Lecture 4: Tensor Product Ansatz - part II

TCM Graduate Lectures

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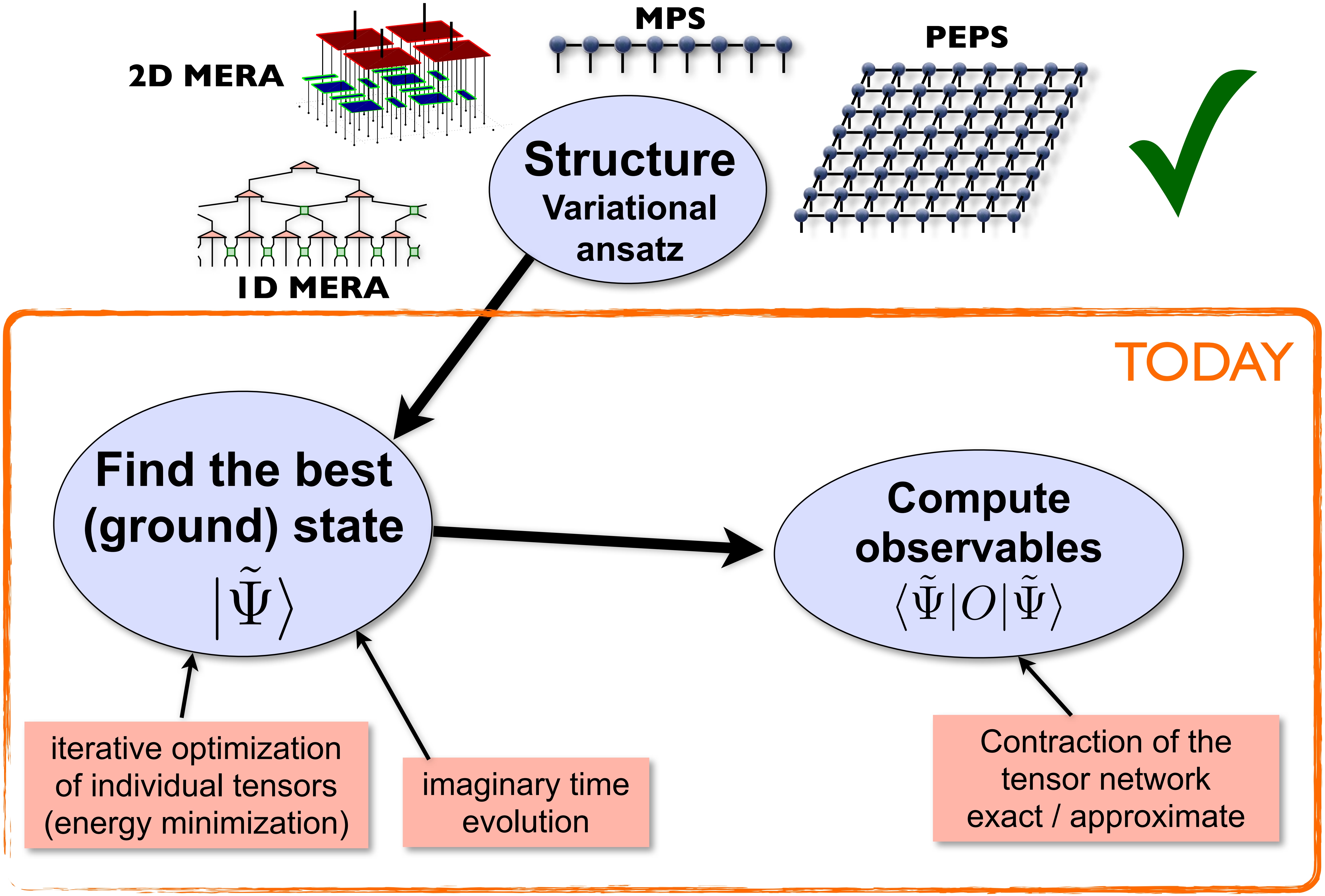
Cavendish Laboratory

Summary: Tensor network algorithms

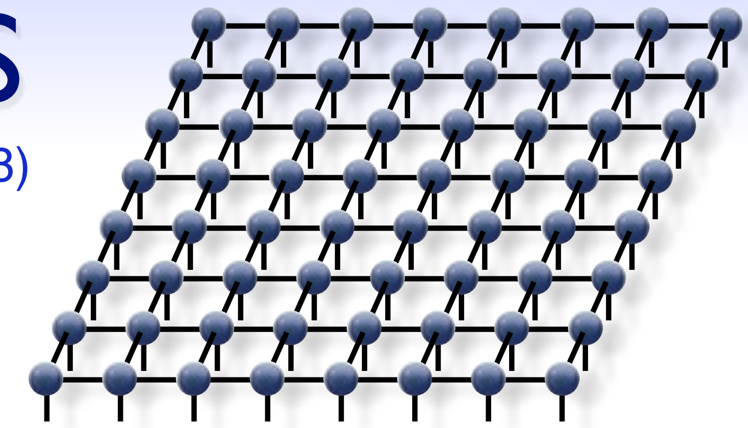


Outline, part II

- Optimization of tensor networks
  - Variational optimization
  - Imaginary-time evolution
- Contraction of tensor networks
  - Basics
  - Approximate contraction of PEPS/iPEPS
- Outlook & Summary

Variational optimization for PEPS

Verstraete, Murg, Cirac, Adv. in Phys. 57, 143 (2008)



1. Select one of the PEPS tensors T

2. Optimize tensor T (leaving all the others fixed) by minimizing the energy:

environment including all Hamiltonian terms

environment from norm term

tensor T reshaped as a vector

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \xrightarrow{\text{minimize}} F\,x = E\,G\,x$$

solve generalized eigenvalue problem

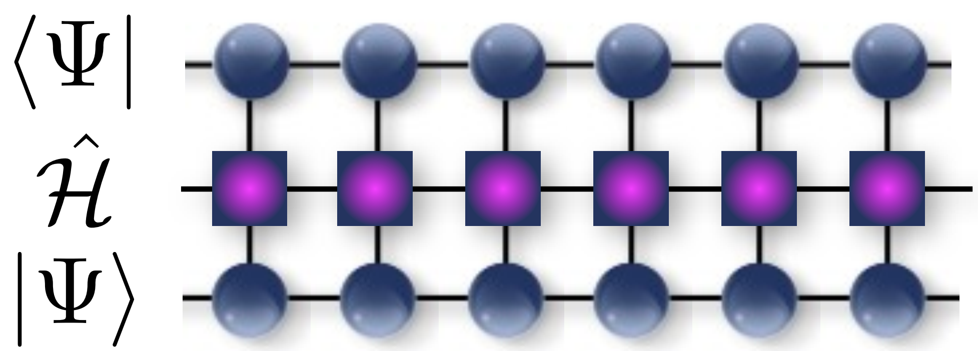
3. Take the next tensor (leave others fixed)

4. Repeat 2-3 iteratively until convergence is reached

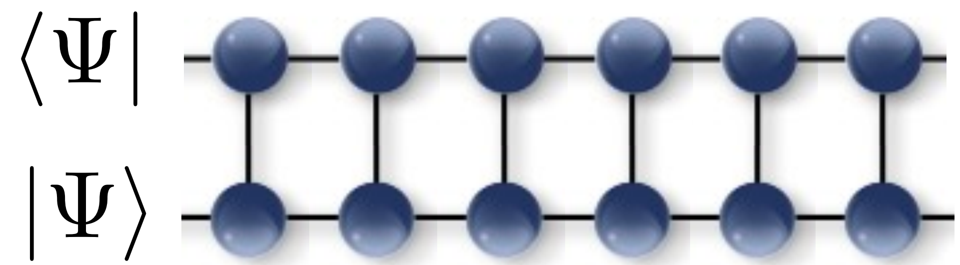
Variational Optimization for MPSs

minimize Energy E, enforcing normalization with a Lagrange multiplier λ

$$\min[\langle\Psi|\hat{\mathcal{H}}|\Psi\rangle - \lambda\langle\Psi|\Psi\rangle]$$



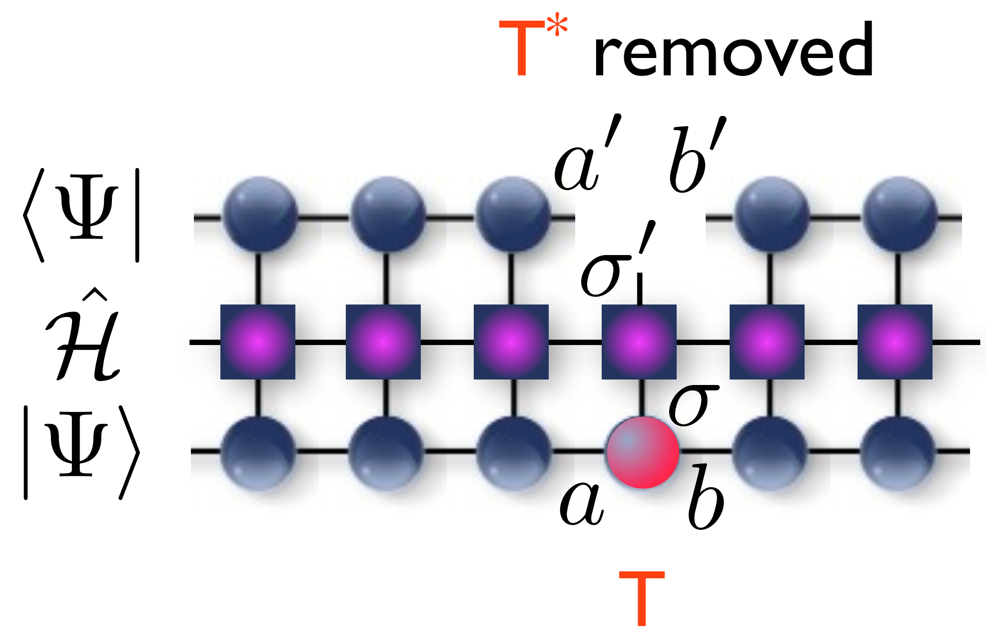
- λ

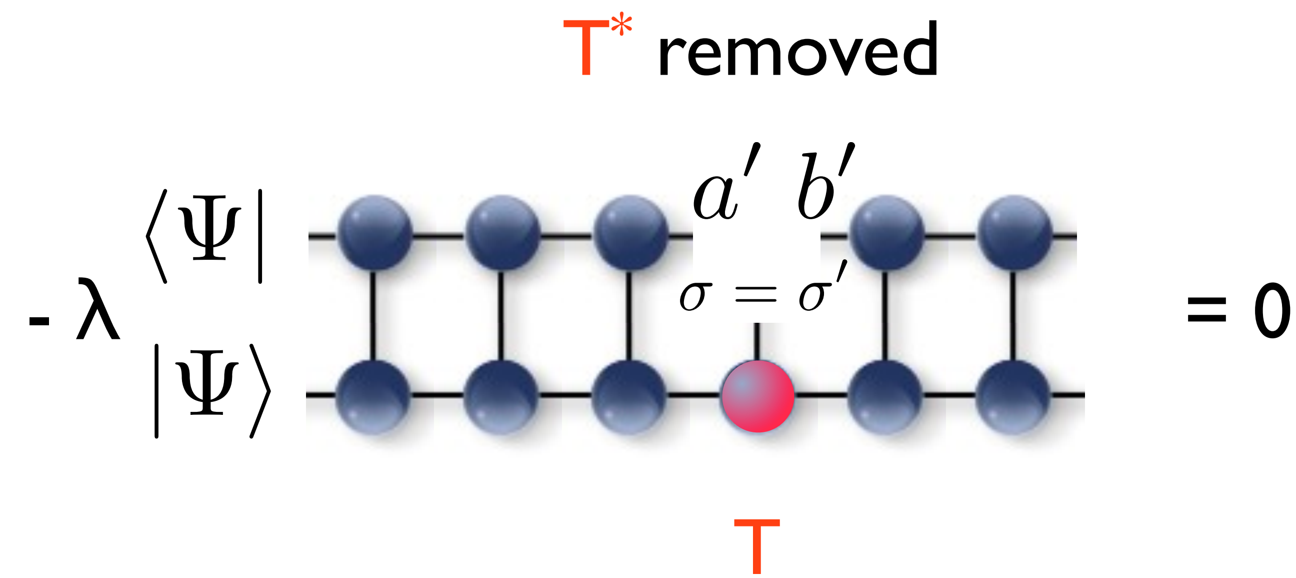


minimize with respect to tensor T: $$\frac{\partial}{\partial T_{\sigma}^{lr\,*}}(\quad \% \quad) = 0$$

Variational Optimization for MPS's

in pictures: $\frac{\partial}{\partial T_{\sigma}^{lr\,*}}(\quad \% \quad) = 0$





read as matrix equation in linearized composite index $\mu = (a\,b\,\sigma)$

$$F_{\mu'\mu} T_{\mu} = \lambda G_{\mu'\mu} T_{\mu} \qquad \text{where} \qquad (G_{\mu'\mu} \propto \delta_{\sigma\sigma'})$$

F, G: remainders of tensor networks with both T and T* cut out

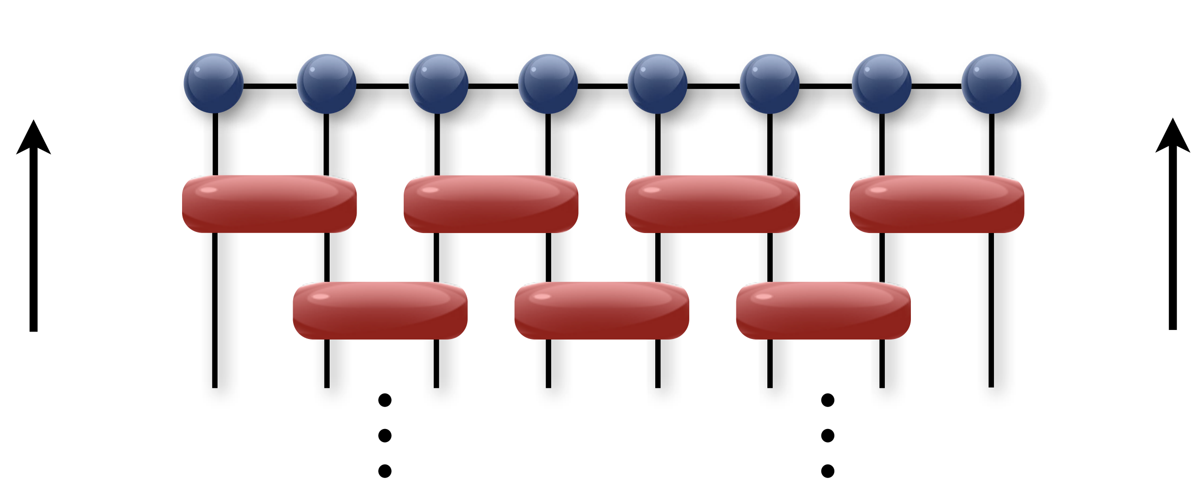
☛ solve for smallest eigenvalue λ_0 and -vector T = new optimized tensor

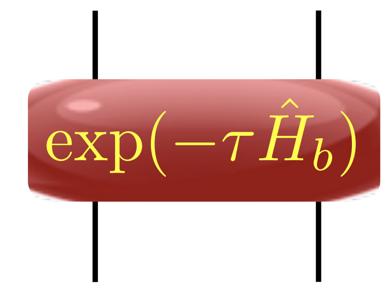
Optimization via imaginary time evolution

- Get the ground state via imaginary time evolution (Trotter-Suzuki)

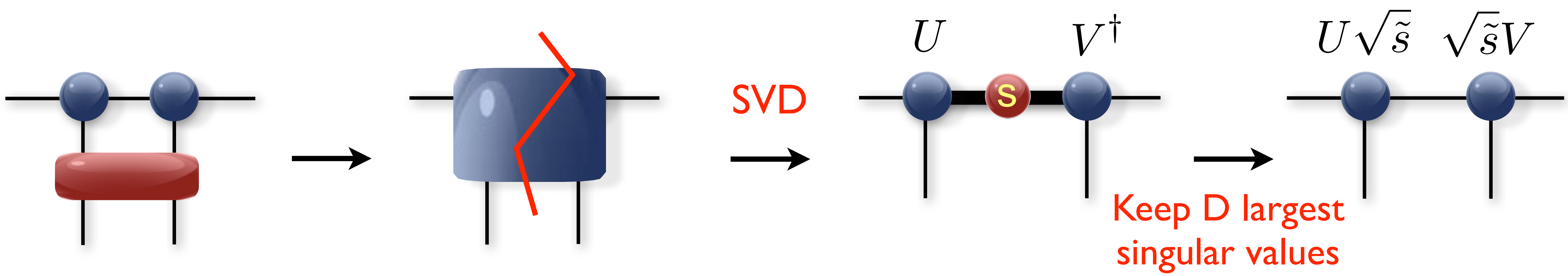
$$\tau = \beta/n$$

$$\exp(-\beta \hat{H}) = \exp(-\beta \sum_b \hat{H}_b) = \left(\exp(-\tau \sum_b \hat{H}_b)\right)^n \approx \left(\prod_b \exp(-\tau \hat{H}_b)\right)^n$$





