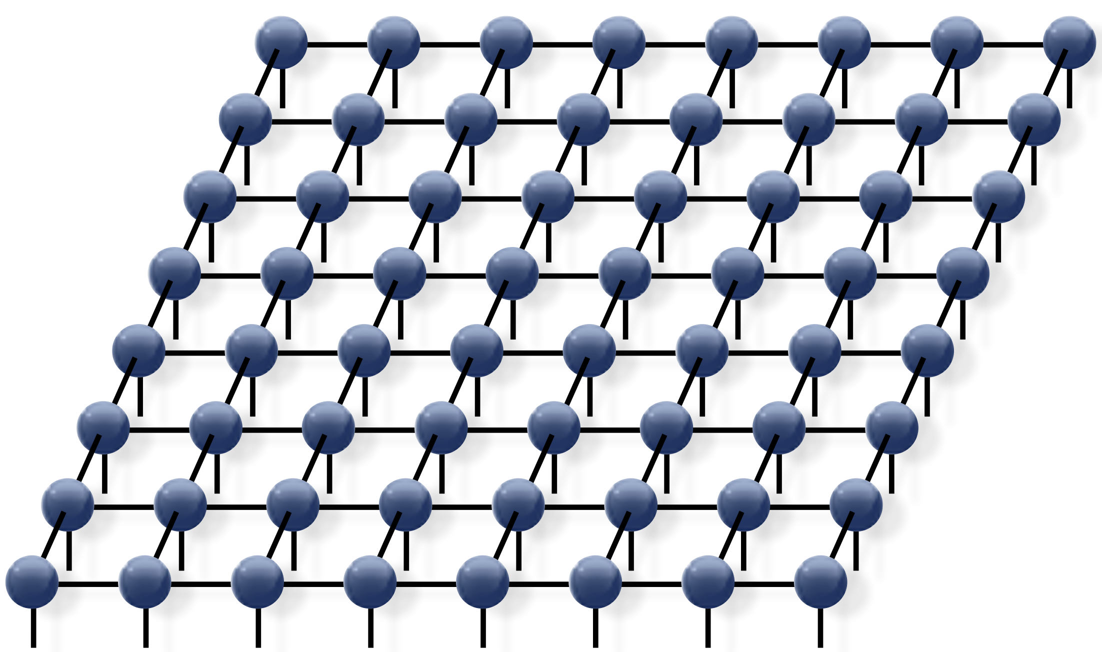
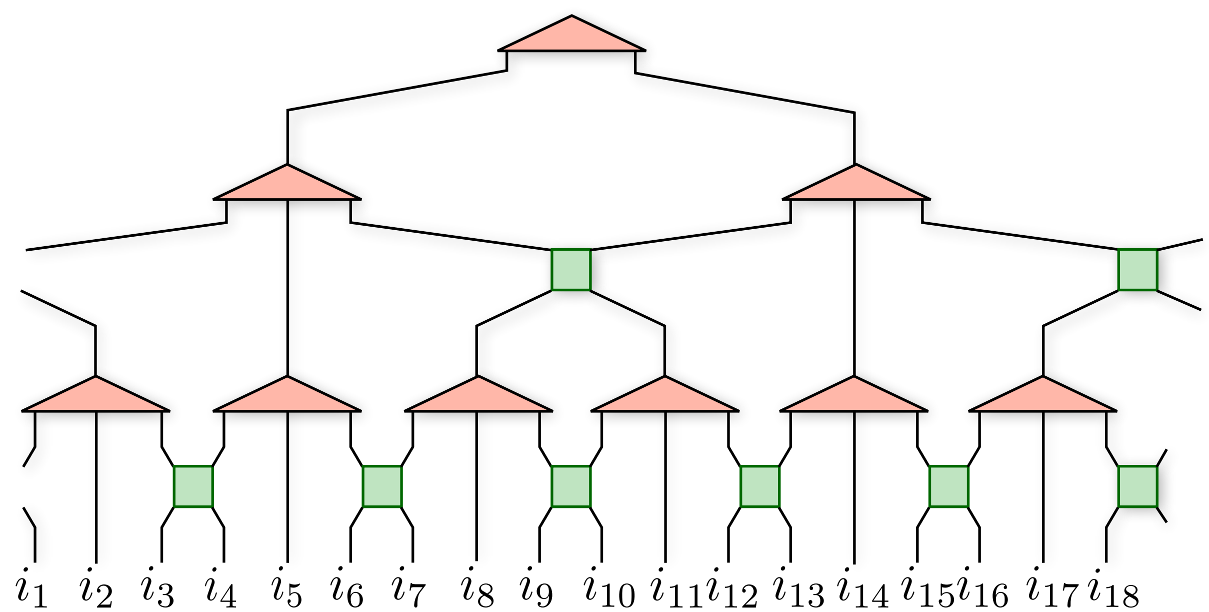
Introduction to (i)PEPS & MERA

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam



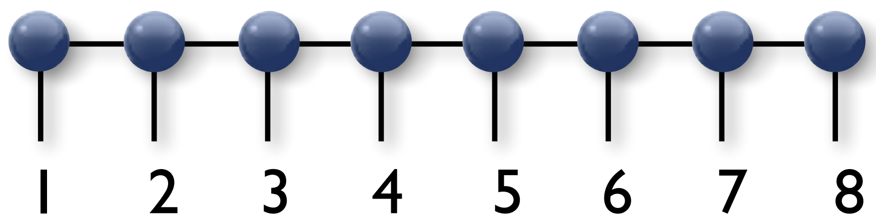


International School on "*Tensor Network based approaches to Quantum Many-Body Systems*", Dresden 2018

Overview: tensor networks in 1D and 2D

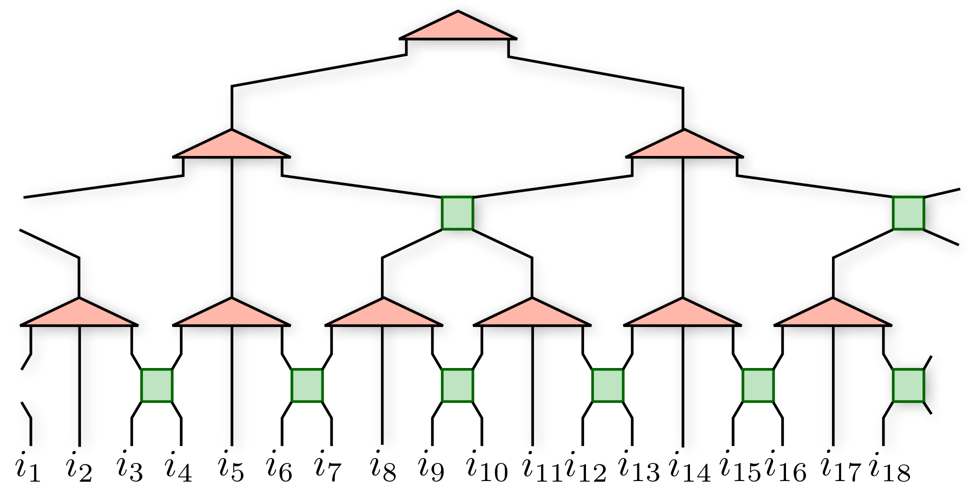
1D

MPS
Matrix-product state



Underlying ansatz of the density-matrix renormalization group (**DMRG**) method

1D MERA
Multi-scale entanglement renormalization ansatz

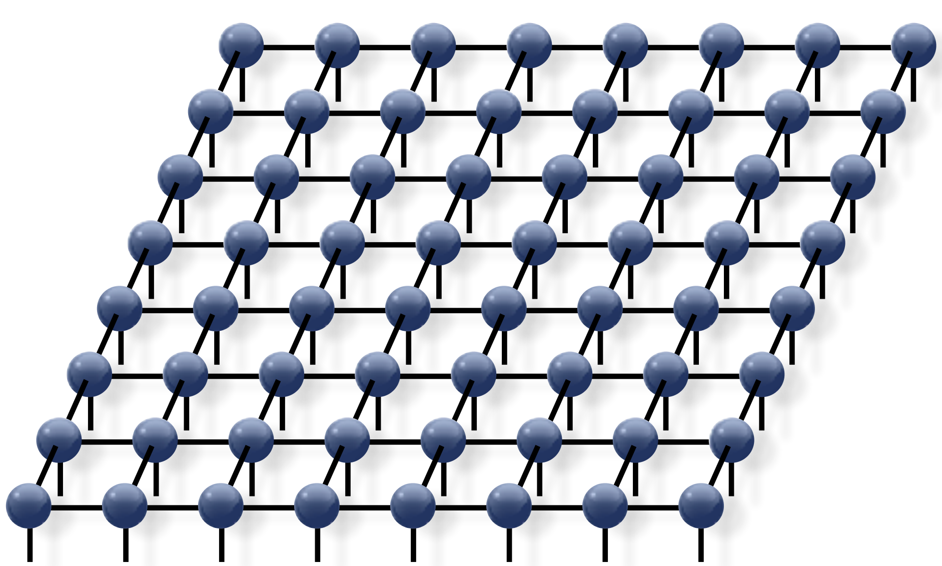


and more

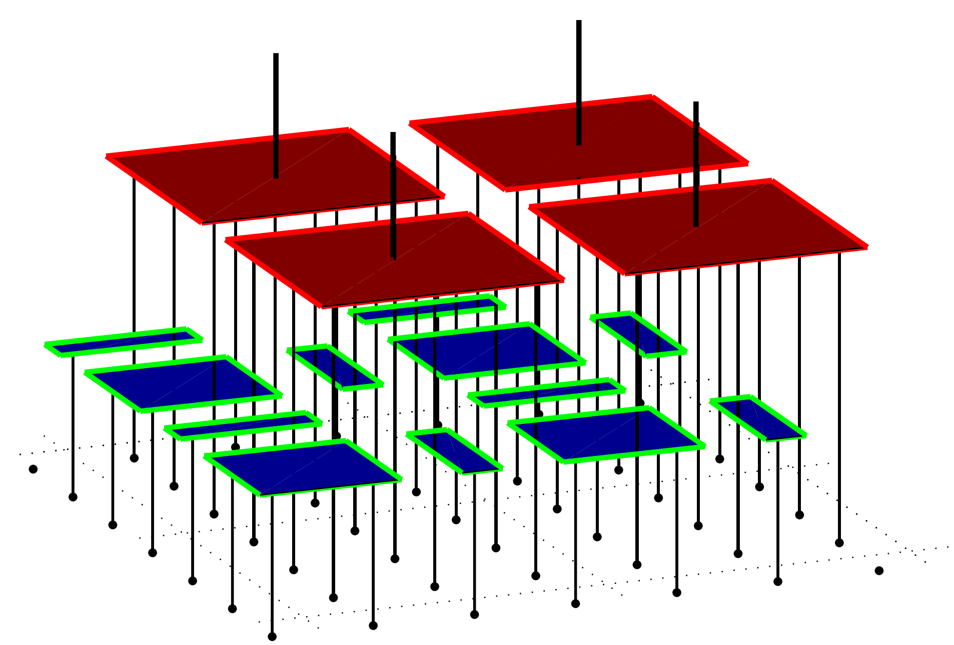
- 1D tree tensor network
- correlator product states
- ...

2D

PEPS
projected entangled-pair state



2D MERA



and more

- Entangled-plaquette states
- 2D tree tensor network
- String-bond states
- ...

Outline

- Part I: Tensor network ansätze
  - ✦ ***Recap***: *main idea of a tensor network ansatz & area law of the entanglement entropy*
  - ✦ *MPS, PEPS & iPEPS, Tree tensor networks, MERA & 2D MERA*
  - ✦ *Classify tensor network ansatz according to its entanglement scaling*
- Part II: Contraction
  - ✦ *Contraction of MPS and the MERA*
  - ✦ *Contraction of PEPS / iPEPS: MPS-MPO approach, corner-transfer-matrix (**CTM**) method, Tensor Renormalization Group (TRG), Tensor network renormalization (TNR)*
  - ✦ *Simple example application: solving the 2D classical Ising model with the CTM method*
- Part III: Optimization
- Part IV: iPEPS application example
- Part V: Finite correlation length scaling
- Outlook & summary

PART I:
Tensor network ansätze

Recap: Tensor network ansatz for a wave function

Lattice: 1 2 3 4 5 6

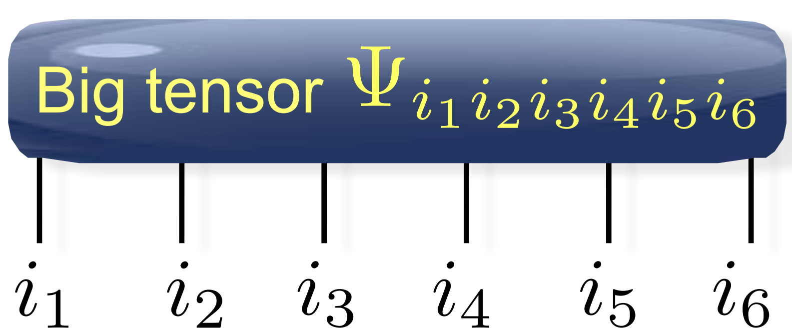
2 basis states per site: $\{|\uparrow\rangle, |\downarrow\rangle\}$

2^6 basis states

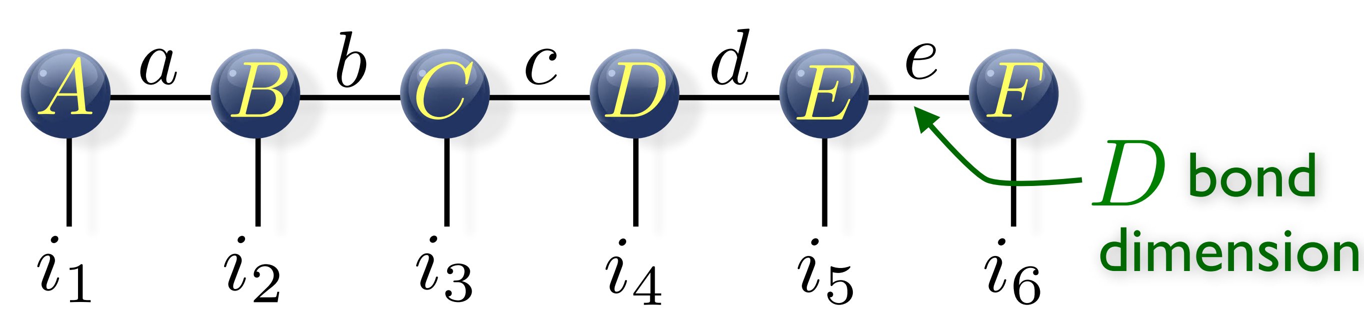
2^6 coefficients

State: $$|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4 i_5 i_6} \Psi_{i_1 i_2 i_3 i_4 i_5 i_6} |i_1 \otimes i_2 \otimes i_3 \otimes i_4 \otimes i_5 \otimes i_6\rangle$$

Tensor/multidimensional array



Tensor network: matrix product state (**MPS**)

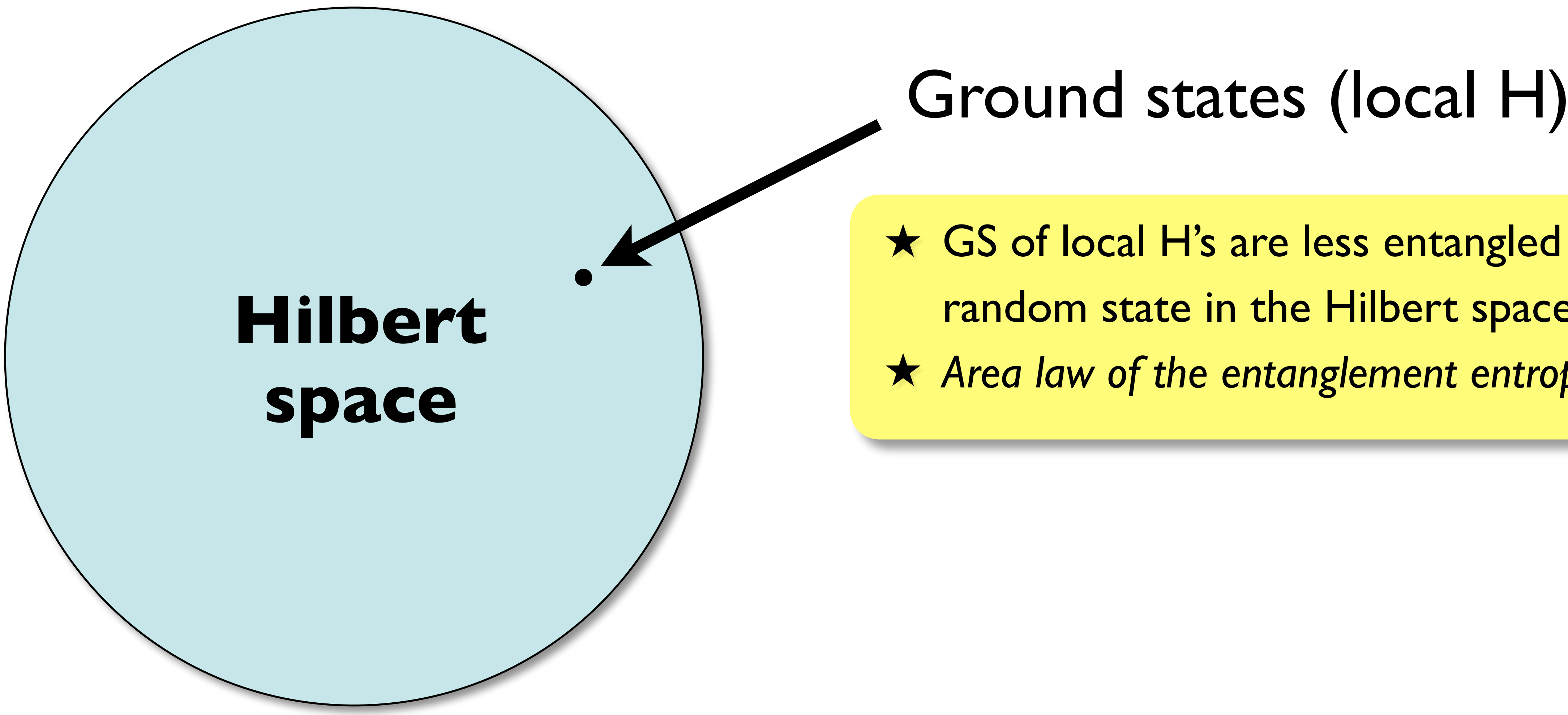


$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6} \approx \sum_{abcde} A^{a}_{i_1} B^{ab}_{i_2} C^{bc}_{i_3} D^{cd}_{i_4} E^{de}_{i_5} F^{e}_{i_6} = \tilde{\Psi}_{i_1 i_2 i_3 i_4 i_5 i_6}$$

exp(N) many numbers **vs** poly(D,N) numbers

Efficient representation!

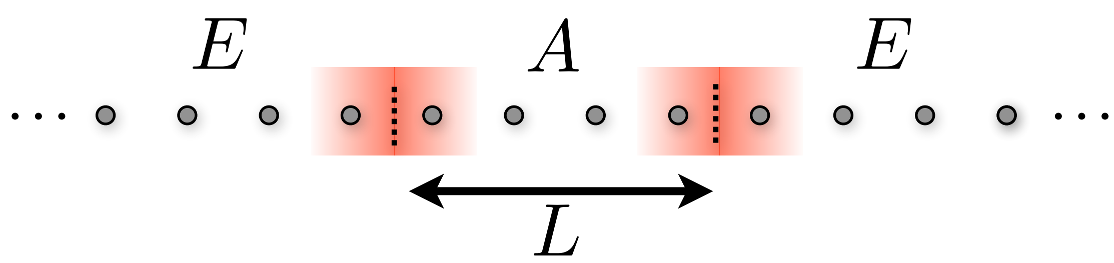
"Corner" of the Hilbert space



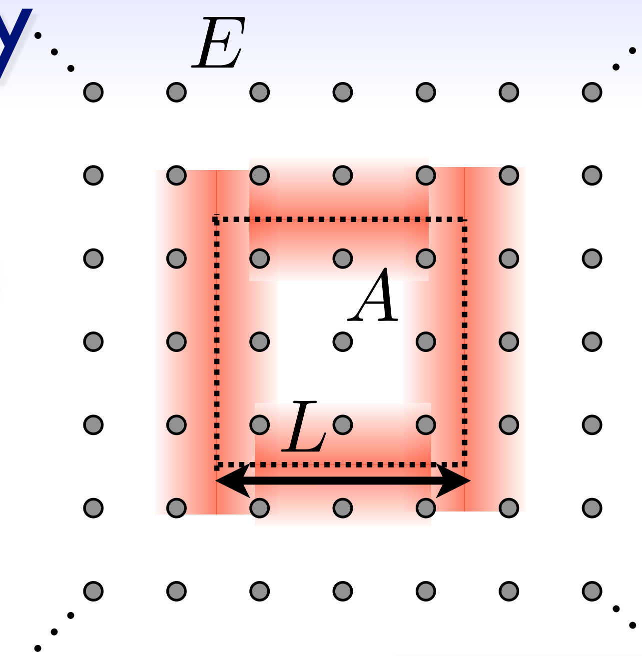
- ★ GS of local H's are less entangled than a random state in the Hilbert space
- ★ *Area law of the entanglement entropy*

Area law of the entanglement entropy

1D



2D



Entanglement entropy $S(A) = -\mathrm{tr}[\rho_A \log \rho_A] = -\sum_i \lambda_i \log \lambda_i$

relevant states
$\chi \sim \exp(S)$

General (random) state

$S(L) \sim L^d$ **(volume)**

Ground state (local Hamiltonian)

$S(L) \sim L^{d-1}$ **(area law)**

Critical ground states:
(all in 1D but not all in 2D)

1D $S(L) \sim \log(L)$

2D $S(L) \sim L \log(L)$

1D $S(L) = const$ $\chi = const$

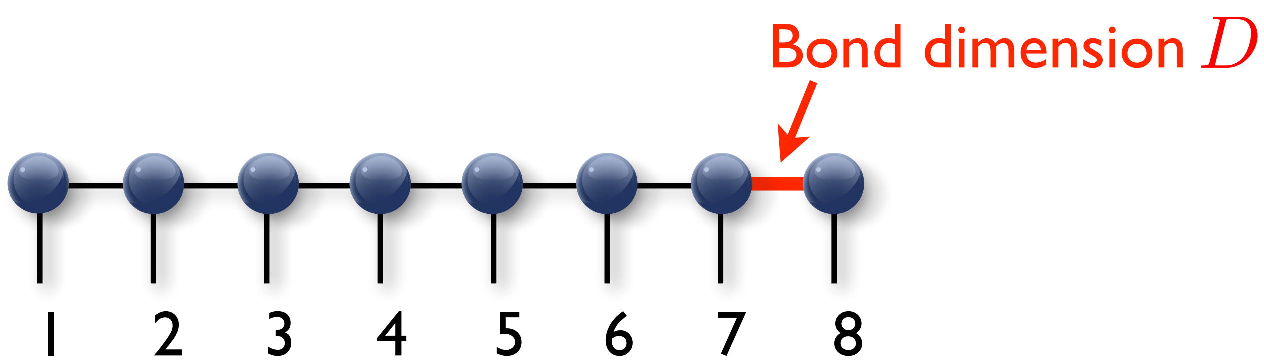
2D $S(L) \sim \alpha L$ $\chi \sim \exp(\alpha L)$

MPS & PEPS

1D

MPS

Matrix-product state



Physical indices (lattices sites)

S. R. White, PRL 69, 2863 (1992)

Fannes et al., CMP 144, 443 (1992)

Östlund, Rommer, PRL 75, 3537 (1995)

✓ Reproduces area-law in 1D

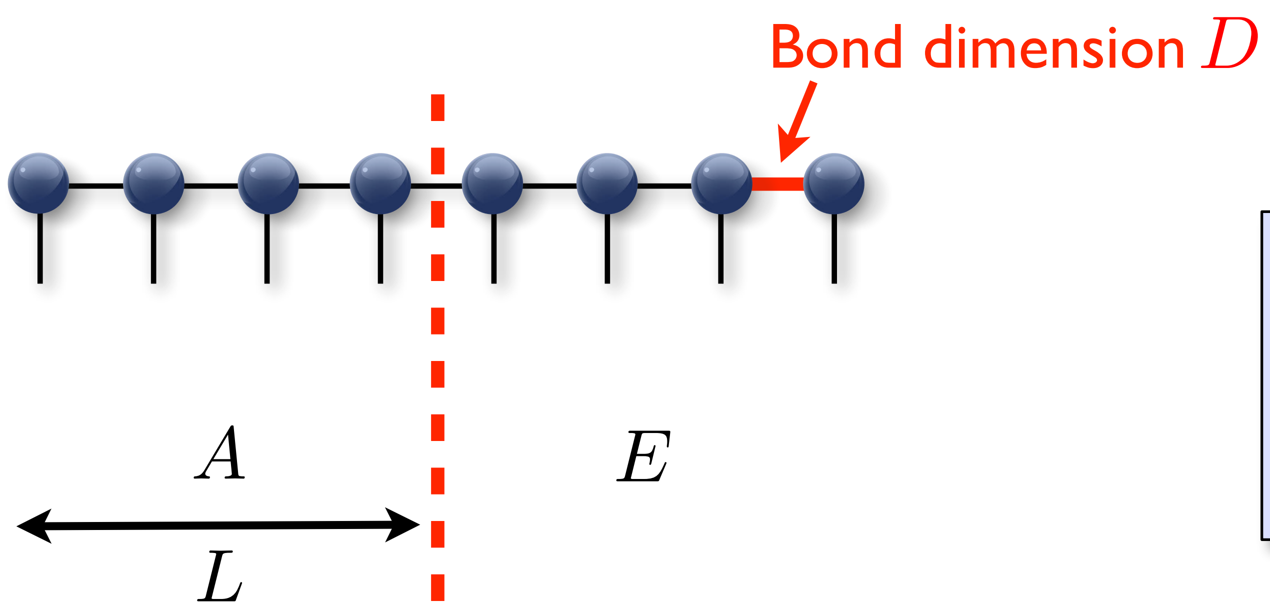
$$S(L) = const$$

MPS & PEPS

1D

MPS

Matrix-product state



➡ One bond can contribute at most log(D) to the entanglement entropy

$$rank(\rho_A) \leq D \longrightarrow S(A) \leq log(D) = const$$

✓ Reproduces area-law in 1D

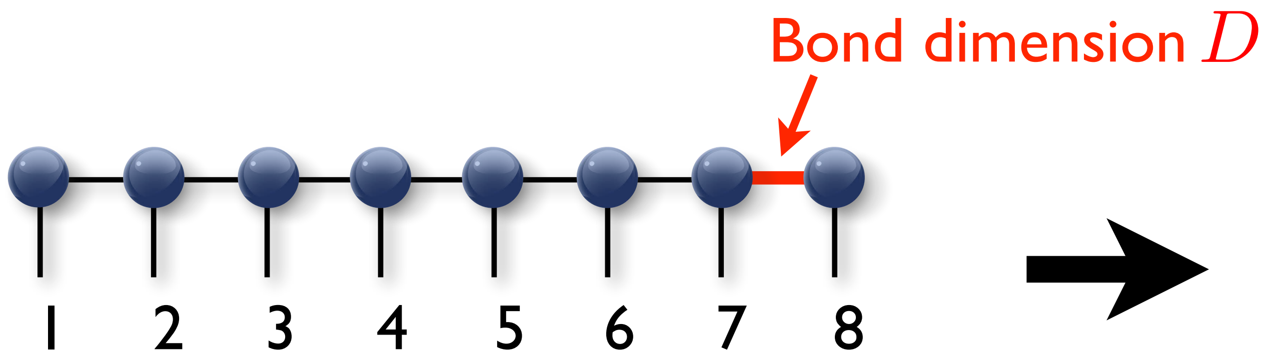
$$S(L) = const$$

MPS & PEPS

1D

MPS

Matrix-product state



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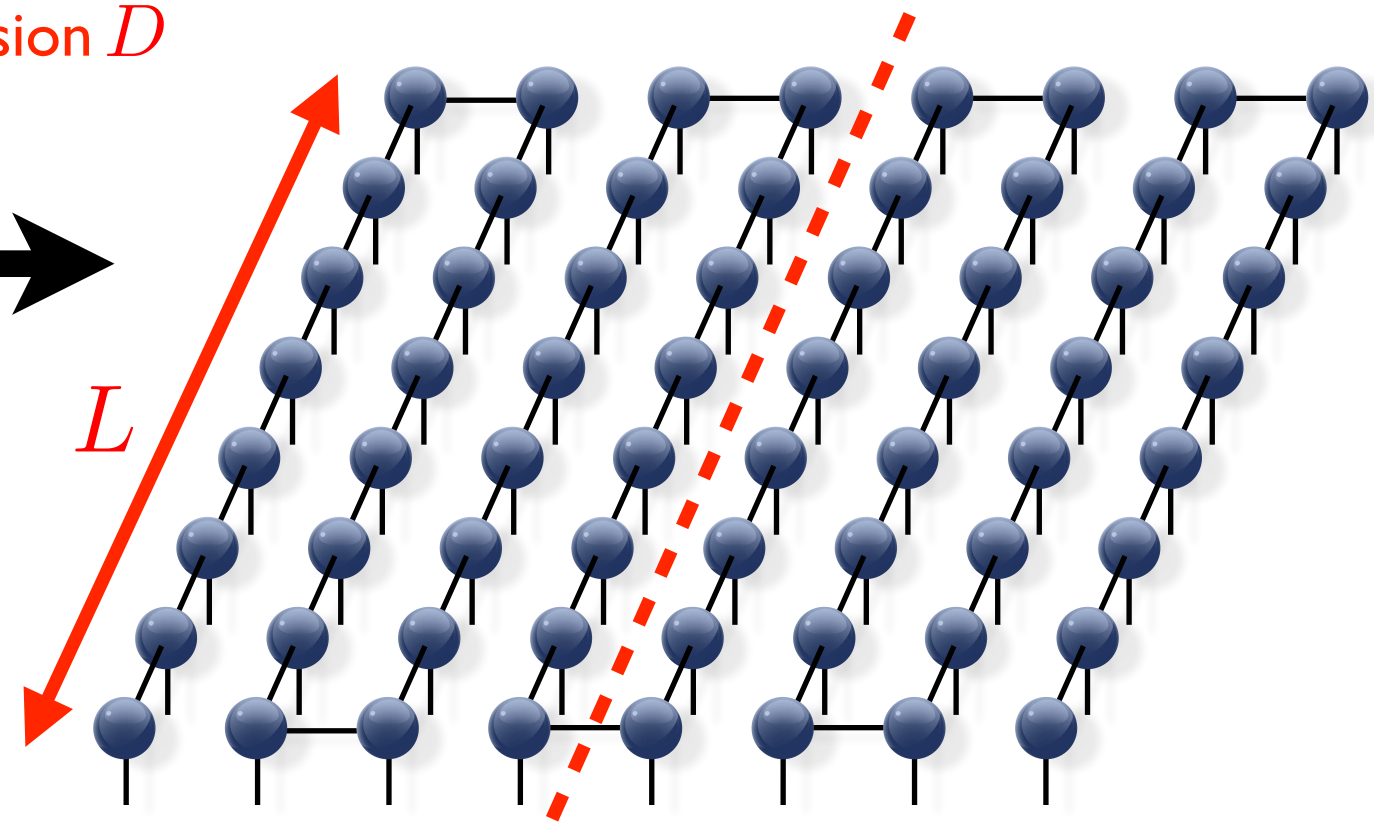
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

can we use an MPS?



!!! Area-law in 2D !!!

$$S(L) \sim L$$

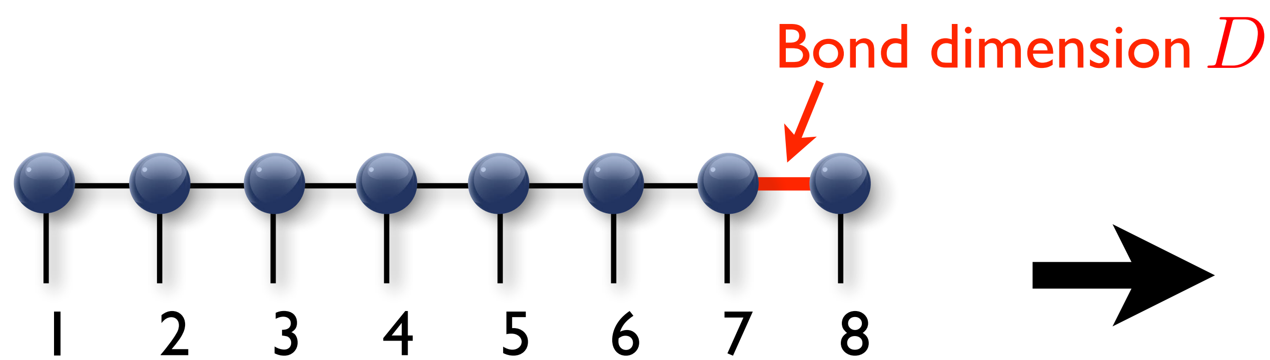
→ $D \sim exp(L)$

MPS & PEPS

1D

MPS

Matrix-product state



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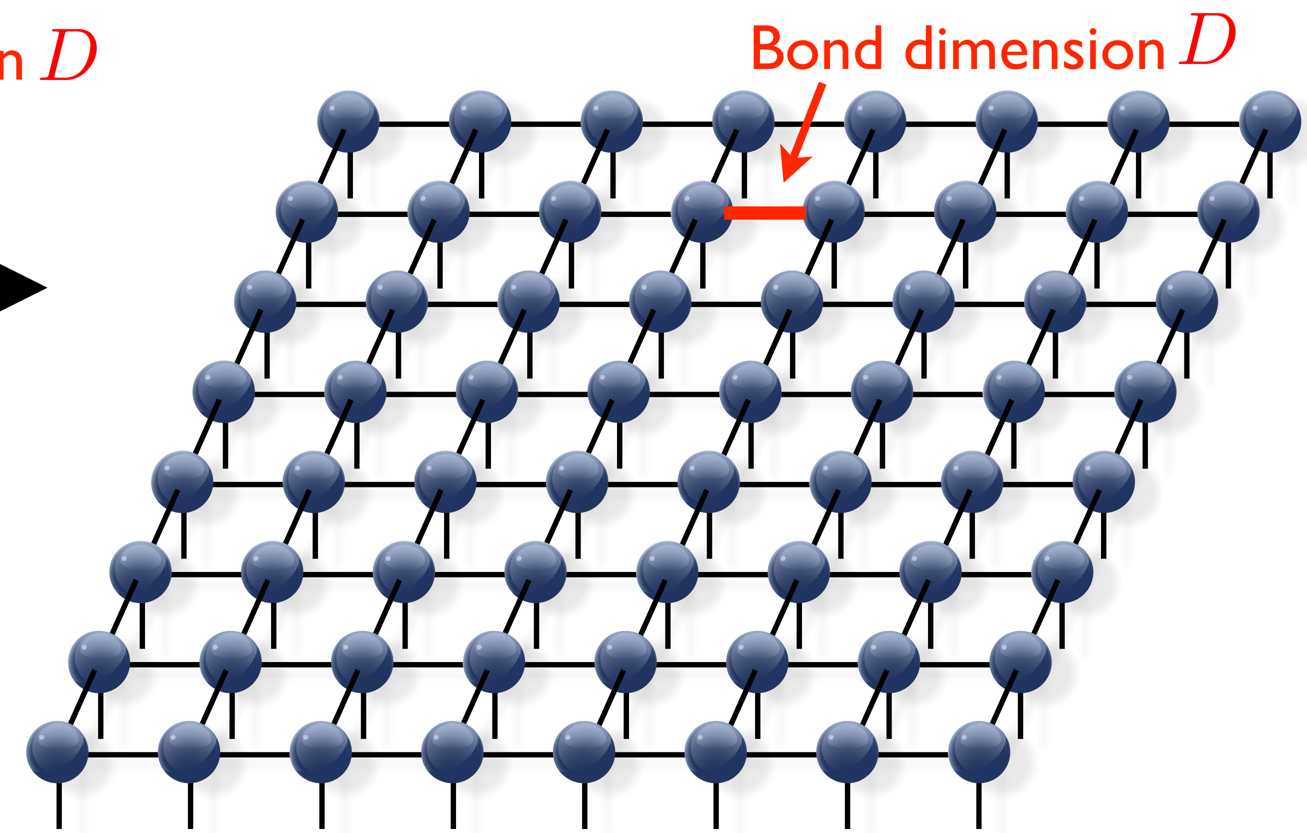
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)

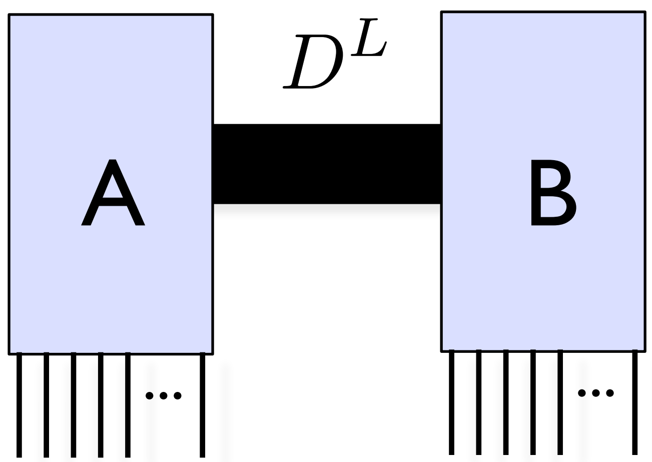


F. Verstraete, J. I. Cirac, cond-mat/0407066
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

✓ Reproduces area-law in 2D

$$S(L) \sim L$$

PEPS: Area law

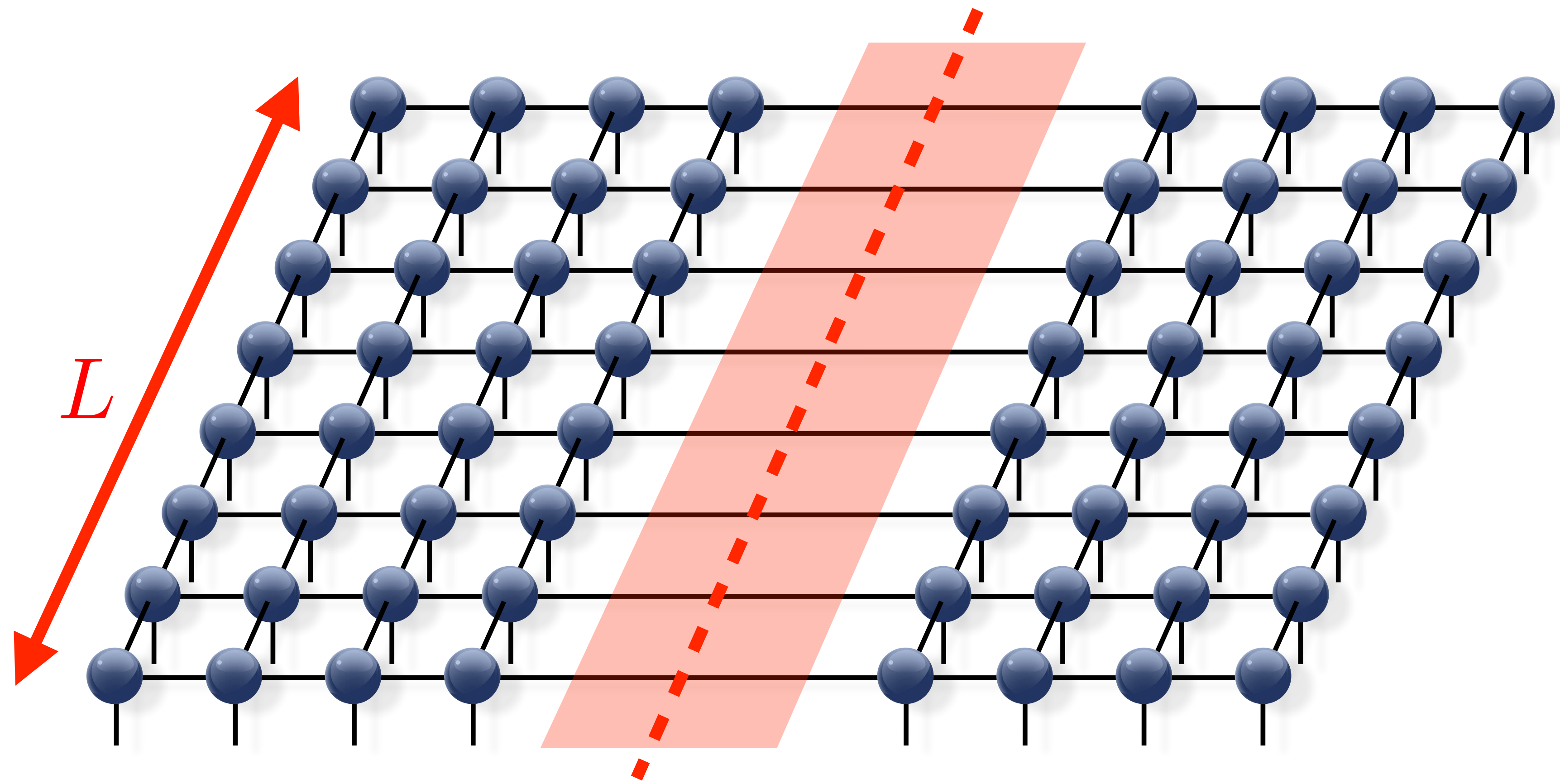


$$S(A) \leq L \log D \sim L$$

each cut auxiliary bond can contribute (at most) log D to the entanglement entropy

The number of cuts scales with the cut length

one “thick” bond of dimension D^L



✓ Reproduces area-law in 2D

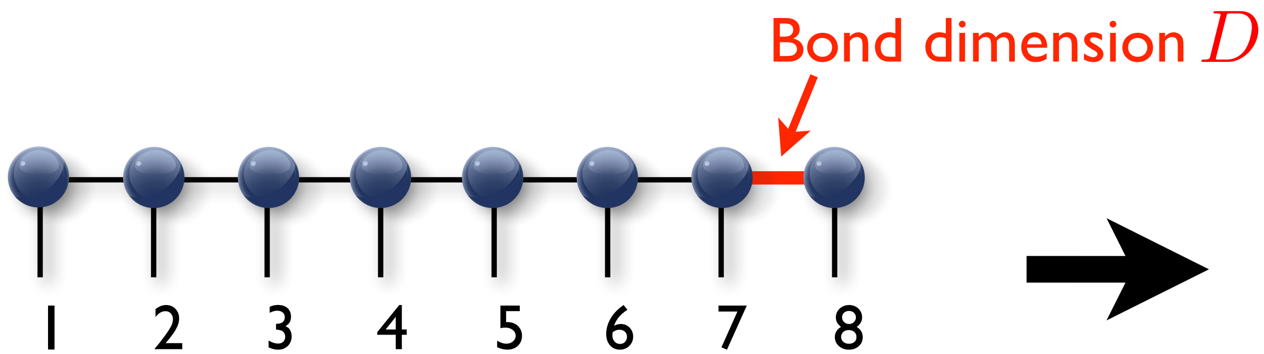
$$S(L) \sim L$$

MPS & PEPS

1D

MPS

Matrix-product state



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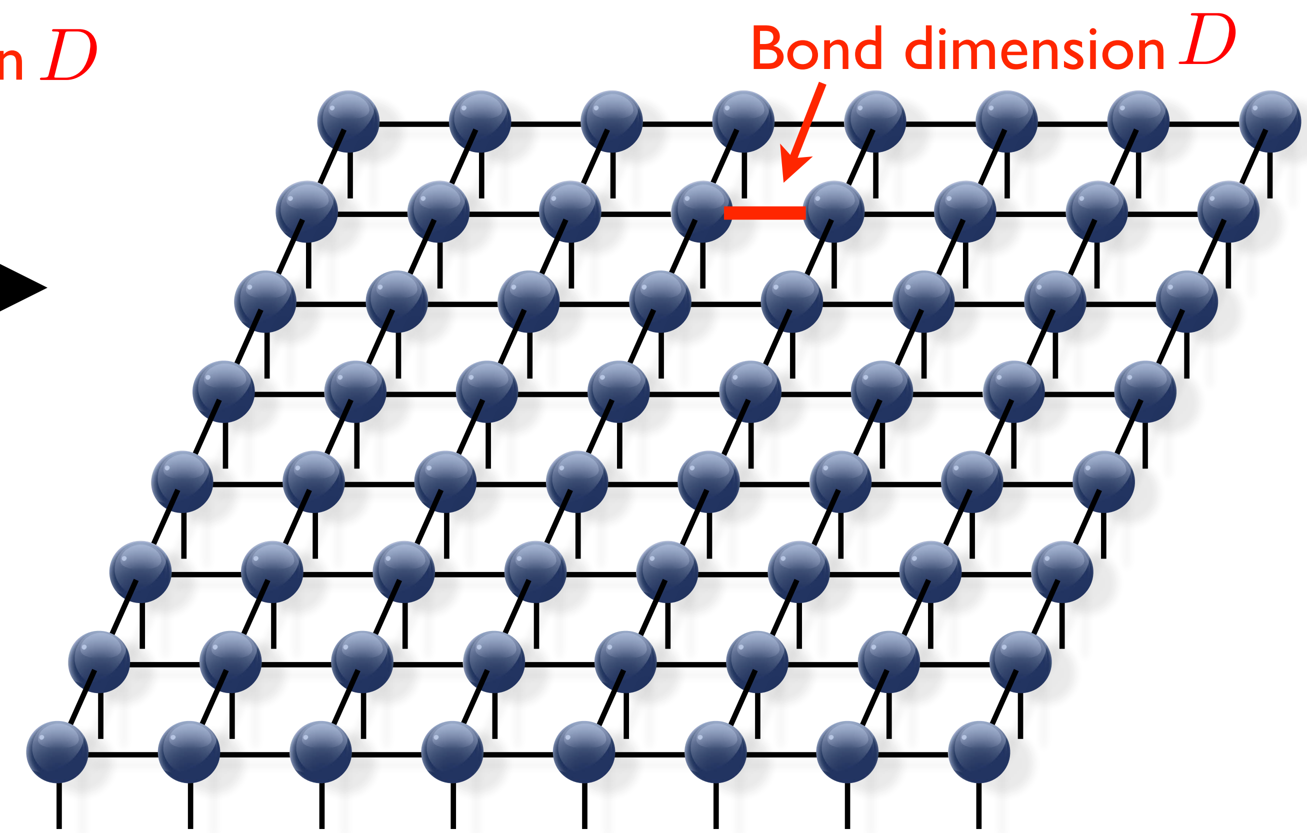
2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



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$$S(L) = const$$

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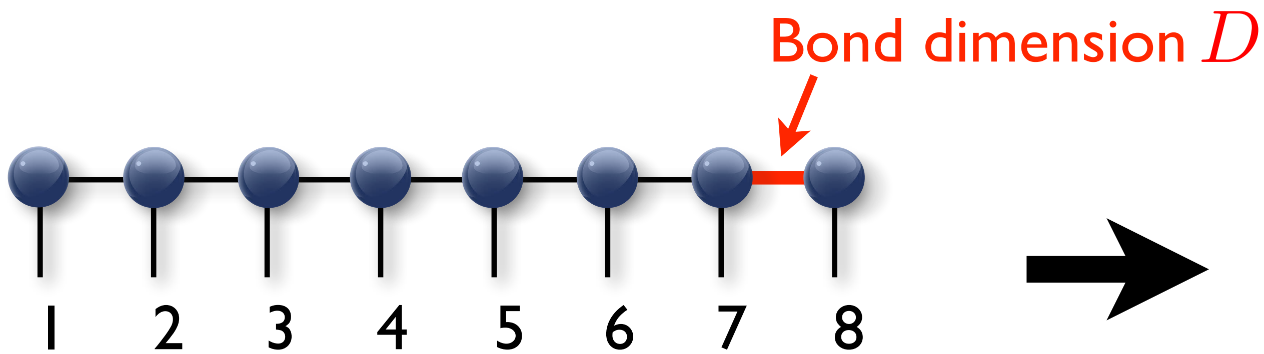
MPS & PEPS

1D

MPS

Matrix-product state



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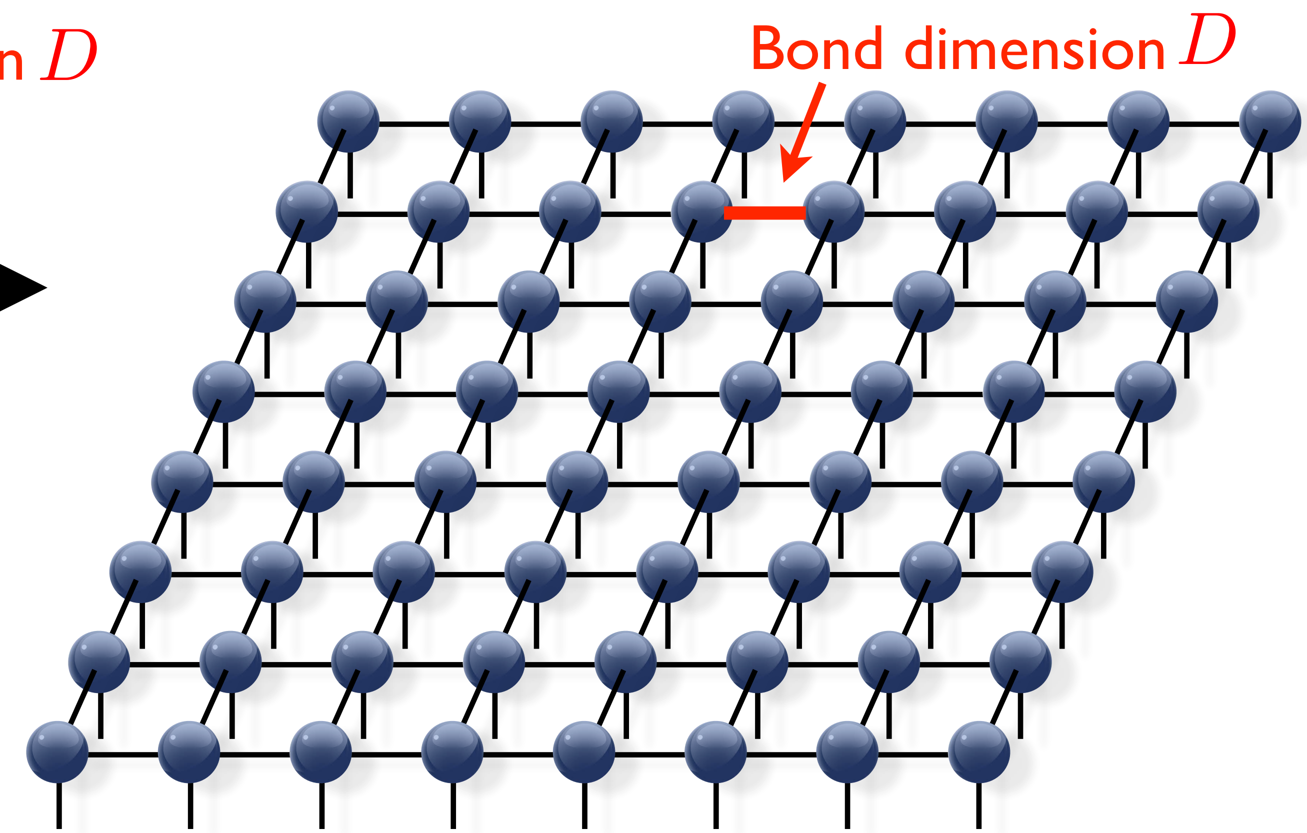
2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



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✓ Reproduces area-law in 2D

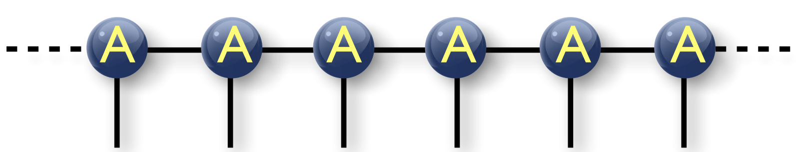
$$S(L) \sim L$$

Infinite PEPS (iPEPS)

1D

iMPS

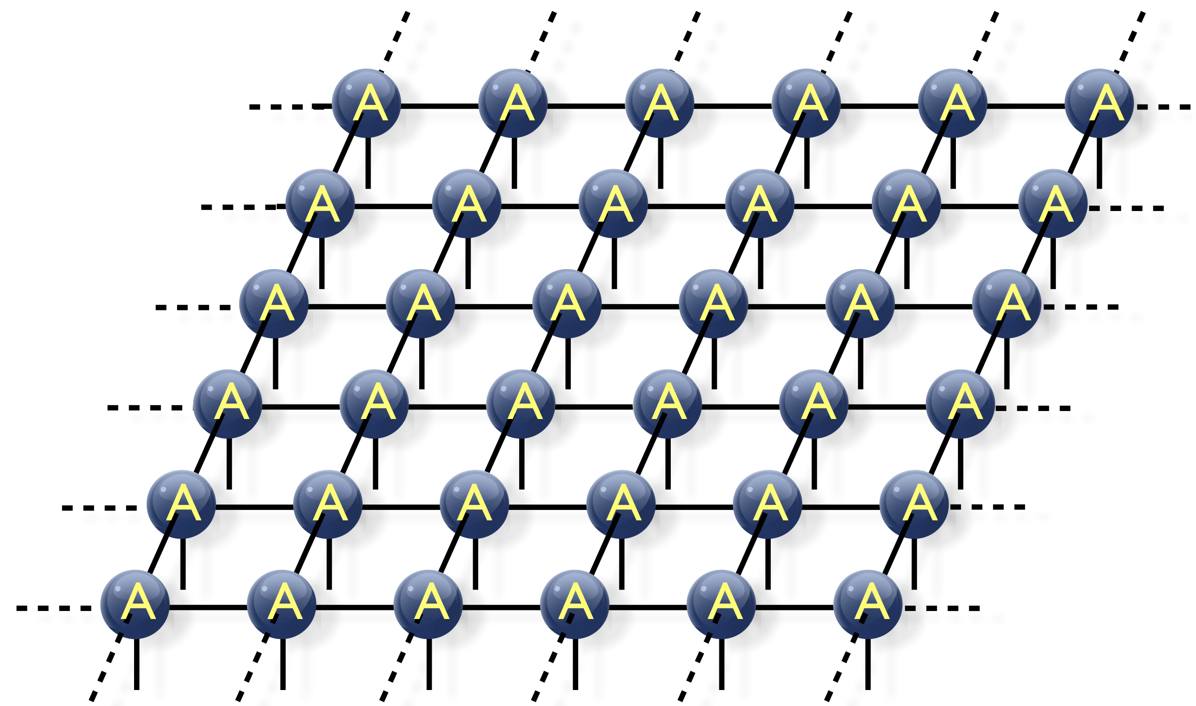
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

Infinite PEPS (iPEPS)

1D

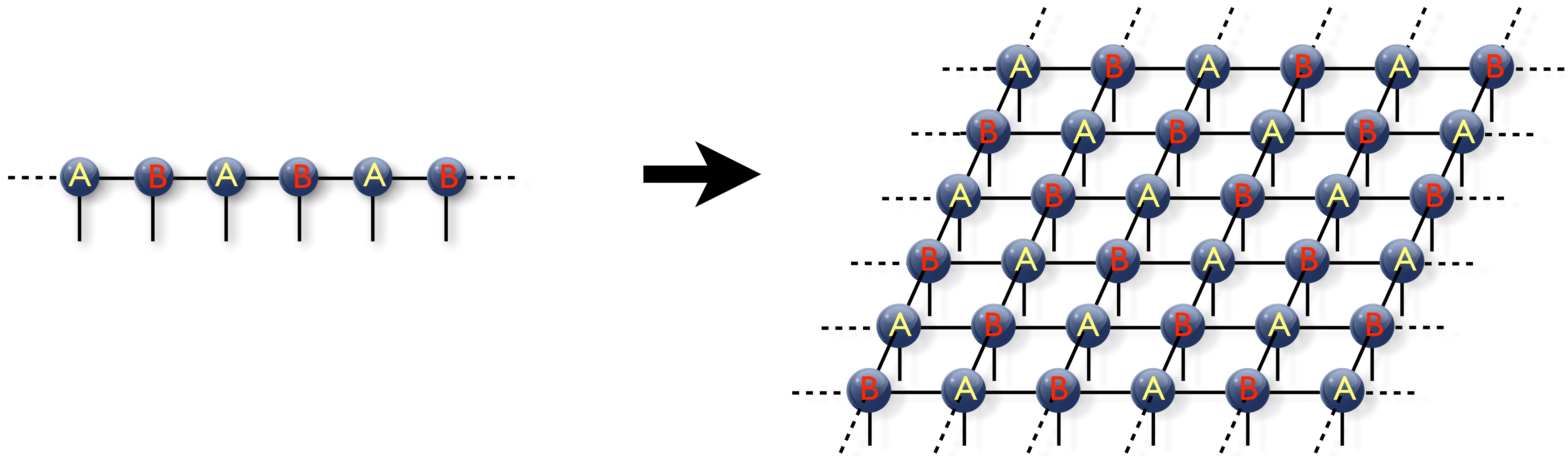
iMPS

infinite matrix-product state

2D

iPEPS

infinite projected entangled-pair state



Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

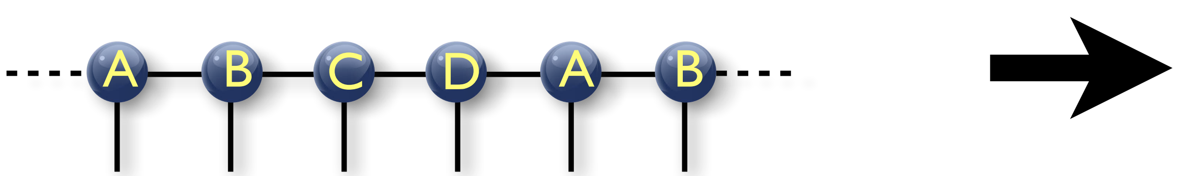
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

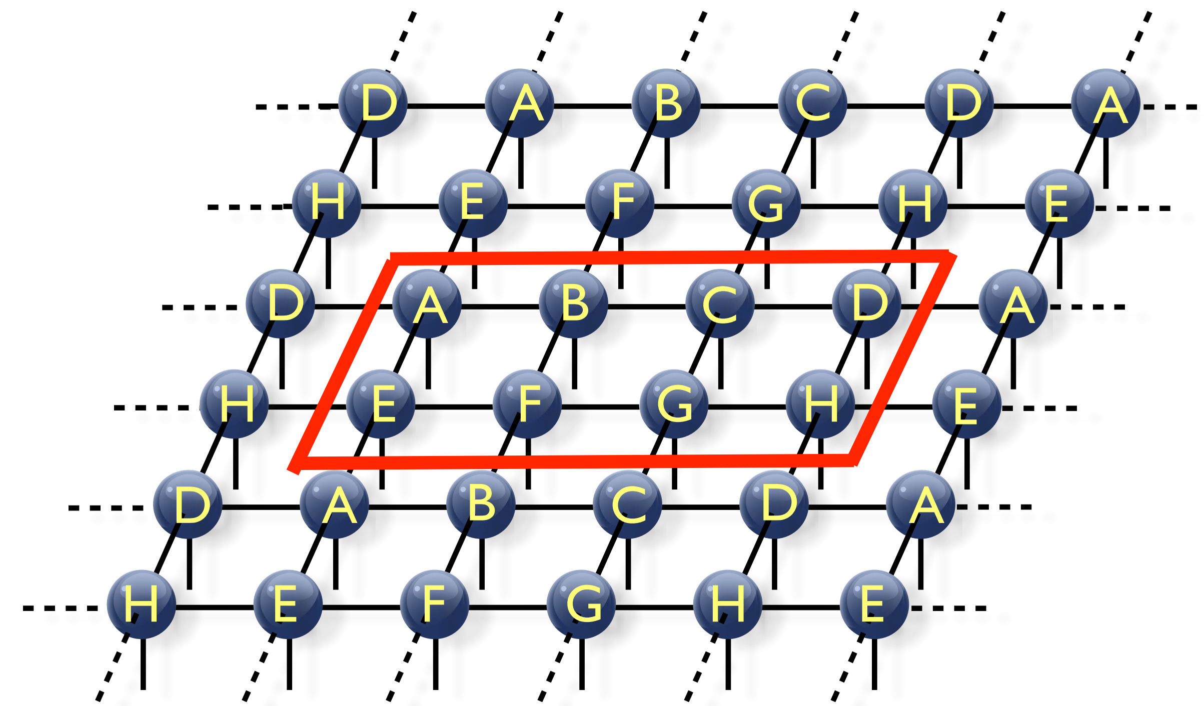
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



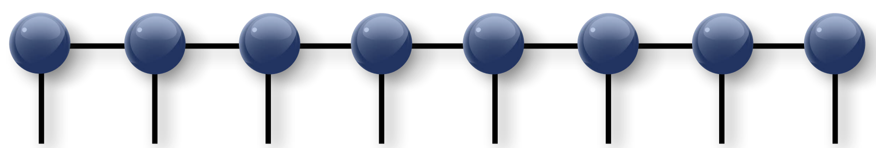
here: 4x2 unit cell

PC, White, Vidal, Troyer, PRB **84** (2011)

★ Run simulations with different unit cell sizes and compare variational energies

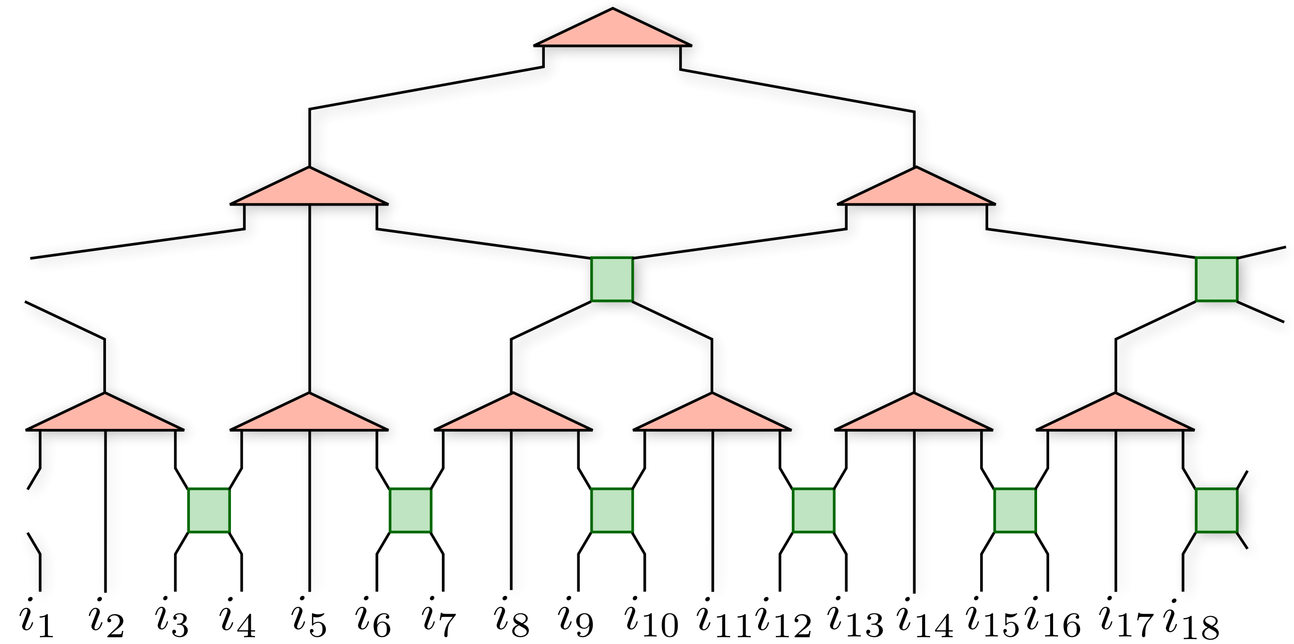
Hierarchical tensor networks (TTN/MERA)

MPS



“flat”

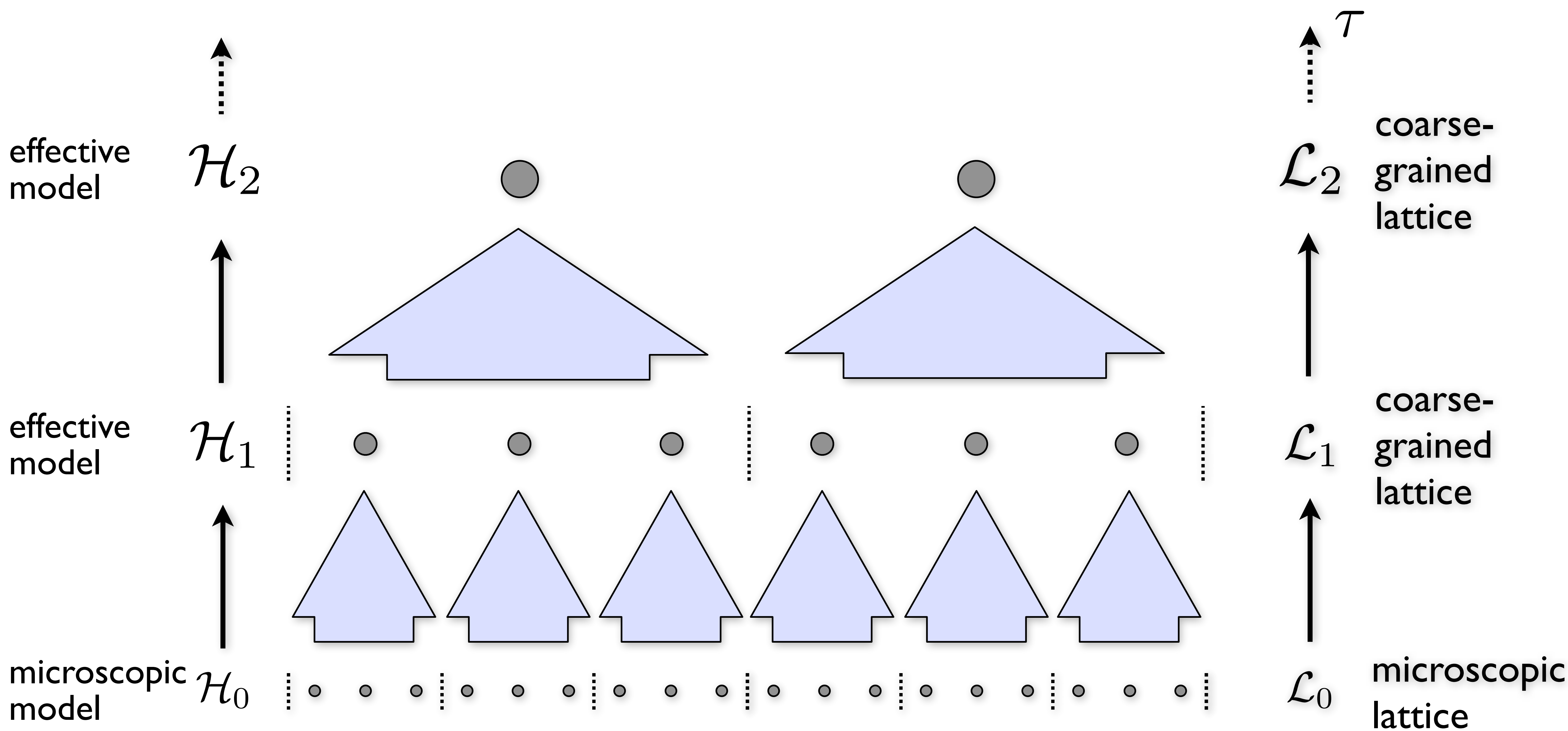
MERA



tensors at different length scales

★ Powerful ansatz for critical systems!
(reproduces S(L) ~ L logL scaling)

Real-space renormalization group transformation

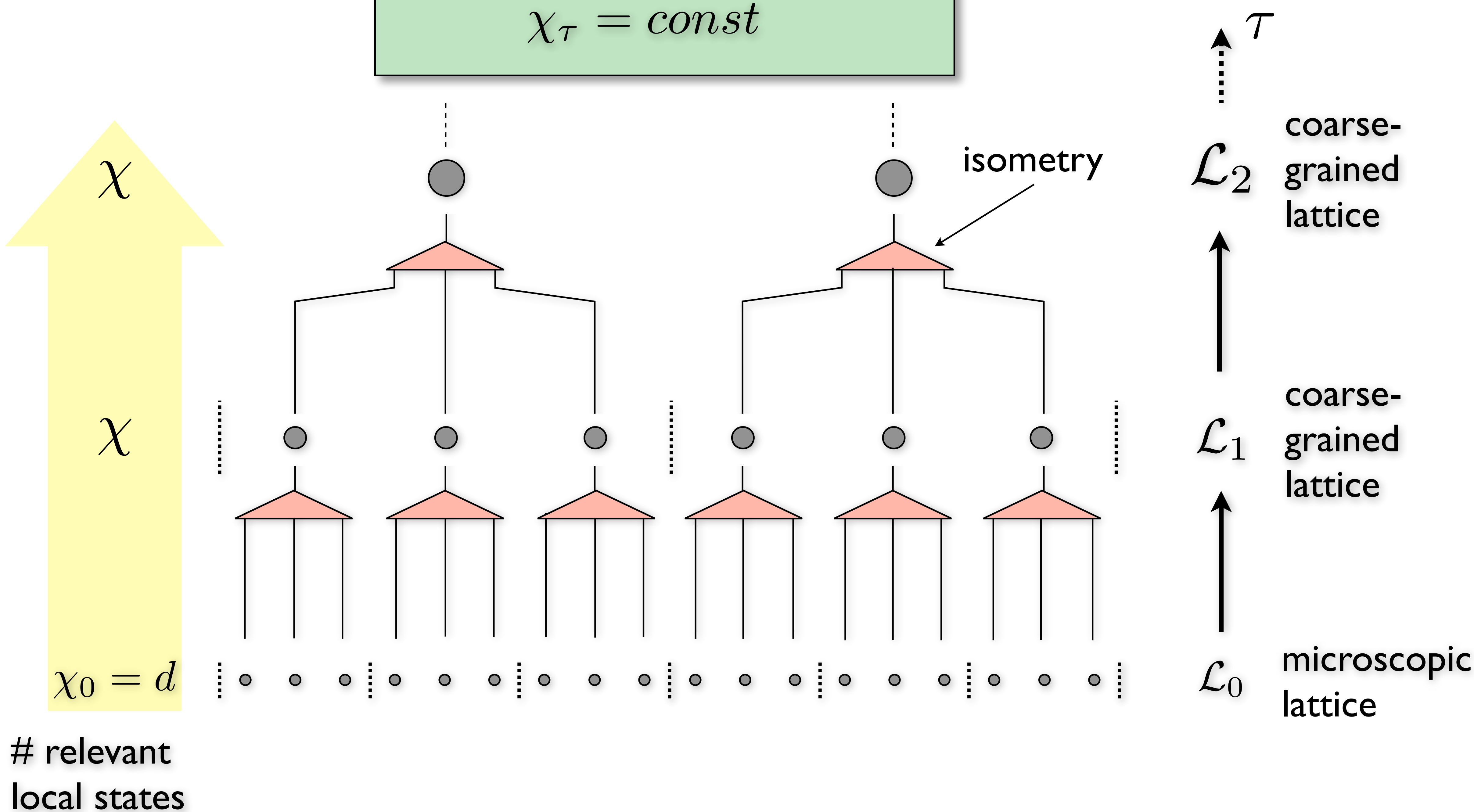


Tree Tensor Network (1D)

