SFB 1143

Tensor Networks (SS2021)

Lecture 18: PEPS optimization and contraction

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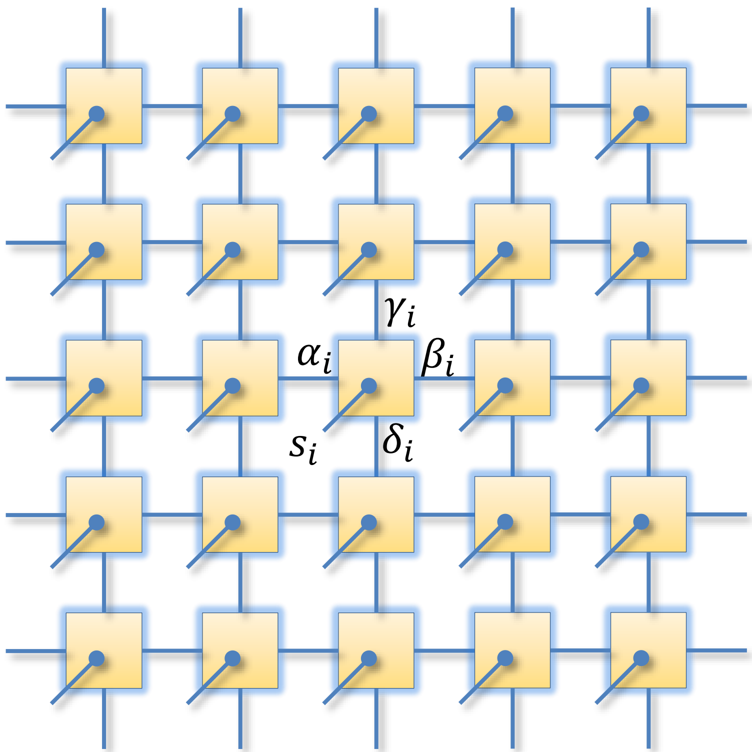
§ 4.2 PEPS: Optimization and contraction

Numerical challenges of PEPS:

- Optimization: finding the best PEPS ansatz for a given Hamiltonian

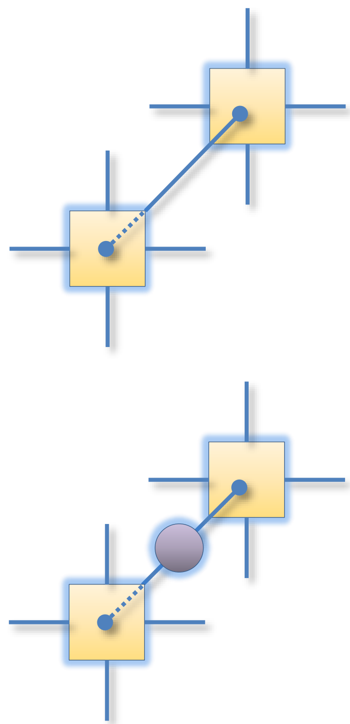
- Contraction: computing physical observables

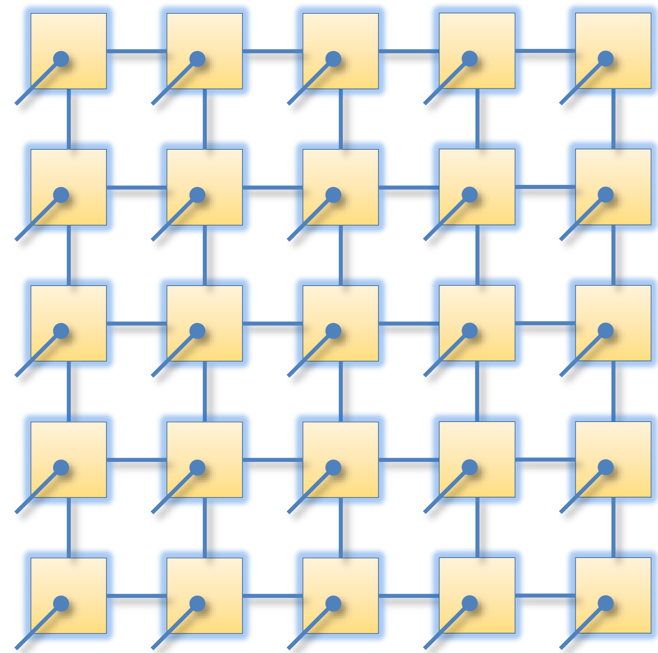


$$|\psi\rangle = \sum_{\{s\}=1}^{d} \left(\sum_{\{\alpha\beta\gamma\delta\}=1}^{D} \cdots A^{s_i}_{\alpha_i\beta_i\gamma_i\delta_i} \cdots \right) | \ldots s_i \ldots \rangle$$