- At each step: apply a two-site operator to a bond and truncate bond back to *D*



Time **E**volving **B**lock **D**ecimation (TEBD) algorithm

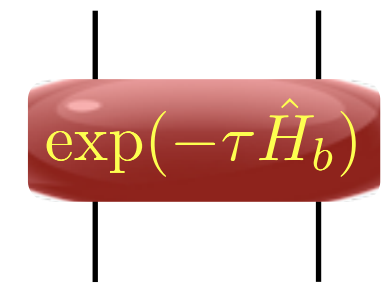
Note: Here I simplified. MPS needs to be in canonical form

Optimization via imaginary time evolution

- Get the ground state via imaginary time evolution (Trotter-Suzuki)

$$\exp(-\beta \hat{H}) = \exp(-\beta \sum_b \hat{H}_b) = \left(\exp(-\tau \sum_b \hat{H}_b) \right)^n \approx \left(\prod_b \exp(-\tau \hat{H}_b) \right)^n \qquad \tau = \beta / n$$

- **2D: same idea:** apply a two-site operator to a bond and truncate bond back to *D* at each step



- **However**, SVD update is not optimal (because of loops in PEPS)!

simple update (SVD)

★ "local" update like in TEBD

★ Cheap, but not optimal (e.g. overestimates magnetization in S=1/2 Heisenberg model)

full update

★ Take the full wave function into account for truncation

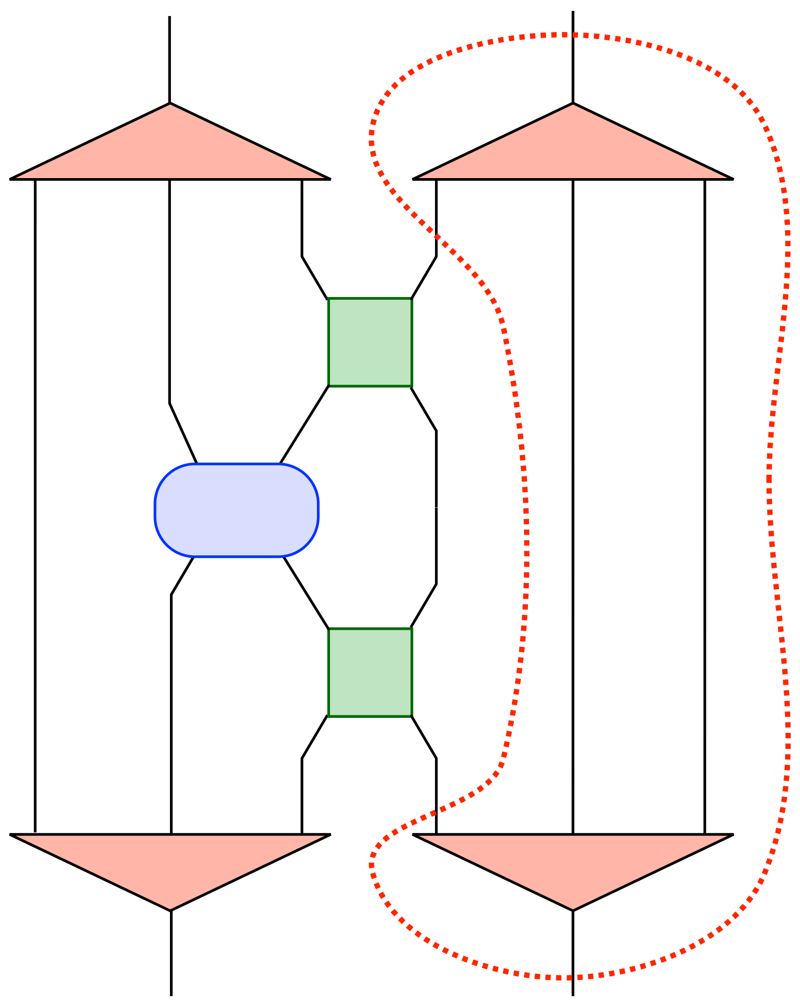
★ optimal, but computationally more expensive

Cluster update Wang, Verstraete, arXiv:1110.4362 (2011)

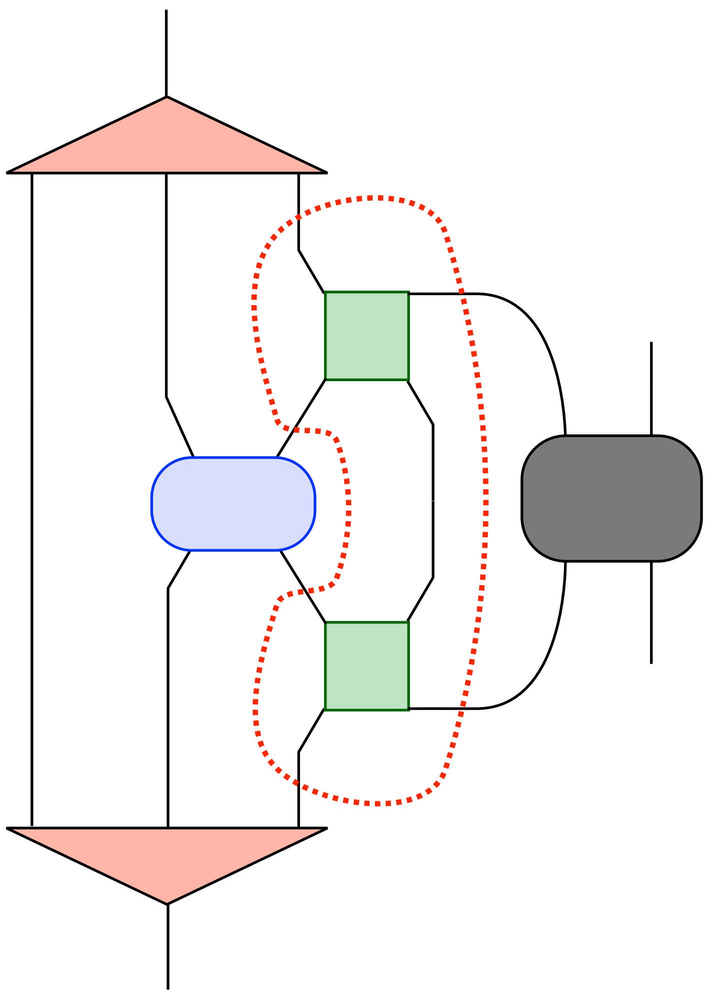
Contracting tensor networks

Contracting a tensor network

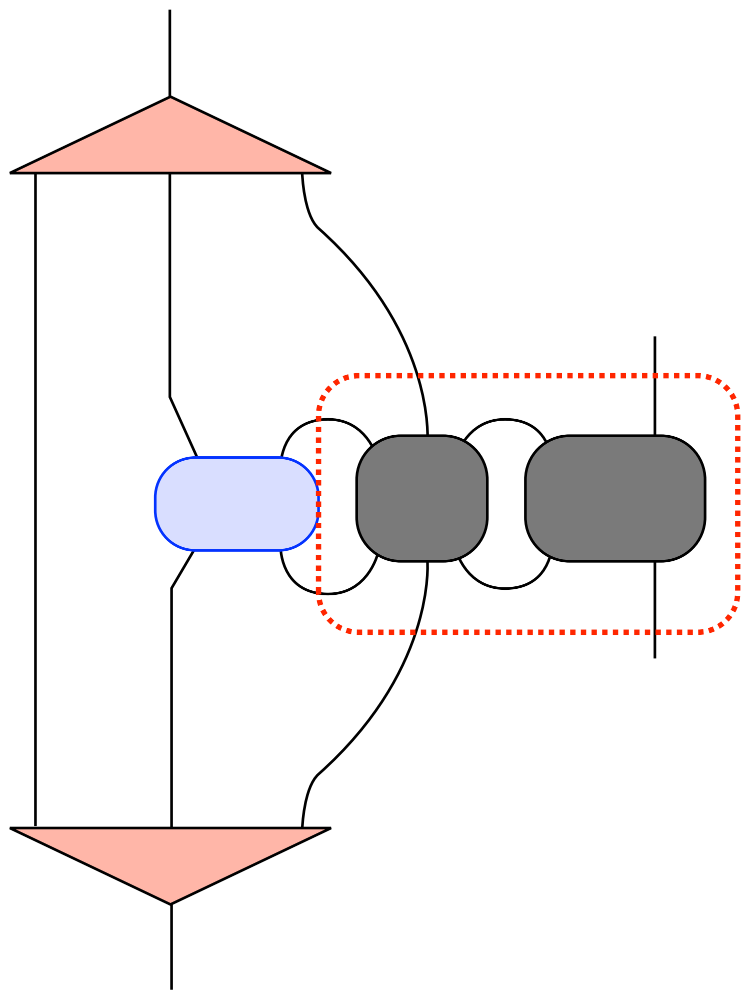
contract tensors pairwise



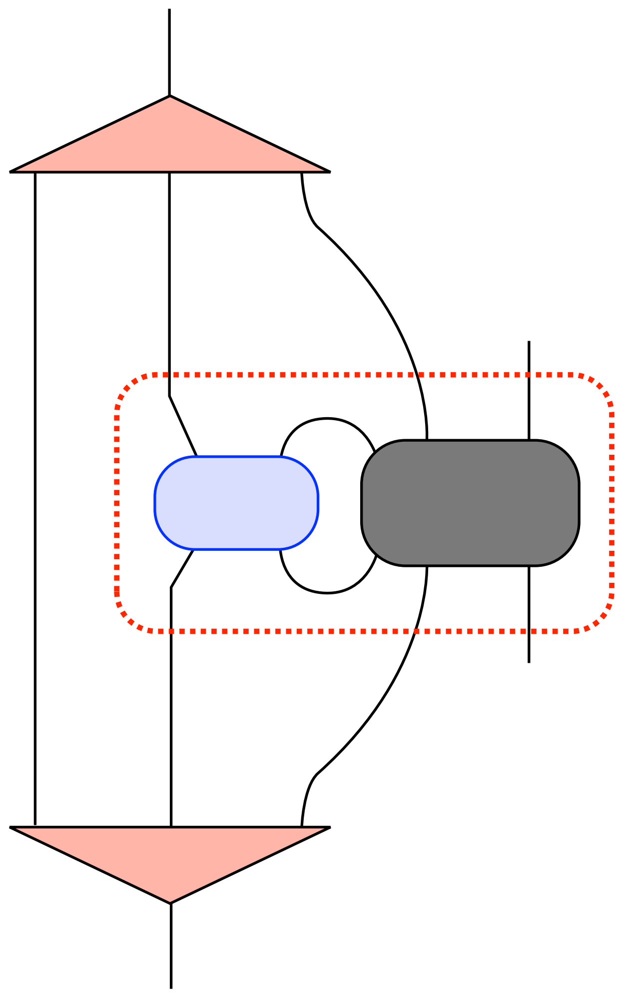
Pairwise contractions...



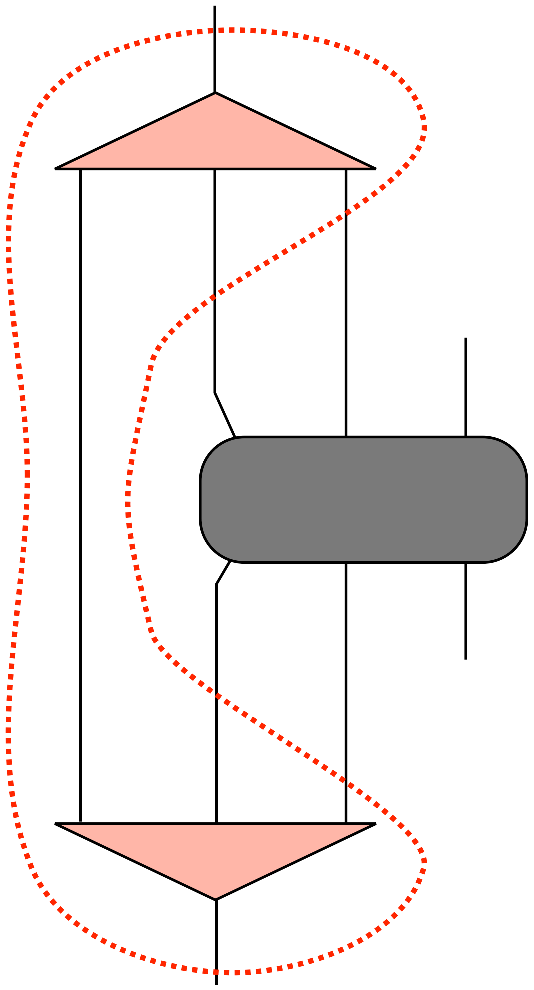
Pairwise contractions...



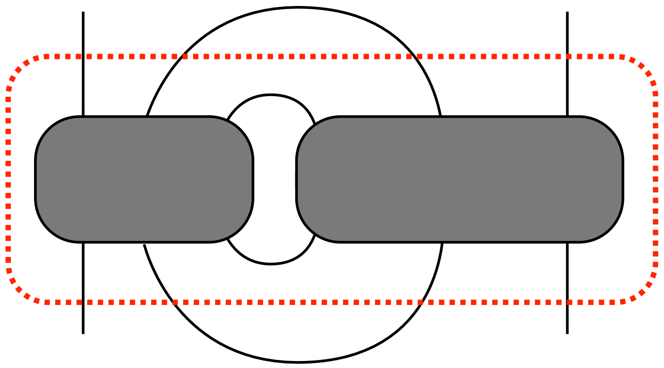
Pairwise contractions...



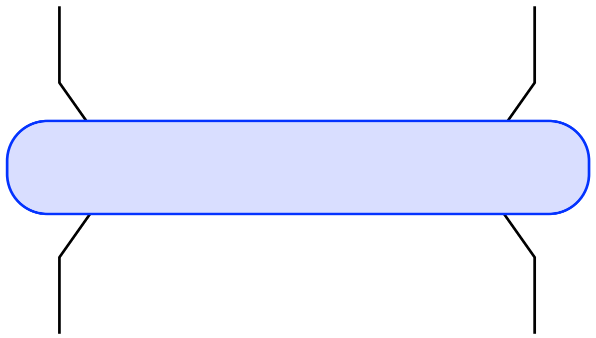
Pairwise contractions...



Pairwise contractions...



Pairwise contractions...

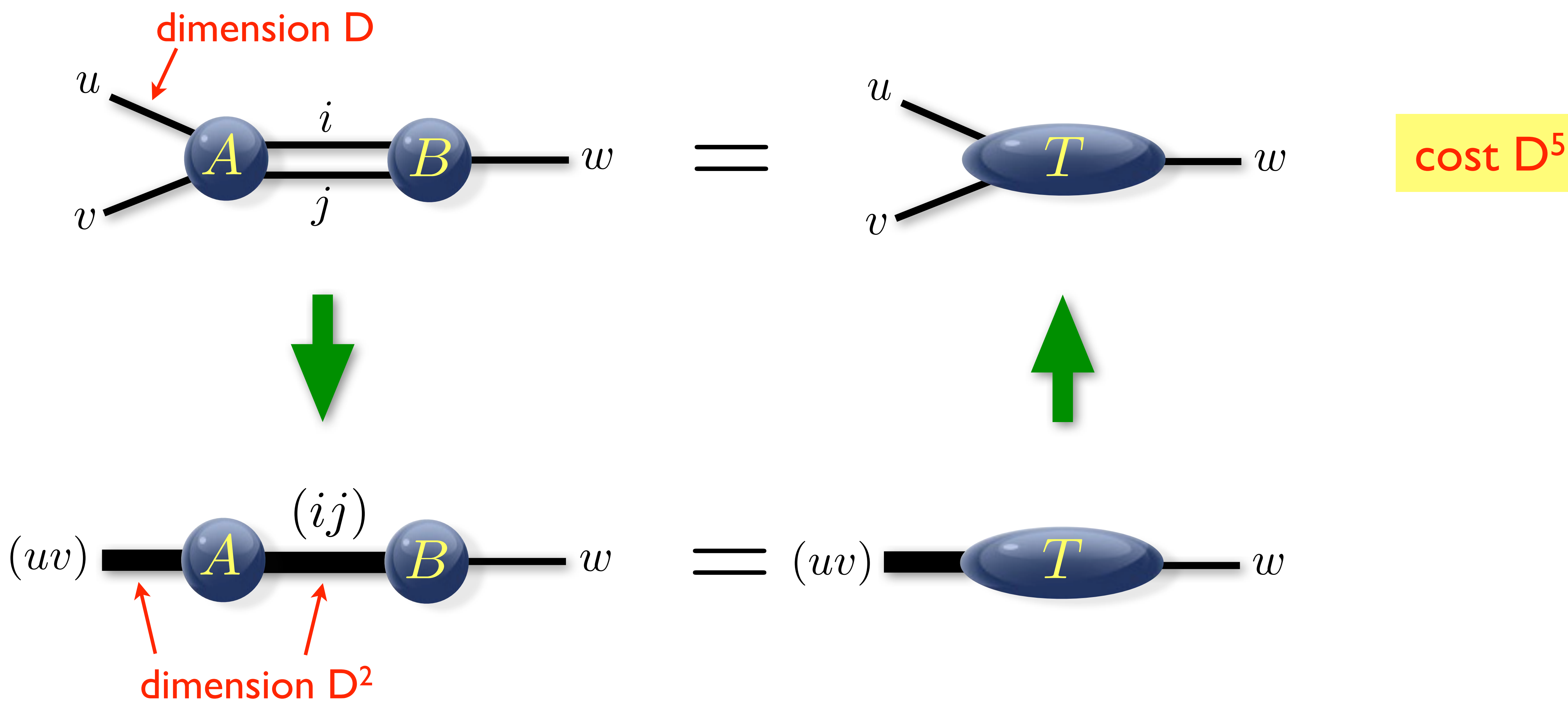


done!

the order of contraction matters for the computational cost!!!

