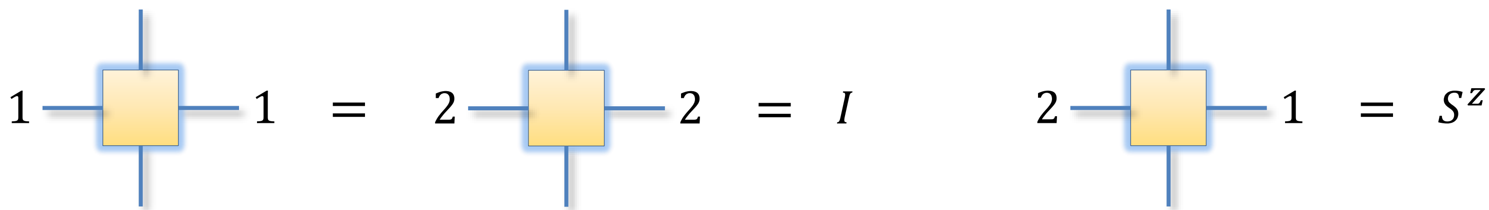
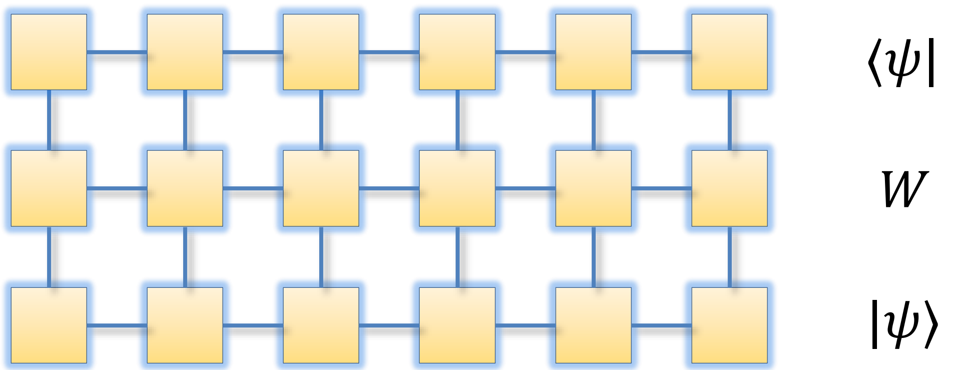
$=$ 



§ 2.1 Matrix Product Operator

- Motivation: It's particularly convenient to compute expectation values (and matrix elements) of MPO within MPS basis!

$$\langle\psi|W|\psi\rangle \; = $$

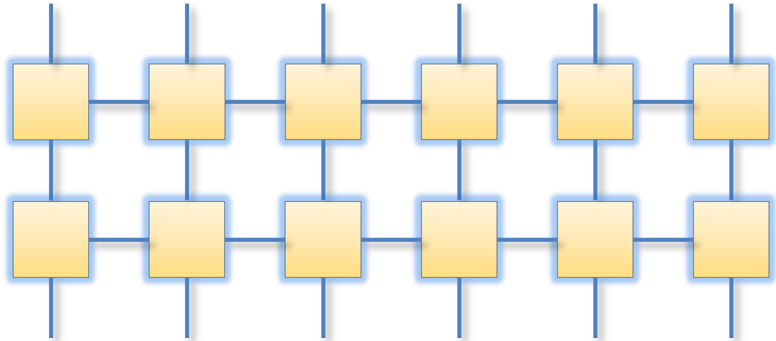


§ 2.1 Matrix Product Operator

What is the MPO form for $S^z_{-q} S^z_q$?

$$S^z_q = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} S^z_j \, e^{-iqj}$$

$$= \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} I & 0 \\ S^z_1 e^{-iq} & I \end{pmatrix} \begin{pmatrix} I & 0 \\ S^z_2 e^{-2iq} & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ S^z_N e^{-iqN} & I \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$S^z_{-q} S^z_q =$ 

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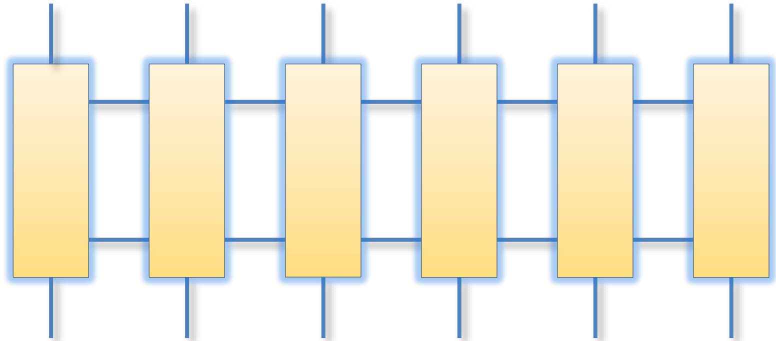
$S^z_{-q}S^z_q =$ 