1D systems (non-critical)

$$S(L) = const$$

$$\chi_\tau = const$$

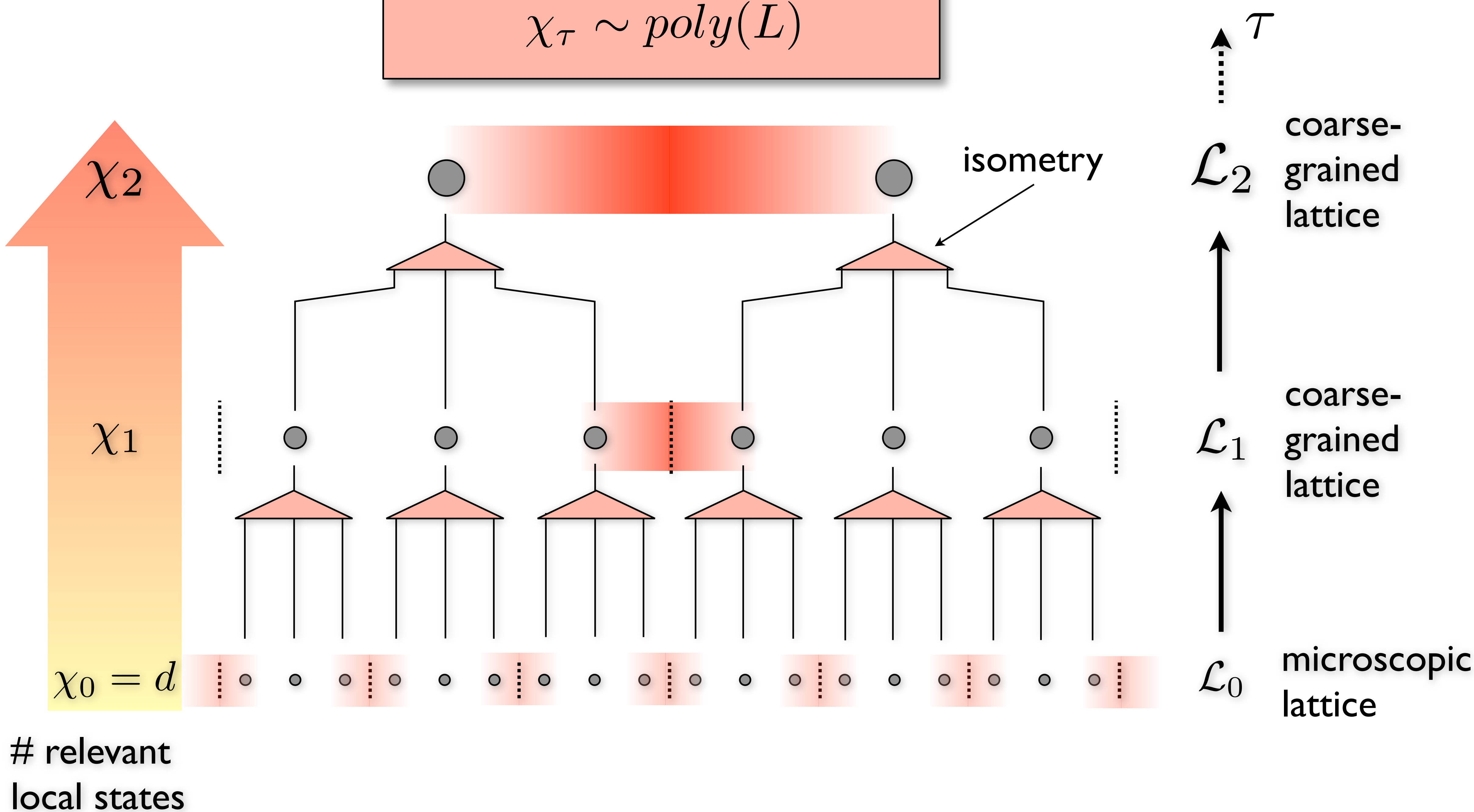


Tree Tensor Network (1D)

1D critical systems

$$S(L) \sim log(L)$$

$$\chi_\tau \sim poly(L)$$



The MERA (The multi-scale entanglement renormalization ansatz)

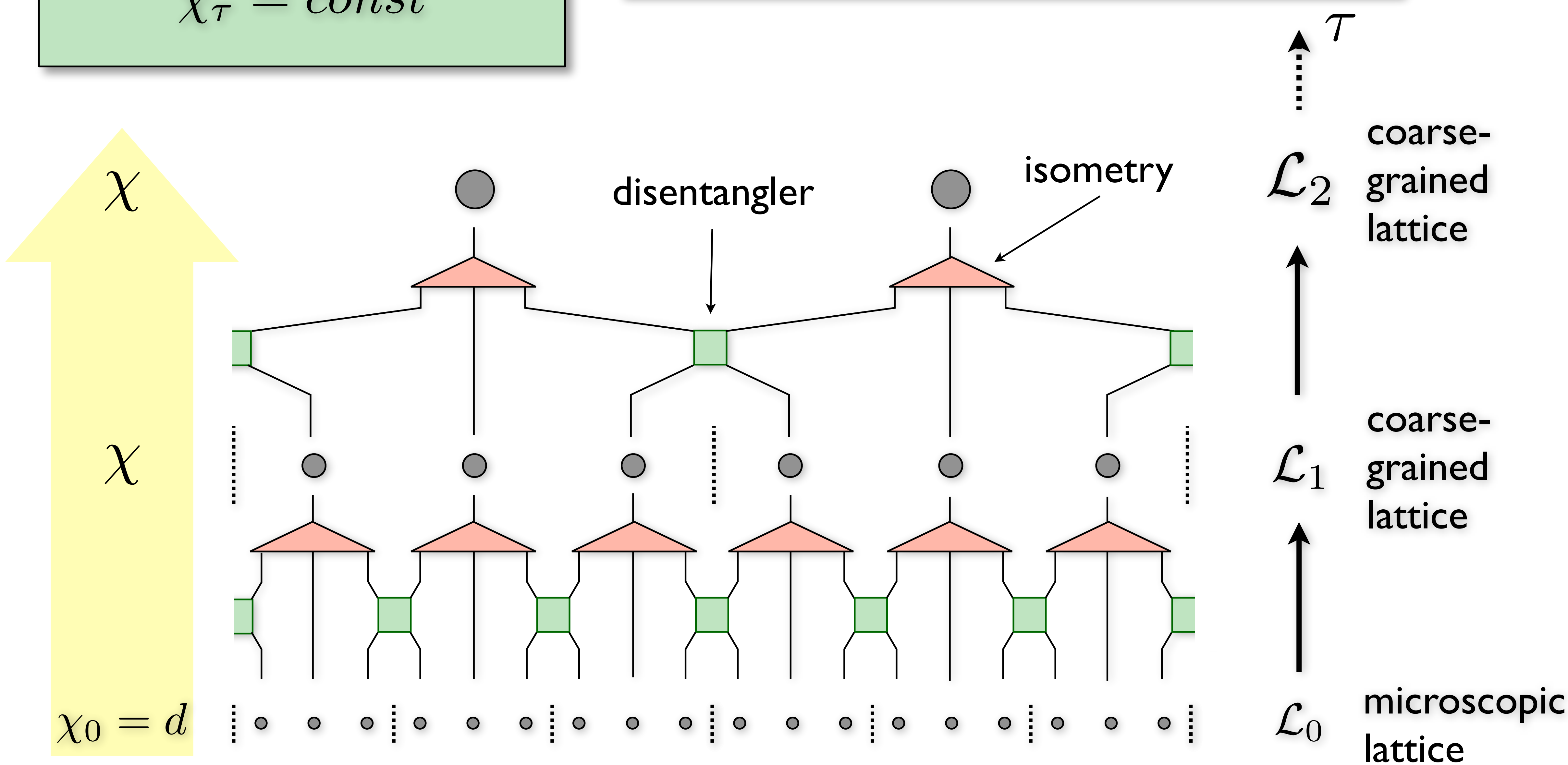
G. Vidal, PRL 99, 220405 (2007)
G. Vidal, PRL 101, 110501 (2008)

1D systems (critical)

$S(L) \sim log(L)$

$\chi_\tau = const$

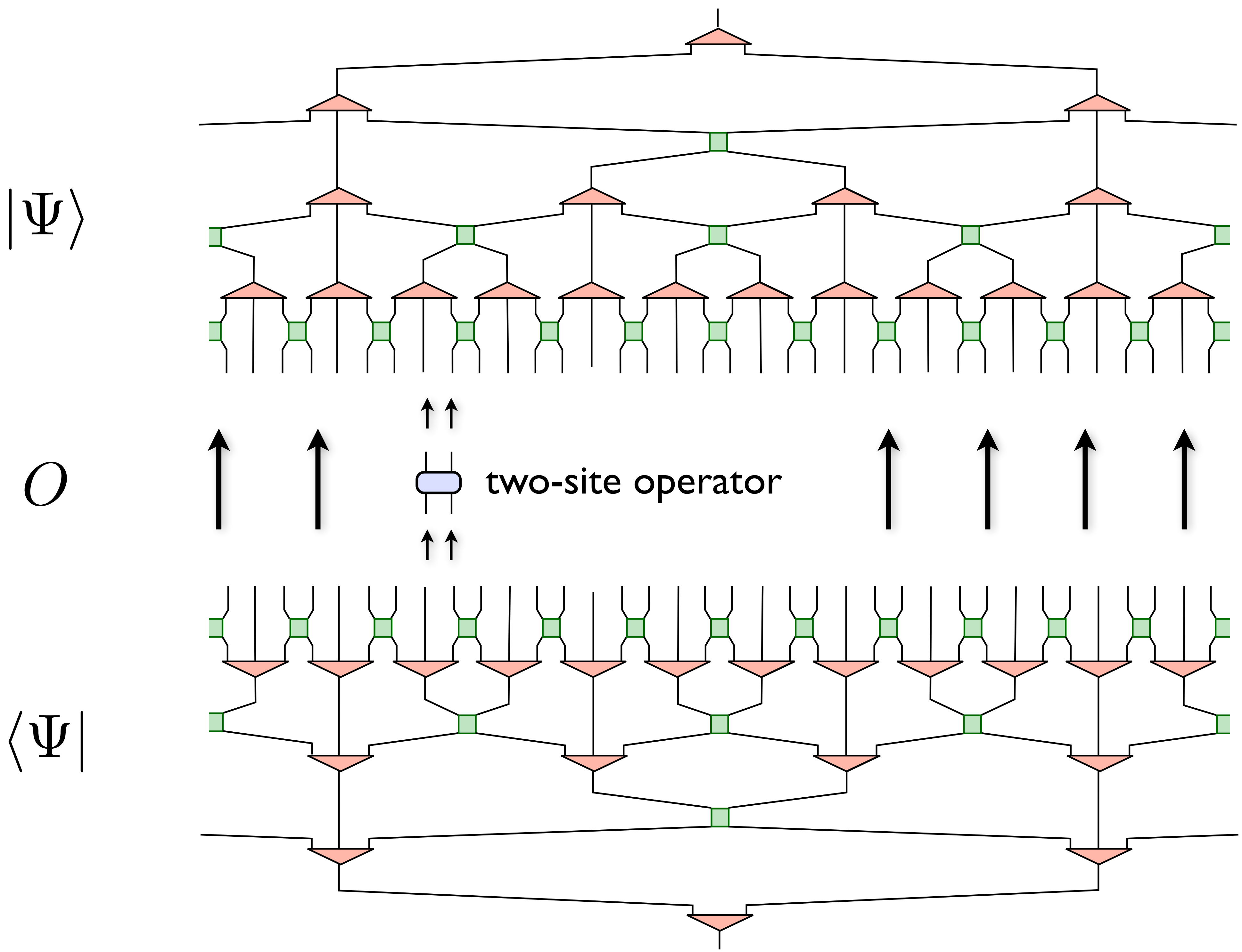
KEY: disentanglers reduce the amount of short-range entanglement



relevant local states

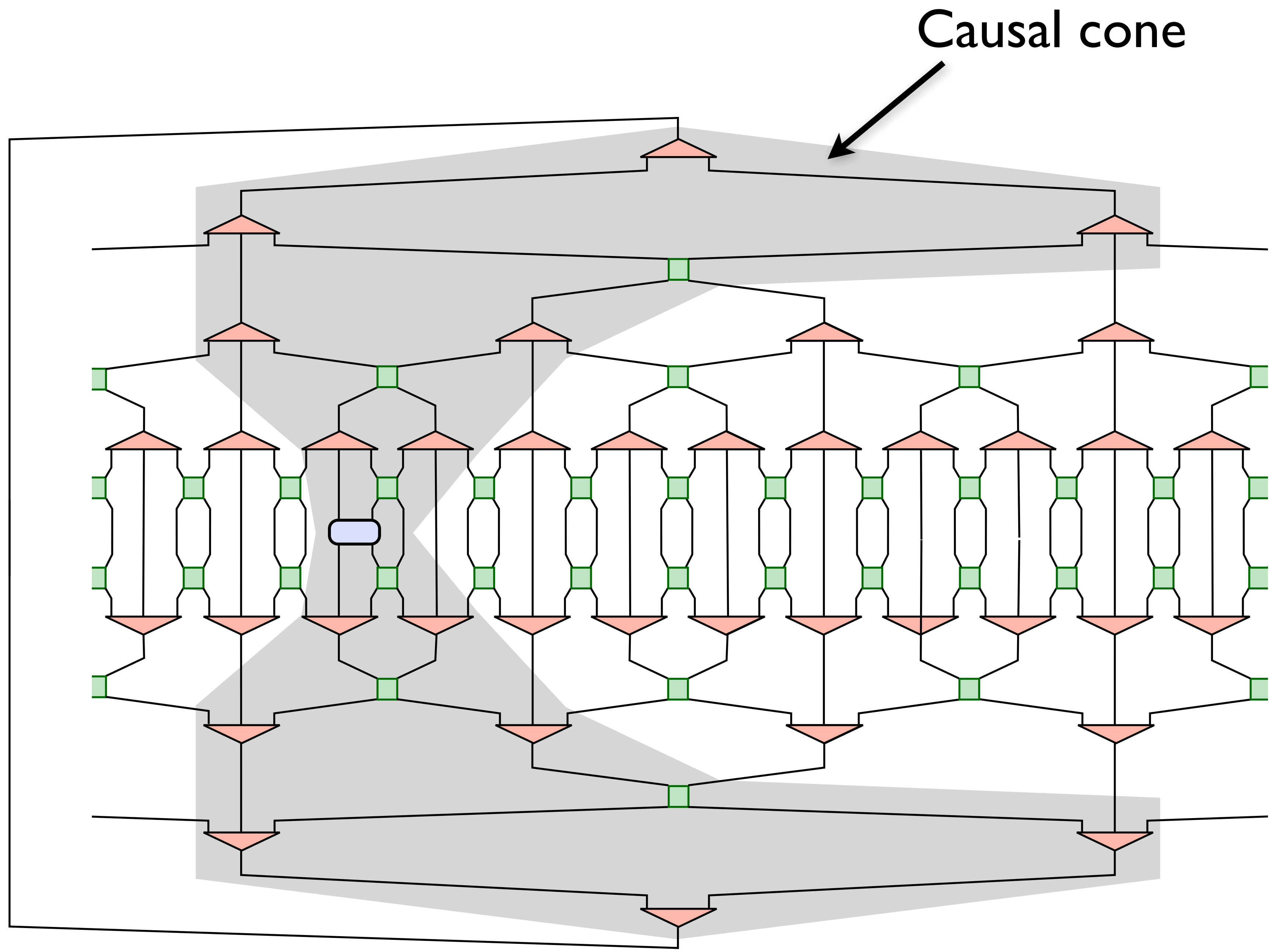
MERA: Properties

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

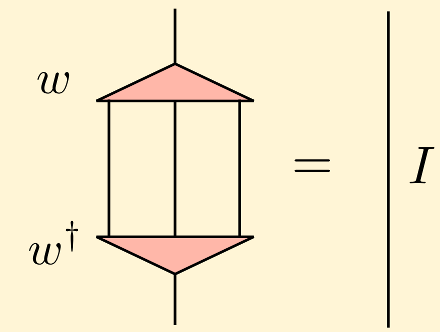


MERA: Properties

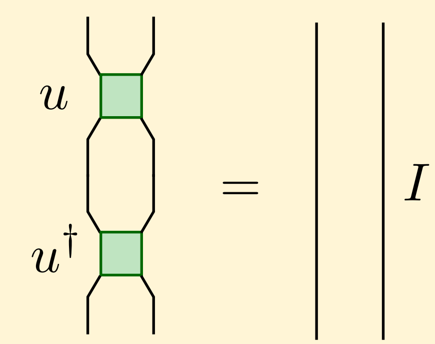
$\langle \Psi | O | \Psi \rangle$



Isometries are *isometric*

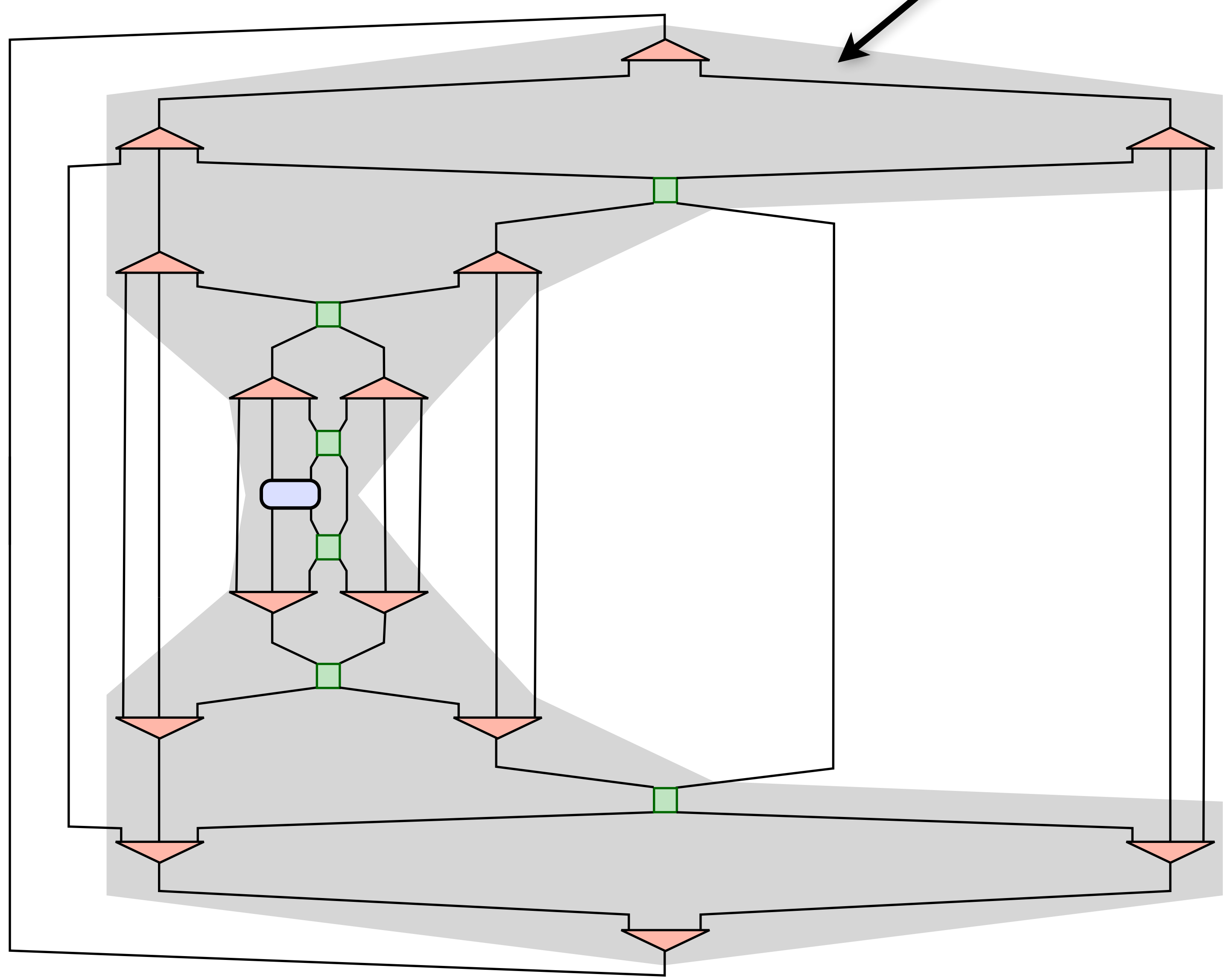


Disentanglers are *unitary*



MERA: Properties

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



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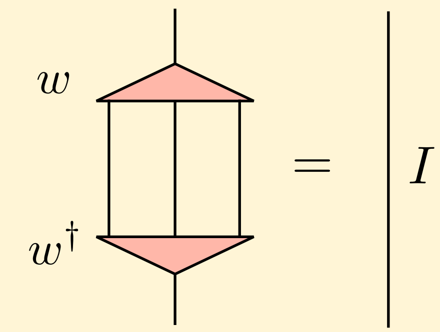
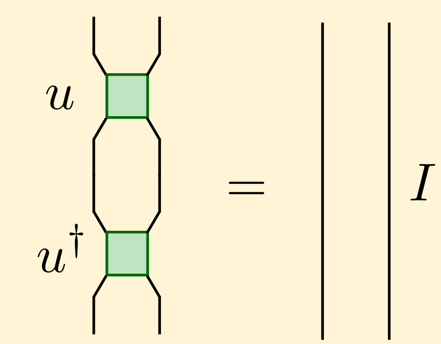


Disentanglers are *unitary*

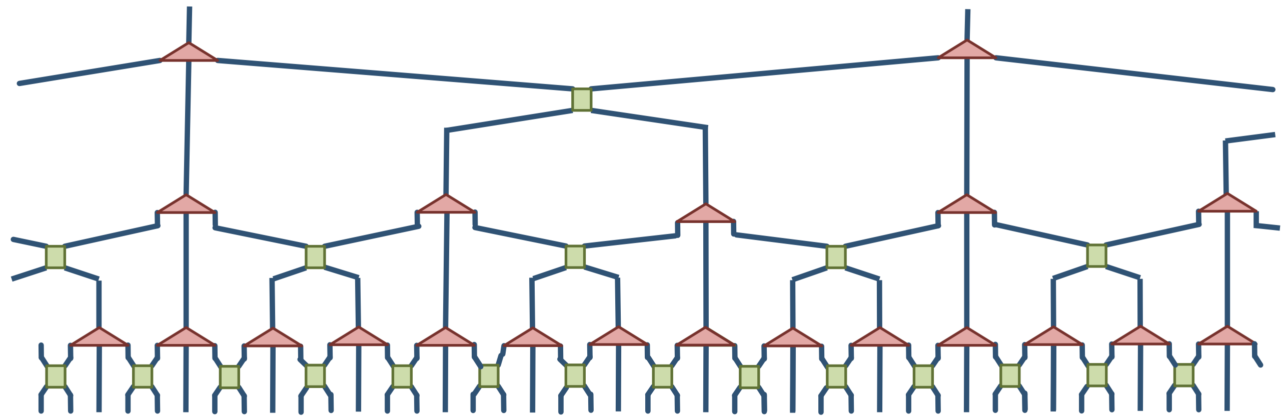


Efficient computation of expectation values of observables!

Different types of MERA's

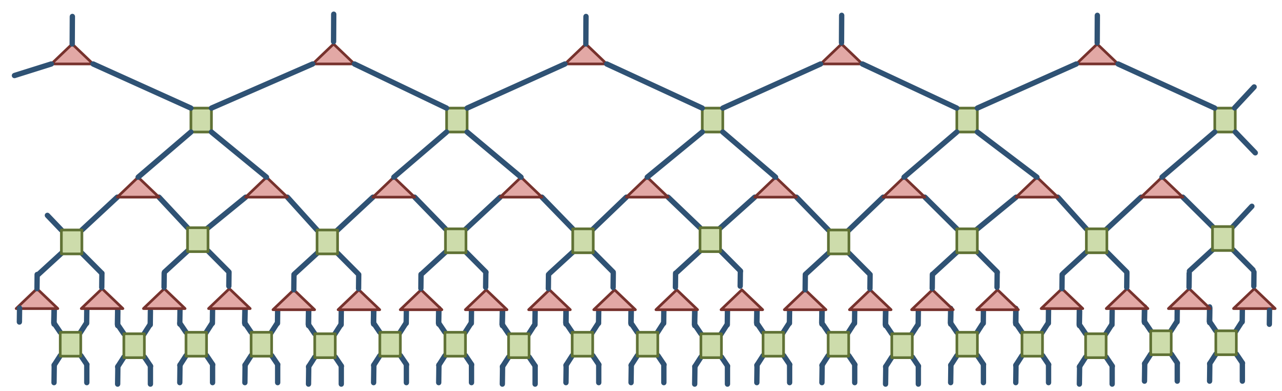
Figures by G. Evenbly

Ternary MERA:
3-to-1 blocking



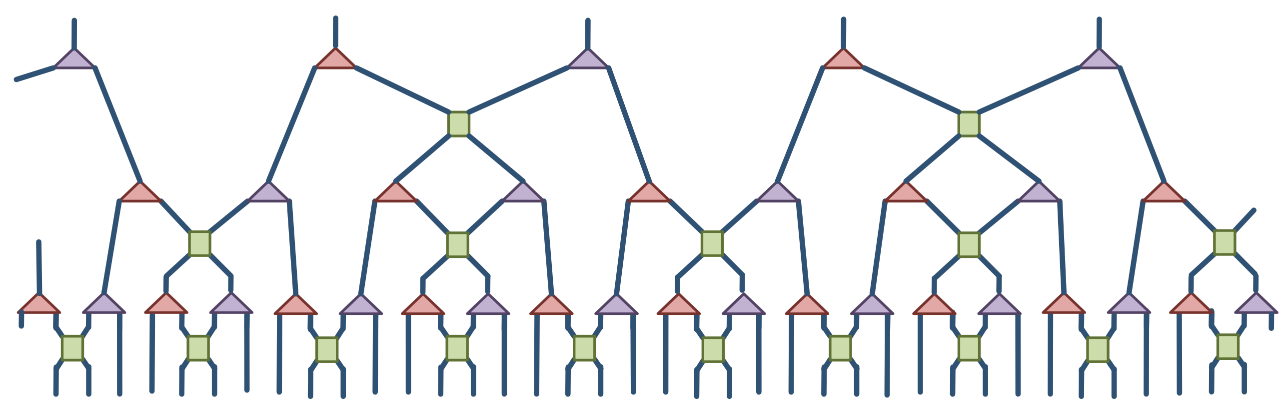
$O(\chi^8)$

Binary MERA:
2-to-1 blocking



$O(\chi^9)$

Modified
binary MERA:
2-to-1 blocking



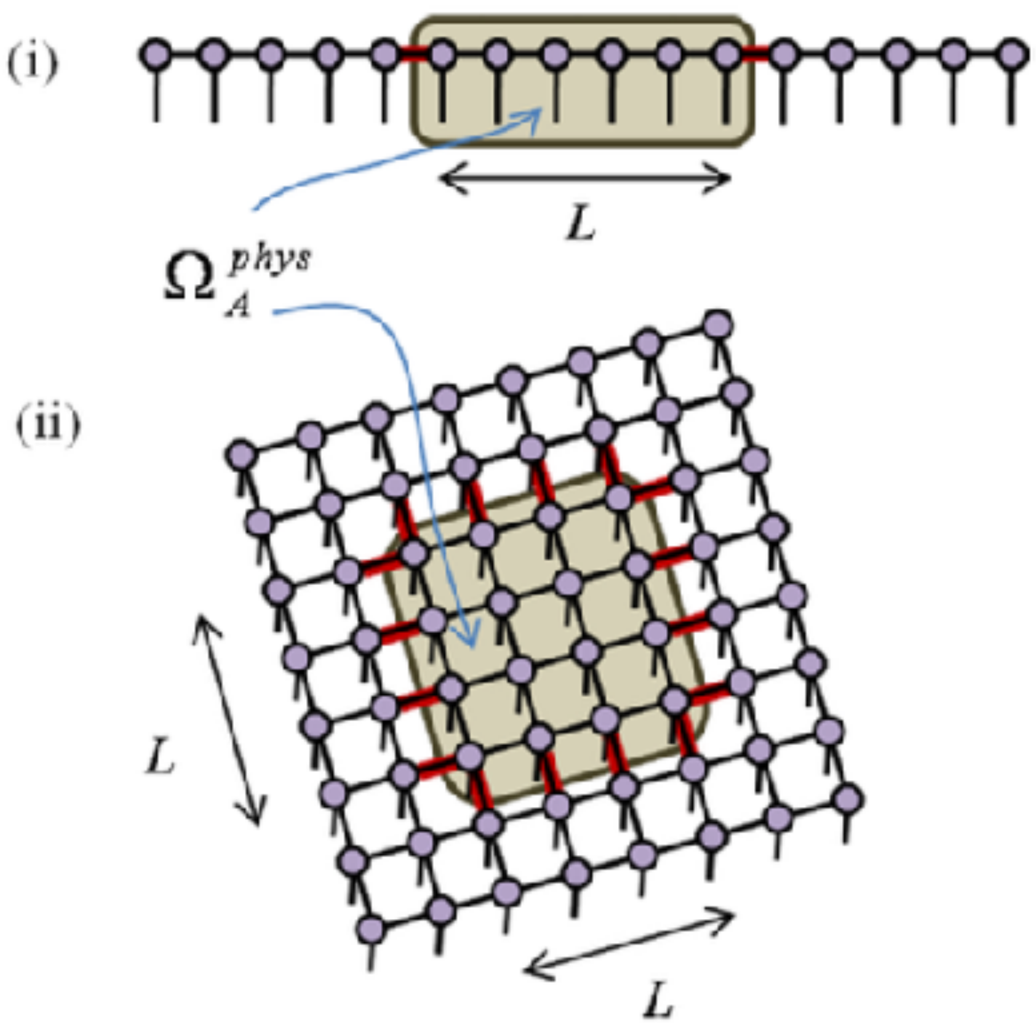
$O(\chi^7)$

TRADEOFF: computational cost vs efficiency of coarse-graining

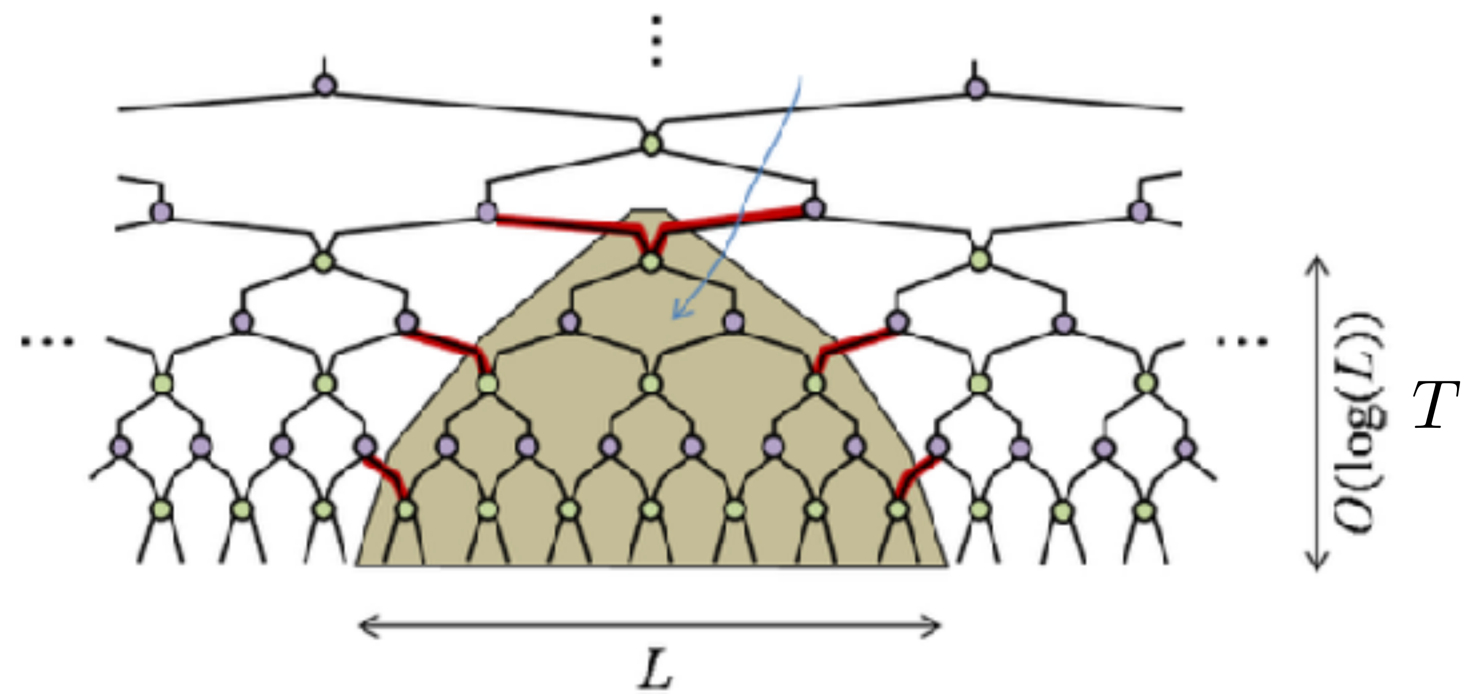
MERA: Entanglement entropy

$$S(A) \leq n(A)\,\log(\chi)$$

$$n(A) = 2 \rightarrow S(A) \sim const$$



$$n(A) = 4L \rightarrow S(A) \sim L$$



$$n(A) \approx 2T \approx 2\log_2 L$$

$$S(A) \sim log(L)$$

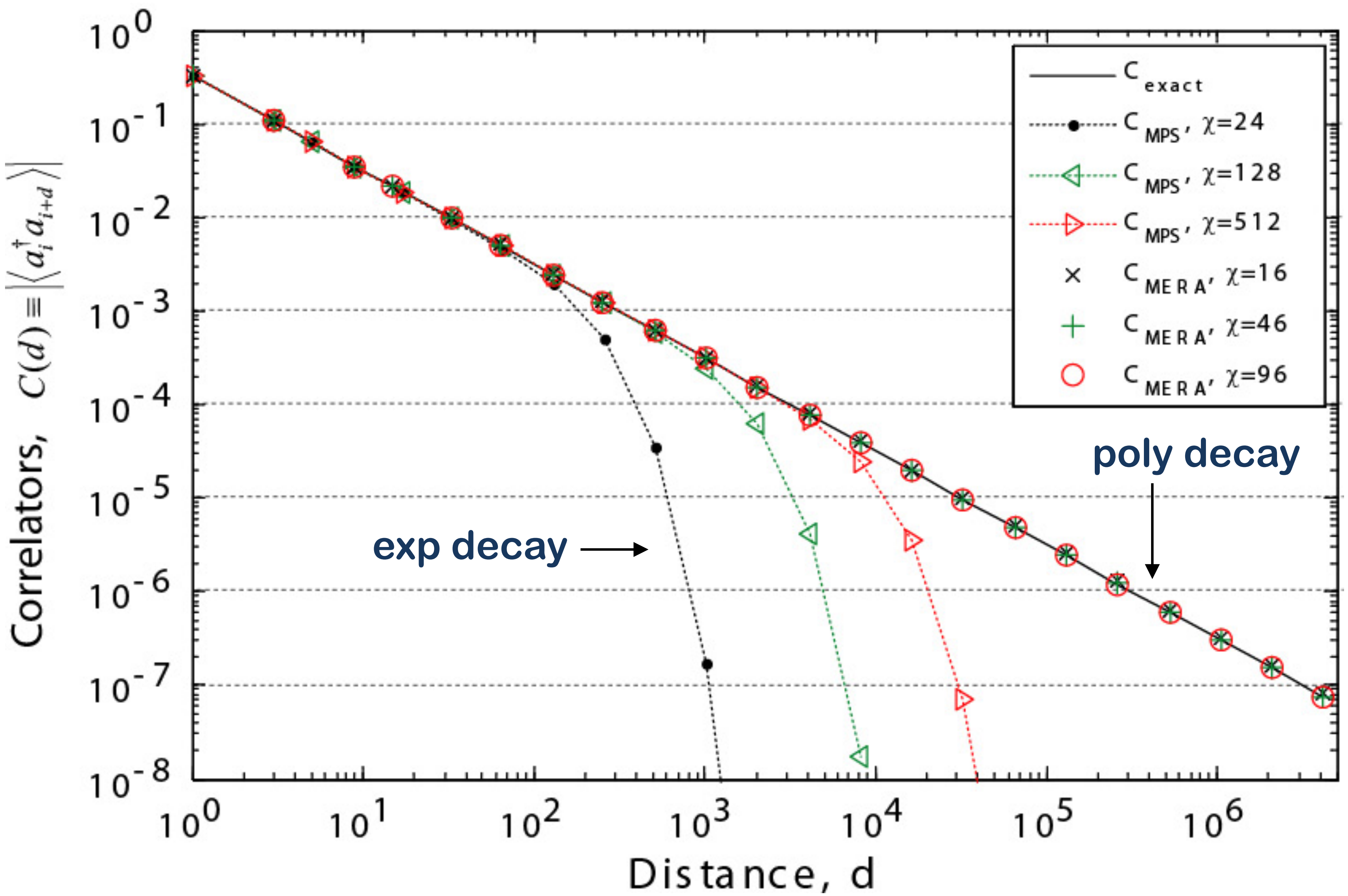
Reproduces log(L) scaling of 1D critical systems

figures from Evenbly & Vidal, J Stat Phys **145** (2011)

Power-law decaying correlations

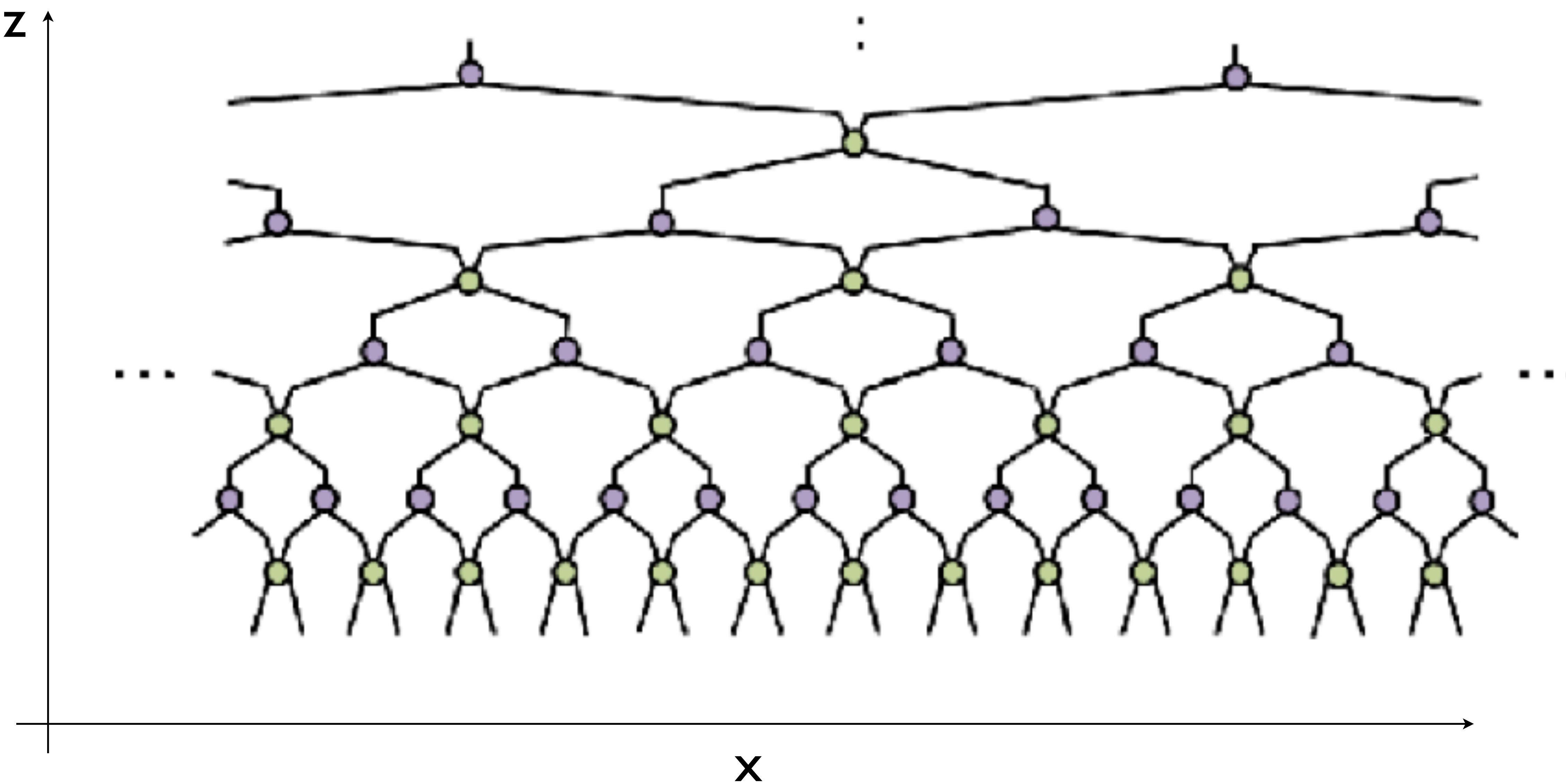
-how accurately do MPS and MERA approximate ground states in terms of correlators?

quantum XX model: (critical, c=1) $$H_{XX} = \sum_r \left(\sigma_r^X \sigma_{r+1}^X + \sigma_r^Y \sigma_{r+1}^Y \right)$$



slide from Glen Evenbly

Scale invariant MERA



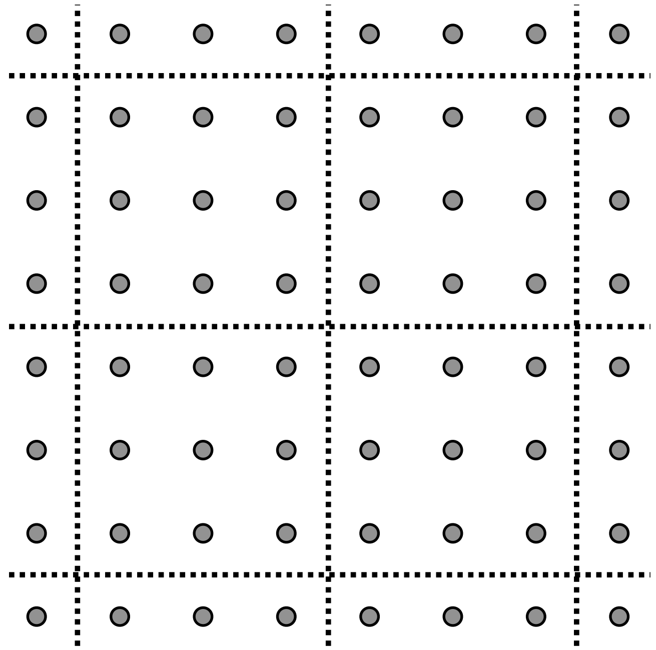
Translational invariance: *same tensors along x*

Scale invariance (at criticality): *same tensors along z*

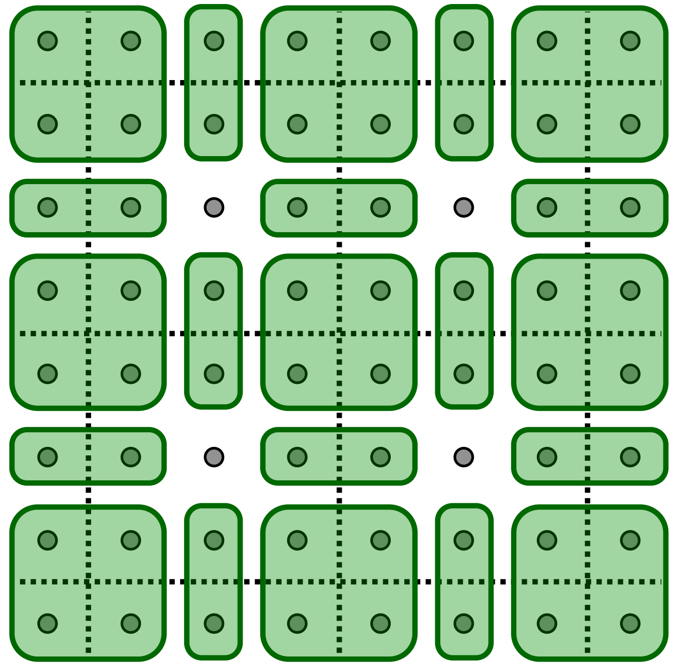
2D MERA (top view)

Evenbly, Vidal. PRL 102, 180406 (2009)

Original lattice



Apply disentanglers

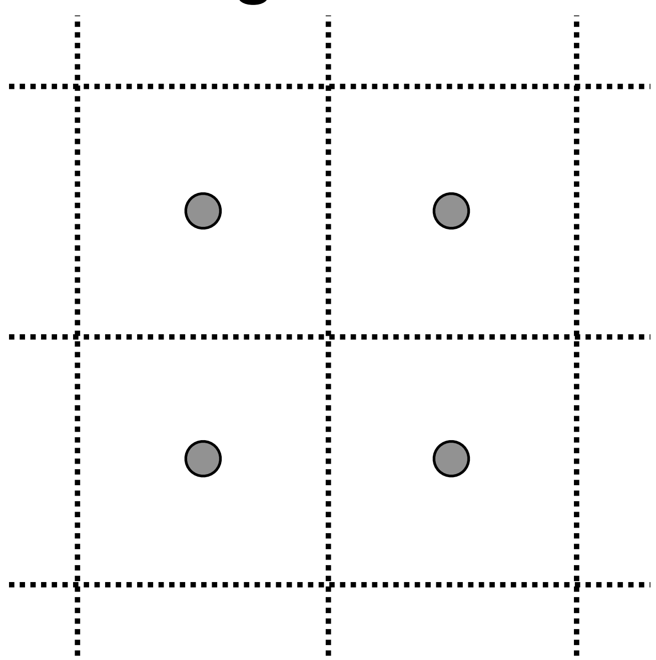


✓ Accounts for area-law in 2D systems

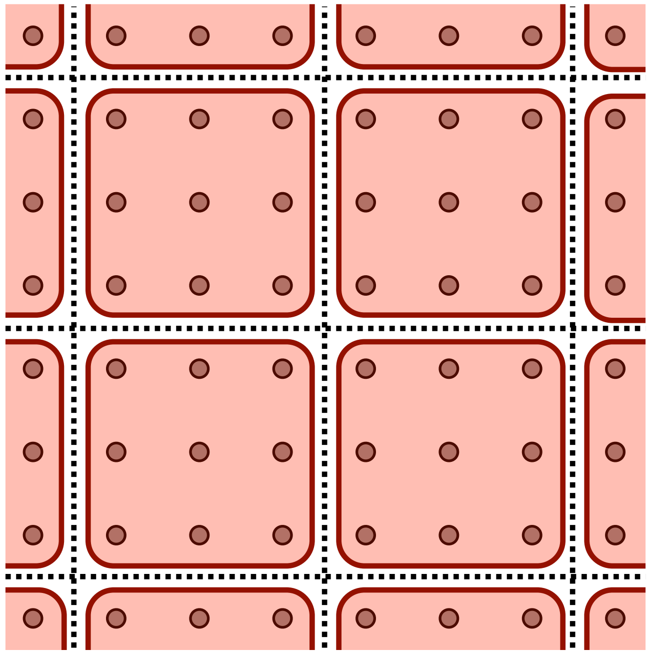
$$S(L) \sim L$$

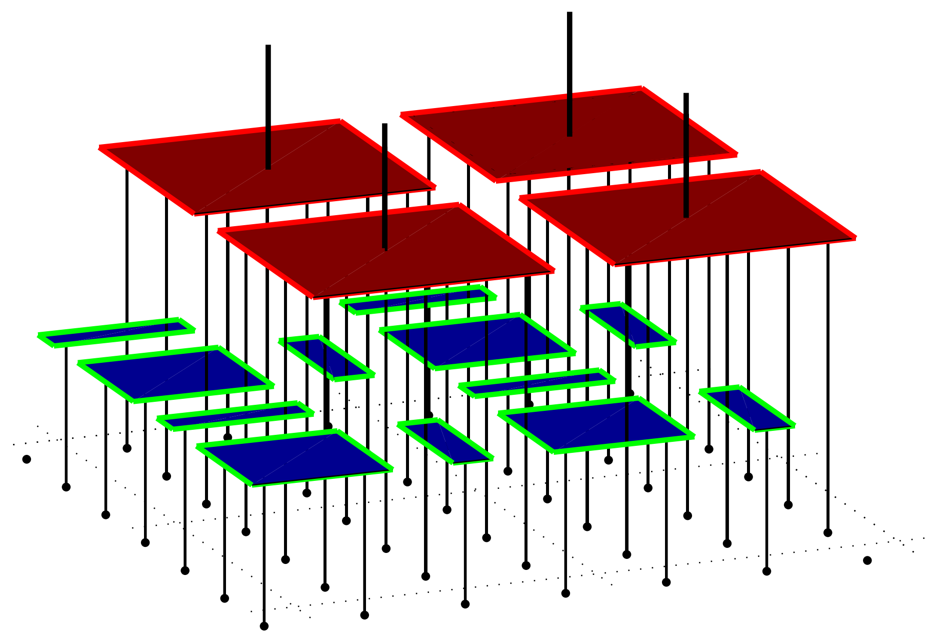
$$\chi_\tau = const$$

Coarse-grained lattice

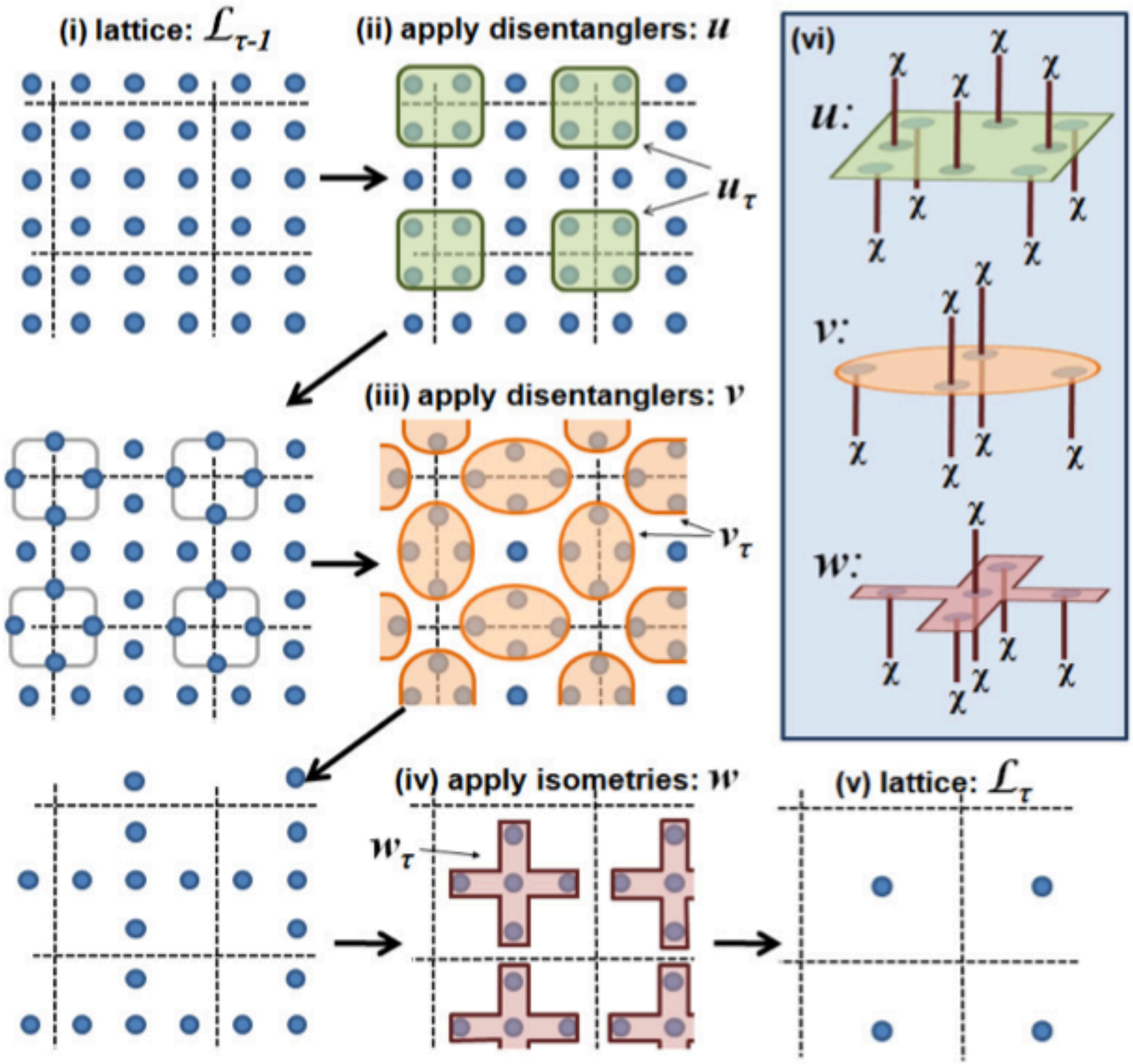


Apply isometries



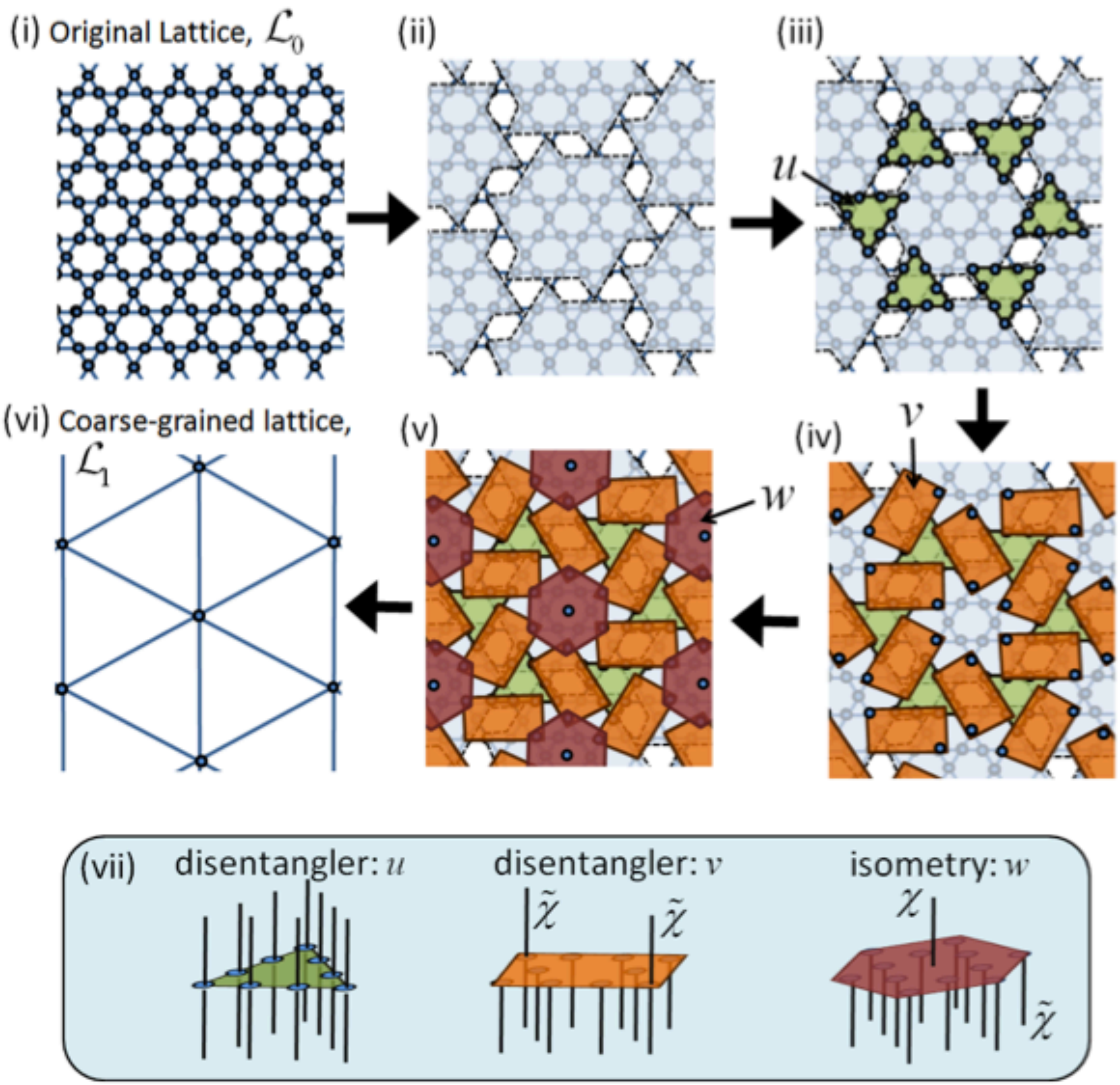


Different structures of the 2D MERA...



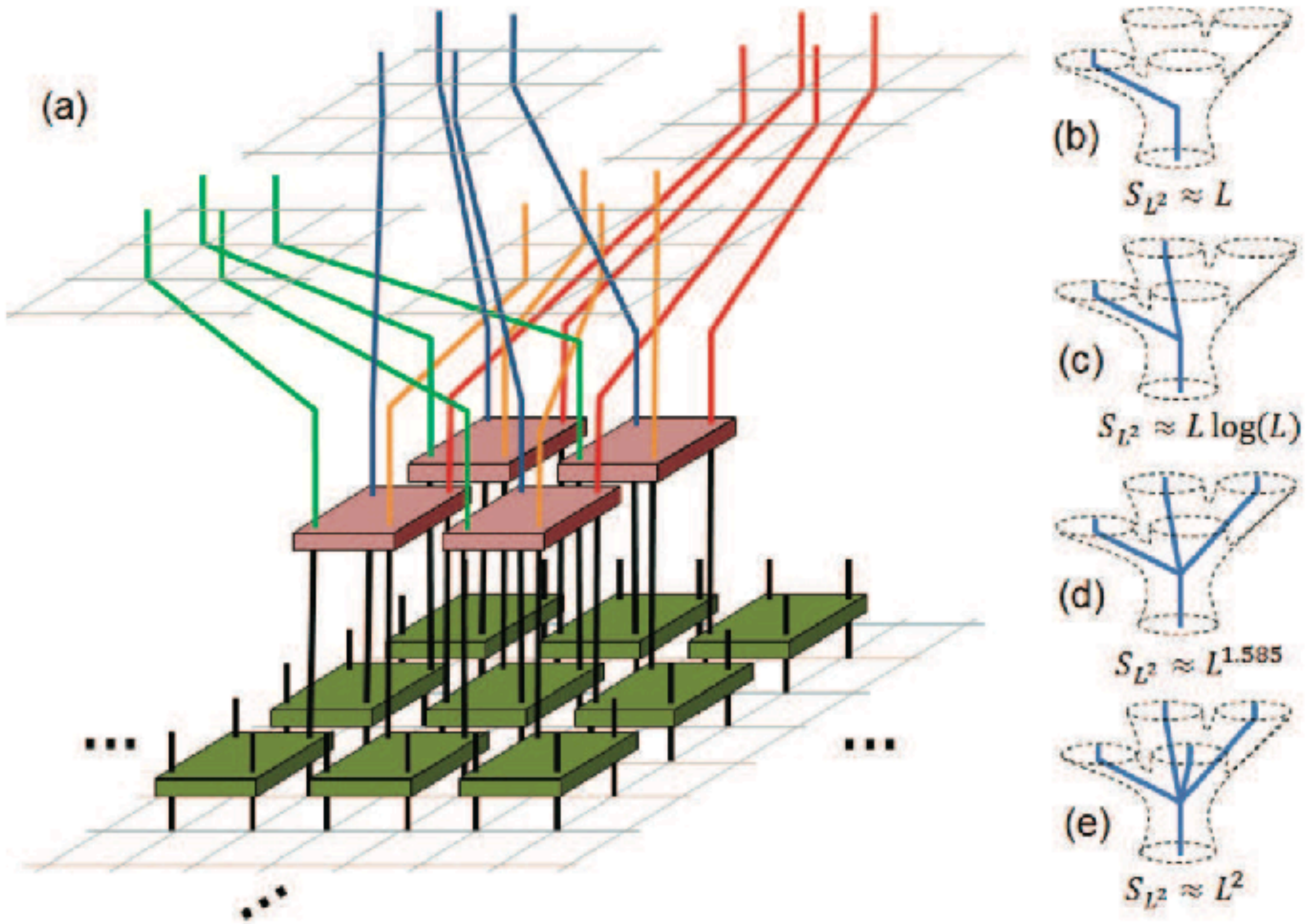
Evenbly & Vidal, PRL **102**, 180406 (2009)

2D MERA on the Kagome lattice



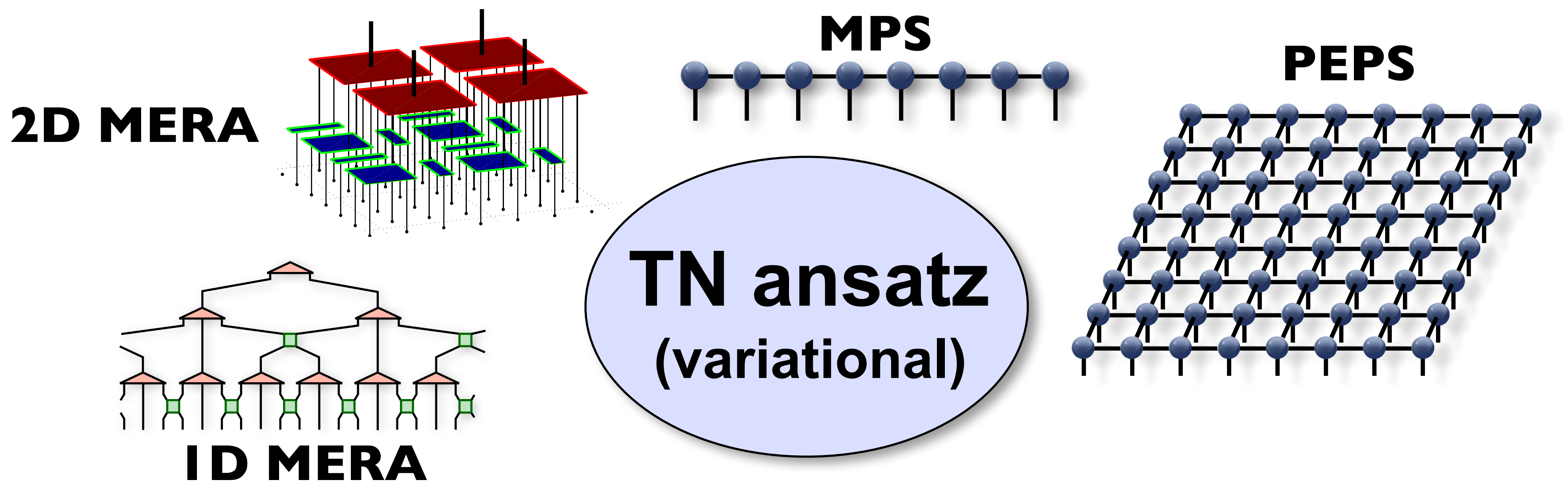
Evenbly & Vidal, PRL 104, 187203 (2010)

Branching MERA: beyond area law scaling in 2D



G. Evenbly and G. Vidal, Physical Review Letters **112**, (2014).

PART I summary: Tensor network ansätze

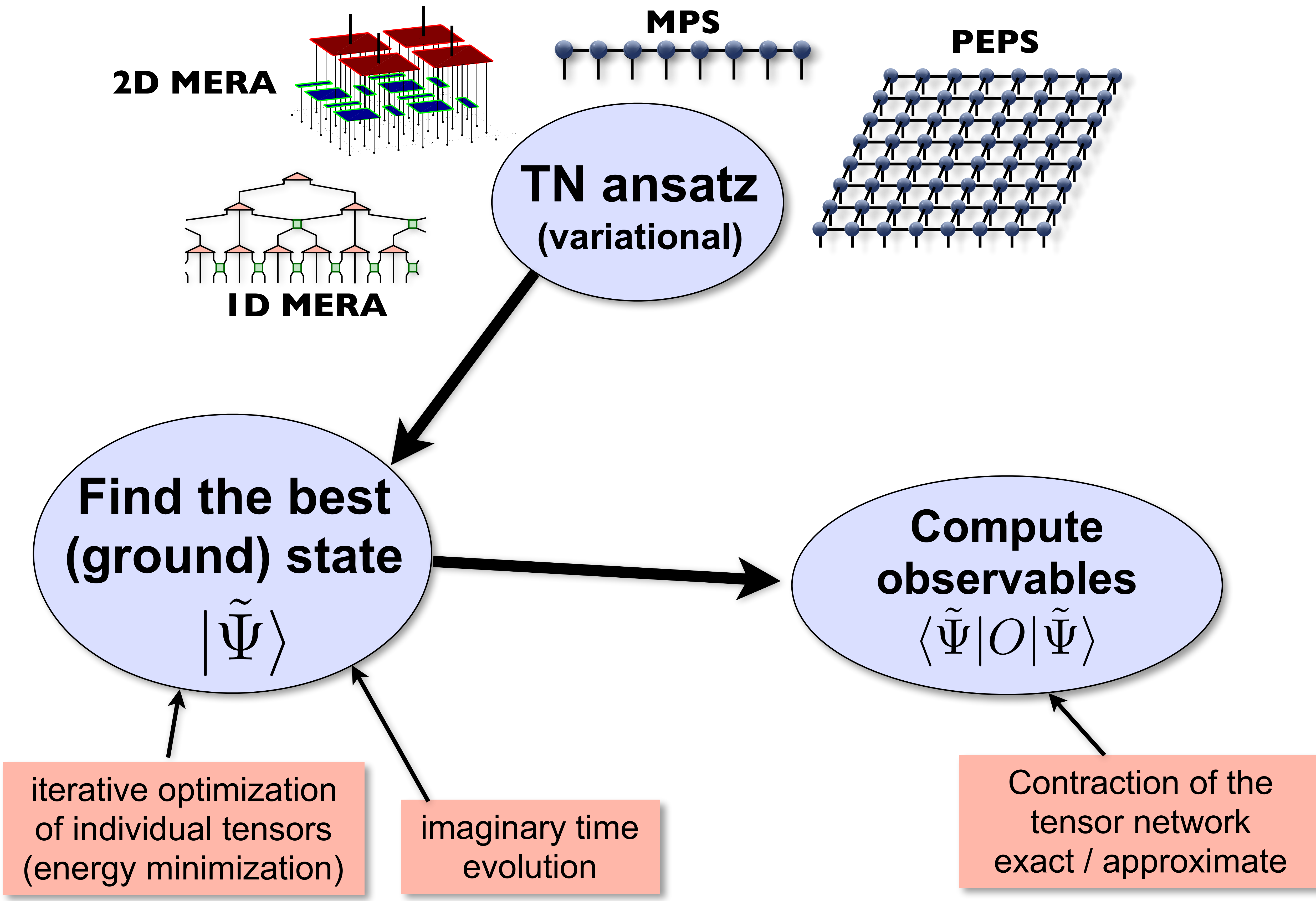


➡ A tensor network ansatz is an efficient variational ansatz for ground states of local H where the accuracy can be systematically controlled with the bond dimension

➡ Different tensor networks can reproduce different entanglement entropy scaling:

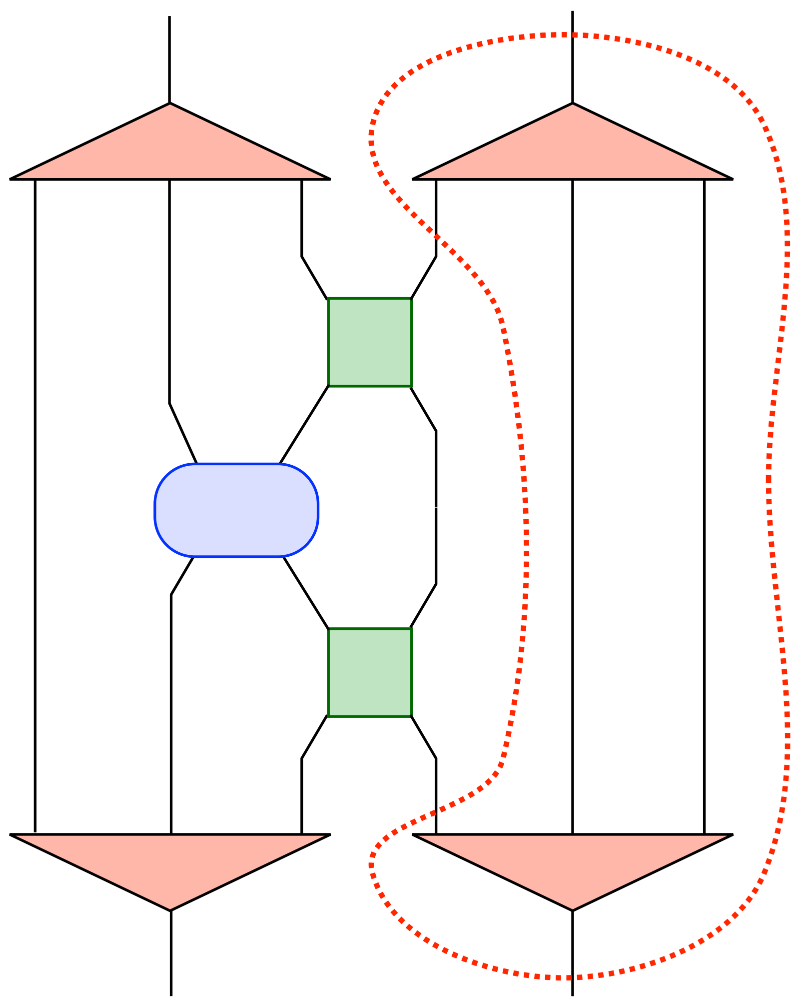
- ★ MPS: area law in 1D
- ★ MERA: log L scaling in 1D (critical systems)
- ★ PEPS/iPEPS: area law in 2D
- ★ 2D MERA: area law in 2D
- ★ branching MERA: beyond area law in 2D (e.g. L log L scaling) (Evenbly & Vidal, 2014)

Overview: Tensor network algorithms (ground state)

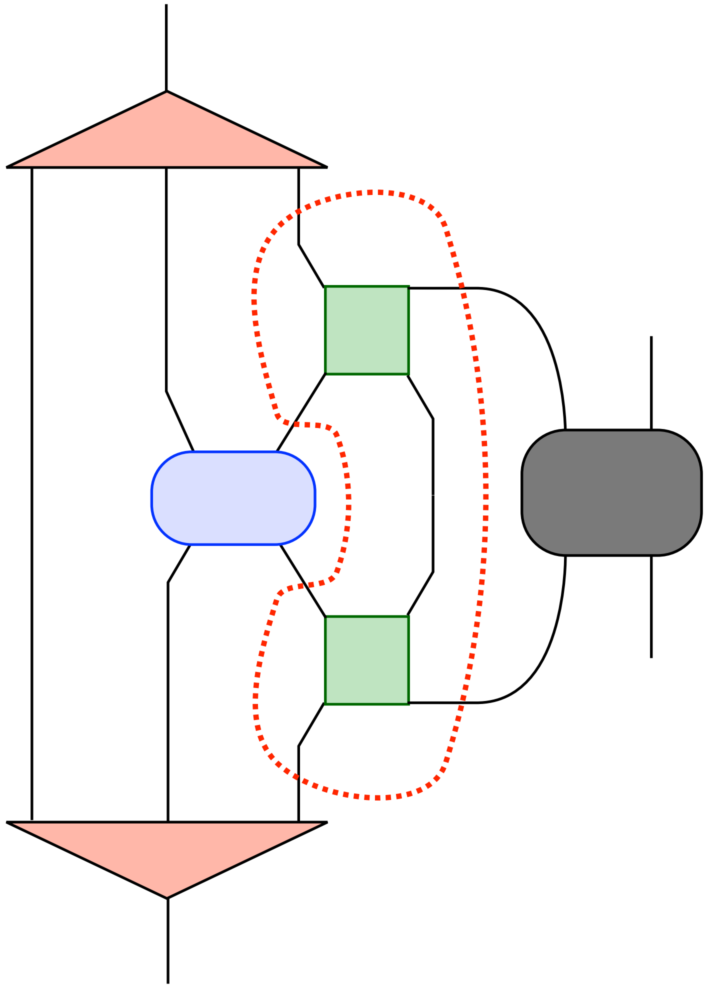


PART II: Contraction

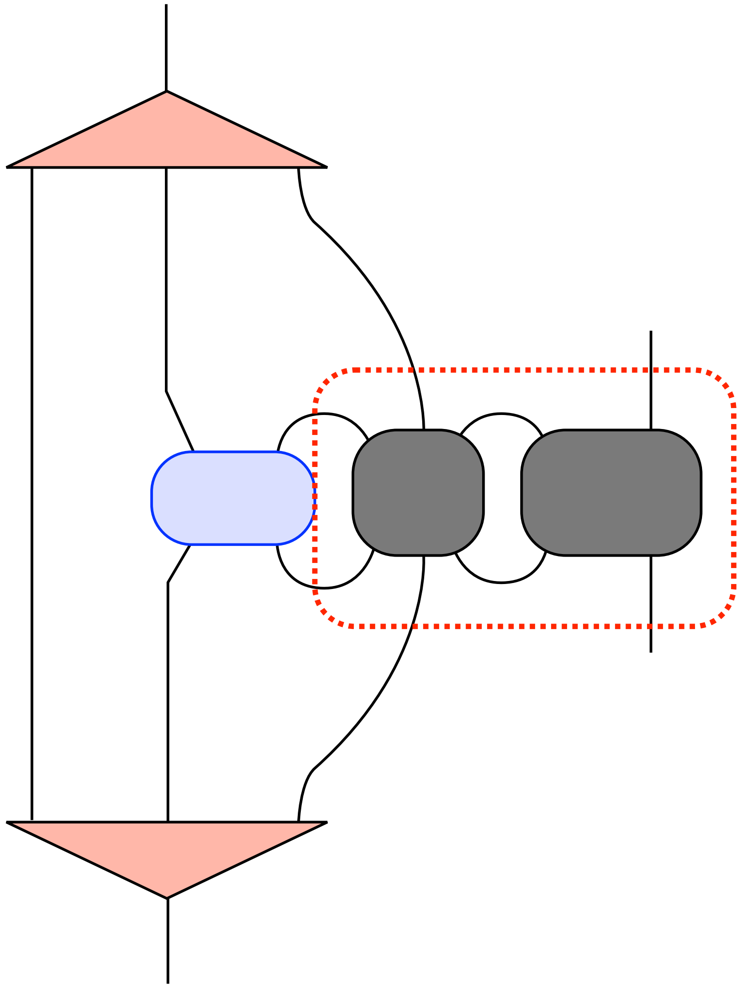
Contracting a tensor network (repetition)



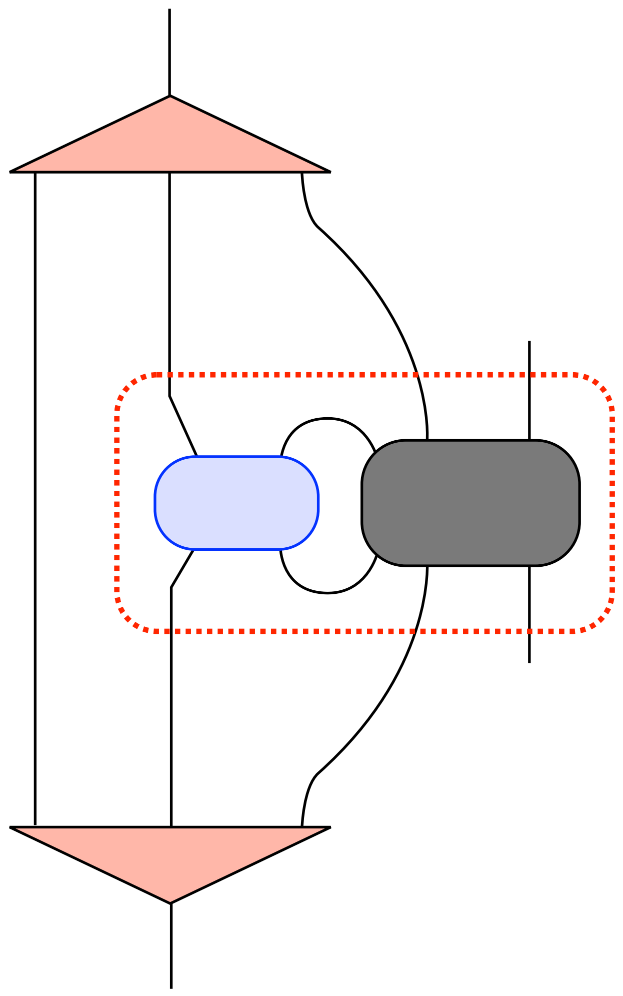
Pairwise contractions...



