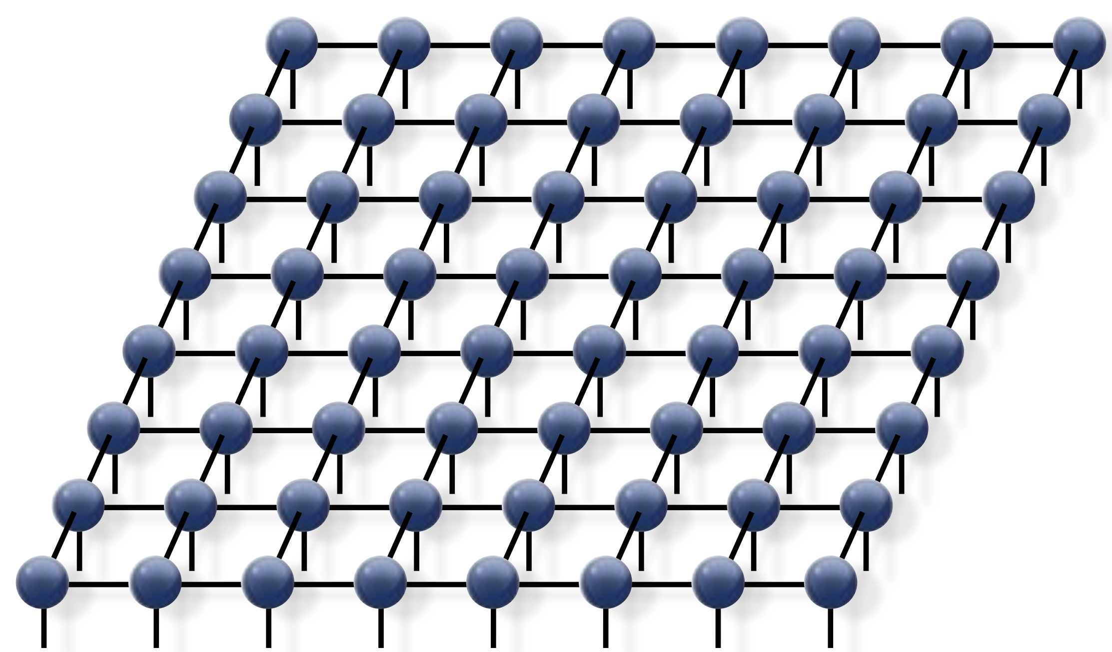
Introduction to (i)PEPS

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam



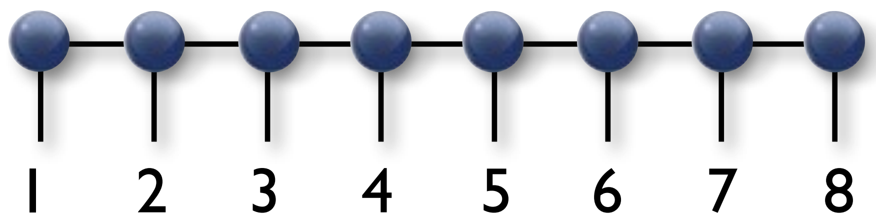
2017 Arnold Sommerfeld School, Munich, Germany

Numerical methods for correlated many-body systems

Overview: tensor networks in 1D and 2D

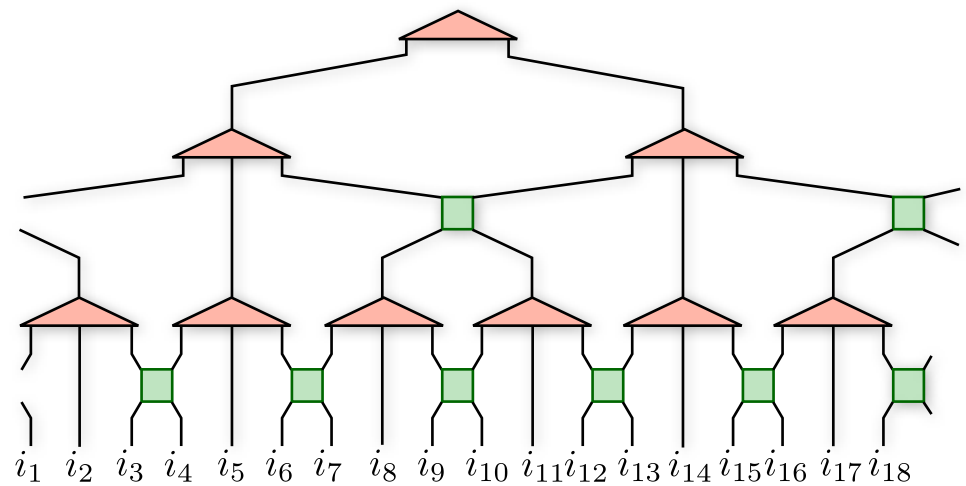
1D

MPS
Matrix-product state



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

1D MERA
Multi-scale entanglement renormalization ansatz

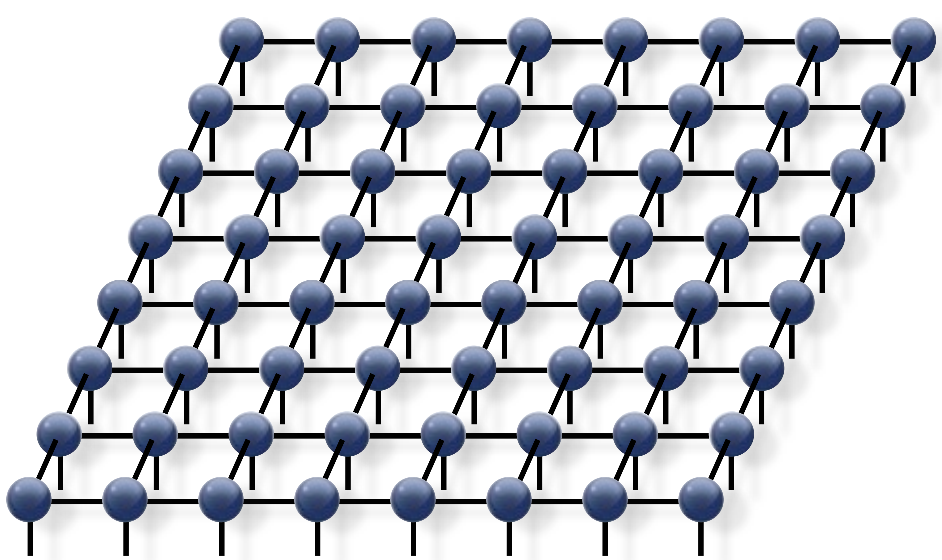


and more

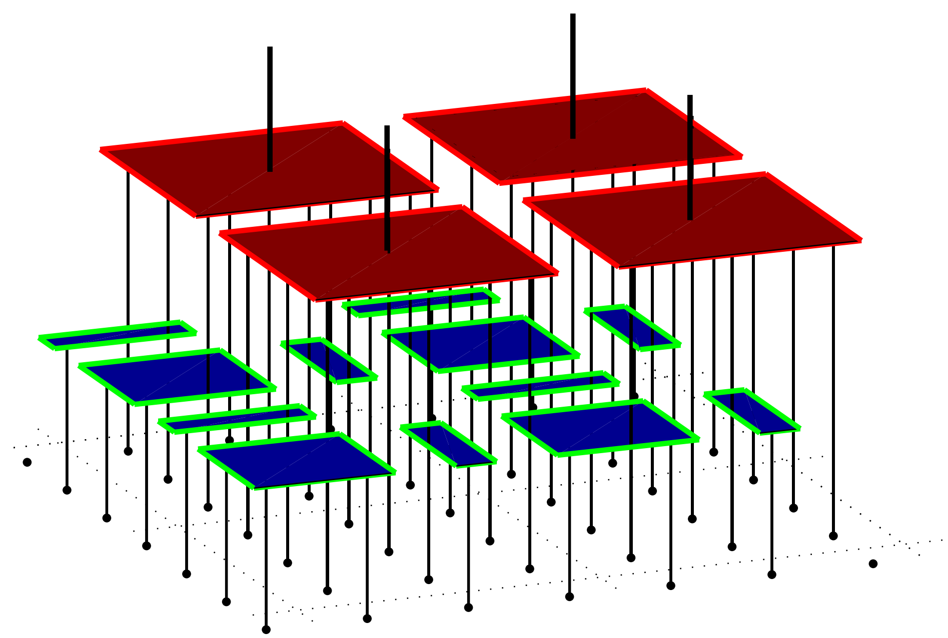
- 1D tree tensor network
- correlator product states
- ...

2D

PEPS
projected entangled-pair state



2D MERA



and more

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

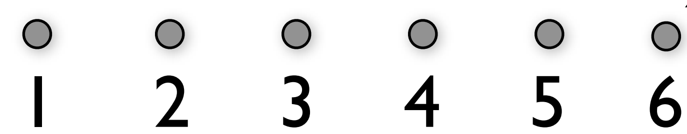
Outline

- Part I: PEPS and iPEPS ansatz
  - ✦ *Recap: area law of the entanglement entropy*
- Part II: Contraction
  - ✦ *MPS-MPO approach, corner-transfer-matrix (**CTM**) method, Tensor Renormalization Group (TRG), Tensor network renormalization (TNR)*
  - ✦ *Simple example: solving the 2D classical Ising model with the CTM method*
- Part III: Optimization
  - ✦ *Imaginary time evolution: simple vs full update*
  - ✦ *Variational optimization (energy minimization)*
- Part IV: iPEPS example application
- Outlook & summary

PART I:
Recap & (i)PEPS ansatz

Recap: Tensor network ansatz for a wave function

Lattice:



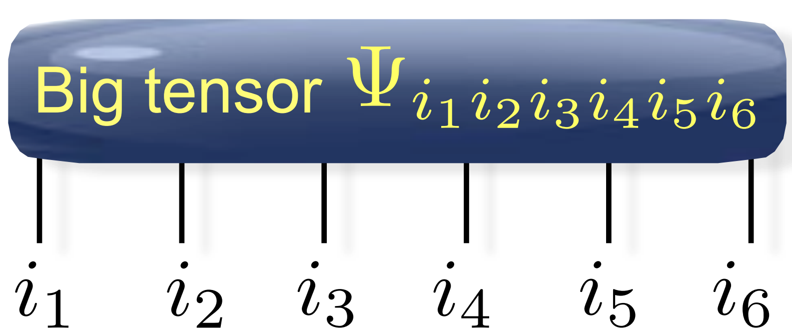
2 basis states per site: $\{|\uparrow\rangle, |\downarrow\rangle\}$

2^6 basis states

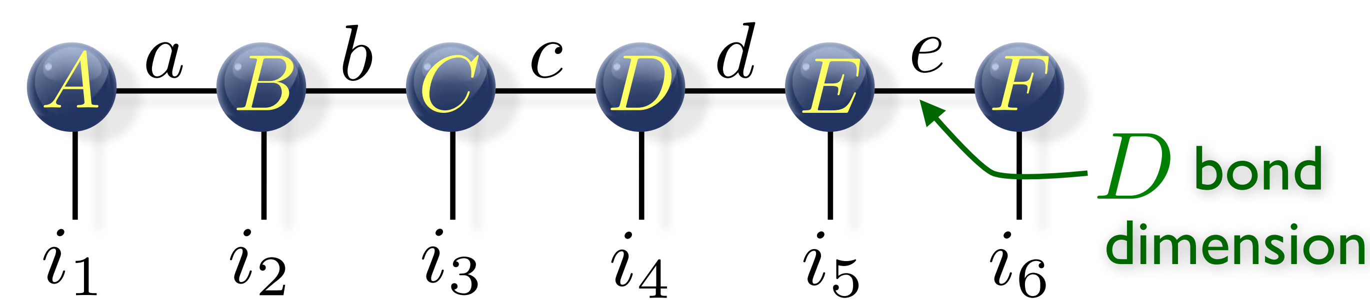
2^6 coefficients

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**)