§ 2.1 Matrix Product Operator

$$H = \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1}$$

$$= \begin{pmatrix} 0 & \frac{1}{2}S_1^- & \frac{1}{2}S_1^+ & S_1^z & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 & 0 & 0 & 0 \\ S_i^+ & 0 & 0 & 0 & 0 \\ S_i^- & 0 & 0 & 0 & 0 \\ S_i^z & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2}S_i^- & \frac{1}{2}S_i^+ & S_i^z & I \end{pmatrix} \cdots \begin{pmatrix} I \\ S_N^+ \\ S_N^- \\ S_N^z \\ 0 \end{pmatrix}$$

§ 2.1 Matrix Product Operator

- How to obtain the MPO representation for a given operator?
  - Construction by hand: inspection + addition of the simplest ones

$$W = W_1 + W_2$$

$$\Rightarrow \quad O = \begin{pmatrix} O_1 & \\ & O_2 \end{pmatrix}$$

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  - Construction by hand: inspection + addition of the simplest ones

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  - Automatic generation: see this link ("AutoMPO" in iTensor) and this paper [Hubig *et al.*, Phys. Rev. B 95, 035129 (2017)].

§ 2.2 Single-site DMRG

- For a given Hamiltonian, we want to find the best variational ansatz within the family of MPS:

$$E(A) = \min_{\{A\}} \frac{\langle \psi(A)|H|\psi(A)\rangle}{\langle \psi(A)|\psi(A)\rangle}$$

- This is a highly nonlinear optimization problem, which is in general rather difficult.

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- Spirit of DMRG: optimize $A^{s_i}_{\alpha_i \beta_i}$ site by site (locally optimal)

S. R. White, Phys. Rev. Lett. 69, 2863 (1992);

U. Schollwöck, Ann. Phys 326, 96 (2011); C. Hubig, PhD Thesis at LMU (2017).

§ 2.2 Single-site DMRG

- Define energy functional:

$$E[A,\bar{A},\lambda] = \langle\psi(A)|H|\psi(A)\rangle - \lambda(\langle\psi(A)|\psi(A)\rangle - 1)$$

Lagrange multiplier

- Energy minimization (with respect to site i):

$$\frac{\partial}{\partial \bar{A}^{s_i}_{\alpha_i\beta_i}} E[A,\bar{A},\lambda] = \frac{\partial}{\partial A^{s_i}_{\alpha_i\beta_i}} E[A,\bar{A},\lambda] = 0$$

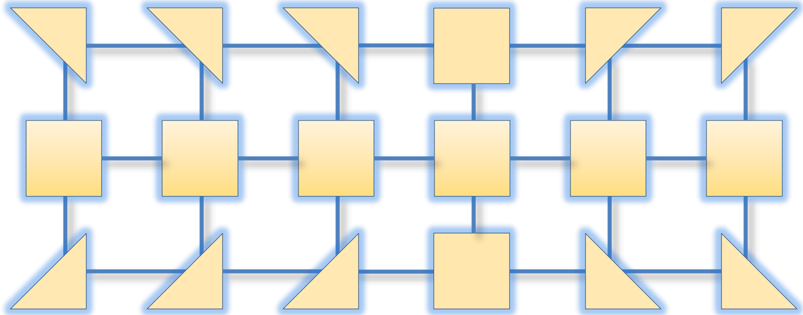
$$\frac{\partial}{\partial \lambda} E[A,\bar{A},\lambda] = 0$$

§ 2.2 Single-site DMRG

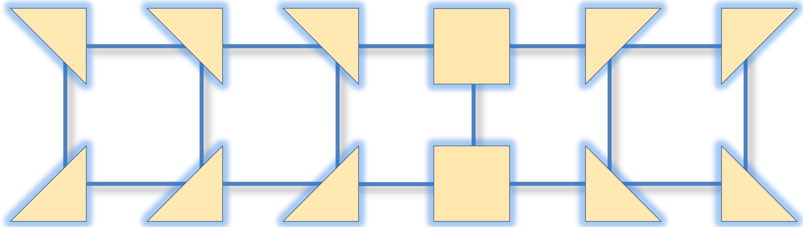
- This is best done with site canonical form (for site i):

$$E[A,\bar{A},\lambda] = \langle\psi(A)|H|\psi(A)\rangle - \lambda(\langle\psi(A)|\psi(A)\rangle - 1)$$