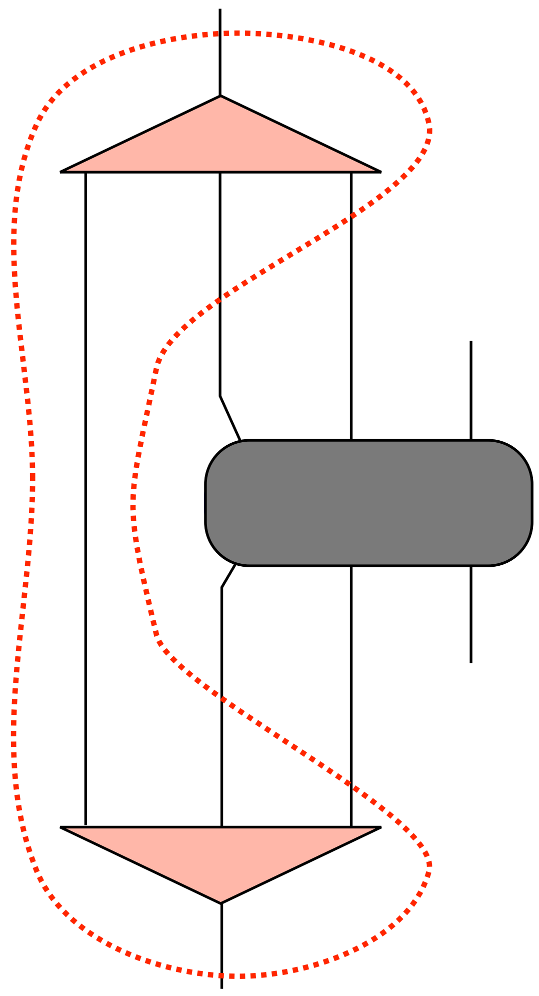
Pairwise contractions...



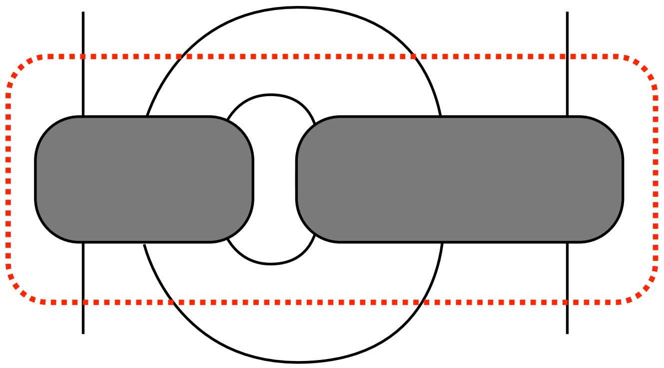
Pairwise contractions...



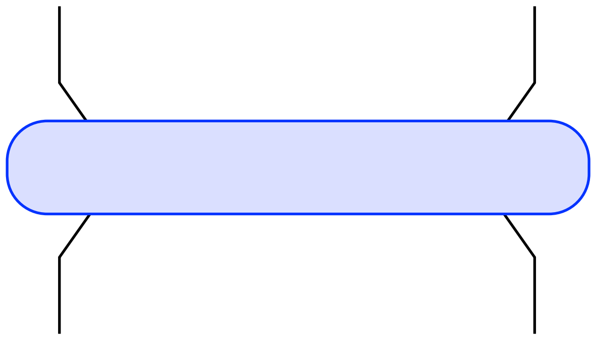
Pairwise contractions...



Pairwise contractions...



Pairwise contractions...

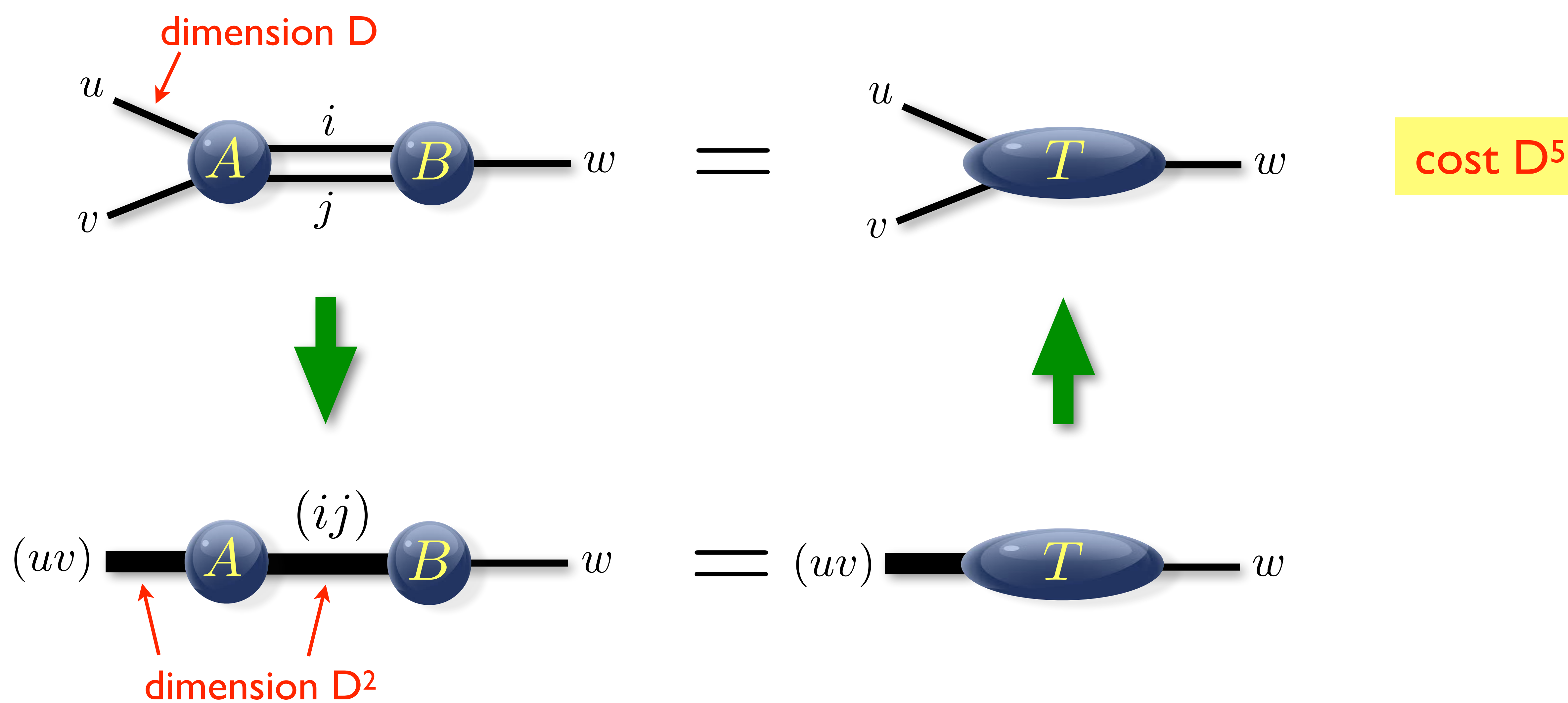


done!

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

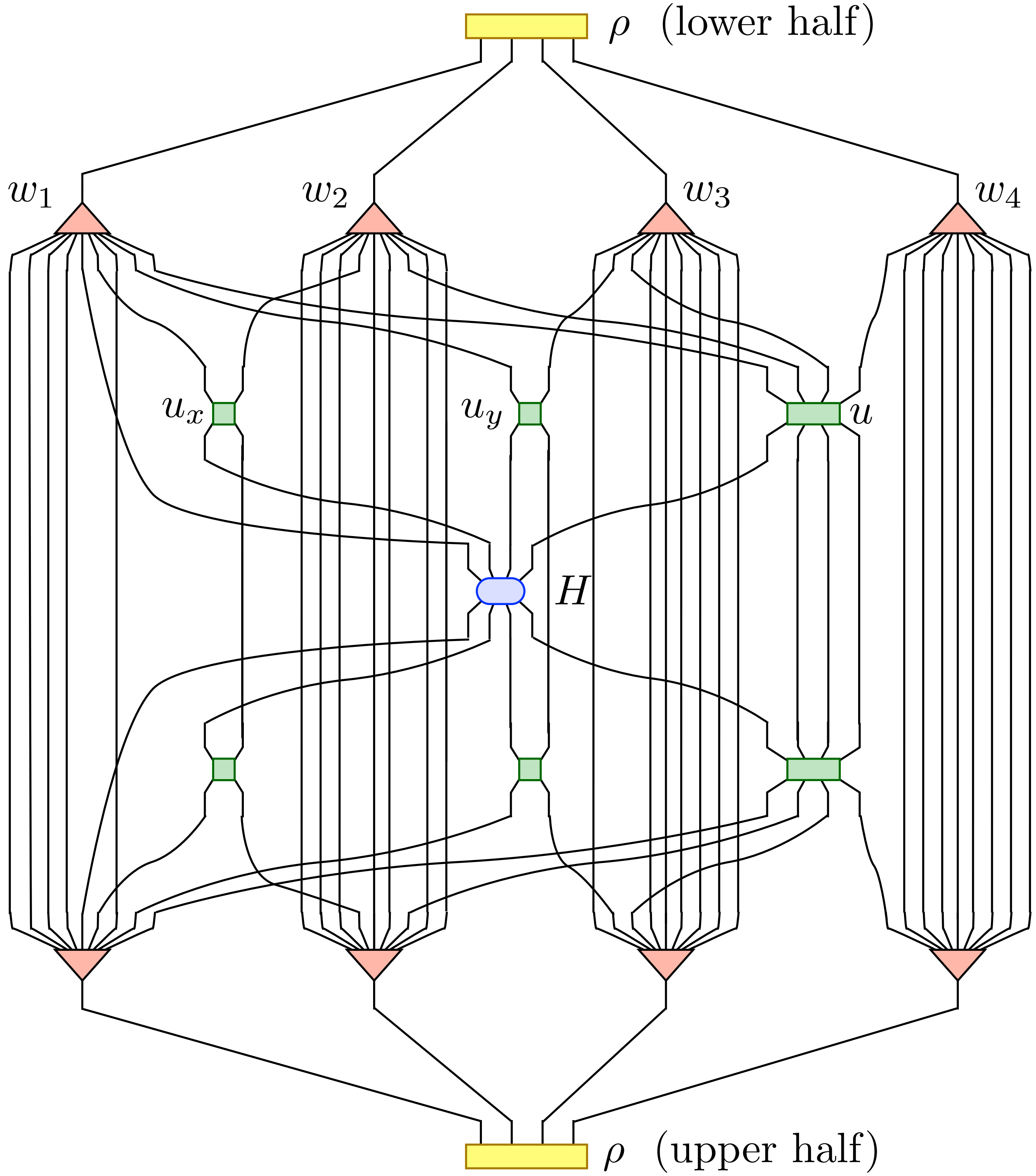
Contracting a tensor network

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



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

Contraction: Example from the 2D MERA



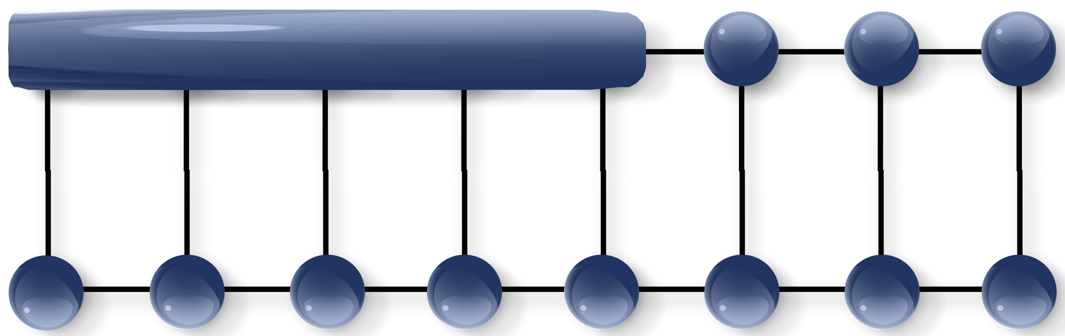
What is the optimal contraction order?

Use program to find optimal contraction, e.g. NETCON:

Pfeifer, Haegeman, Verstraete, PRE 90 (2014)

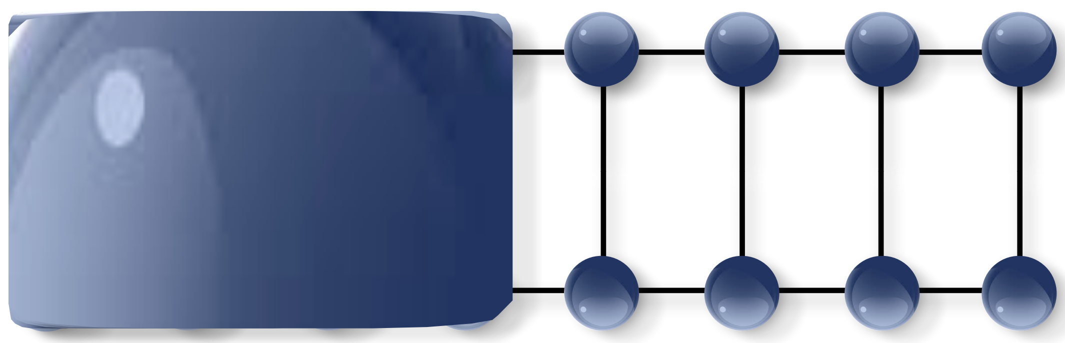
Contracting an MPS

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



BAD!

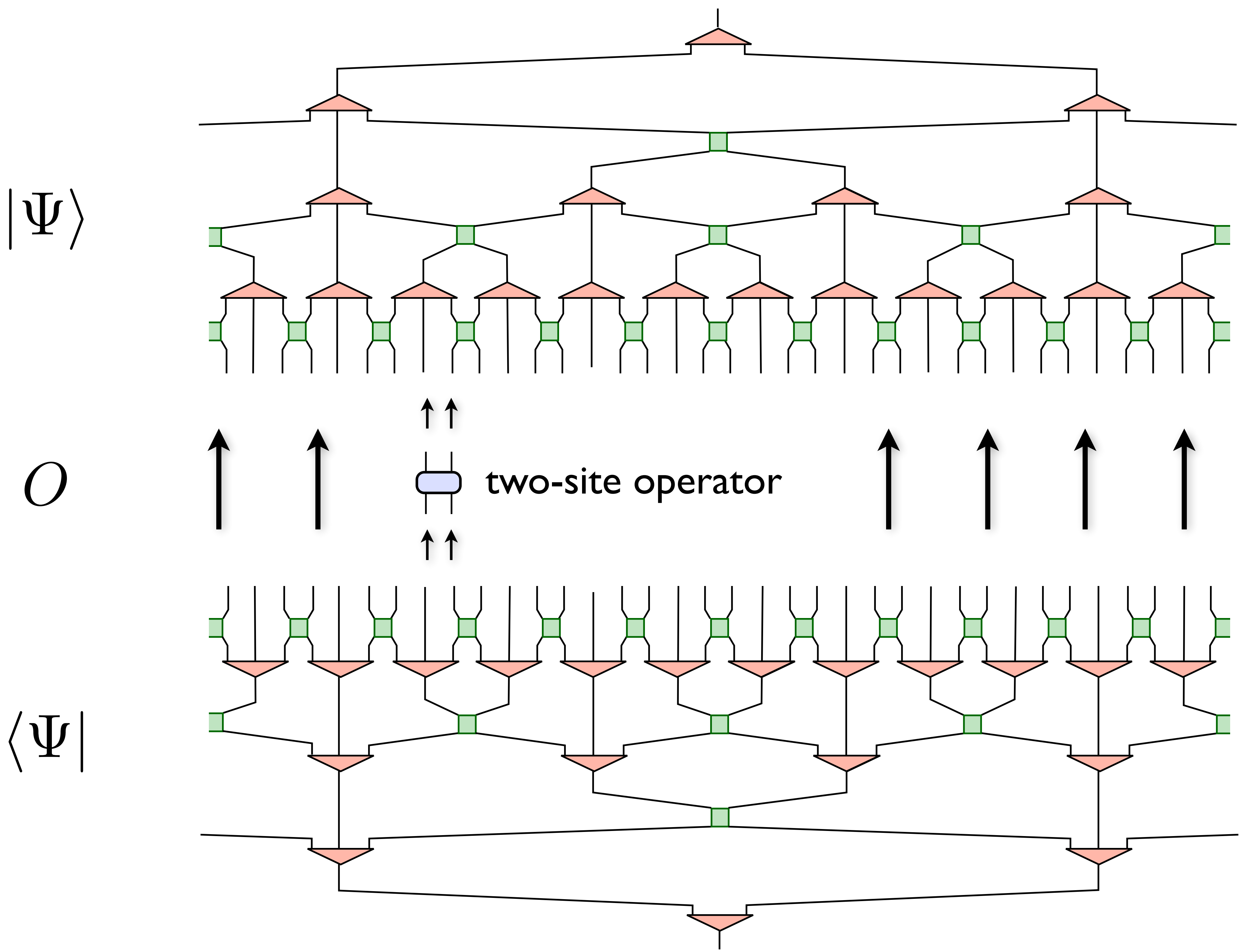
$\langle\Psi|\Psi\rangle =$



Good!

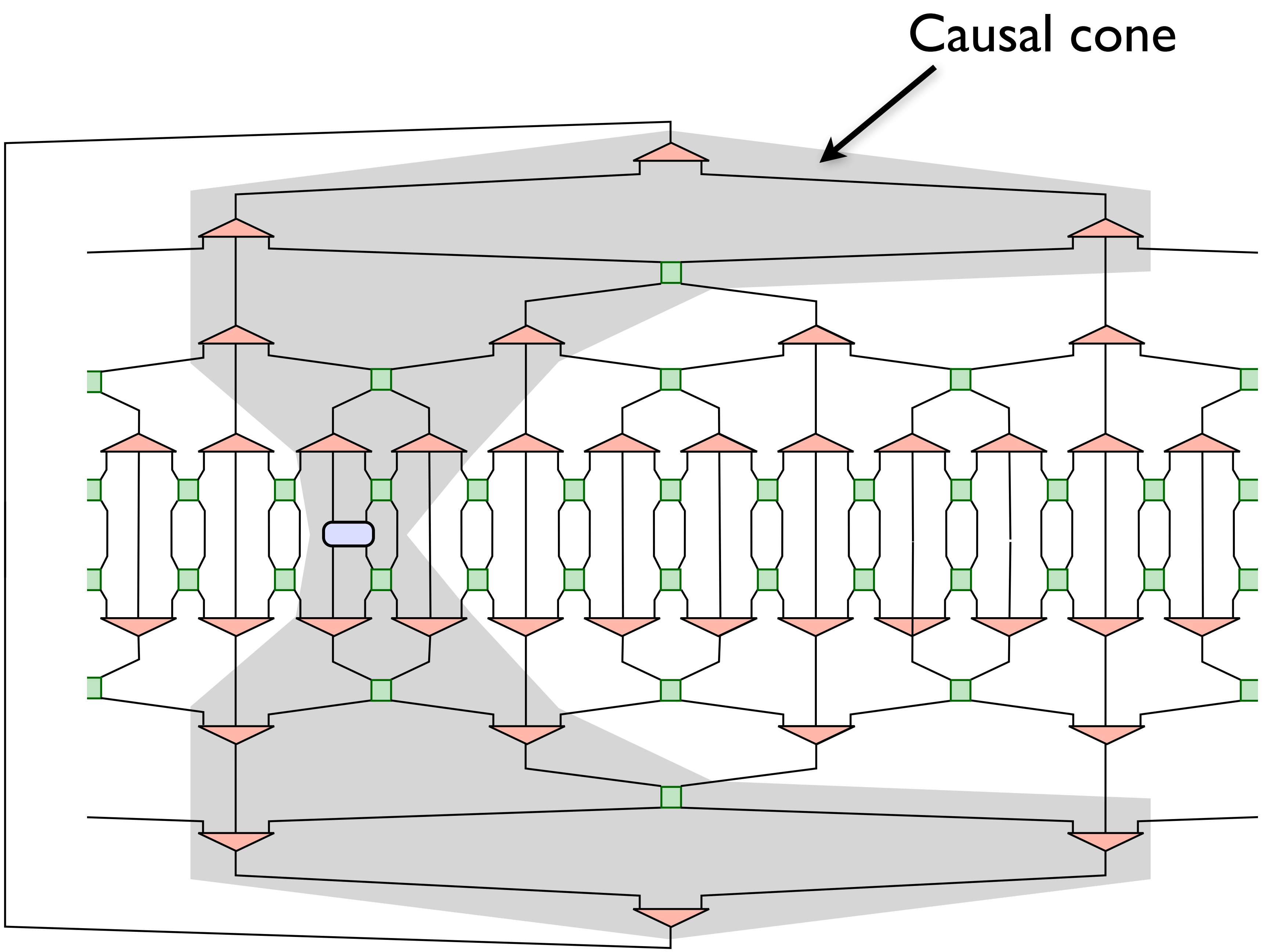
MERA: Contraction

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

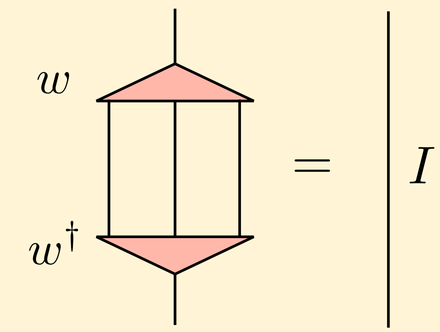


MERA: Contraction

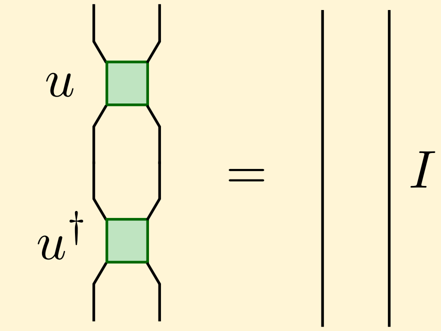
$\langle \Psi | O | \Psi \rangle$



Isometries are *isometric*

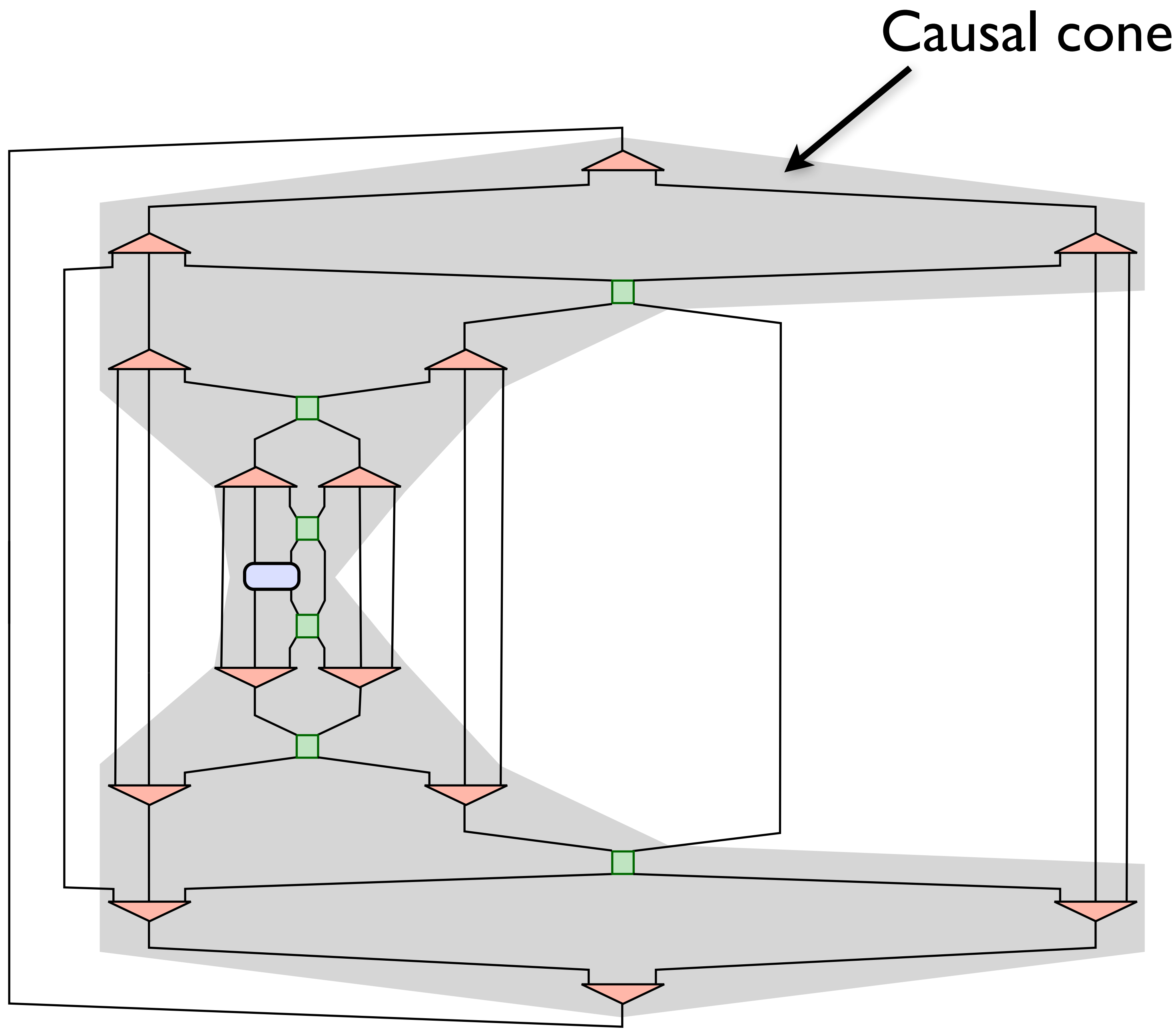


Disentanglers are *unitary*

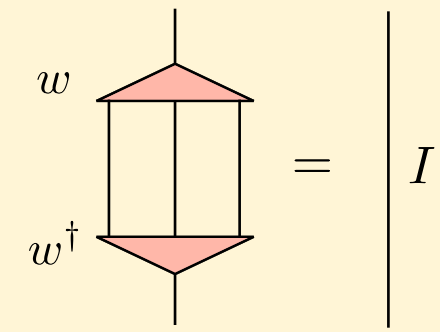


MERA: Contraction

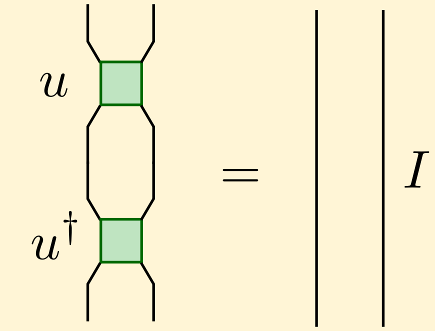
$\langle \Psi | O | \Psi \rangle$



Isometries are *isometric*

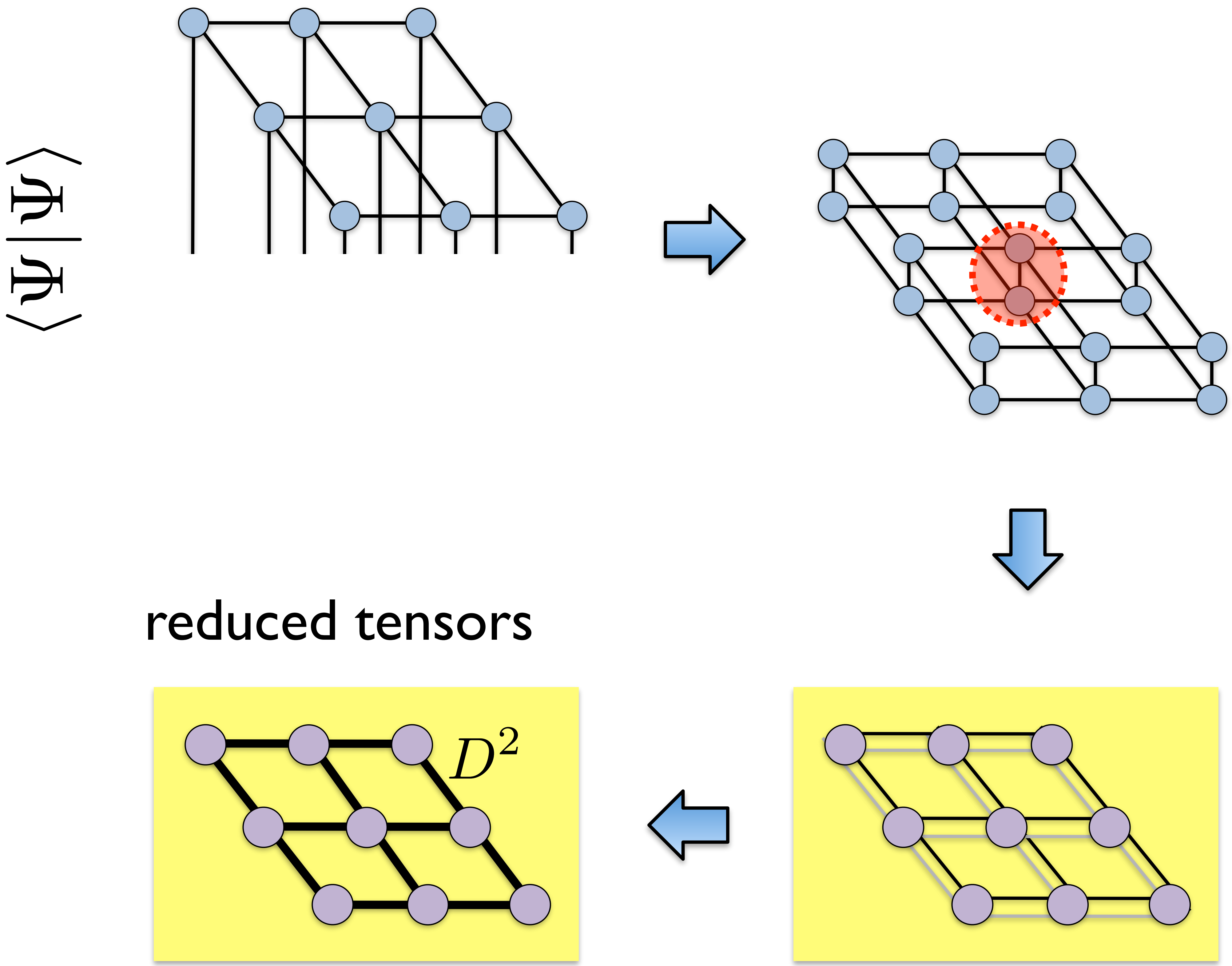


Disentanglers are *unitary*

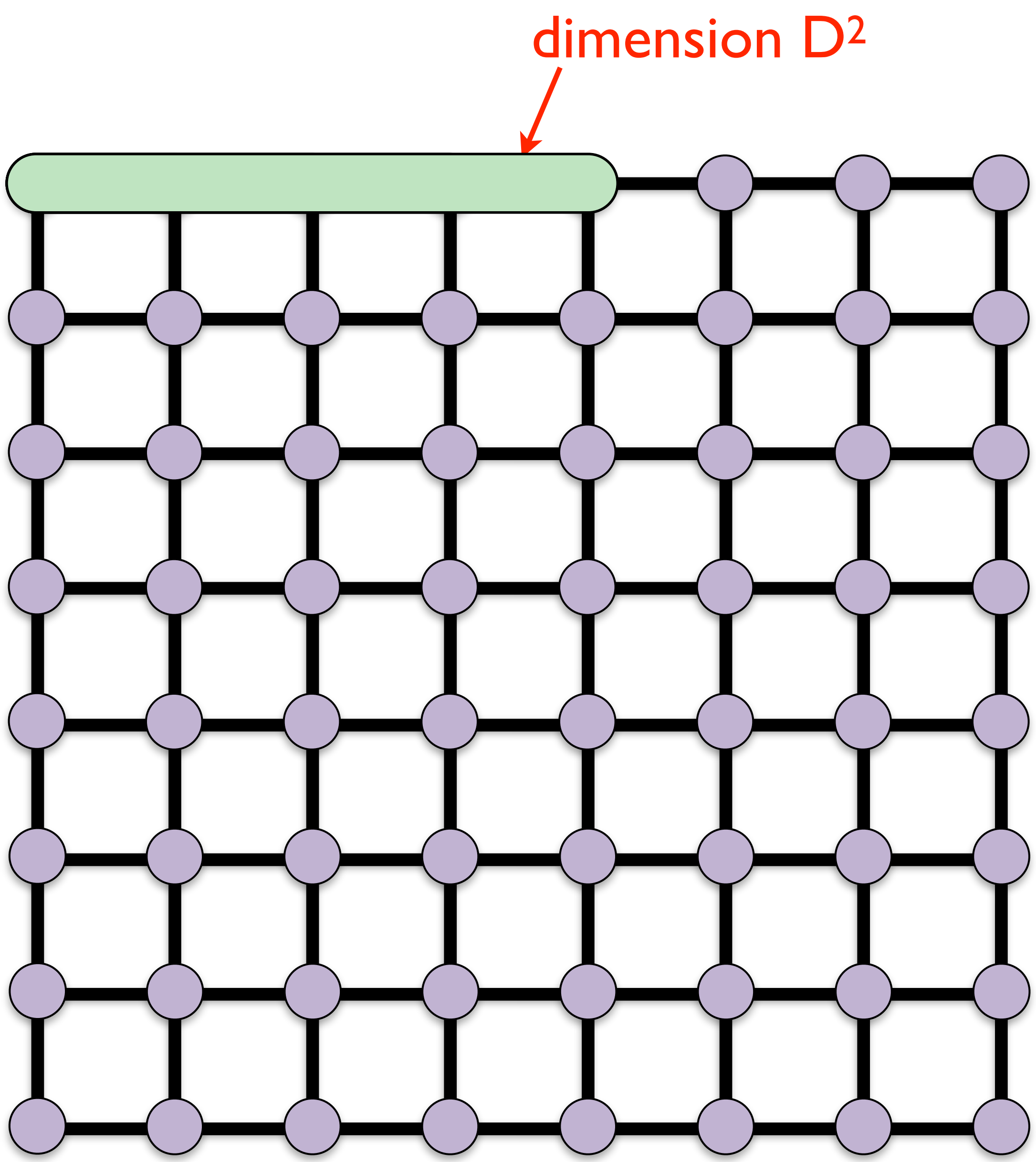


Efficient computation of expectation values of observables!

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^{2L}

Exponentially increasing with L!

NOT EFFICIENT

Contracting the PEPS

★ Exact contraction of an PEPS is exponentially hard!

→ *use controlled approximate contraction scheme*

MPS-MPO-based approaches

Murg,Verstraete,Cirac, PRA75 '07
Jordan,et al. PRL79 (2008)
Haegeman & Verstraete (2017)
…

Corner transfer matrix method

Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)
Fishman et al, arxiv:1711:05881
…

TRG

Tensor Renormalization Group
(variants: HOTRG, SRG, HOSRG)

Levin, Nave, PRL99 (2007)
Xie et al. PRL 103 (2009)
Xie et al. PRB 86 (2012), …

↓

TNR

Tensor Network Renormalization
Evenbly & Vidal, PRL 115 (2015)

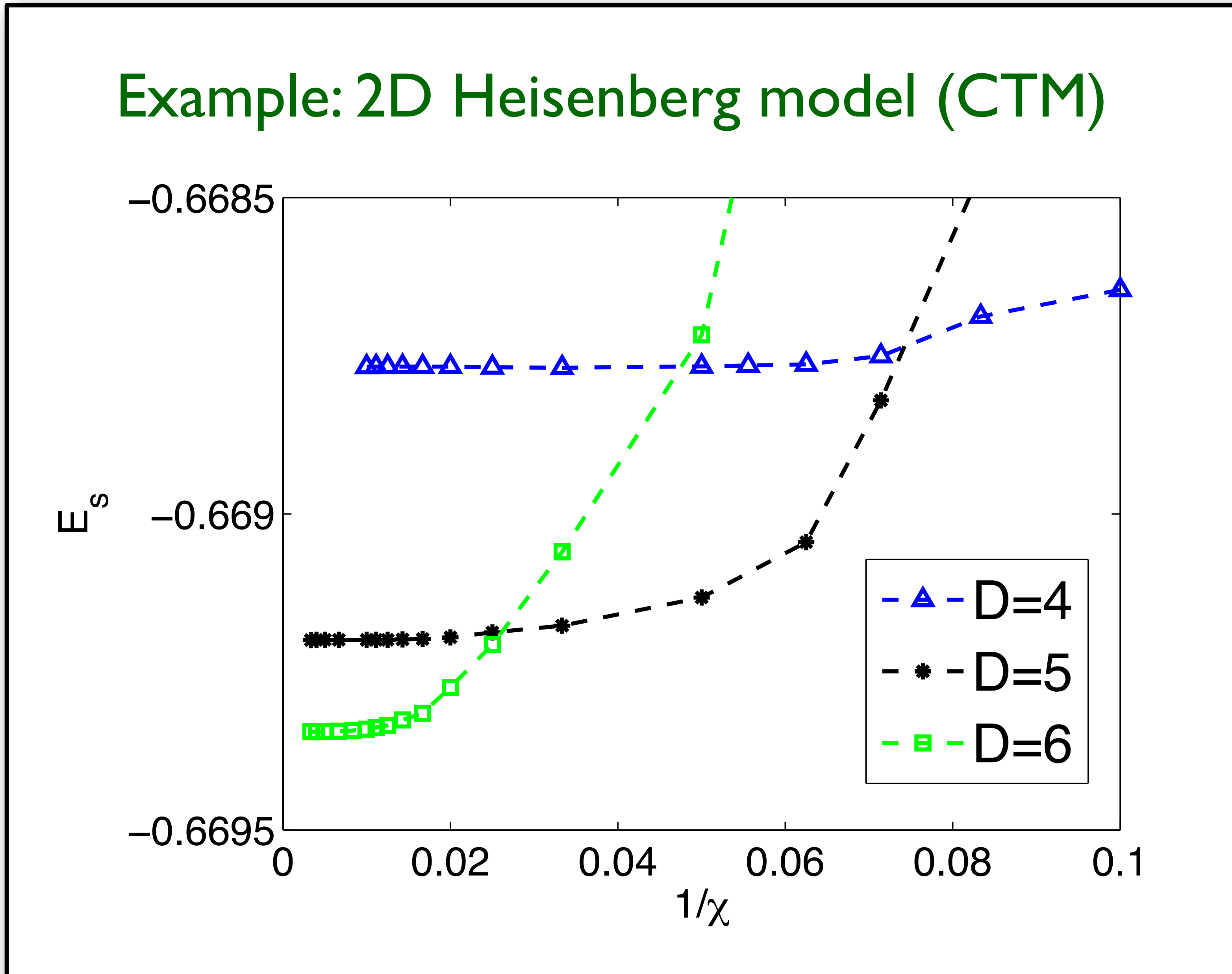
Loop-TNR:
Yang, Gu & Wen, PRL 118 (2017)

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

★ Convergence in χ needs to be carefully checked

★ Overall cost: $\mathcal{O}(D^{10\ldots14})$ with $\chi \sim D^2$

Contracting the PEPS



★ Fast convergence

★ Effect of finite D is much larger!

★ Be careful with "variational" energy!!!

Contracting the PEPS

★ Exact contraction of an PEPS is exponentially hard!

→ *use controlled approximate contraction scheme*

MPS-MPO-based approaches

Murg,Verstraete,Cirac, PRA75 '07
Jordan,et al. PRL79 (2008)
Haegeman & Verstraete (2017)
…

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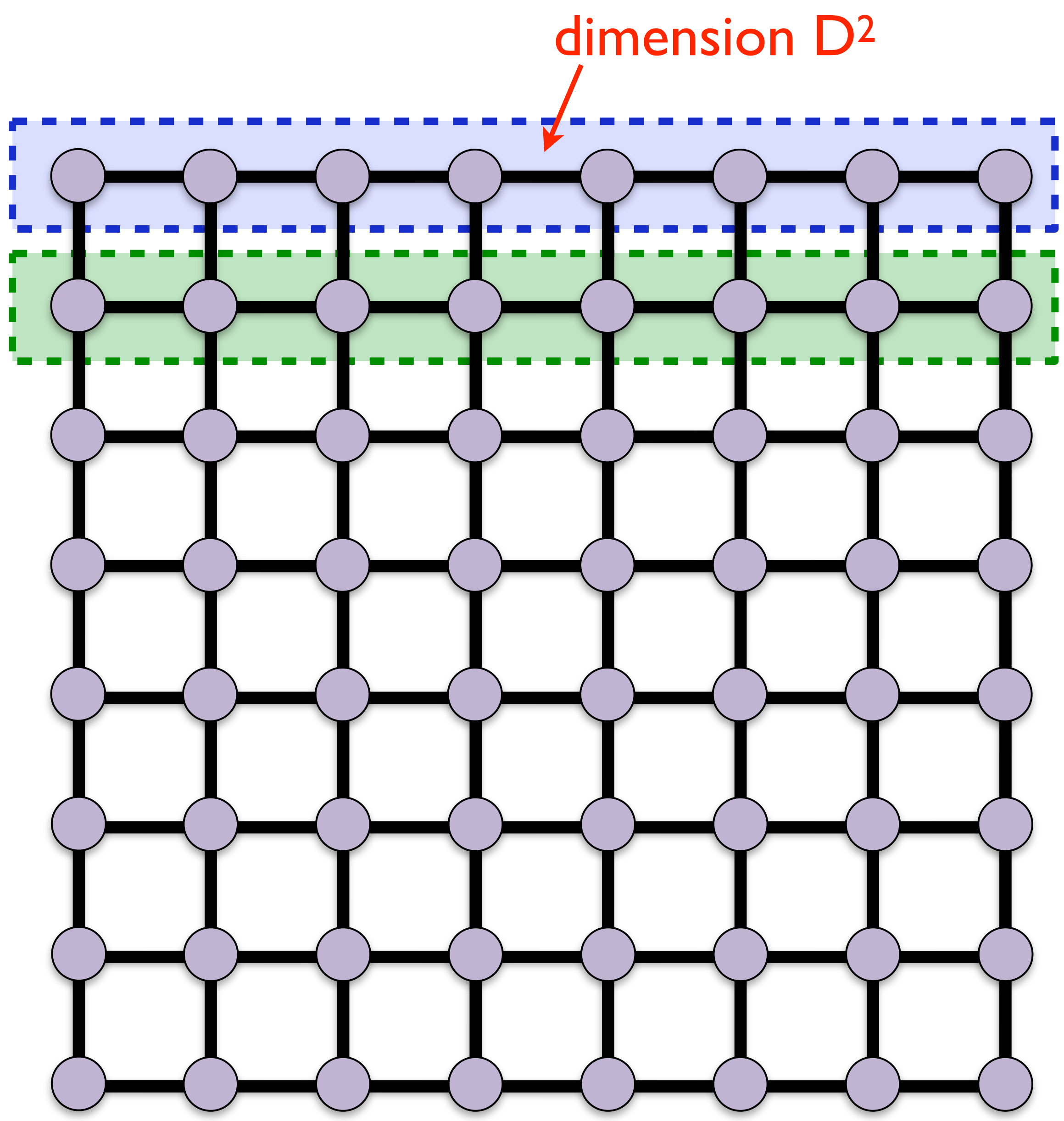
Contracting the PEPS using an MPS

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

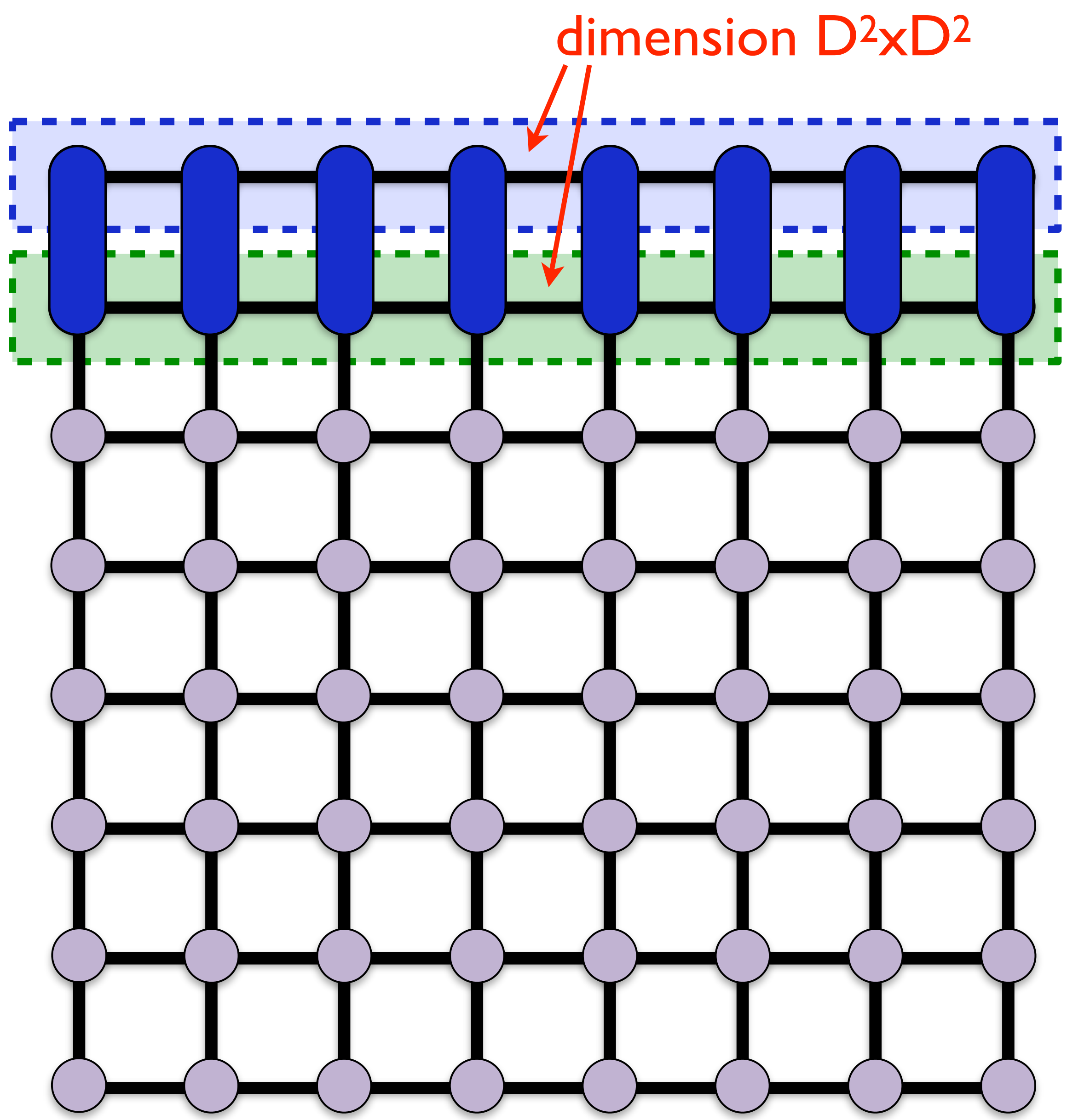


this is an MPS

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

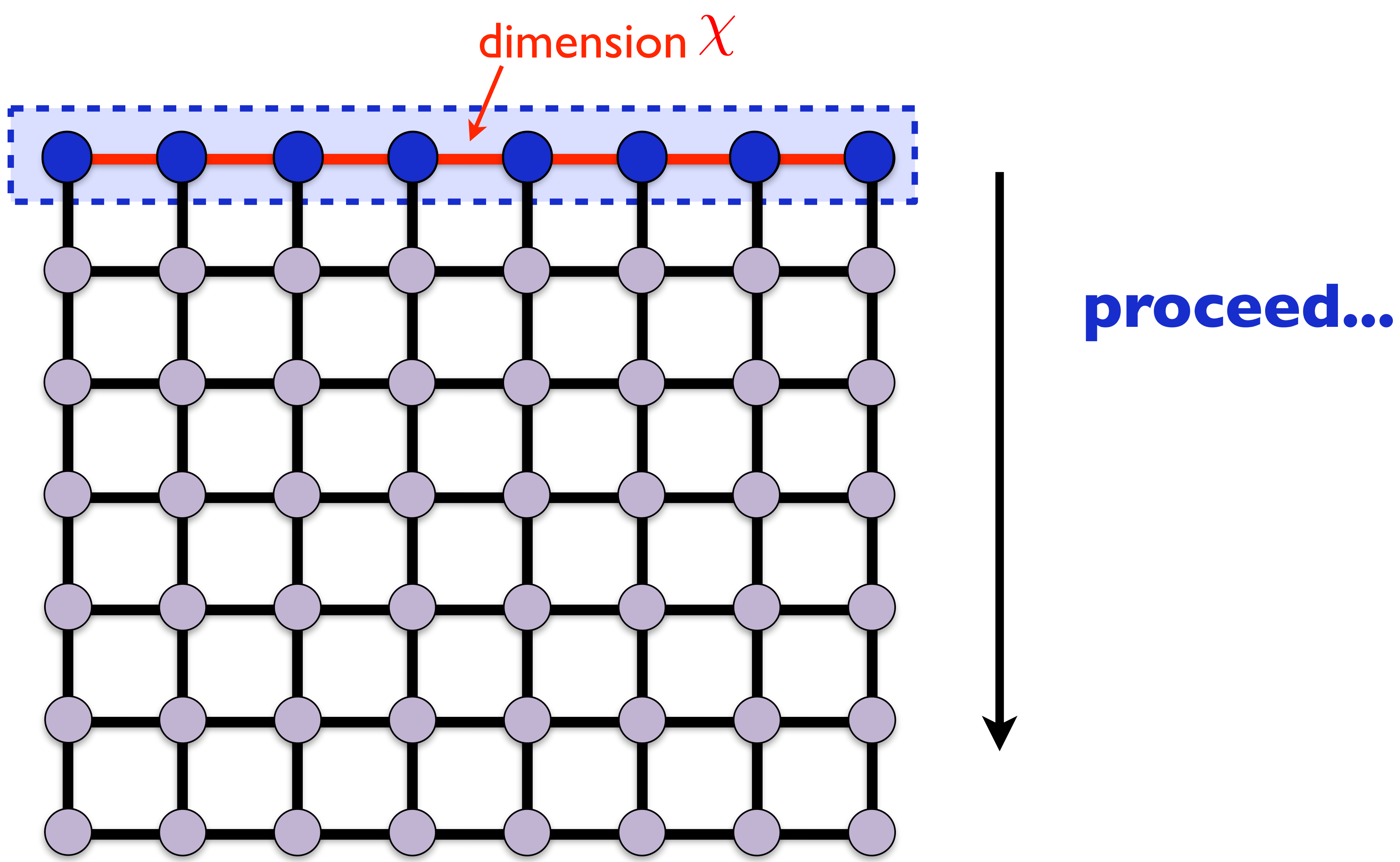
truncate the bonds to χ

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

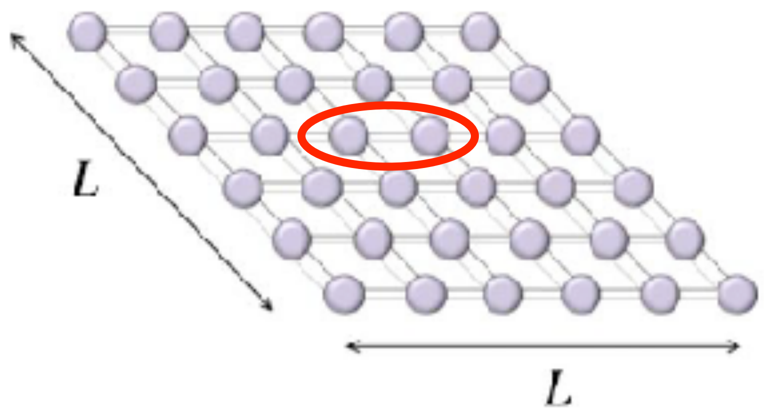
Verstraete, Murg, Cirac, Adv. in Phys. 57, 143 (2008)

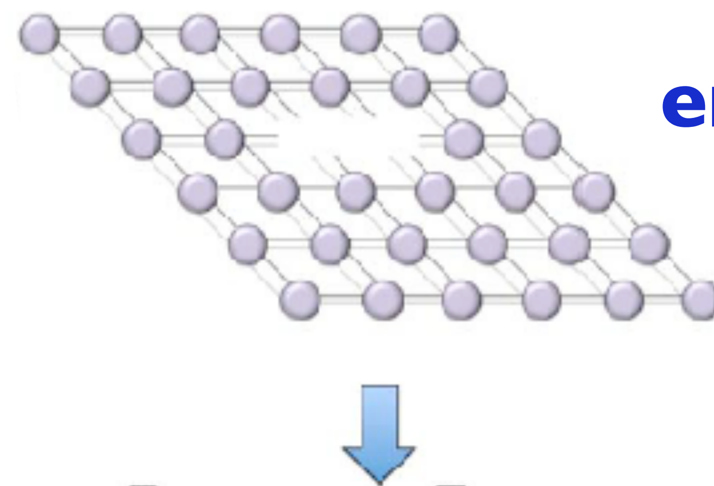


★ We can do this from several directions

★ Similar procedure when computing an expectation value

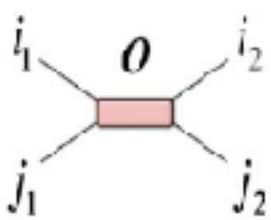
Compute expectation values

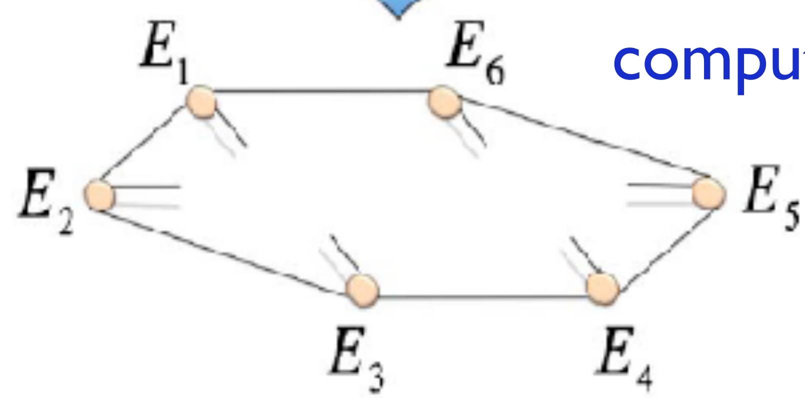


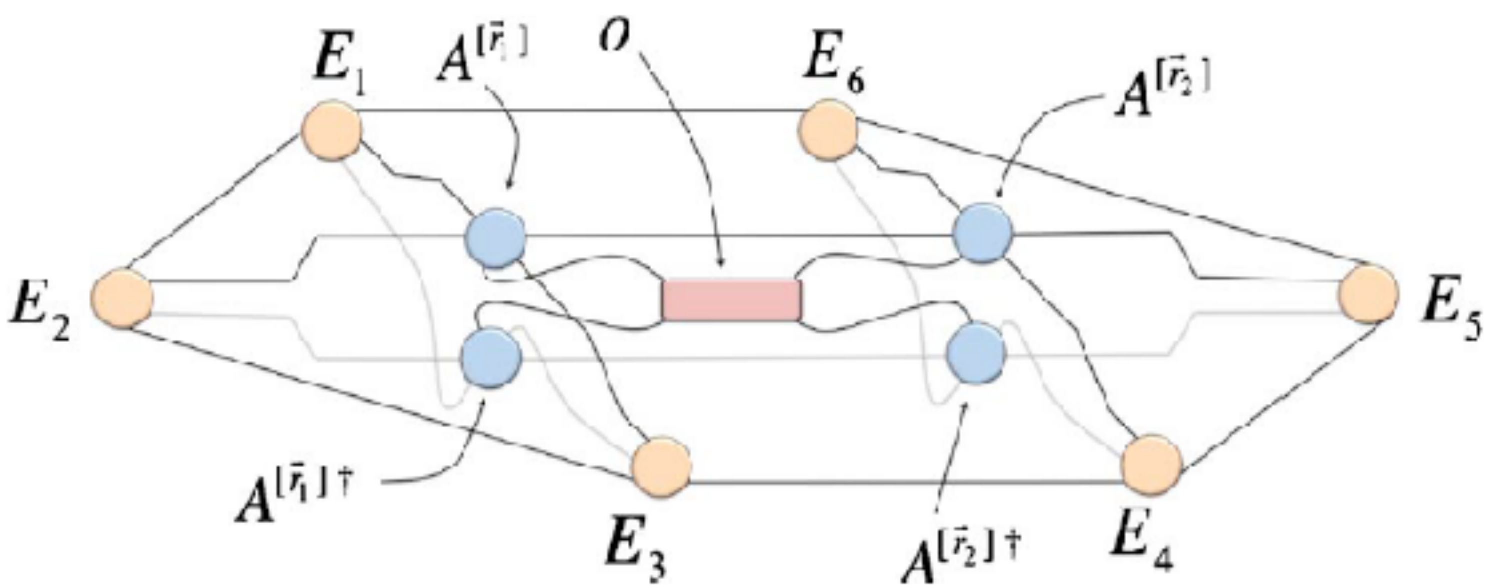


environment

compute environment approximately







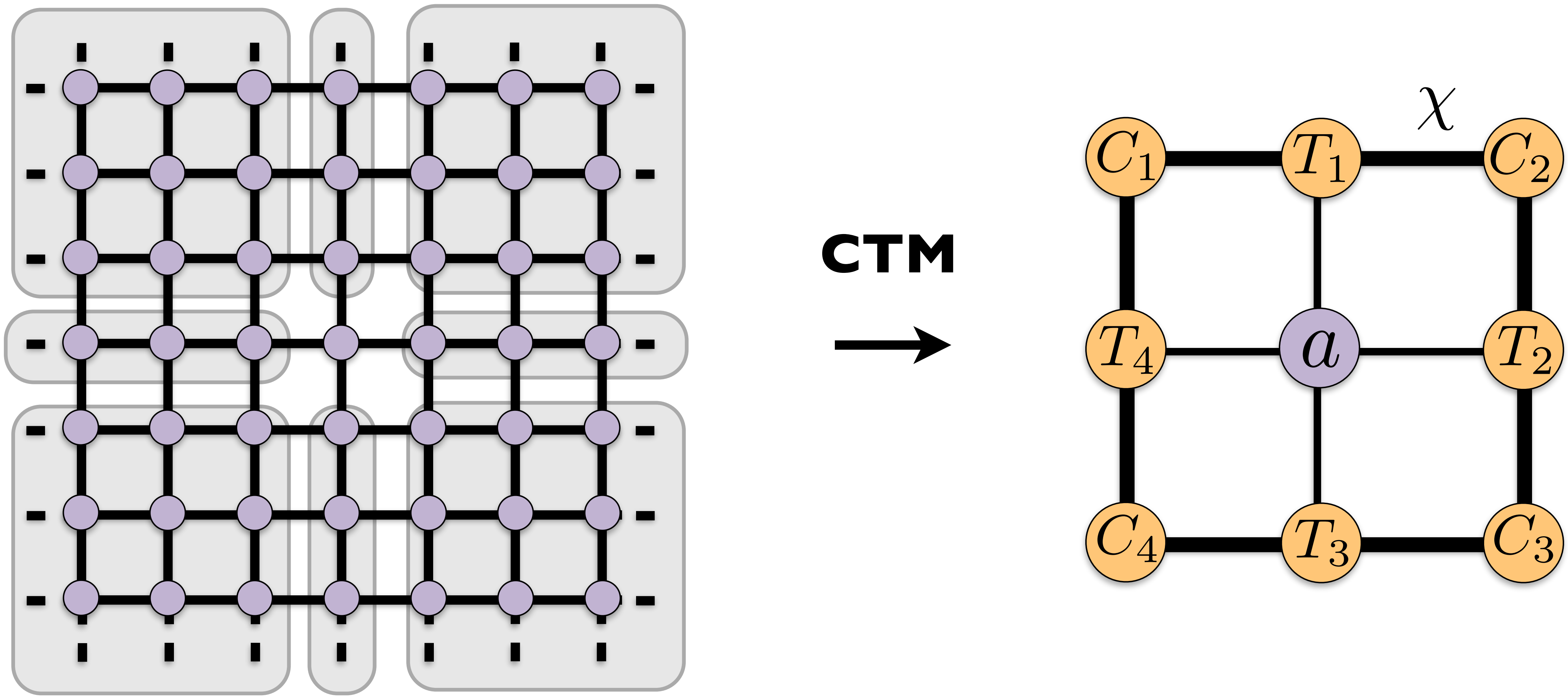
Connect two-body operator

Contract this network!