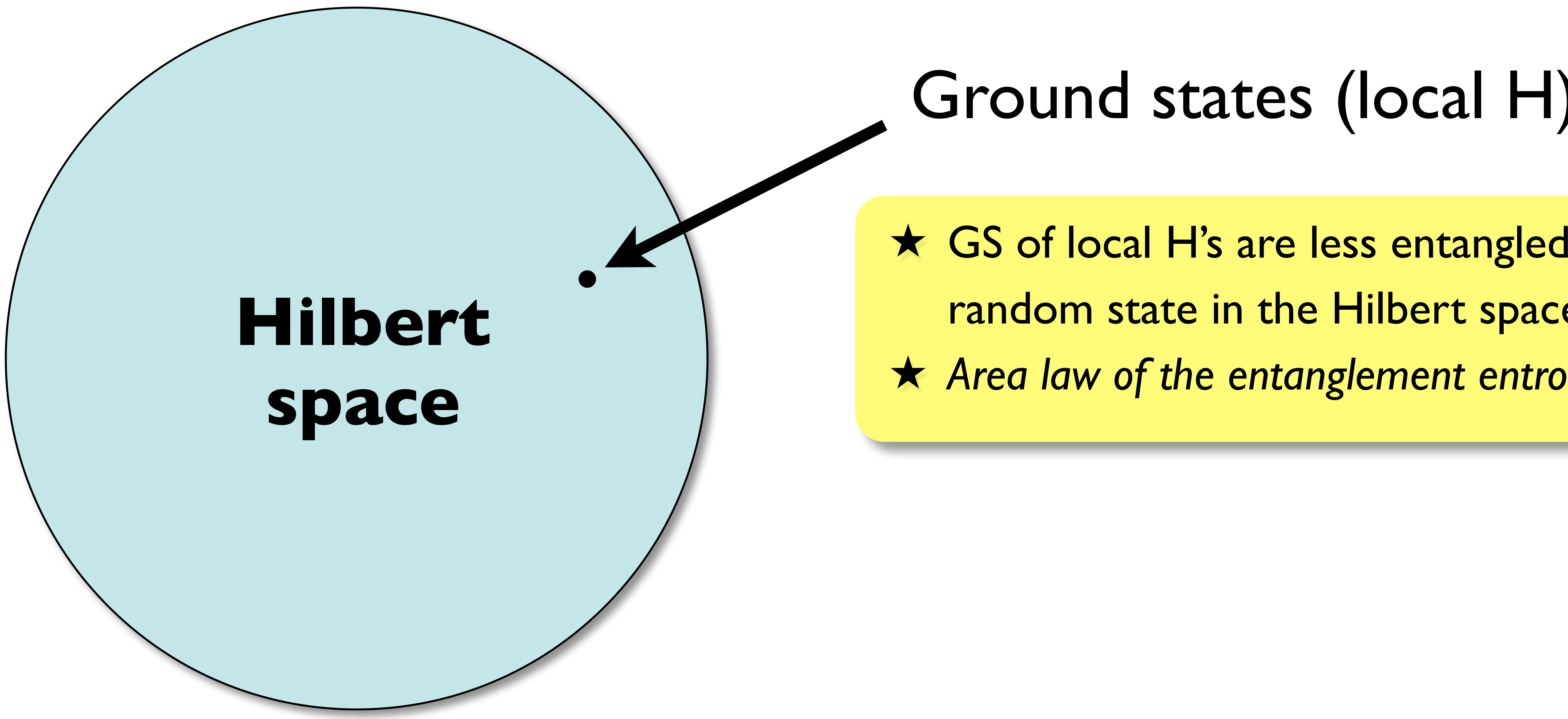


$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6} \approx \sum_{abcde} A^{a}_{i_1} B^{ab}_{i_2} C^{bc}_{i_3} D^{cd}_{i_4} E^{de}_{i_5} F^{e}_{i_6} = \tilde{\Psi}_{i_1 i_2 i_3 i_4 i_5 i_6}$$

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

Efficient representation!

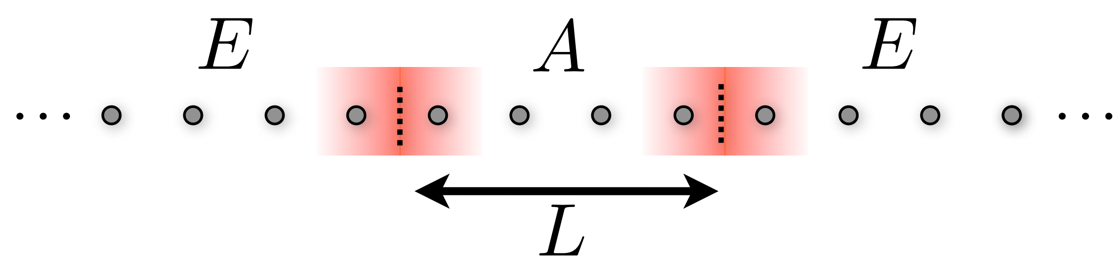
"Corner" of the Hilbert space



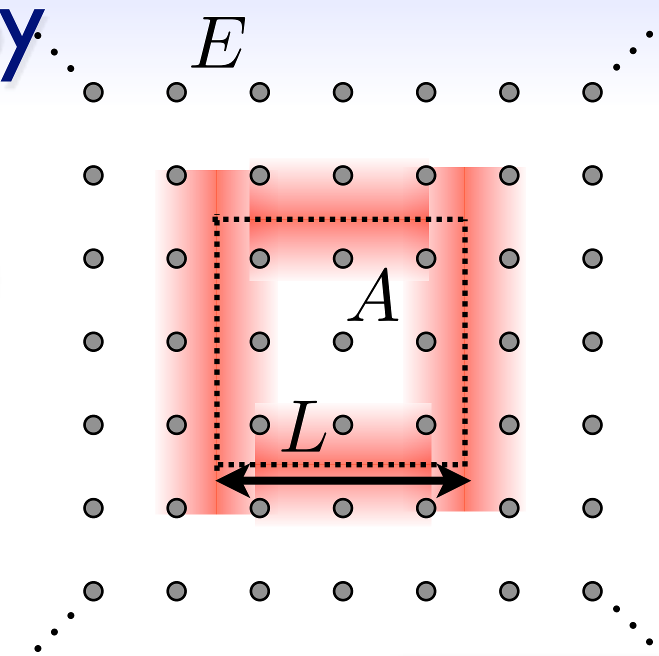
- ★ GS of local H's are less entangled than a random state in the Hilbert space
- ★ *Area law of the entanglement entropy*

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

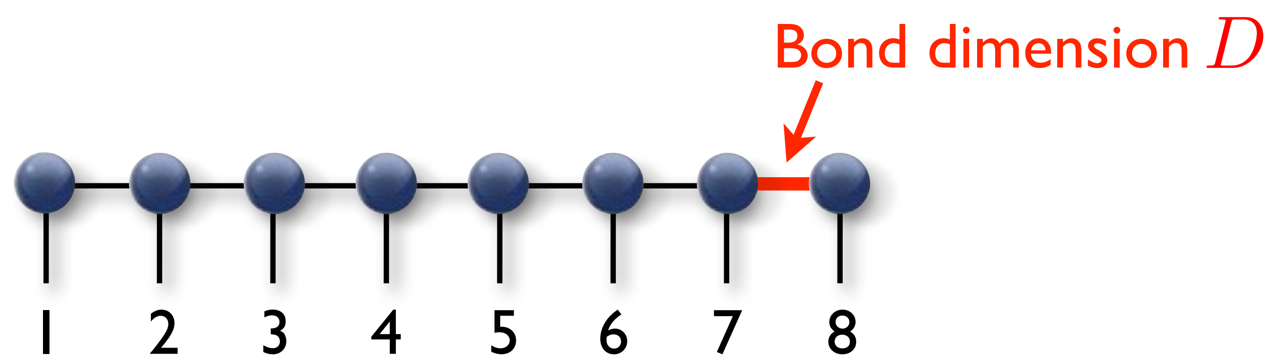
2D $S(L) \sim \alpha L$ $\chi \sim \exp(\alpha L)$