Contracting a tensor network

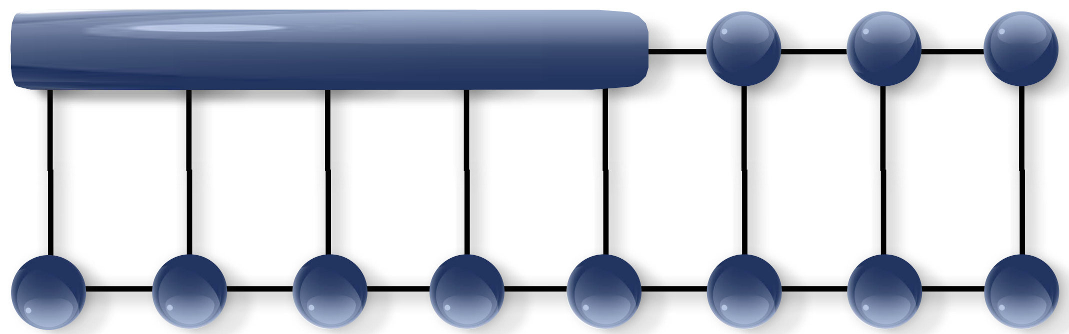
★ Reshape tensors into matrices and multiply them with optimized routines (BLAS)



★ Computational cost: multiply the dimensions of all legs (connected legs only once)

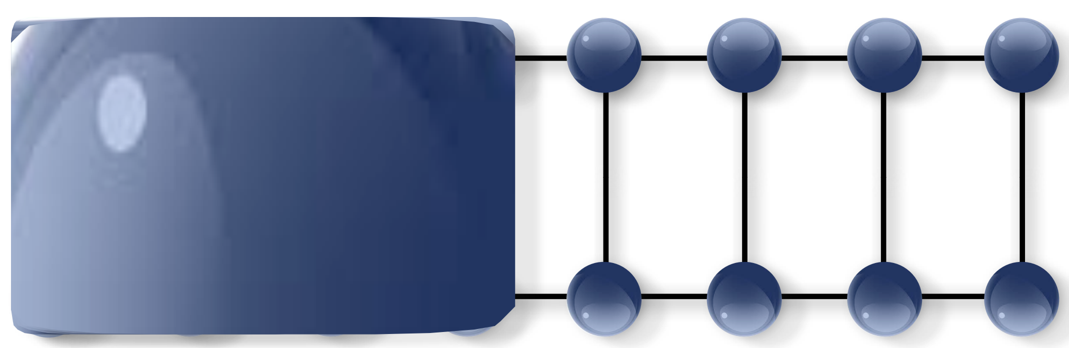
Contracting an MPS

$\langle \Psi | \Psi \rangle =$



BAD!

$\langle \Psi | \Psi \rangle =$

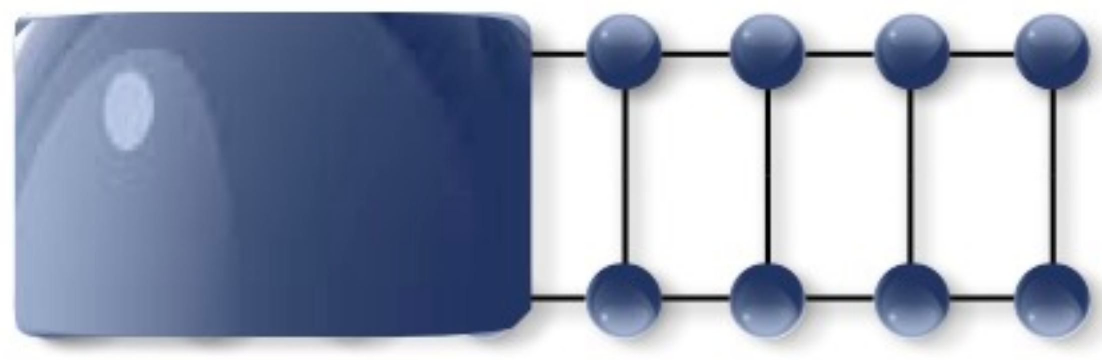


Good!

Relation to Transfer Matrix

Norm

$\langle \Psi | \Psi \rangle$ =

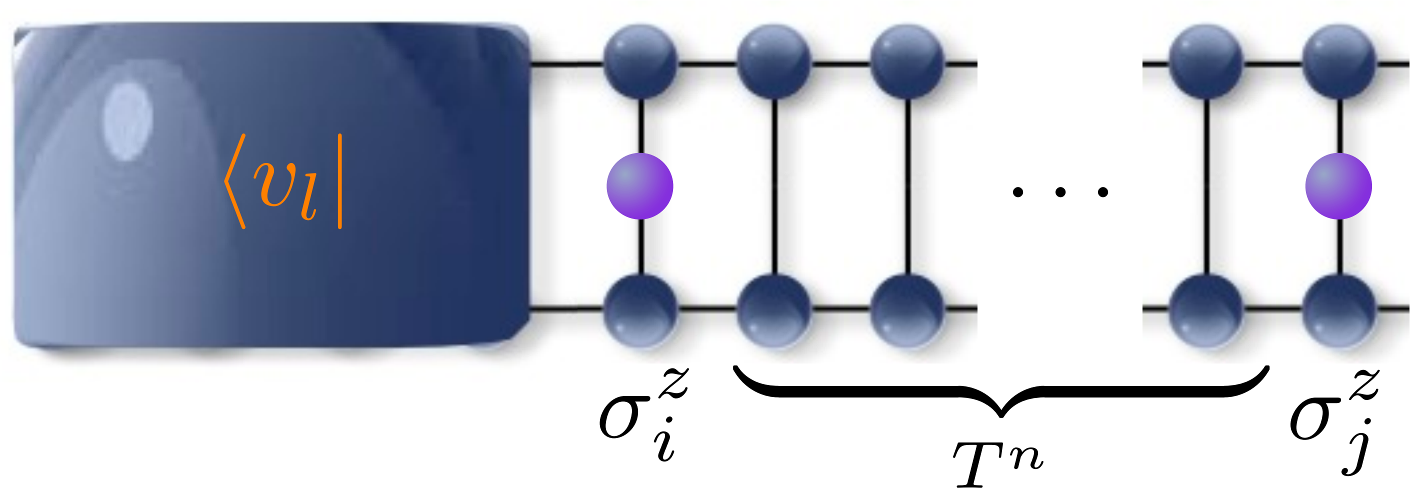


d=D^2 vector D^2 x D^2 matrix

$\langle v_l' |$ =

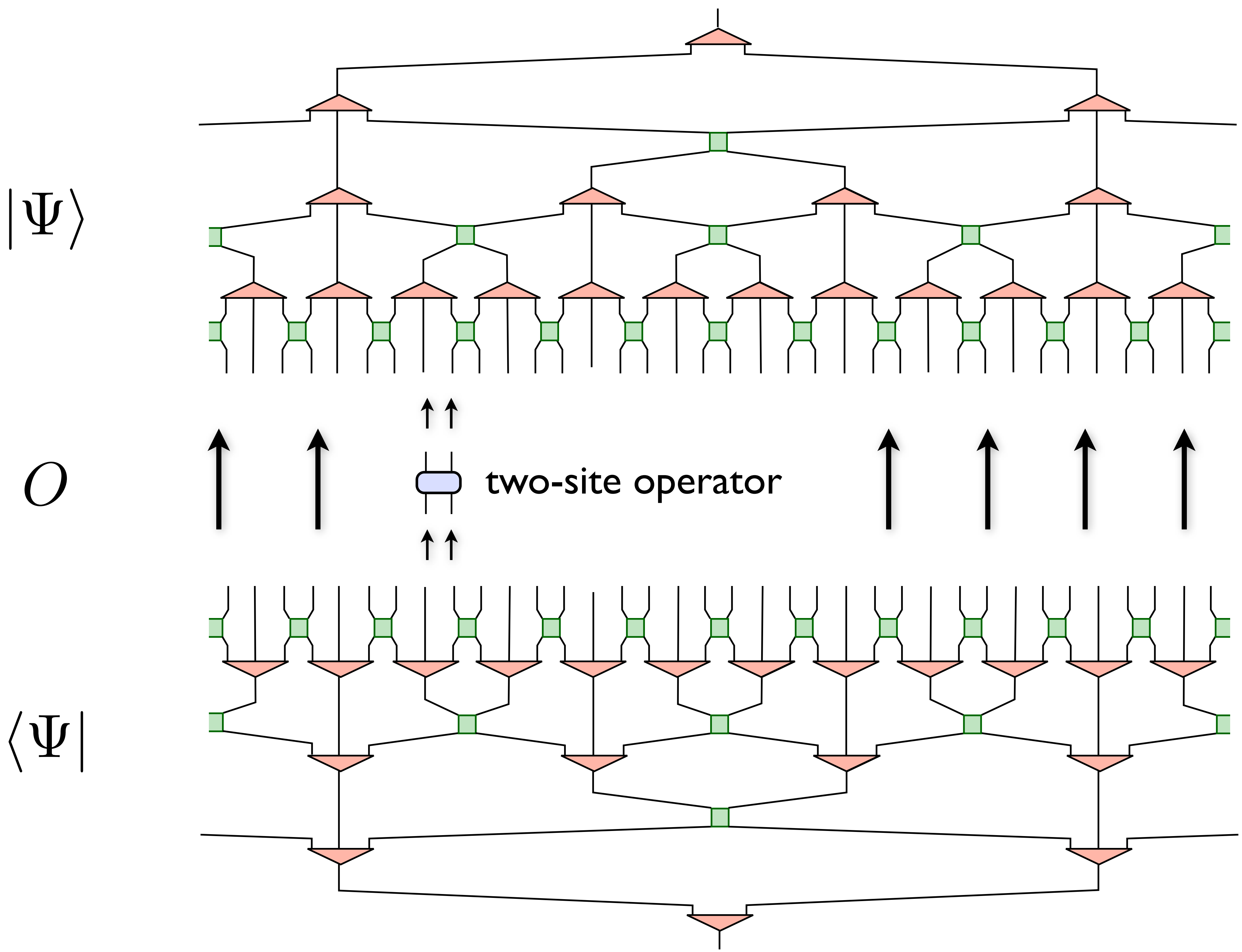
each rung acts as a transfer matrix T !