$=$



$-\lambda($

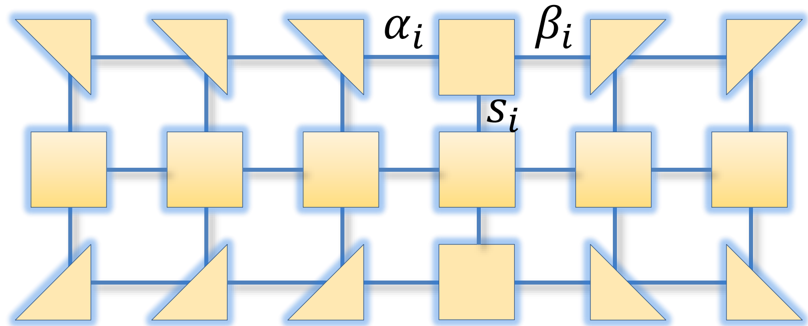


$-1)$

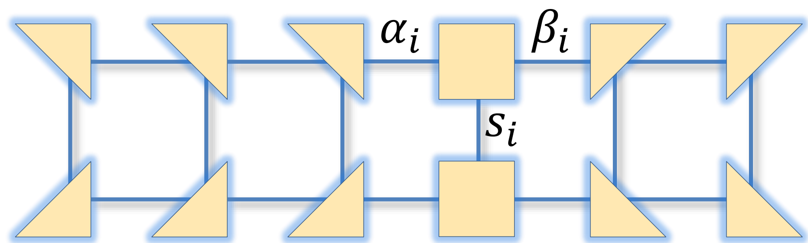
§ 2.2 Single-site DMRG

- This is best done with site canonical form (for site i):

$$\frac{\partial}{\partial \bar{A}^{s_i}_{\alpha_i \beta_i}} E[A, \bar{A}, \lambda] = \frac{\partial}{\partial \bar{A}^{s_i}_{\alpha_i \beta_i}}$$



$$-\lambda \frac{\partial}{\partial \bar{A}^{s_i}_{\alpha_i \beta_i}}$$



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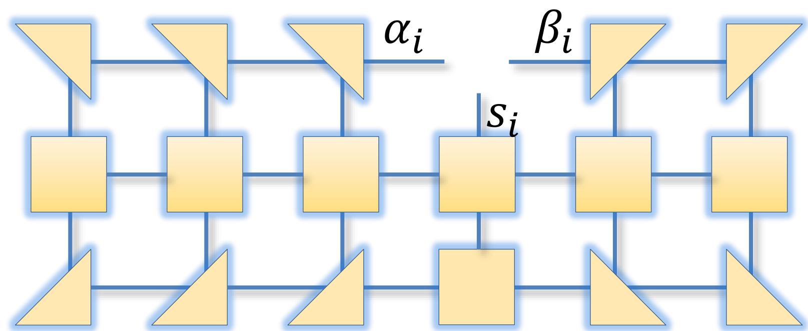
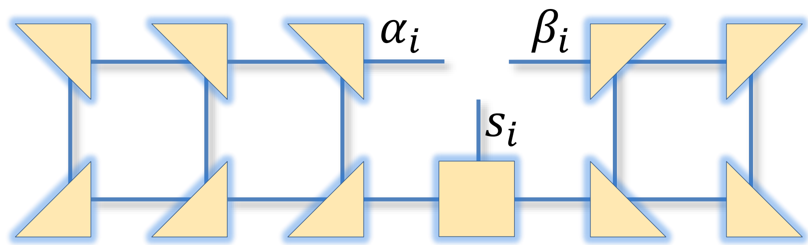
- This is best done with site canonical form (for site i):

$$\frac{\partial}{\partial \bar{A}^{s_i}_{\alpha_i \beta_i}} E[A, \bar{A}, \lambda] =$$