§ 4.2 PEPS: Optimization and contraction

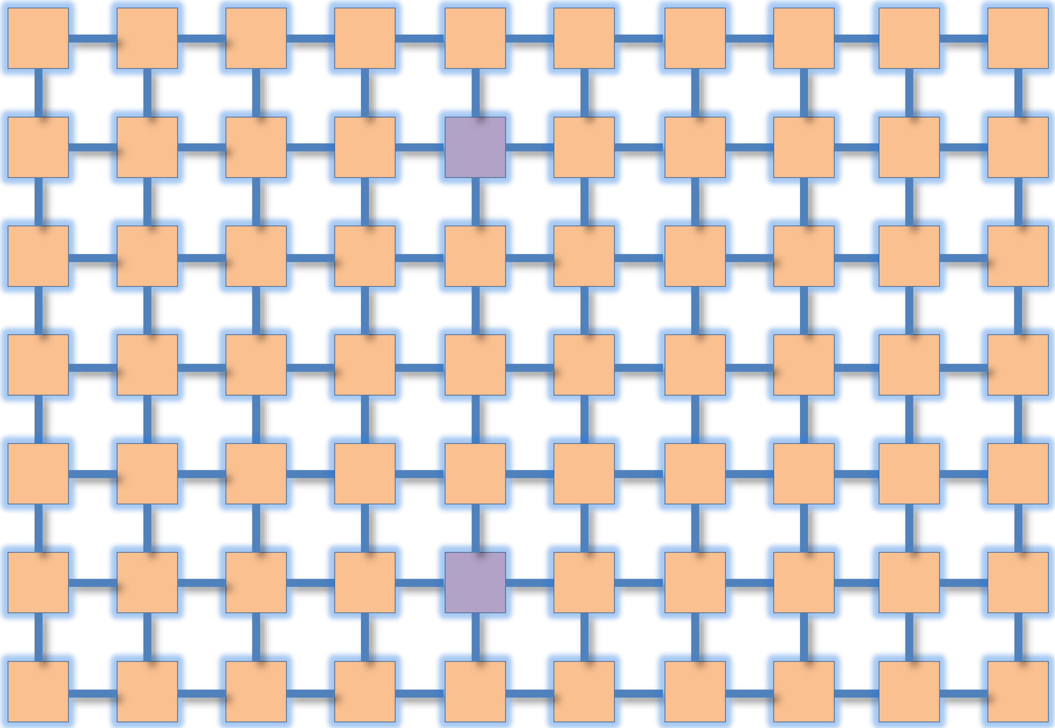
$\langle\psi|O_iO_j|\psi\rangle$





§ 4.2 PEPS: Optimization and contraction

$\langle\psi|O_i O_j|\psi\rangle =$



Exact contraction: #P hard!

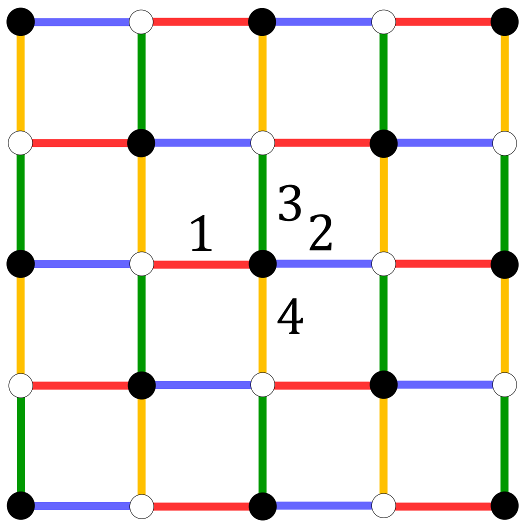
§ 4.2 PEPS: Optimization and contraction

- Finite PEPS algorithm:

Imaginary time evolution:

$$\lim_{\tau\to\infty} e^{-\tau H}|\psi\rangle \to |\psi(D)\rangle$$

$$e^{-\delta\tau H} \approx e^{-\delta\tau H_1} e^{-\delta\tau H_2} \times e^{-\delta\tau H_3} e^{-\delta\tau H_4} + O(\delta\tau^2)$$

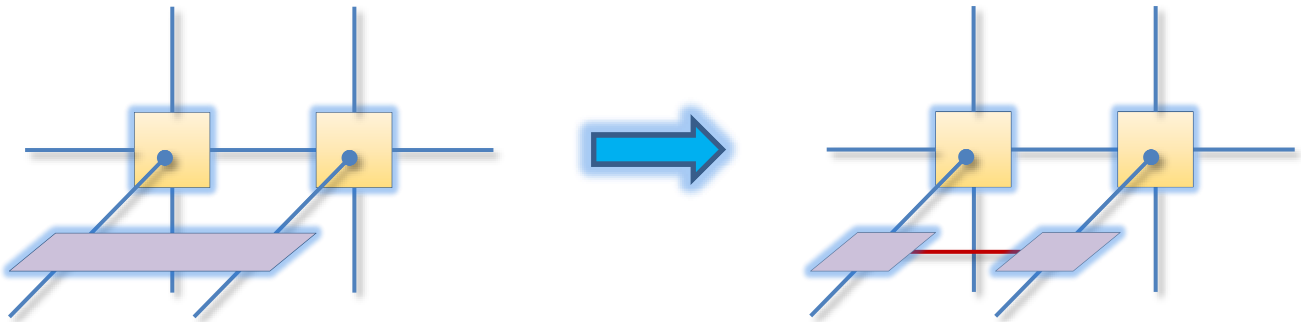


F. Verstraete & J. I. Cirac, cond-mat/0407066;

V. Murg, F. Verstraete & J. I. Cirac, Phys. Rev. A 75, 033605 (2007).

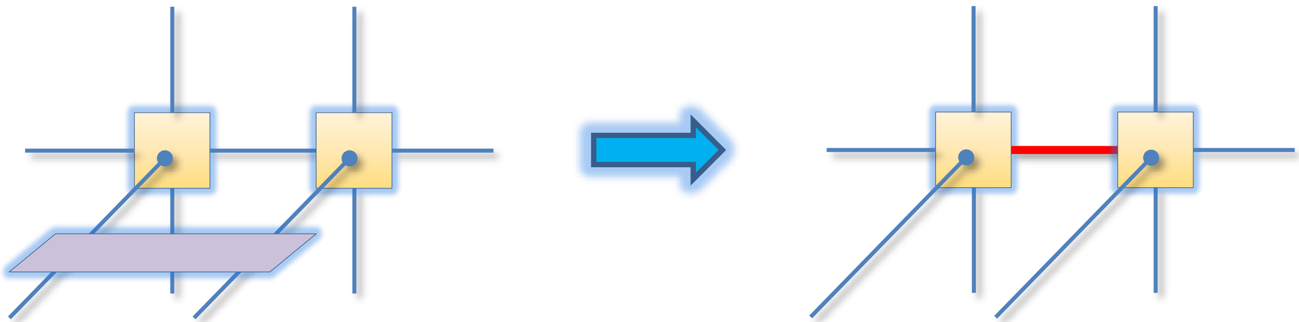
§ 4.2 PEPS: Optimization and contraction

Evolve PEPS with small imaginary-time steps:



§ 4.2 PEPS: Optimization and contraction

Evolve PEPS with small imaginary-time steps:



Bond dimension increased from D to d^2D!