Correlation functions for two sites

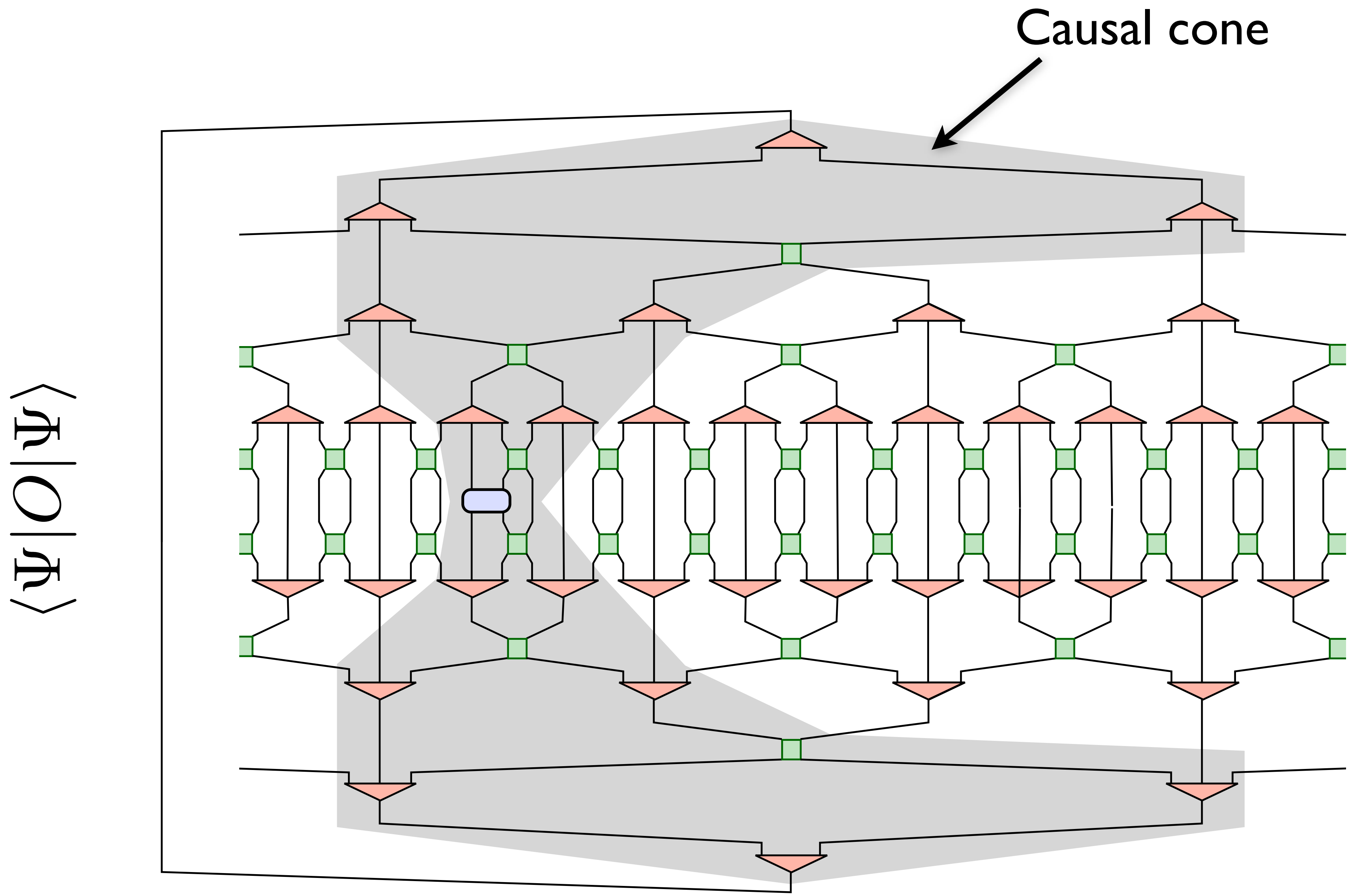


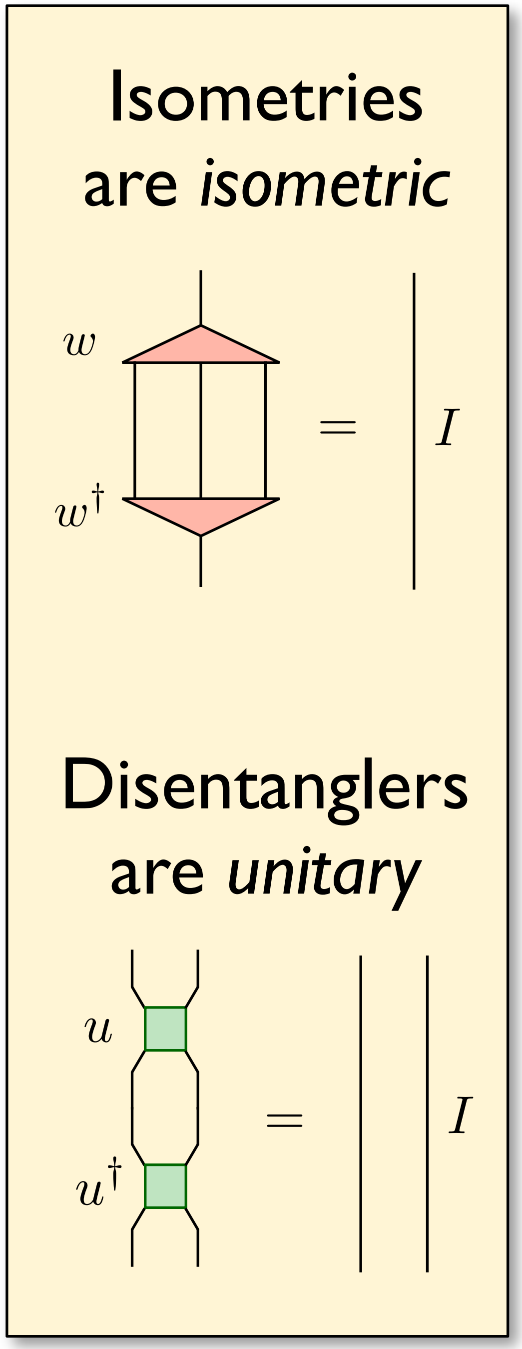
MERA: Properties

Let's compute $\langle \Psi | O | \Psi \rangle$ $\qquad O$: two-site operator

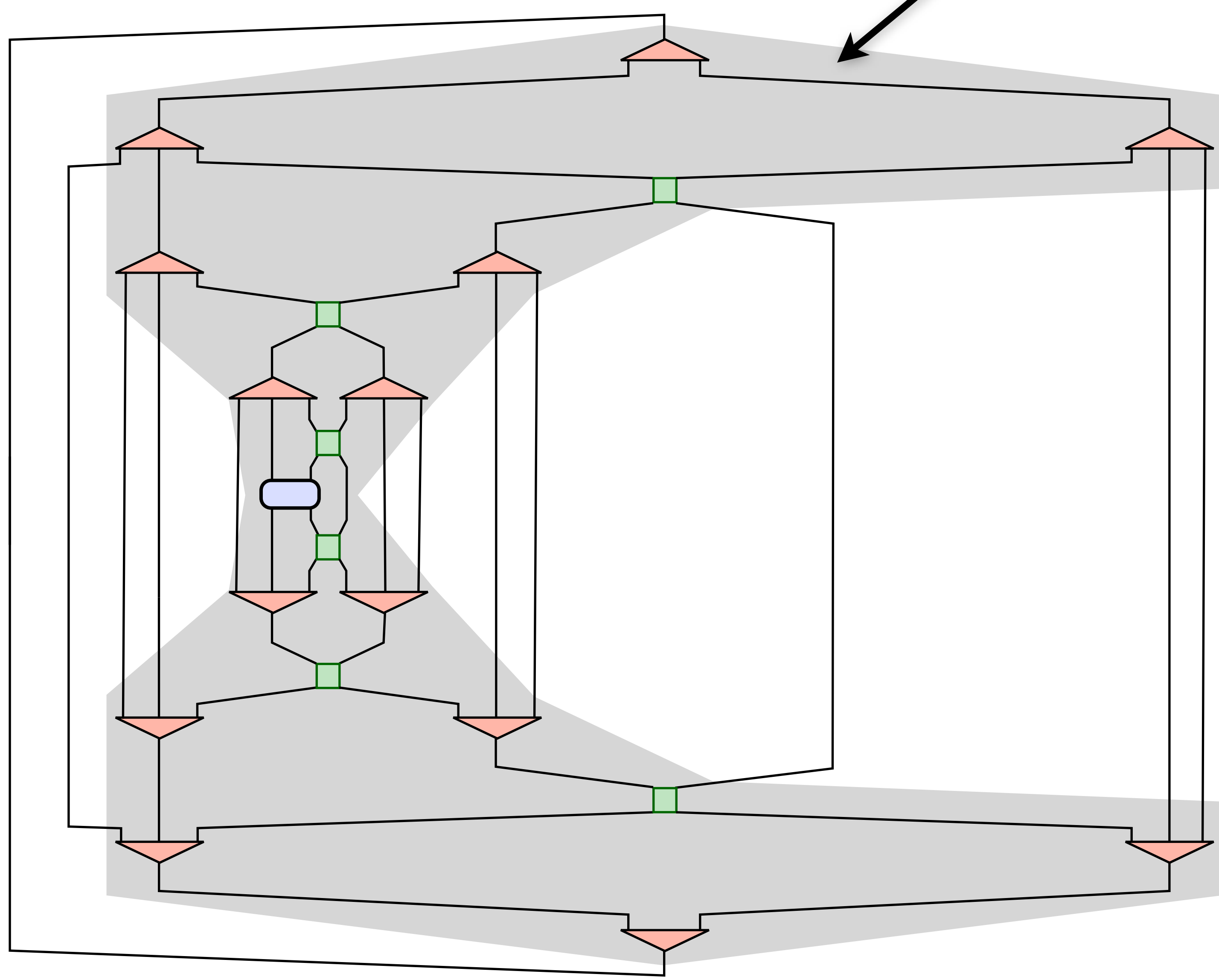


MERA: Contraction



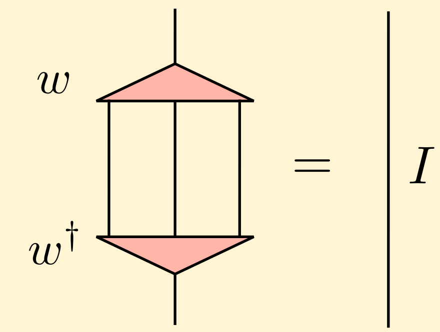


MERA: Contraction

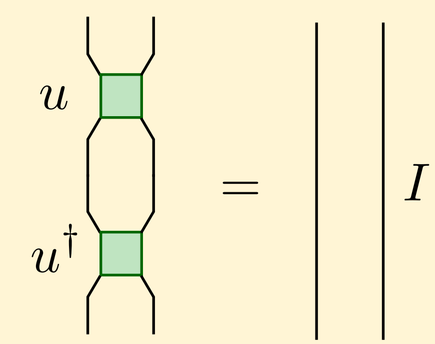


$\langle \Psi | O | \Psi \rangle$

Isometries are *isometric*

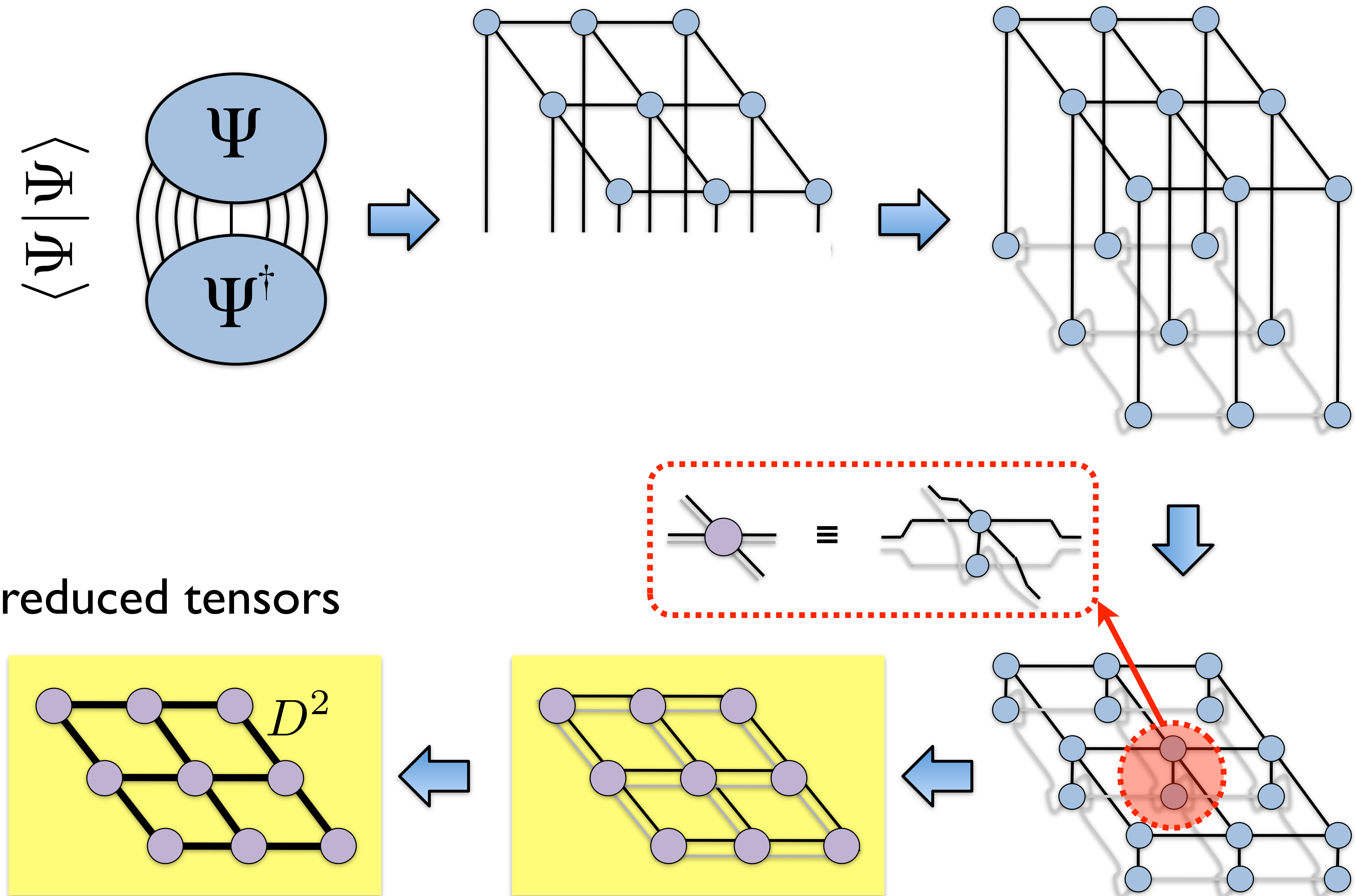


Disentanglers are *unitary*

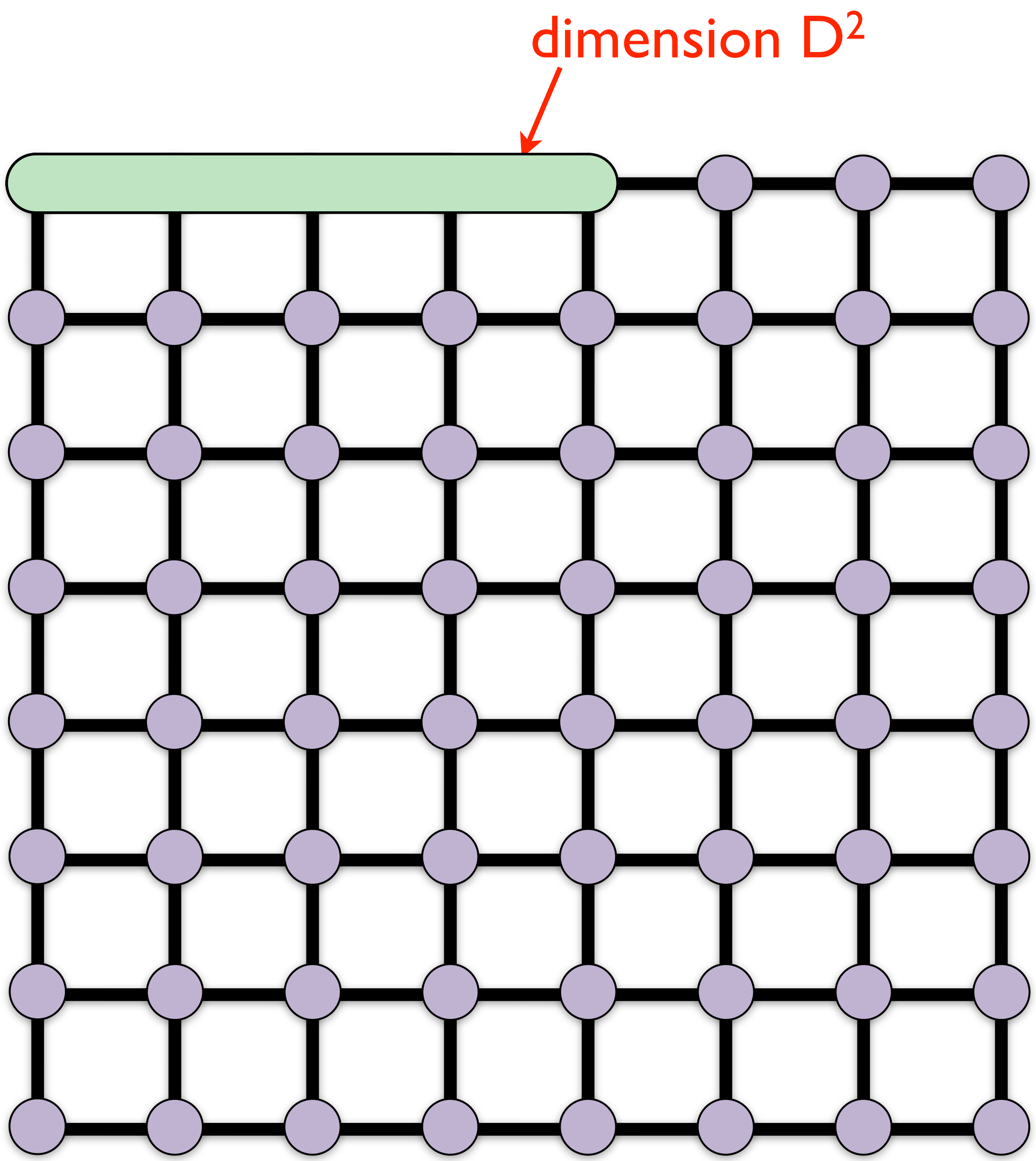


Efficient computation of expectation values of observables!

Contracting the PEPS



Contracting the PEPS



Problem: how do we contract this??

no matter how we contract, we will get intermediate tensors with O(L) legs

number of coefficients D^L

Exponentially increasing with L!

NOT EFFICIENT

Contracting the PEPS

★ Exact contraction of an PEPS is exponentially hard!

→ *need approximate contraction scheme*

MPS-based approach

Murg,Verstraete,Cirac, PRA75 '07
Jordan,et al. PRL79 (2008)

Corner transfer matrix method

Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)

TRG

Tensor Renormalization Group

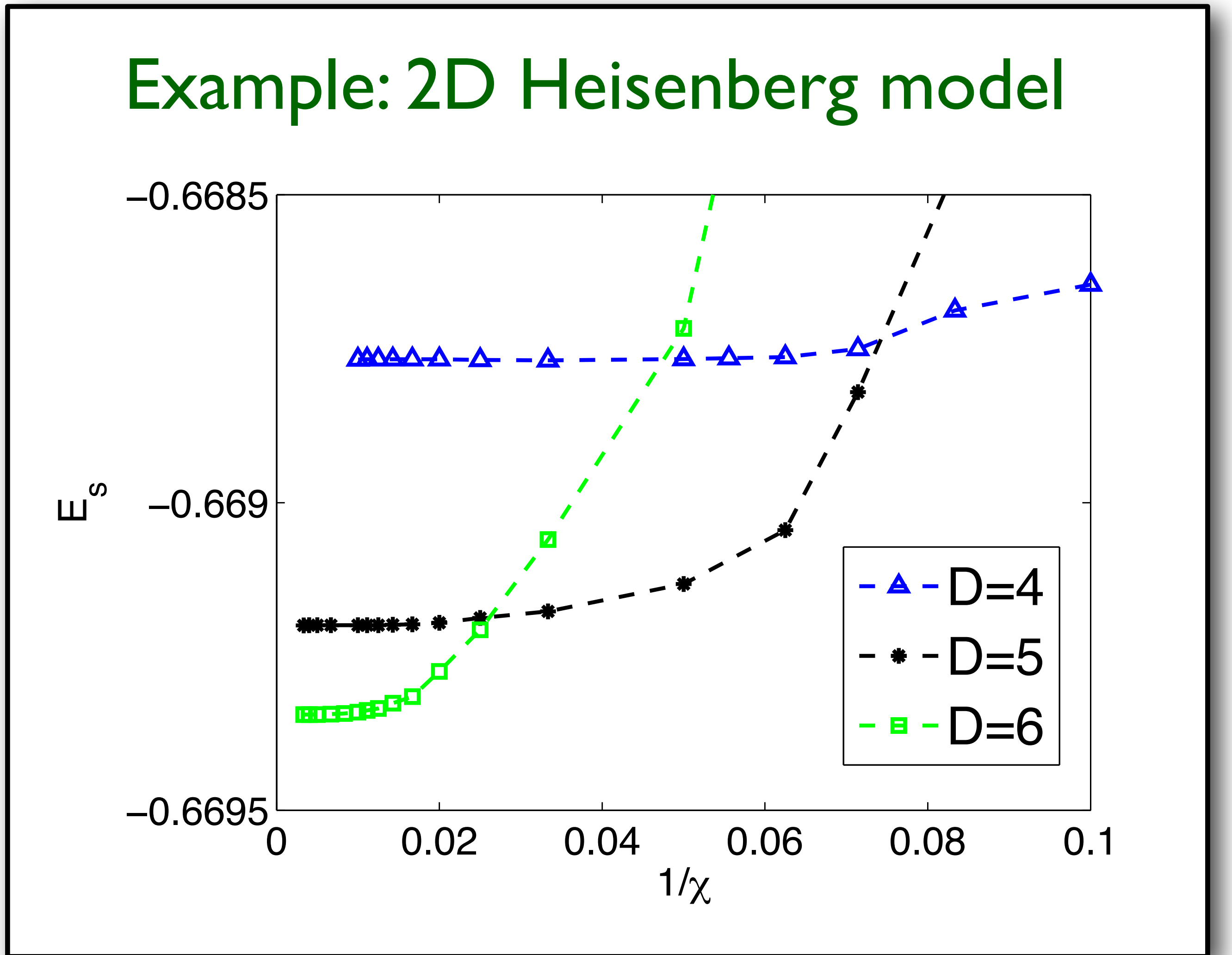
Gu, Levin, Wen, B78, (2008)
Levin, Nave, PRL99 (2007)
Xie et al. PRL 103, (2009)