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

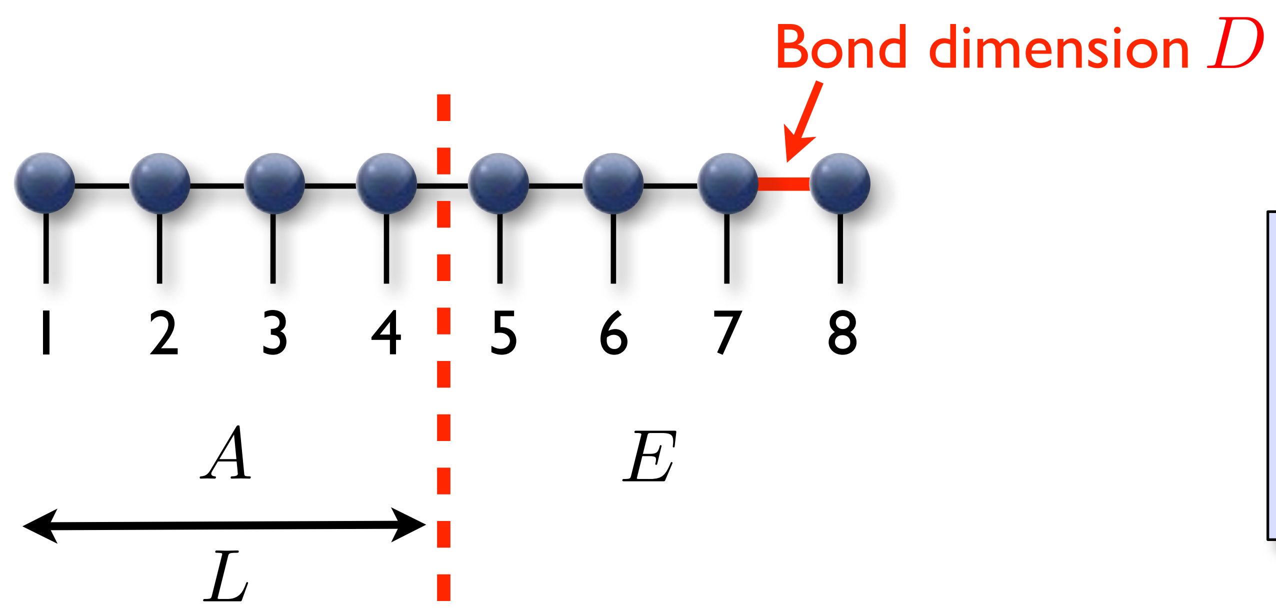
$$S(L) = const$$

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

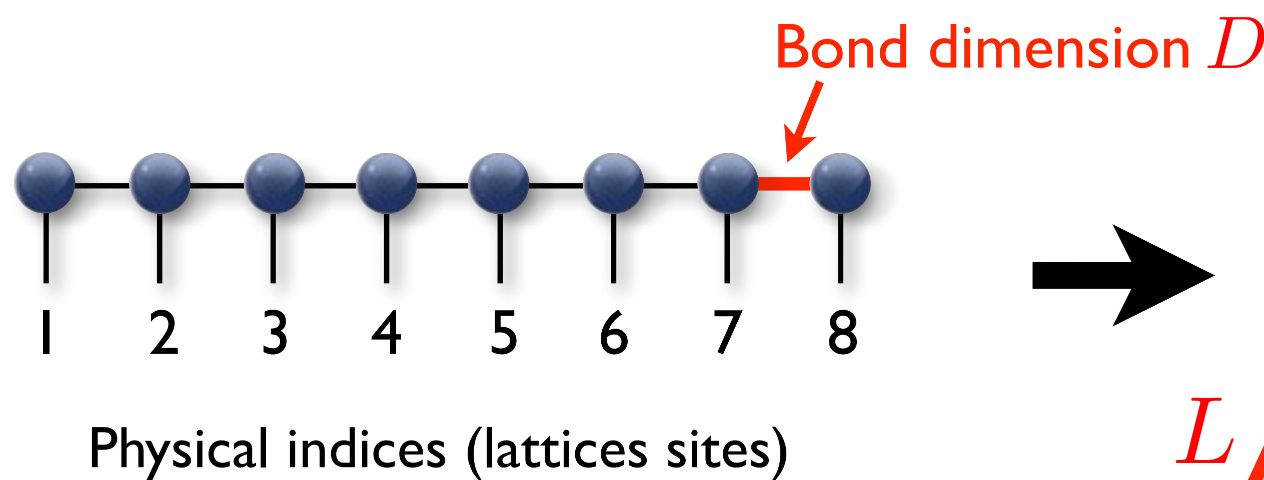
$$S(L) = const$$

MPS & PEPS

1D

MPS

Matrix-product state



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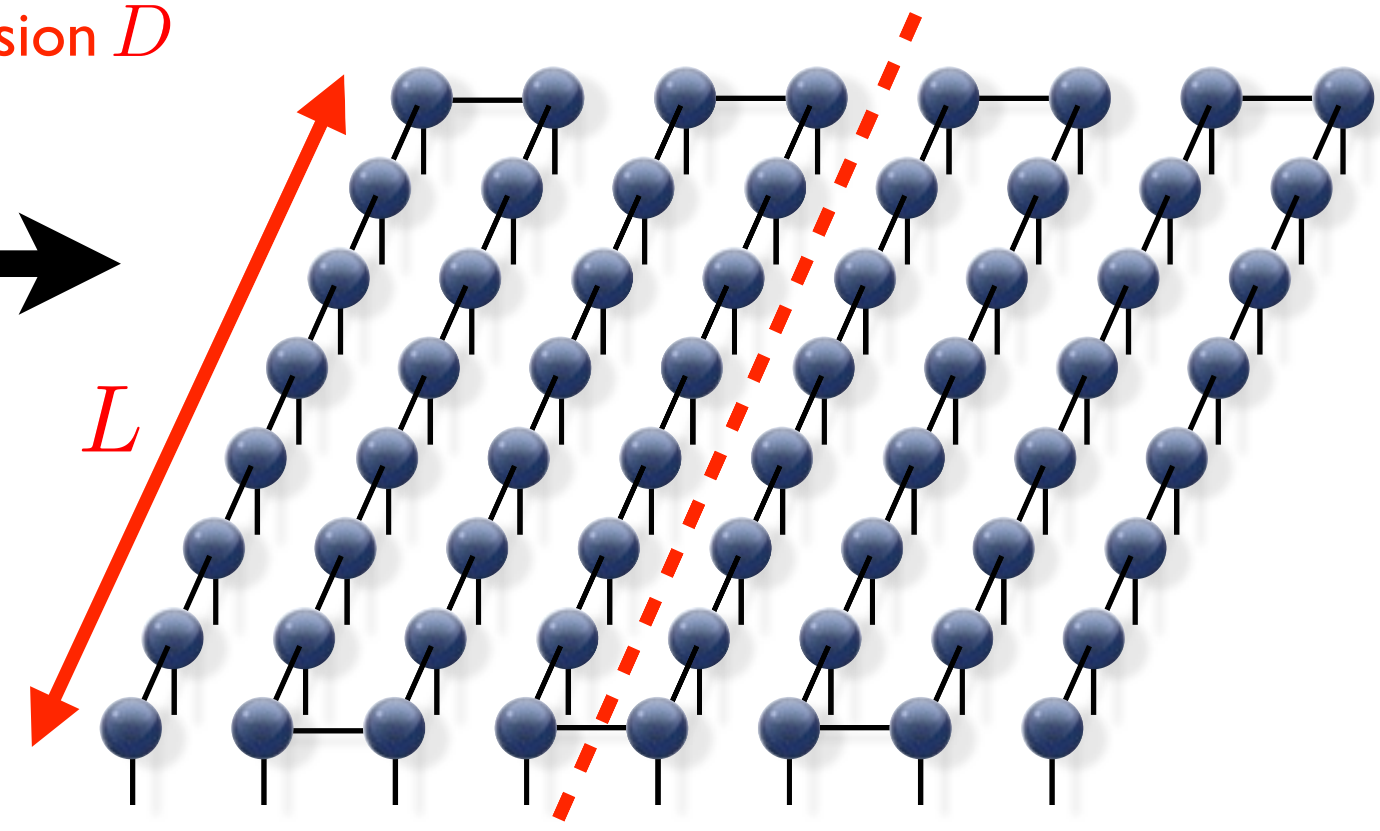
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

can we use an MPS?



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

$$S(L) \sim L$$

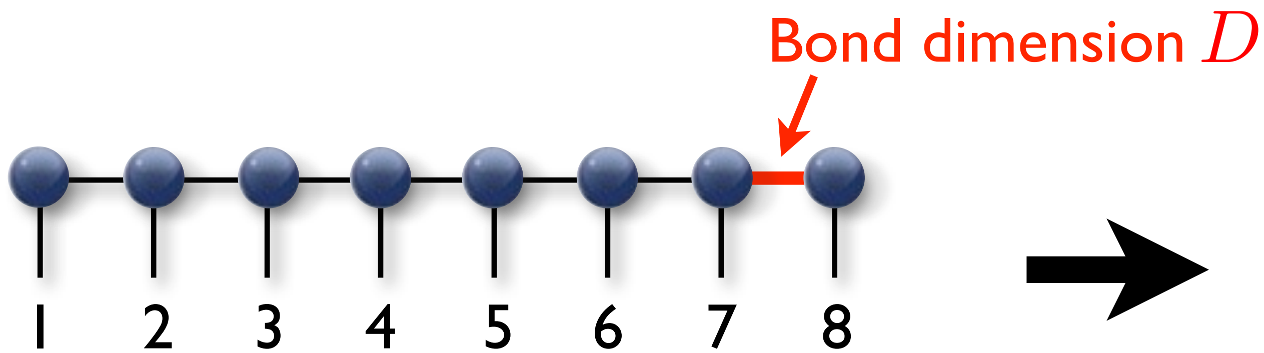
$$\rightarrow D \sim exp(L)$$

MPS & PEPS

1D

MPS

Matrix-product state



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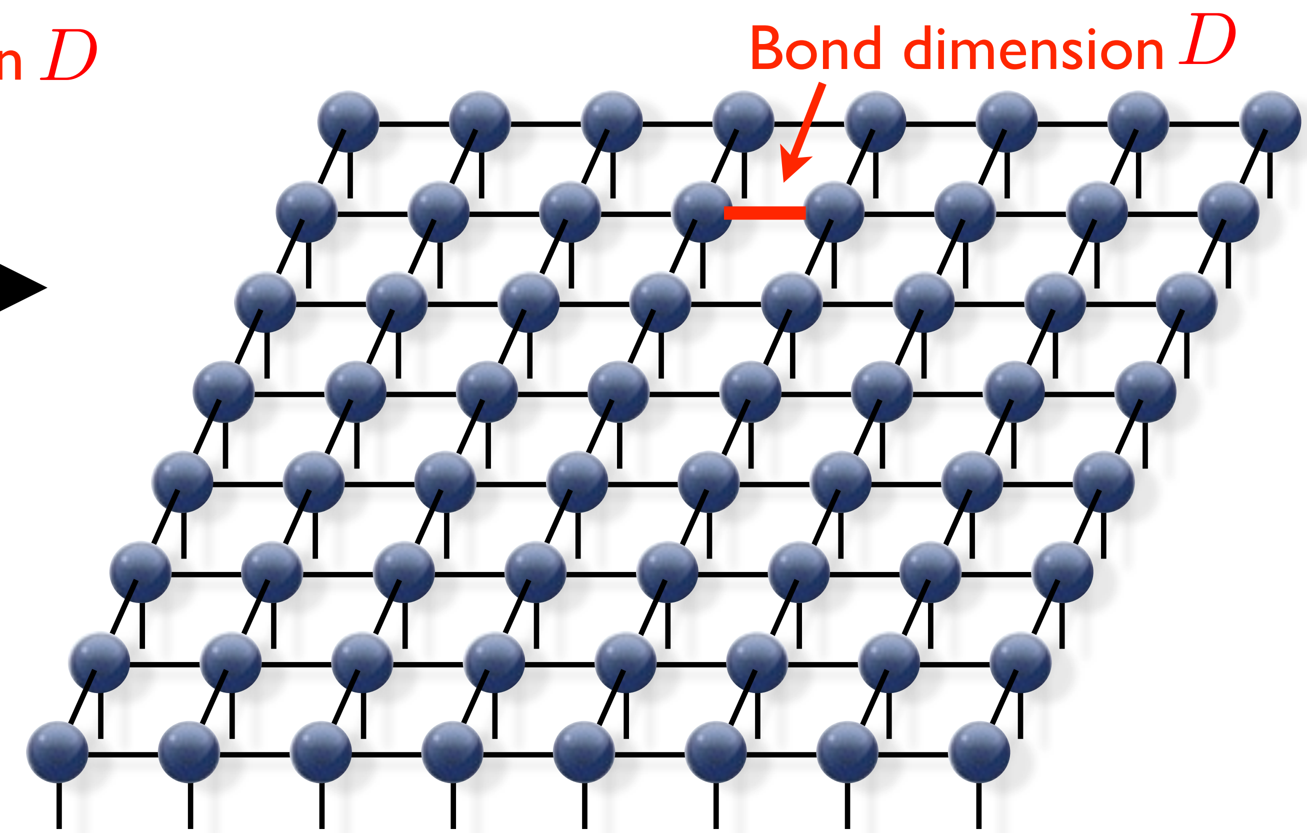
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)