§ 4.2 PEPS: Optimization and contraction

Truncation: $|\psi_B\rangle \Rightarrow |\psi_A\rangle$ bond dimension from d^2D to D

- Find $|\psi_A\rangle$ such that $K = \||\psi_A\rangle - |\psi_B\rangle\|^2$ is minimized:

$$K = \langle\psi_A|\psi_A\rangle + \langle\psi_B|\psi_B\rangle - \langle\psi_A|\psi_B\rangle - \langle\psi_B|\psi_A\rangle$$

§ 4.2 PEPS: Optimization and contraction

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- Carry out the local optimization site by site (i.e. DMRG-like):

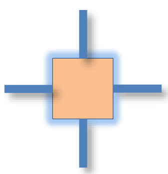
$$\langle\psi_A|\psi_A\rangle = \mathbf{A}_i^\dagger \mathbf{N}_i \mathbf{A}_i$$

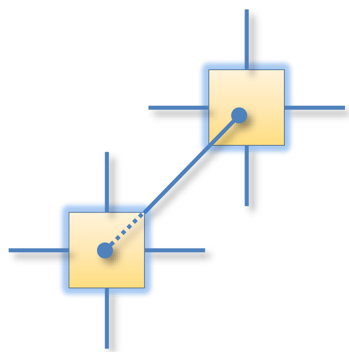
$$\langle\psi_A|\psi_B\rangle = \mathbf{A}_i^\dagger \mathbf{W}_i$$

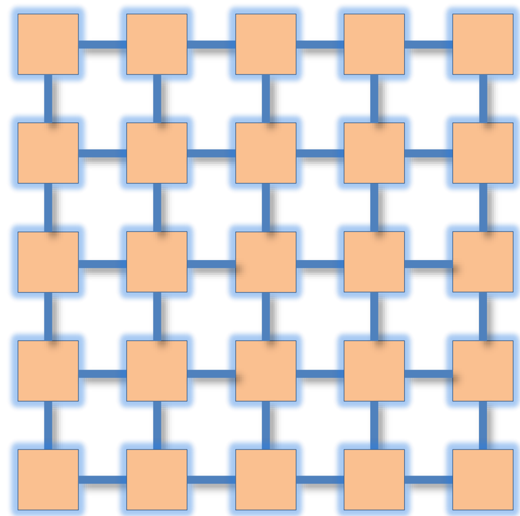
$$\frac{\partial K}{\partial \bar{A}^{s_i}_{\alpha_i\beta_i\gamma_i\delta_i}} = 0 \Rightarrow \mathbf{N}_i \mathbf{A}_i = \mathbf{W}_i$$