★ Accuracy of the approximate contraction is controlled by "boundary dimension" χ

★ Convergence in χ needs to be carefully checked

★ Overall cost: $\mathcal{O}(D^{10\ldots12})$ with $\chi \sim D^2$

Contracting the PEPS



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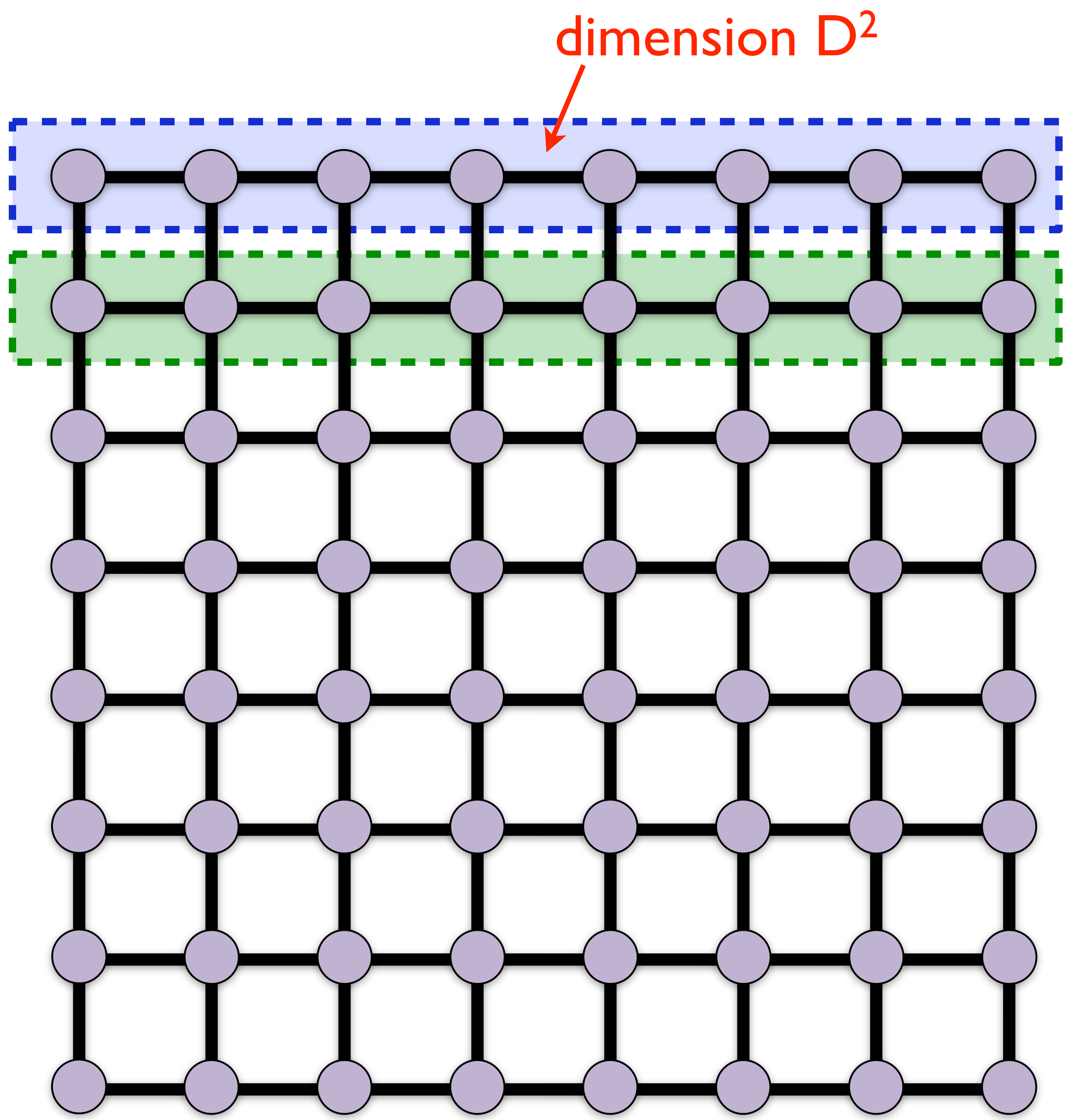
Contracting the PEPS using an MPS

Verstraete, Murg, Cirac, Adv. in Phys. 57, 143 (2008)

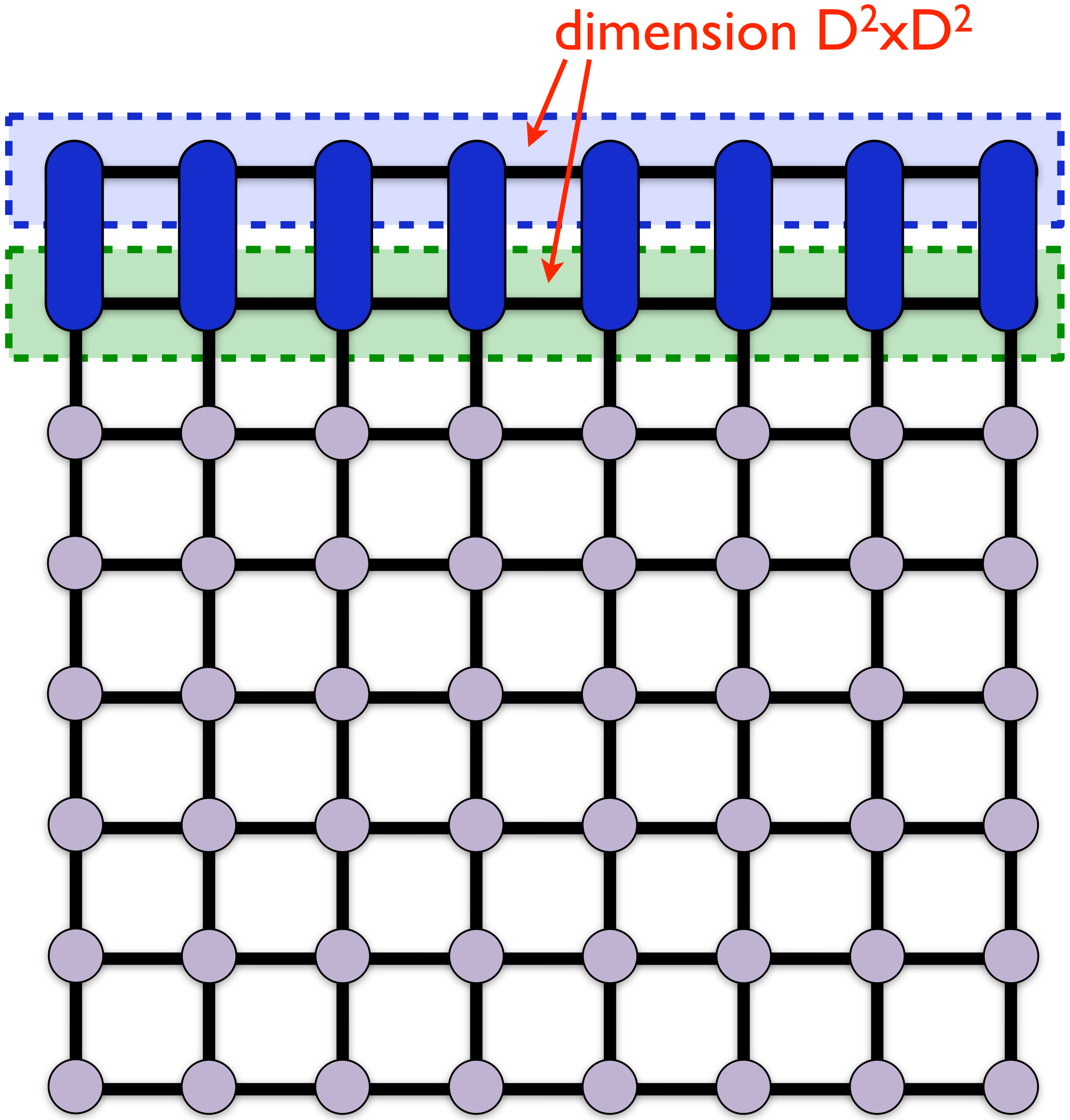


this is an MPS

this is an MPO (matrix product operator)

Contracting the PEPS using an MPS

Verstraete, Murg, Cirac, Adv. in Phys. 57, 143 (2008)



this is an MPS with bond dimension $D^2 xD^2$

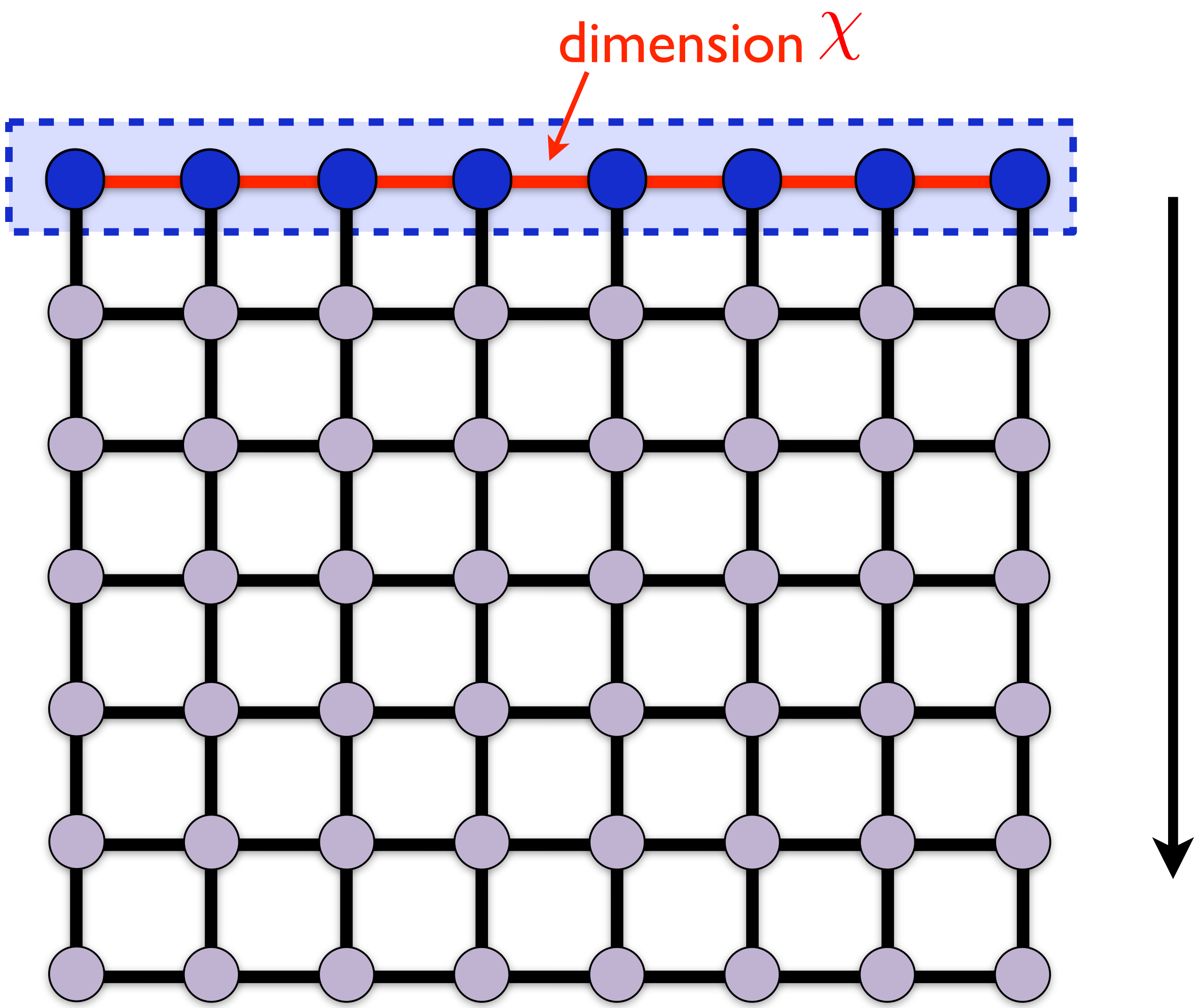
truncate the bonds to χ

there are different techniques for the efficient MPO-MPS multiplication (SVD, variational optimization, zip-up algorithm...)

Schollwöck, Annals of Physics 326, 96 (2011)
Stoudenmire, White, New J. of Phys. 12, 055026 (2010).

Contracting the PEPS using an MPS

Verstraete, Murg, Cirac, Adv. in Phys. 57, 143 (2008)

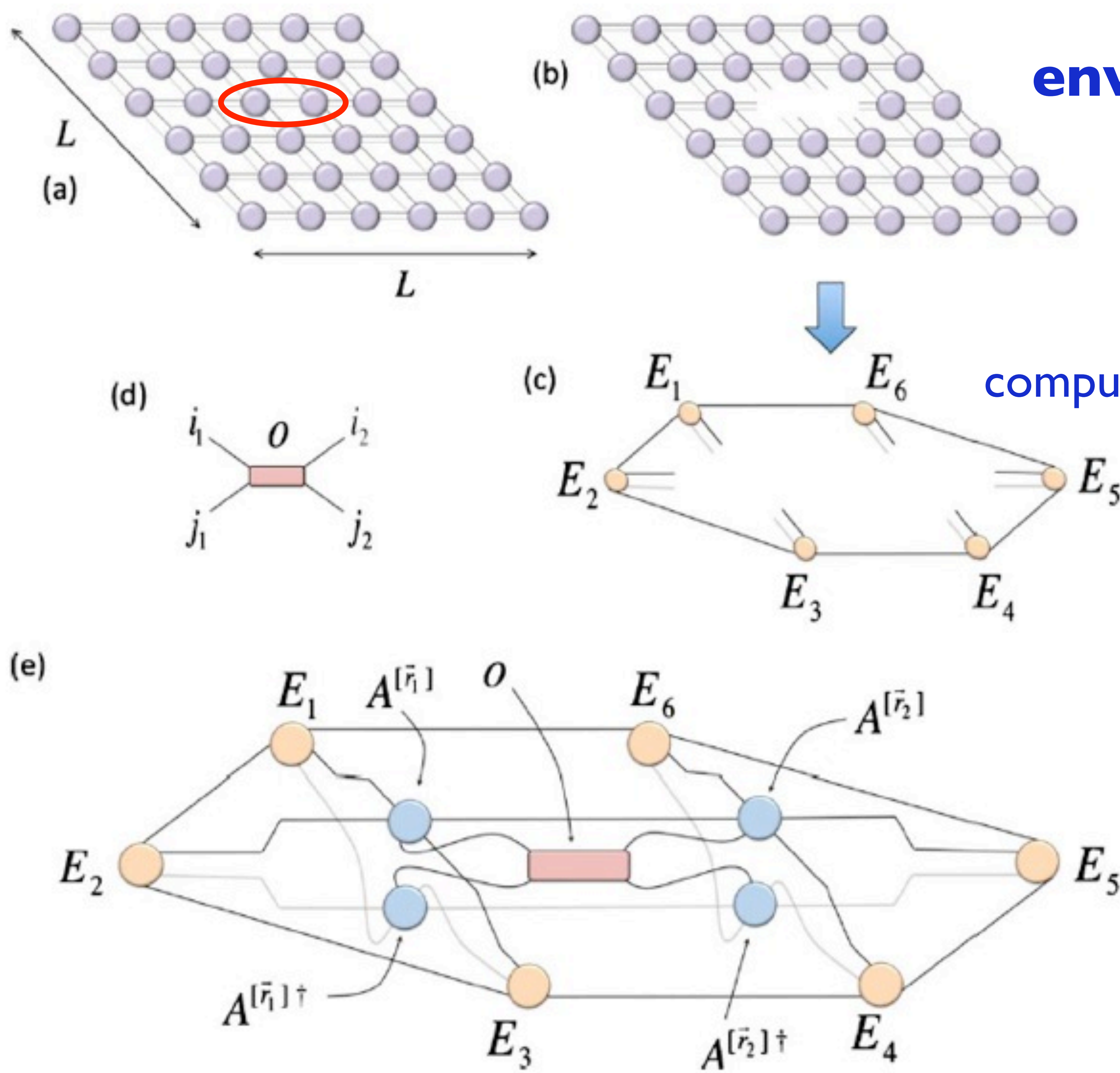


proceed...