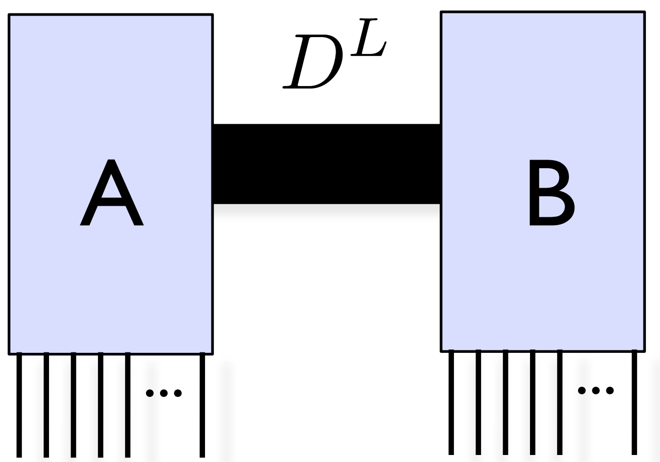


F. Verstraete, J. I. Cirac, cond-mat/0407066
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

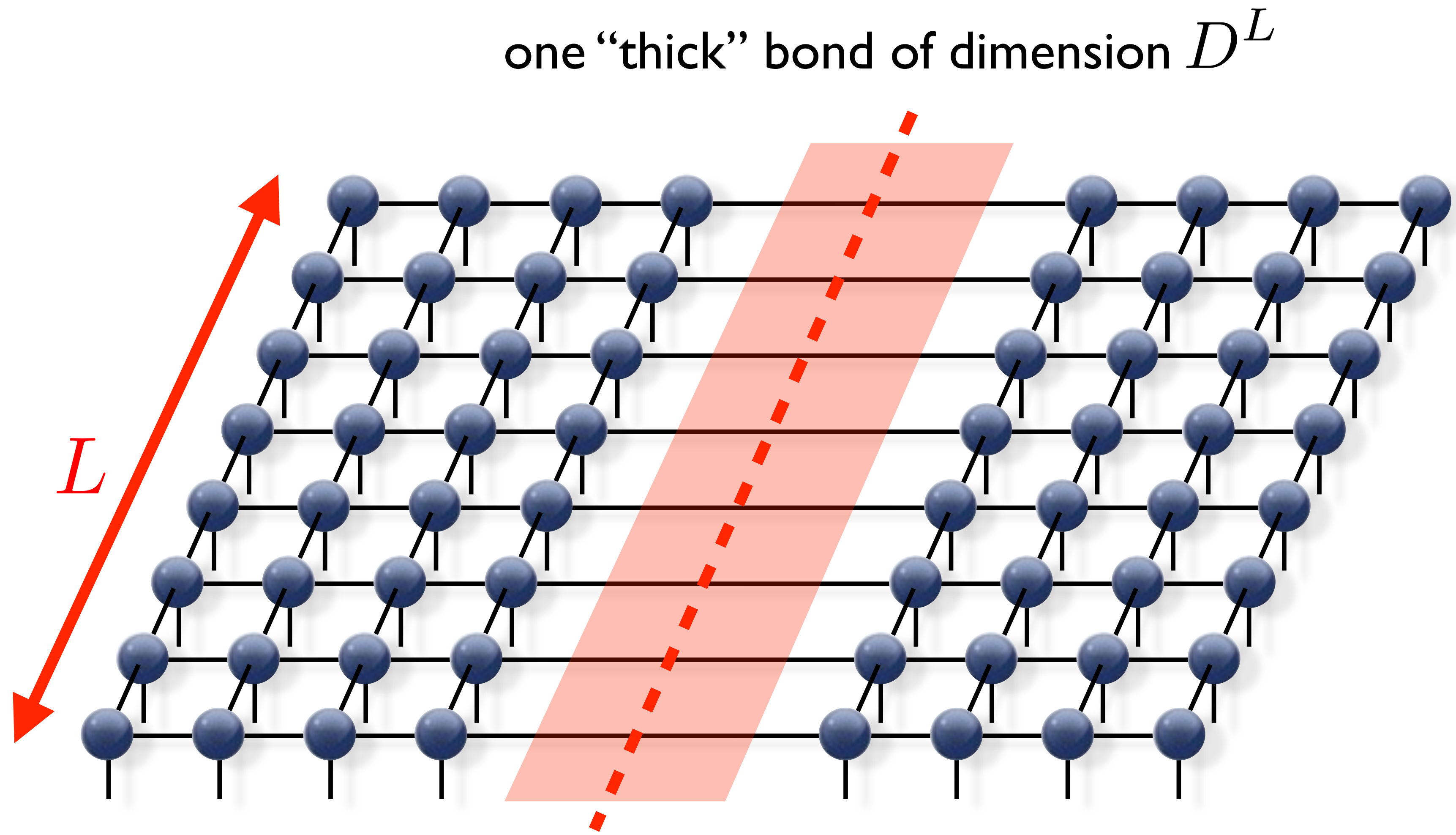
✓ Reproduces area-law in 2D

$$S(L) \sim L$$

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

✓ Reproduces area-law in 2D

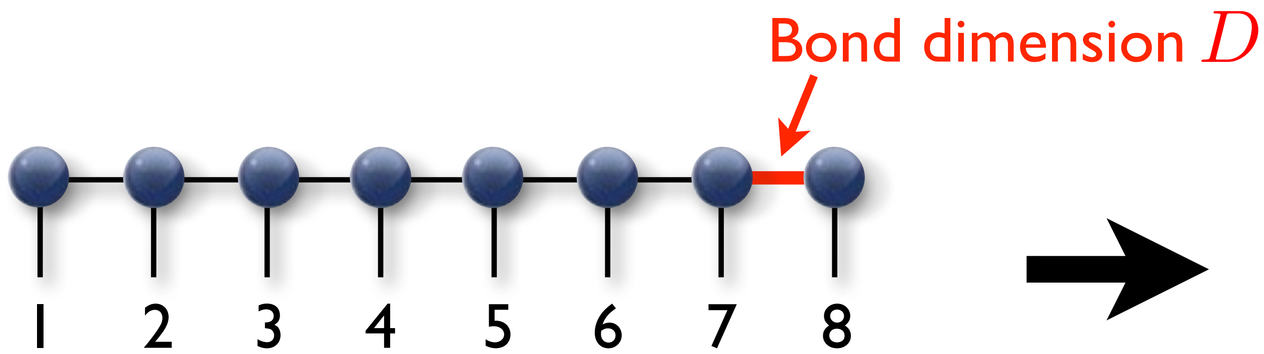
$$S(L) \sim L$$

MPS & PEPS

1D

MPS

Matrix-product state



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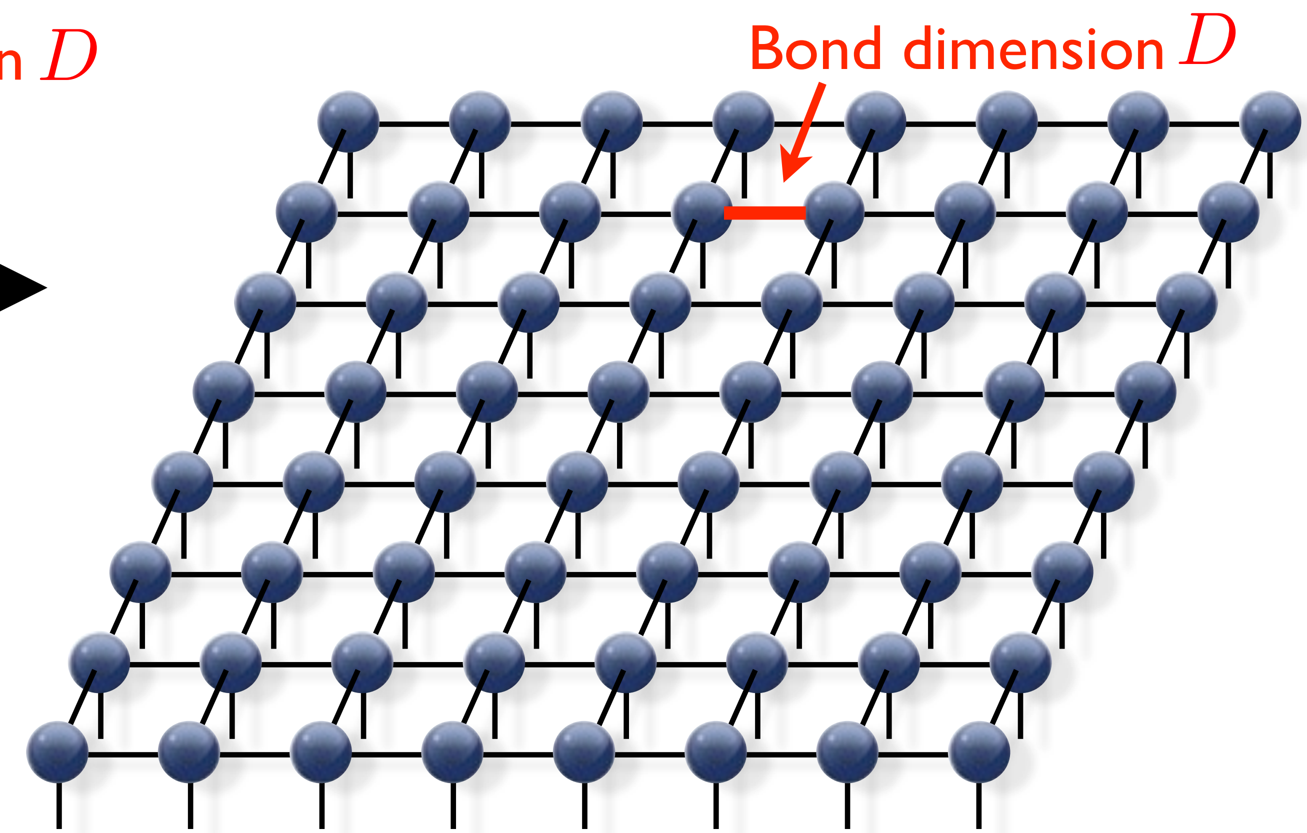
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



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✓ Reproduces area-law in 2D

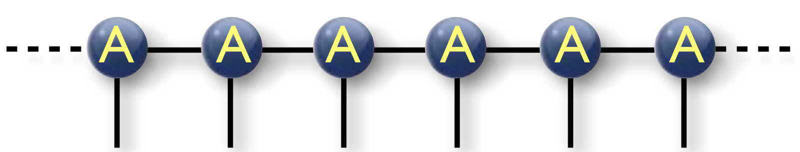
$$S(L) \sim L$$

Infinite PEPS (iPEPS)

1D

iMPS

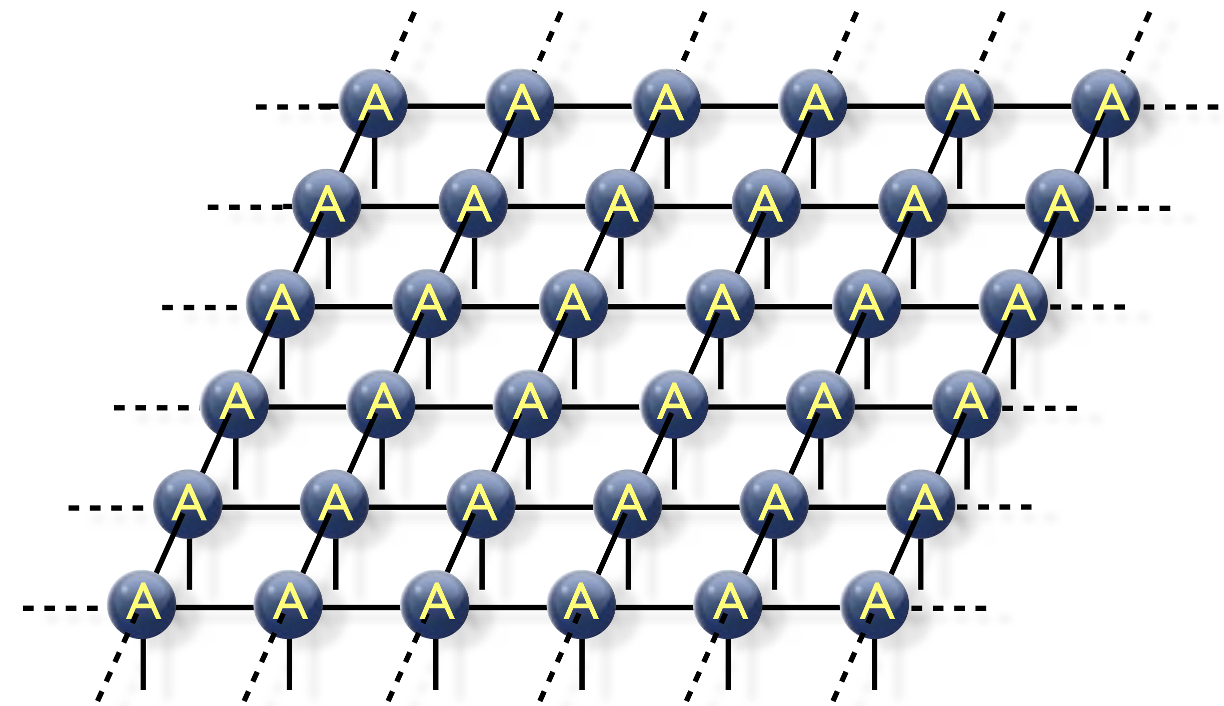
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

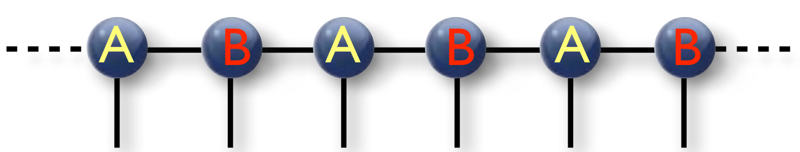
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

Infinite PEPS (iPEPS)

1D

iMPS

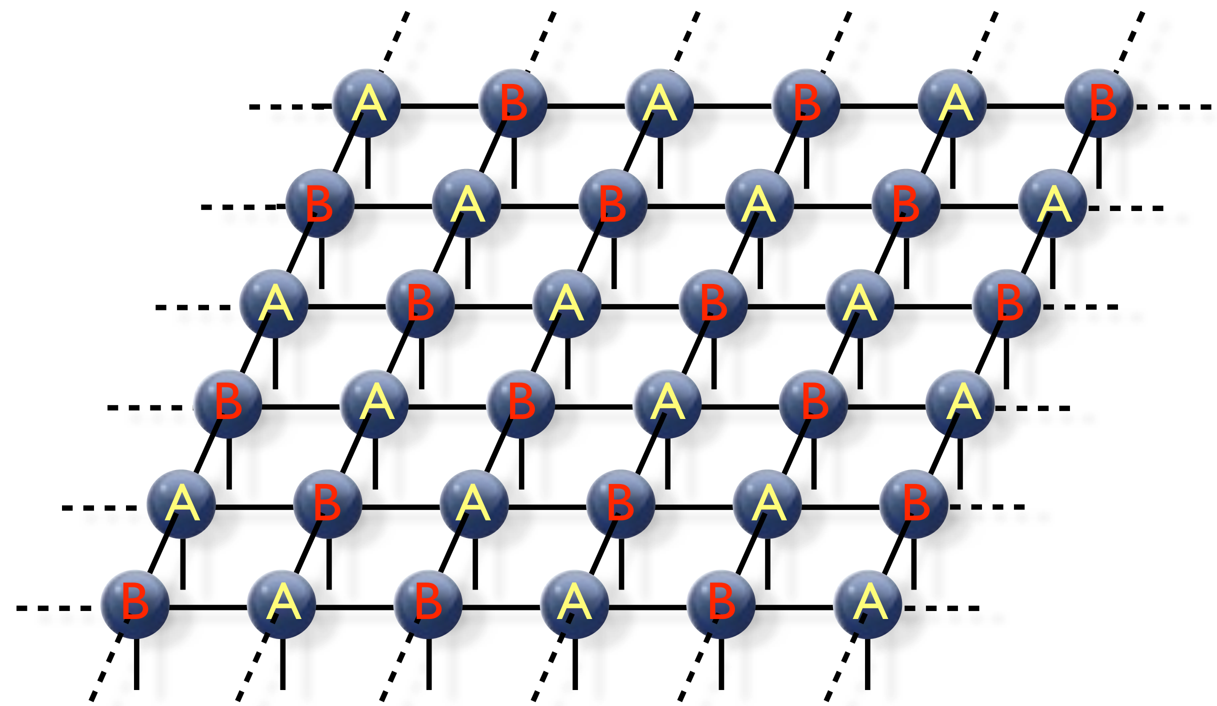
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

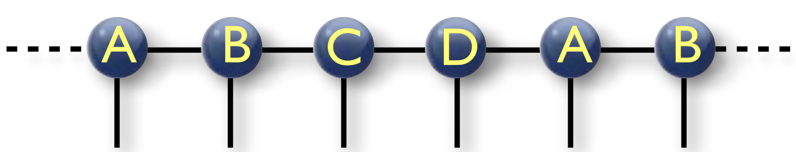
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