$$-\lambda$$



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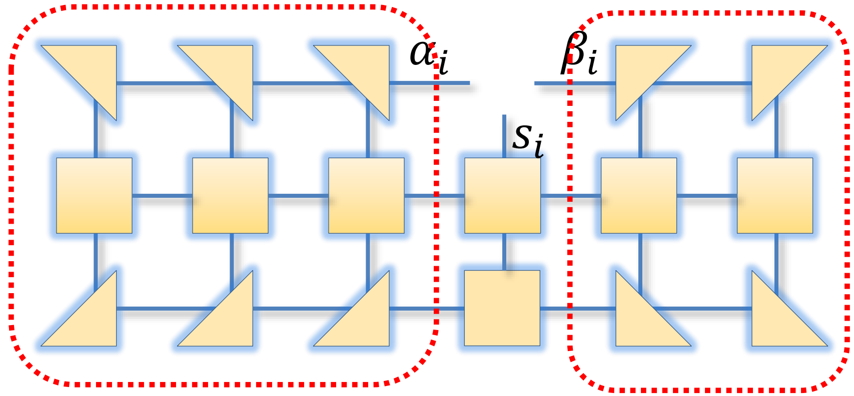

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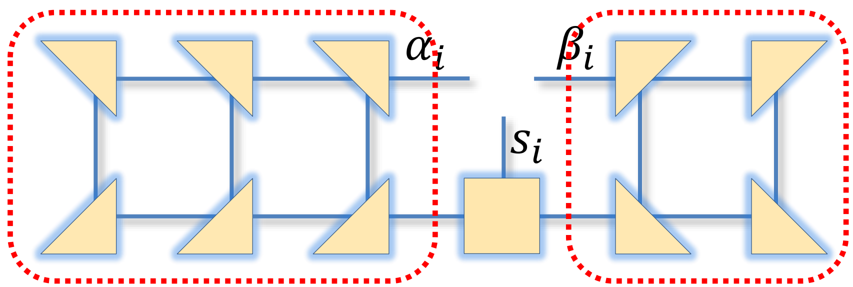

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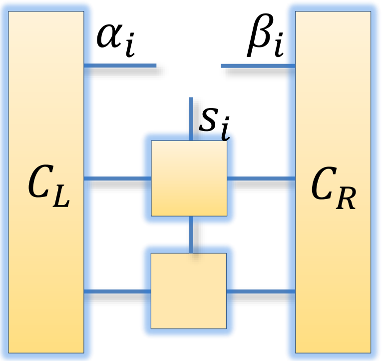

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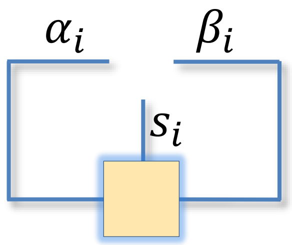
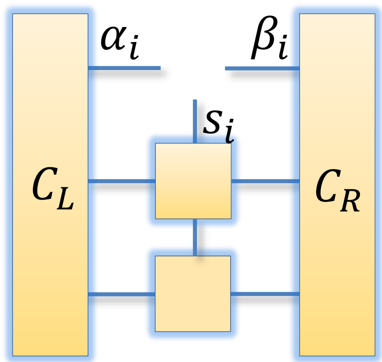


§ 2.2 Single-site DMRG

$$\frac{\partial}{\partial \bar{A}^{s_i}_{\alpha_i \beta_i}} E[A, \bar{A}, \lambda] =$$



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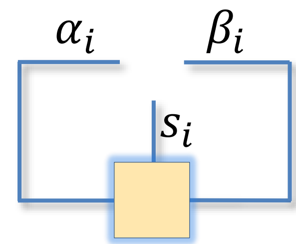
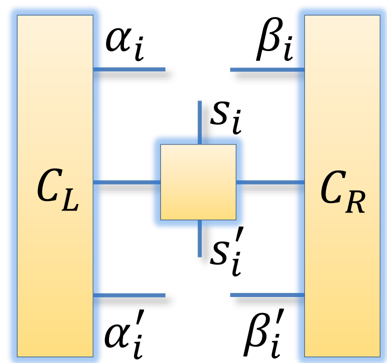


$$= 0$$

Effective Hamiltonian:

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



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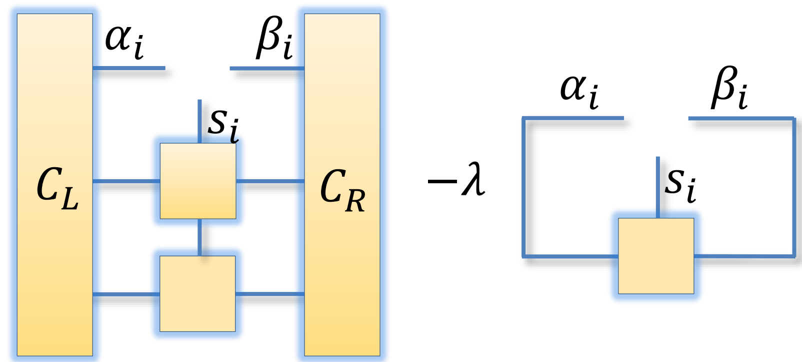
$$\frac{\partial}{\partial \bar{A}^{s_i}_{\alpha_i \beta_i}} E[A, \bar{A}, \lambda] =$$



$$= 0$$

Standard eigenvalue problem!

$$\sum_{\alpha_i' \beta_i' s_i'} (H_{\text{eff}})_{(\alpha_i \beta_i s_i);(\alpha_i' \beta_i' s_i')} A_{\alpha_i' \beta_i' s_i'} = \lambda A_{\alpha_i \beta_i s_i} \quad \Rightarrow \quad H_{\text{eff}} A = \lambda A$$

§ 2.2 Single-site DMRG

Standard eigenvalue problem (at site i):

$$H_{\text{eff}} A = \lambda A \qquad A^\dagger A = 1$$

- Keep the lowest eigenvalue λ_{min} and its corresponding (normalized) eigenvector $A^{s_i}_{\alpha_i \beta_i}$.

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$A^\dagger A = 1$

- Keep the lowest eigenvalue λ_{min} and its corresponding (normalized) eigenvector $A^{s_i}_{\alpha_i \beta_i}$.

variational ground-state energy
(see next slide)

This ensures normalization:

$$\frac{\partial}{\partial \lambda} E[A, \bar{A}, \lambda] = \langle \psi | \psi \rangle - 1 = 0$$

§ 2.2 Single-site DMRG

Standard eigenvalue problem (at site i):

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- Keep the lowest eigenvalue $\lambda_{\min}$ and its corresponding (normalized) eigenvector $A^{s_i}_{\alpha_i \beta_i}$.

variational ground-state energy (see next slide)

This ensures normalization:

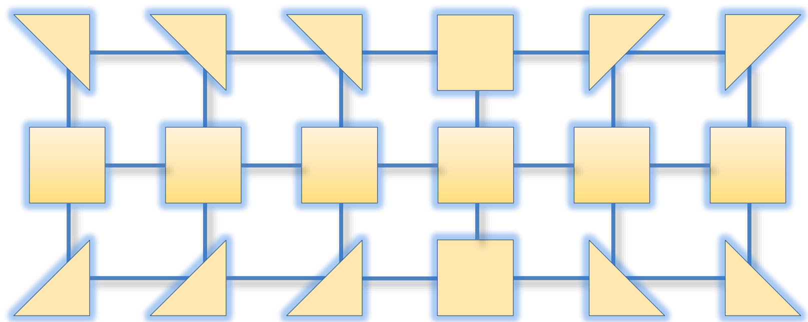
$$\frac{\partial}{\partial \lambda} E[A, \bar{A}, \lambda] = \langle \psi | \psi \rangle - 1 = 0$$

- Use Lanczos algorithm (next lecture), since H_{eff} is a large matrix and only its lowest eigenvalue/eigenvector is needed.

§ 2.2 Single-site DMRG

Substitute the obtained solution $A^{s_i}_{\alpha_i\beta_i}$ into the energy functional:

$$E[A,\bar{A},\lambda] = \langle\psi(A)|H|\psi(A)\rangle - \lambda(\langle\psi(A)|\psi(A)\rangle - 1)$$

$=$ 

$= \lambda_{\min}$ (So $\lambda_{\min}$ is already the variational energy!)

§ 2.2 Single-site DMRG

Workflow:

- Generate a random MPS (to initialize DMRG).

- Start with site 1: bring the MPS into site canonical form (at site 1), optimize the MPS tensor at site 1 (by diagonalizing the effective Hamiltonian), save the variational energy (to compare with the variational energies in the next steps), use the obtained MPS tensor to calculate/update the environment tensors C_L and C_R (this saves computing time).

- Go to site 2, repeat the above steps for site 1.

- Do the same for site 3, site 4, … , site N, site $N-1$, … , site 1, ...

- Sweep a few times, until the variational energy is converged.