★ We can do this from several directions

★ Similar procedure when computing an expectation value

Compute expectation values



environment

compute environment approximately

Connect two-body operator

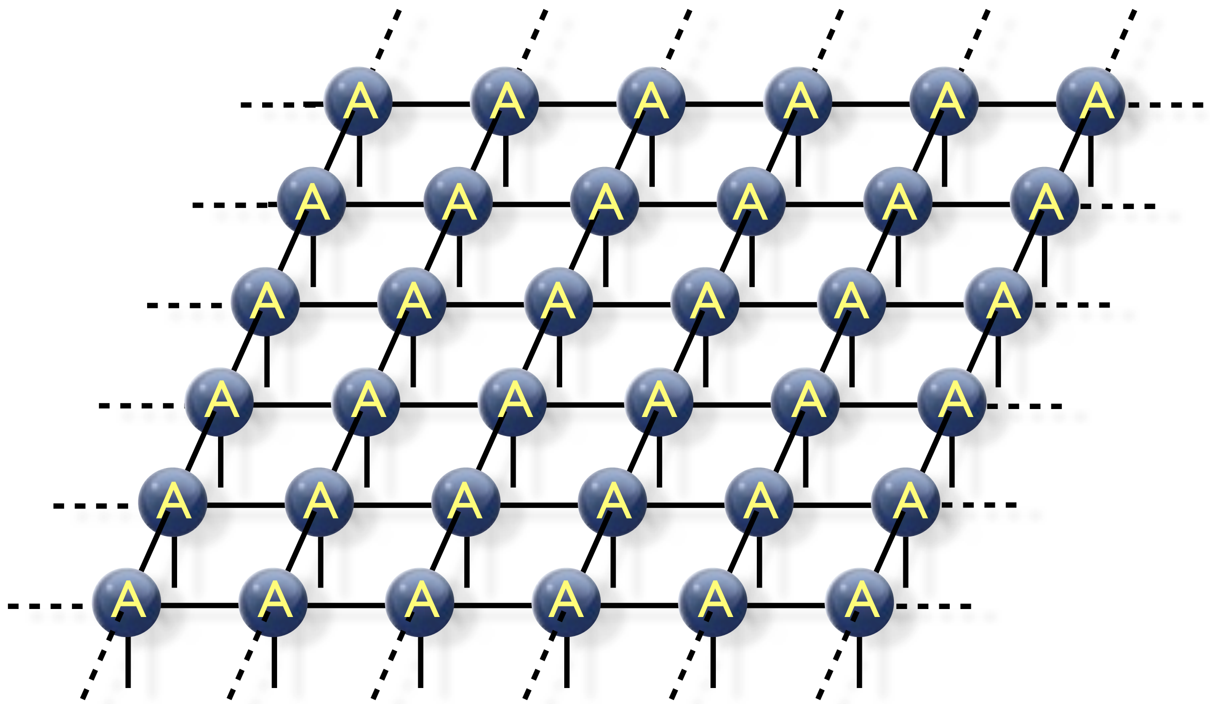
Contract this network!

Figure taken from Corboz, Orús, Bauer, Vidal, PRB 81, 165104 (2010)

Contracting the iPEPS using the corner transfer matrix

iPEPS

infinite projected entangled-pair state



open boundaries, but "infinitely" far away

Contracting the iPEPS using the corner transfer matrix

Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)

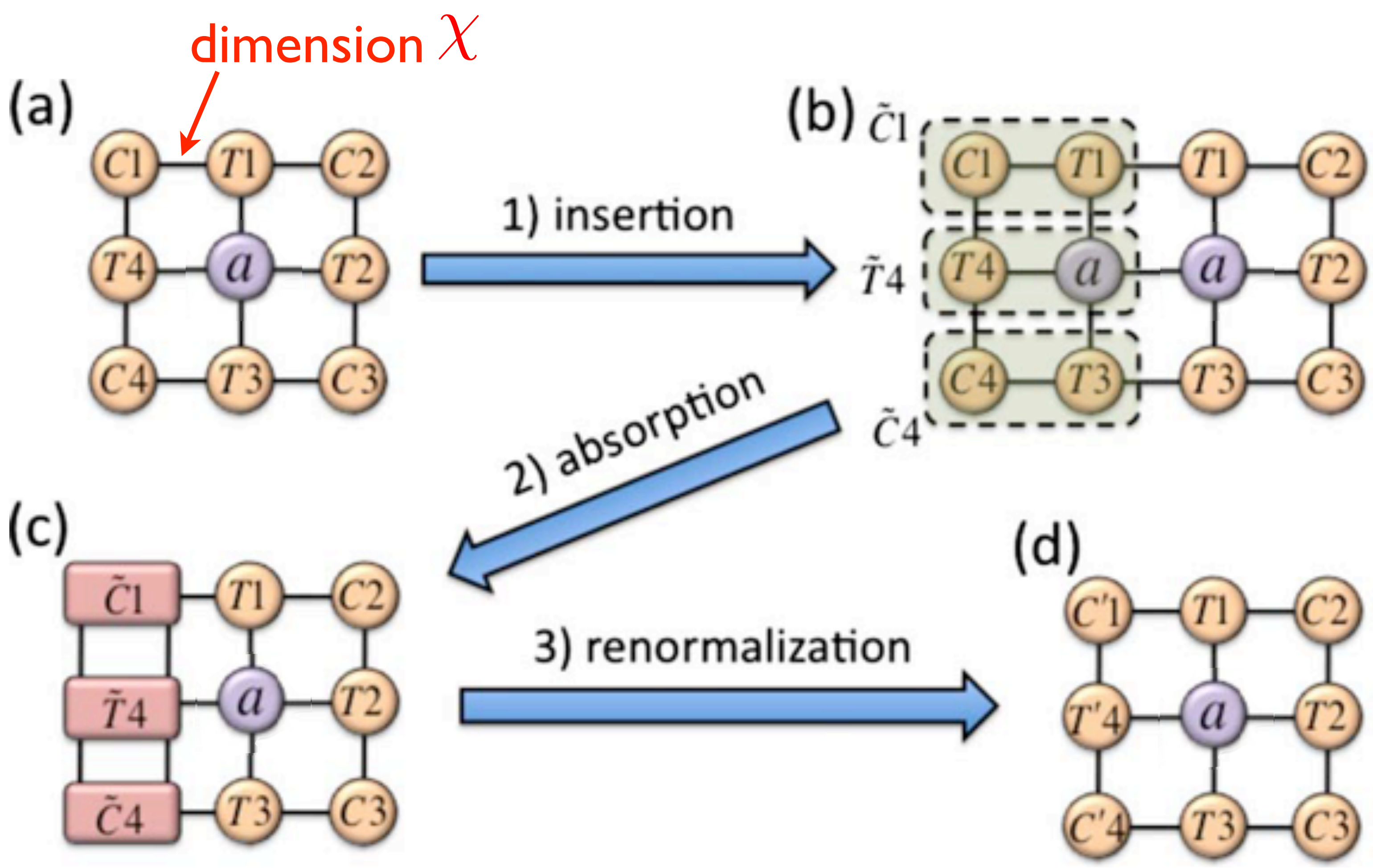


figure taken from Orus, Vidal, PRB 80 (2009)

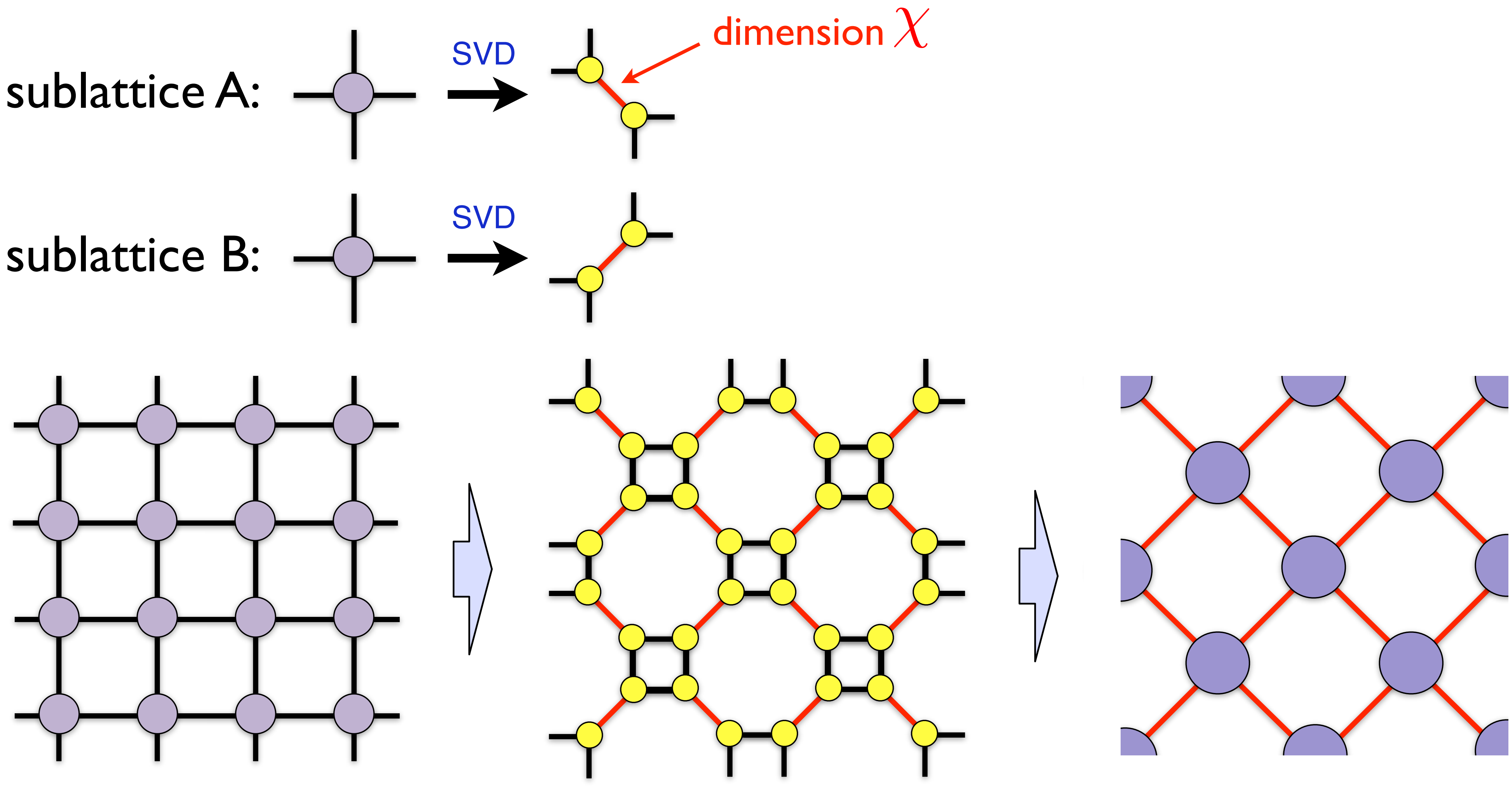
- ★ Let the system grow in all directions.
- ★ Repeat until convergence is reached
- ★ The boundary tensors form the **environment**
- ★ Can be generalized to arbitrary unit cell sizes

Corboz, et al., PRB 84 (2011)

Contracting the PEPS/iPEPS using TRG

Tensor **R**enormalization **G**roup

Gu, Levin, Wen, B78, (2008)
Levin, Nave, PRL99 (2007)
Xie et al. PRL 103, (2009)



- ★ Contract PEPS with periodic boundary conditions
- ★ Finite or infinite systems
- ★ Related schemes: SRG, HOTRG, HOSRG, ...

Contracting the PEPS

★ Exact contraction of an PEPS is exponentially hard!

→ *need approximate contraction scheme*

MPS-based approach

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★ Accuracy of the approximate contraction is controlled by "boundary dimension" χ

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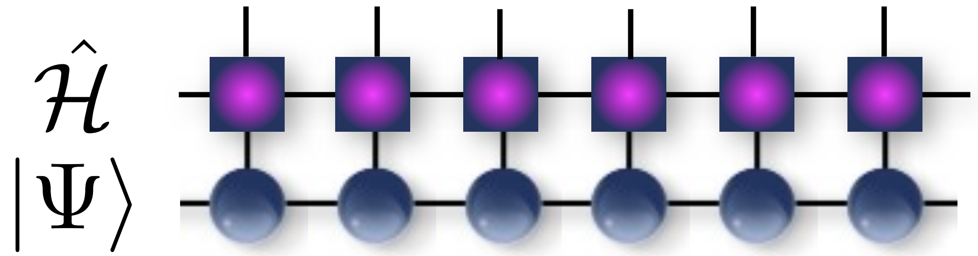
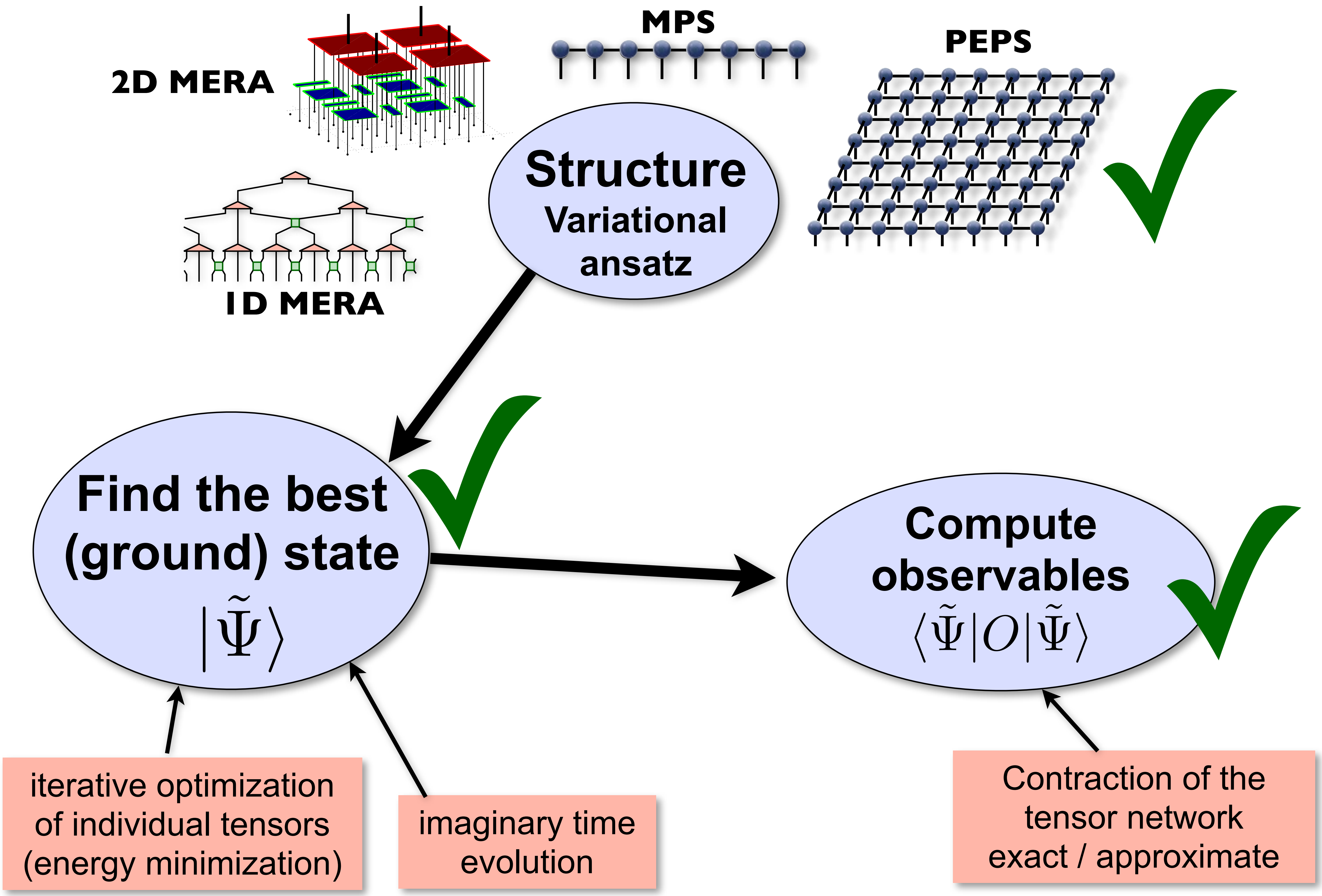
★ Overall cost: $\mathcal{O}(D^{10\ldots12})$ with $\chi \sim D^2$

Expressing the Hamiltonian as a MPO



- on the blackboard...