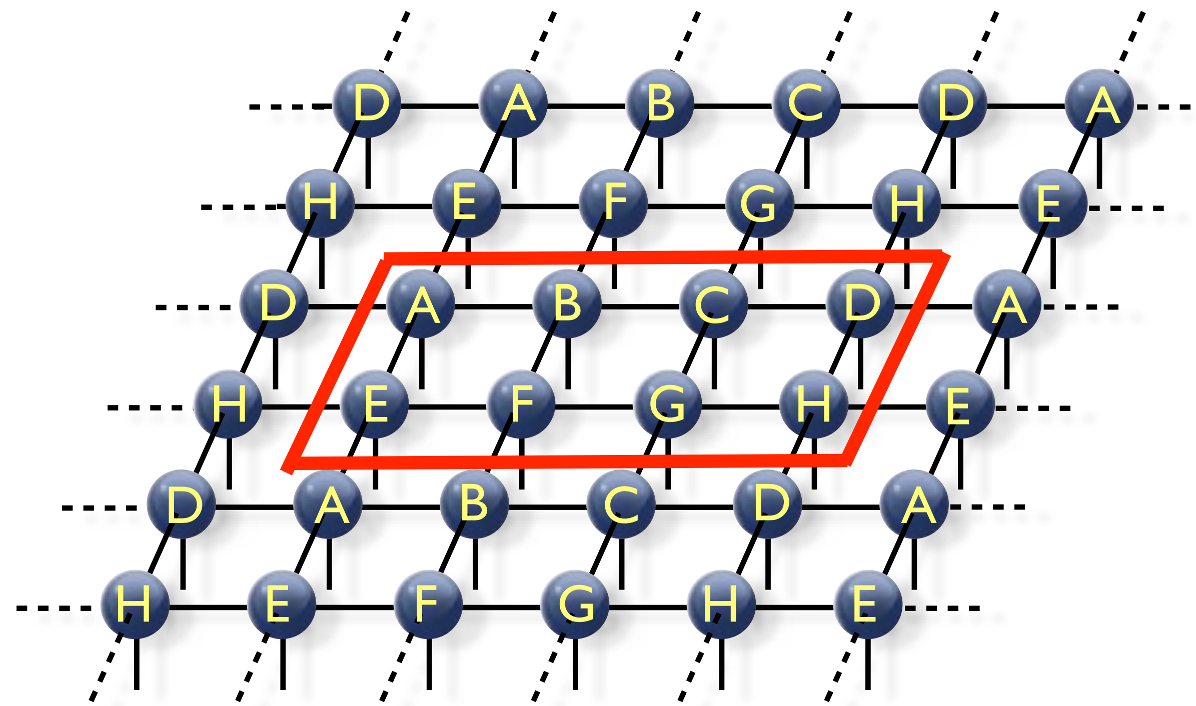
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors

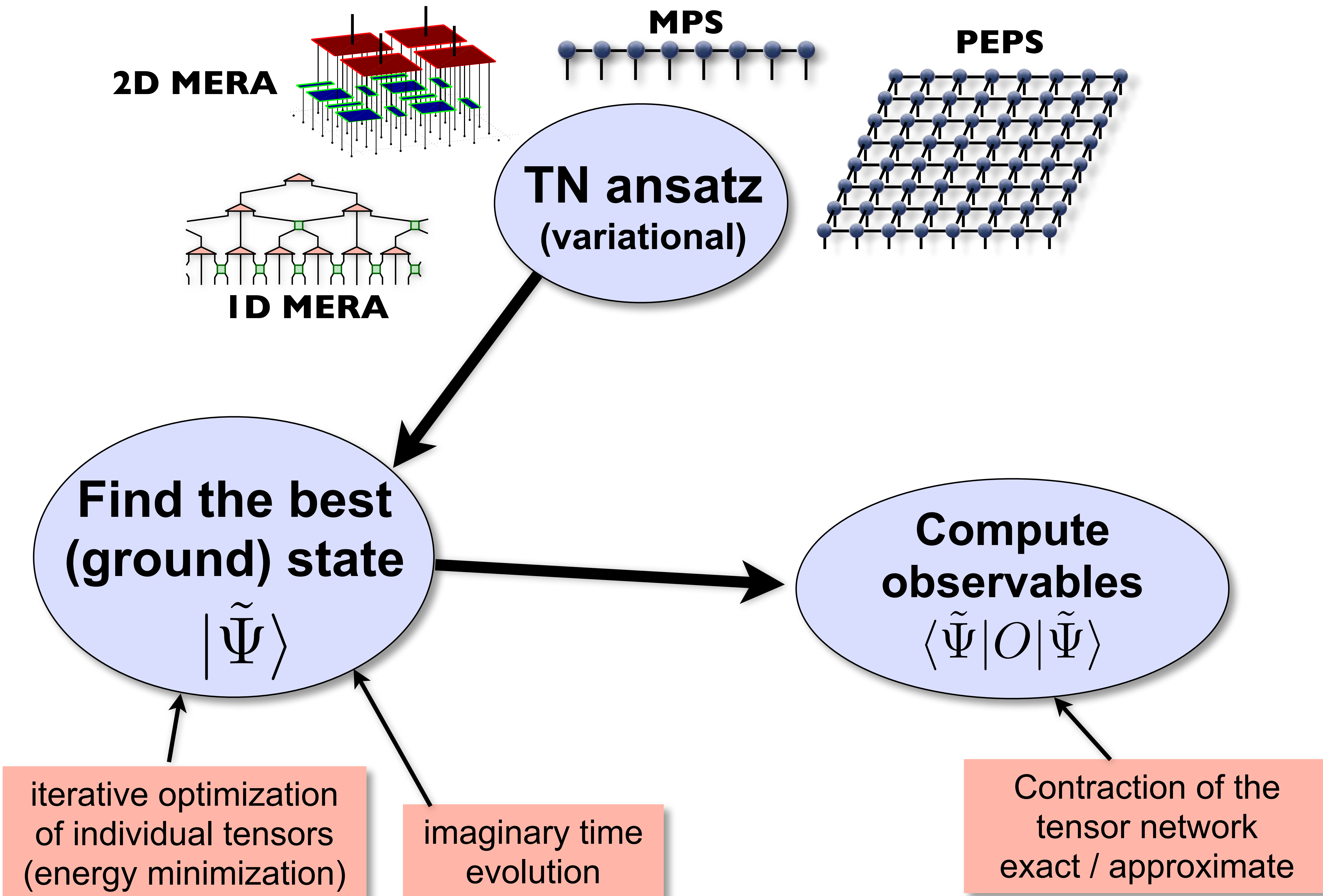


here: 4x2 unit cell

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

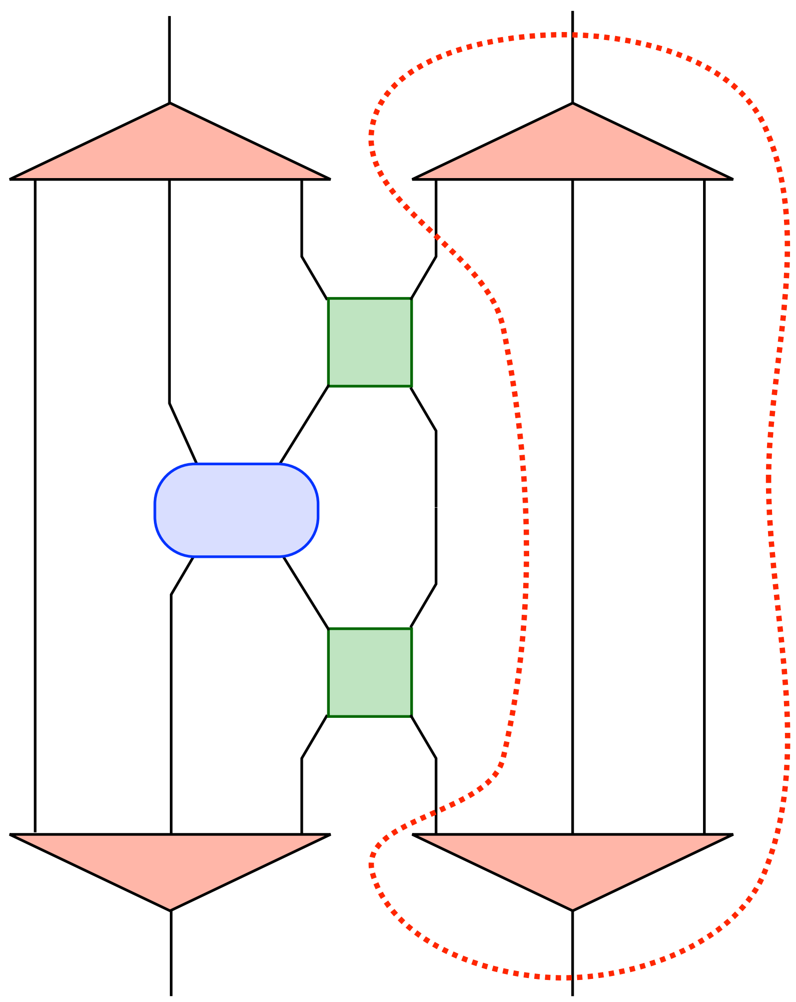
★ Run simulations with different unit cell sizes and compare variational energies

Overview: Tensor network algorithms (ground state)

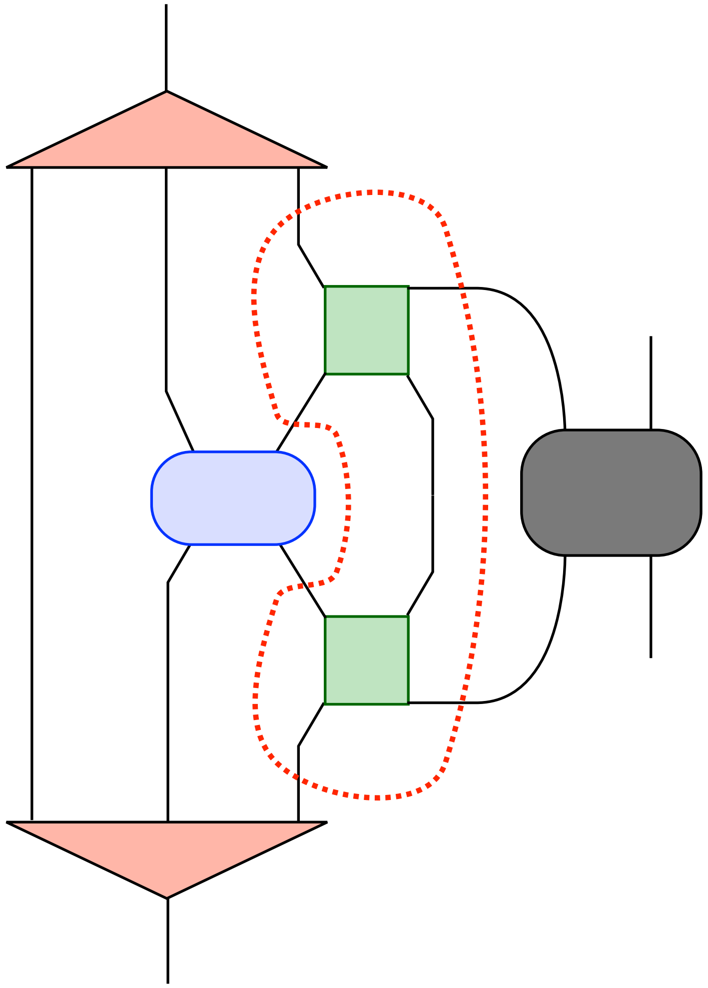


PART II: Contraction

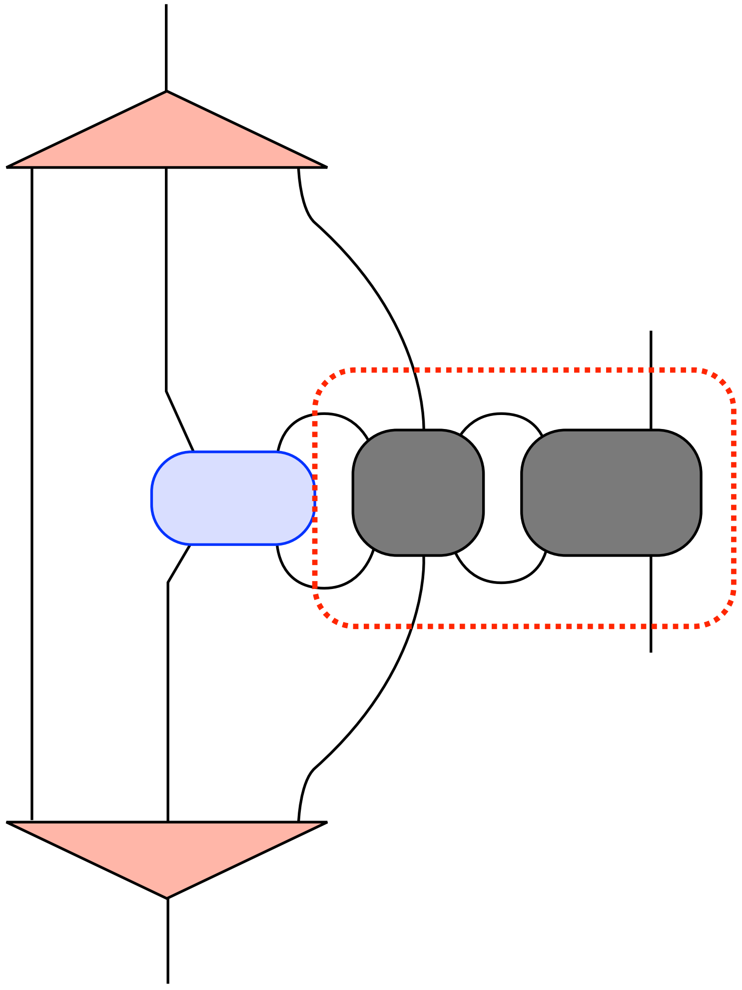
Contracting a tensor network (repetition)