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

Contracting the iPEPS using the corner transfer matrix method

Nishino, Okunishi, JPSJ65 (1996)



- Environment tensors account for infinite system around a bulk site
- CTM: Compute environment in an iterative way
- Accuracy can be systematically controlled with χ

Contracting the iPEPS using the corner transfer matrix method

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

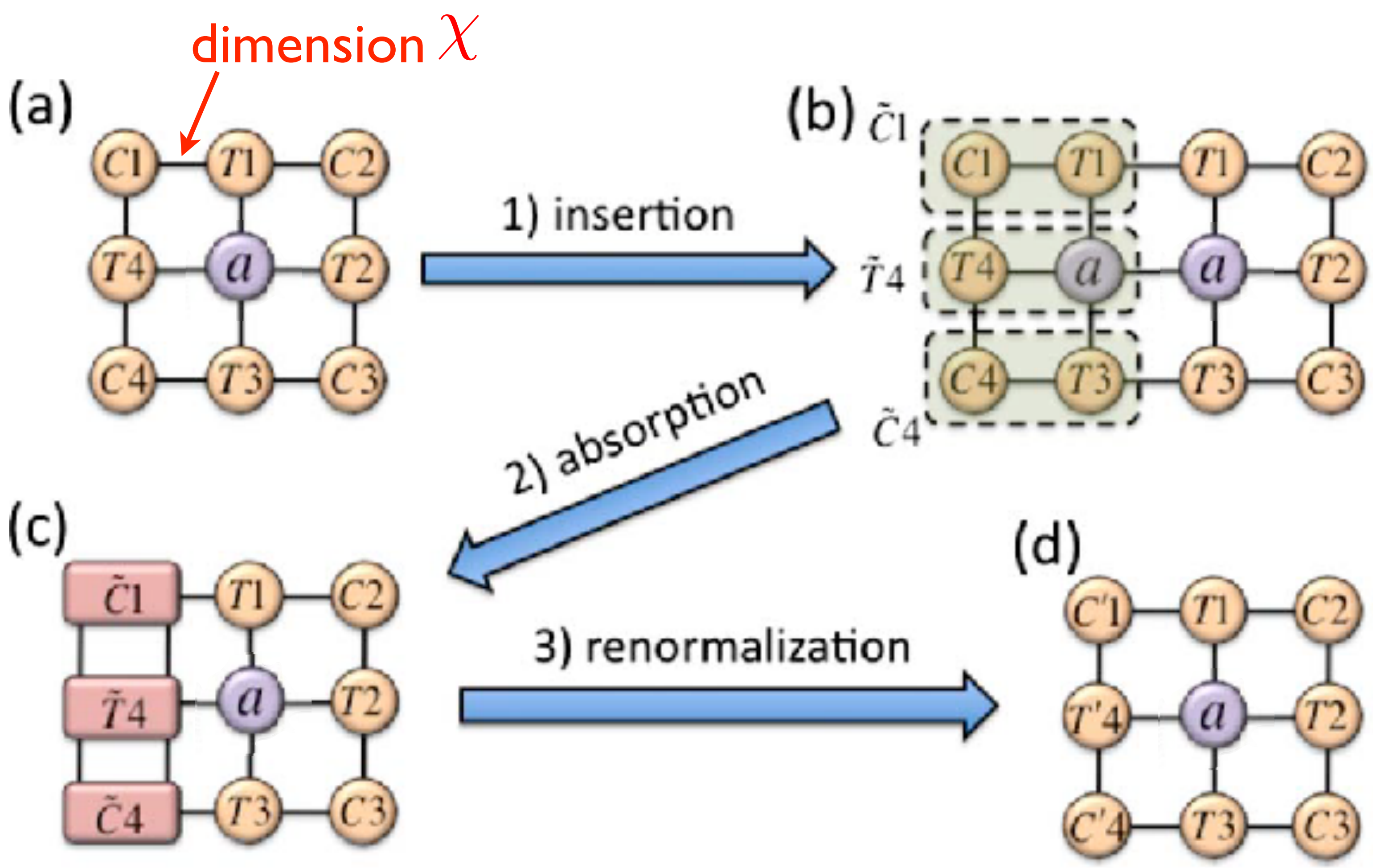
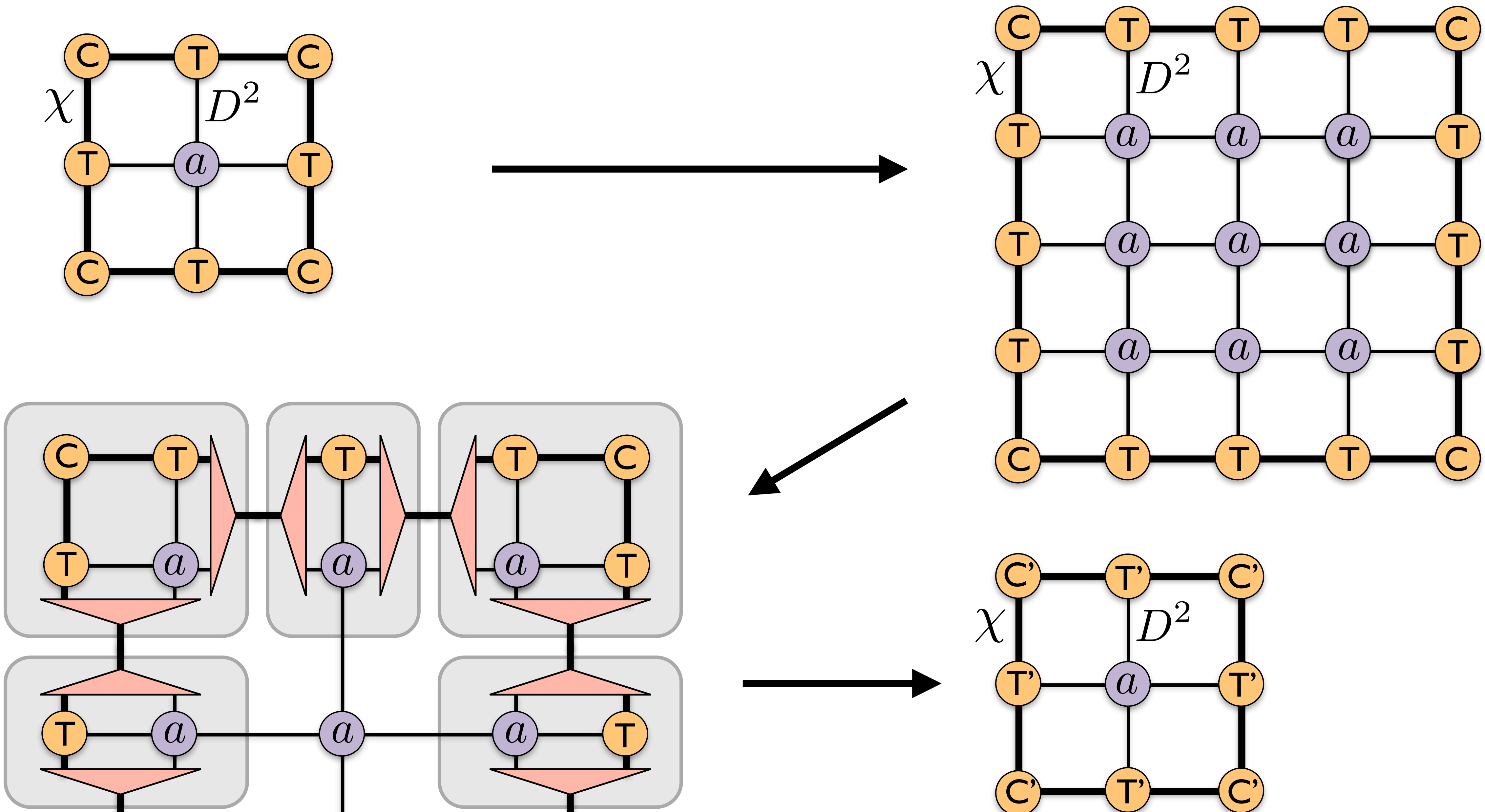
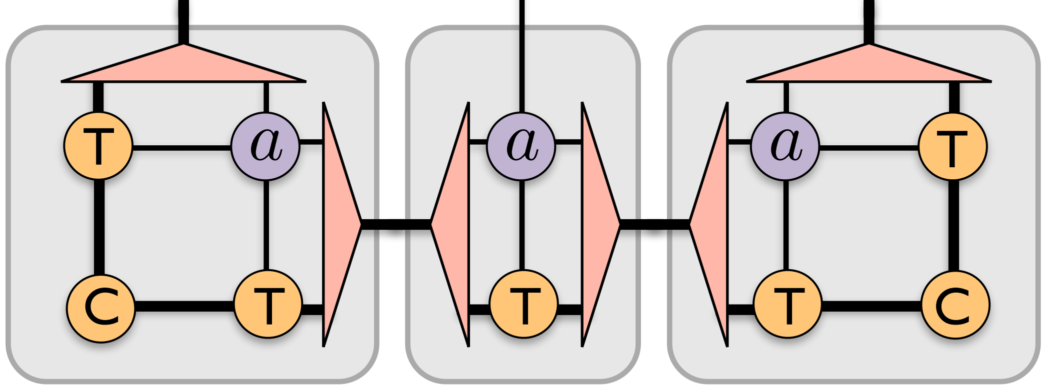


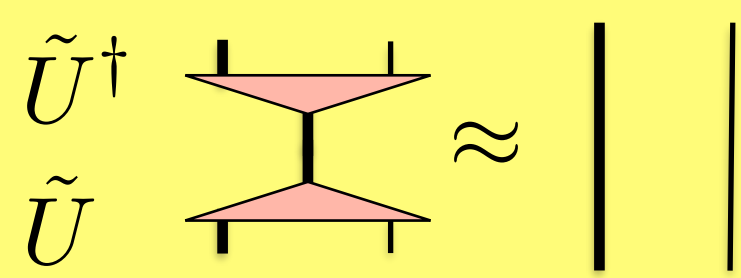
figure taken from Orus, Vidal, PRB 80 (2009)

- ★ 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)

Simplest case: rotational symmetric tensors

Nishino, Okunishi, JPSJ65 (1996)

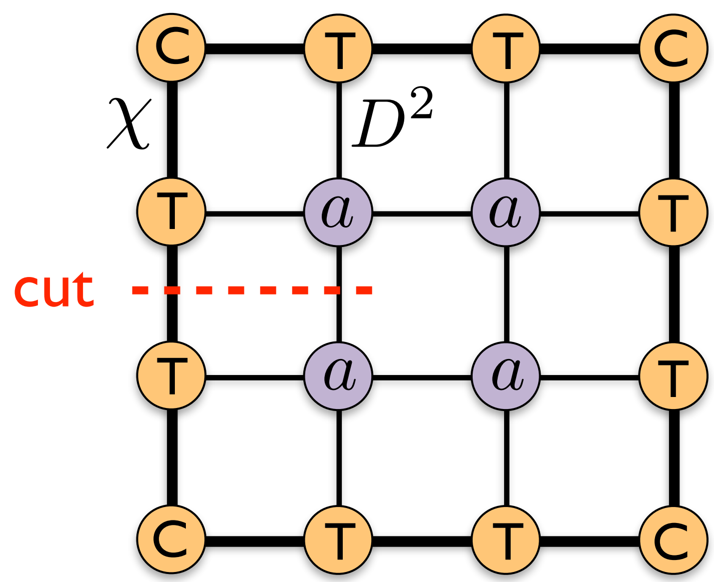





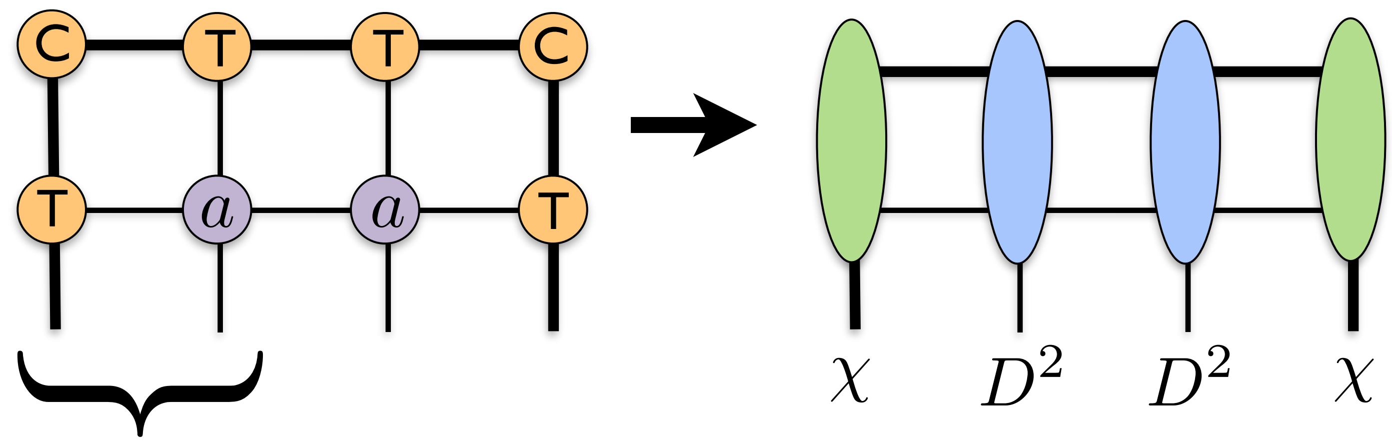
Approximate resolution of the identity (in the relevant subspace)

Simplest case: rotational symmetric tensors

Nishino, Okunishi, JPSJ65 (1996)



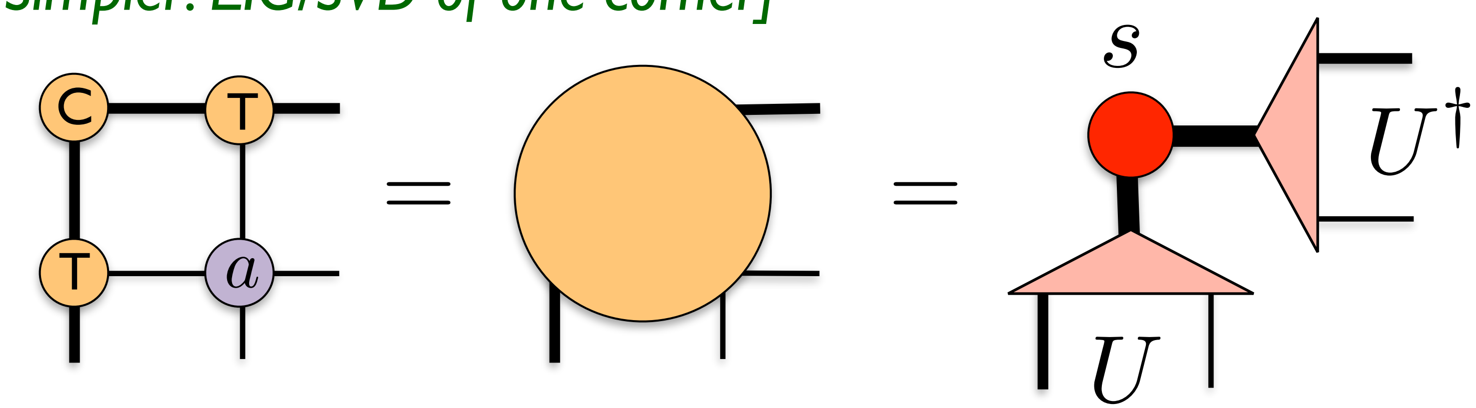
$"\rho_{left}"$



Relevant subspace?

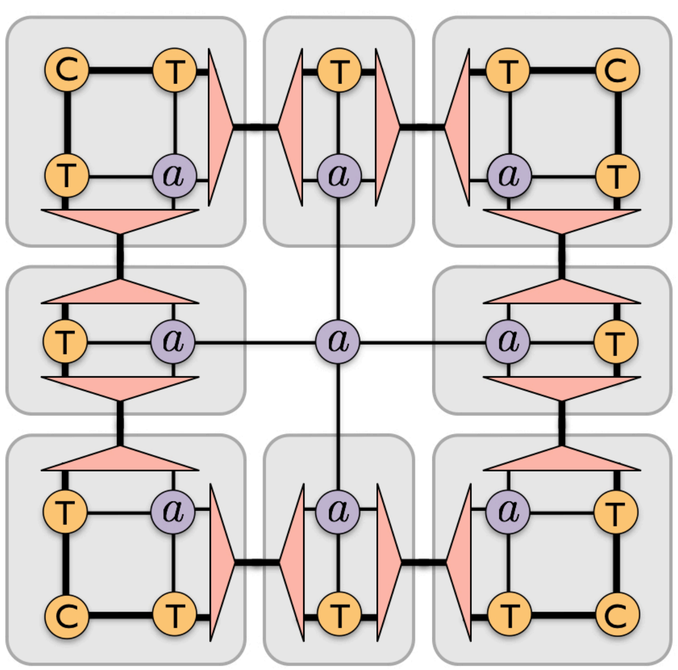
DMRG: Eigenvectors with largest eigenvalues of ρ_{left}

[Simpler: EIG/SVD of one corner]

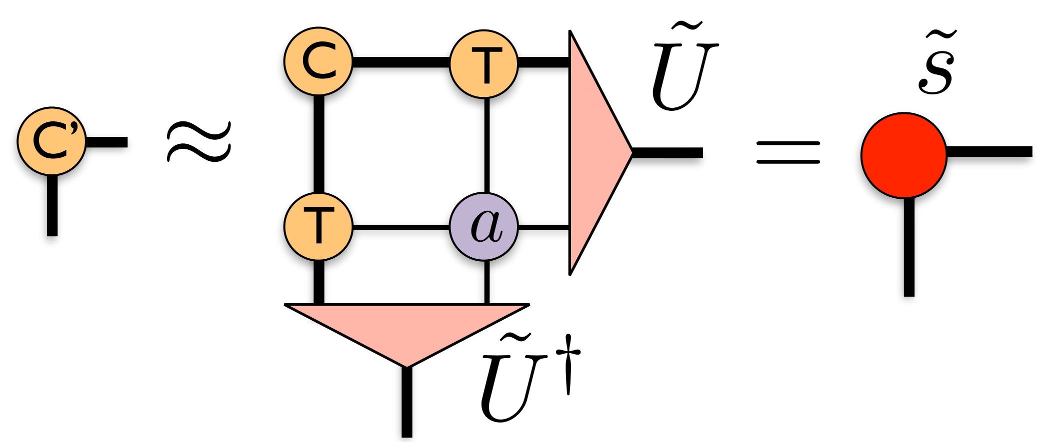


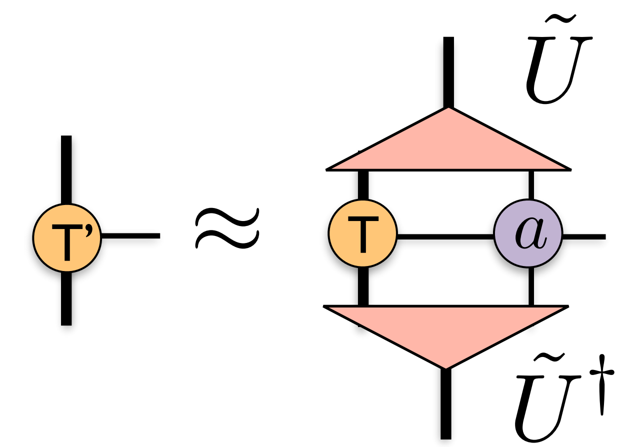
How can we best truncate from

$\chi D^2 \rightarrow \chi$

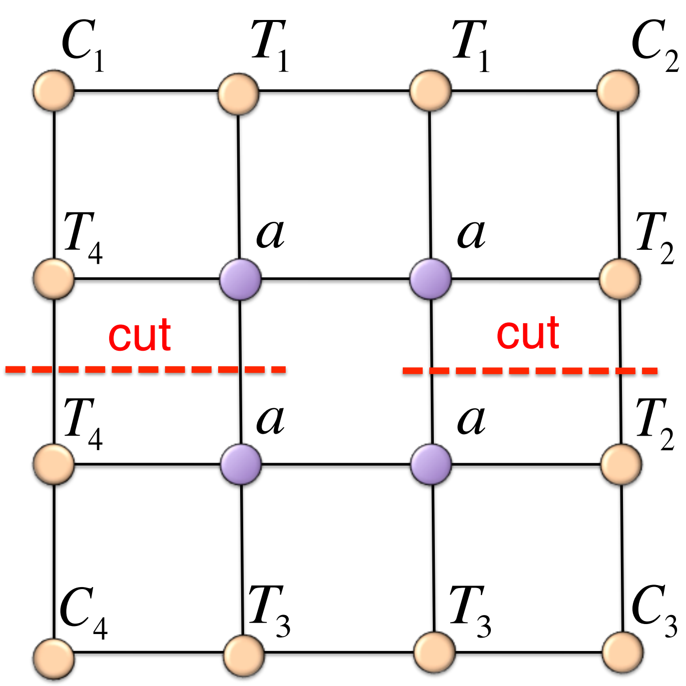


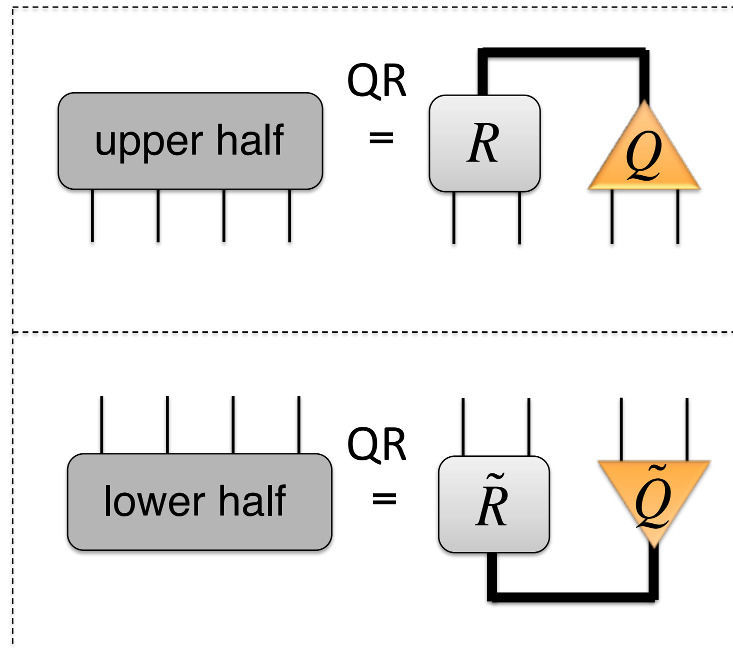
Renormalized tensors: keep only χ states with largest weight



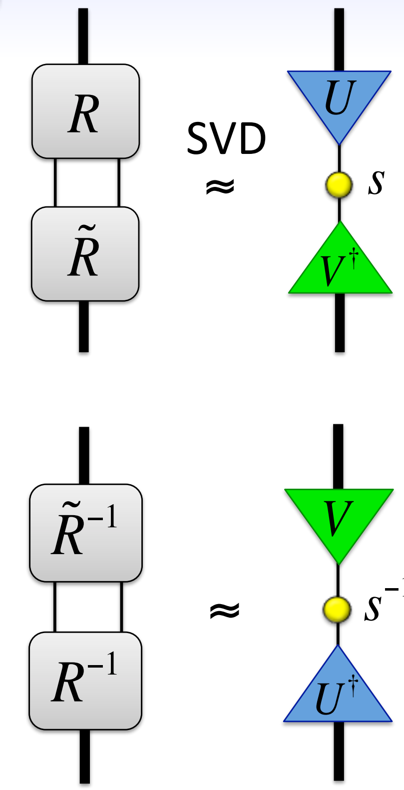


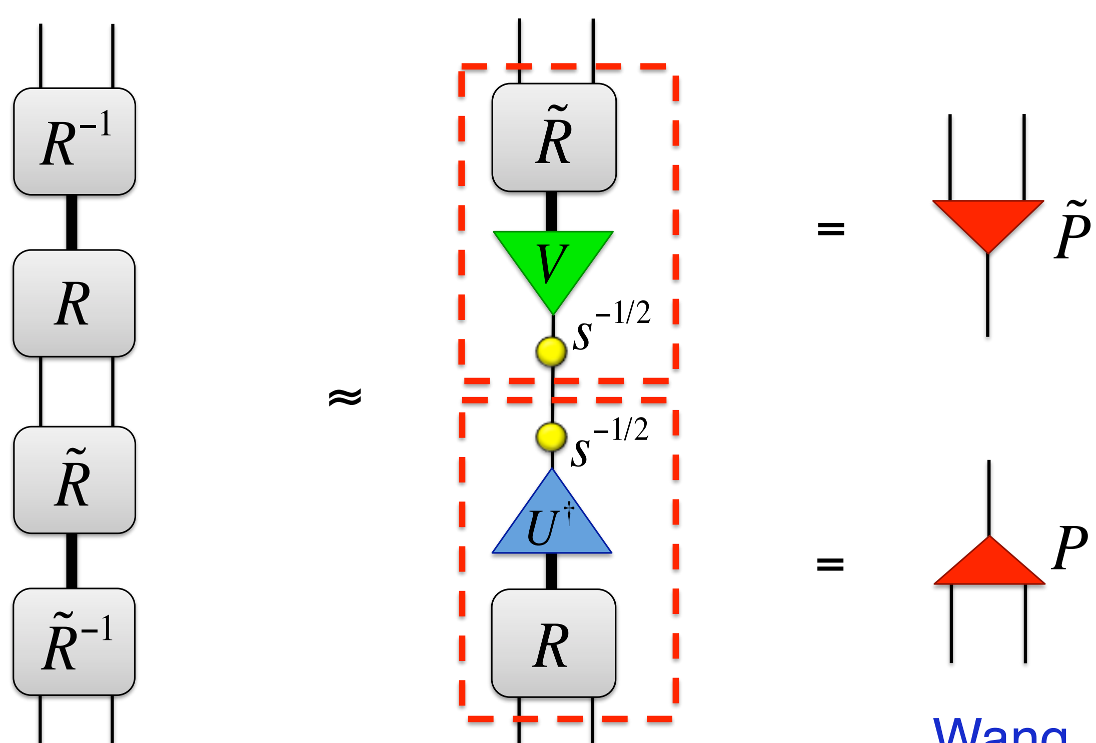
General case: Renormalization step (left move)





alternatively: only use upper left and lower left corners

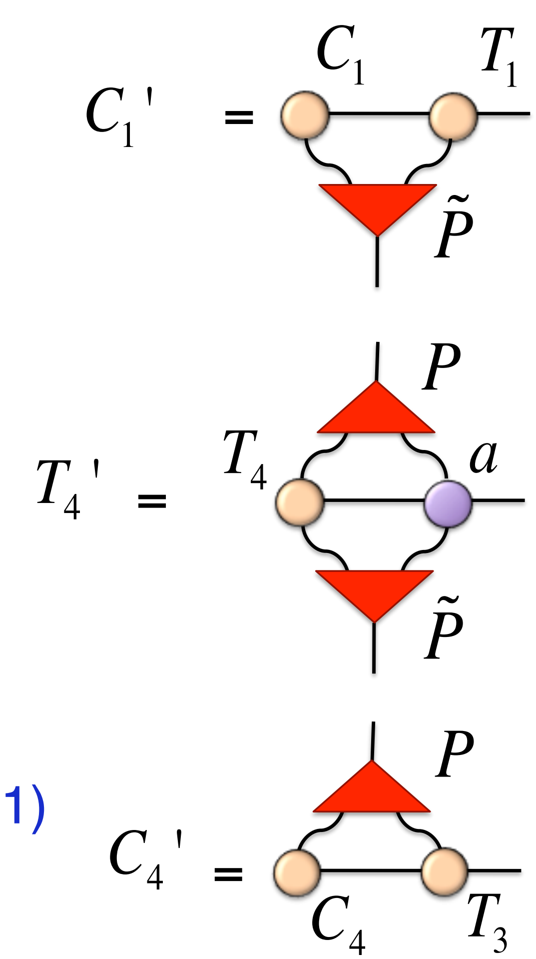




identity

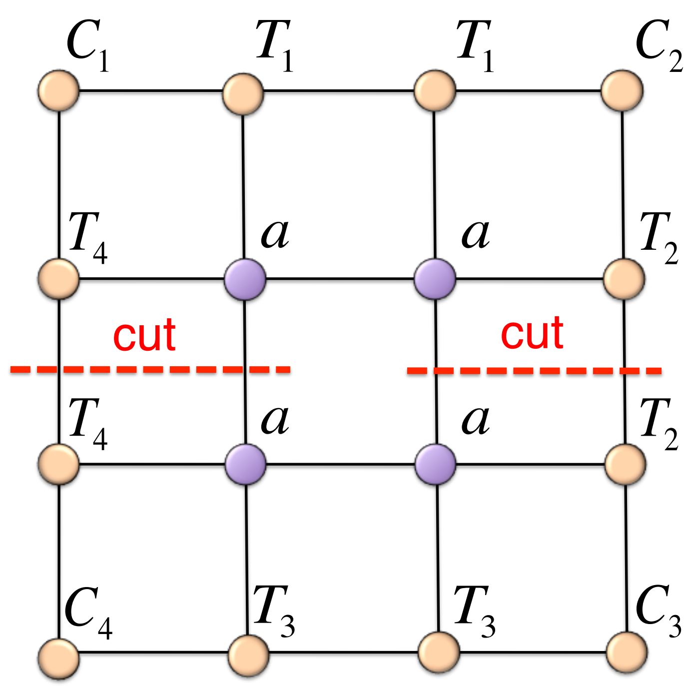
approx. identity

projectors onto relevant subspace

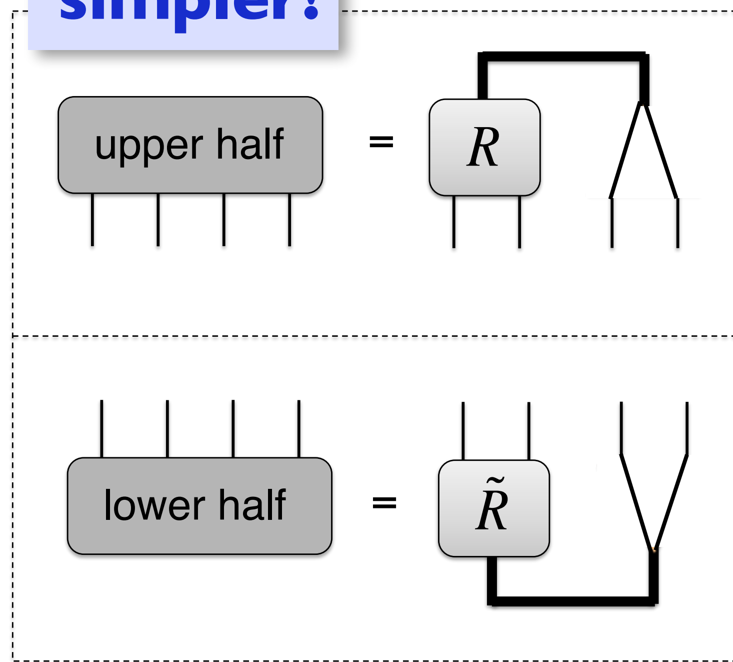


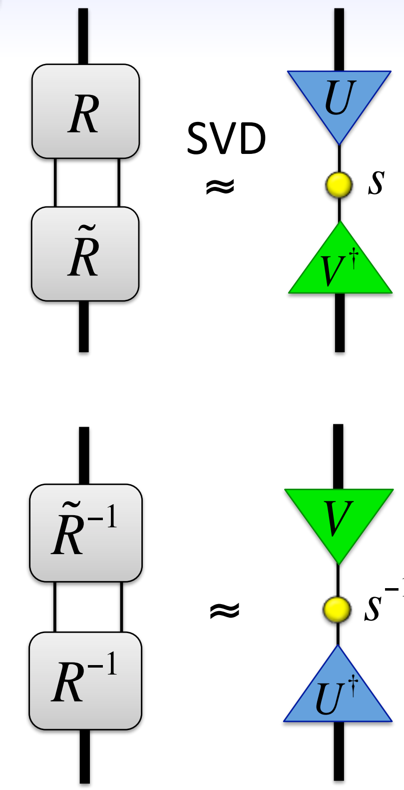
Wang, Pižorn & Verstraete, PRB 83 (2011)
Huang, Chen & Kao, PRB 86 (2012)
PC, Rice, Troyer, PRL 113 (2014)

General case: Renormalization step (left move)

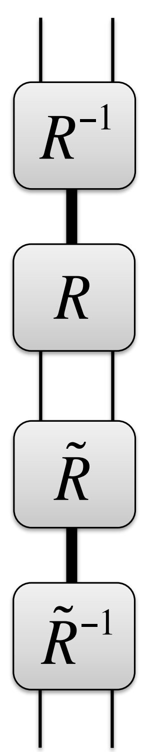


simpler!

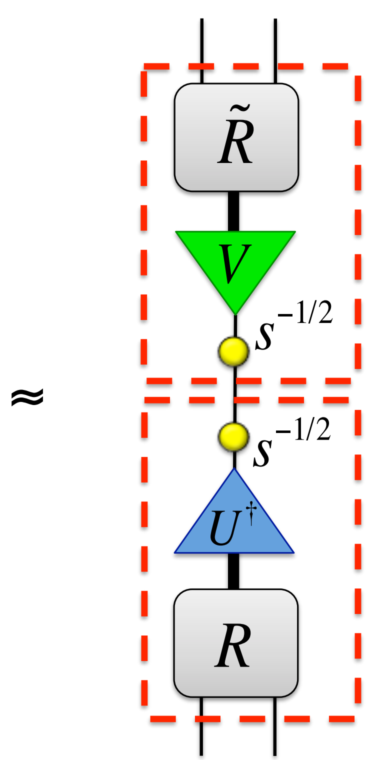




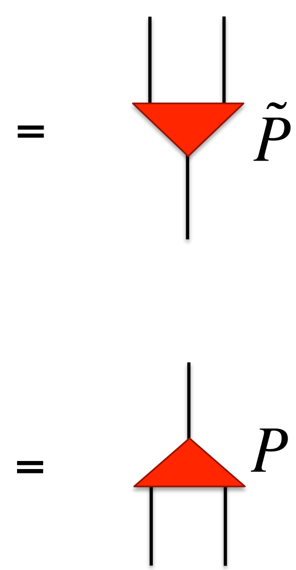
QR is actually not required!
T. Okubo, private comm.



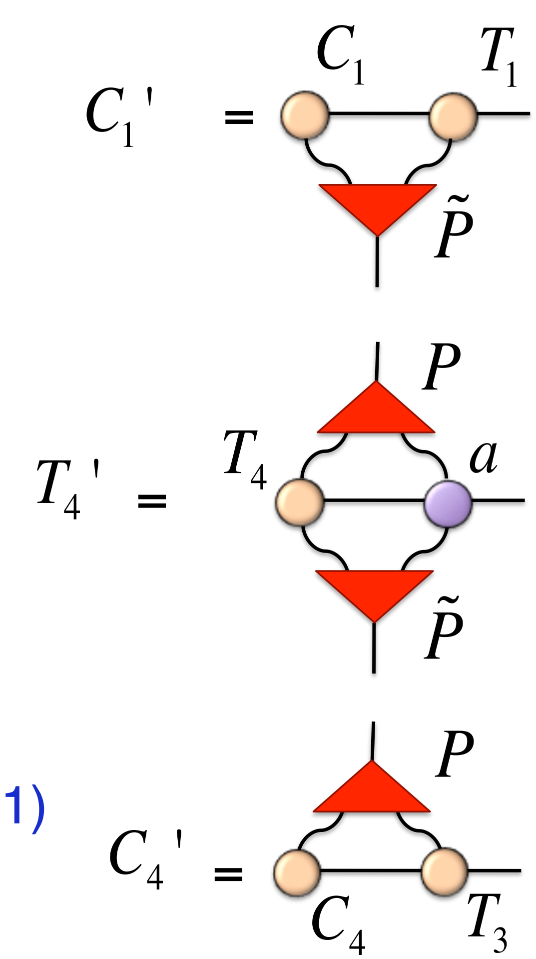
identity



approx. identity



projectors onto relevant subspace

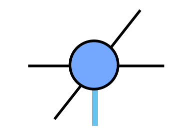


Wang, Pižorn & Verstraete, PRB 83 (2011)
Huang, Chen & Kao, PRB 86 (2012)
PC, Rice, Troyer, PRL 113 (2014)

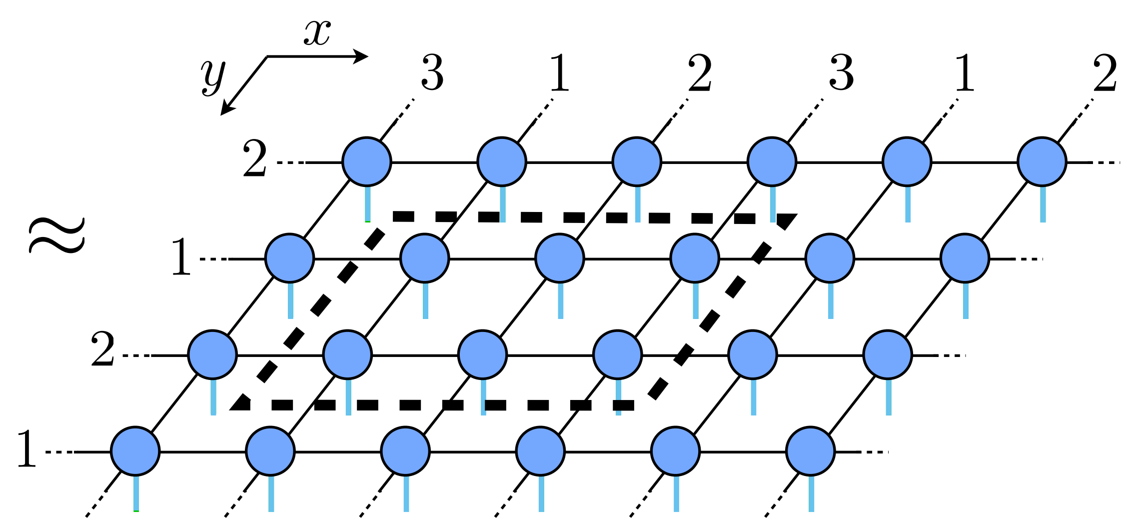
CTM with larger unit cells

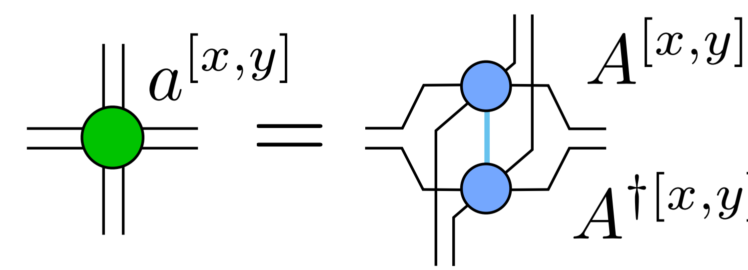
PC, White, Vidal, Troyer, PRB **84** (2011)

★ Each tensor has coordinates with respect to the unit cell: $A^{[x,y]}$

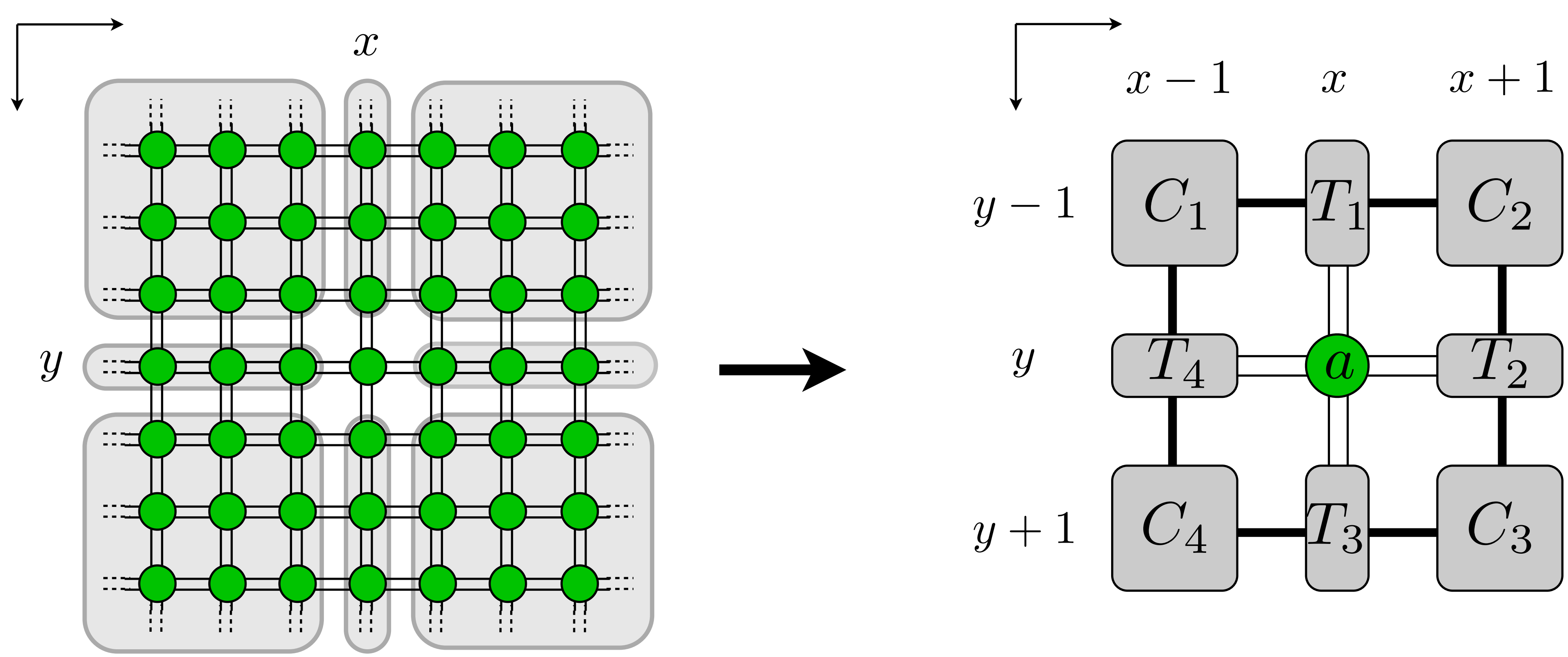


$|\Psi\rangle \approx$



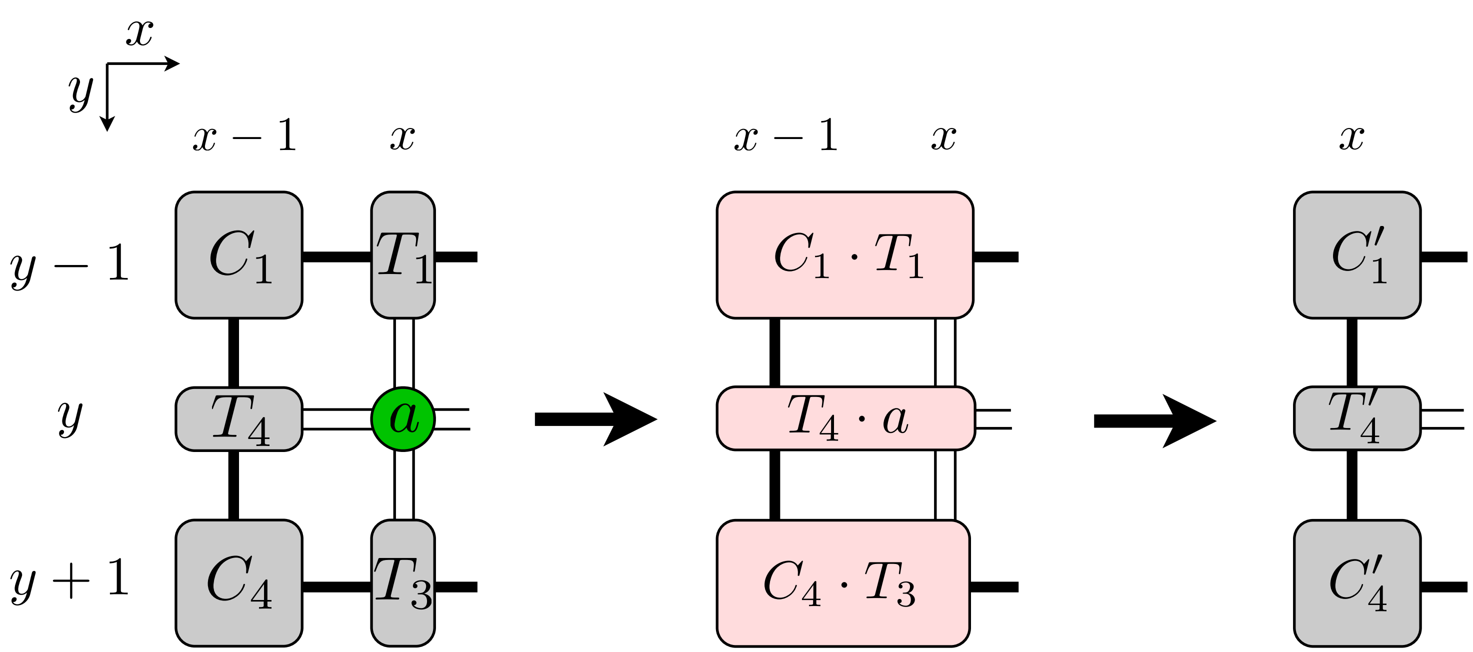


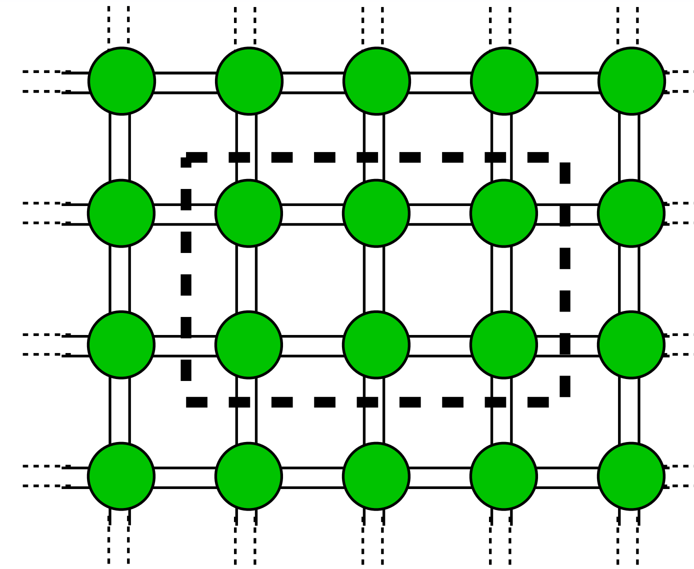
★ Keep a copy of every environment tensors C_1, ... C_4, T_1, ..., T_4 for each coordinate

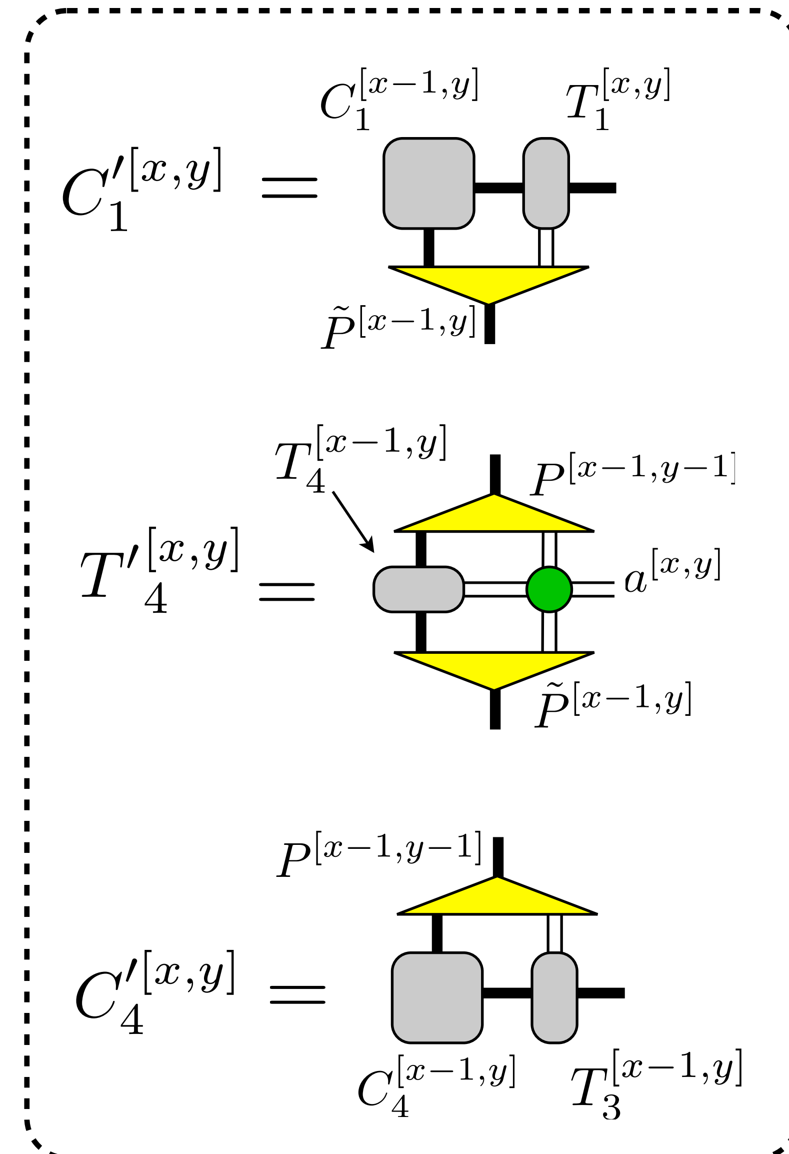


CTM with larger unit cells

Left move for $L_x \times L_y$ cell: *do for all x and y!*



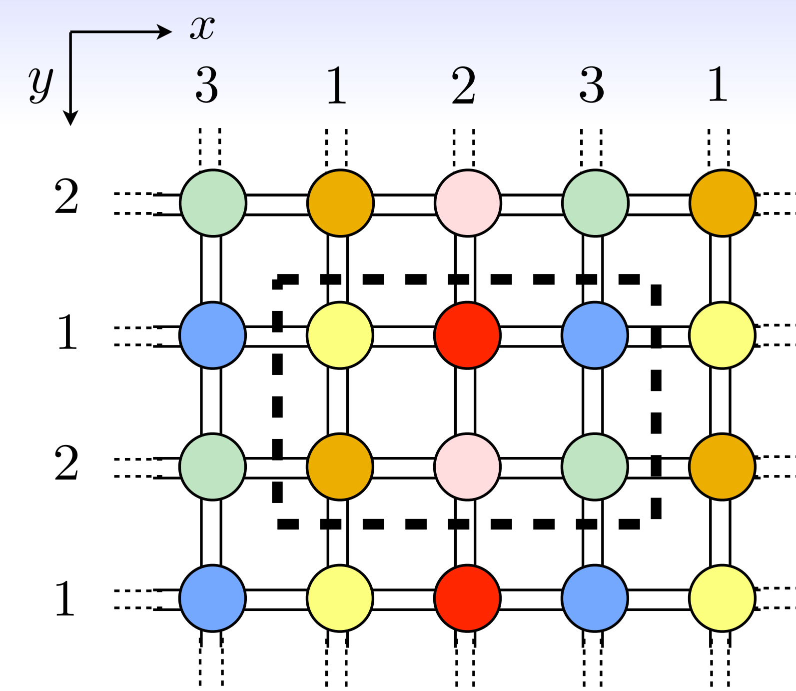


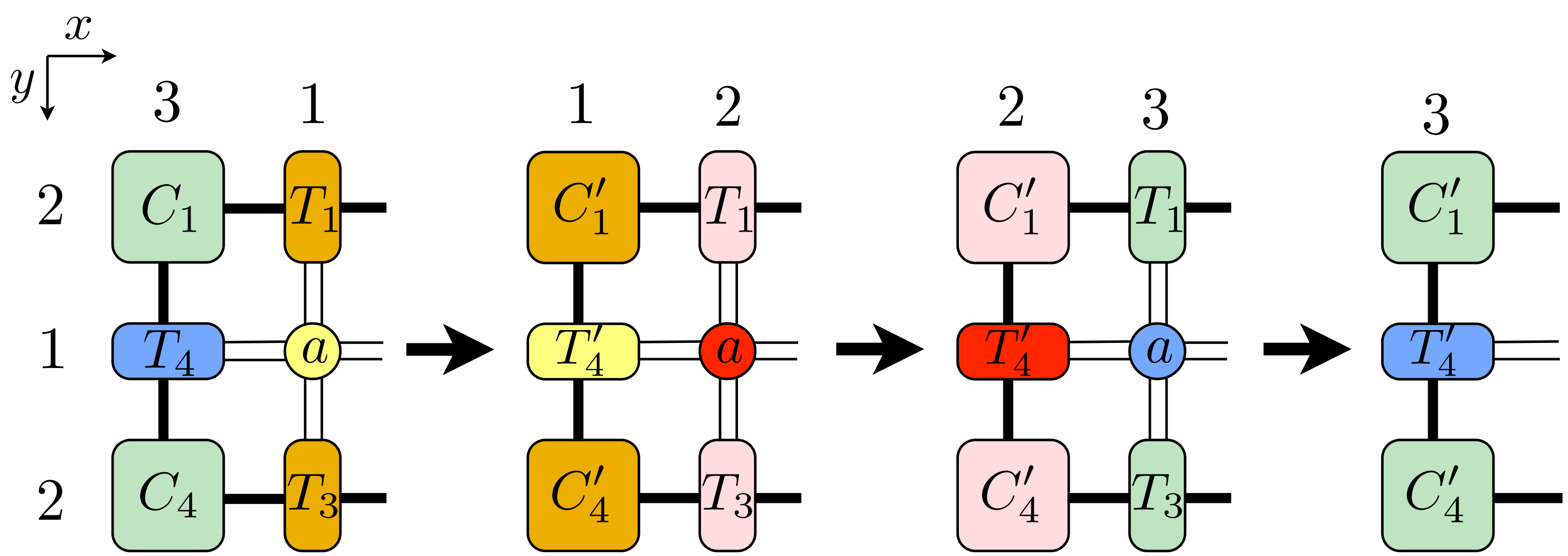


- Do for all $x \in [1, L_x]$
  - Do for all $y \in [1, L_y]$
    - Compute projectors $P^{[x-1,y]}$, $\tilde{P}^{[x-1,y]}$
  - Do for all $y \in [1, L_y]$
    - Compute updated environment tensors: $C_1'^{[x,y]}$, $C_4'^{[x,y]}$, $T_4'^{[x,y]}$

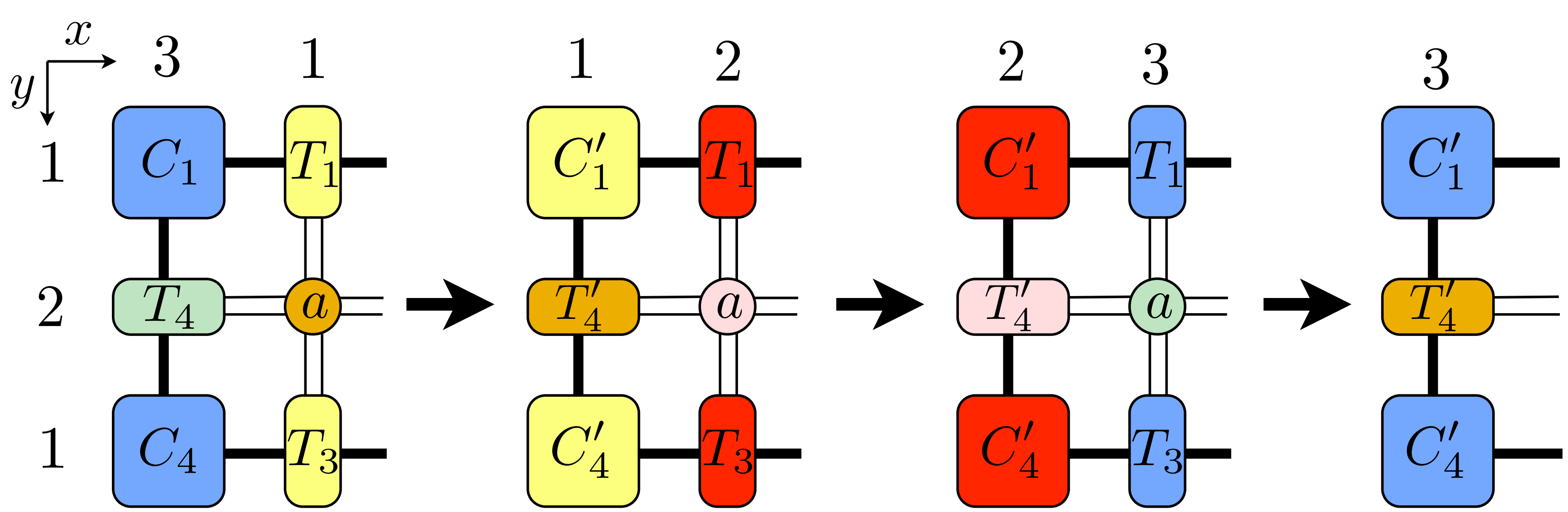
CTM with larger unit cells

Left move for $L_x \times L_y$ cell: *do for all y and x!*





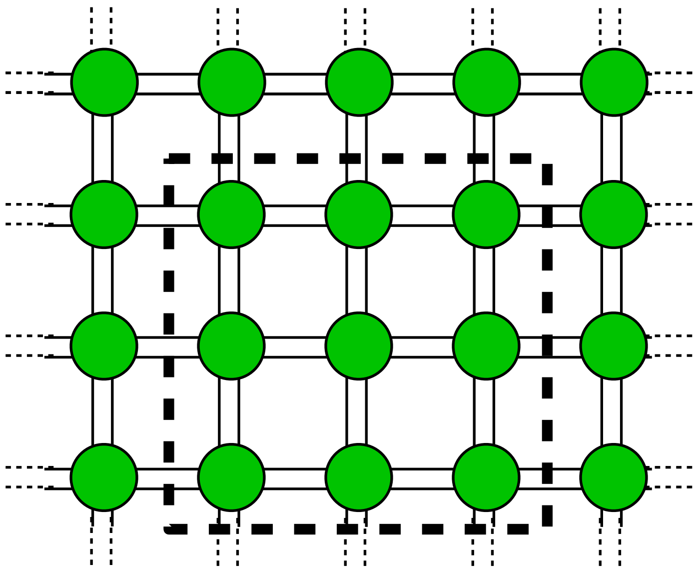
Completed left move of entire unit cell!



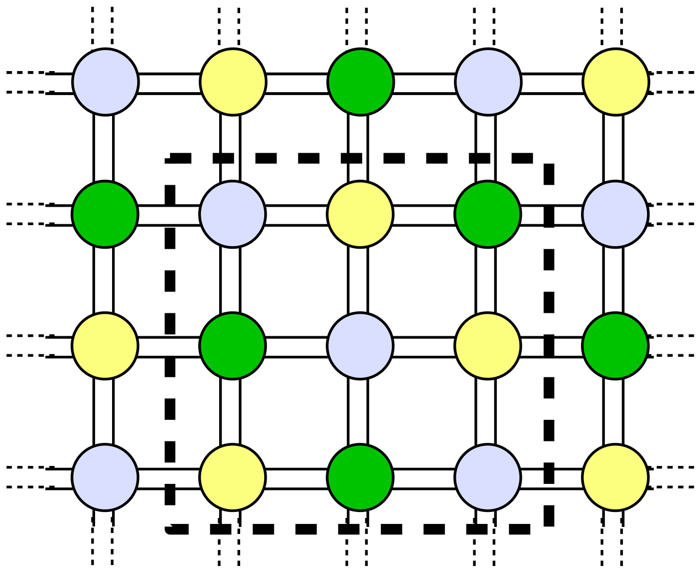
CTM with larger unit cells

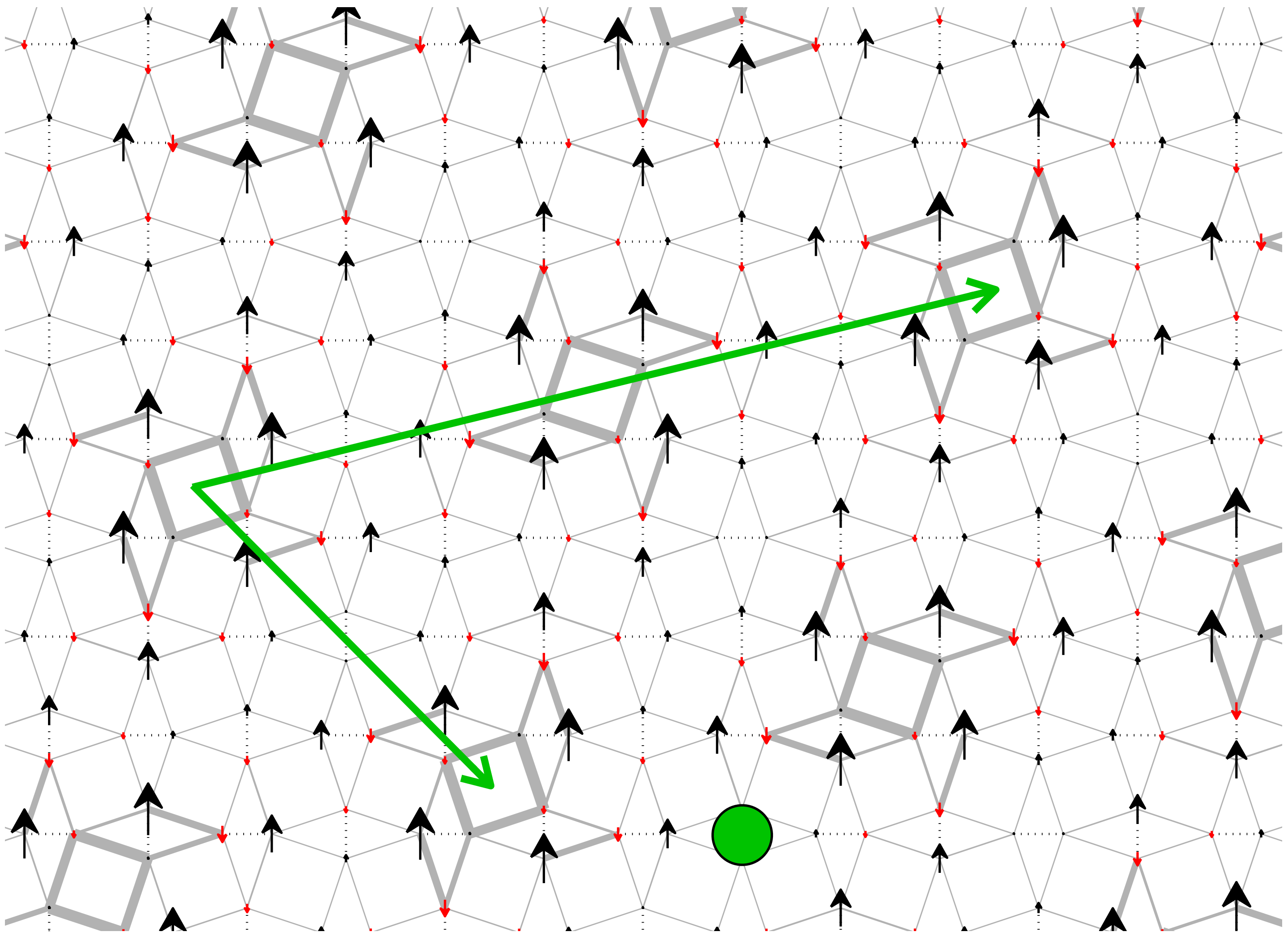
Other shapes than rectangular cell possible:

All 9 tensors different:



Only 3 different tensors:





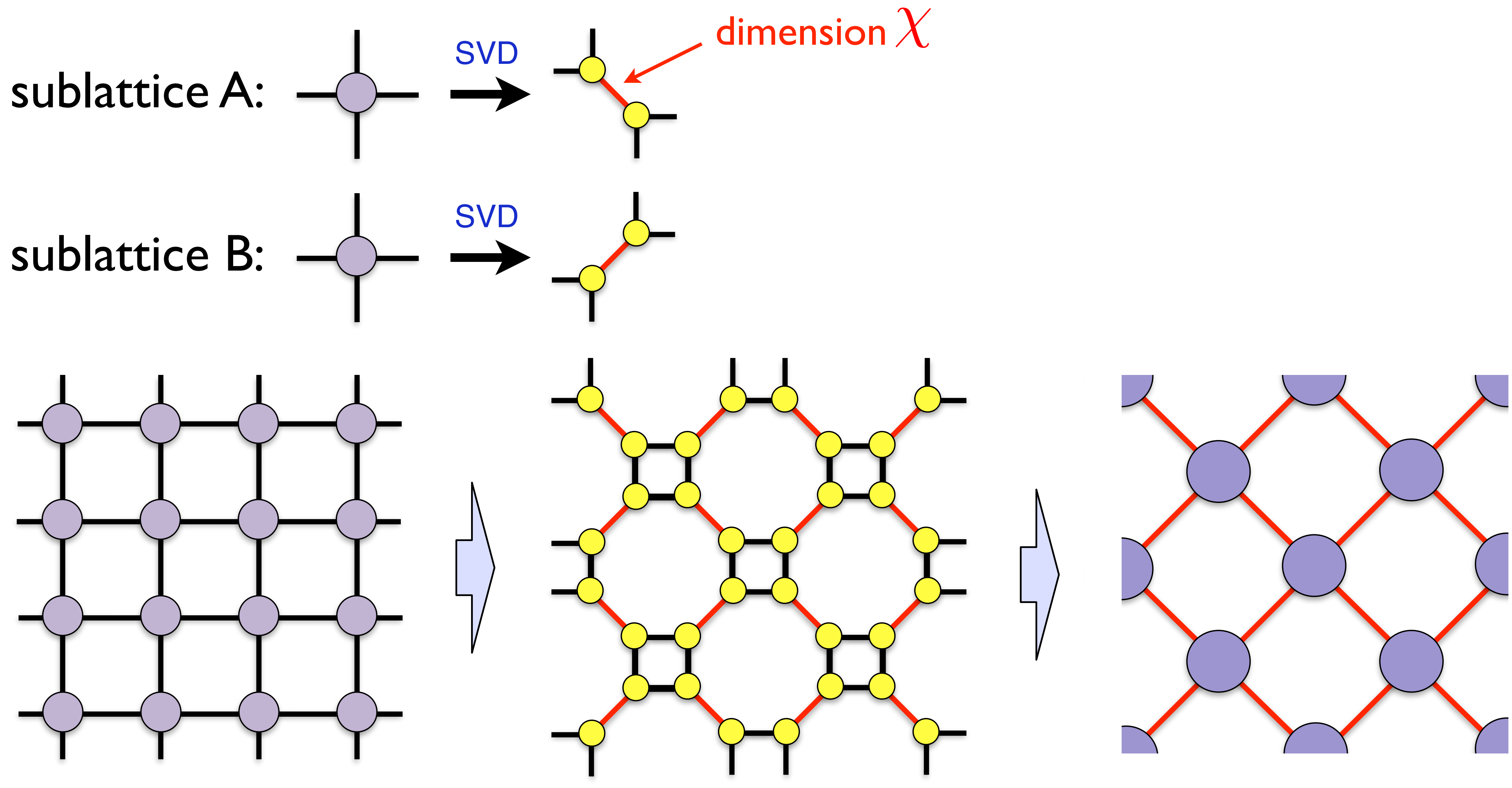
Unit cell with 30 tensors (60 sites)

(example: Shastry-Sutherland model)

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)

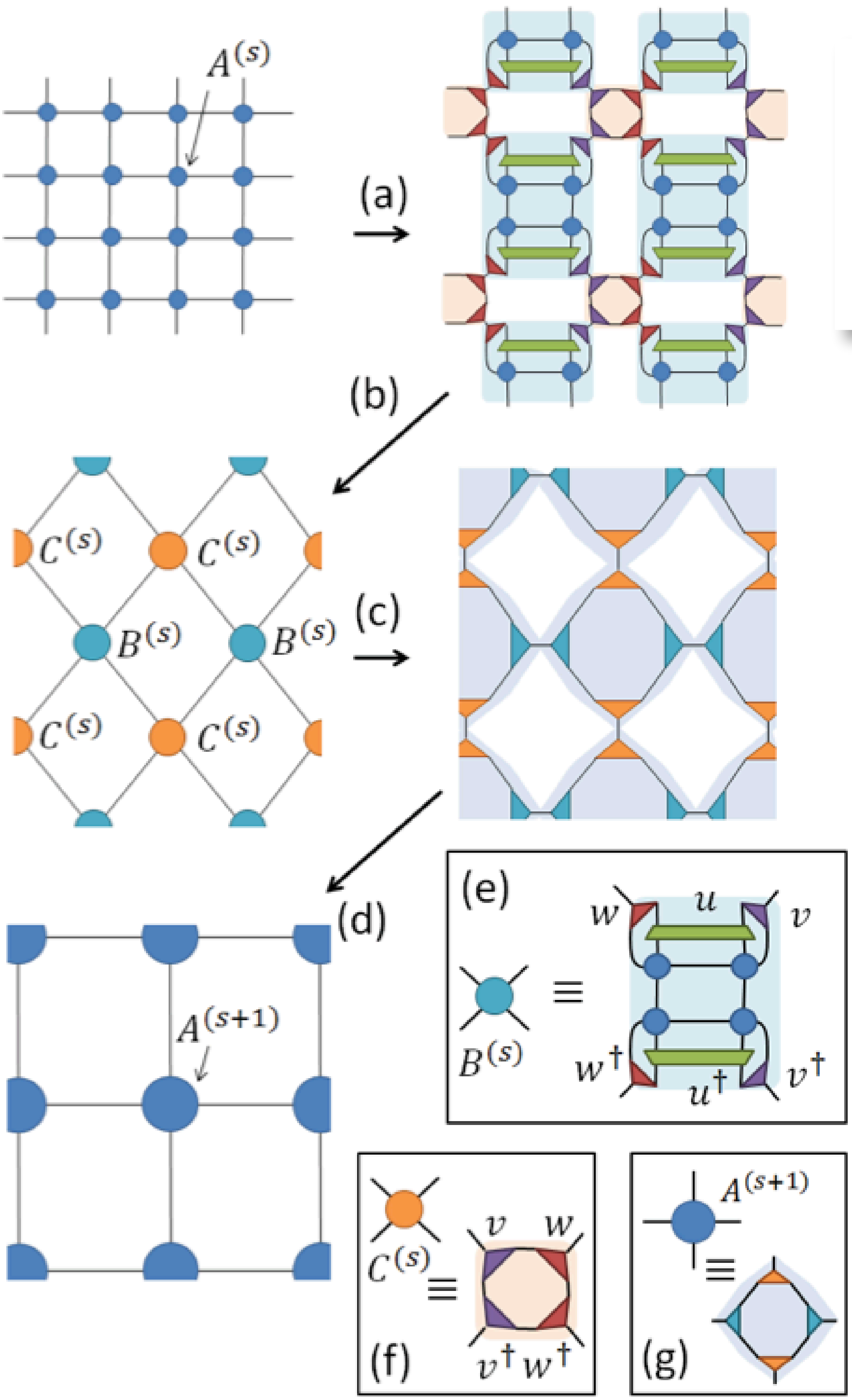


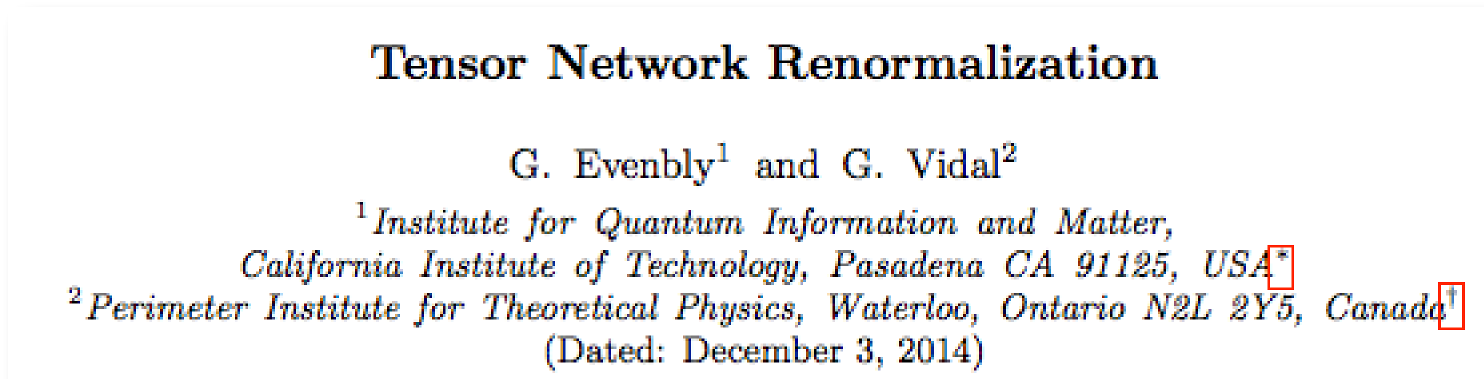
★ Contract PEPS with periodic boundary conditions

★ Finite or infinite systems

★ Related schemes: SRG, HOTRG, HOSRG, ...

More recent: Tensor network renormalization




Tensor Network Renormalization

G. Evenbly[1] and G. Vidal[2]

[1]Institute for Quantum Information and Matter, California Institute of Technology, Pasadena CA 91125, USA*
[2]Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada†
(Dated: December 3, 2014)

Evenbly & Vidal, PRL 115 (2015)

- ★ Additional ingredient: **Disentanglers**
- ★ Remove short-range entanglement at each coarse-graining step (key idea of the **MERA)**
- ★ Faster convergence with chi
- ★ Especially important for **critical** systems
- ★ Another variant: Loop-TNR:
  Yang, Gu & Wen, PRL 118 (2017)

Contracting the PEPS

★ Exact contraction of an PEPS is exponentially hard!