§ 4.2 PEPS: Optimization and contraction

$\langle \psi_A | \psi_A \rangle$

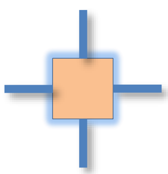


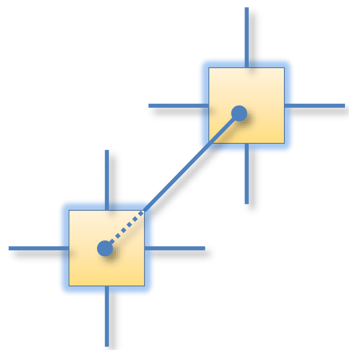


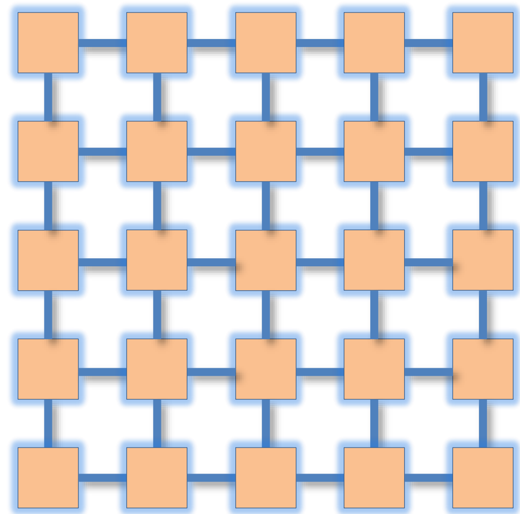


§ 4.2 PEPS: Optimization and contraction

$\langle \psi_A | \psi_A \rangle$







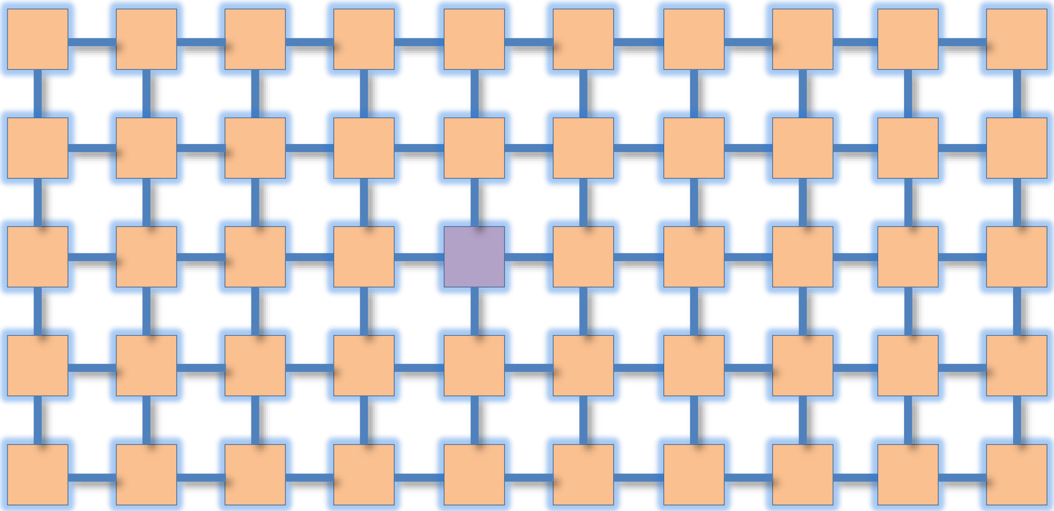
$$\mathbf{N}_i = \frac{\partial \langle \psi_A | \psi_A \rangle}{\partial \bar{A}^{s_i}_{\alpha_i \beta_i \gamma_i \delta_i}}$$

($\mathbf{W}_i$ similar)

$\bar{A}^{s_i}_{\alpha_i \beta_i \gamma_i \delta_i}$ removed in the double-layer tensor network!

§ 4.2 PEPS: Optimization and contraction

- Compute $\mathbf{N}_i$ and $\mathbf{W}_i$: MPO-MPS evolution



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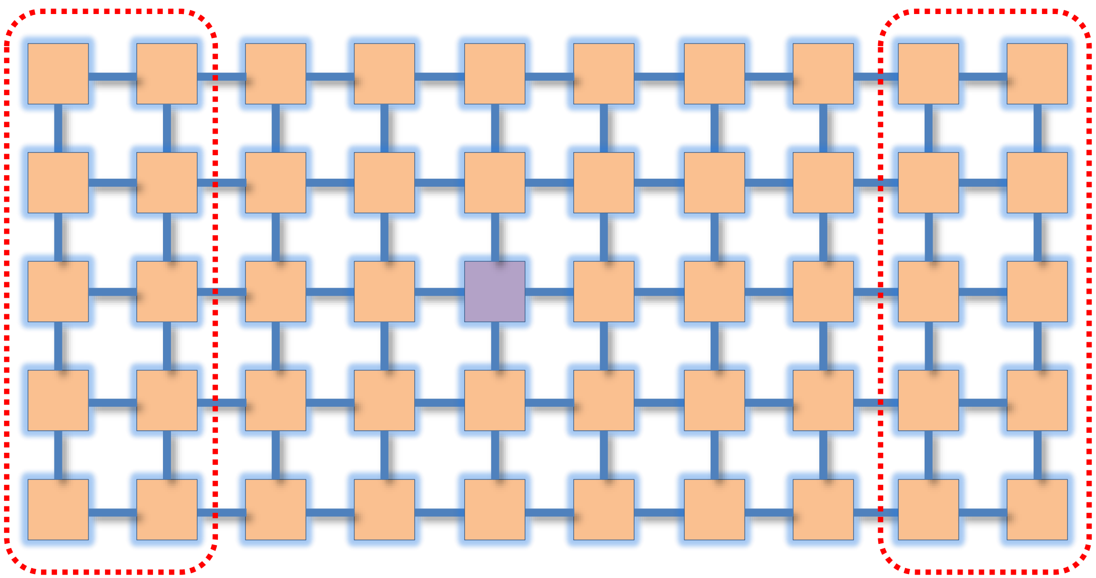