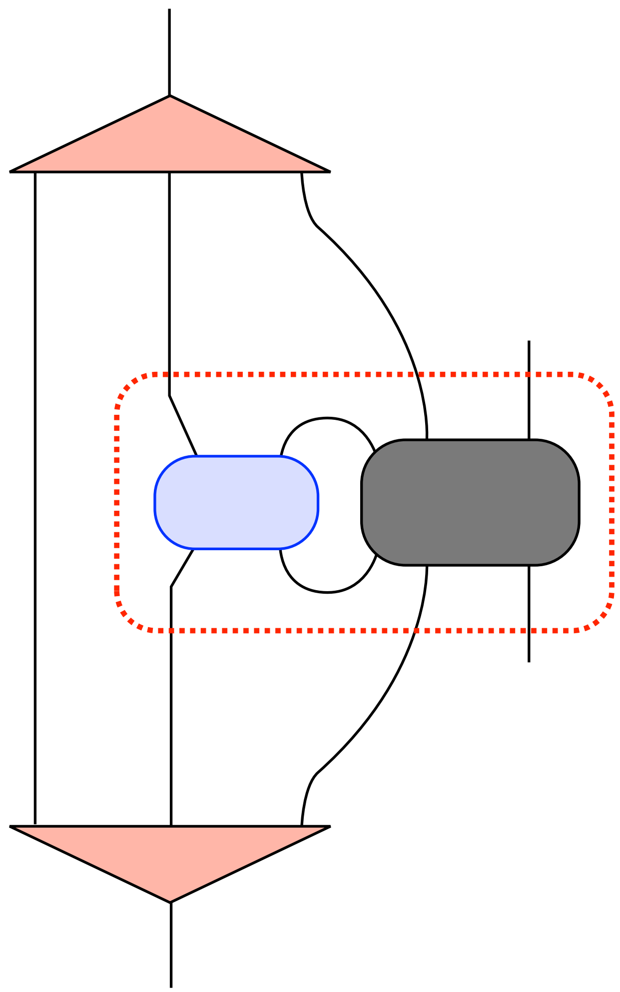
Pairwise contractions...



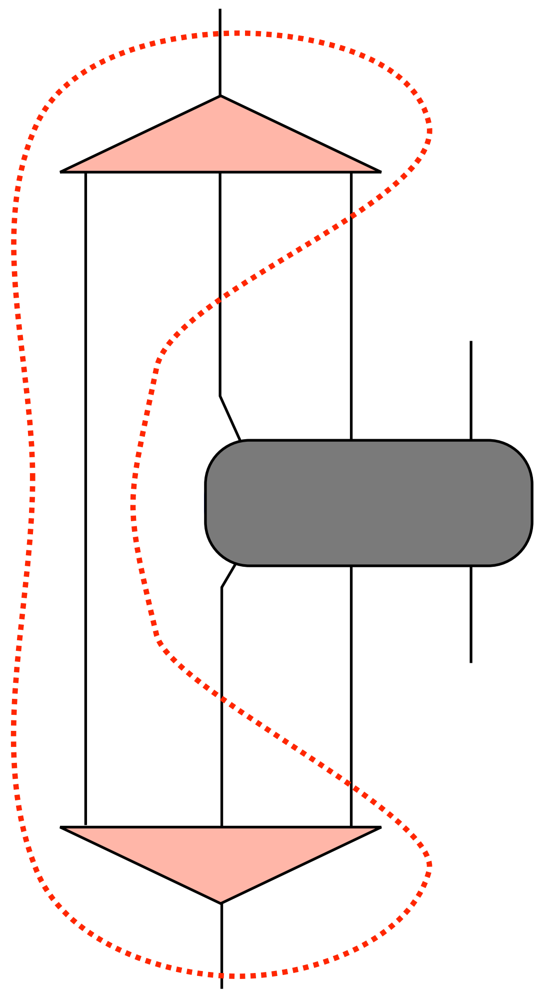
Pairwise contractions...



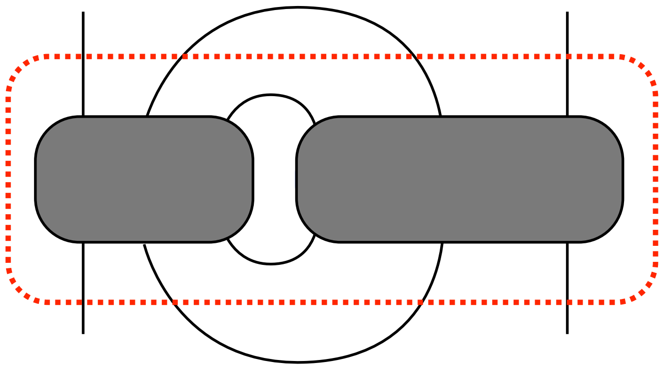
Pairwise contractions...



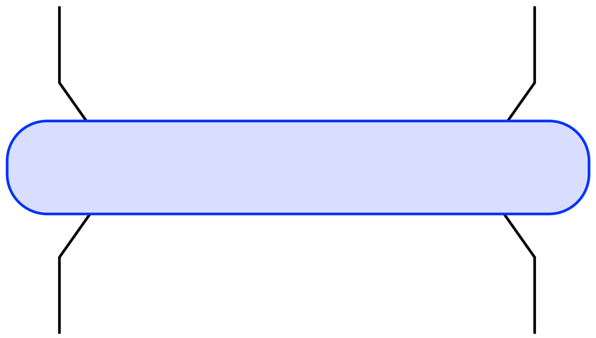
Pairwise contractions...



Pairwise contractions...



Pairwise contractions...

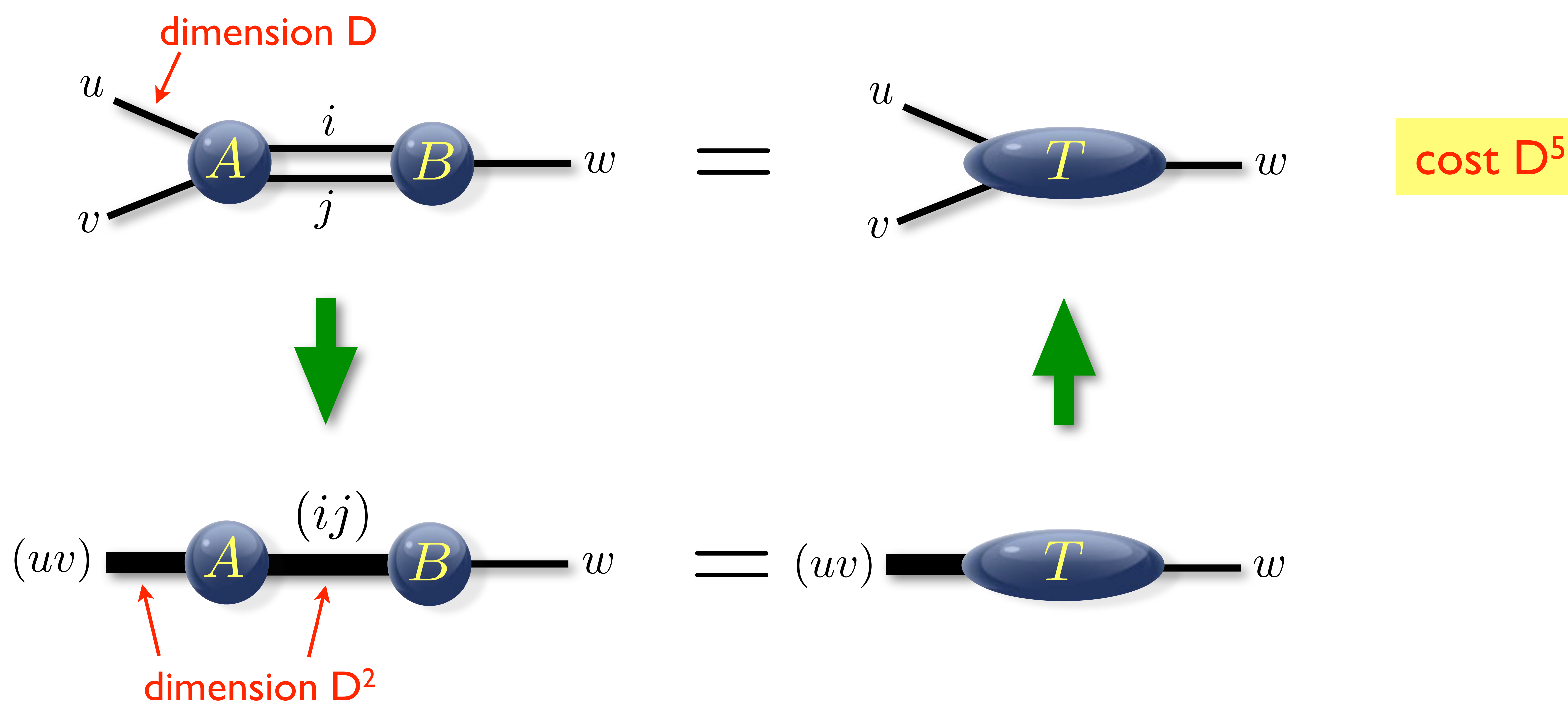


done!

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

Contracting a tensor network

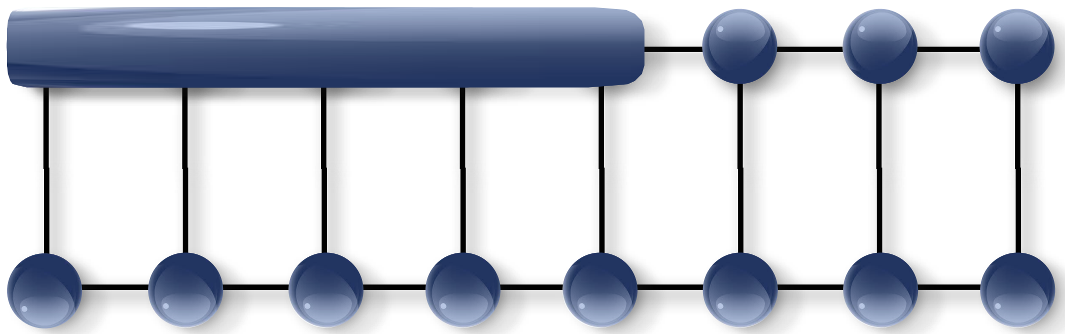
★ Reshape tensors into matrices and multiply them with optimized routines (BLAS)