→ *use controlled approximate contraction scheme*

MPS-MPO-based approaches

Murg,Verstraete,Cirac, PRA75 '07
Jordan,et al. PRL79 (2008)
Haegeman & Verstraete (2017)
…

Corner transfer matrix method

Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)
Fishman et al, arxiv:1711:05881
…

TRG

Tensor Renormalization Group
(variants: HOTRG, SRG, HOSRG)

Levin, Nave, PRL99 (2007)
Xie et al. PRL 103 (2009)
Xie et al. PRB 86 (2012), …

↓

TNR

Tensor Network Renormalization

Evenbly & Vidal, PRL 115 (2015)

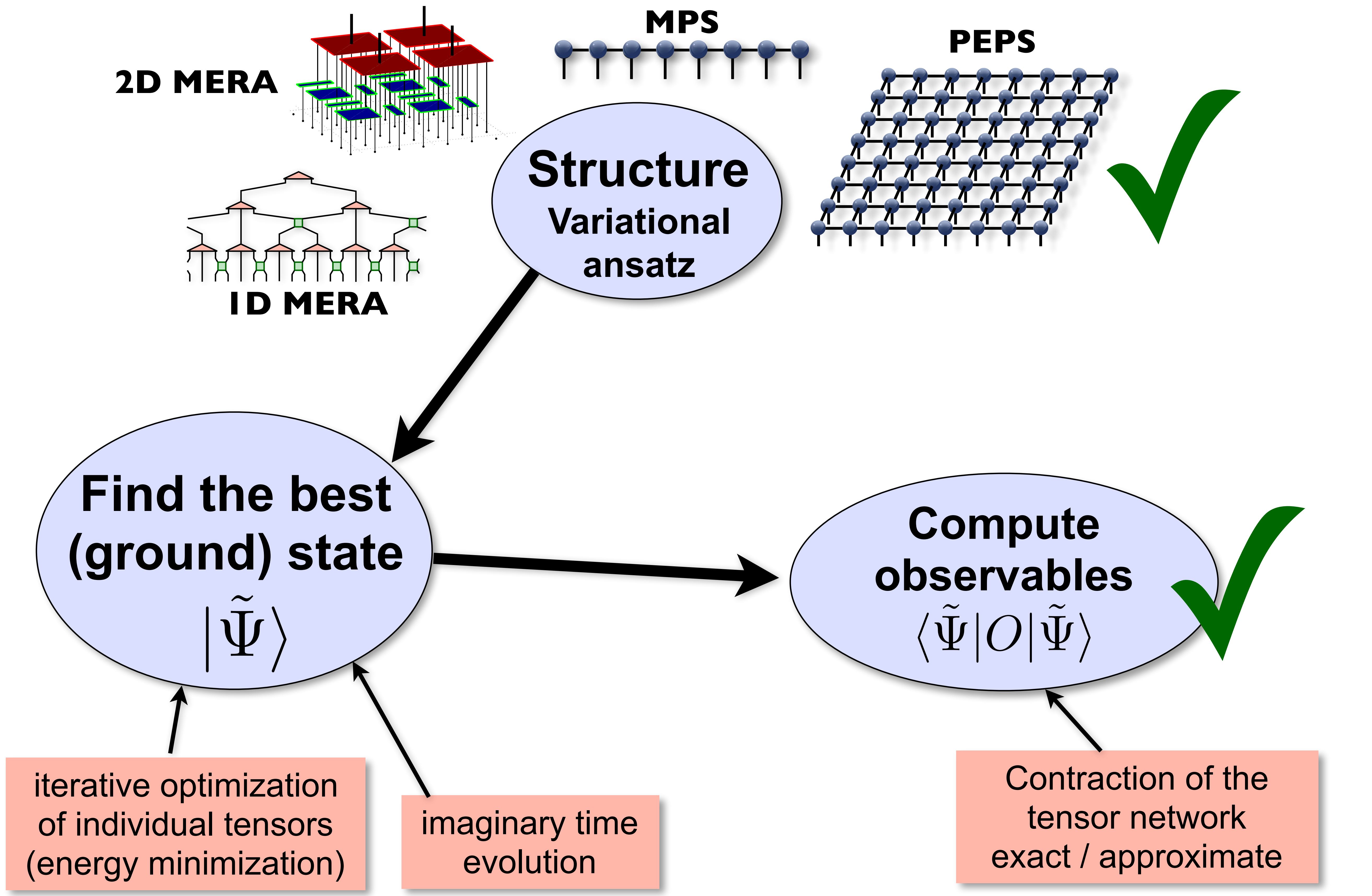
Loop-TNR:
Yang, Gu & Wen, PRL 118 (2017)

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

★ Convergence in χ needs to be carefully checked

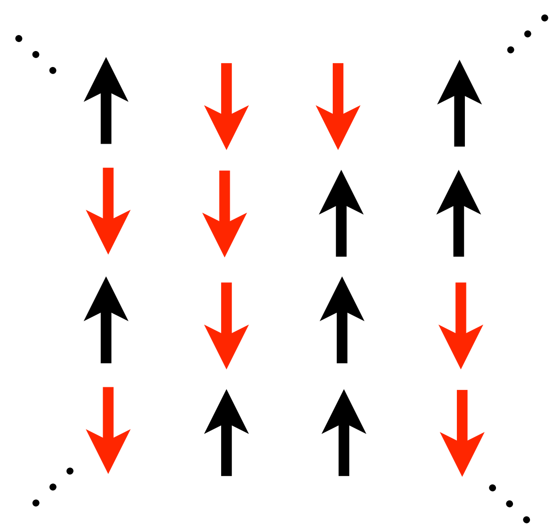
★ Overall cost: $\mathcal{O}(D^{10\dots 14})$ with $\chi \sim D^2$

Summary: Tensor network algorithm for ground state

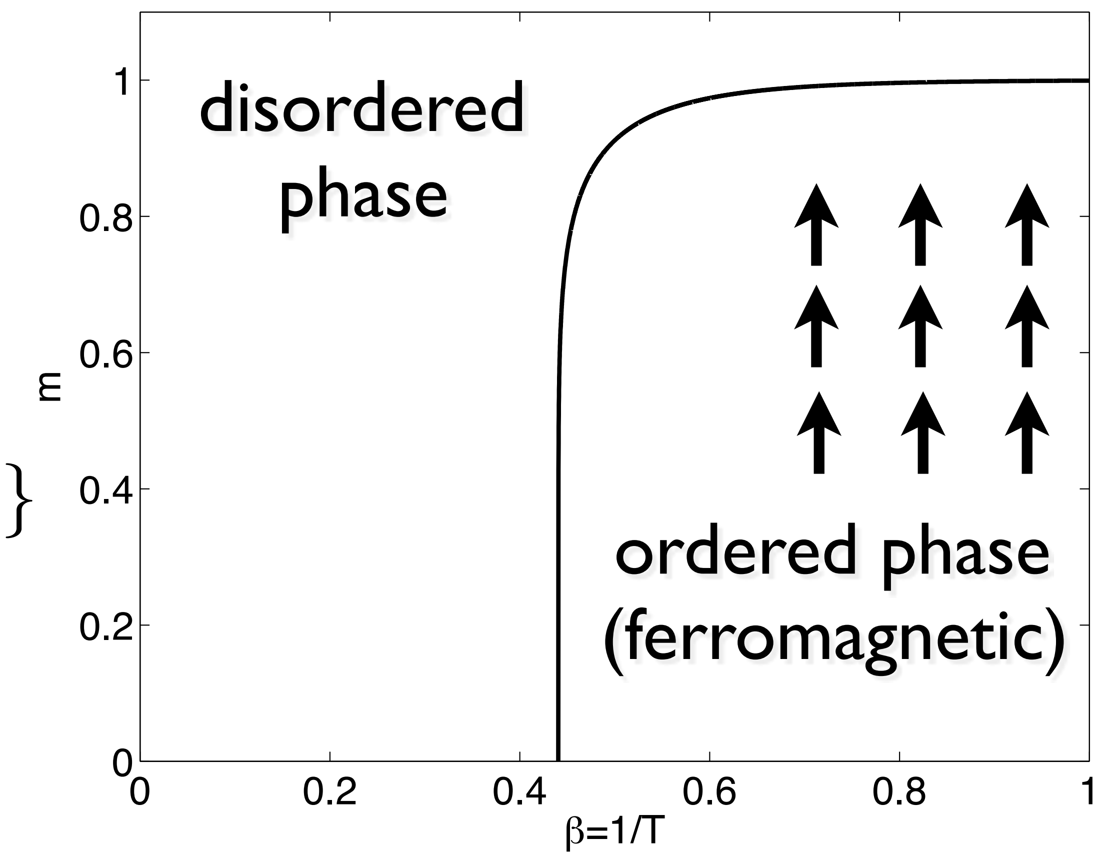


Simple example / exercise

Example: CTM method for the classical 2D Ising model



$s_i \in \{+1, -1\}$



$$H = \sum_{\langle i,j \rangle} H_b(s_i, s_j) = -\sum_{\langle i,j \rangle} s_i s_j,$$

$$\beta_c = \log(1+\sqrt{2})/2 \approx 0.44069$$

Partition function:

$$Z(\beta) = \sum_{\{c\}} \exp(-\beta H(c)) = \sum_{\{c\}} \prod_{\langle i,j \rangle} \exp(-\beta H_b(s_i, s_j))$$

GOAL: Compute m using tensor network methods

Magnetization per site:

$$m(\beta) = \frac{\sum_{\{c\}} s_r \exp(-\beta H(c))}{Z}$$

Exact solution:

$$= (1 - [\sinh(2\beta)]^{-4})^{1/8}, \quad \text{for } \beta > \beta_c$$

Represent partition function as a 2D TN

$$Q_{s_i s_j} = \exp(-\beta H_b(s_i, s_j)) = \begin{pmatrix} e^{\beta} & e^{-\beta} \\ e^{-\beta} & e^{\beta} \end{pmatrix}$$

$$Z(\beta) = \sum_{\{c\}} \exp(-\beta H(c)) = \sum_{\{c\}} \prod_{\langle i,j \rangle} \exp(-\beta H_b(s_i, s_j))$$

$$a_{ijkl} = \sum_s \left(\sqrt{Q}\right)_{is} \left(\sqrt{Q}\right)_{js} \left(\sqrt{Q}\right)_{ks} \left(\sqrt{Q}\right)_{ls}$$

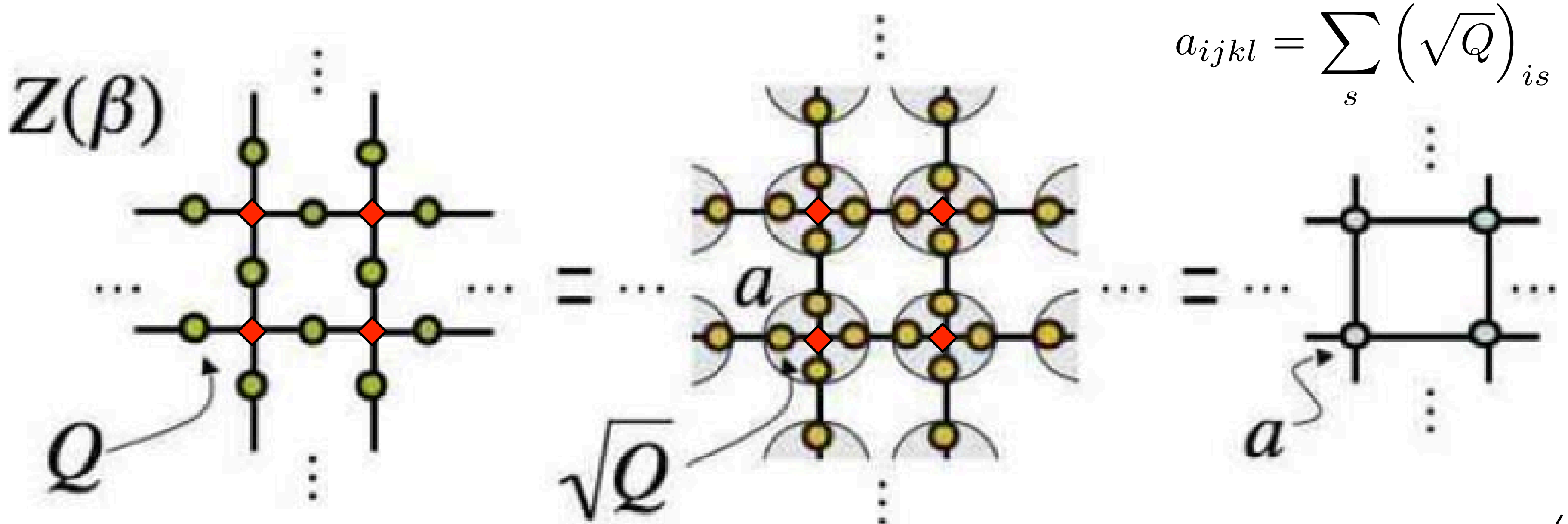
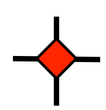


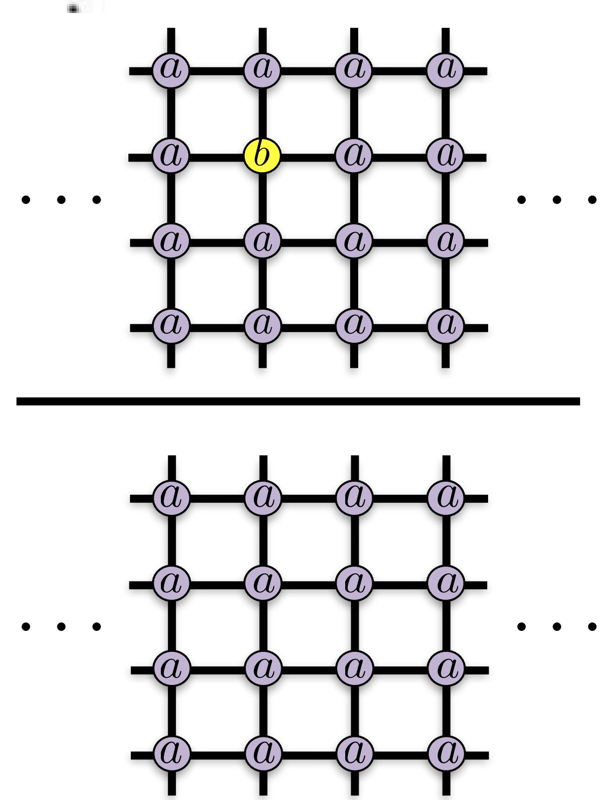
Figure taken from Orús & Vidal, PRB 78, 155117 (2008).

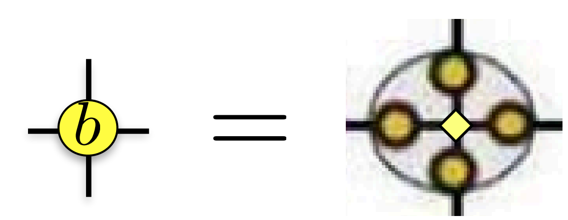


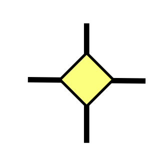
$g_{ijkl} = \delta_{ijkl}$

$$b_{ijkl} = \sum_s s \left(\sqrt{Q}\right)_{is} \left(\sqrt{Q}\right)_{js} \left(\sqrt{Q}\right)_{ks} \left(\sqrt{Q}\right)_{ls}$$

$$m(\beta) = \frac{\sum_{\{c\}} s_r \exp(-\beta H(c))}{Z} =$$



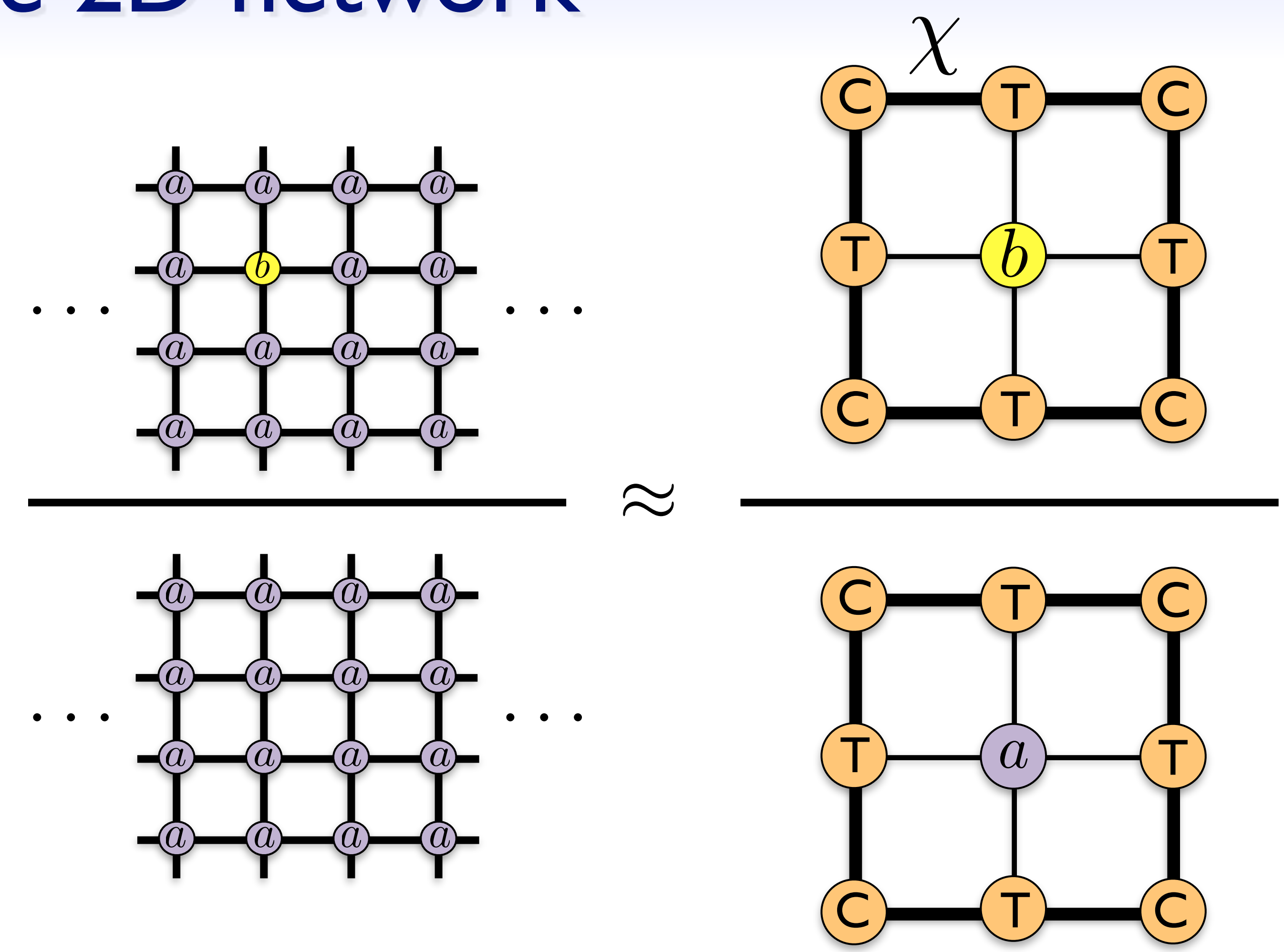




$g'_{ijkl} = s_i \delta_{ijkl}$

Use CTM to contract the 2D network

$$m(\beta) = \frac{\sum_{\{c\}} s_r \exp(-\beta H(c))}{Z} =$$



- Compute environment tensors C and T iteratively (CTM)
- Here: symmetric case: all corner/edge tensors the same and

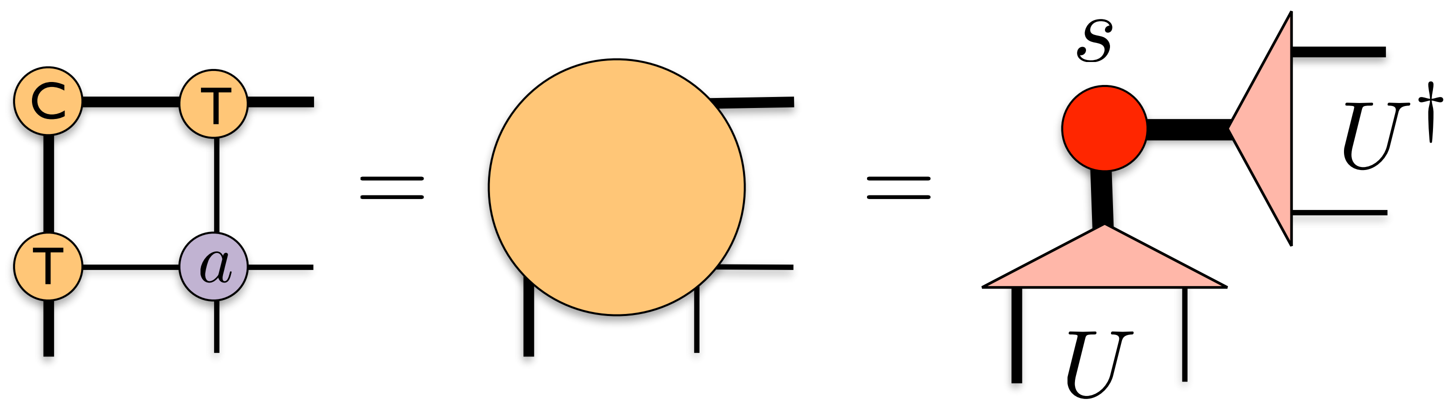
$$C_{ij} = C_{ji} \qquad T^k_{ij} = T^k_{ji}$$

- Start with random (symmetric) C and T, e.g. with $\chi_0 = 2$

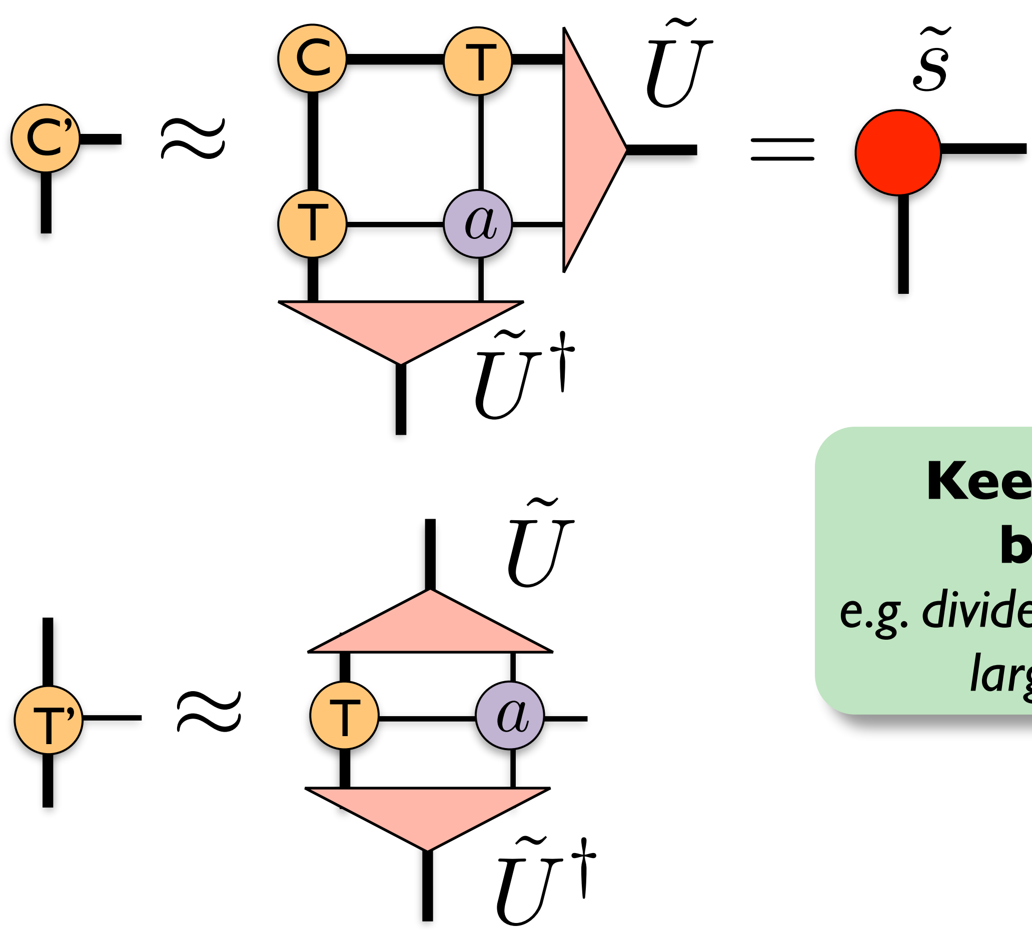
CTM for rotational/mirror symmetric tensors

Nishino, Okunishi, JPSJ65 (1996)

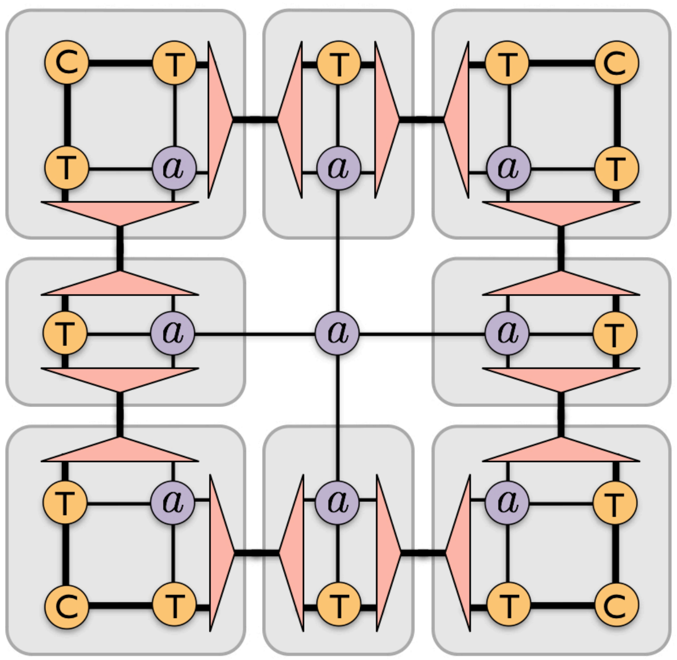
Eigenvalue decomposition of corner



Renormalized tensors: keep only χ states with largest weights



Keep numbers bounded:
e.g. divide each tensor by its largest element

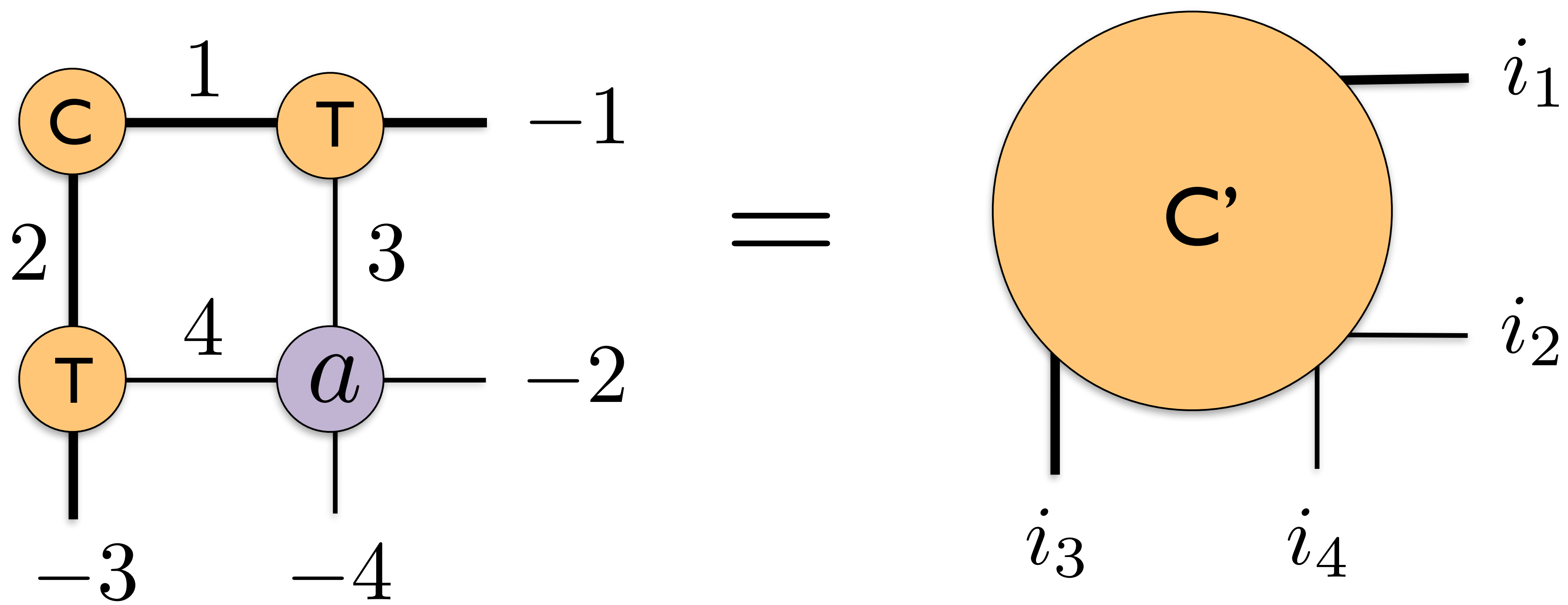


CTM algorithm summary

- Start with random (symmetric) C and T, e.g. with $\chi_0 = 2$
- Do CTM renormalization steps, keeping (at most) a boundary dimension χ
  - *The method is converged once the change* $\sum_k |s_k - s'_k| < tol$
    where s_k *(truncated & normalized) are the singular values of corner C*
  - *Due to round-off errors the tensors might not be perfectly symmetric anymore. For better numerical stability, symmetrize matrix before doing svd/eig.*
- Once convergence is reached, quantities of interest (e.g. m) can be computed using the converged environment tensors C and T
- **Try it out: this is an ideal starting point to get into 2D TN!**
- **See MATLAB solution code: https://tinyurl.com/ybtpqoeq**

Contracting TNs using NCON

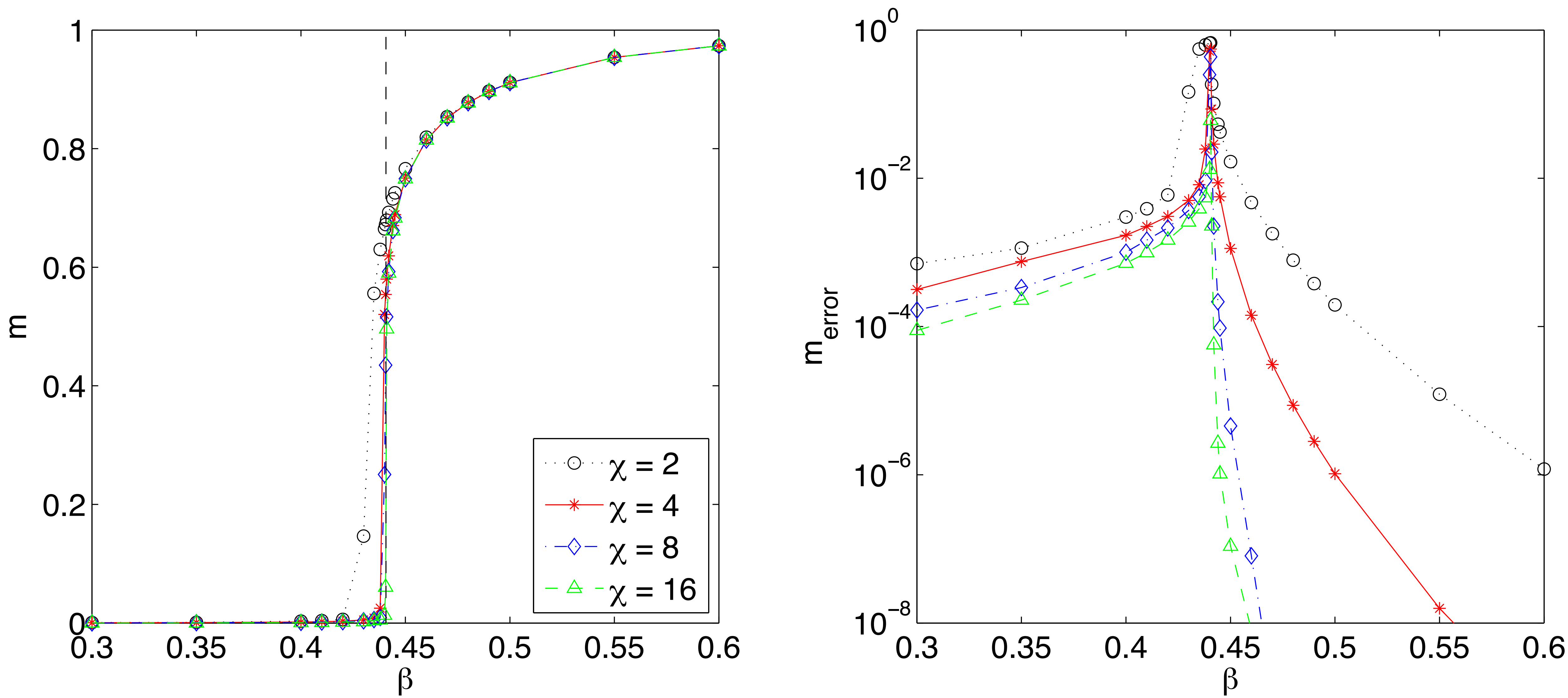
- NCON: Network contractor to conveniently contract TNs
- Written by R. N. C. Pfeifer, G. Evenbly, S. Singh, and G. Vidal, arXiv:1402.0939
- Example:



- Code: Cp = ncon({C, T, T, a},{[1 2], [-1 1 3], [2 -3 4], [-2 3 4 -4]});

- Complicated networks can be contracted in an easy way **in a single line!**

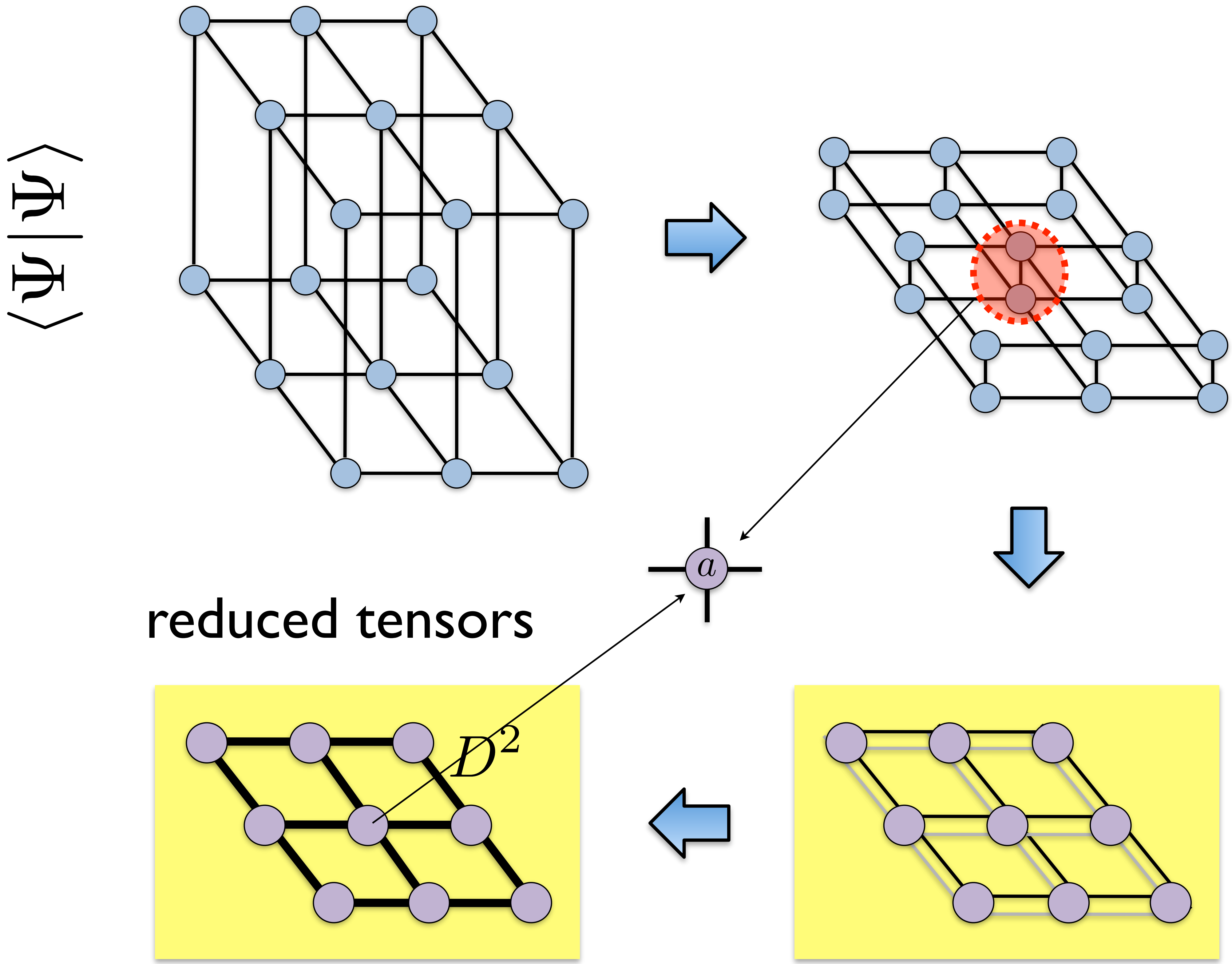
Results



1
0.8
0.6
0.4
0.2
0
m
0.3
0.35
0.4
0.45
0.5
0.55
0.6
β
χ = 2
χ = 4
χ = 8
χ = 16
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
m_{error}
0.3
0.35
0.4
0.45
0.5
0.55
0.6
β

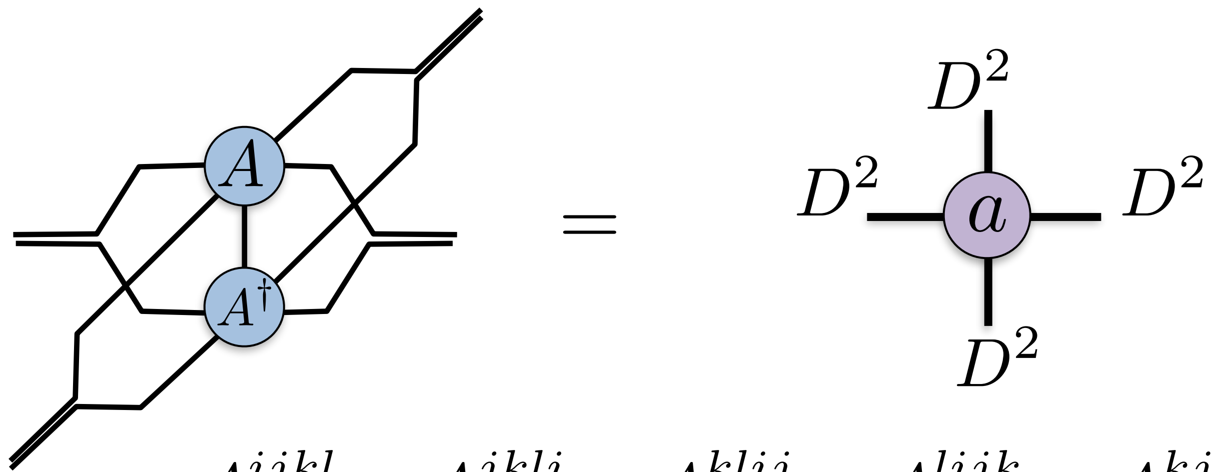
Ex 2: CTM for the symmetric quantum case (D=2)

- Remember PEPS/iPEPS contraction:



Ex 2: CTM for the symmetric quantum case (D=2)

- Consider an iPEPS tensor from a translational+rotational invariant system

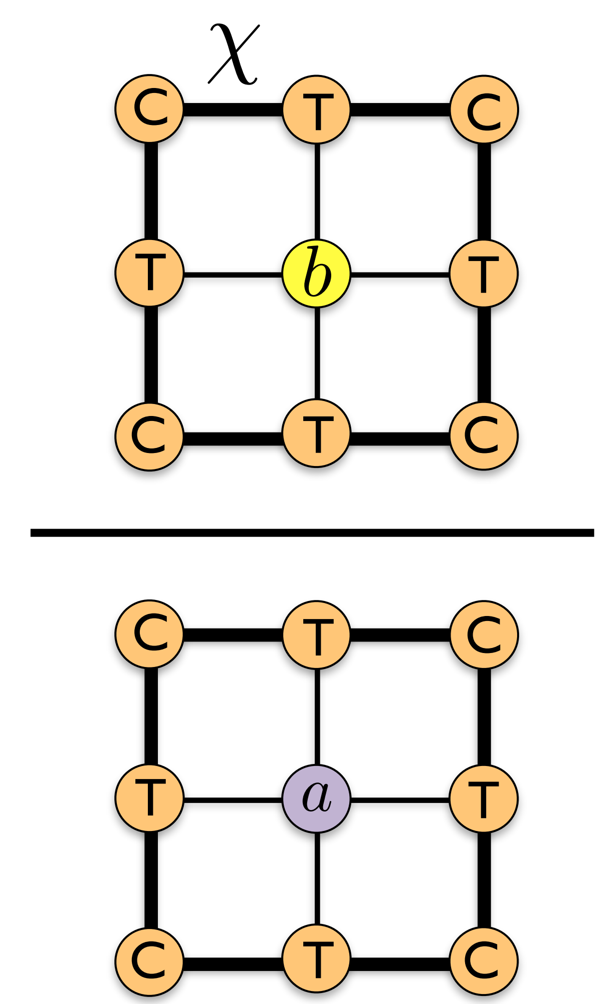


$$A_p^{ijkl} = A_p^{jkli} = A_p^{klij} = A_p^{lijk} = A_p^{kjil} = A_p^{ilkj}$$

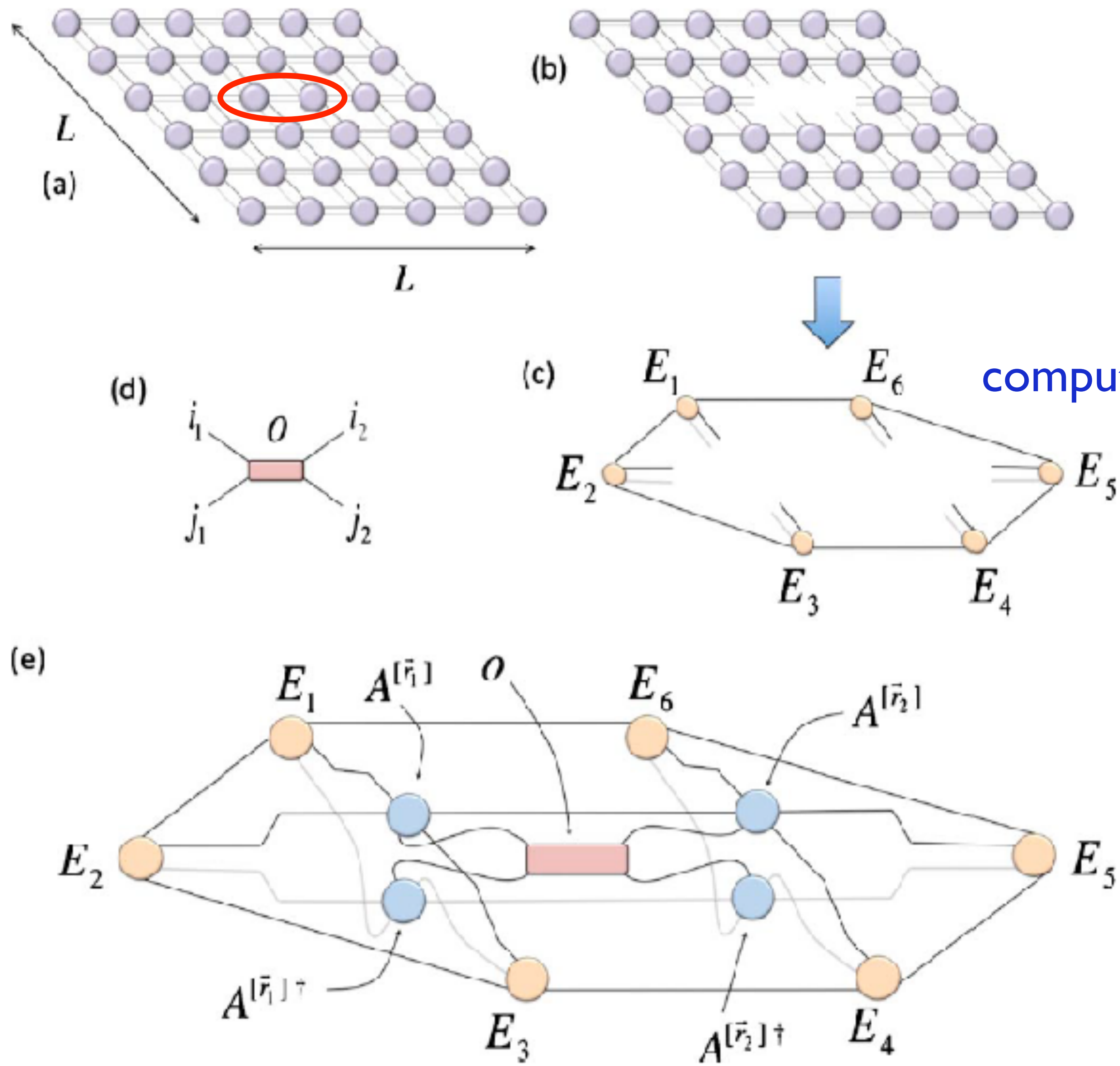
- For D=2: 12 free parameters c

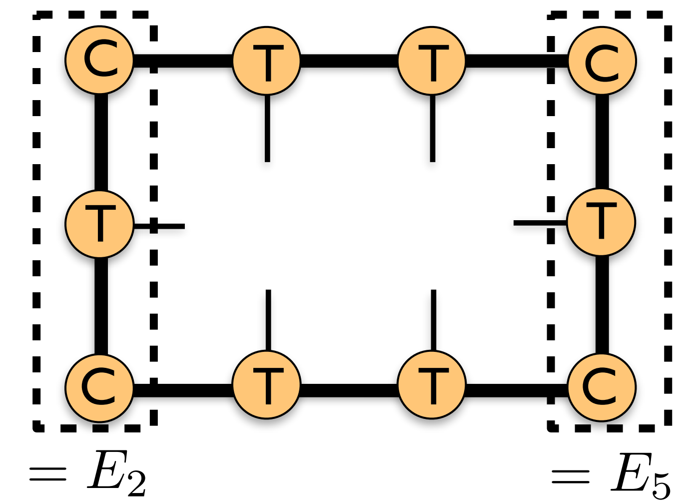
- Compute environment tensors as in the classical case

- Compute expectation values: $\langle O \rangle = \dfrac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx$



Compute expectation values (2-site operators)





compute environment approximately

Connect two-body operator

or leave physical indices open to compute 2-site reduced density matrix

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

Play around with the D=2 quantum case...

- Consider 2D transverse Ising model: $H = -\sum_{\langle i,j \rangle} \sigma_z^i \sigma_z^j - \lambda \sum_i \sigma_x^i$
- Critical point: $\lambda_c \approx 3.0444$
- Write a function to compute the energy for a given iPEPS tensor A(c)
- You can try different random guesses and see how the energy changes...
- Try a brute-force minimization (works fine here since "only" 12 parameters) using some standard routine (e.g fmincon from MATLAB).
  Since the norm does not matter we can limit the search [-1,1] for all parameters

```
x1 = ones(1,12);
opts.TolFun=1e-8;
opts.MaxFunEvals=10000;
[cres,Eres] = fmincon(@get_E,c,[],[],[],[],-x1,x1,[],opts);
```

Example values:

λ	E_{bond}
1	-1.06283
2	-1.25565
3	-1.59727
4	-2.06688

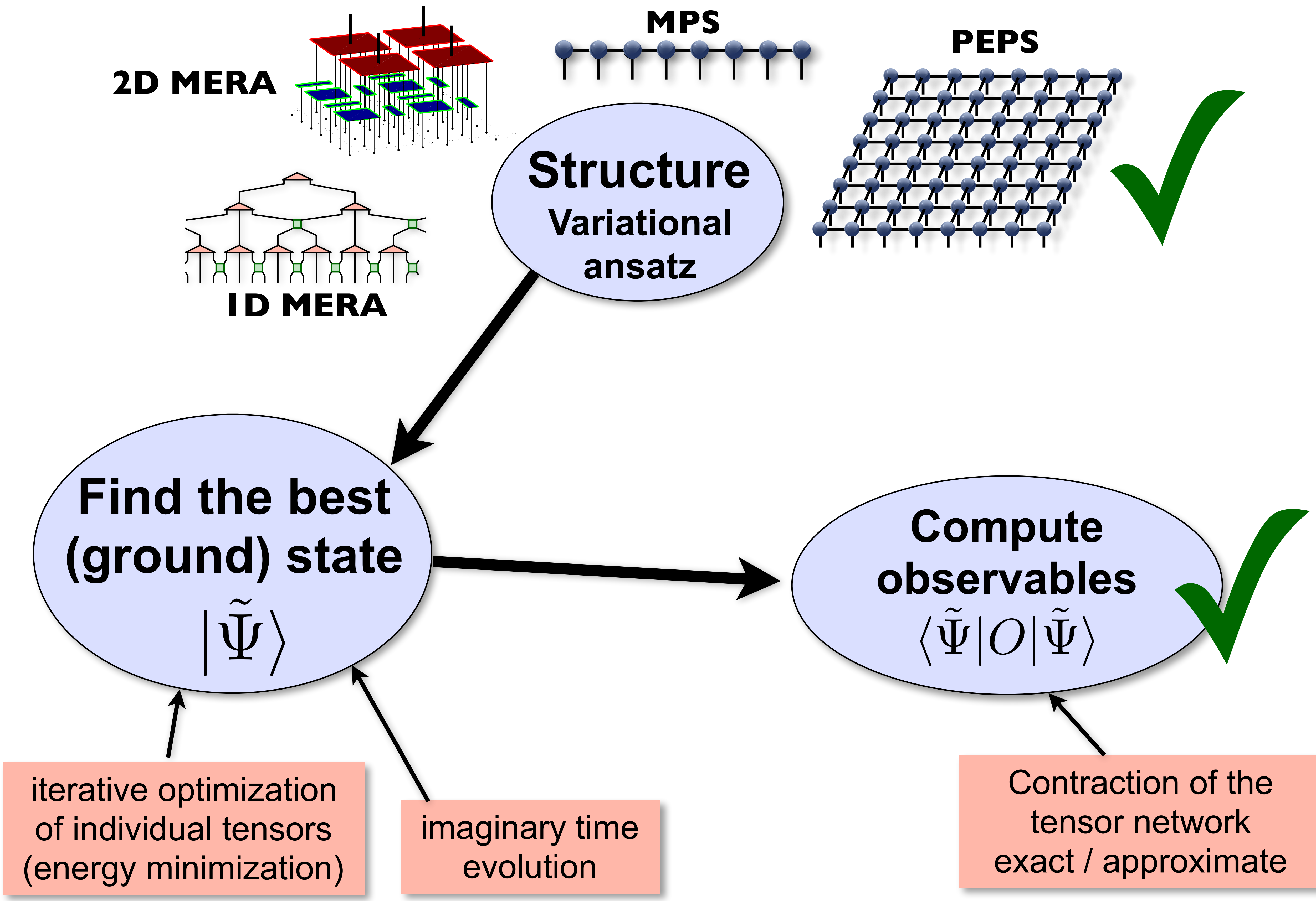
Outline

- Part I: Tensor network ansaetze
- Part II: Contraction

- Part III: Optimization (PEPS + iPEPS)
  - *Imaginary time evolution: simple vs full optimization*
  - *Variational optimization (energy minimization)*
- Part IV: iPEPS application example
  - *Shastry-Sutherland model*
- Part V: Finite correlation length scaling
  - *Accurate study of continuous phase transitions and order parameter extrapolation*
- Outlook & summary

PART III: Optimization

Summary: Tensor network algorithm for ground state

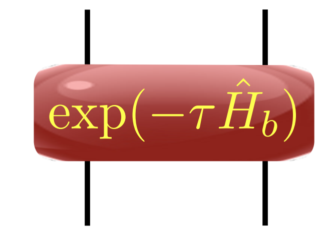


Optimization via imaginary time evolution

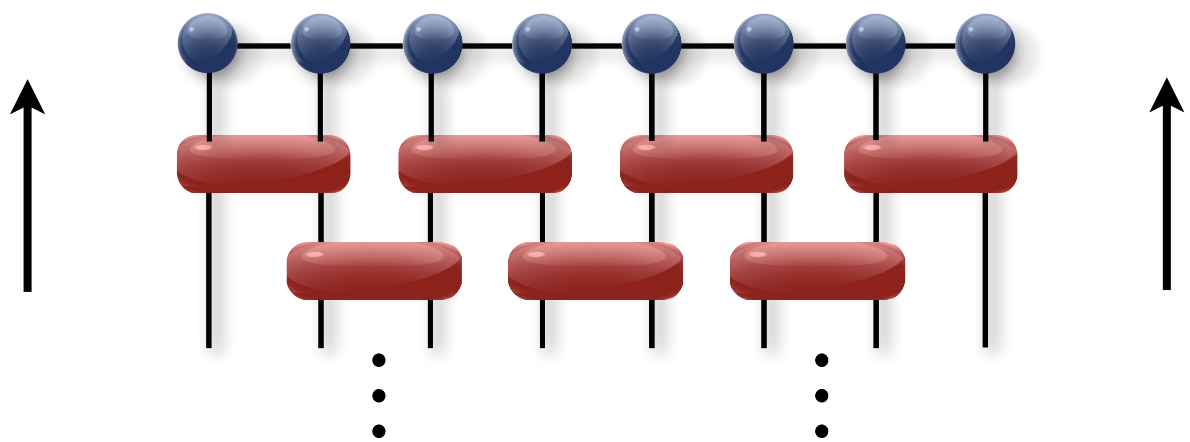
- Idea: $\exp(-\beta\hat{H})|\Psi_i\rangle \xrightarrow{\beta\to\infty} |\Psi_{GS}\rangle$

Trotter-Suzuki decomposition:

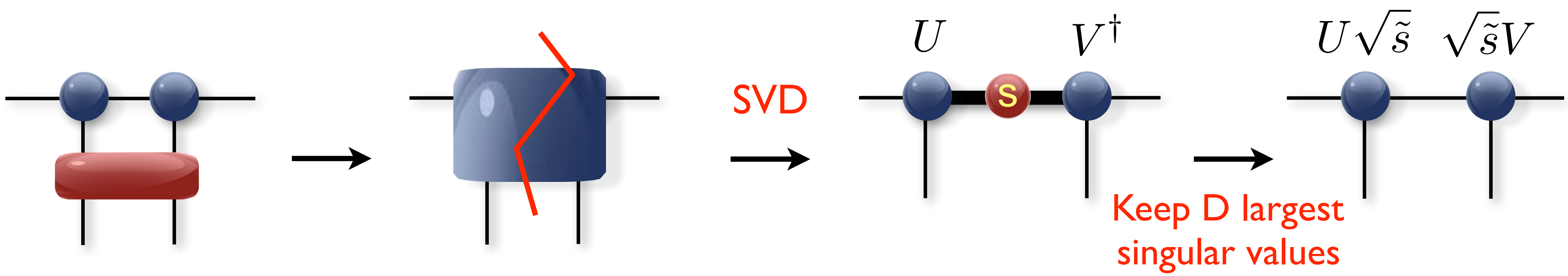
$$\exp(-\beta\hat{H}) = \exp(-\beta\sum_b \hat{H}_b) = \left(\exp(-\tau\sum_b \hat{H}_b)\right)^n \approx \left(\prod_b \exp(-\tau\hat{H}_b)\right)^n \qquad \tau = \beta/n$$



- 1D:



- 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: MPS needs to be in canonical form

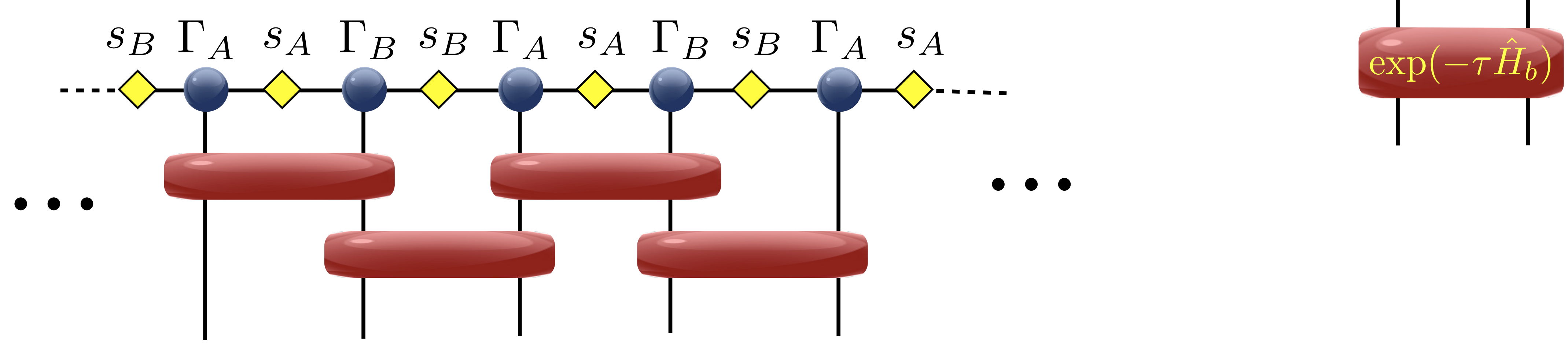
Optimization via imaginary time evolution

- Idea: $\exp(-\beta \hat{H})|\Psi_i\rangle \xrightarrow{\beta \to \infty} |\Psi_{GS}\rangle$

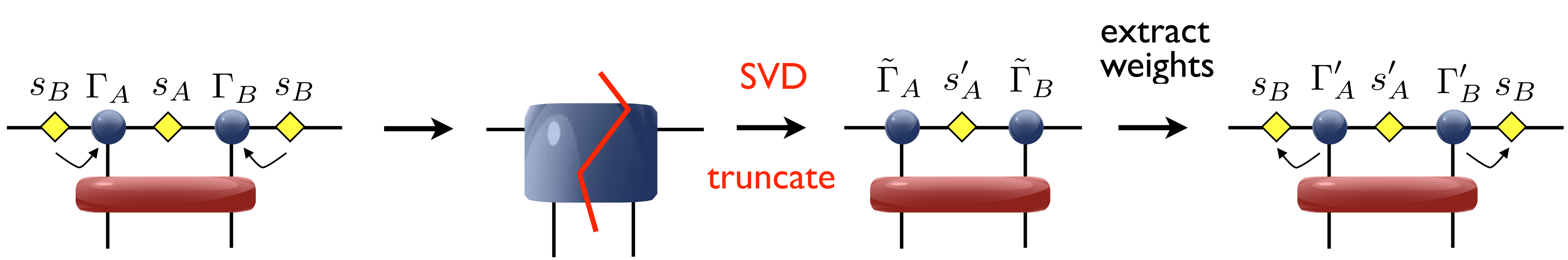
Trotter-Suzuki decomposition:

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

- 1D:

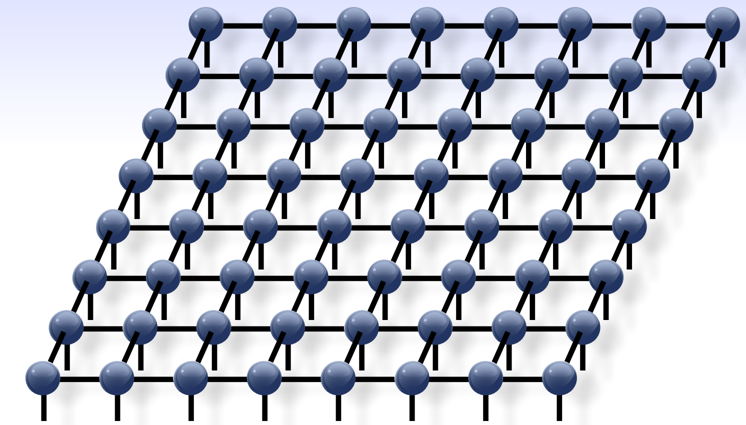


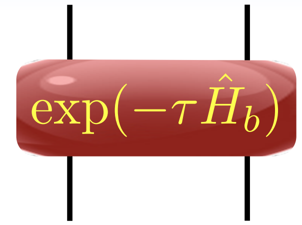
- At each step: apply a two-site operator to a bond and truncate bond back to *D*



infinite **T**ime **E**volving **B**lock **D**ecimation (iTEBD)

Optimization via imaginary time evolution



- **2D: same idea:** apply  to a bond and truncate bond back to *D*

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

simple update (SVD)

Jiang et al, PRL 101 (2008)

★ "local" update like in TEBD

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

full update

Jordan et al, PRL 101 (2008)

★ Take the full wave function into account for truncation

★ optimal, but computationally more expensive

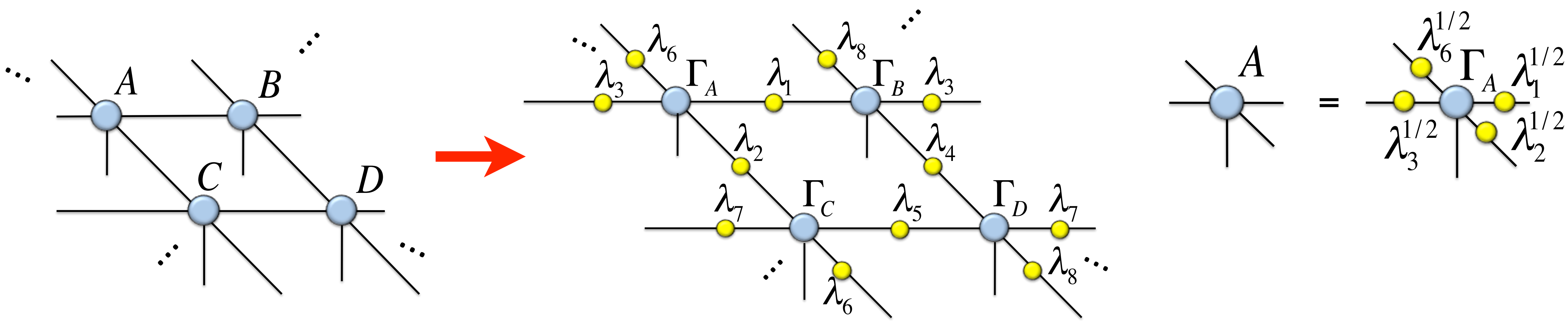
★ Fast-full update [Phien et al, PRB 92 (2015)]

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

Optimization: simple update

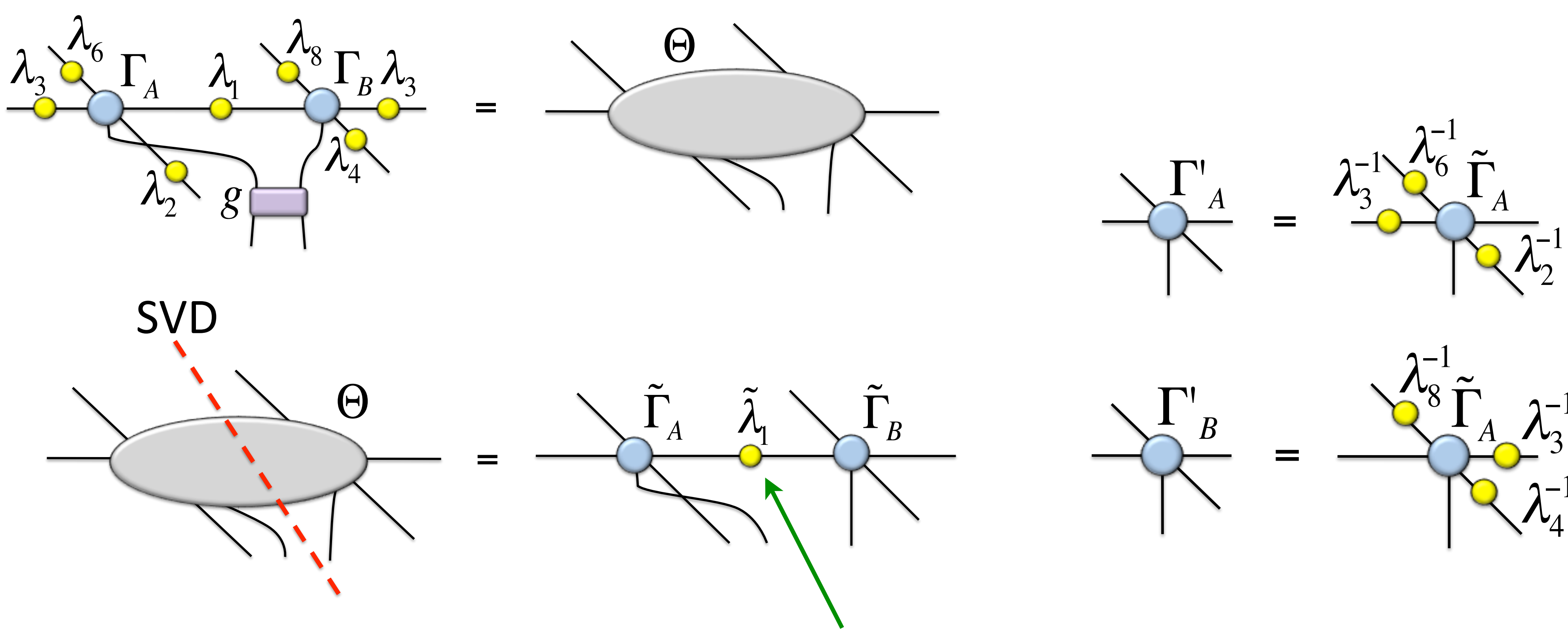
Jiang, et al., PRL 101, 090603 (2008)

- iPEPS with "weights" on the bonds (takes environment effectively into account)



- Update works like in 1D with iTEBD (infinite time-evolving block decimation)

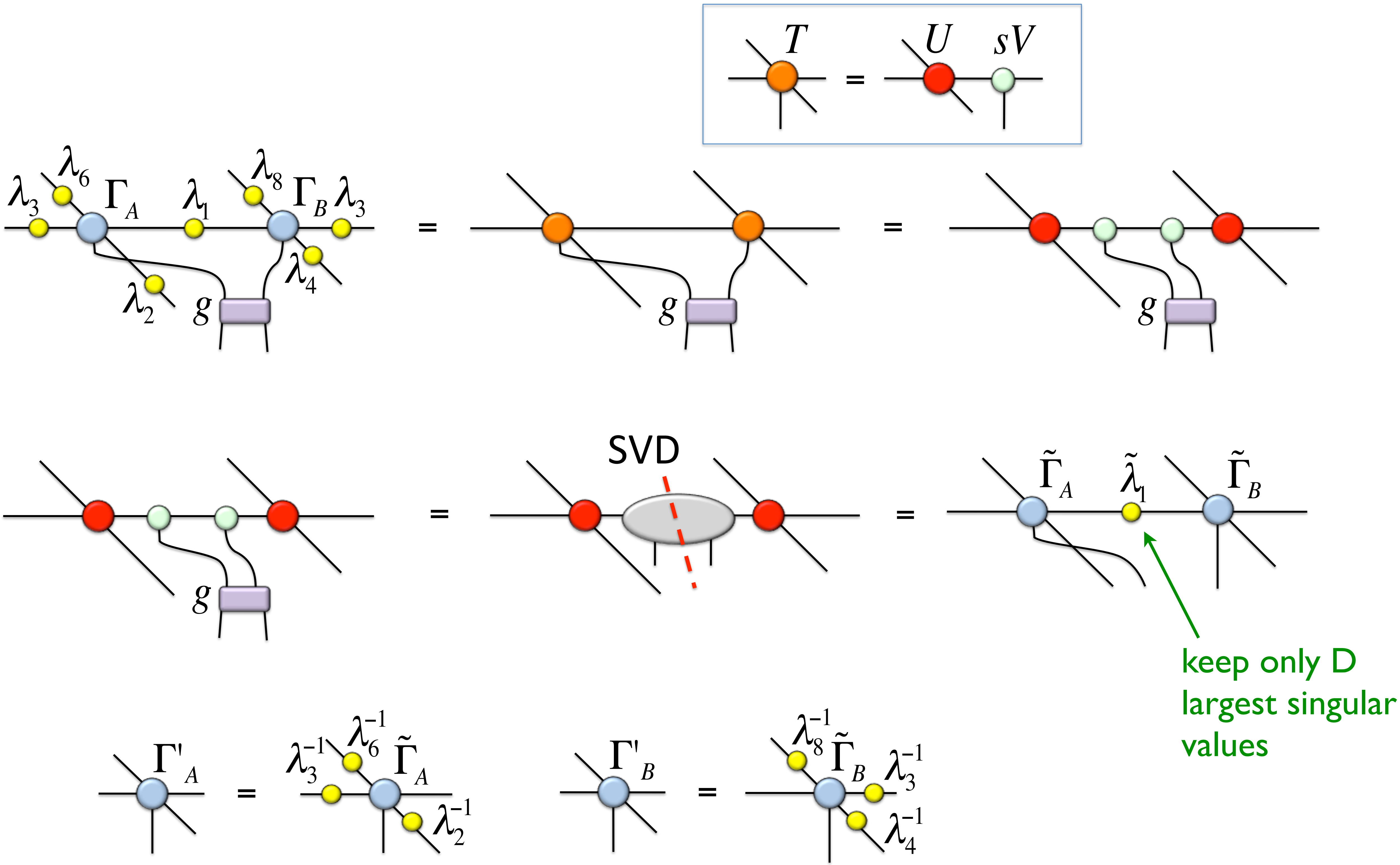
G. Vidal, PRL 91, 147902 (2003)



keep only D largest singular values

Trick to make it cheaper

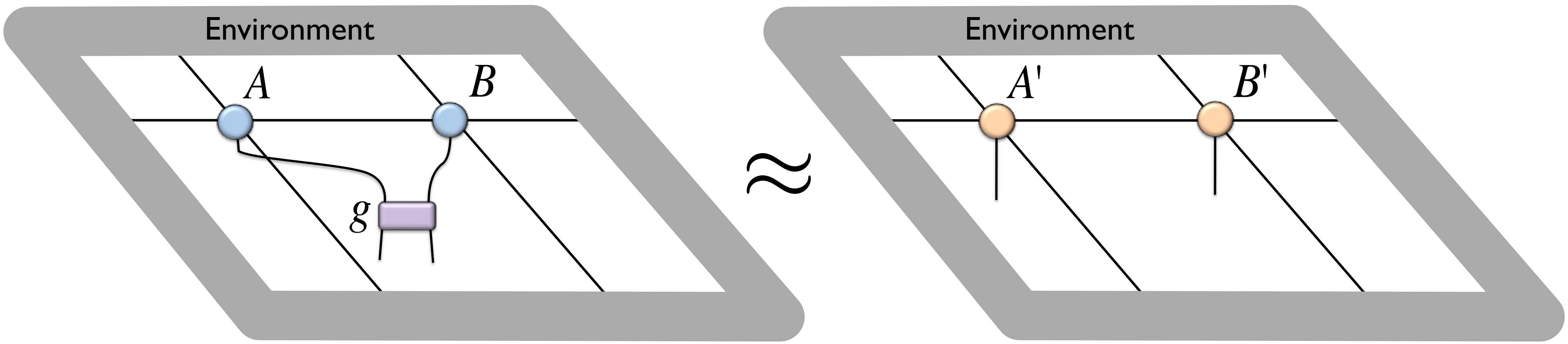
- Idea: Split off the part of the tensor which is updated



Optimization: full update

Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)
Corboz, Orus, Bauer, Vidal, PRB 81, 165104 (2010)

- Approximate old PEPS + gate with a new PEPS with bond dimension D



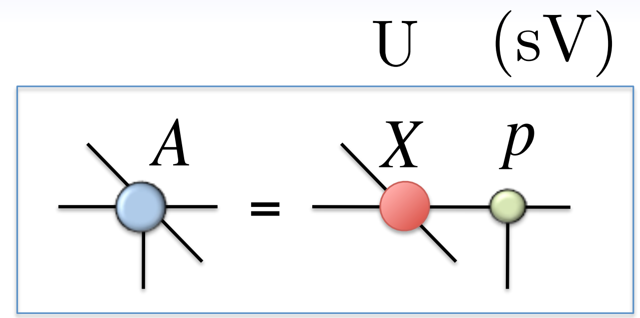
$$|\tilde{\Psi}\rangle = g|\Psi\rangle \qquad \approx \qquad |\Psi'\rangle$$

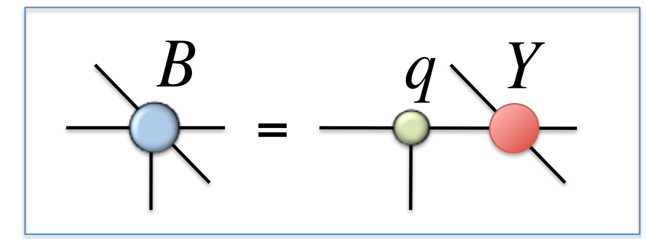
- Minimize $\quad || \, |\tilde{\Psi}\rangle - |\Psi'\rangle \, ||^2 = \langle\tilde{\Psi}|\tilde{\Psi}\rangle + \langle\Psi'|\Psi'\rangle - \langle\tilde{\Psi}|\Psi'\rangle - \langle\Psi'|\tilde{\Psi}\rangle$

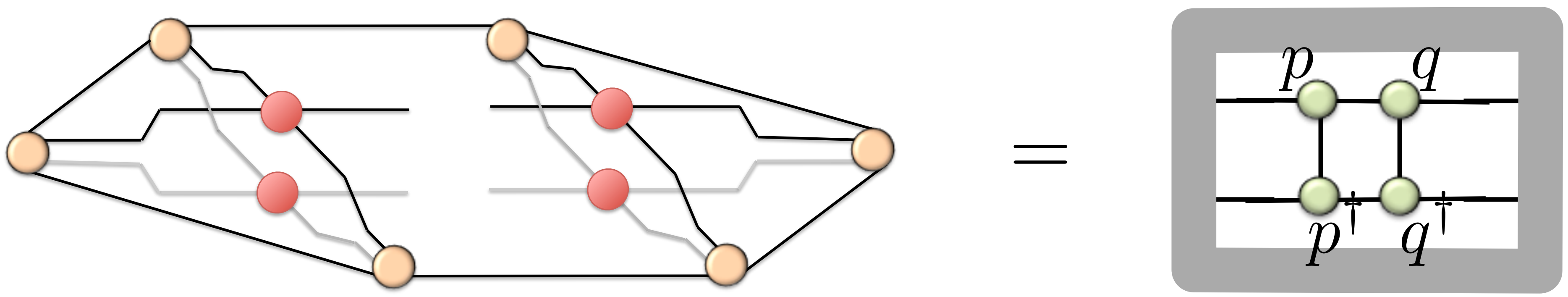
- Iteratively / CG / Newton / ...