§ 4.2 PEPS: Optimization and contraction

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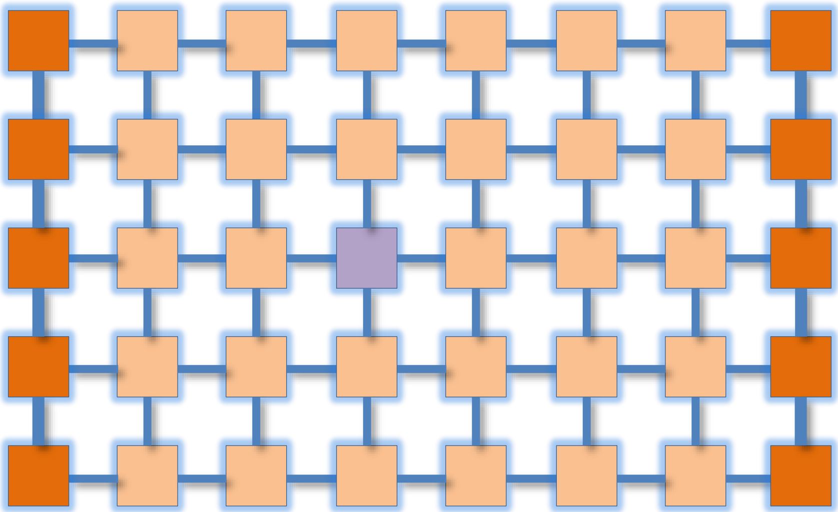

§ 4.2 PEPS: Optimization and contraction

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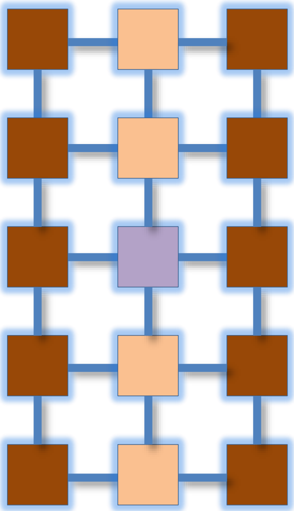
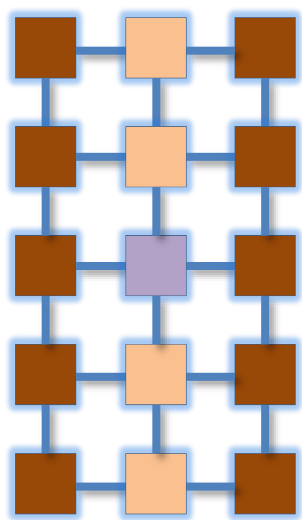


§ 4.2 PEPS: Optimization and contraction

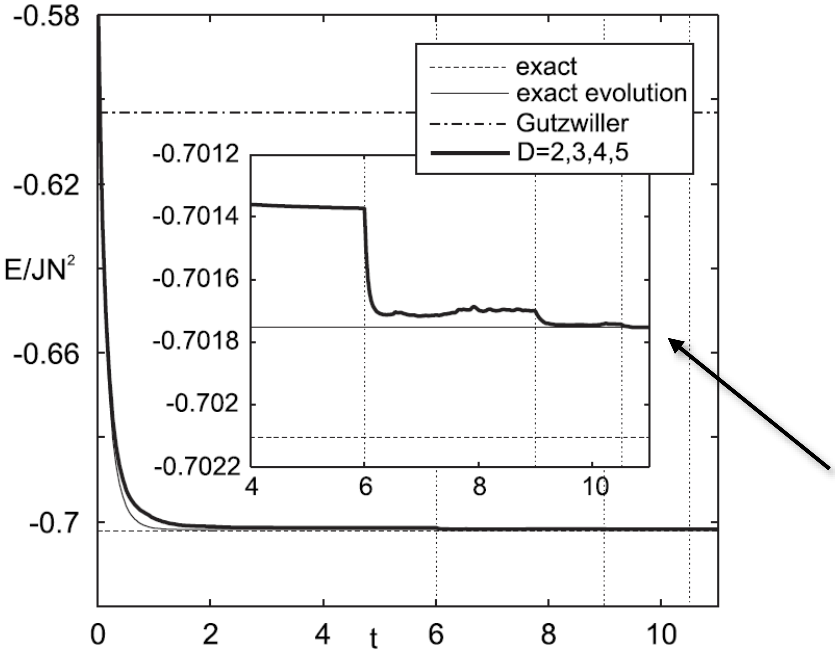
➢ Compute $\mathbf{N}_i$ and $\mathbf{W}_i$: MPO-MPS evolution



For large system sizes and/or large bond dimensions, the computation of environment tensors can only be done approximately!