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

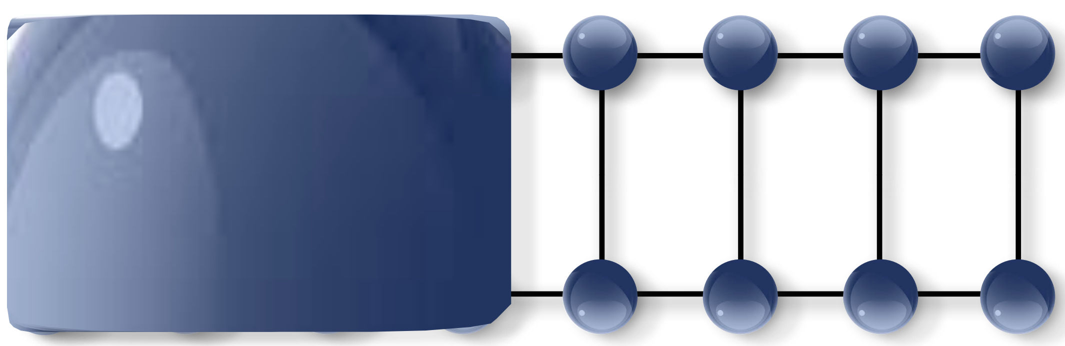
Contracting an MPS

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



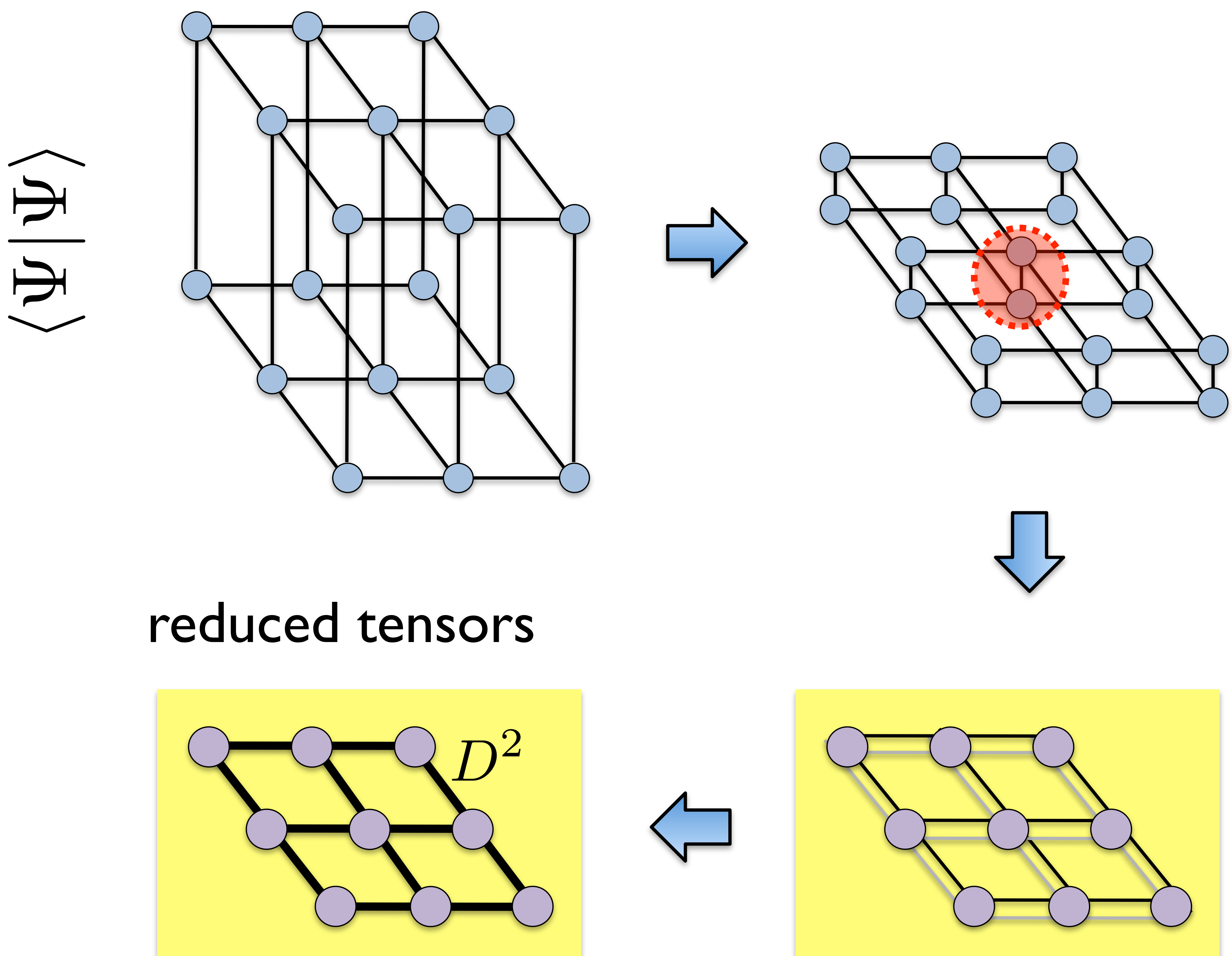
BAD!

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



Good!

Contracting the PEPS



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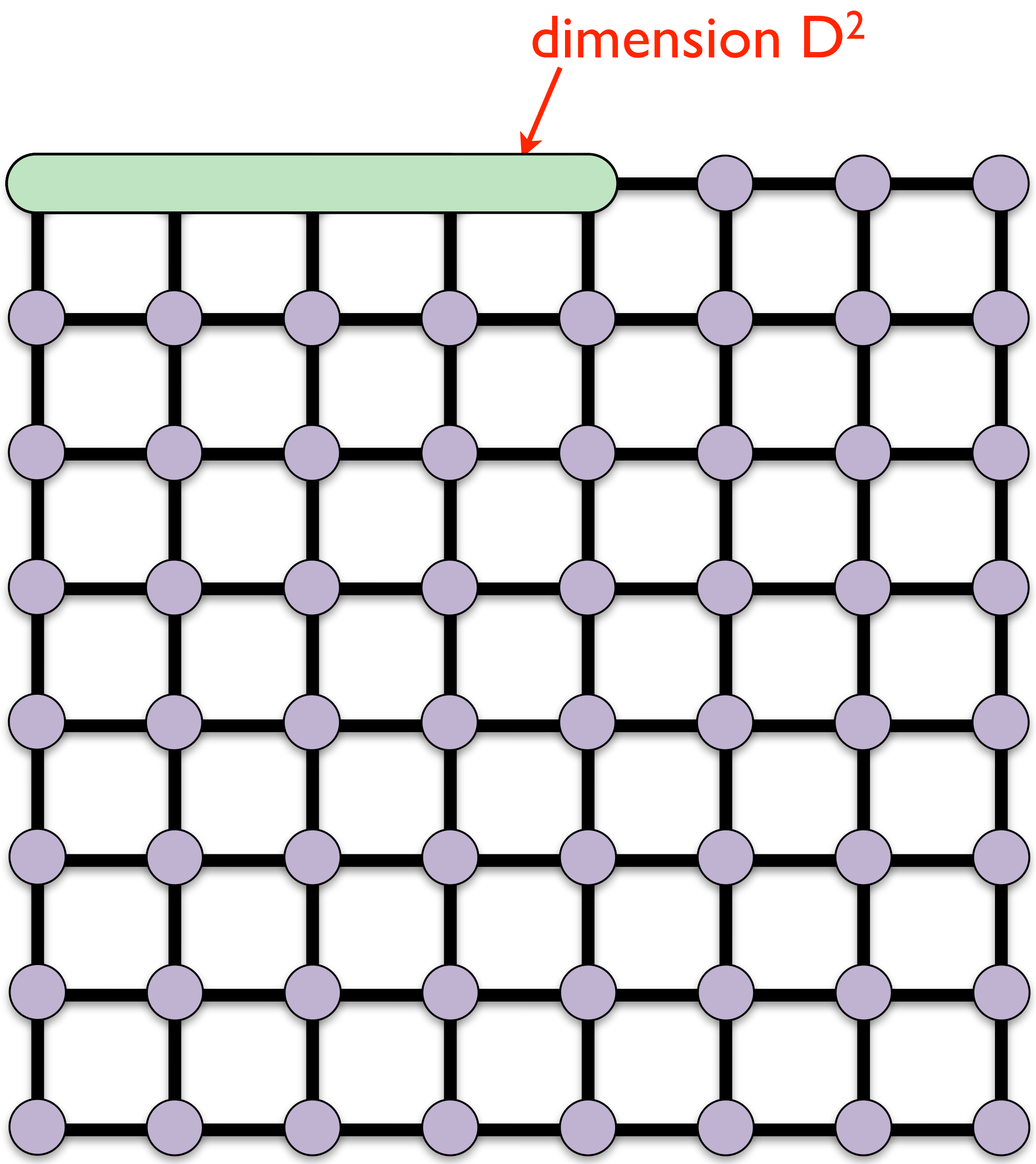


Problem: how do we contract this??

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

Corner transfer matrix method
Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)

TRG
Tensor Renormalization Group
(+HOTRG, SRG, HOSRG)
Levin, Nave, PRL99 (2007)
Xie et al. PRL 103, (2009)

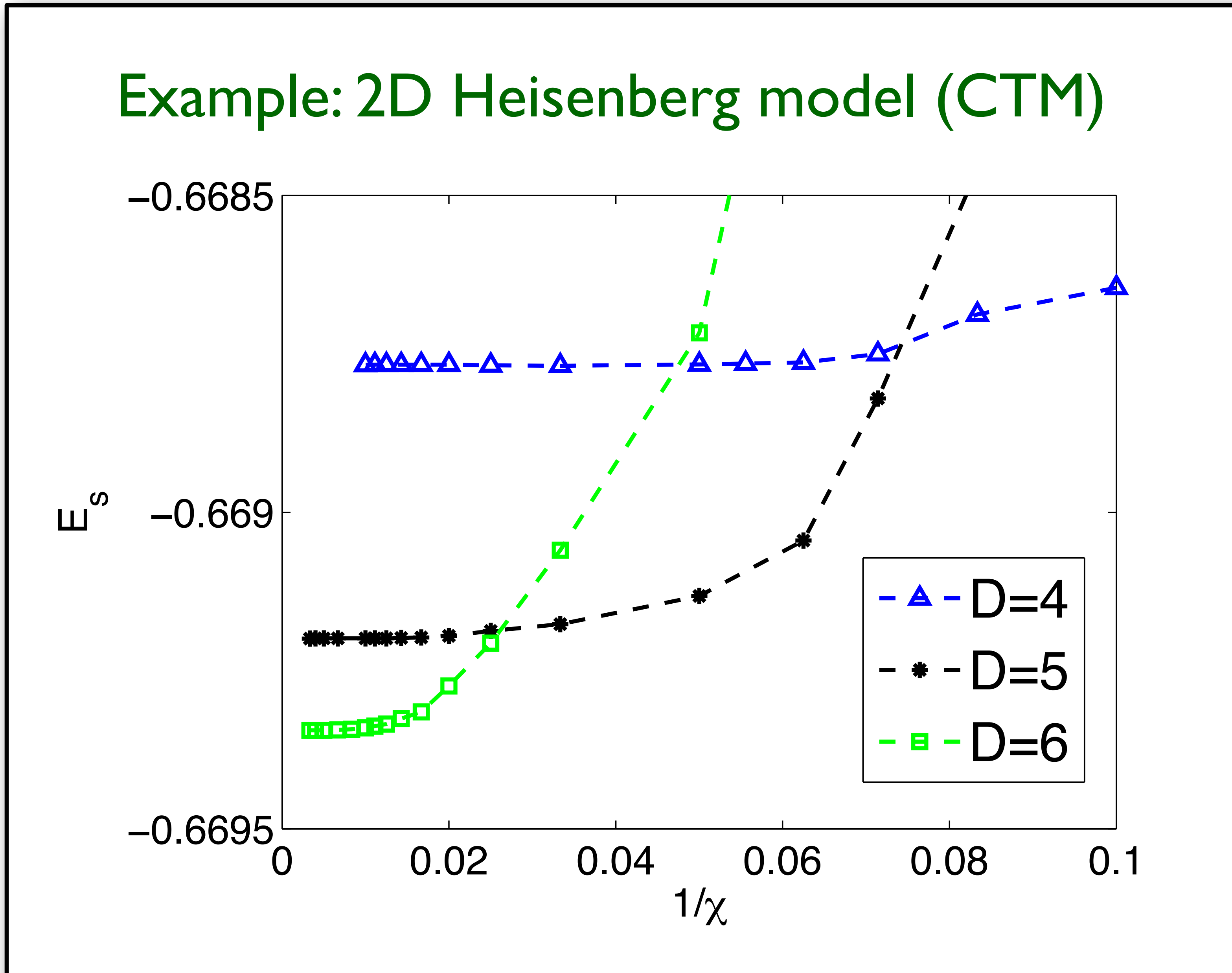
TNR
Tensor Network Renormalization
Evenbly & Vidal, PRL 115 (2015)
Loop-TNR:
Yang, Gu & Wen, arXiv:1512.04938

★ 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

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→ *use controlled approximate contraction scheme*