Summary: Tensor network algorithms

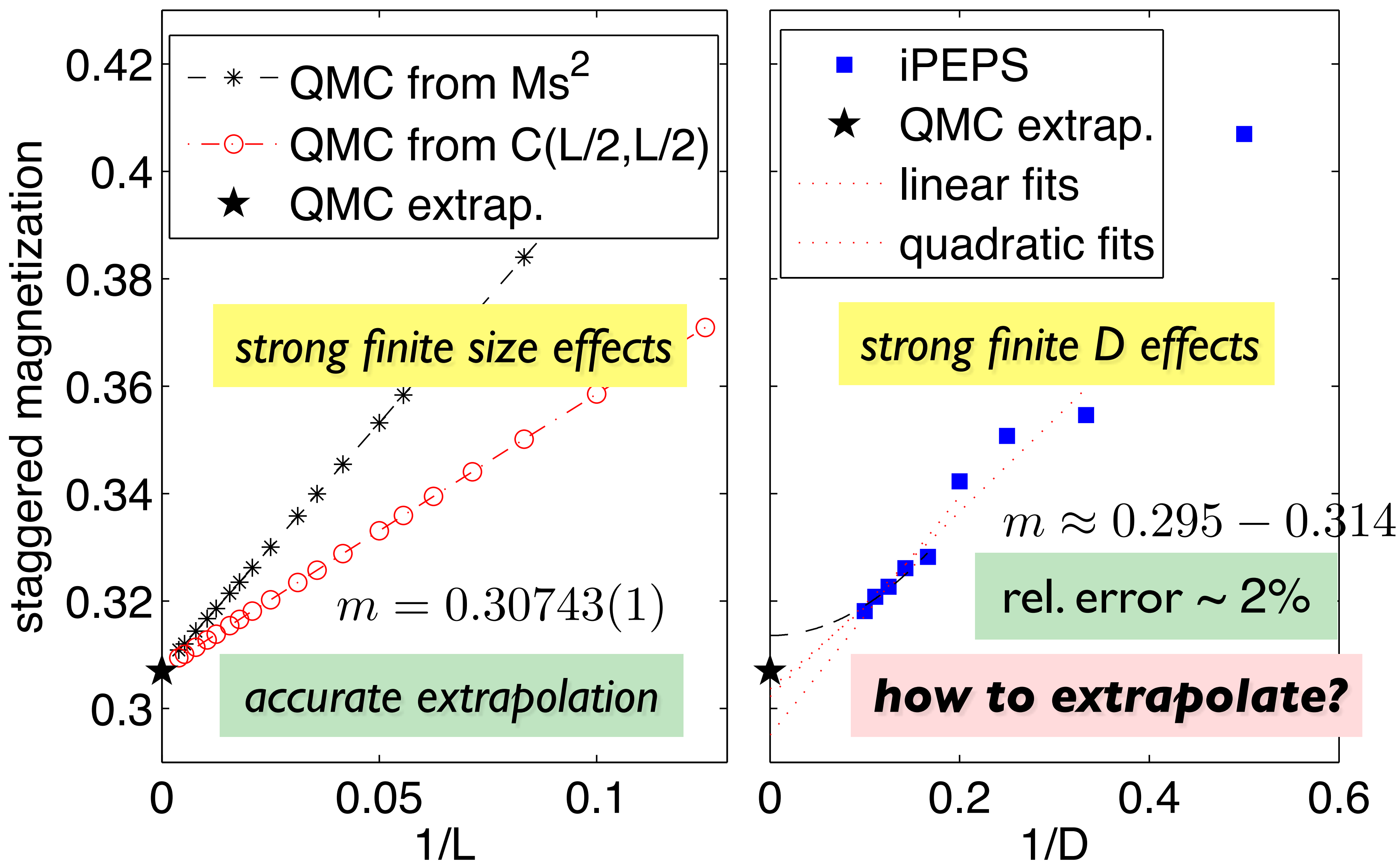


A Benchmark: Heisenberg model

Energy: QMC (extrap.): -0.669437(5)J A. Sandvik, PRB56, 11678 (1997)

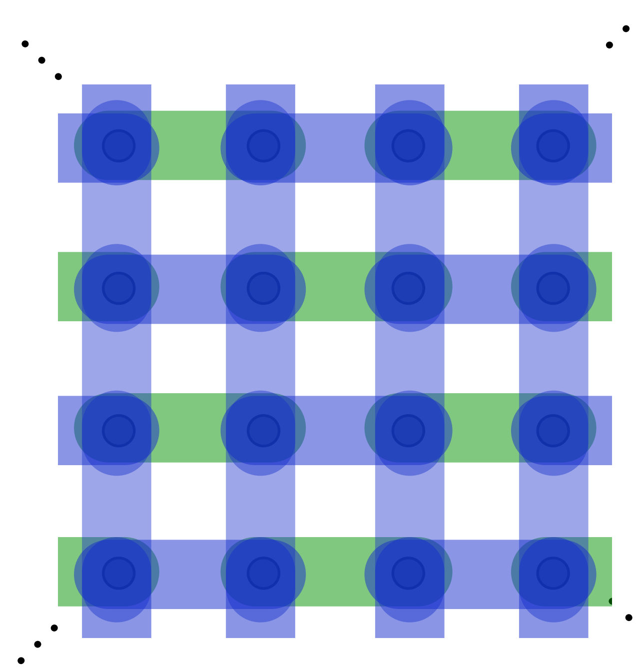
iPEPS (D=10): -0.66939J rel. error < 10^{-4}

QMC study: Sandvik & Evertz, PRB82, 024407 (2010): system sizes up to 256x256

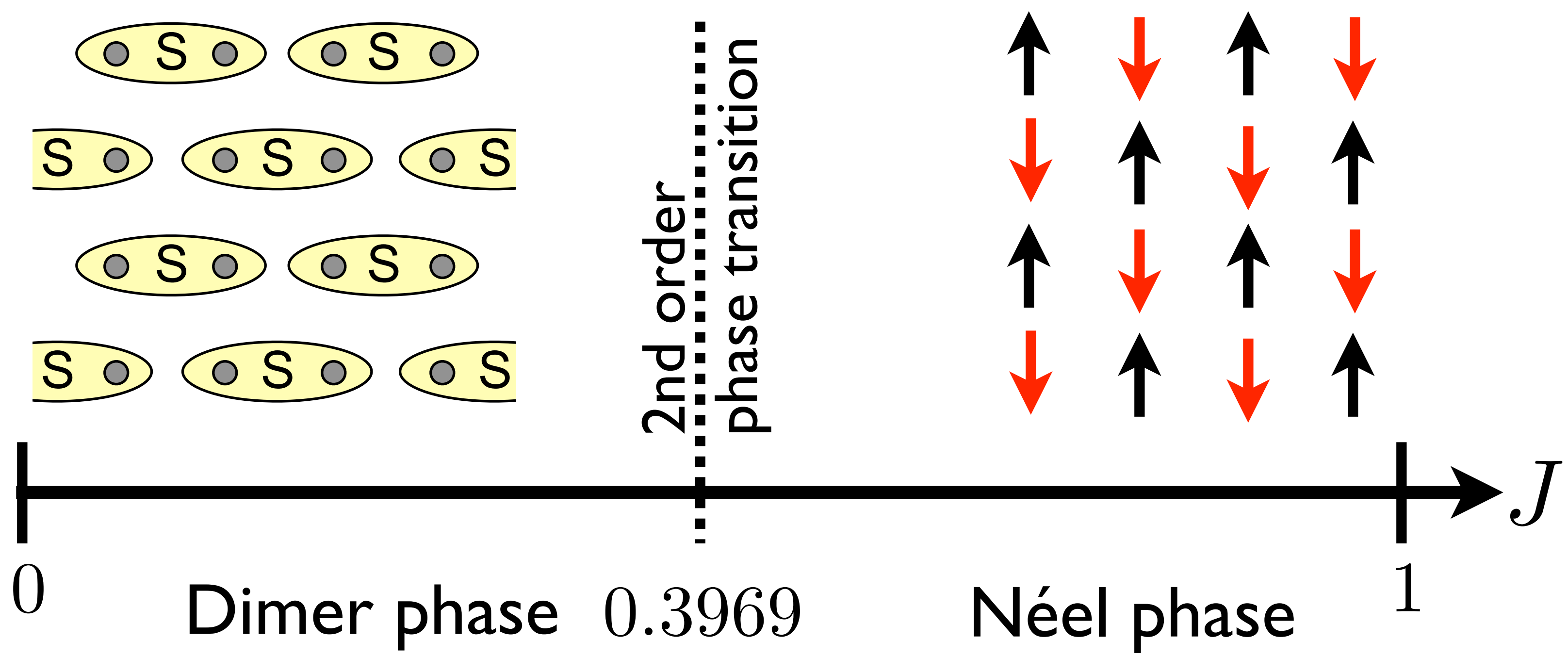


Distinguish between ordered / disordered phase?

$$H = J \sum_{\langle i,j \rangle_A} S_i S_j + \sum_{\langle i,j \rangle_B} S_i S_j$$



Phase diagram

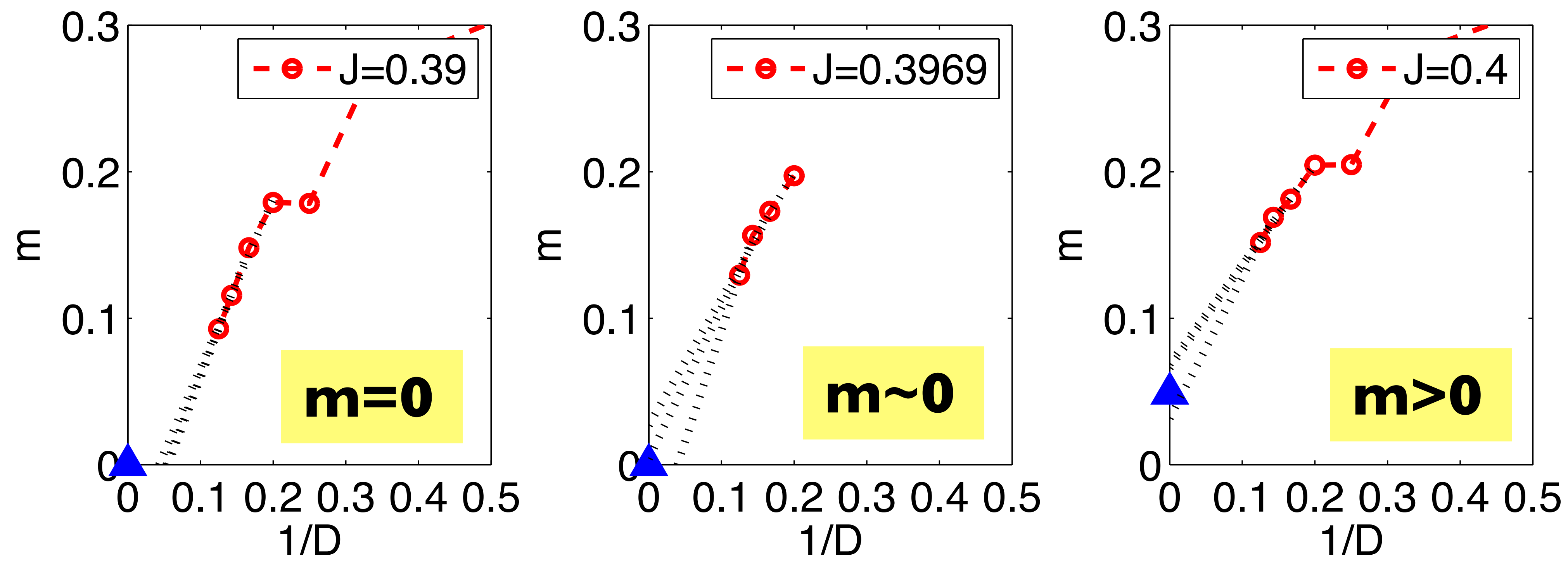


m=0

m>0

Wenzel, Janke, PRB 79 (2009)

Distinguish between ordered / disordered phase?



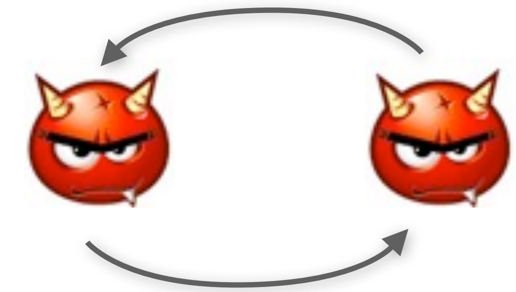
★ Extrapolations in D are important to distinguish between ordered phase and a disordered one!

★ A better understanding how to accurately extrapolate in D would be very useful

Fermionic tensor networks

Breakthrough in 2009: Fermions with 2D tensor networks

How to take fermionic statistics into account?



$$\hat{c}_i \hat{c}_j = -\hat{c}_j \hat{c}_i$$

fermionic operators *anti*commute

Different formulations:

P. Corboz, G. Evenbly, F. Verstraete, G. Vidal, Phys. Rev. A 81, 010303(R) (2010)

C. V. Kraus, N. Schuch, F. Verstraete, J. I. Cirac, Phys. Rev. A 81, 052338 (2010)

C. Pineda, T. Barthel, and J. Eisert, Phys. Rev. A 81, 050303(R) (2010)

P. Corboz and G. Vidal, Phys. Rev. B 80, 165129 (2009)

T. Barthel, C. Pineda, and J. Eisert, Phys. Rev. A 80, 042333 (2009)

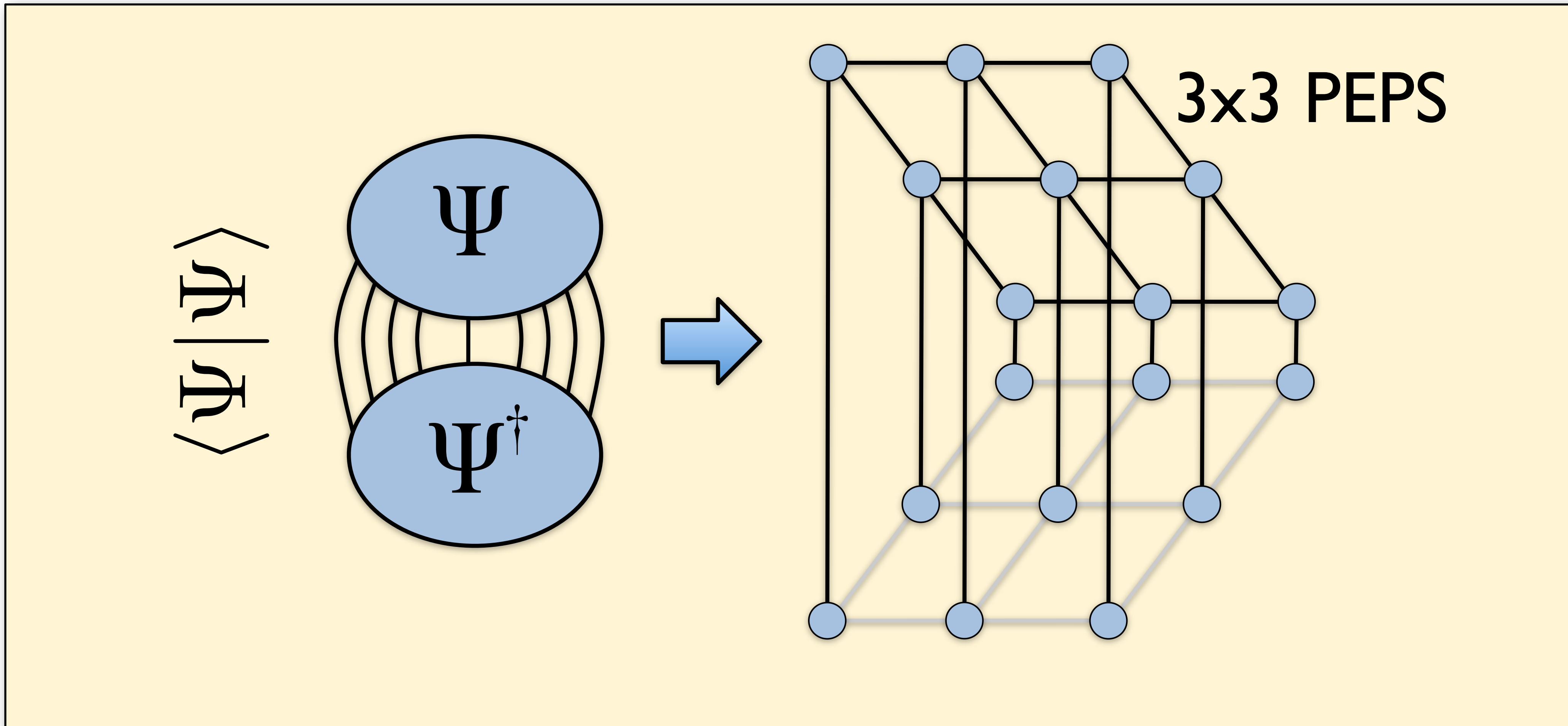
Q.-Q. Shi, S.-H. Li, J.-H. Zhao, and H.-Q. Zhou, arXiv:0907.5520