§ 4.2 PEPS: Optimization and contraction

$$H = -J\sum_{\langle i,j\rangle}(a_i^\dagger a_j + \text{H.c.}) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \sum_i V_i \hat{n}_i$$



2D square lattice, 4×4

4 hardcore bosons

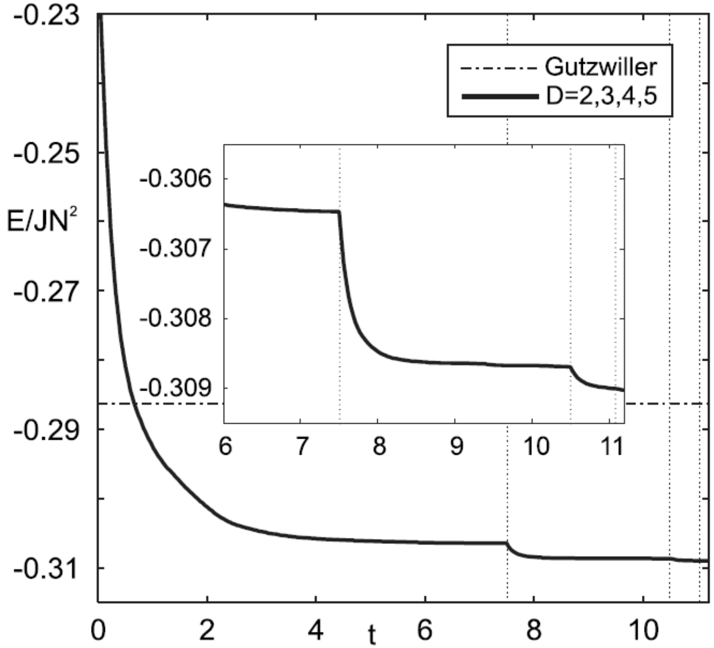
$V_0/J = 36 \quad \delta\tau = 0.03$

error $\sim 10^{-5}$

V. Murg, F. Verstraete & J. I. Cirac, Phys. Rev. A 75, 033605 (2007).

§ 4.2 PEPS: Optimization and contraction

$$H = -J\sum_{\langle i,j\rangle}(a_i^\dagger a_j + \mathrm{H.c.}) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \sum_i V_i\hat{n}_i$$



2D square lattice, 11×11

14 hardcore bosons

$V_0/J = 100 \quad \delta\tau = 0.03$

V. Murg, F. Verstraete & J. I. Cirac, Phys. Rev. A 75, 033605 (2007).

§ 4.2 PEPS: Optimization and contraction

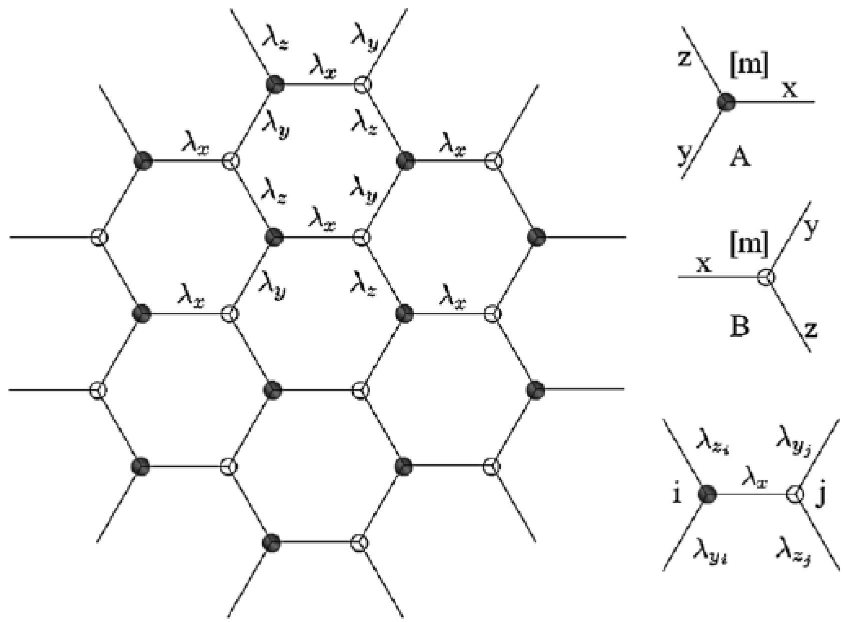
- Infinite PEPS algorithm: simple update