Full-update: details

- Split off the part of the tensor which is updated







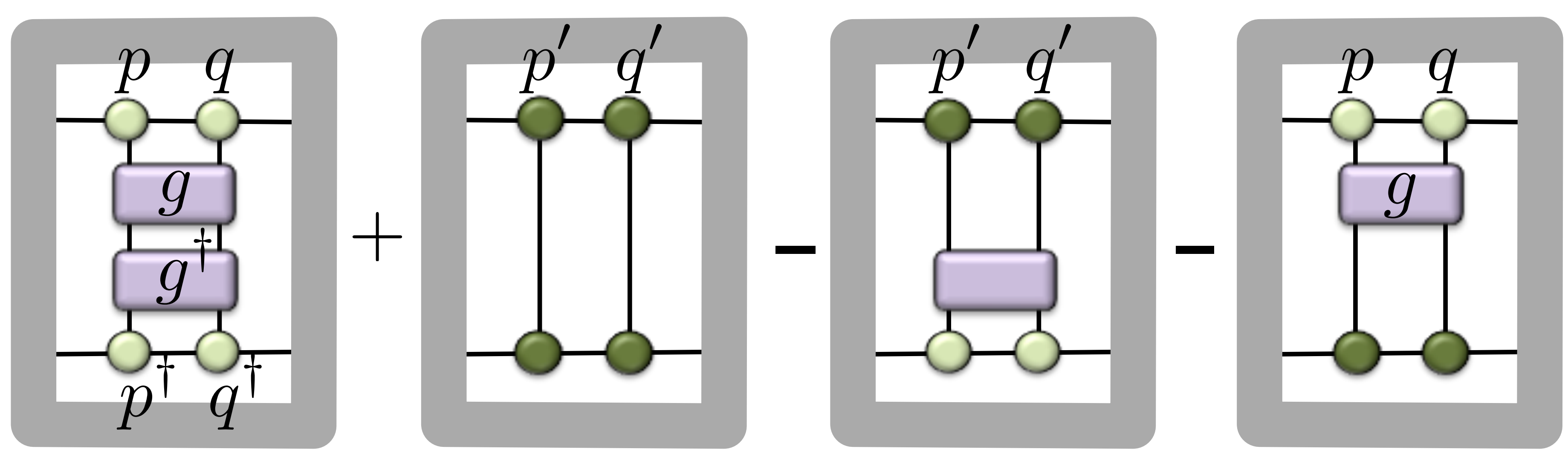
Environment of p and q tensors

$$|\tilde{\Psi}\rangle = g|\Psi(p,q)\rangle \approx |\Psi'(p',q')\rangle$$

find new p', and q' to minimize: $|| \; |\tilde{\Psi}\rangle - |\Psi'\rangle \; ||^2$

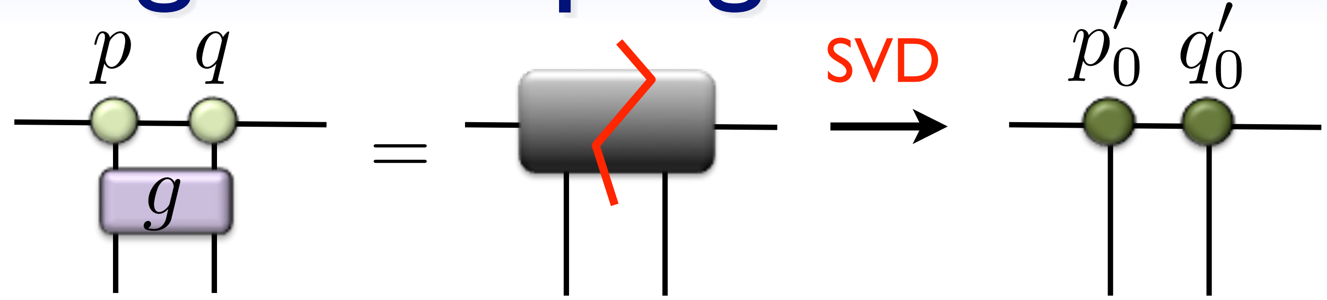
$$d(p',q') = \langle\tilde{\Psi}|\tilde{\Psi}\rangle + \langle\Psi'|\Psi'\rangle - \langle\tilde{\Psi}|\Psi'\rangle - \langle\Psi'|\tilde{\Psi}\rangle$$

"Cost-function"

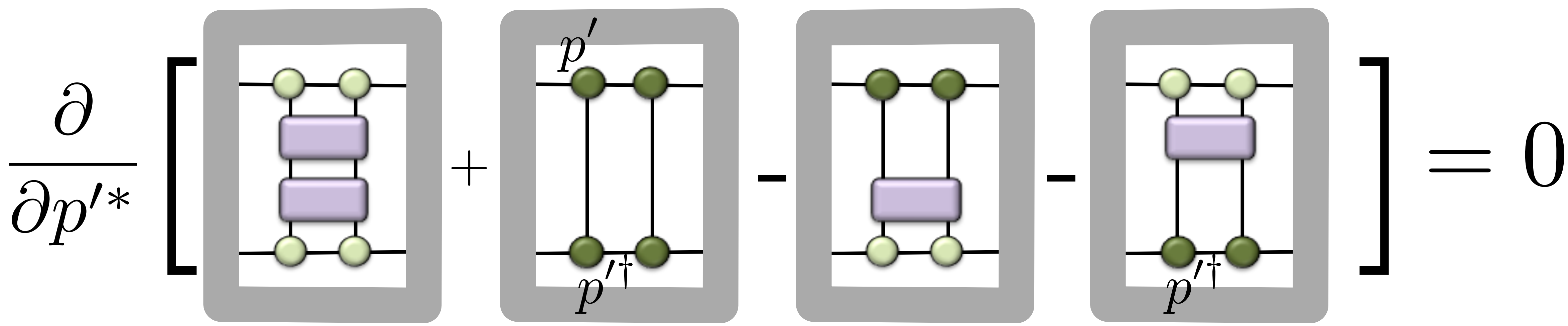


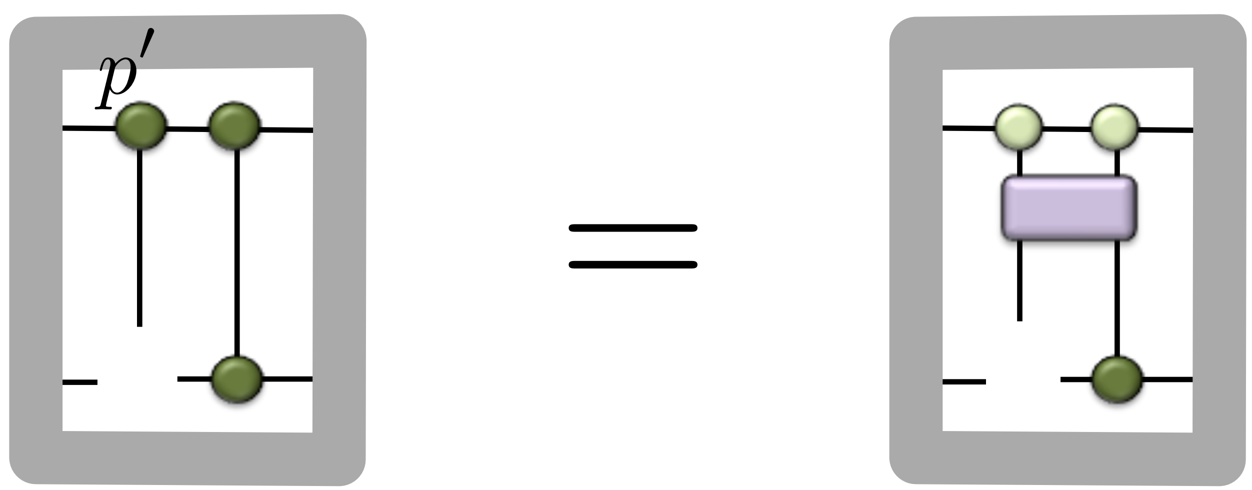
Finding p' and q' through sweeping

- Initial guess with SVD:



- Keep q' fixed and optimize with respect to p' $\frac{\partial}{\partial p'^*} d(p', q') = 0$

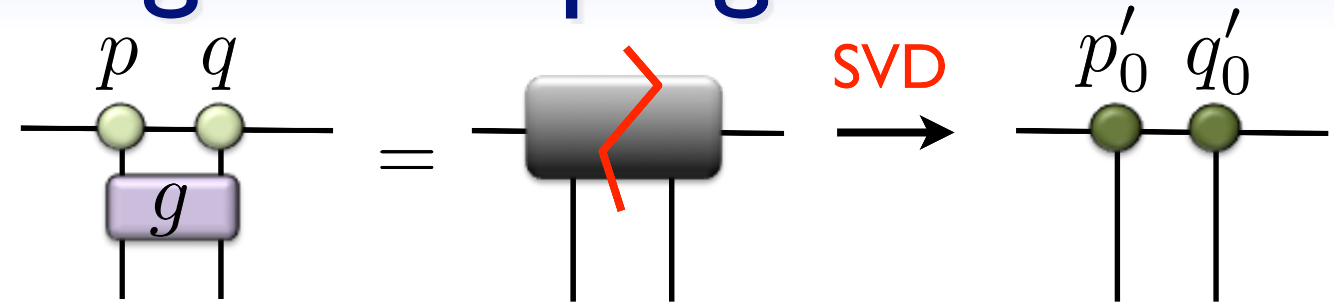




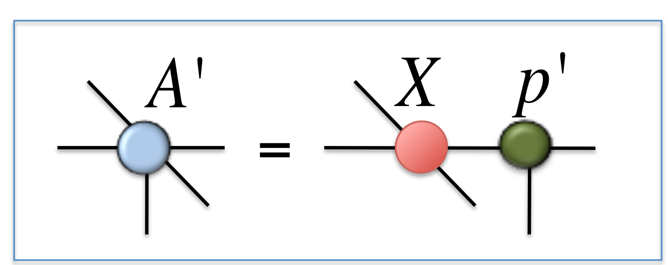
- Solve linear system: $Mp' = b \rightarrow$ **new p'**

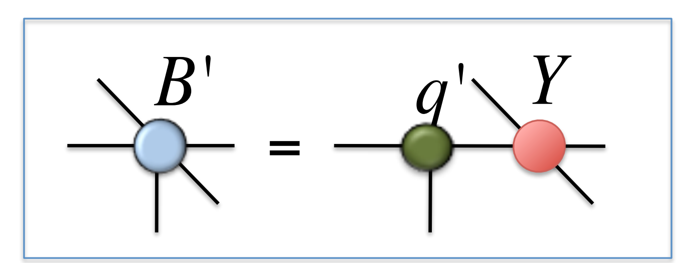
Finding p' and q' through sweeping

- Initial guess with SVD:



- Keep q' fixed and optimize with respect to p': $$\frac{\partial}{\partial p'^*} d(p', q') = 0$$
- Solve linear system: $$M p' = b \quad \longrightarrow$$ **new p'**
- Keep p' fixed and optimize with respect to q': $$\frac{\partial}{\partial q'^*} d(p', q') = 0$$
- Solve linear system: $$\tilde{M} q' = \tilde{b} \quad \longrightarrow$$ **new q'**
- Repeat above until convergence in $d(p', q')$
- Retrieve full tensors again:

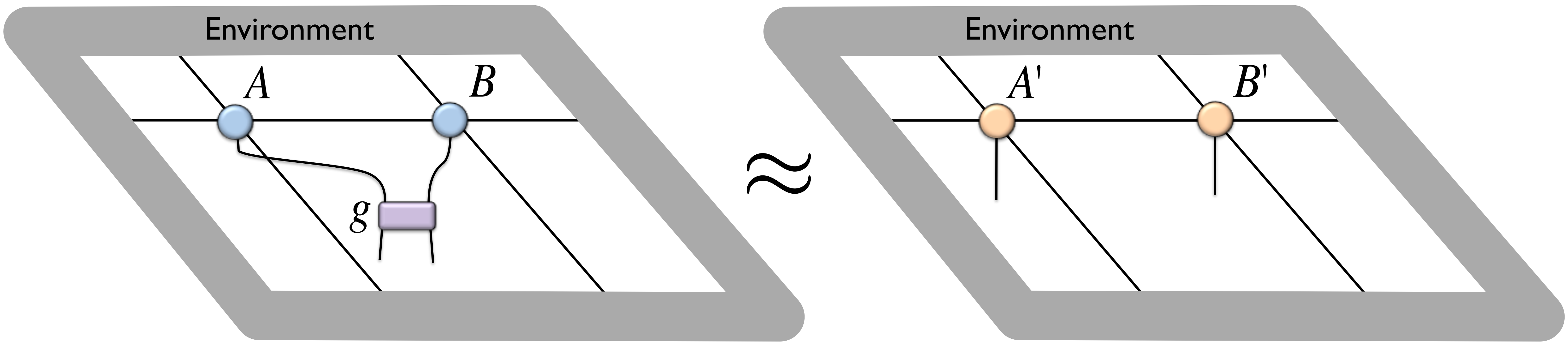




Optimization: full update

Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)
Corboz, Orus, Bauer, Vidal, PRB 81, 165104 (2010)

- Approximate old PEPS + gate with a new PEPS with bond dimension D



$$|\tilde{\Psi}\rangle = g|\Psi\rangle \quad \approx \quad |\Psi'\rangle$$

- Minimize $|| \, |\tilde{\Psi}\rangle - |\Psi'\rangle \, ||^2 = \langle\tilde{\Psi}|\tilde{\Psi}\rangle + \langle\Psi'|\Psi'\rangle - \langle\tilde{\Psi}|\Psi'\rangle - \langle\Psi'|\tilde{\Psi}\rangle$
- Iteratively / CG / Newton / ...
- The full wave function is taken into account for the truncation!
- At each step the environment has to be computed! expensive... but optimal!

Optimization: simple vs full update

simple update

★ "local" update like in TEBD

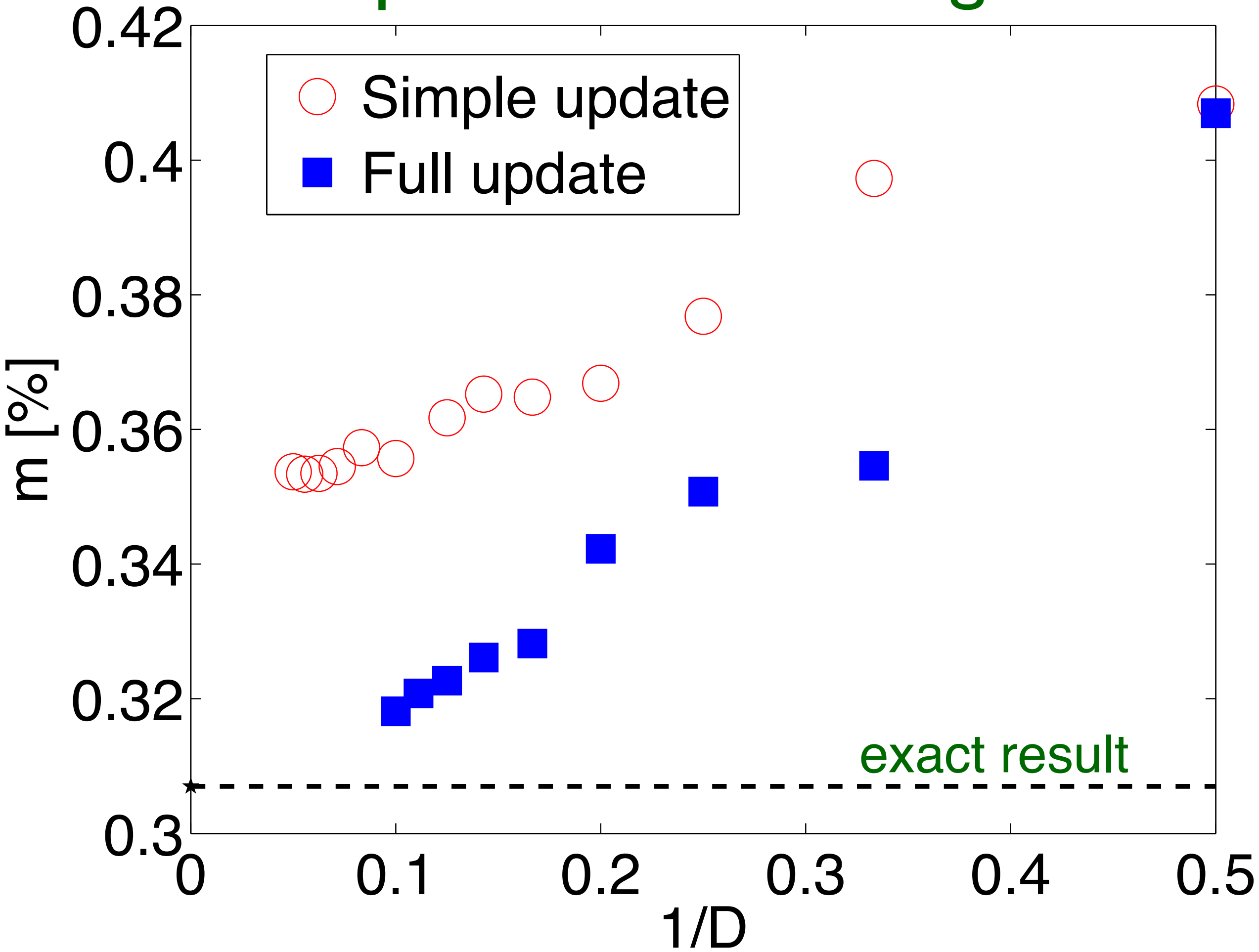
★ Cheap, but not optimal (e.g. overestimates magnetization in S=1/2 Heisenberg model)

full update

★ Take the full wave function into account for truncation

★ optimal, but computationally more expensive

Example: 2D Heisenberg model

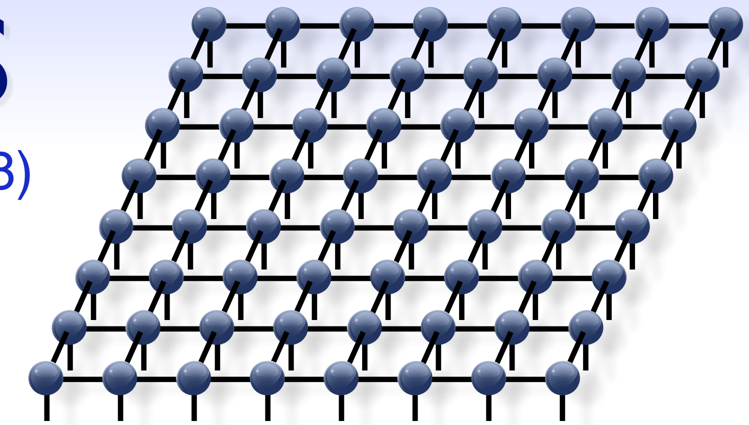


- Combine the two: Use simple update to get an initial state for the full update

- Don't compute environment from scratch but recycle previous one
  → **fast full update** Phien, Bengua, Tuan, PC, Orus, PRB 92 (2015)

Variational optimization for PEPS

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



1. Select one of the PEPS tensors A

2. Optimize tensor A (keeping all the others fixed) by minimizing the energy:

tensor network including all Hamiltonian terms

tensor network from norm term

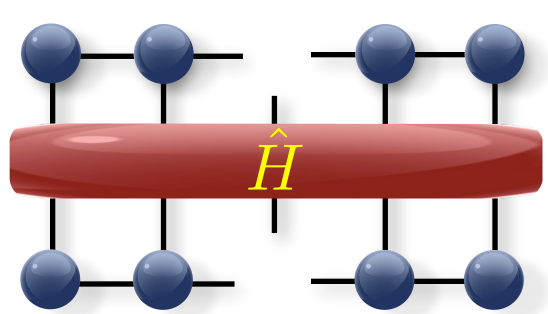
tensor A reshaped as a vector

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

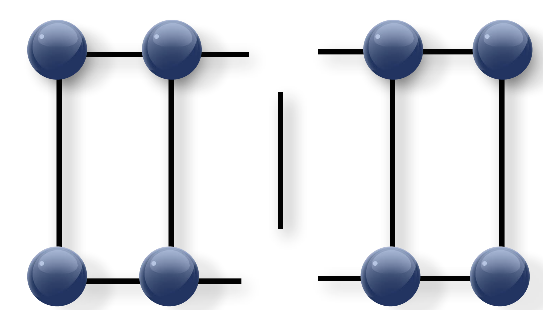
solve generalized eigenvalue problem

$\mathbf{H} =$

in 1D:

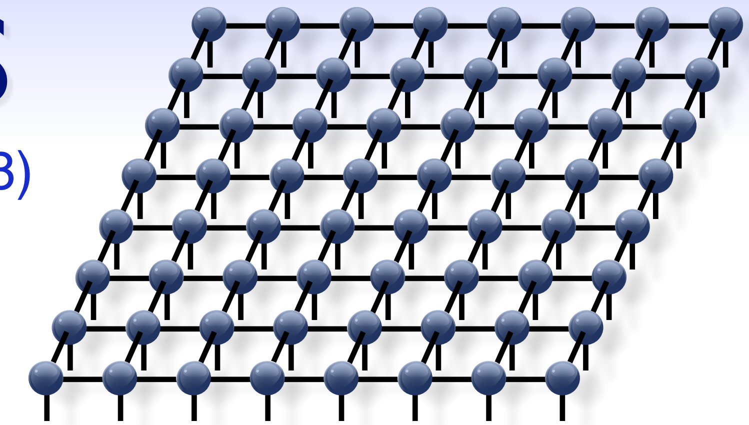


$\mathbf{N} =$



Variational optimization for PEPS

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



1. Select one of the PEPS tensors A

2. Optimize tensor A (keeping all the others fixed) by minimizing the energy:

tensor network including all Hamiltonian terms

tensor network from norm term

tensor A reshaped as a vector

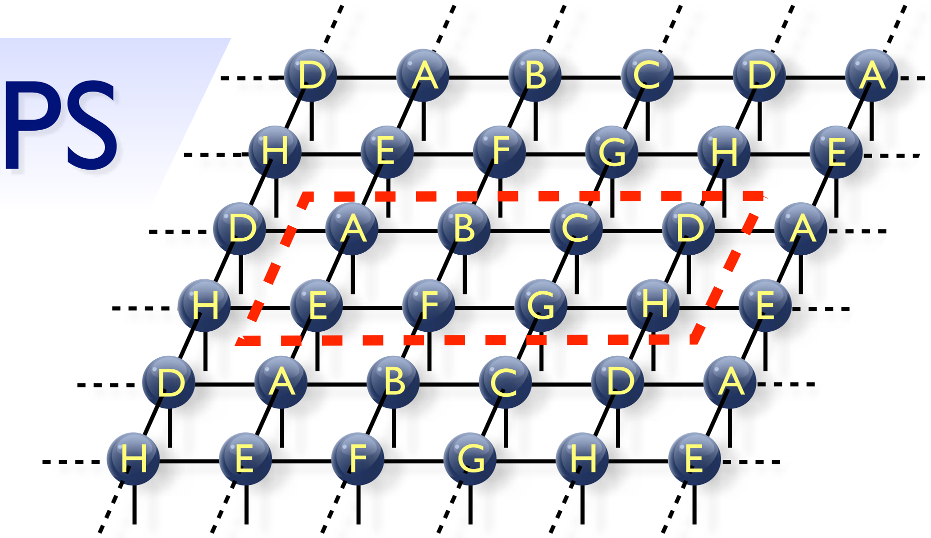
$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \xrightarrow{\text{minimize}} \mathbf{H}\, x = E\, \mathbf{N}\, x$$

solve generalized eigenvalue problem

3. Take the next tensor and optimize (keeping other tensors fixed)

4. Repeat 2-3 iteratively until convergence is reached

Variational optimization for iPEPS



Main challenges:

1. Need to take into account infinitely many Hamiltonian contributions

- ✦ Solution: use corner-transfer matrix method [PC, PRB 94 (2016)]
- ✦ Alternative: use "channel-environments" [Vanderstraeten et al, PRB 92; PRB 94 (2016)]
- ✦ Or: Use PEPO (similar to 3D classical) [cf. Nishino et al. Prog. Theor. Phys 105 (2001)]

2. Tensor A appears infinitely many times! (Min. problem highly non-linear)

- ✦ Take adaptive linear combination of old and new tensor [PC, PRB 94 (2016)] [see also Nishino et al. Prog. Theor. Phys 105 (2001), Gendiar et al. PTR 110 (2003)]
- ✦ Alternative: use CG approach [Vanderstraeten, Haegeman, PC, Verstraete, PRB 94 (2016)]

tensor network including all Hamiltonian terms

tensor network from norm term

tensor A reshaped as a vector

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

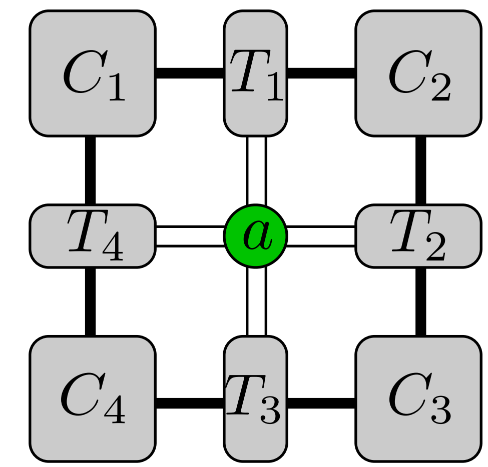
H-environment

tensor network including all Hamiltonian terms

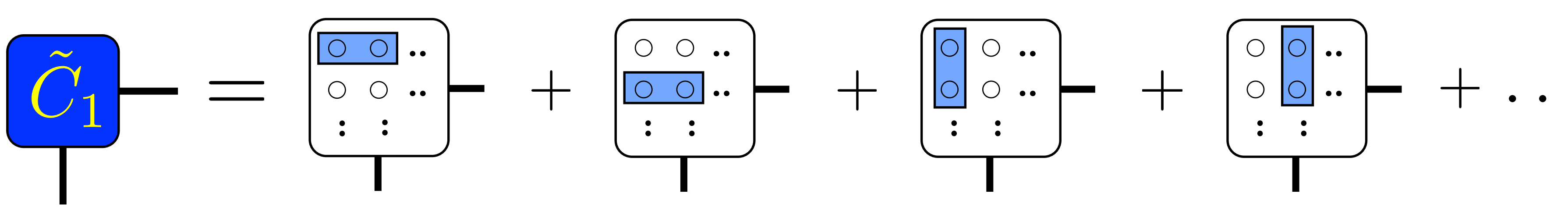
tensor network from norm ✓

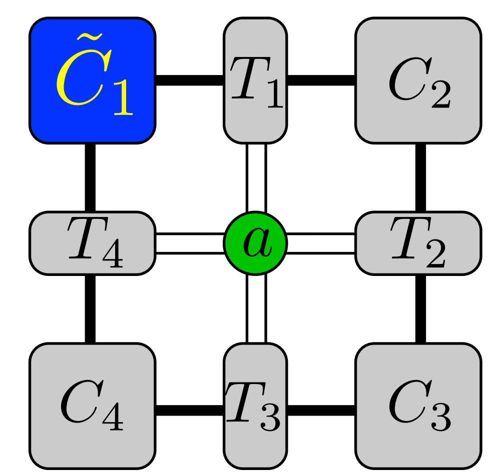
$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \xrightarrow{\text{minimize}} \mathbf{H}\, x = E\, \mathbf{N}\, x$$

But how about H ??



- Need additional **H**-environment tensors:

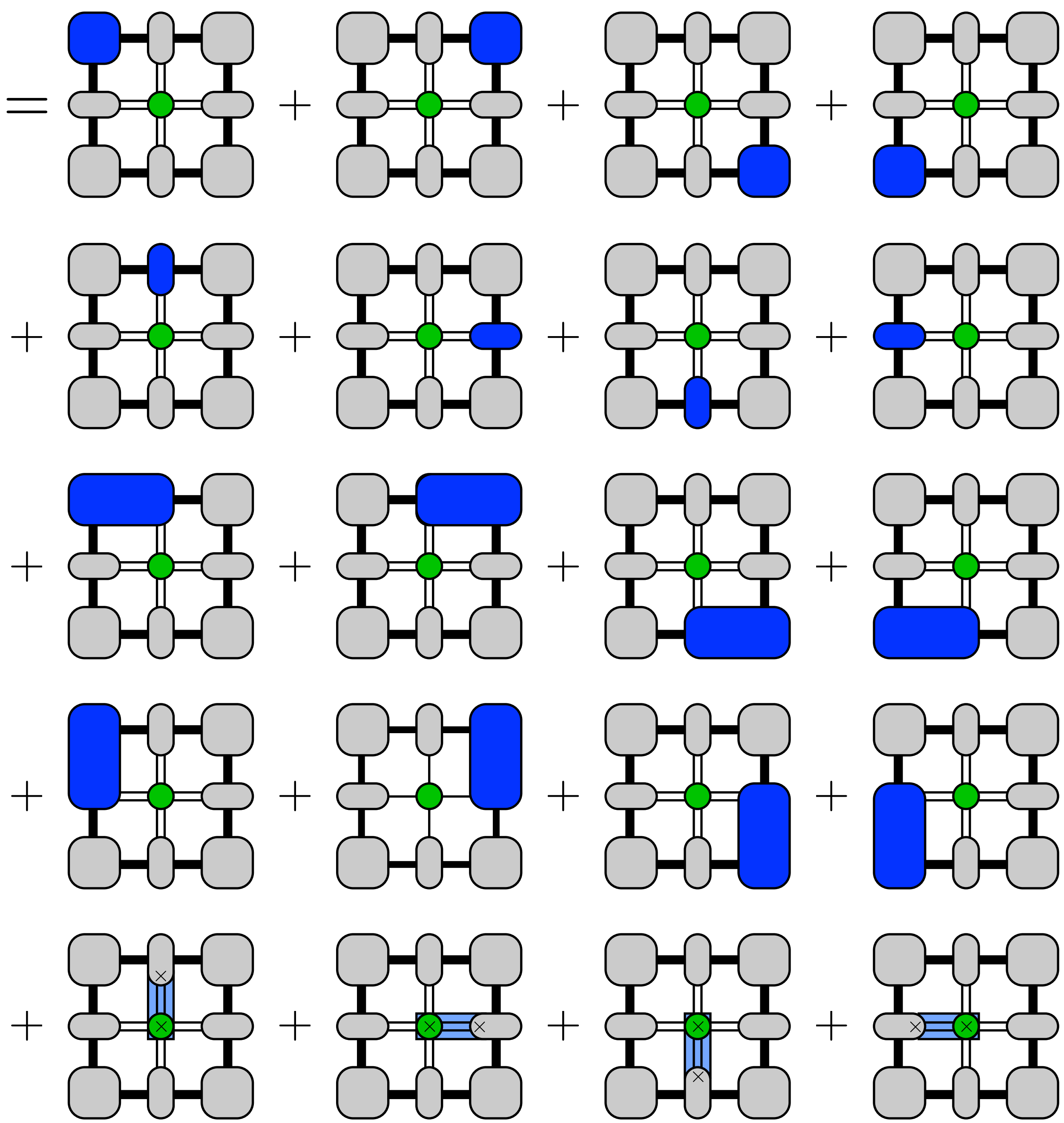




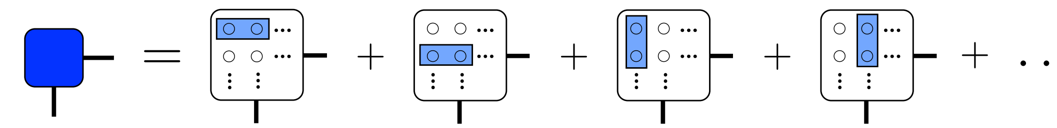
➡ taking into account all Hamiltonian contributions in the infinite upper left corner

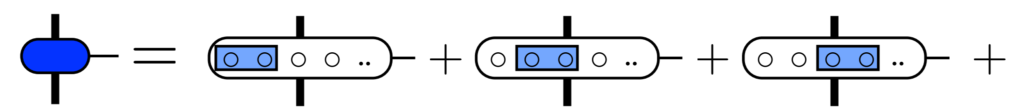
H-environment

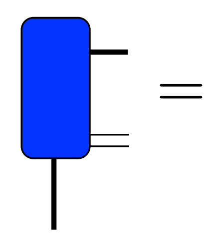
$$\langle \Psi | \hat{H} | \Psi \rangle =$$



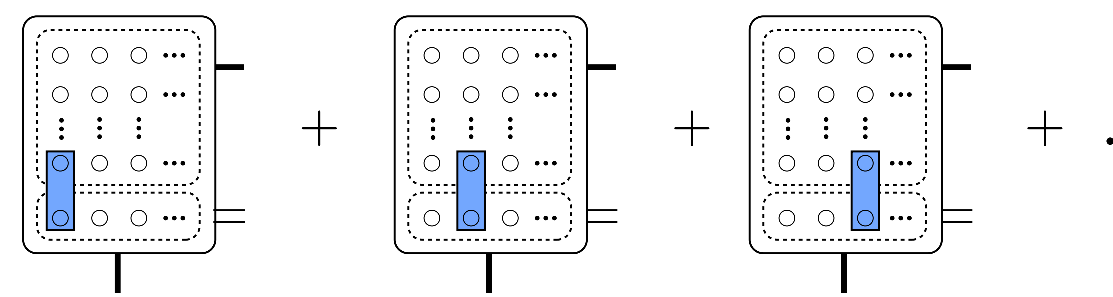
Corner terms







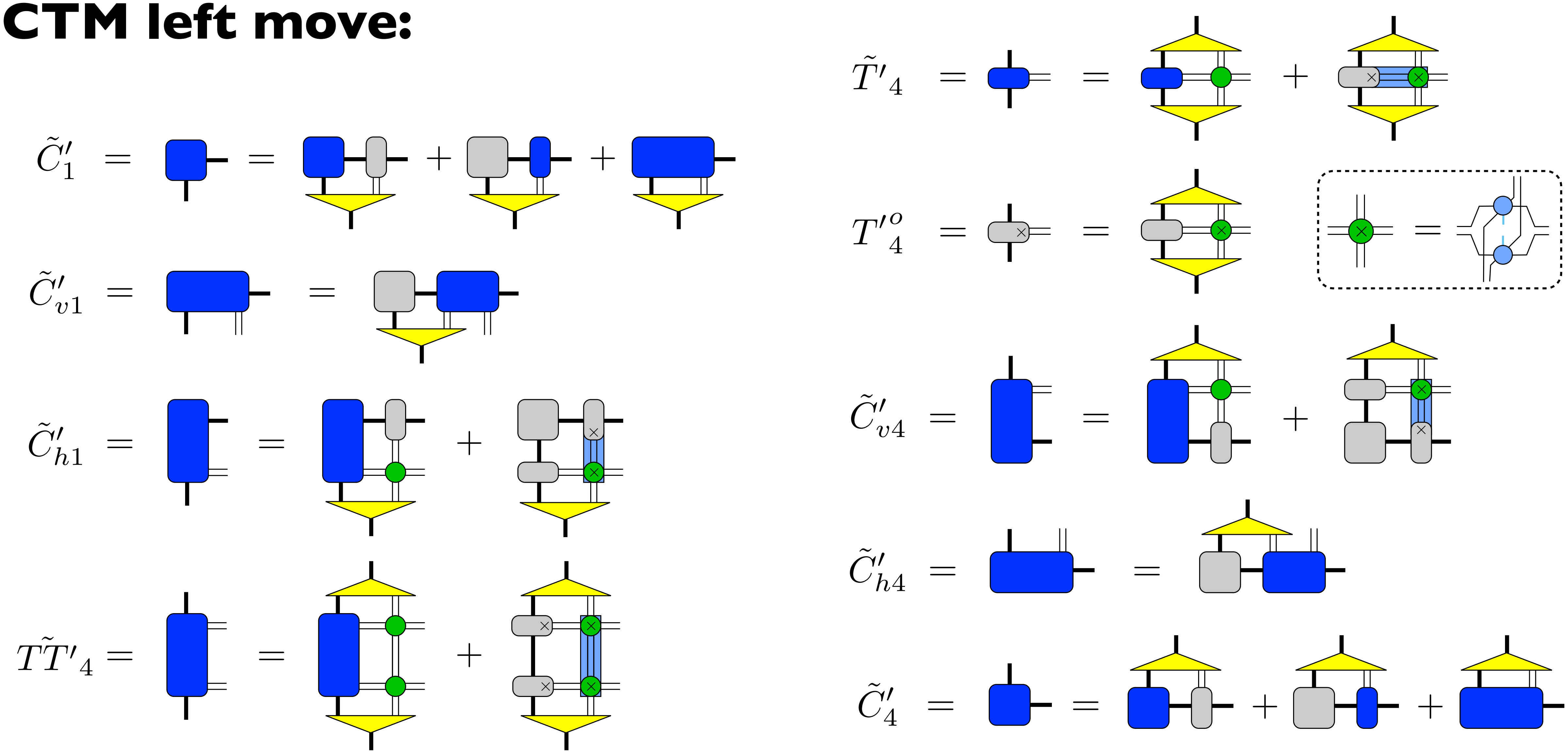
Terms between a corner and an edge tensor



Local terms

H-environment: bookkeeping

CTM left move:



... and similarly for right-, top-, bottom-move

- We can sum up all Hamiltonian contributions in an iterative way

Practical scheme

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

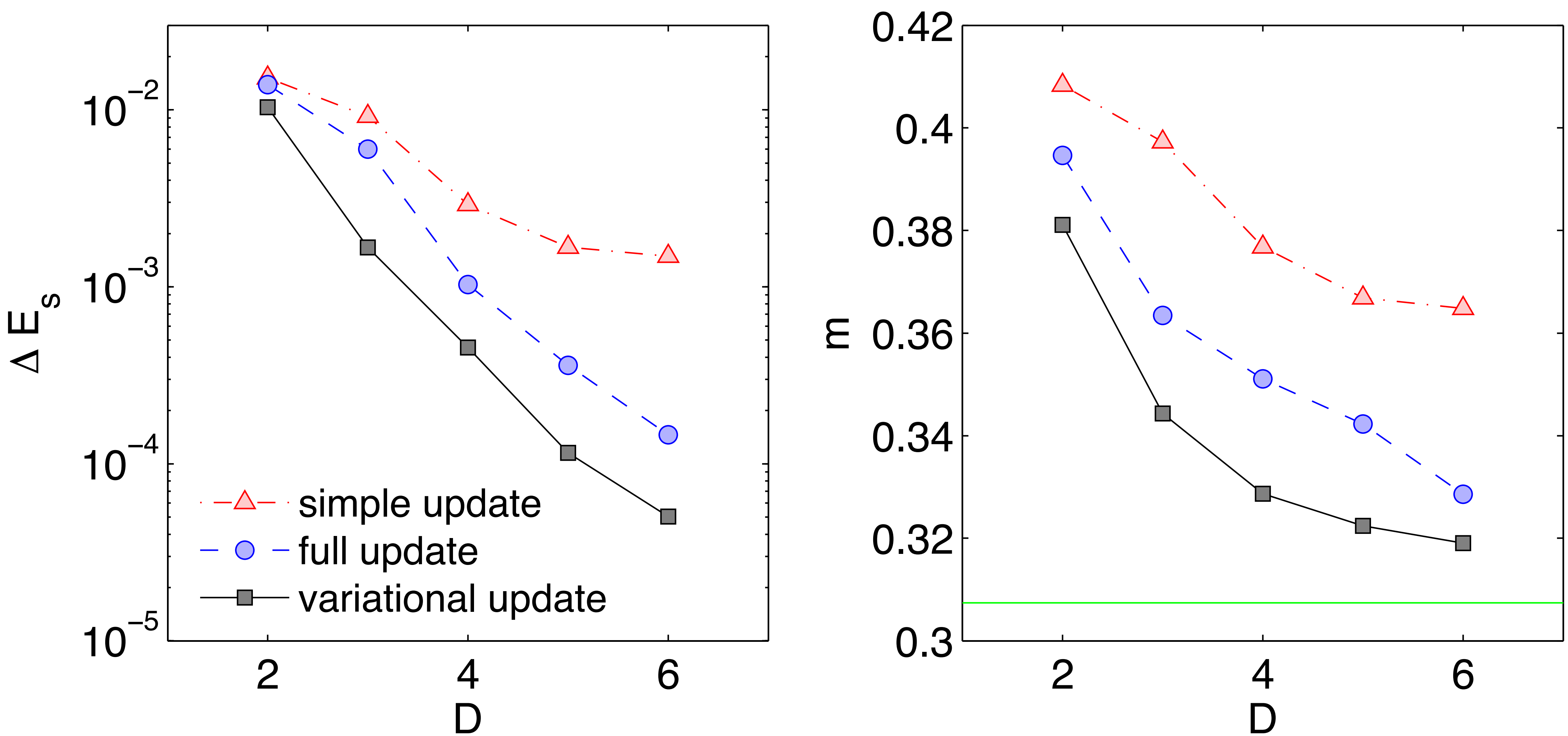
tensor A reshaped as a vector

- However, the solution $\tilde{A}$ of the GEVP is NOT the optimum
- Make ansatz for solution A' see also [Nishino et al. PTR 105 (2001)]

$$A'(\lambda)^{[x,y]} = \tilde{A}^{[x,y]} \sin \lambda\pi - A^{[x,y]} \cos \lambda\pi .$$

- Find $\lambda \in [0.5, 1.5]$ which minimizes $E(\lambda)$ (using only a few steps)
- Repeat iteratively for all tensors in the unit cell

Comparison: Heisenberg model



- Energy and order parameter are substantially improved with the variational optimization
- **Highest** accuracy (D=6): -0.66941
- Extrapolated QMC result: -0.66944 [Sandvik&Evertz 2010]

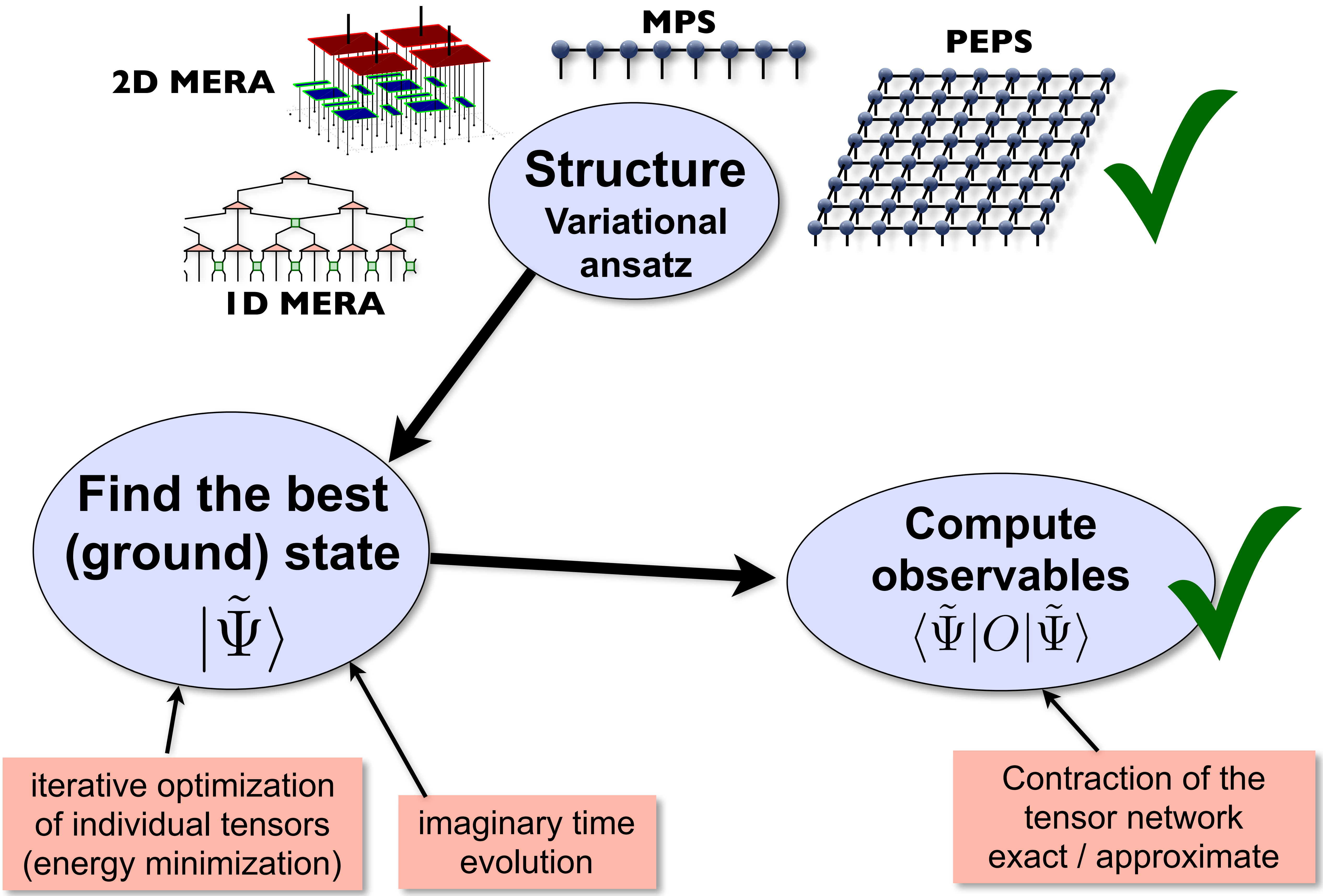
Summary: optimization in iPEPS

- Imaginary time evolution
  - ✦ Simple update: cheap and simple, but not accurate
    Jiang et al, PRL 101 (2008)
  - ✦ Cluster update: improved accuracy
    Wang et al, arXiv:1110.4362
  - ✦ Full update: high accuracy, more expensive
    Jordan et al, PRL 101 (2008)
  - ✦ Fast-full update: high accuracy, cheaper than FU
    Phien et al, PRB 92 (2015)

+ COMBINATIONS!

- Energy minimization / variational
  - ✦ DMRG-like sweeping: **higher accuracy**, similar cost as FFU
    PC, PRB 94 (2016)
  - ✦ CG-approach: **higher accuracy**, similar cost as FFU
    Vanderstraeten, Haegeman, PC, and Verstraete, PRB 94 (2016)
  - ✦ See also variational optimization in the context of 3D classical models
    Nishino et al. Prog. Theor. Phys 105 (2001), Gendiar et al. Prog. Theor. Phys 110 (2003)
  - ✦ ... more to explore...!

Summary: Tensor network algorithms (ground state)



Part IV: iPEPS application example

Overview: iPEPS simulations

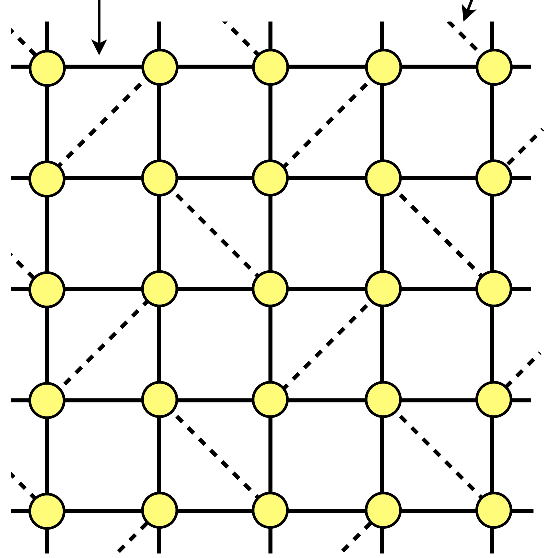
- interacting spinless fermions
  - honeycomb & square lattice
- t-J model & Hubbard model
  - square lattice
- SU(N) Heisenberg models
  - N=3 square, triangular, kagome & honeycomb lattice
  - N=4 square, honeycomb & checkerboard lattice
  - N=5 square lattice
  - N=6 honeycomb lattice
- frustrated spin systems
  - Shastry-Sutherland model
  - Heisenberg model on kagome lattice
  - Bilinear-biquadratic S=1 Heisenberg model
  - Kitaev-Heisenberg model
  - J1-J2 Heisenberg model
- and many more...

iPEPS is a very **competitive** variational method!

Find new physics thanks to (largely) unbiased simulations

The Shastry-Sutherland model

$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\text{dimer}}} S_i \cdot S_j$$

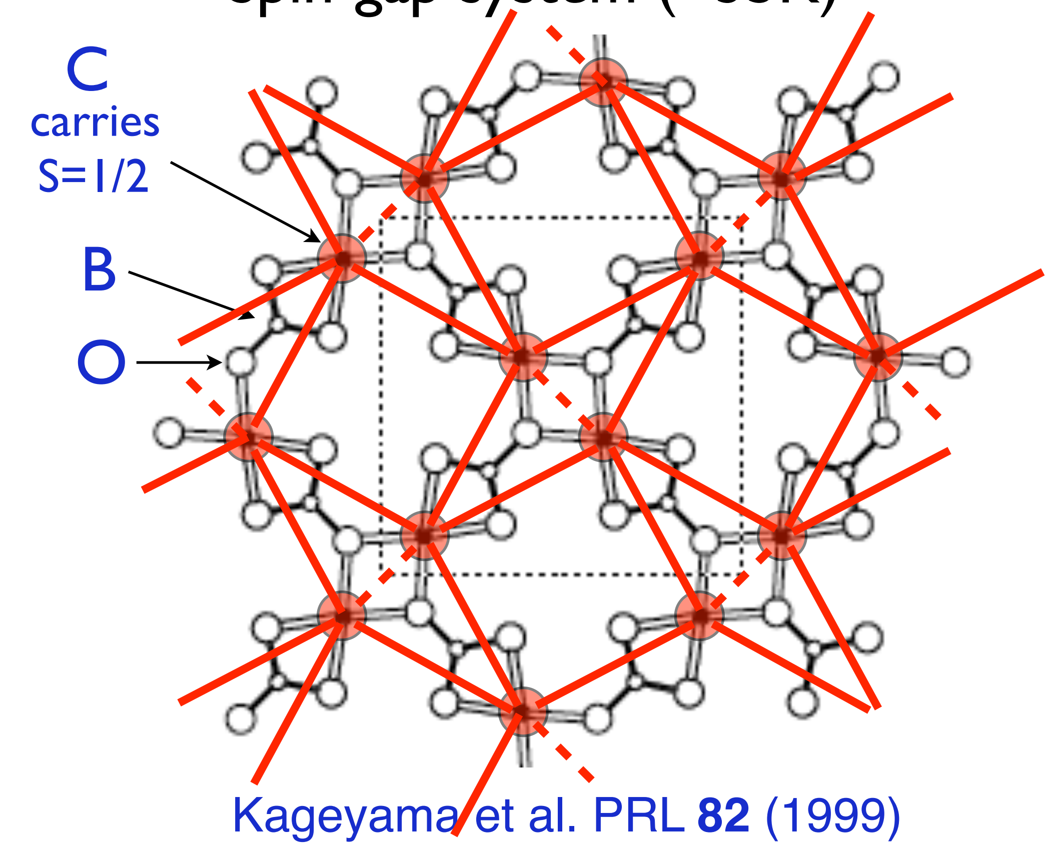


Shastry & Sutherland, Physica B+C **108** (1981).

same lattice!

$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



Kageyama et al. PRL **82** (1999)

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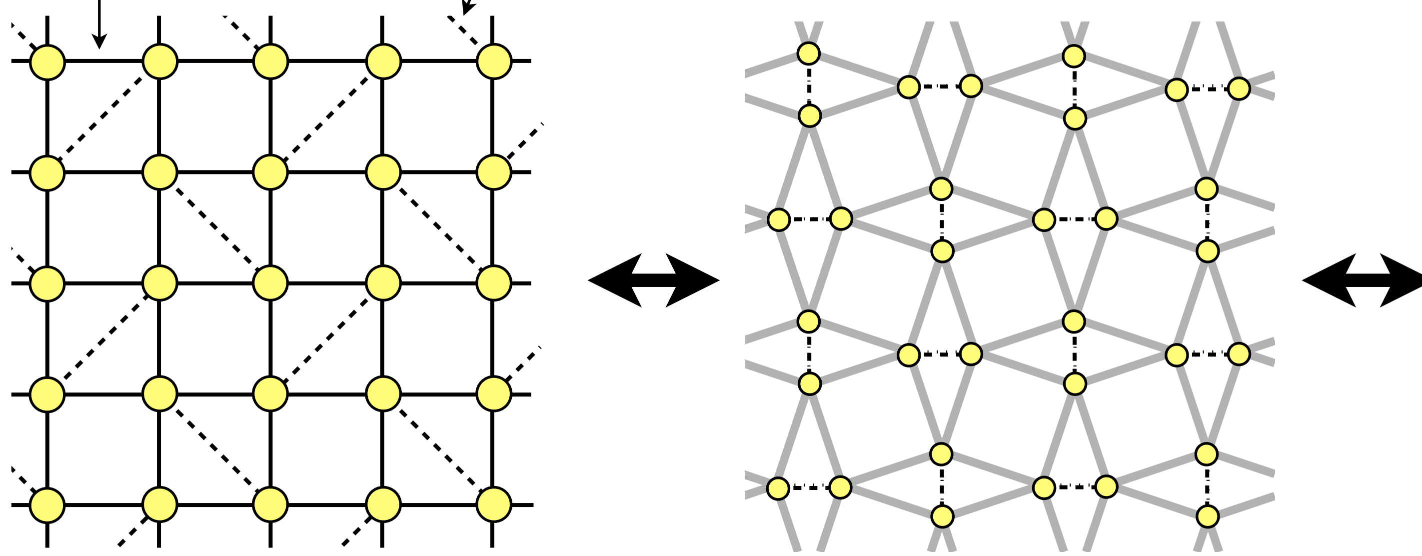
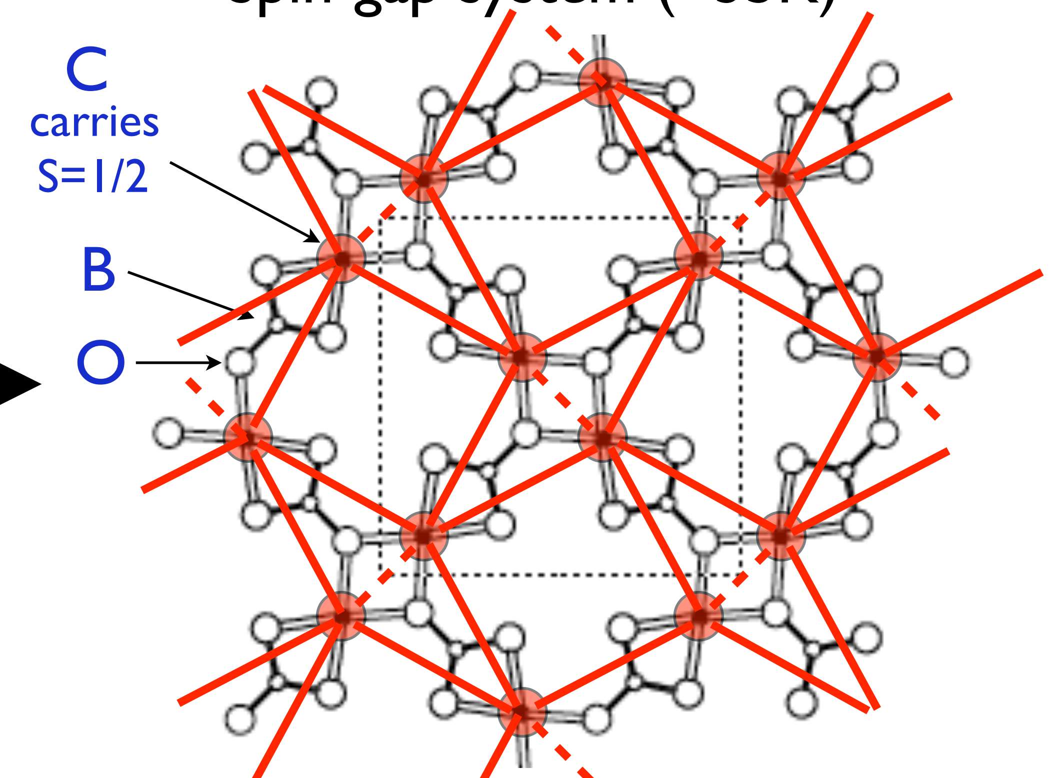
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j$$



$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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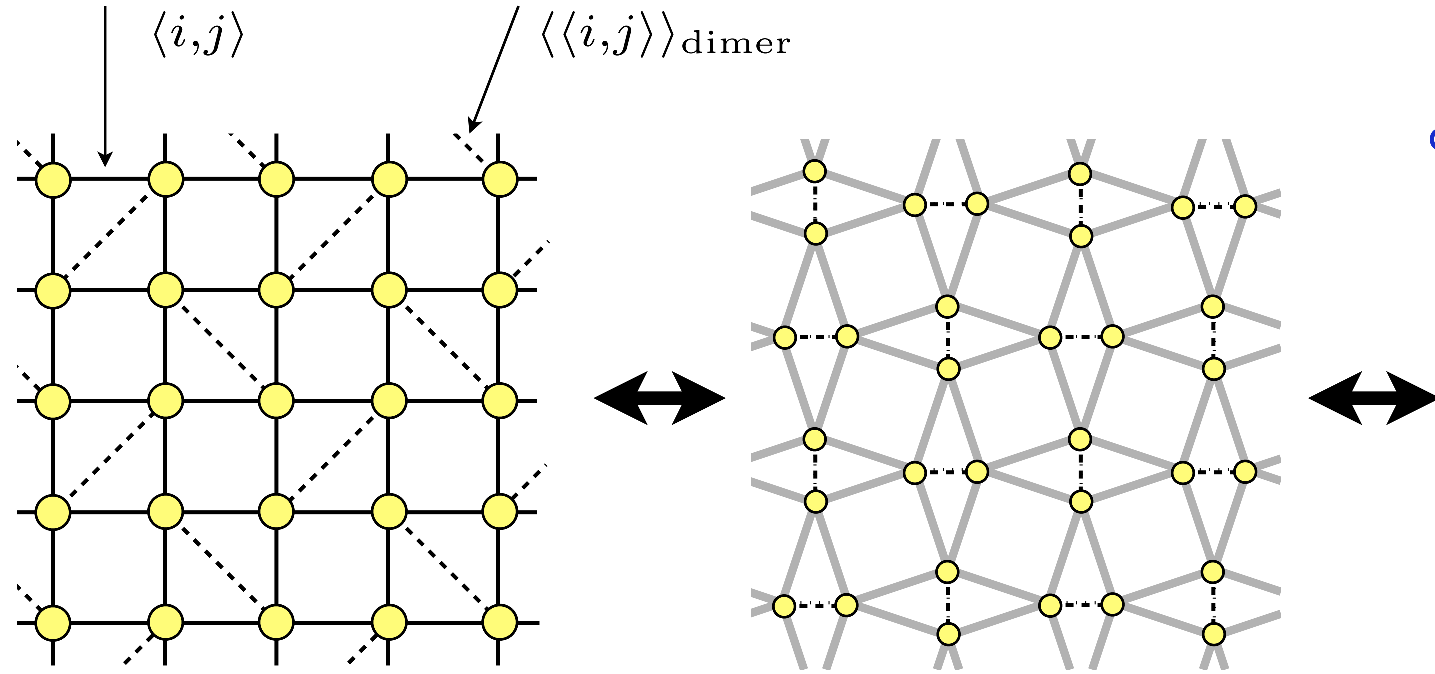
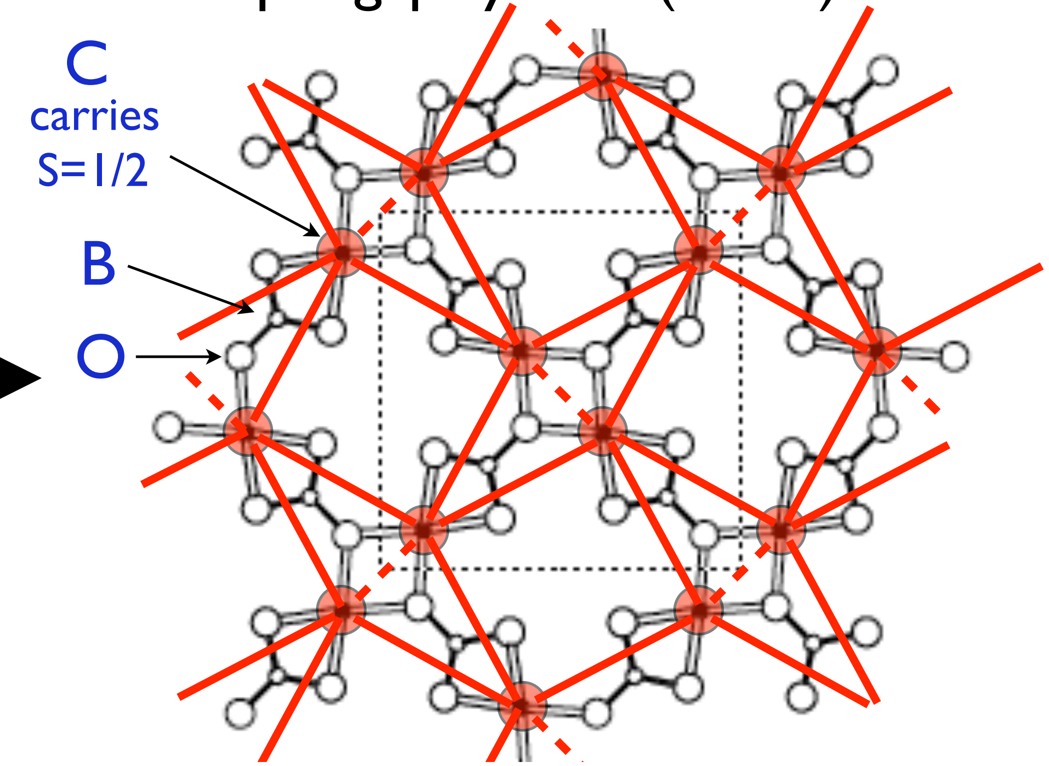
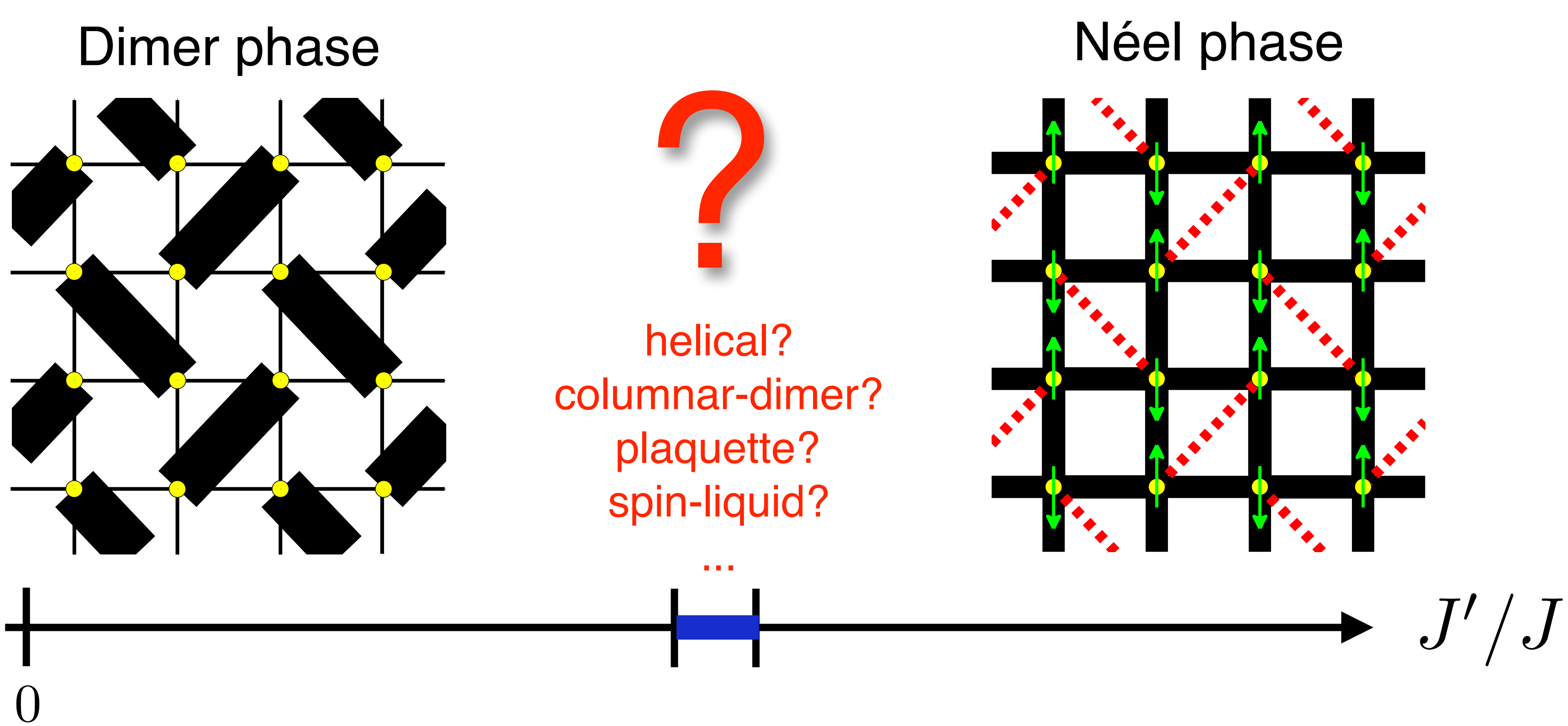


$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



Kageyama et al. PRL **82** (1999)