P. Corboz, R. Orus, B.Bauer, G. Vidal, PRB 81, 165104 (2010)

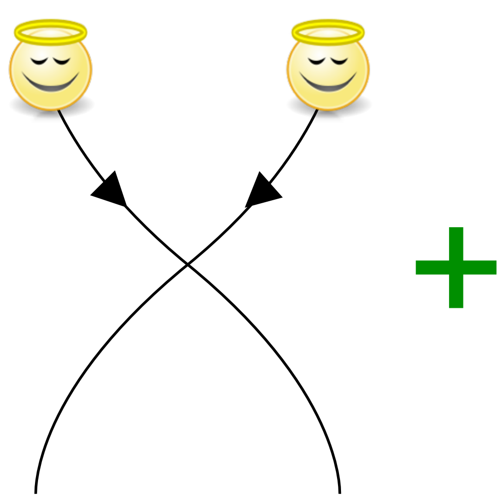
I. Pizorn, F. Verstraete, Phys. Rev. B 81, 245110 (2010)

Z.-C. Gu, F. Verstraete, X.-G. Wen. arXiv:1004.2563

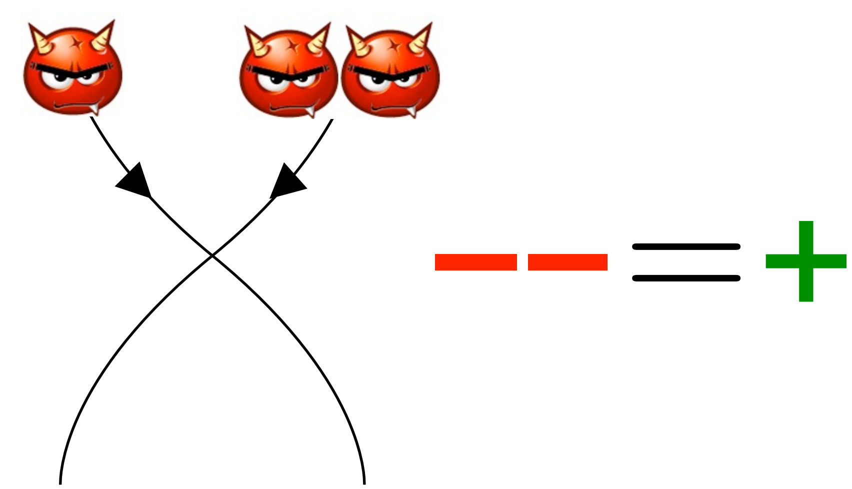
Bosons vs Fermions



Crossings in a tensor network



ignore crossings

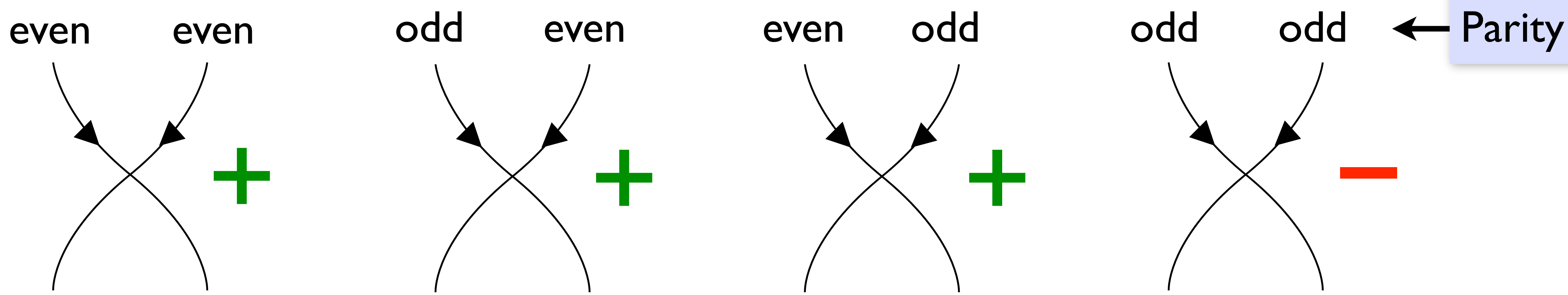


take care!

The swap tensor

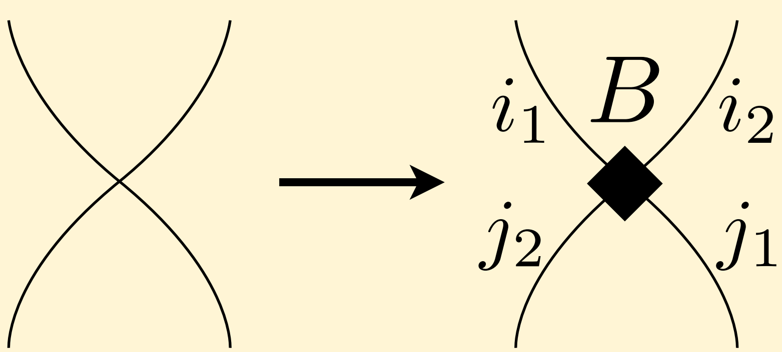
Fermions

RULE:



Parity P of a state: $\begin{cases} P = +1 & \text{(even parity), even number of fermions} \\ P = -1 & \text{(odd parity), odd number of fermions} \end{cases}$

Replace crossing by **swap tensor**



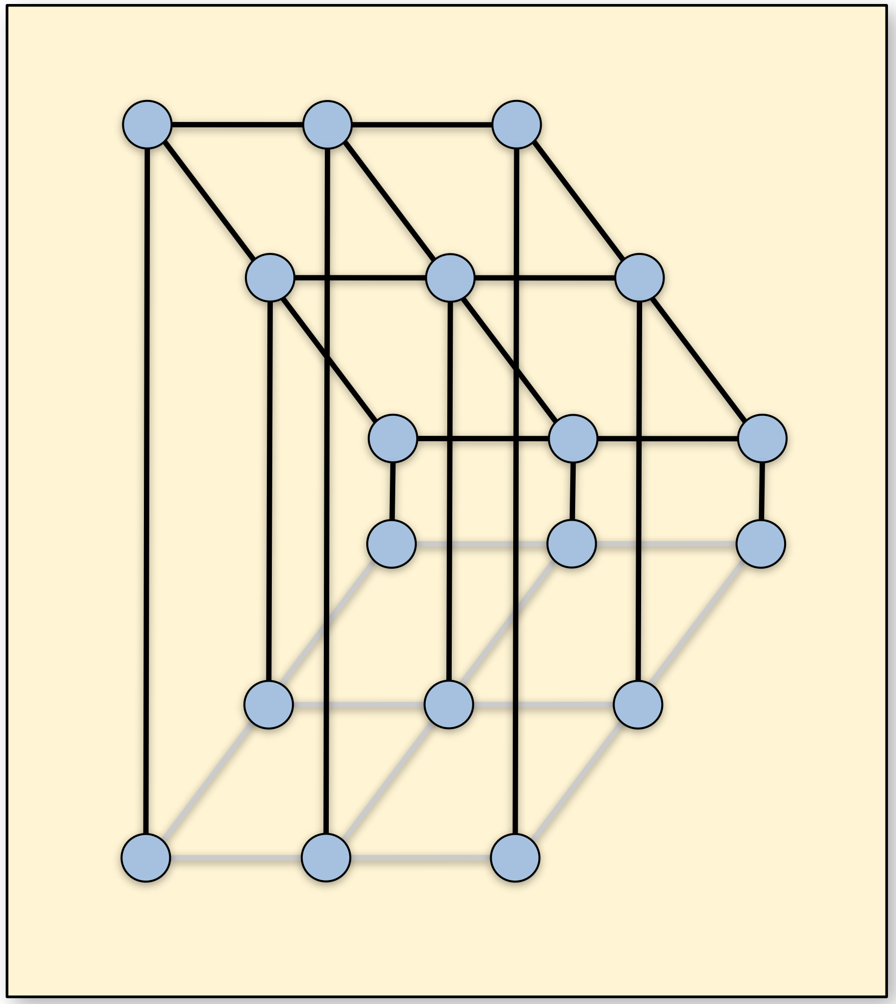
$$B^{i_1 i_2}_{j_2 j_1} = \delta_{i_1,j_1}\delta_{i_2,j_2} S(P(i_1), P(i_2))$$

$$S(P(i_1), P(i_2)) = \begin{cases} -1 & \text{if } P(i_1) = P(i_2) = -1 \\ +1 & \text{otherwise} \end{cases}$$

Use **parity** preserving tensors: $T_{i_1 i_2 \ldots i_M} = 0$ if $P(i_1)P(i_2)\ldots P(i_M) \neq 1$

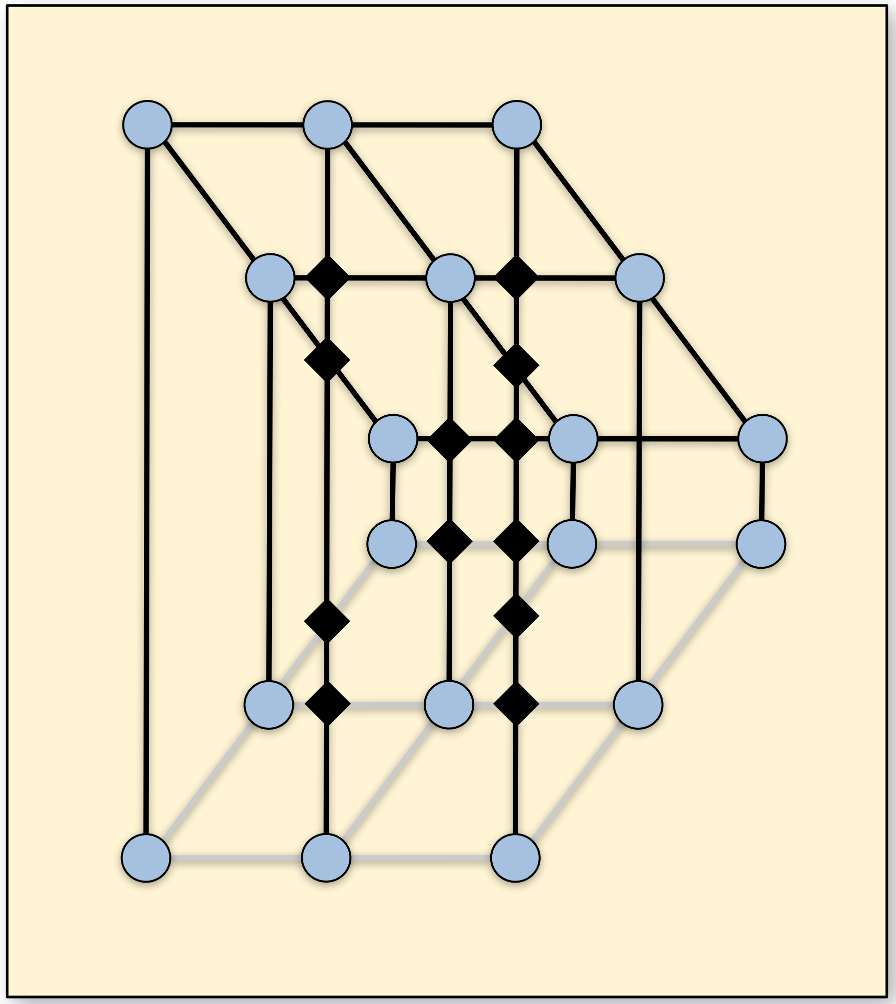
Example

Bosonic tensor network



→

Fermionic tensor network

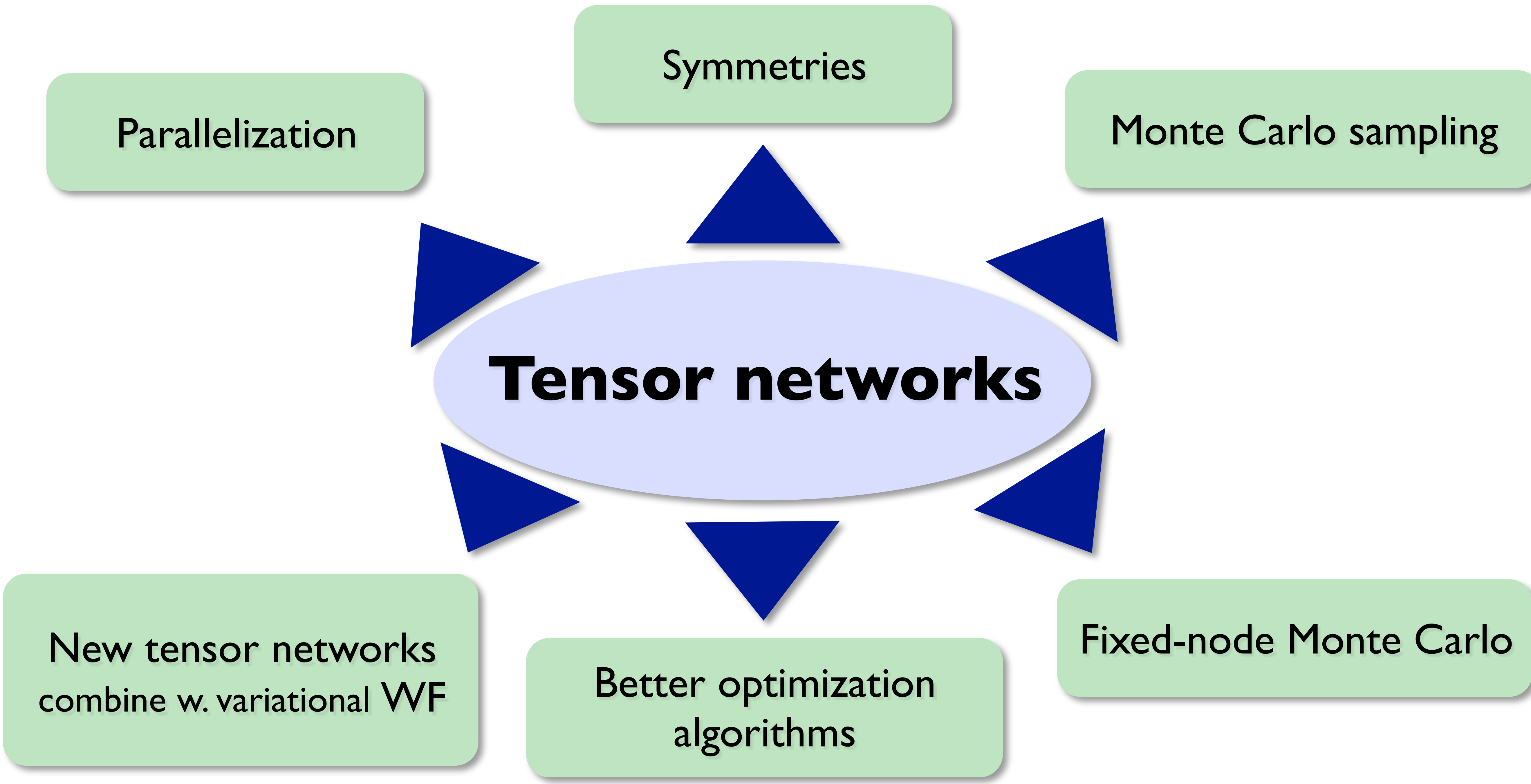


Simple rules!

Same computational cost!

Outlook

Improvements of tensor networks methods



Conclusion: Tensor network algorithms

- Variational ansatz where the accuracy can be systematically controlled
- Simulate bosonic, (frustrated) spin and fermionic systems

✓ **1D**: State-of-the-art (MPS, DMRG)

✓ **2D**: A lot of progress in recent years!

- ★ iPEPS can outperform state-of-the-art variational methods!
- ★ cMPS (not discussed) evolving as state of the art for fractional QHE

➡ **Tensor networks yield promising routes to solve challenging open problems in 2D**