2D analog of iTEBD:

$$\lim_{\tau\to\infty} e^{-\tau H}|\psi\rangle \to |\psi(D)\rangle$$

$$e^{-\delta\tau H} \approx e^{-\delta\tau H_1} e^{-\delta\tau H_2}$$

$$\times\, e^{-\delta\tau H_3} + O(\delta\tau^2)$$

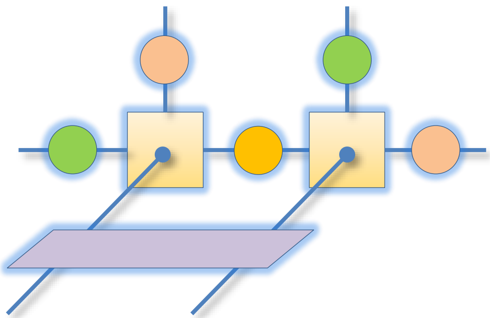


$$\lambda_{x,y,z} > 0$$

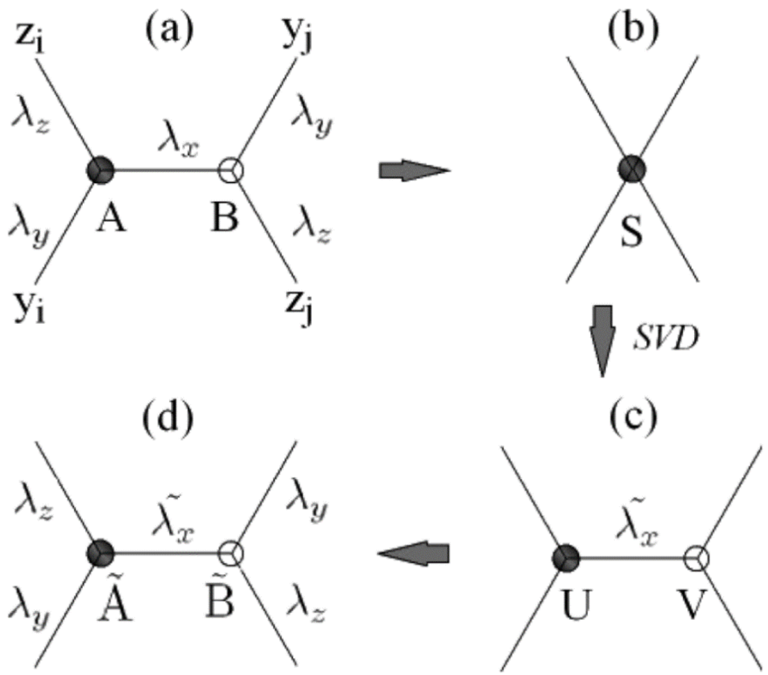
H. C. Jiang, Z. Y. Weng & T. Xiang, Phys. Rev. Lett. 101, 090603 (2008).

§ 4.2 PEPS: Optimization and contraction

- Infinite PEPS algorithm: simple update



Local update!



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§ 4.2 PEPS: Optimization and contraction

Spin-1/2 Heisenberg model on the honeycomb lattice: $H = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$

TABLE I. The ground state energy per site E and the staggered magnetization M in the zero field limit as a function of D.

D	E	M
3	−0.5365	0.249
4	−0.5456	0.228
5	−0.5488	0.220
6	−0.5513	0.206
7	−0.5490	0.216
8	−0.5506	0.212

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§ 4.2 PEPS: Optimization and contraction

Spin-1/2 Heisenberg model on the honeycomb lattice: $H = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$

TABLE II. Comparison of our results with those obtained by other approaches for the ground state energy per site E and the staggered magnetization M of the Heisenberg model with $h = 0$.

Method	E	M
Spin wave [12]	−0.5489	0.24
Series expansion [13]	−0.5443	0.27
Monte Carlo [14]	−0.5450	0.22
Ours $D = 8$	−0.5506	0.21 ± 0.01

H. C. Jiang, Z. Y. Weng & T. Xiang, Phys. Rev. Lett. 101, 090603 (2008).