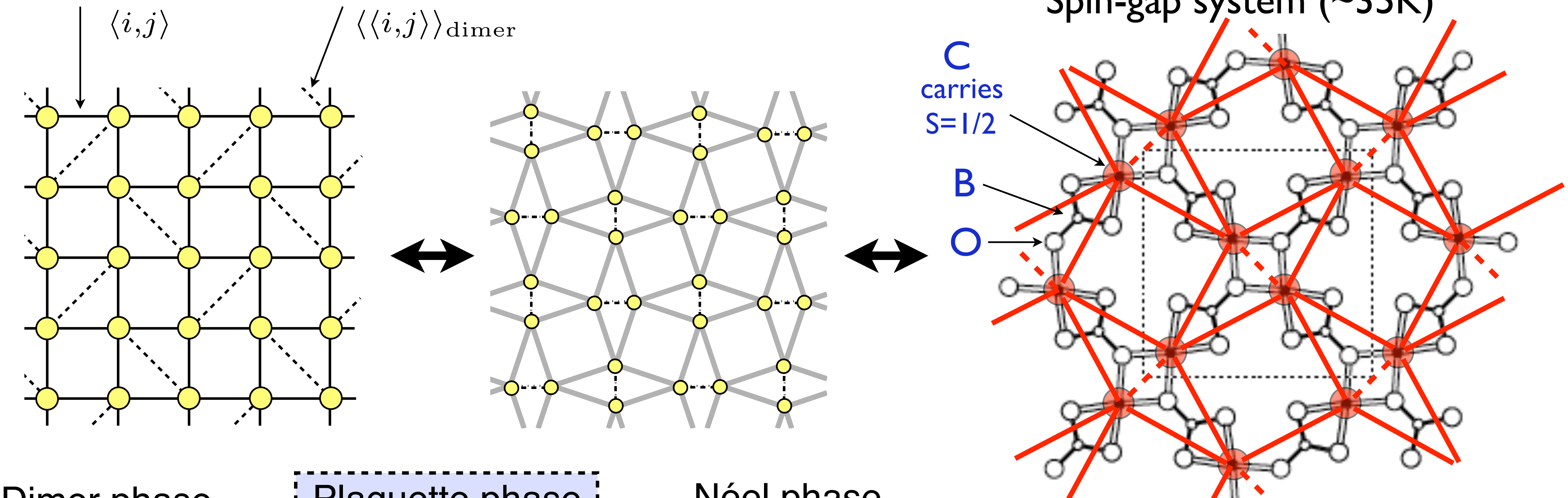


The Shastry-Sutherland model

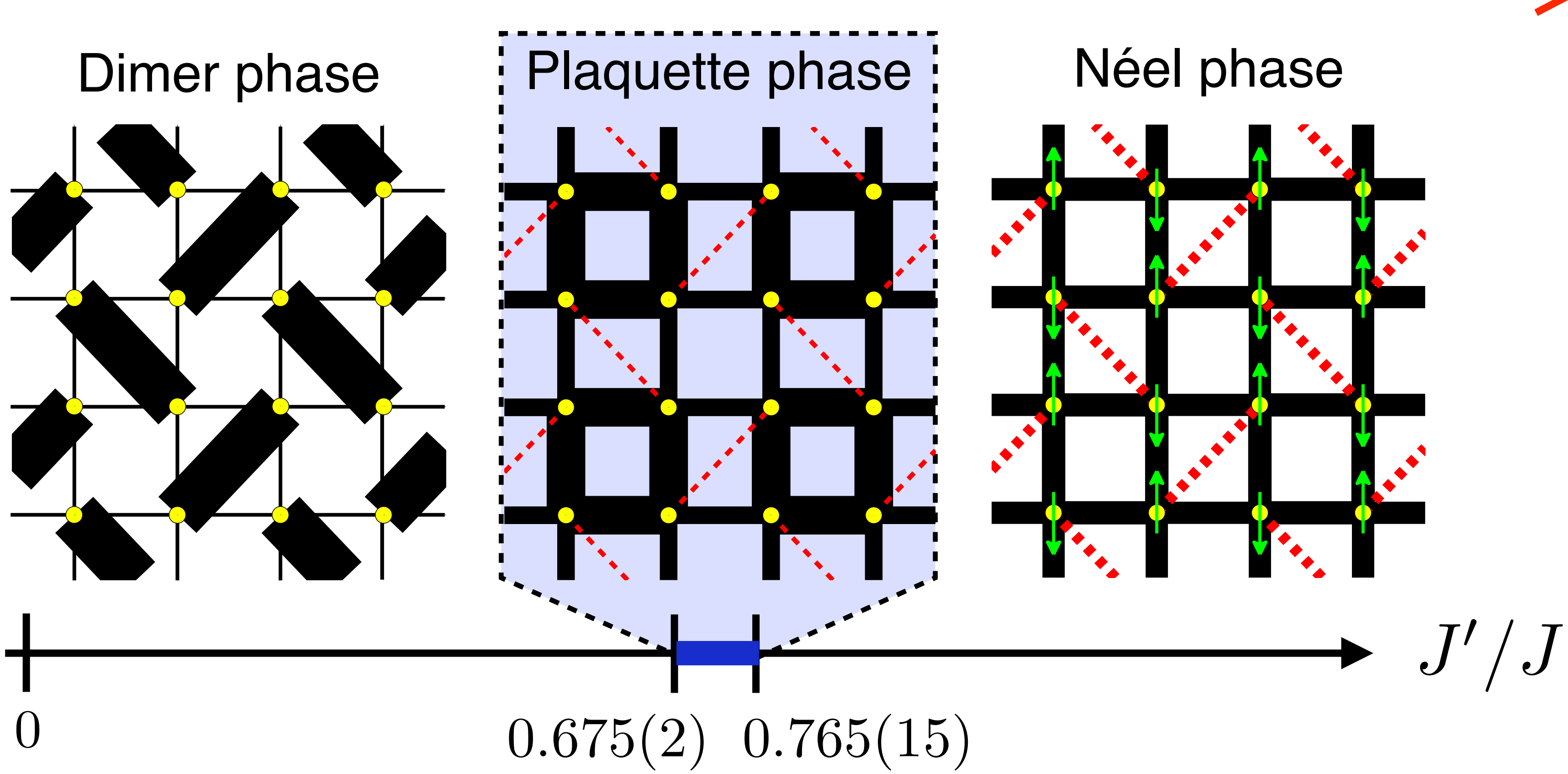
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\text{dimer}}} S_i \cdot S_j$$

$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



Kageyama et al. PRL **82** (1999)



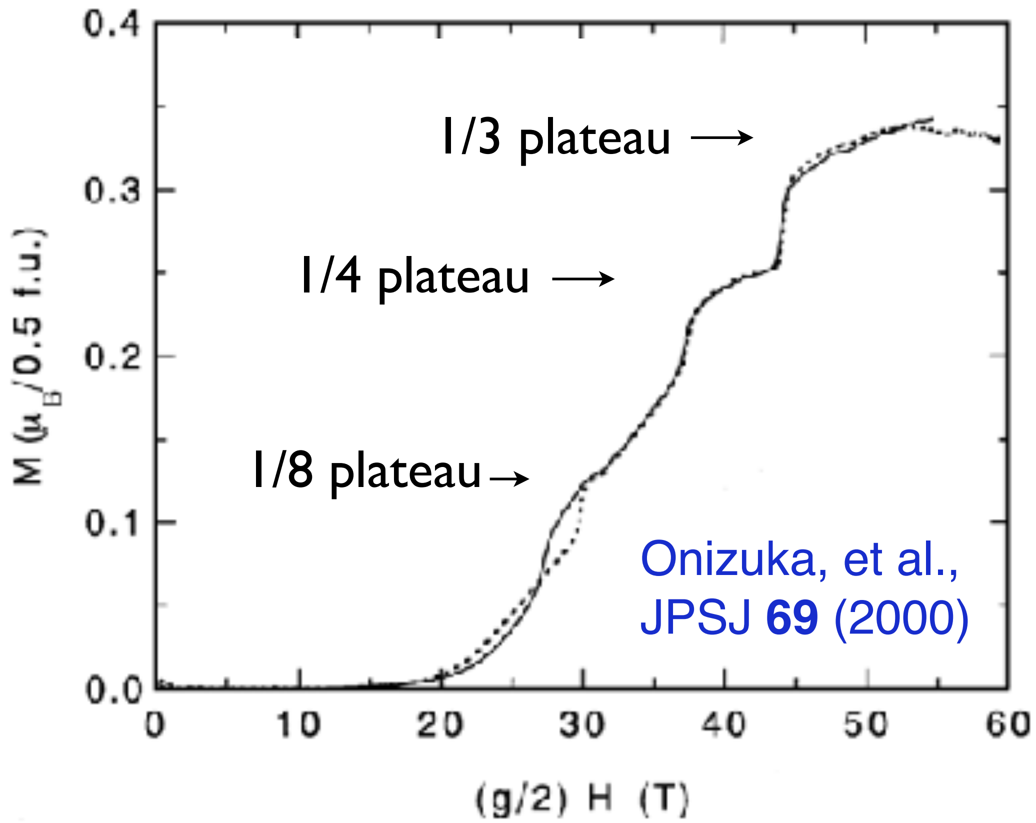
Corboz and Mila, PRB **87** (2013)

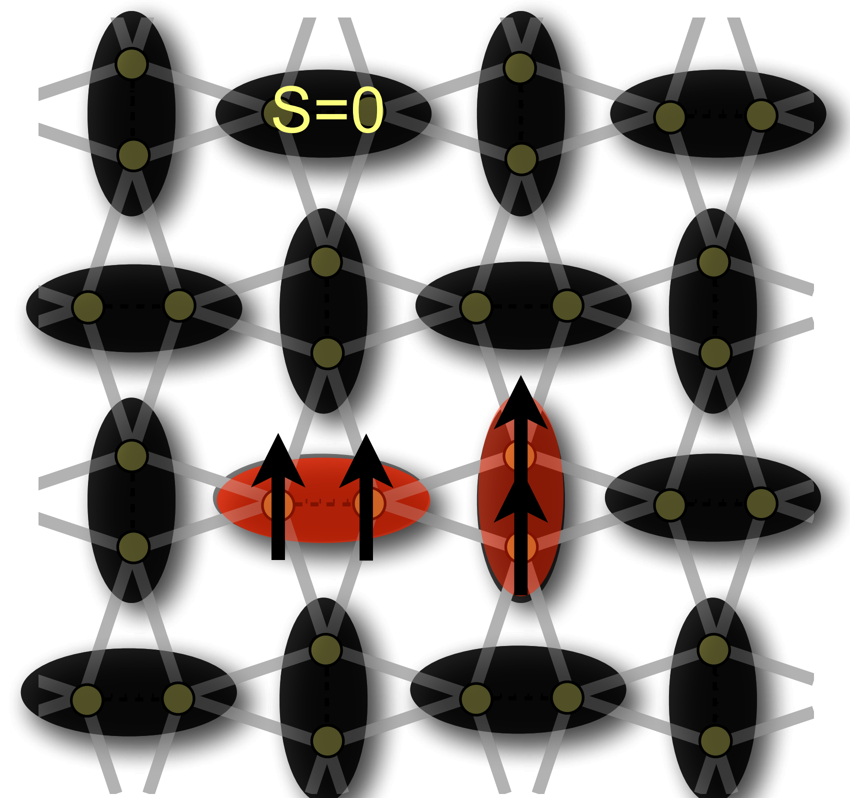
previously found in:

Koga and Kawakami, PRL **84** (2000)
Takushima et al., JPSJ **70** (2001)
Chung et al, PRB **64** (2001)
Läuchli et al, PRB **66** (2002)

Magnetization plateaus

$SrCu_2(BO_3)_2$ in a magnetic field exhibits several magnetization plateaus





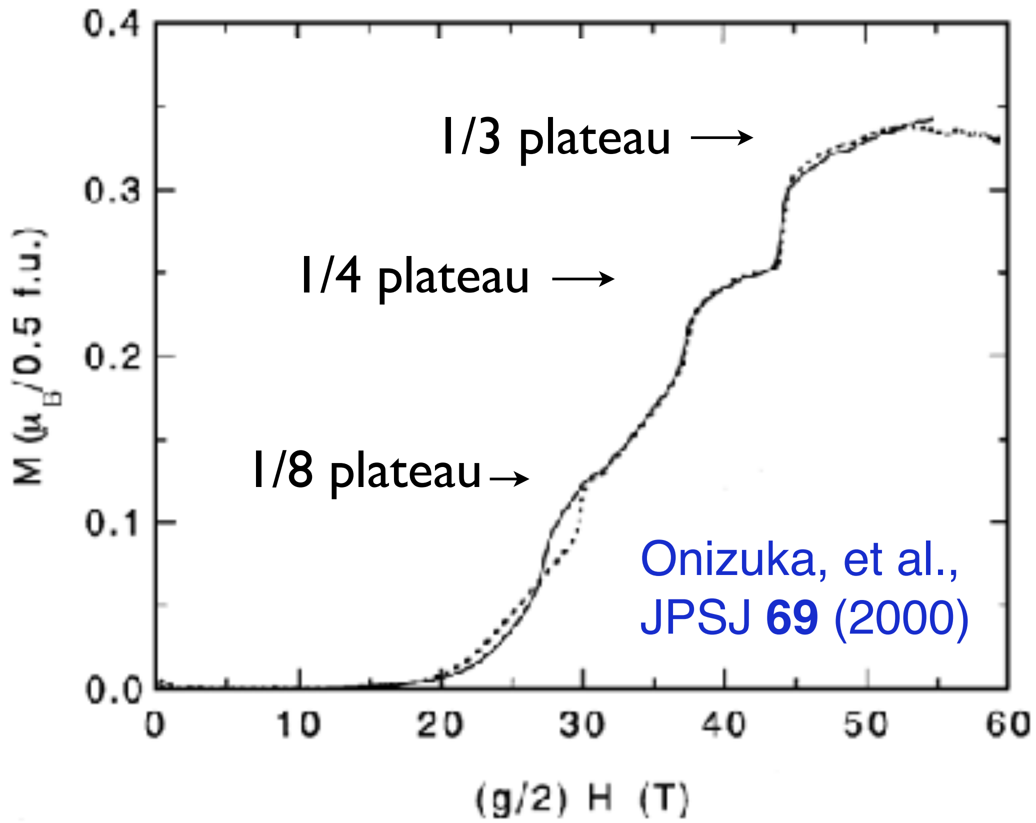
The SSM has almost localized triplet excitations [Miyahara&Ueda'99, Kageyama et al. '00]

Triplets repel each other
(on the mean-field level)

Common belief: The magnetization plateaus corresponds to *crystals of localized triplets*! (Mott insulators)

Magnetization plateaus

$SrCu_2(BO_3)_2$ in a magnetic field exhibits several magnetization plateaus



The SSM has almost localized triplet excitations [Miyahara&Ueda'99, Kageyama et al. '00]

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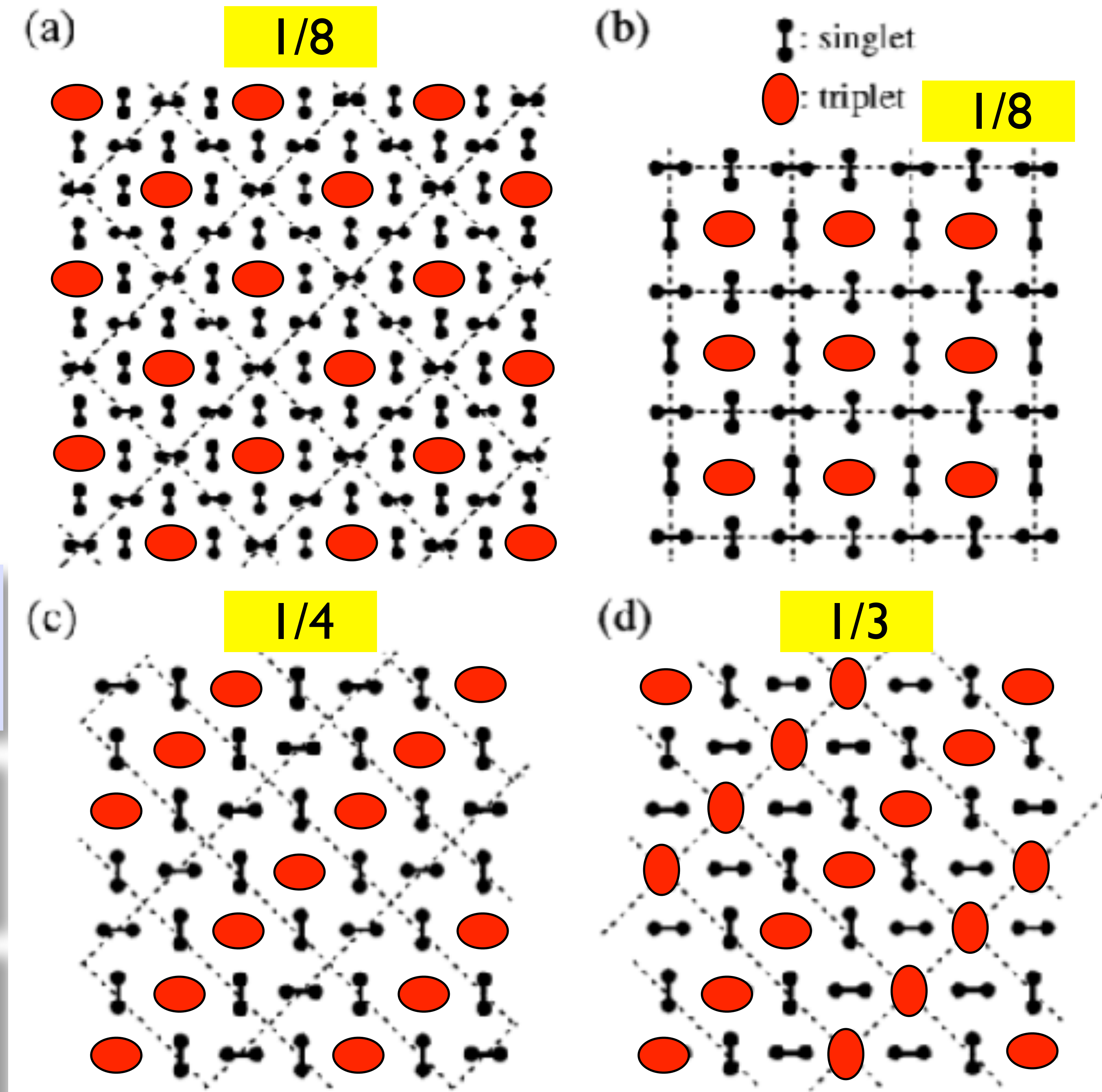
Crystals of localized triplets



Onizuka, et al., JPSJ **69** (2000)

Magnetization plateaus

- Many experiments and theoretical works over the last 15 years
- Experiments: 1/8, 2/15, 1/6, 1/4, 1/3, 1/2
- Theory: 1/9, 2/15, 1/6, 1/4, 1/3, 1/2

- What about the 1/8 plateau?
- Complicated structures for the 2/15 plateau...
- Big puzzle for many years...

Kageyama et al, PRL **82** (1999)
Onizuka et al, JPSJ **69** (2000)
Kageyama et al, PRL **84** (2000)
Kodama et al, Science **298** (2002)
Takigawa et al, Physica **27** (2004)
Levy et al, EPL **81** (2008)
Sebastian et al, PNAS **105** (2008)
Isaev et al, PRL **103** (2009)
Jaime et al, PNAS **109** (2012)
Takigawa et al, PRL **110** (2013)
Matsuda et al, PRL **111** (2013)
Miyahara and K. Ueda, PRL **82** (1999)
Momoi and Totsuka, PRB **61** (2000)
Momoi and Totsuka, PRB **62** (2000)
Fukumoto and Oguchi, JPSJ **69** (2000)
Fukumoto, JPSJ **70** (2001)
Miyahara and Ueda, JPCM **15** (2003)
Miyahara, Becca and Mila, PRB **68** (2003)
Dorier, Schmidt, and Mila, PRL **101** (2008)
Abendschein & Capponi, PRL **101** (2008)
Takigawa et al, JPSJ **79** (2010).
Nemec et al, PRB **86** (2012).
Lou et al, arXiv:1212.1999.
...

★ Ideal problem for iPEPS: simulating large unit cell embedded in infinite system and compare variational energies of the proposed crystals

BUT!

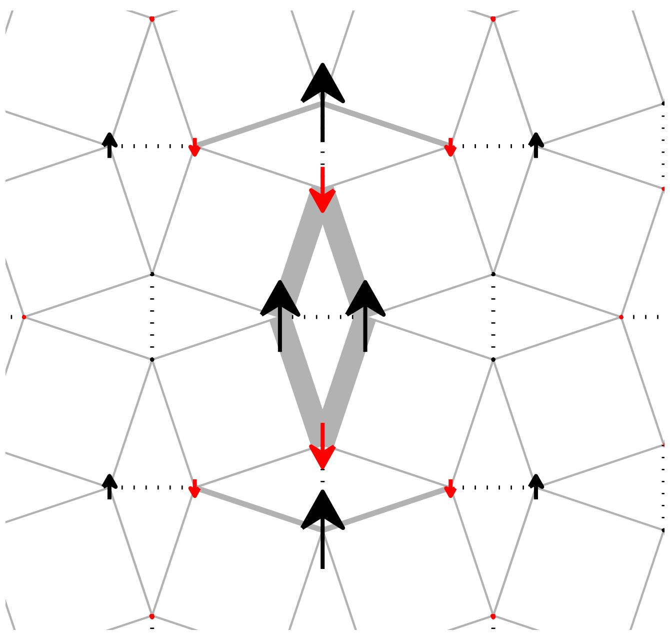
SURPRISE!

iPEPS simulations of the SSM in a magnetic field

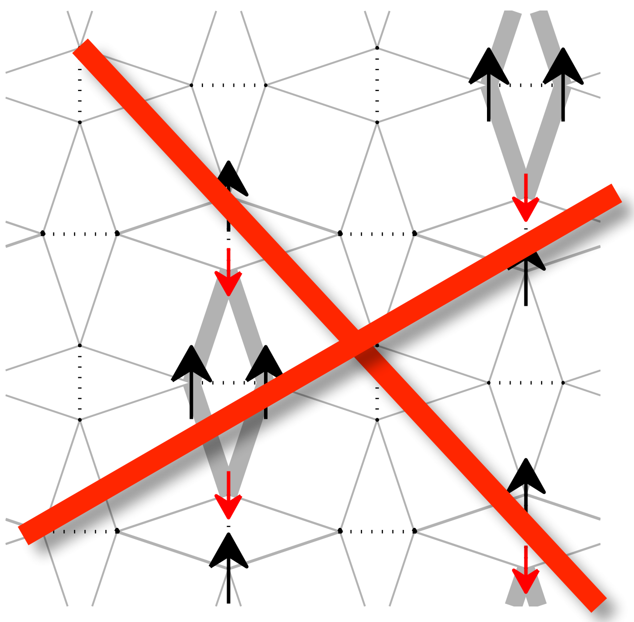
PC, F. Mila, PRL **112** (2014)

- The assumption that plateaus correspond to crystals of triplets is wrong!

(for the plateaus below 1/4)

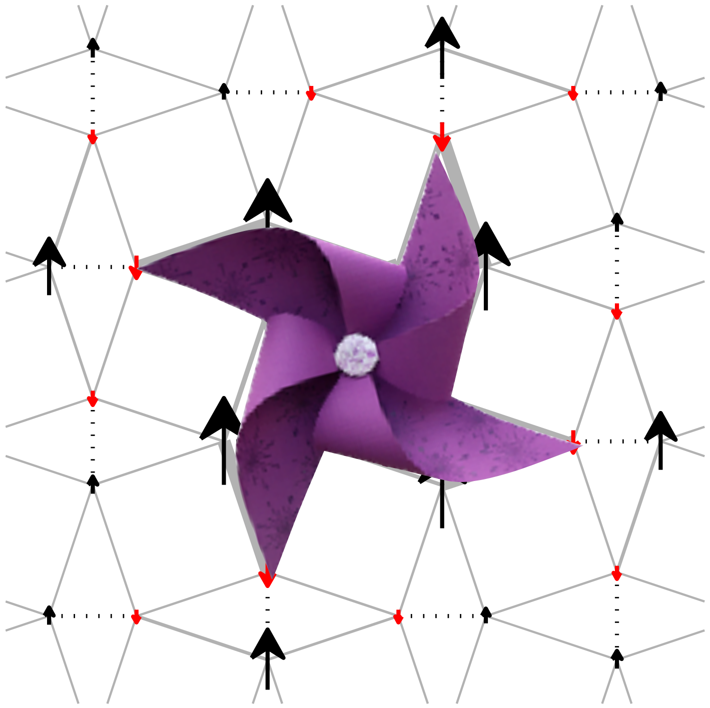


spin structure of 1 localized triplet in a 4x4 cell



expected spin structure of 2 localized triplets in a 4x4 cell

small D (mean-field result)



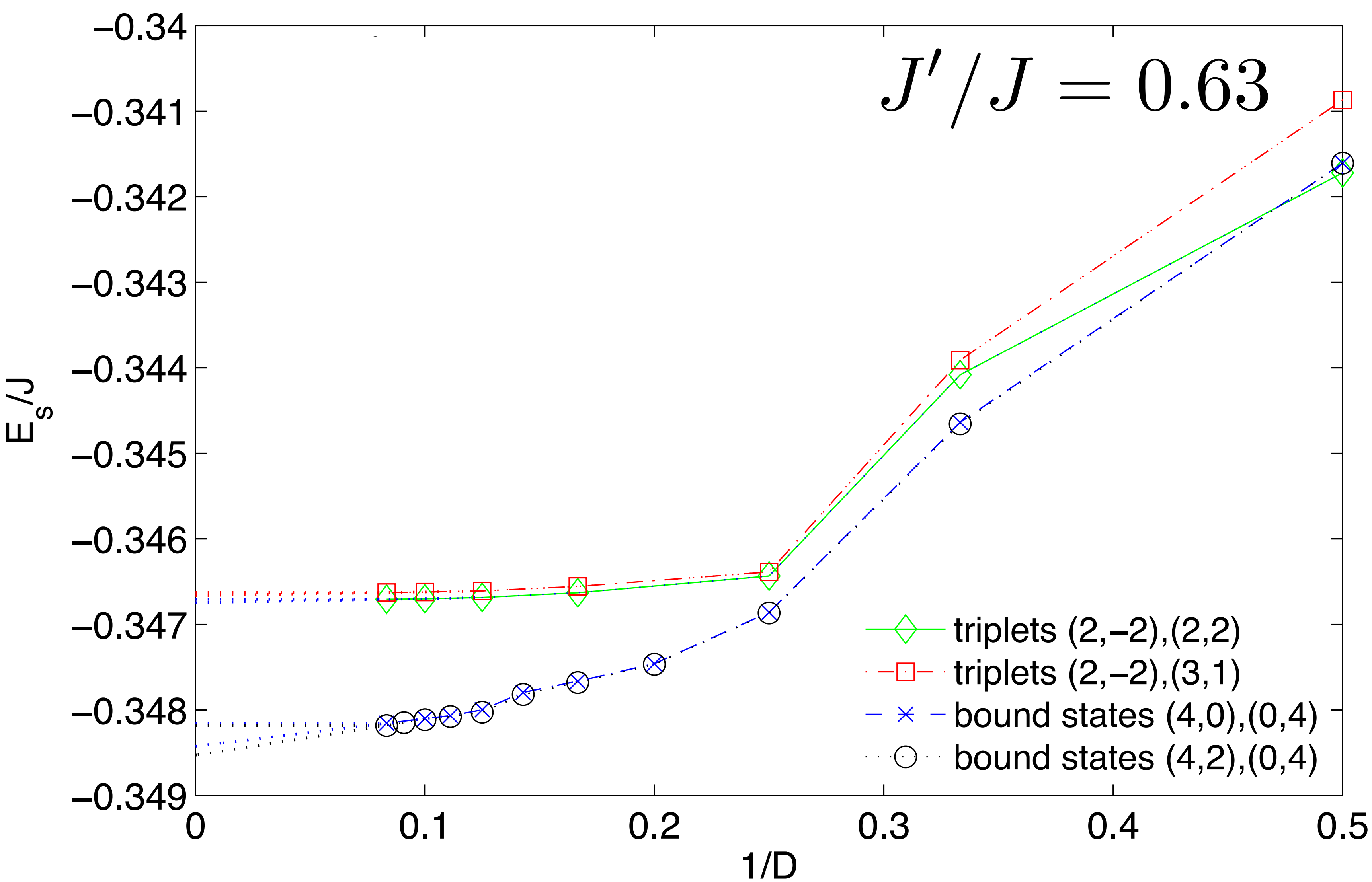
spin structure of a Sz=2 excitation in a 4x4 cell

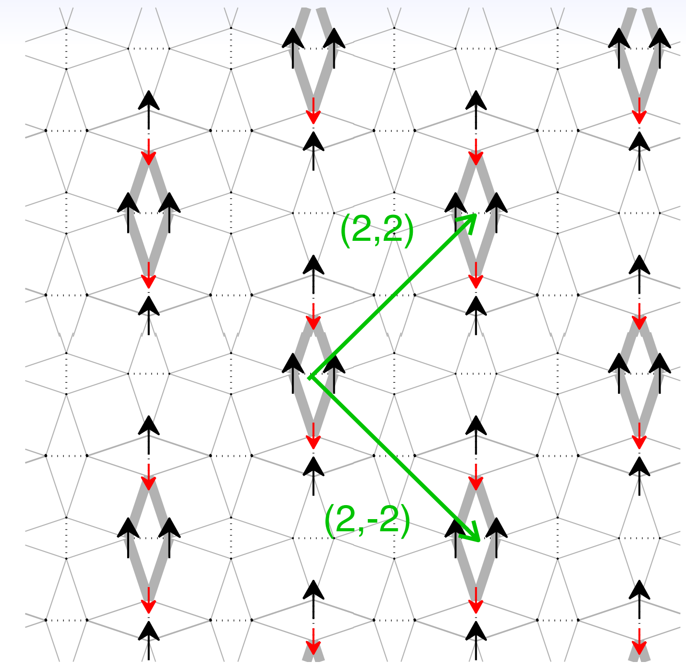
obtained with iPEPS for D>4

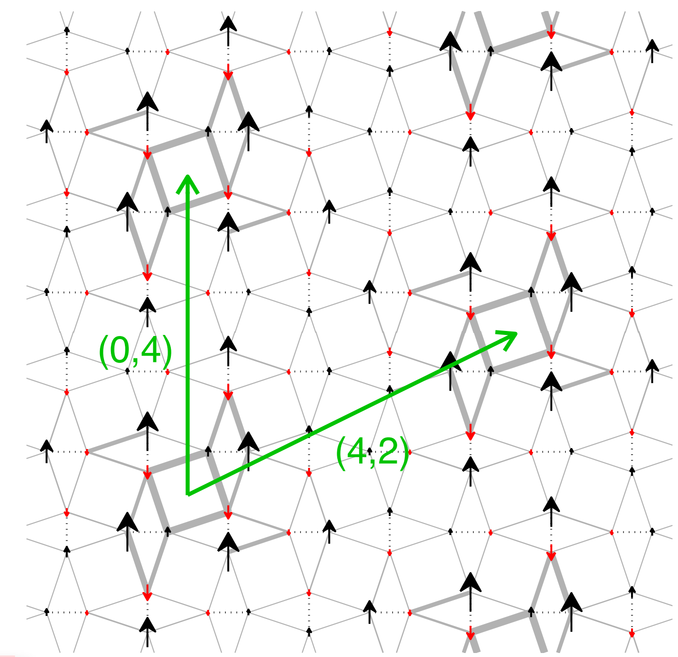
Bound state of two triplets!

- Crystals of bound states instead of crystals of triplets!!

Example: 1/8 plateau

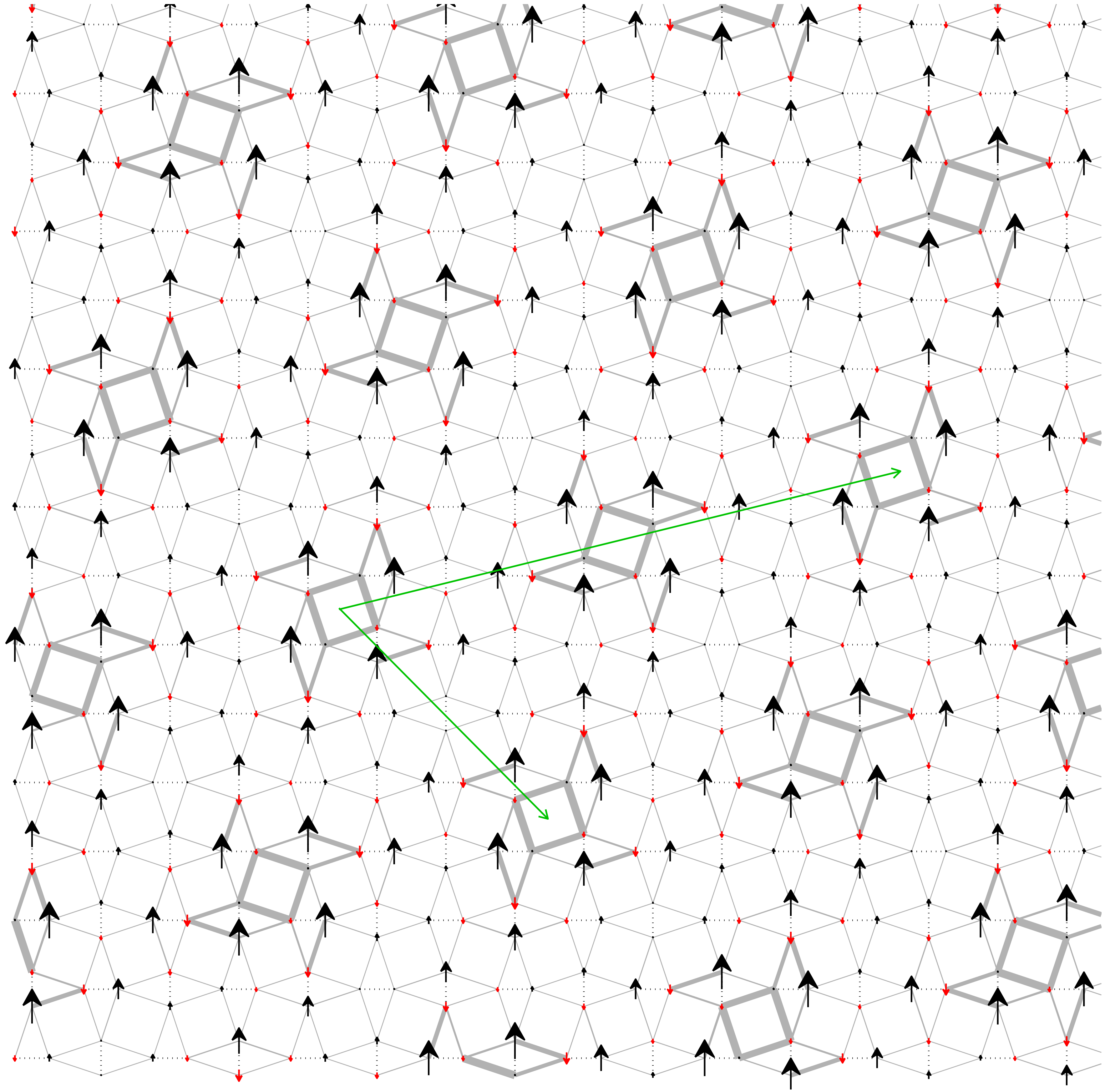






- All the proposed triplet crystals have a higher energy than the crystals made of bound states!
- Similar results found for other plateaus below 1/4

2/15 plateau

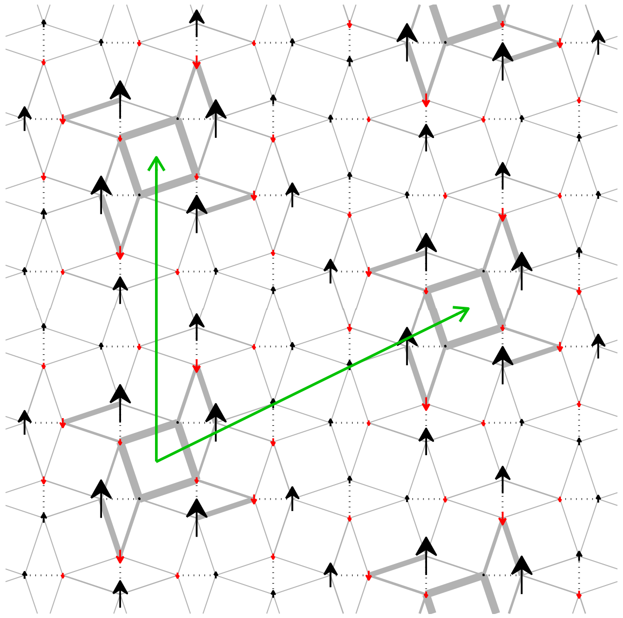


Unit cell with 30 tensors (60 sites)

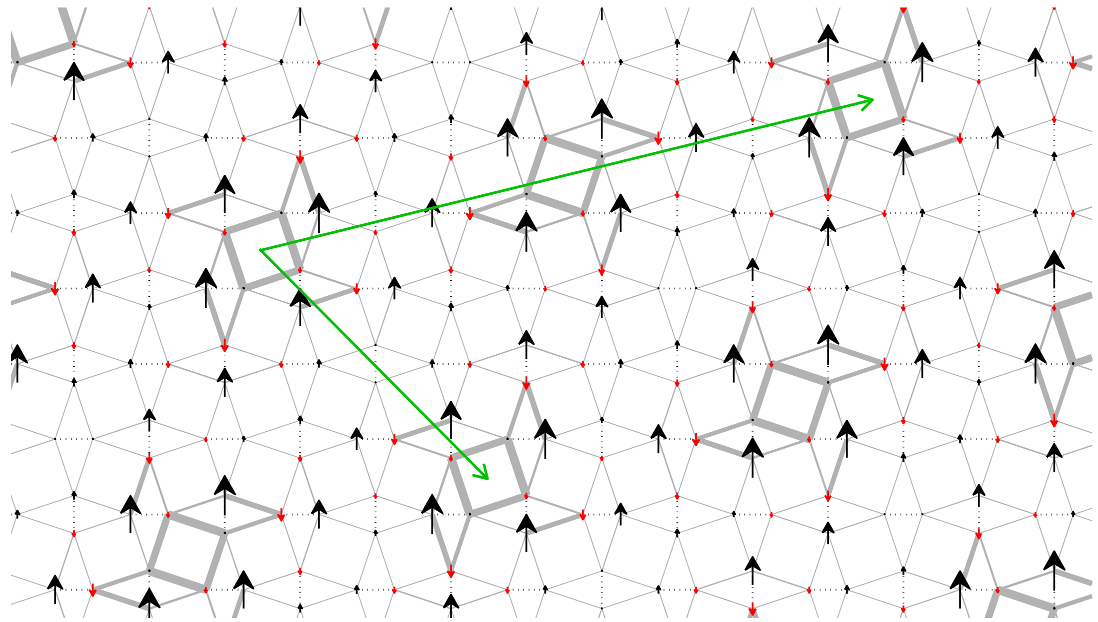
Regular pattern of bound states!

Computing the energies of all possible crystals

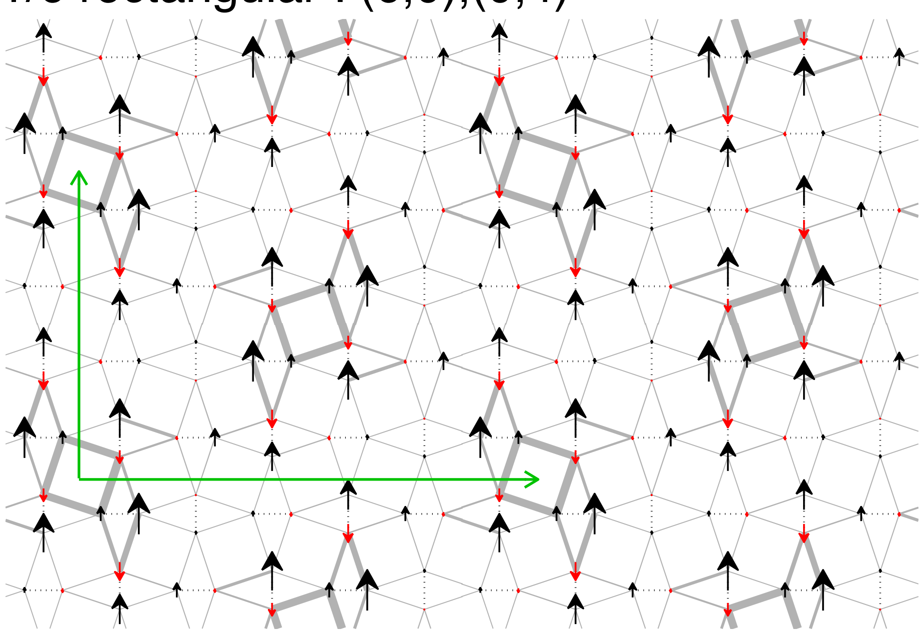
1/8 rhomboid : (4,2),(0,4)



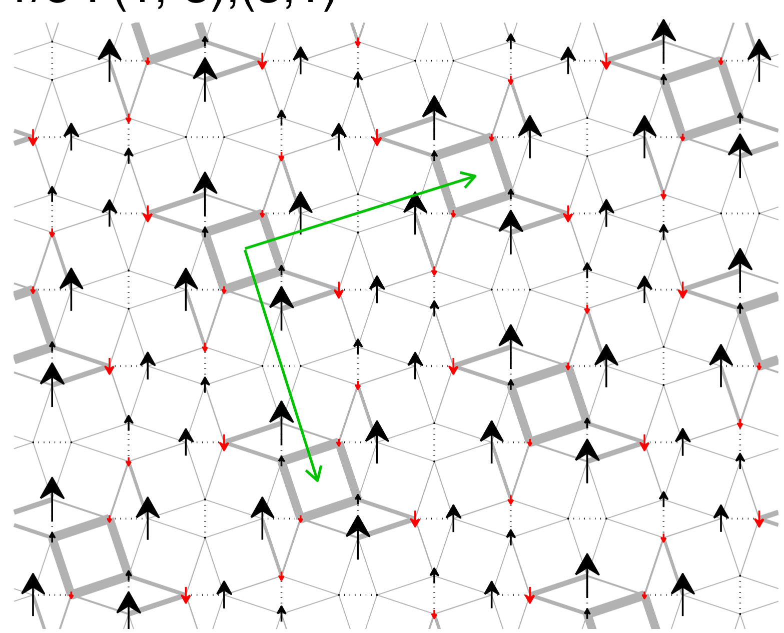
2/15 : (3,-3),(8,2)



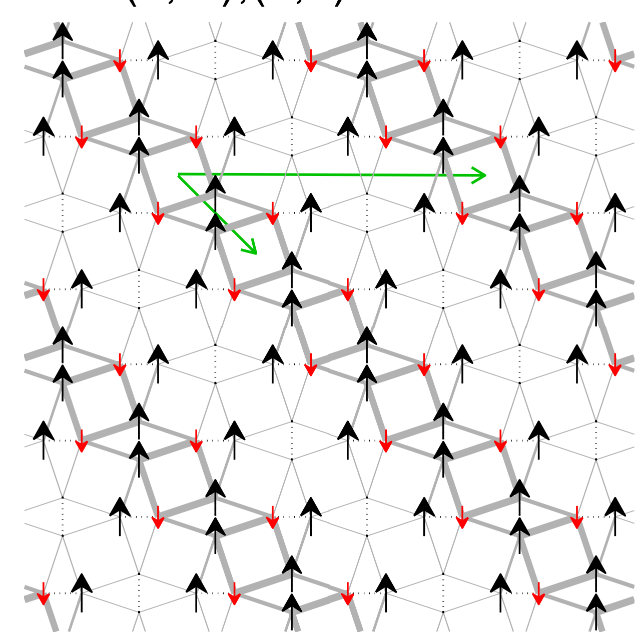
1/6 rectangular : (6,0),(0,4)



1/5 : (1,-3),(3,1)

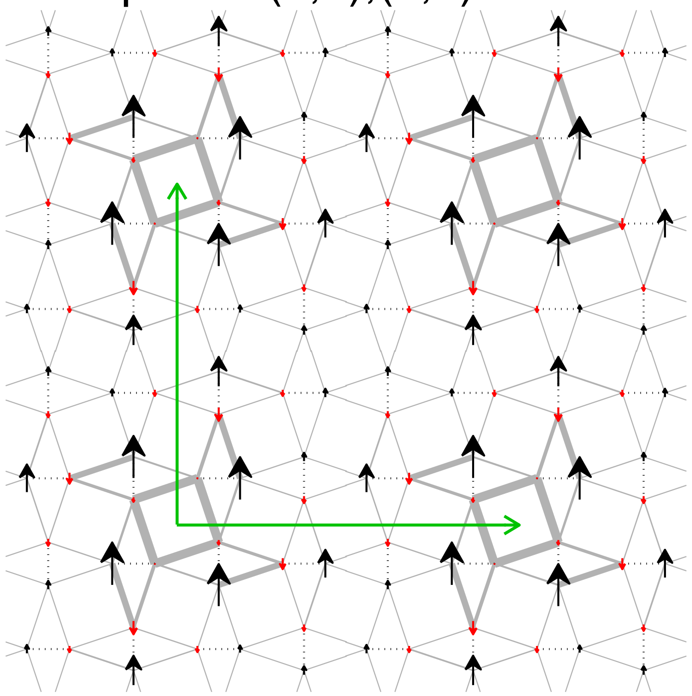


1/4 : (1,-1),(4,0)

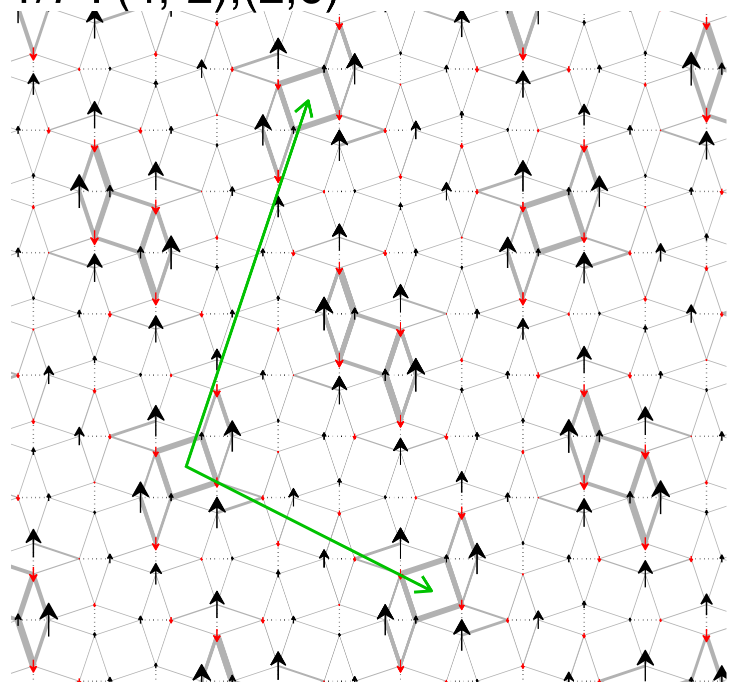


Computing the energies of all possible crystals

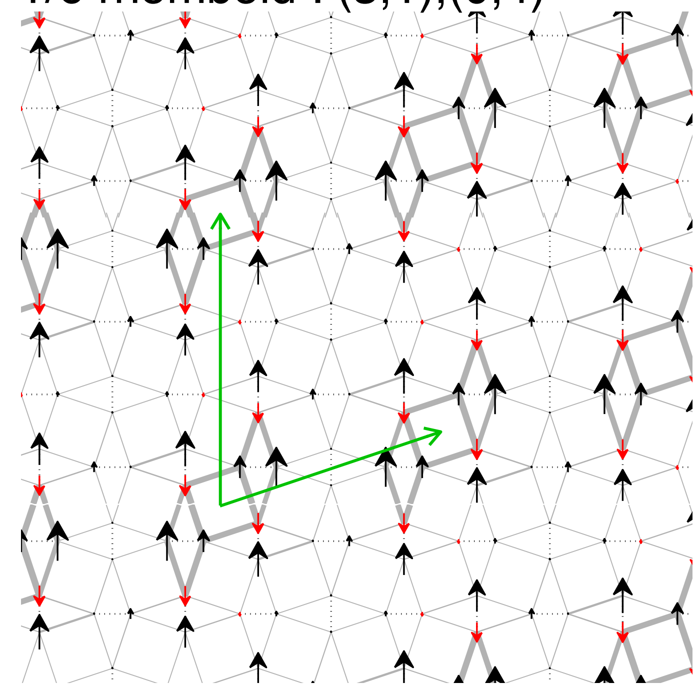
1/8 square : (4,0),(0,4)



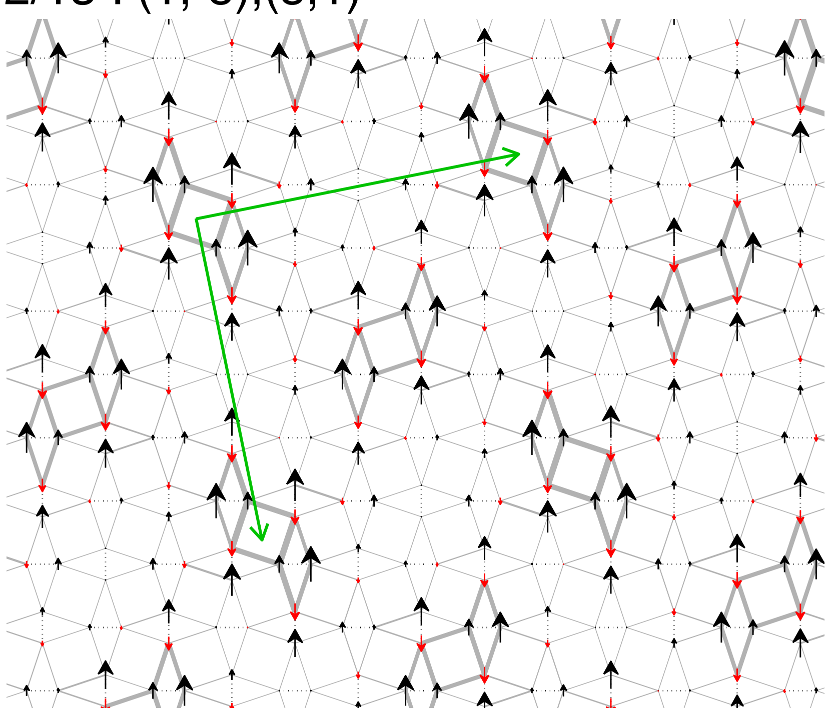
1/7 : (4,-2),(2,6)



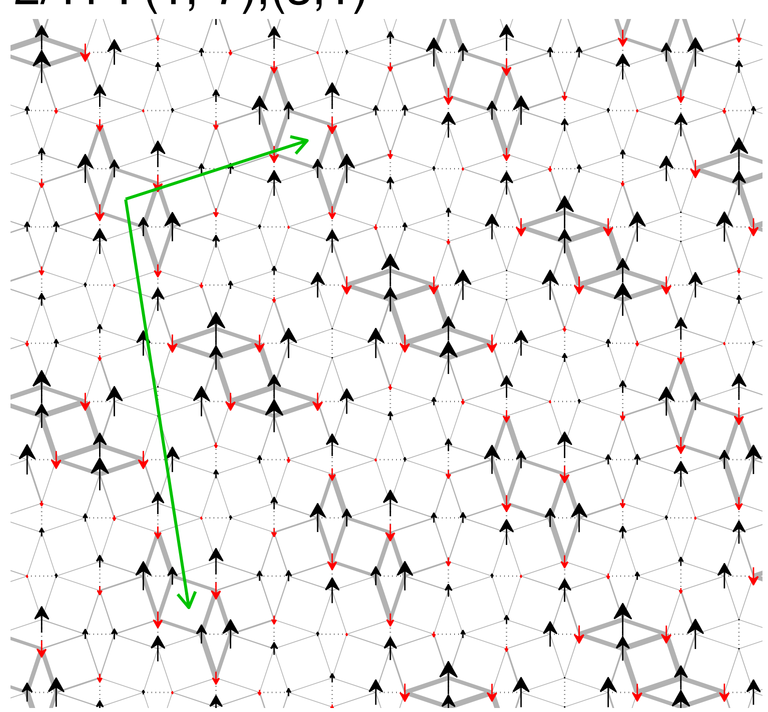
1/6 rhomboid : (3,1),(0,4)



2/13 : (1,-5),(5,1)

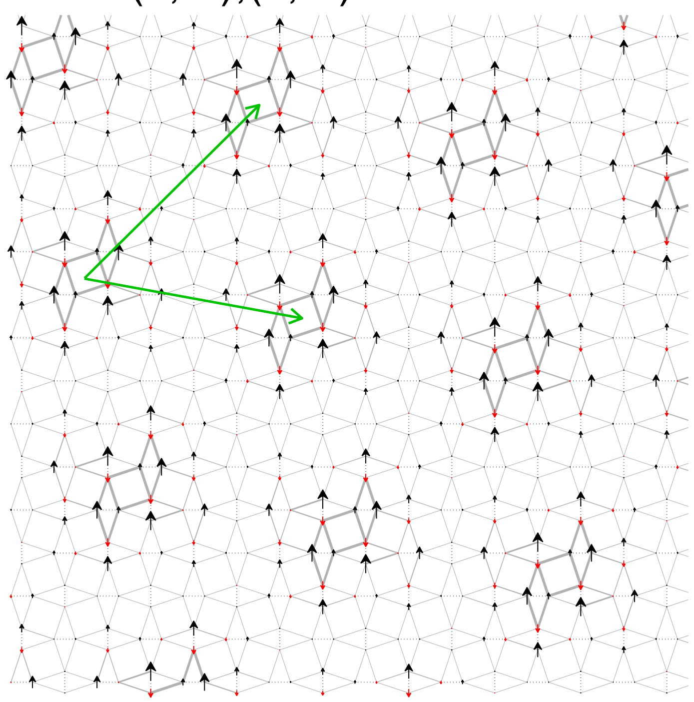


2/11 : (1,-7),(3,1)

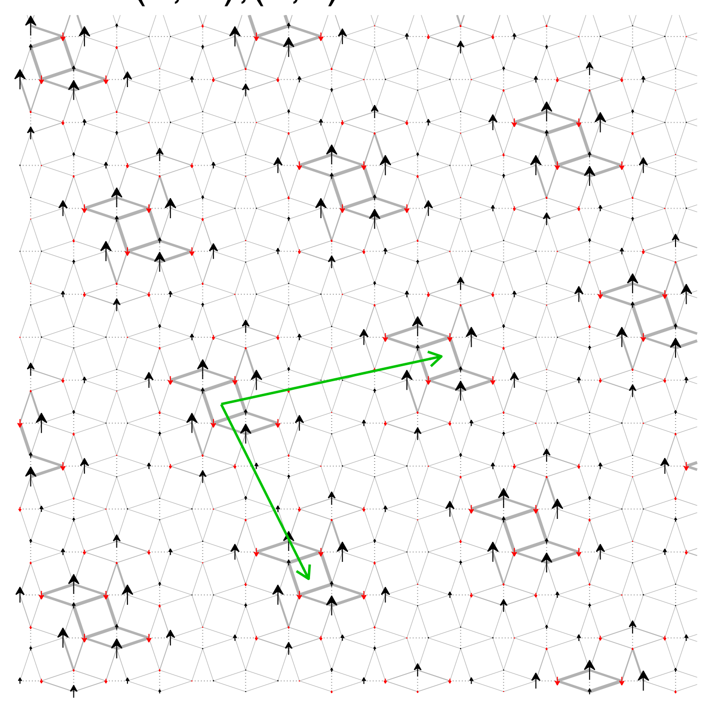


Computing the energies of all possible crystals

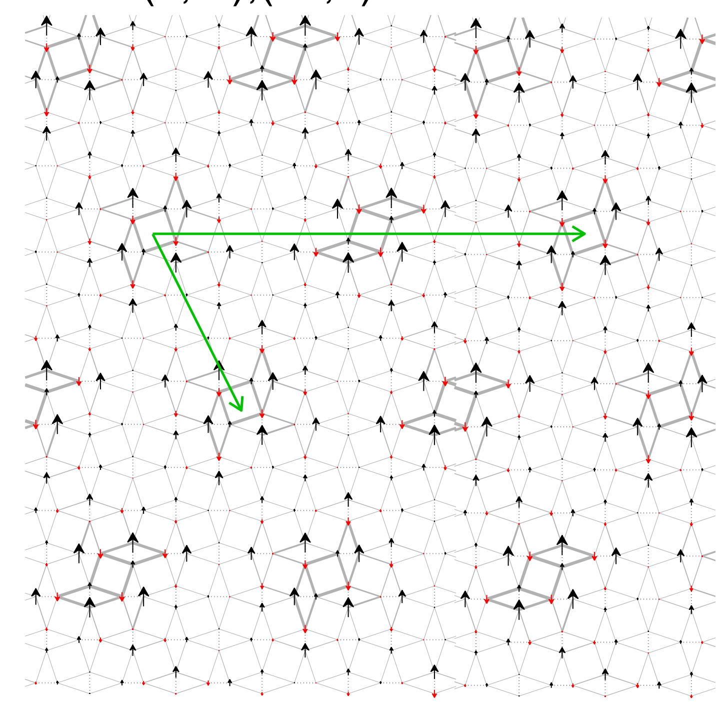
1/12 : (1,-5),(5,-1)



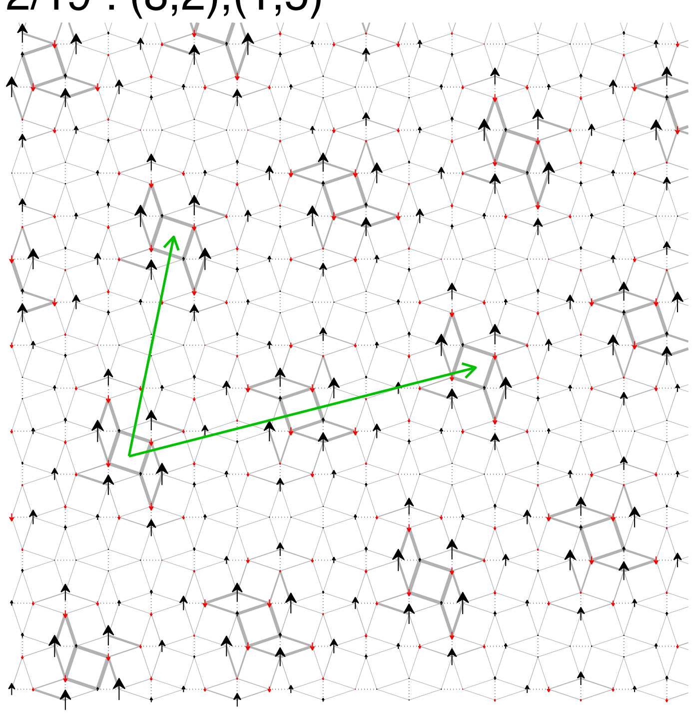
1/11 : (2,-4),(5,1)



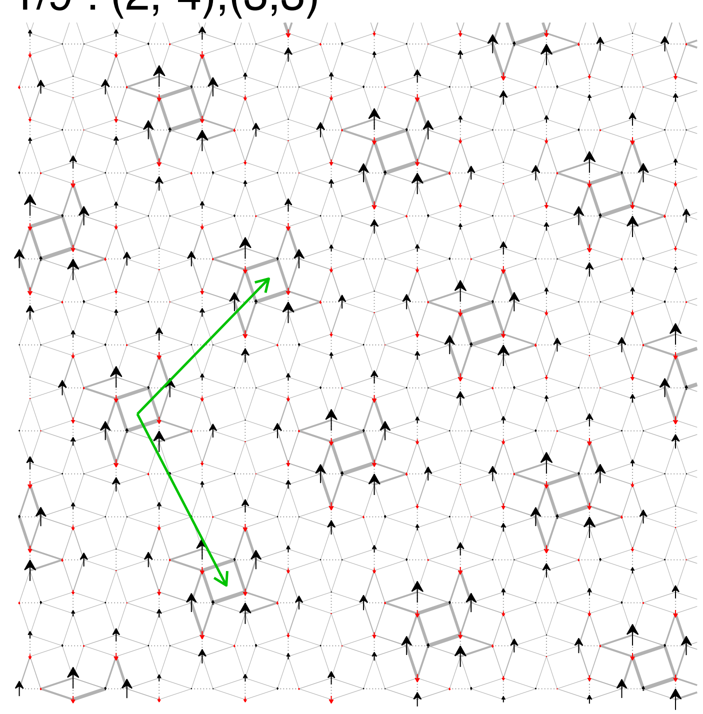
1/10 : (2,-4),(10,0)



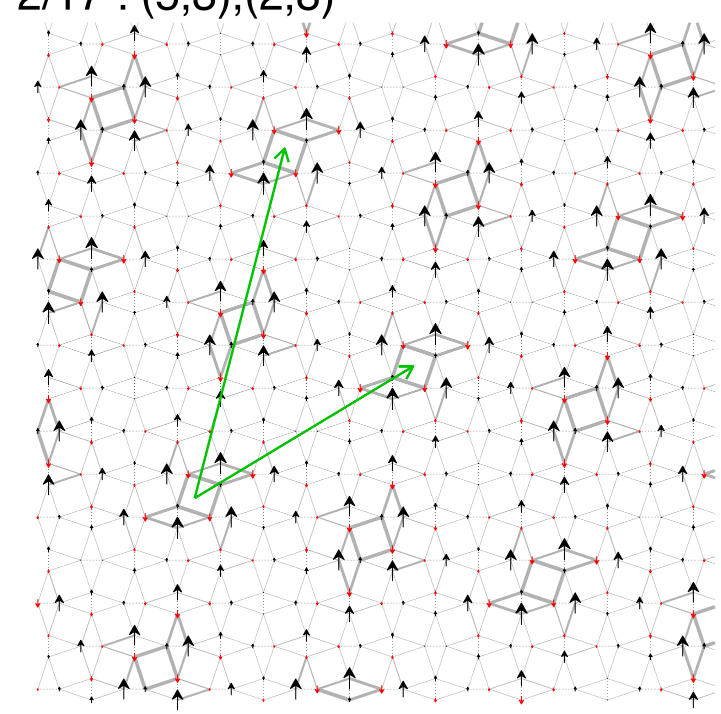
2/19 : (8,2),(1,5)



1/9 : (2,-4),(3,3)

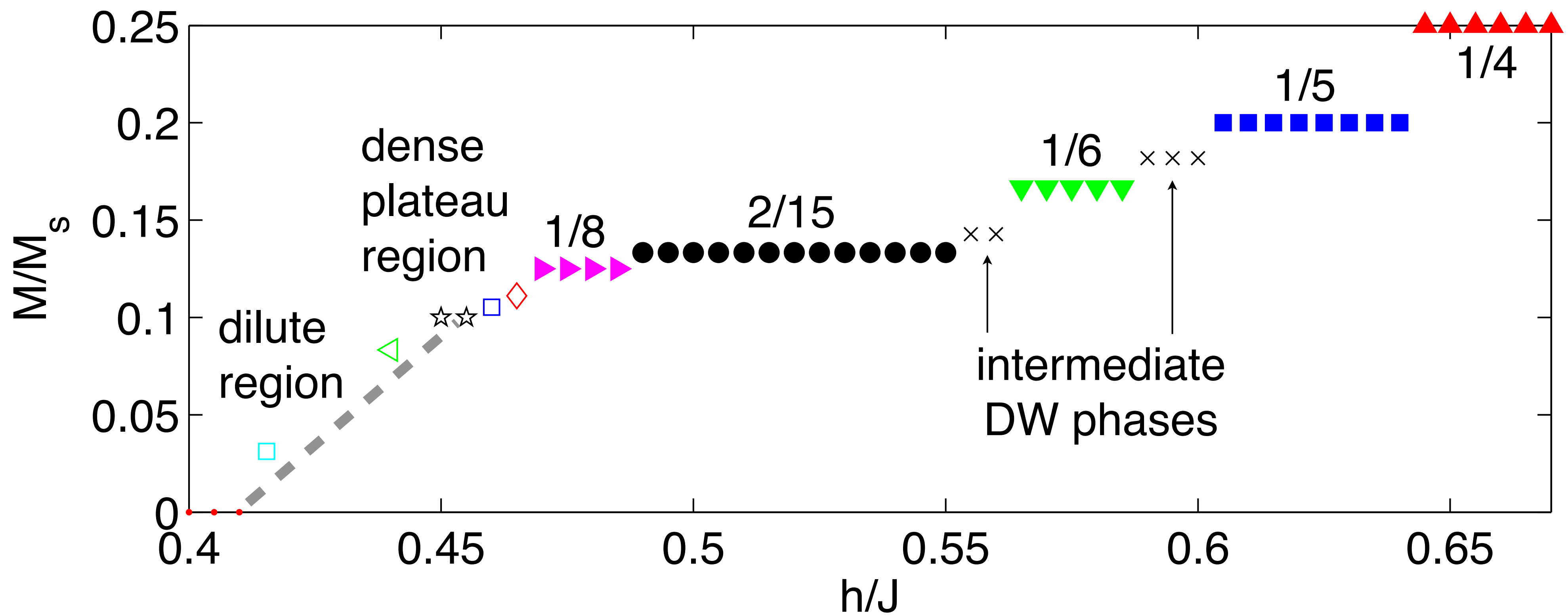


2/17 : (5,3),(2,8)



Magnetization curve obtained with iPEPS

PC, F. Mila, PRL **112** (2014)



$J'/J = 0.63$

★ Sizable plateaus found at: 1/8, 2/15, 1/6, 1/5, 1/4, 1/3, 1/2

[1/5 plateau vanishes upon adding a small (but realistic) DM interaction]

★ **Sequence in agreement with experiments**

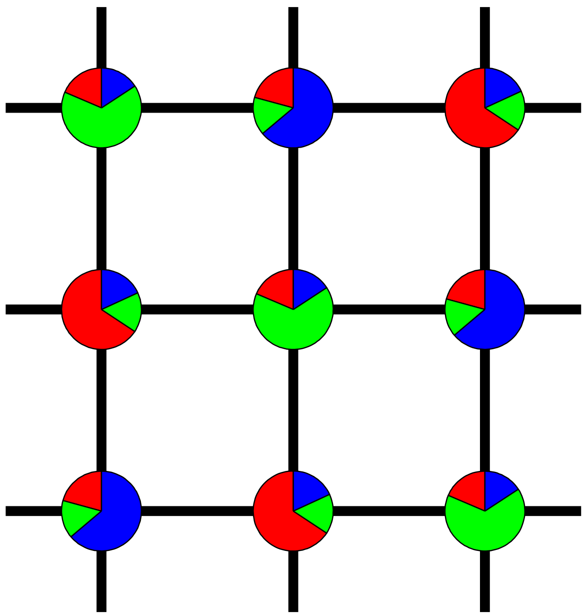
★ New understanding of the magnetization process in $SrCu_2(BO_3)_2$

- see also related work: SSM in high fields: Matsuda et al. PRL **111** (2013)

SU(N) Heisenberg models

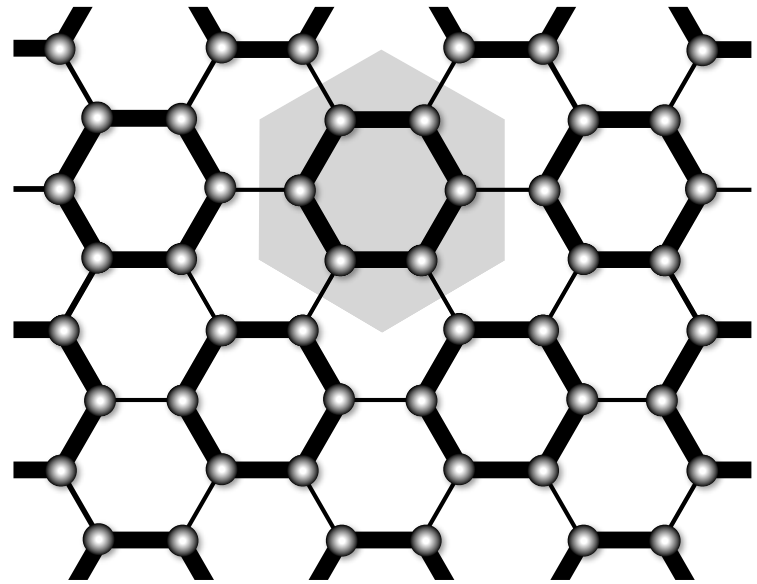
SU(3) square/triangular: *3-sublattice Néel order*

Bauer, PC, et al., PRB **85** (2012)



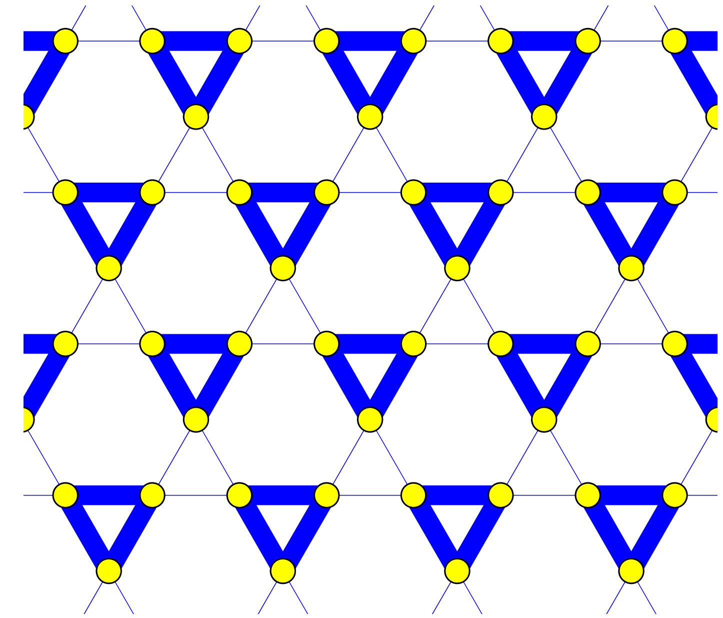
SU(3) honeycomb: *Plaquette state*

Zhao, Xu, Chen, Wei, Qin, Zhang, Xiang, PRB **85** (2012);
PC, Läuchli, Penc, Mila, PRB **87** (2013)



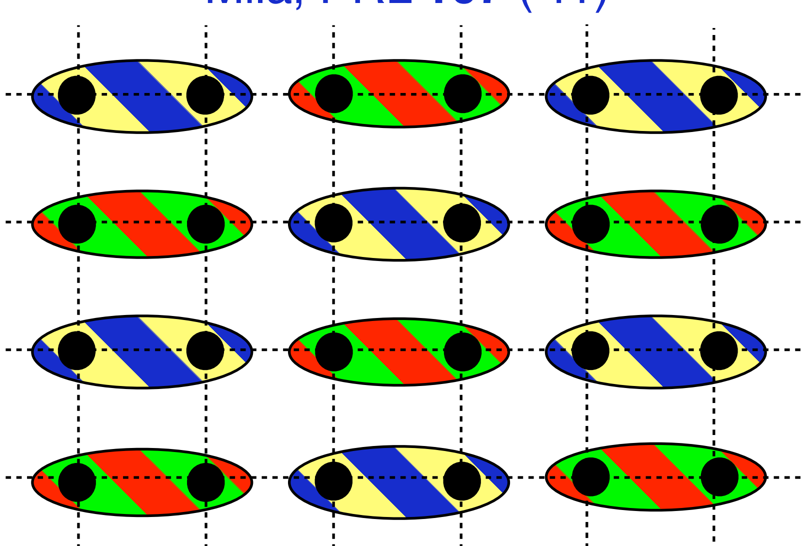
SU(3) kagome: *Simplex solid state*

PC, Penc, Mila, Läuchli, PRB **86** (2012)



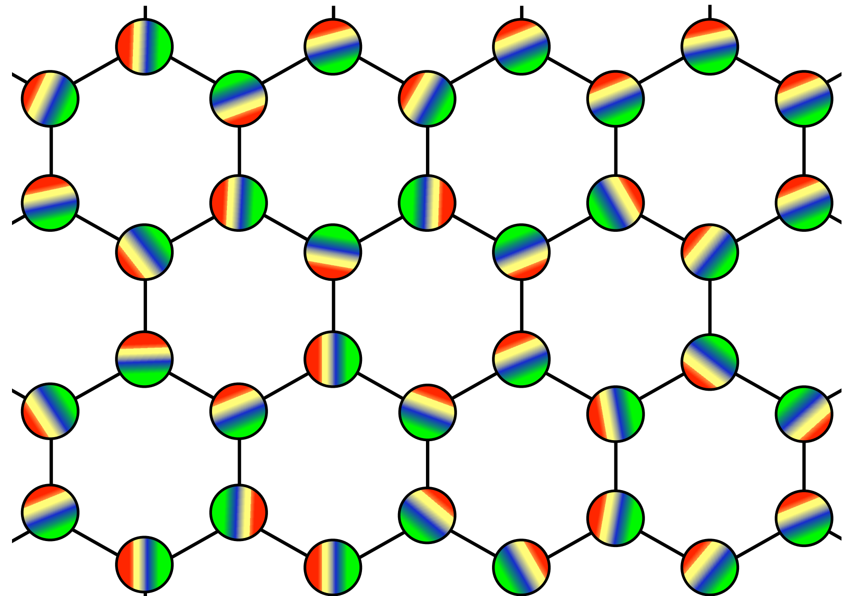
SU(4) square: *Dimer-Néel order*

PC, Läuchli, Penc, Troyer, Mila, PRL **107** ('11)



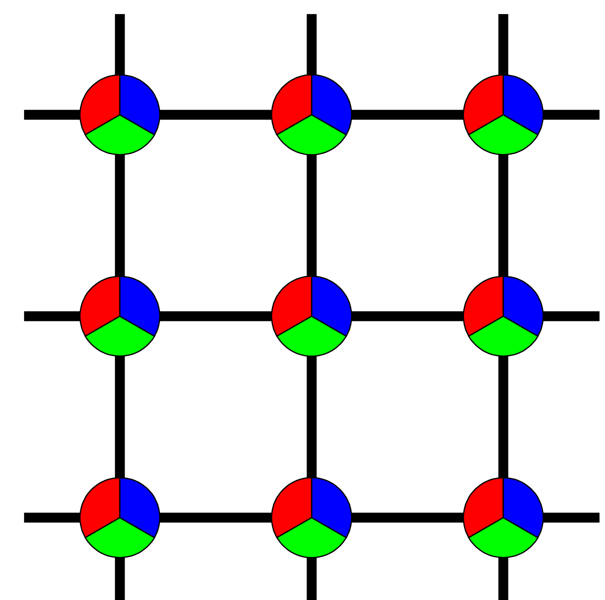
SU(4) honeycomb: *spin-orbital (4-color) liquid*

PC, Lajkó, Läuchli, Penc, Mila, PRX **2** ('12)



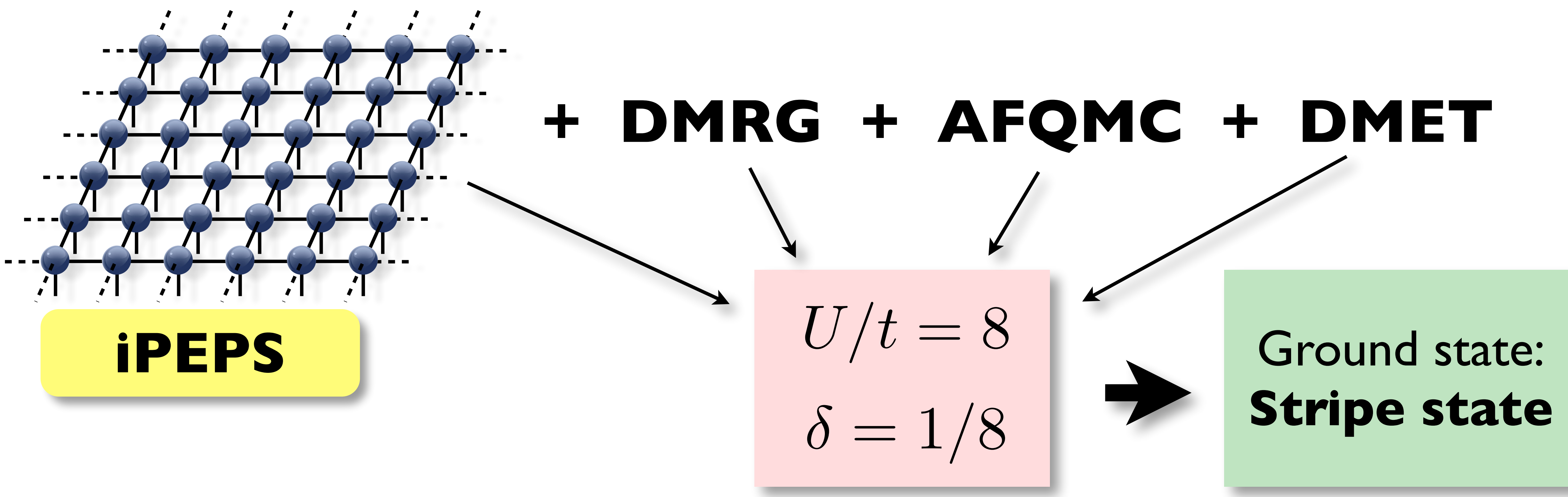
3-color quantum Potts: *superfluid phases*

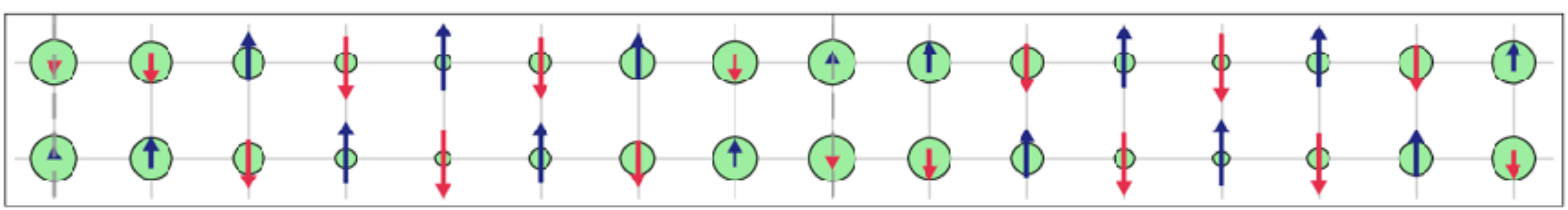
Messio, PC, Mila, PRB **88** (2013)



Stripe order in the 2D Hubbard model

Boxiao Zheng, Chia-Min Chung, PC, Georg Ehlers, Ming-Pu Qin, Reinhard Noack, Hao Shi, Steven White, Shiwei Zhang, Garnet Chan, Science 358, 1155 (2017)

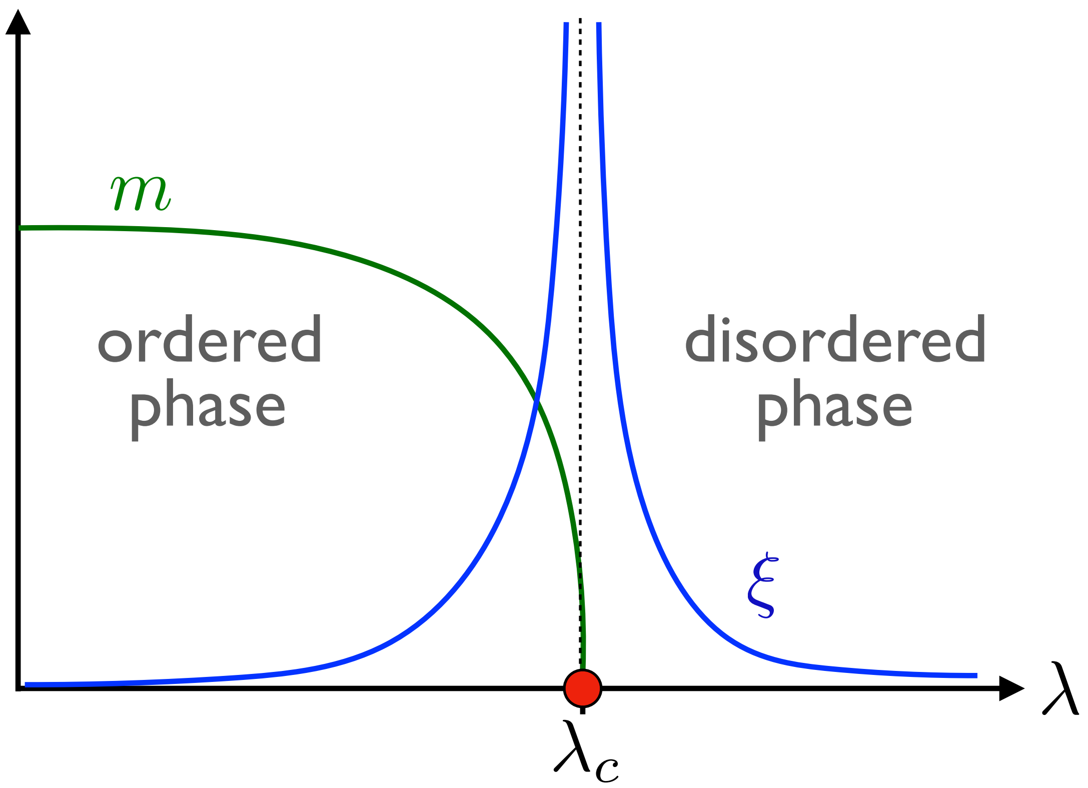




Part V
Finite correlation length scaling:

study of continuous phase transitions +
extrapolation of order parameters

Motivation: study of quantum phase transitions



$$m \sim |g|^{\beta}$$

$$\xi \sim |g|^{-\nu}$$

$$g = \frac{\lambda - \lambda_c}{\lambda_c}$$

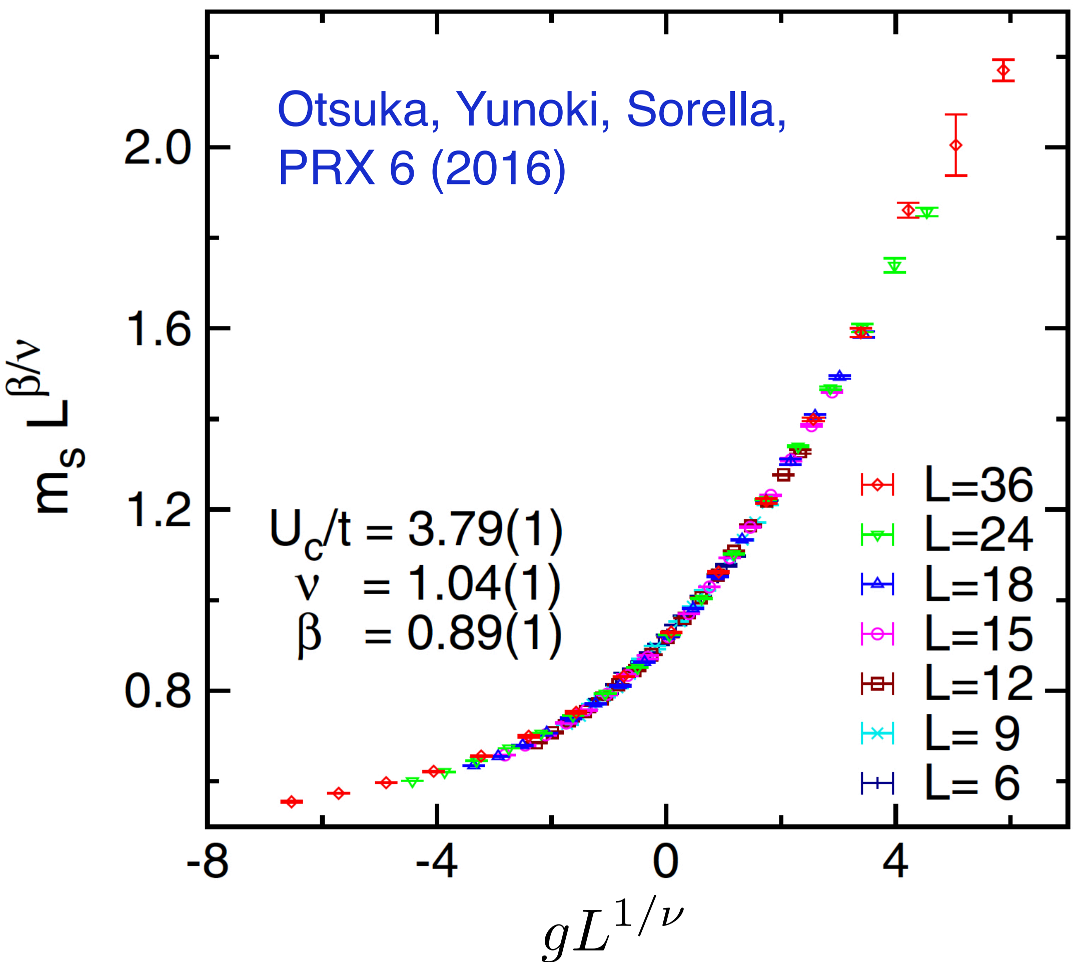
Critical coupling?

Universal critical exponents?

Challenging!

- Strong finite size effects in the vicinity of the critical point
- Powerful approach: *finite size scaling:* $m(g, L) = L^{-\beta/\nu} \mathcal{F}(g L^{1/\nu})$

Motivation: study of quantum phase transitions



$$m \sim |g|^{\beta}$$

$$\xi \sim |g|^{-\nu}$$

$$g = \frac{\lambda - \lambda_c}{\lambda_c}$$

- Strong finite size effects in the vicinity of the critical point
- Powerful approach: *finite size scaling:* $m(g, L) = L^{-\beta/\nu}\mathcal{F}(gL^{1/\nu})$
- Need an accurate method to obtain data for sufficiently large system sizes

Goal:

use iPEPS to study 2D quantum phase transitions

$$L \to \xi_D$$

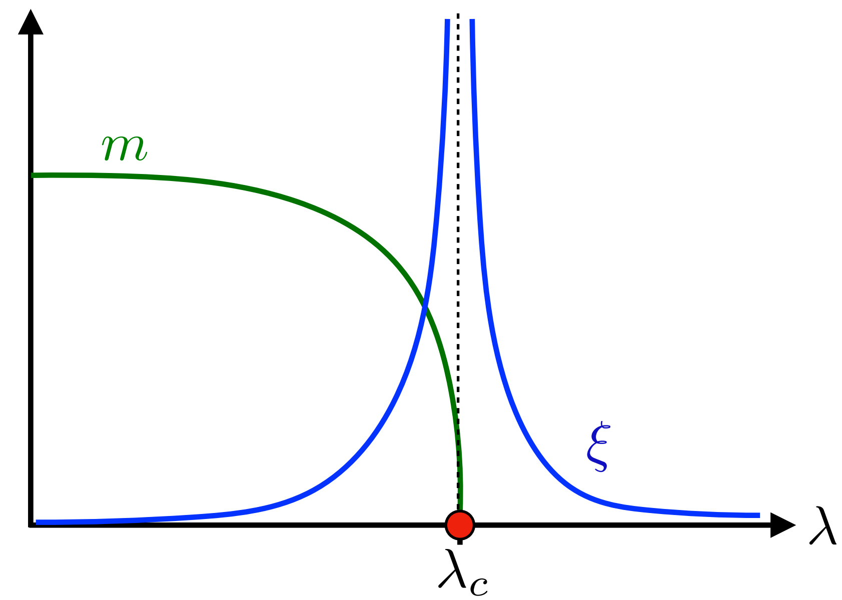
finite correlation length scaling

PC, P. Czarnik, G. Kapteijns, L. Tagliacozzo, PRX 8 (2018)

see also: M. Rader and A. M. Läuchli, PRX 8 (2018)

Finite correlation length scaling in 1D (iMPS)

- iMPS with finite D can only represent states with a finite correlation length
- Correlation length at the critical point: ξ_D
- ξ_D acts as a cut-off on the diverging correlation length, similarly to a finite L



$$m(g,L) = L^{-\beta/\nu}\mathcal{F}(gL^{1/\nu}) \quad \longleftrightarrow \quad m(g,D) = \xi_D^{-\beta/\nu}\mathcal{M}(g\xi_D^{1/\nu})$$

Finite size scaling ansatz — *Finite correlation length scaling ansatz*

Tagliacozzo, de Oliveira, Iblisdir & Latorre, PRB 78 (2008)
Pollmann, Mukerjee, Turner & Moore, PRL 102 (2009)
Pirvu, Vidal, Verstraete & Tagliacozzo, PRB 86 (2012)

- Similar idea for 2D tensor networks for 2D classical partition functions

Nishino, Okunishi, Kikuchi, Phys. Lett. A 213 (1996)

$$m(g,\chi) = \xi_\chi^{-\beta/\nu}\mathcal{M}(g\xi_\chi^{1/\nu})$$

χ: bond dimension for contraction

How about in (2+1)D with iPEPS?

- iPEPS: There exist critical states with a finite D

see e.g. Kraus et al. PRA 81 (2010), Verstraete et al. PRL 96 (2006)

- However, these are 2D classical states or ground states of generalized Rokhsar-Kivelson Hamiltonians at the critical point which can effectively be described by a (2+0)D CFT

see e.g. Henley, JPCM 16 (2004); Ardonne, Fendley & Fradkin, Ann. Phys. 310 (2004); Castelnovo, Chamon, Mudry & Pujol, Ann. Phys. 318 (2005); Isakov, et al. PRB 83 (2011)

- For Lorentz-invariant critical points (2+1D): no example of a critical iPEPS is known

Dynamical critical exponent: $z = 1$ $\xi_{time} \sim \xi_{space}^{z} \sim \xi_{space}$

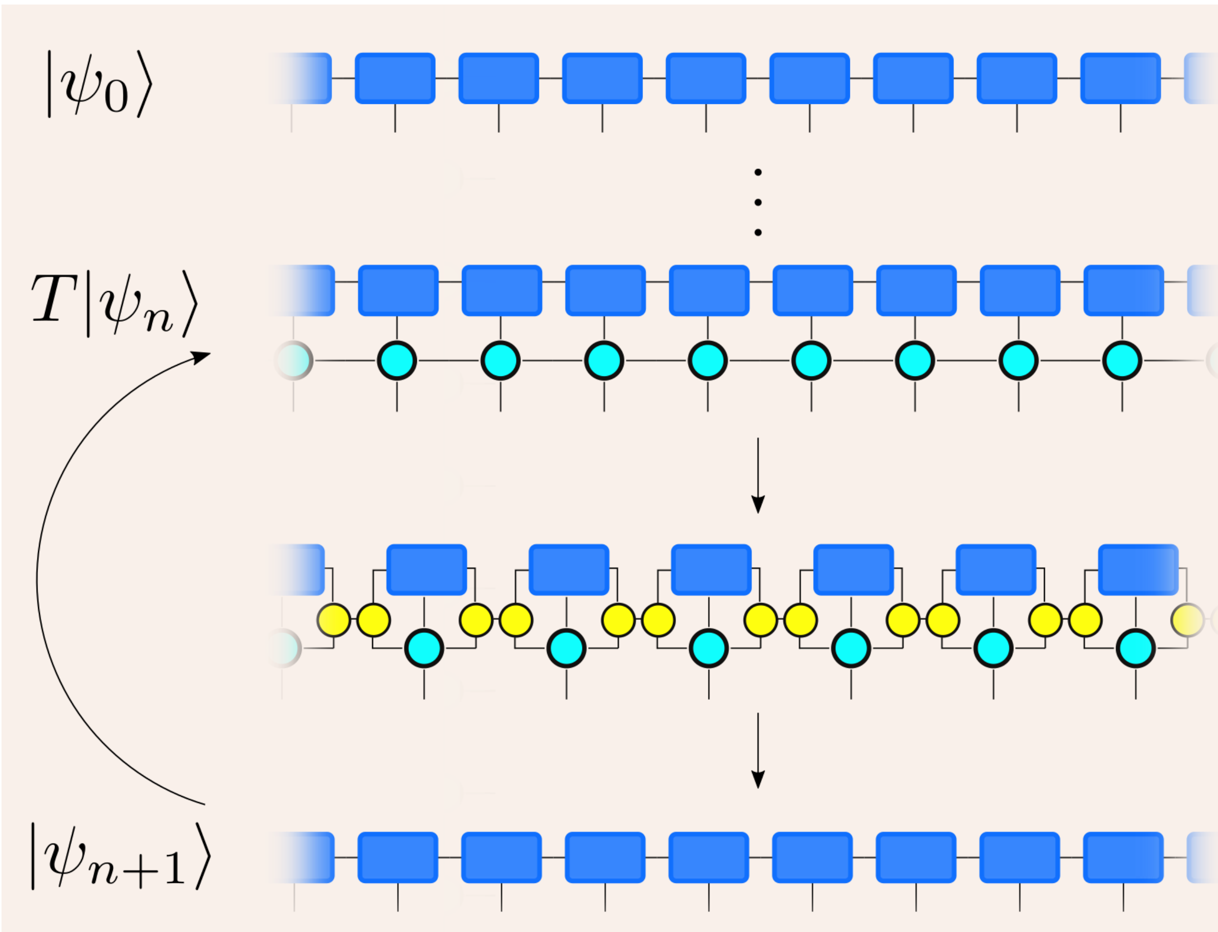
- All simulations suggest: $D \rightarrow \xi_D$ *despite that these states obey an area law!*

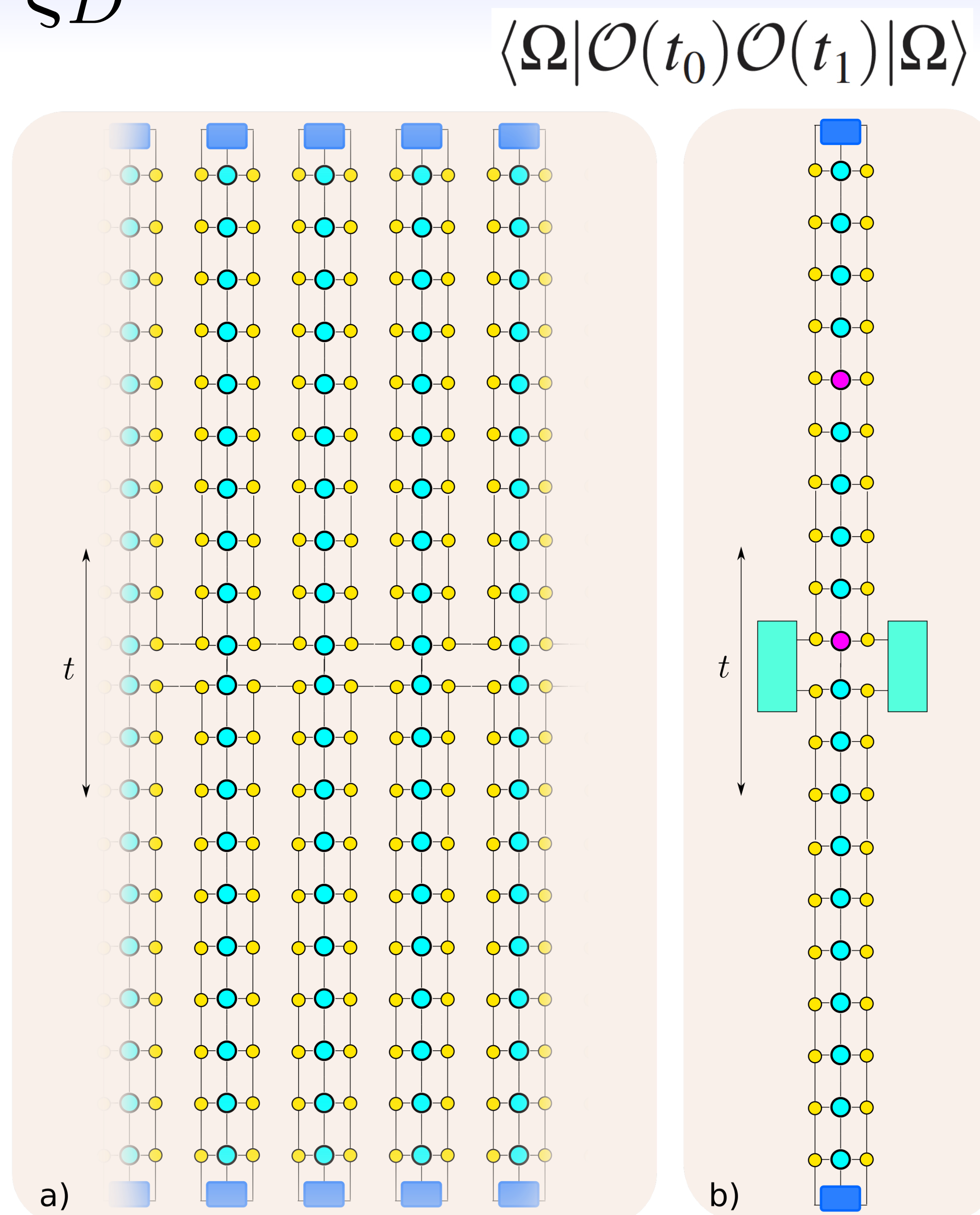
- *Example of a state with an area law which cannot be represented with finite D*

★ We can apply finite correlation length scaling also in 2D!

Intuitive argument why $D \to \xi_D$

Consider imaginary time evolution:





Channel in the time-direction has an MPS structure: $D \to \xi_{time}$

Lorentz invariance: $\xi_{space} \sim \xi_{time}$ → $D \to \xi_{space}$

The best finite D state tries to reproduce Lorentz invariance

Finite correlation length scaling with iPEPS

- Complication: there are two bond dimensions:

Bond dimension of the TN ansatz:

$$D \to \xi_D$$

Boundary dimension in contraction:

$$\chi \to \xi_\chi$$

- Scaling ansatz: $m(g, D, \chi) = \xi_D^{-\beta/\nu} \mathcal{M}(g\xi_D^{1/\nu}, \xi_D/\xi_\chi)$
- Simplify: eliminate χ dependence by taking $\chi \to \infty$ limit
- Now same as in MPS (1D) case:

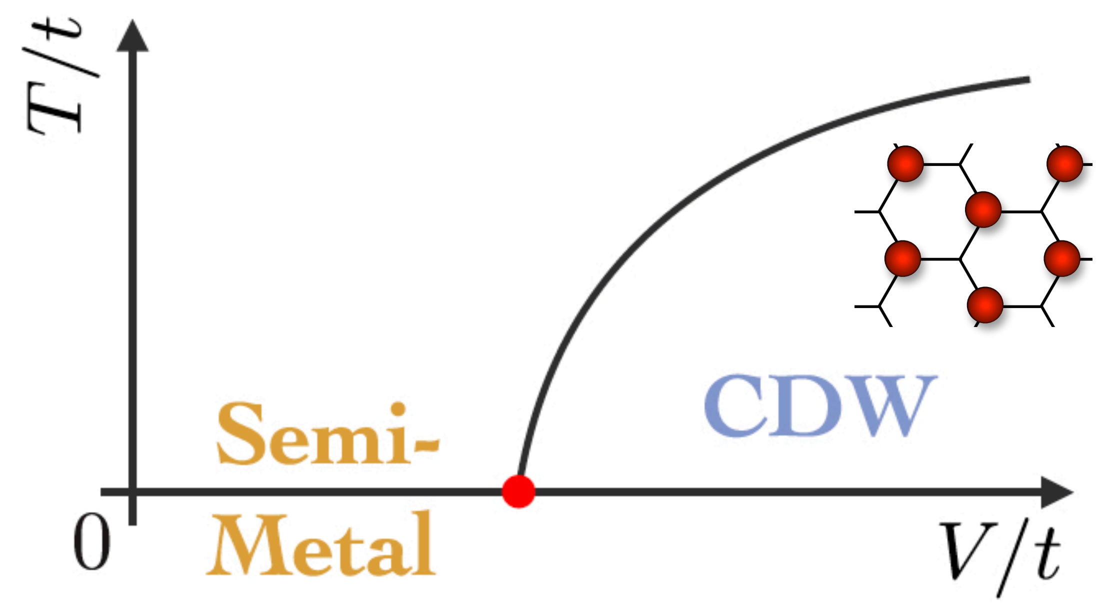
$$m(g, D) = \xi_D^{-\beta/\nu} \mathcal{M}(g\xi_D^{1/\nu})$$

Benchmark example: spinless fermions on honeycomb lattice

- Model:

$$\hat{H} = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \left[\hat{c}^\dagger_{\mathbf{i}} \hat{c}_{\mathbf{j}} + h.c. \right] + V \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \hat{n}_{\mathbf{i}} \hat{n}_{\mathbf{j}}$$

at half filling



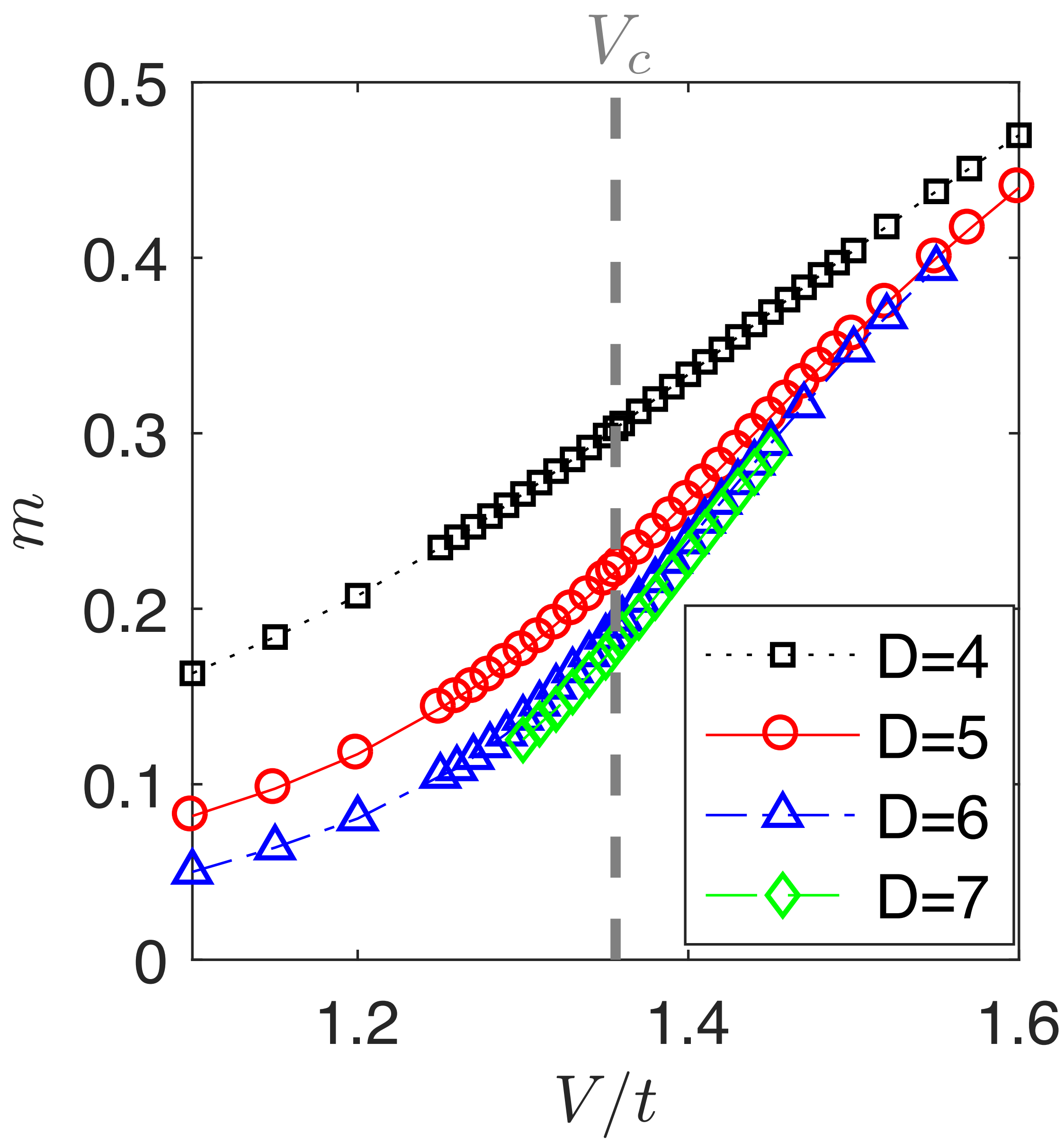
Wang, PC, Troyer, NJP 16 (2014)

- Continuous PT between a semi-metal phase and charge-density wave phase (CDW) *(Chiral Ising Gross-Neveu universality class with z=1)*

- No sign problem in Quantum Monte Carlo!

Huffman, Chandrasekharan, PRB 89 (2014); Wang, PC, Troyer, NJP 16 (2014); Li, Jiang, Yao, NJP 17 (2015); Wang, Iazzi, PC & Troyer, PRB 91 (2015); Wang, Liu, Troyer PRB 93 155117 (2016); Hesselmann & Wessel, PRB 93 (2016)

Benchmark example: spinless fermions on honeycomb lattice



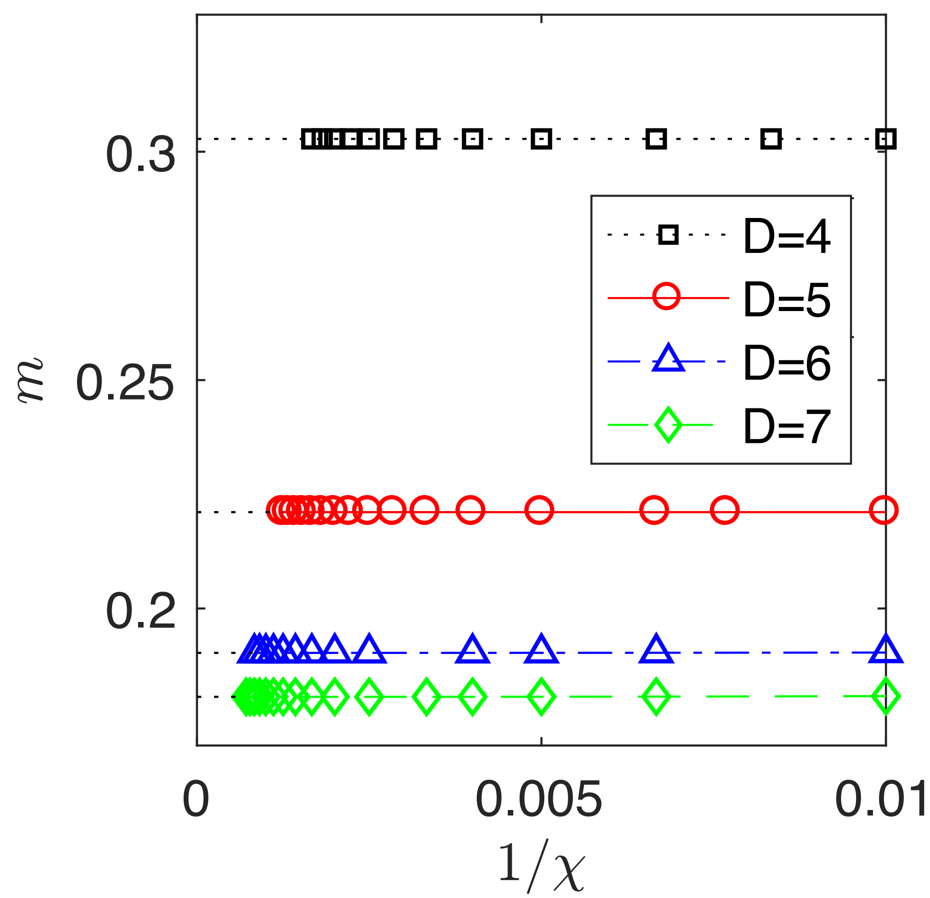
CDW order parameter:

$$m = |n_A - n_B|$$

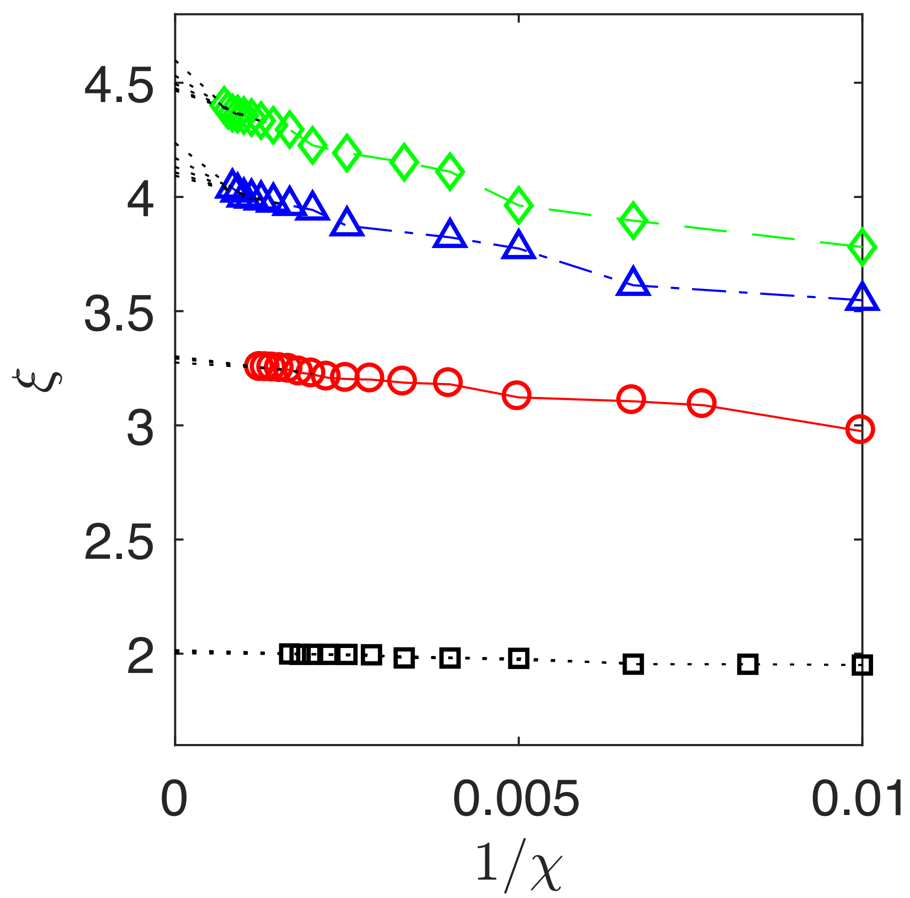
- Finite size effects get weaker with increasing D

χ - dependence

Order parameter



Correlation length



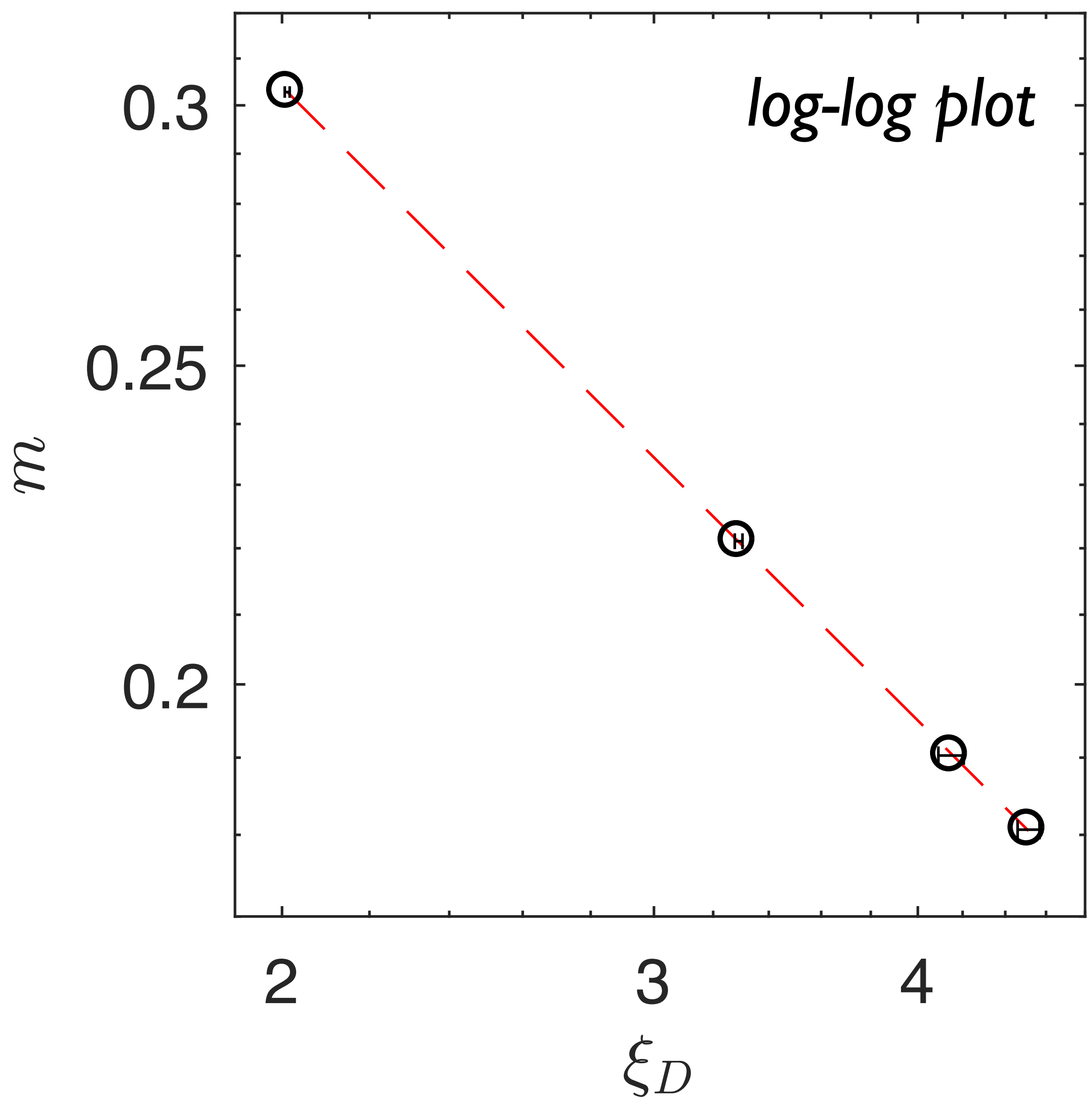
- Weak χ dependence

- Stronger χ dependence

  ➡ extrapolate in $1/\chi$

Scaling ansatz at the critical point, $V_c/t = 1.356$

$$m(g=0, D) = \xi_D^{-\beta/\nu}\mathcal{M}(0\cdot\xi_D^{1/\nu}) \sim \xi_D^{-\beta/\nu} \qquad g = (V - V_c)/V_c$$



- Linear fit to log-log plot yields

  $\beta/\nu = 0.64(2)$

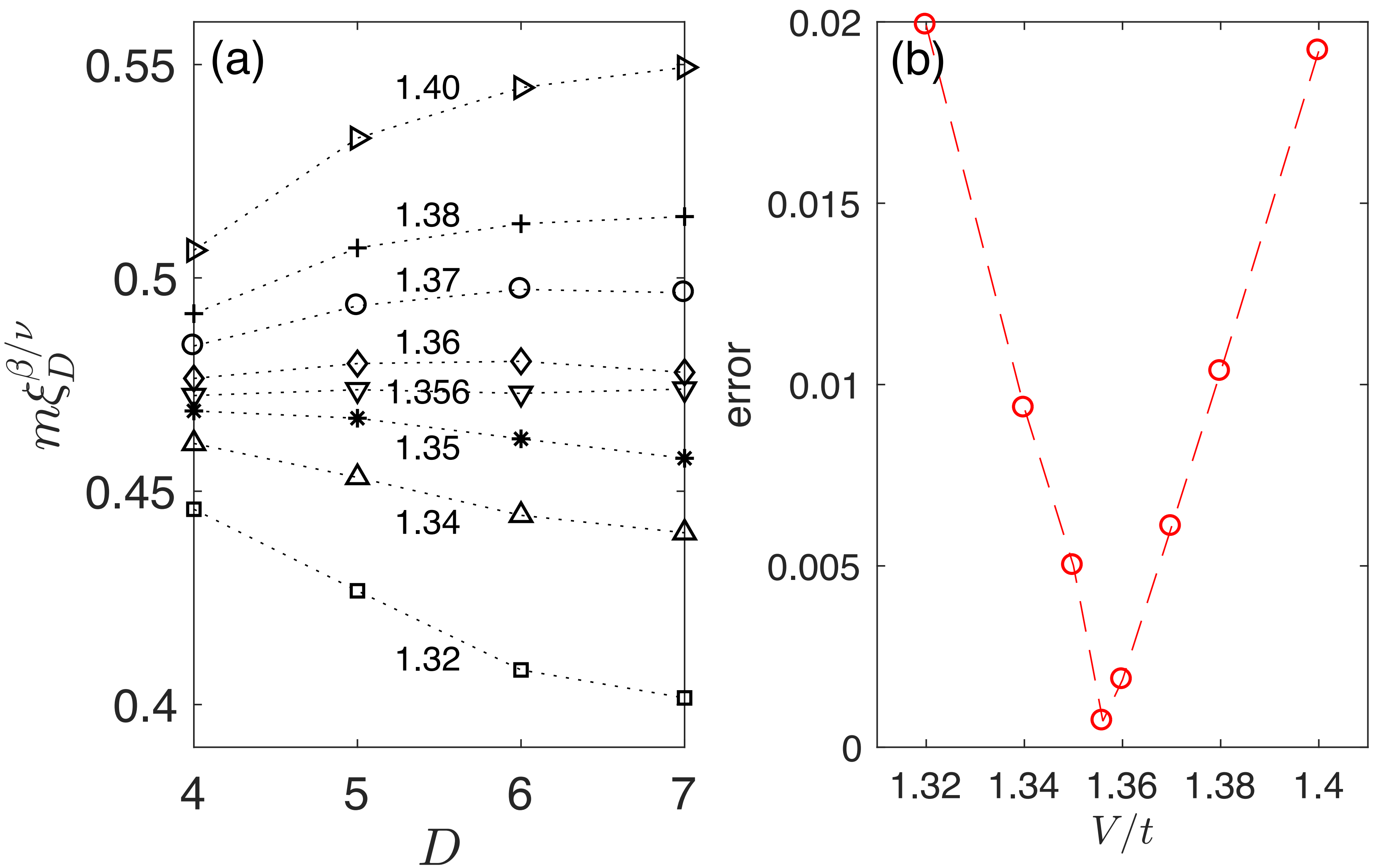
- In agreement with QMC:

  $\beta/\nu = 0.65(4)$

  Wang, PC, Troyer, NJP16 (2014)

Finding V_c with fixed $\beta/\nu = 0.64$

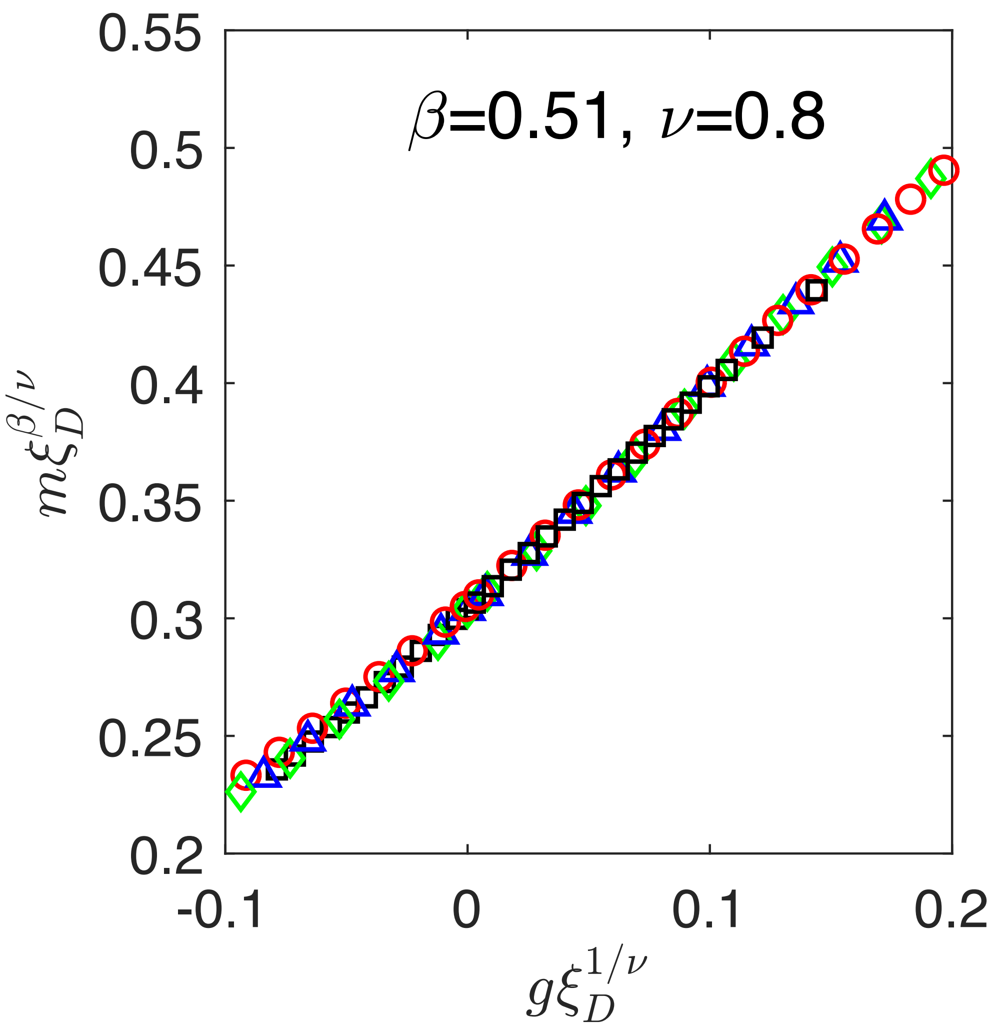
$$m(g, D)\,\xi_D^{\beta/\nu} = \mathcal{M}(g\xi_D^{1/\nu}) \qquad y = m(g=0, D)\,\xi_D^{\beta/\nu} = const$$



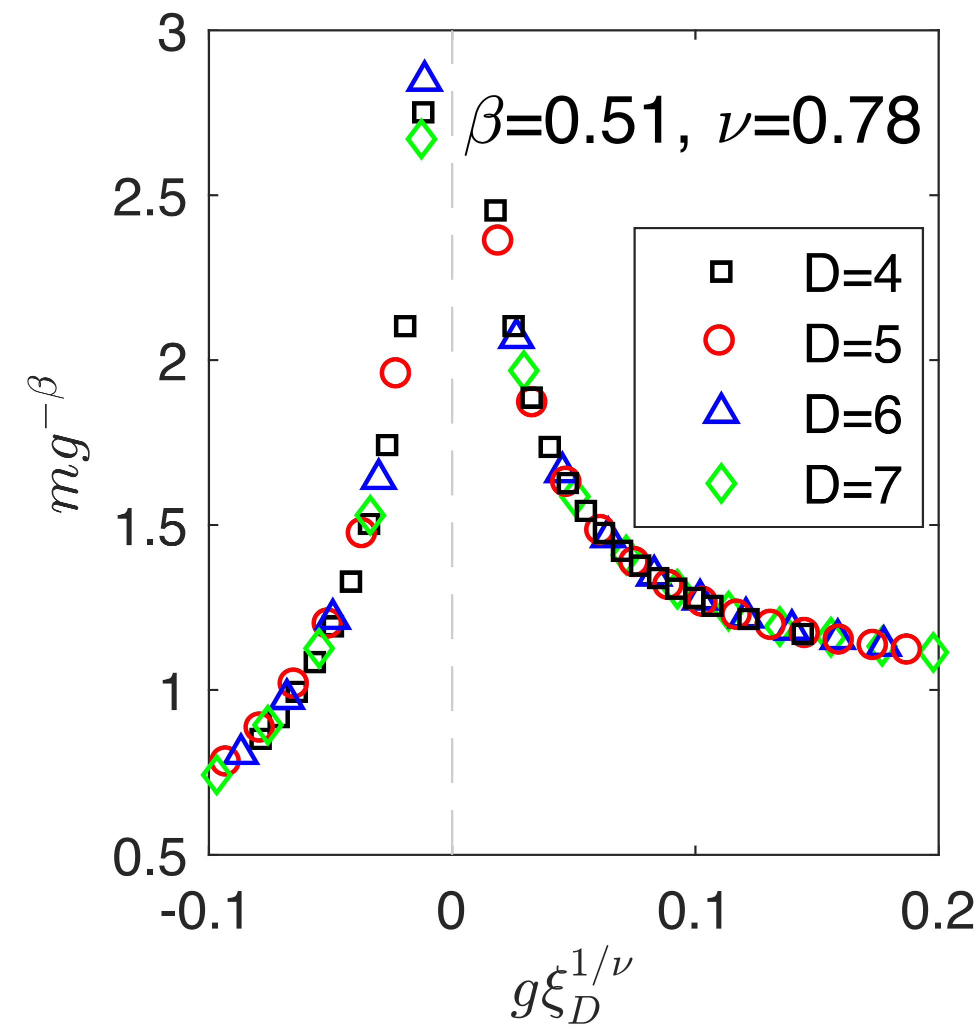
- $V_c/t = 1.356(4)$, consistent with QMC: $V_c/t = 1.356(1)$

Data collapse

$$m(g,D)\,\xi_D^{\beta/\nu} = \mathcal{M}(g\xi_D^{1/\nu})$$



$$m(g,D)\,g^{-\beta} = \tilde{\mathcal{M}}(g\xi_D^{1/\nu})$$



iPEPS: $\beta = 0.51(1) \qquad \nu = 0.79(2)$

QMC: $\beta = 0.52(3) \qquad \nu = 0.80(3)$

Wang, PC, Troyer, NJP16 (2014)

How to determine V_c directly?

- Derive ansatz including derivative of m:

$$m(g, D) = \xi_D^{-\beta/\nu} \mathcal{M}(g\xi_D^{1/\nu})$$

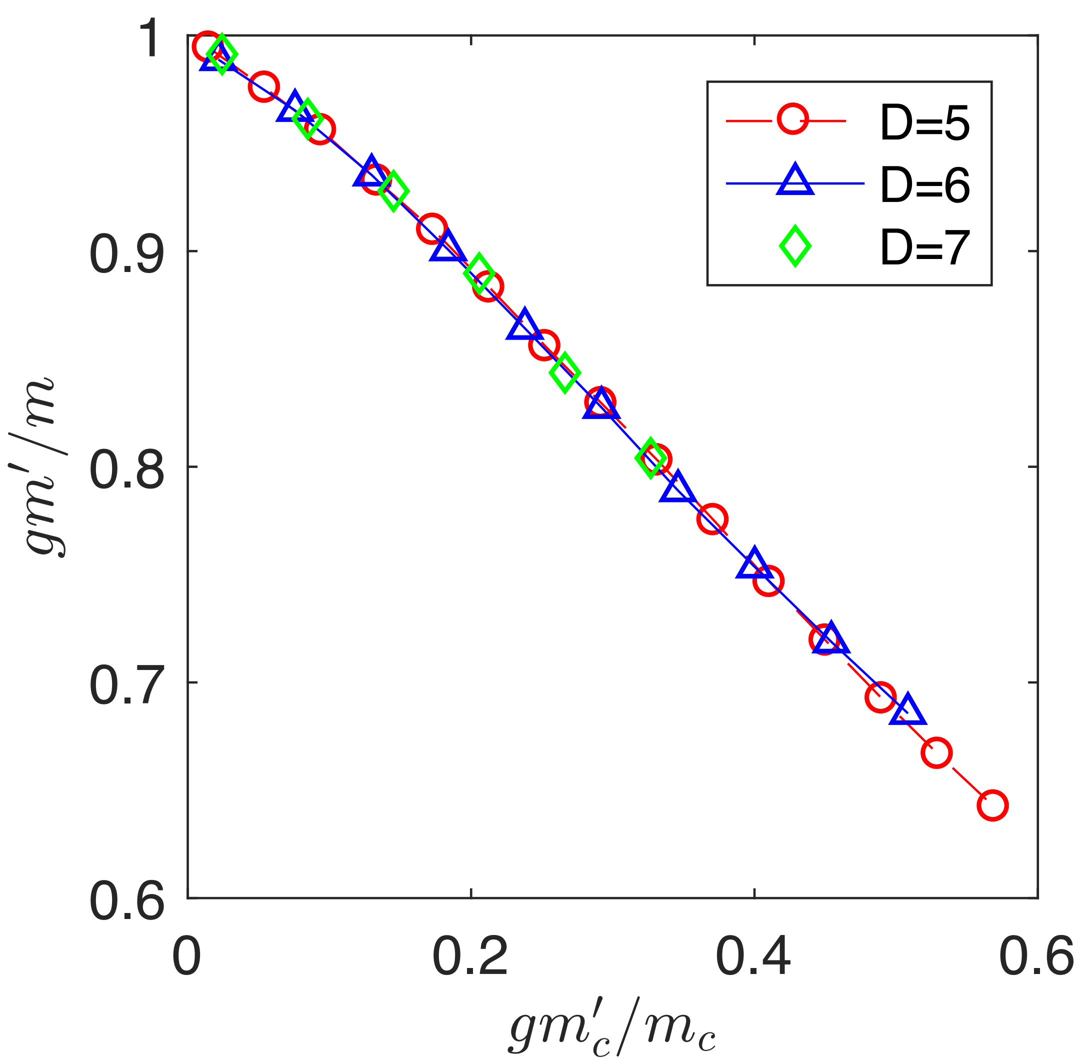
$$m'(g, D) = \xi_D^{-(\beta-1)/\nu} \mathcal{M}'(g\xi_D^{1/\nu})$$

$$\frac{m_c'(D)}{m_c(D)} := \frac{m'(g=0, D)}{m(g=0, D)} \sim \xi_D^{1/\nu}$$

$$\mathcal{M}(g\xi_D^{1/\nu}) \sim \mathcal{P}\left(g\frac{m_c'(D)}{m_c(D)}\right)$$

$$g\frac{m'(g, D)}{m(g, D)} = \mathcal{P}\left(g\frac{m_c'(D)}{m_c(D)}\right)$$

m'/m - approach



iPEPS: $V_c/t = 1.356(2)$

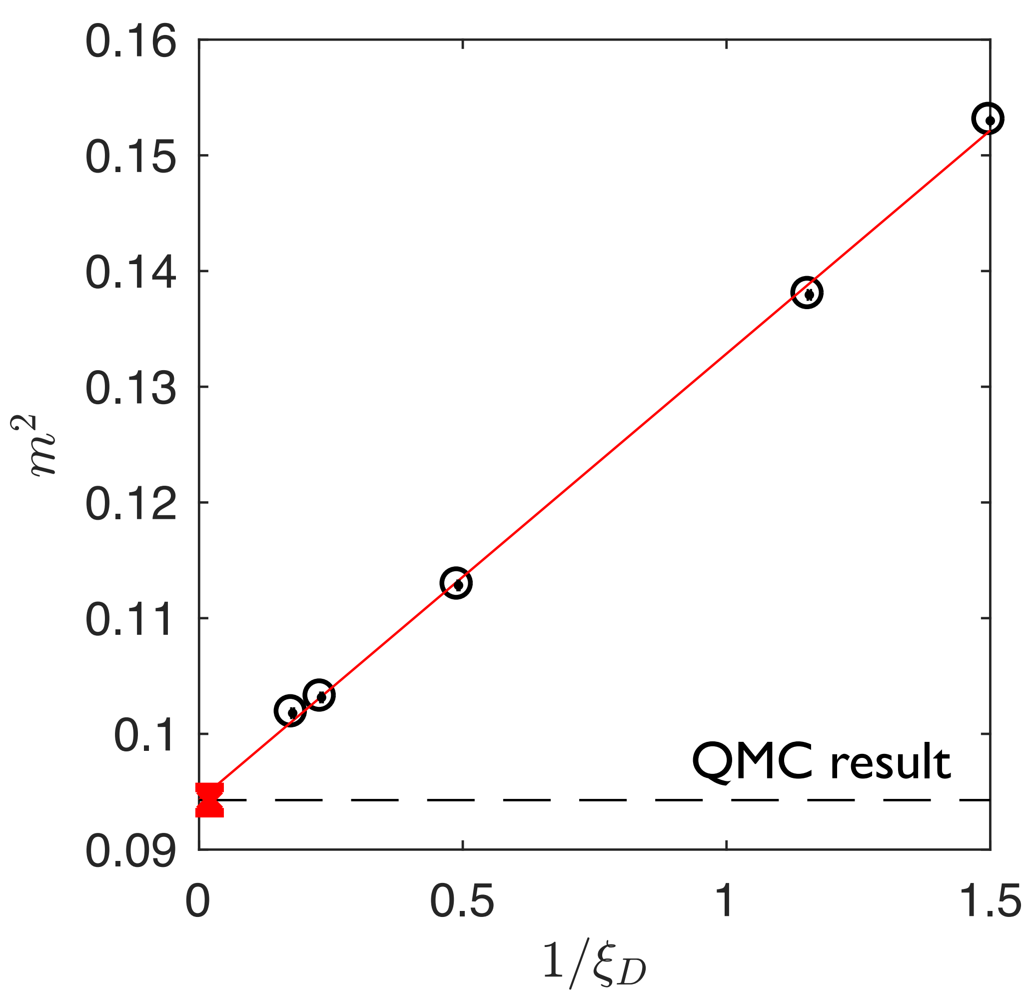
QMC: $V_c/t = 1.356(1)$

Wang, PC, Troyer, NJP16 (2014)

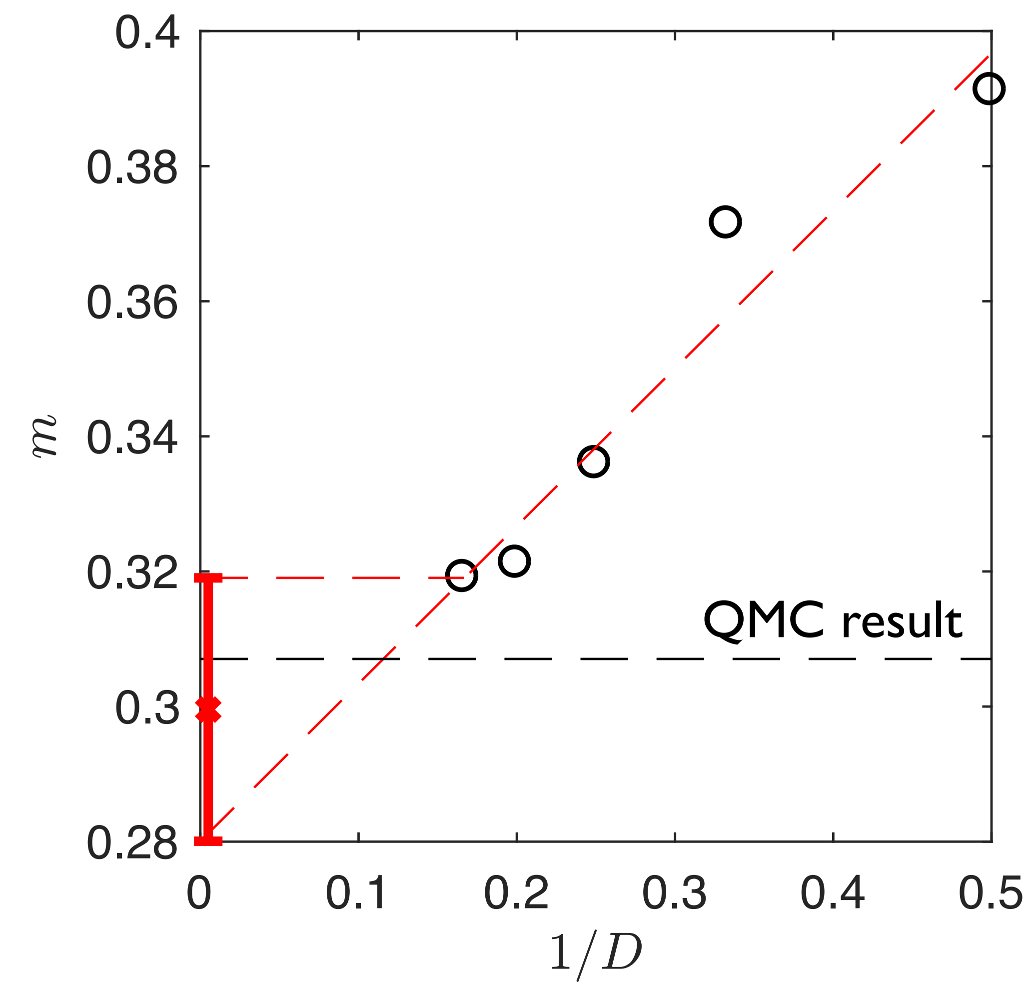
Extrapolation of order parameter: 2D Heisenberg model

- Use FCL scaling to extrapolate the order parameter in gapless system

Extrapolation in $1/\xi_D$



$1/D$ extrapolation



iPEPS: $m = 0.307 \pm 0.002$

QMC: $m = 0.30743(1)$

Sandvik & Evertz (2010)

Strong improvement compared to "naive" 1/D extrapolation!

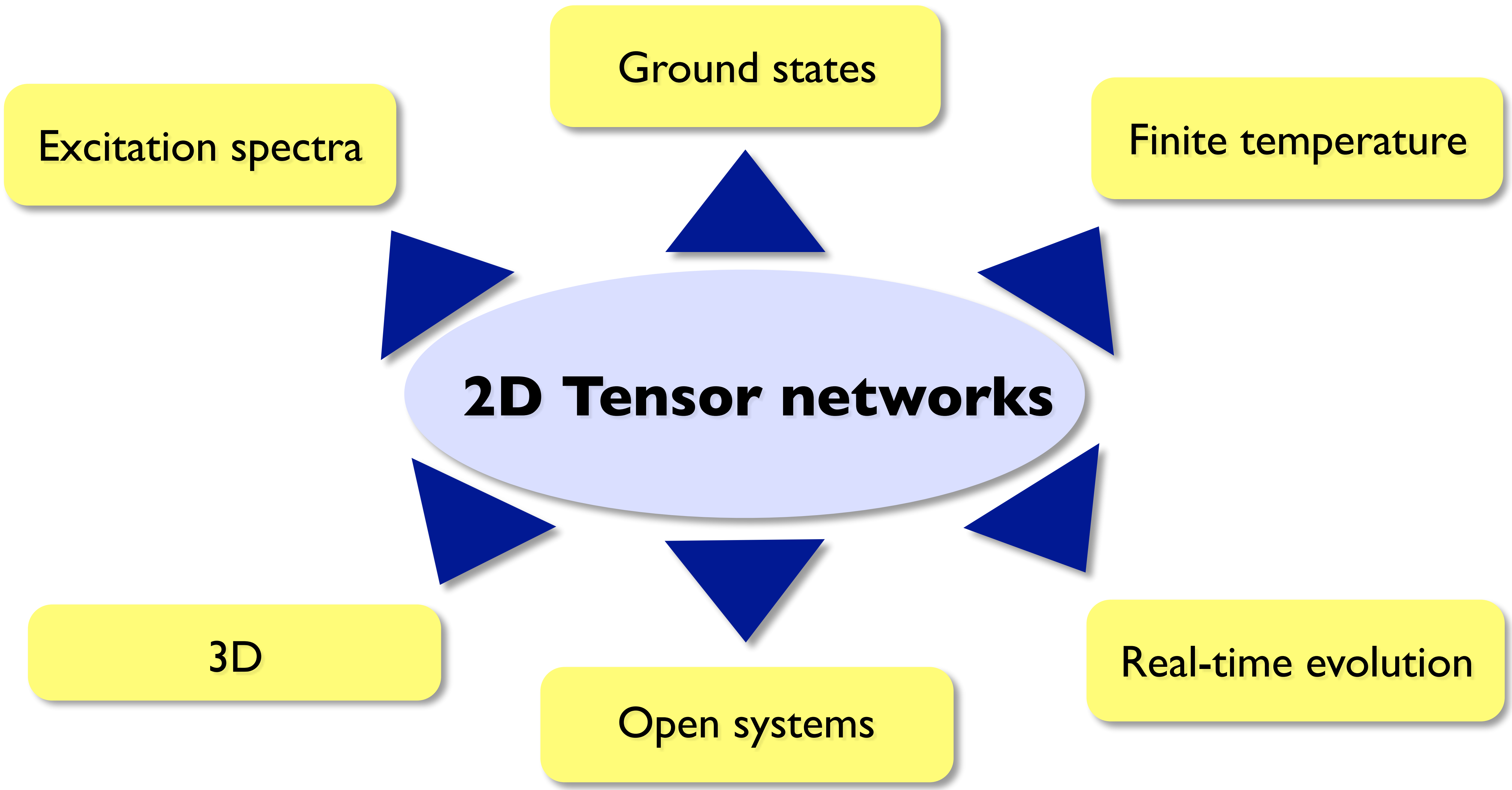
Summary: finite correlation length scaling with iPEPS

- ✓ Study quantum phase transitions (Lorentz-invariant QCP) using finite correlation length scaling with iPEPS
- ✓ Benchmark: Critical coupling and exponents in agreement with QMC
- ✓ m'/m approach: determine critical coupling
- ✓ Use ξ_D to extrapolate order parameters in gapless systems
- ✓ Promising approach for critical systems out of reach by QMC

PC, P. Czarnik, G. Kapteijns, L. Tagliacozzo, PRX 8 (2018)
M. Rader and A. M. Läuchli, PRX 8 (2018)

Outlook & summary

Extensions of 2D tensor networks methods



Summary

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

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

★ iPEPS has become a powerful tool to study challenging problems

★ Shastry-Sutherland model: new understanding of the magnetization process in $SrCu_2(BO_3)_2$

★ Finite correlation length scaling: systematic study of 2nd order phase transitions

✓ Big room for improvement & many possible extensions!

➡ **It's an exciting time to work on tensor networks!**

Thank you for your attention!