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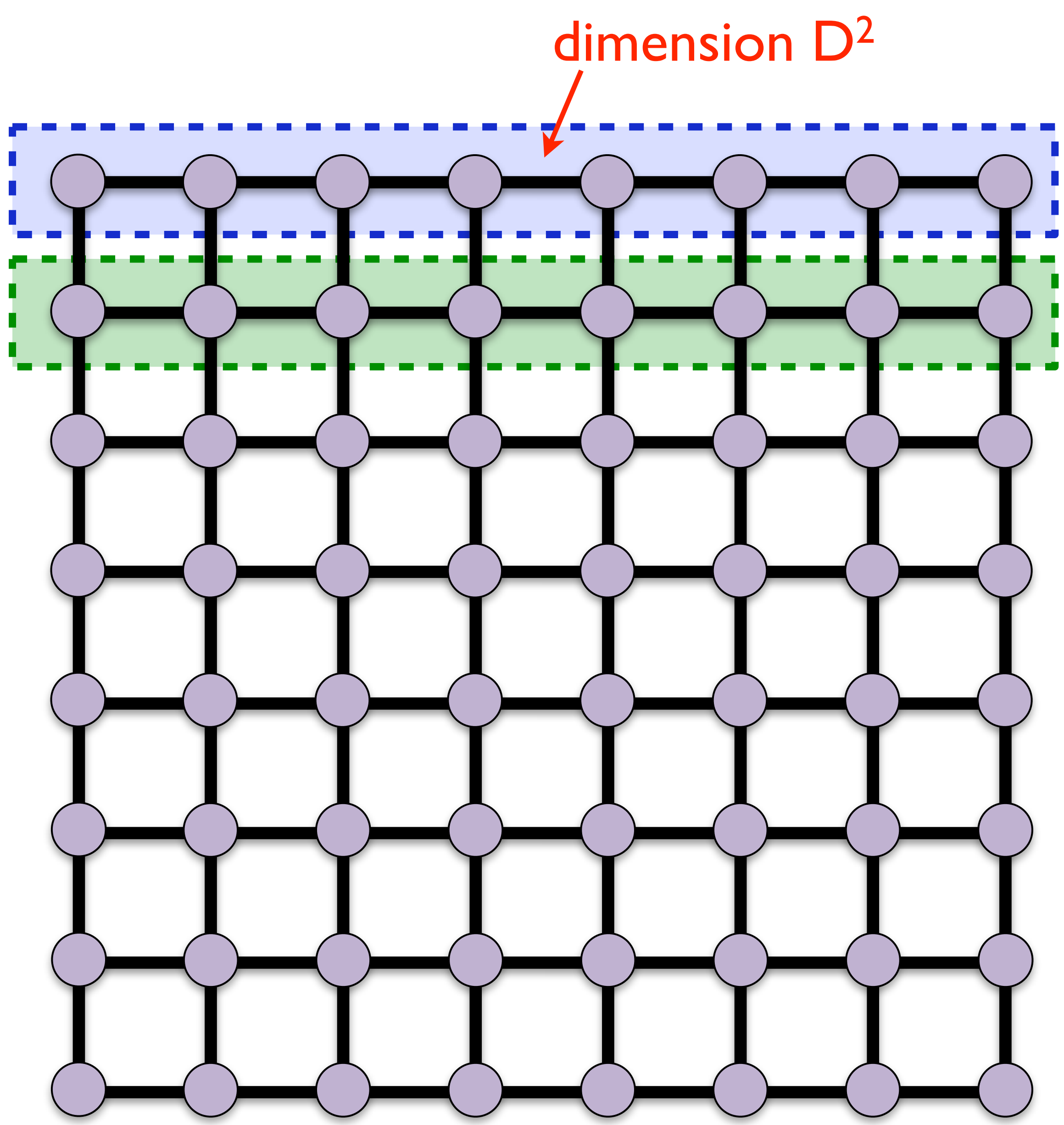
Contracting the PEPS using an MPS

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

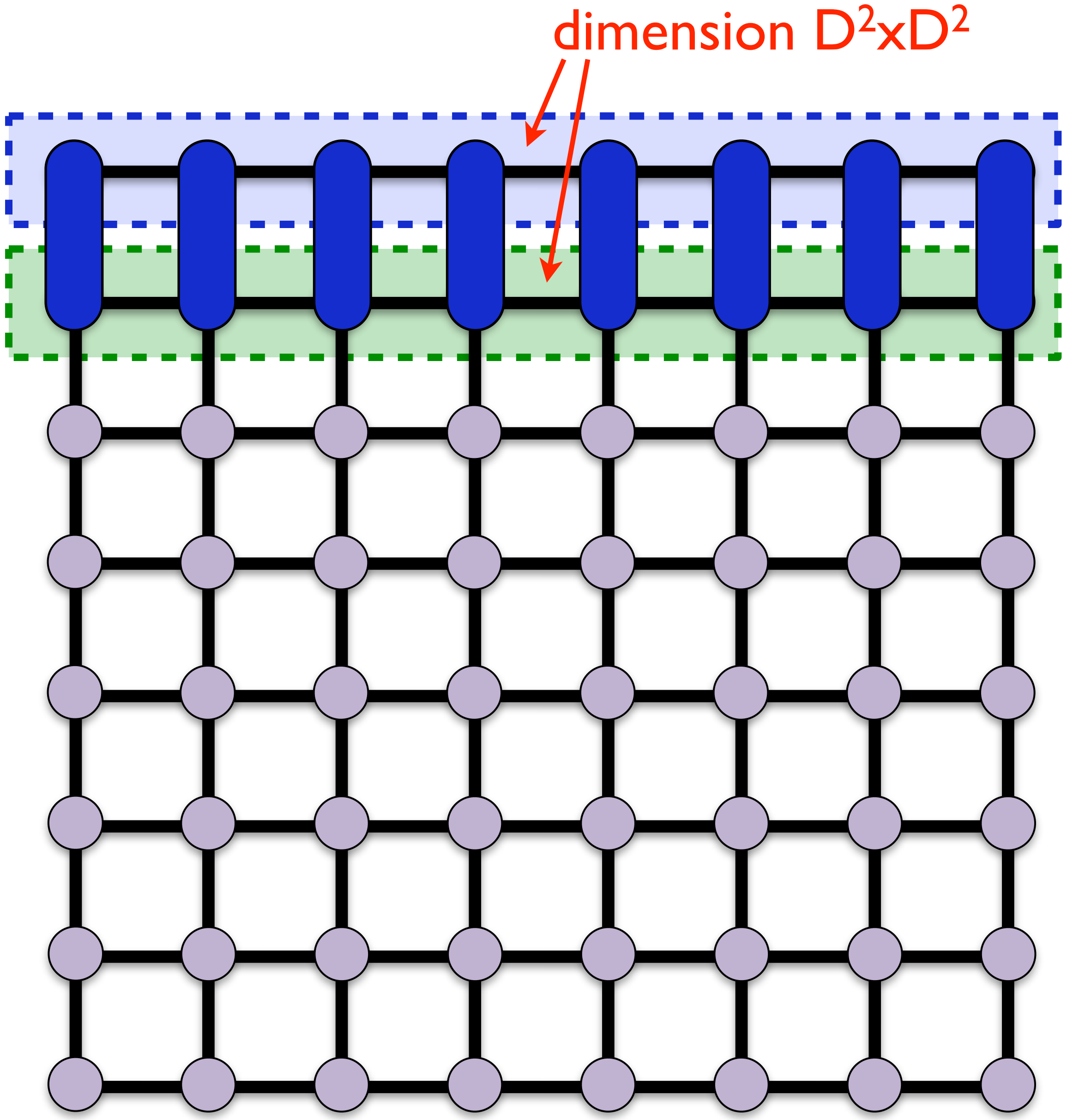


this is an MPS

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 $D^2 x D^2$

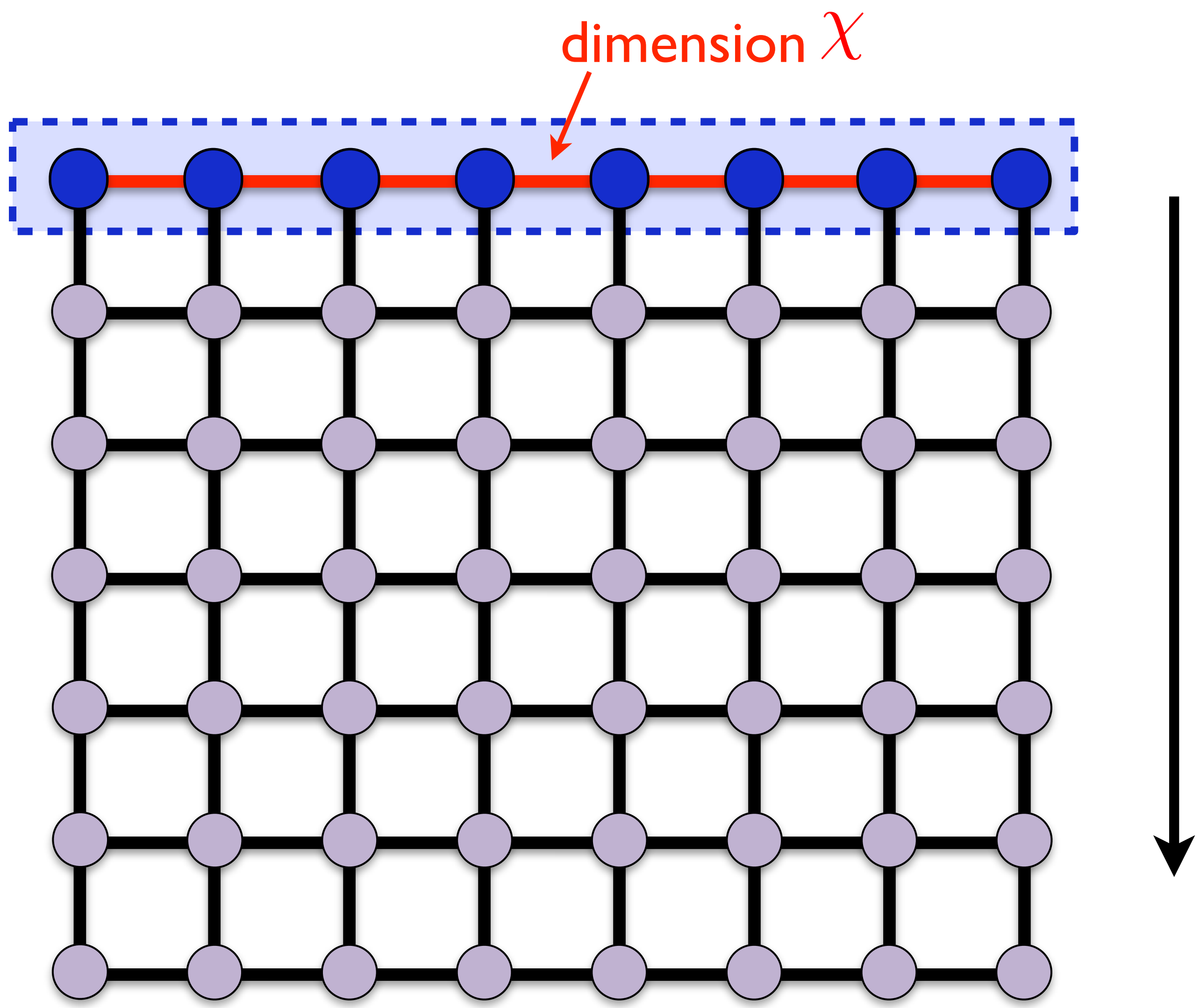
truncate the bonds to χ

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

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

Contracting the PEPS using an MPS

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

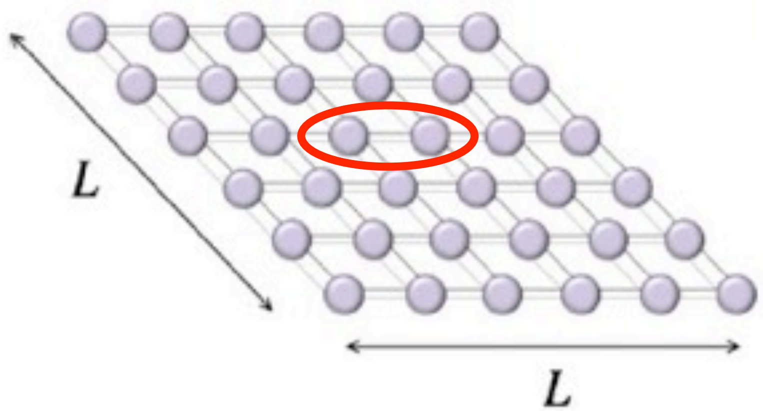


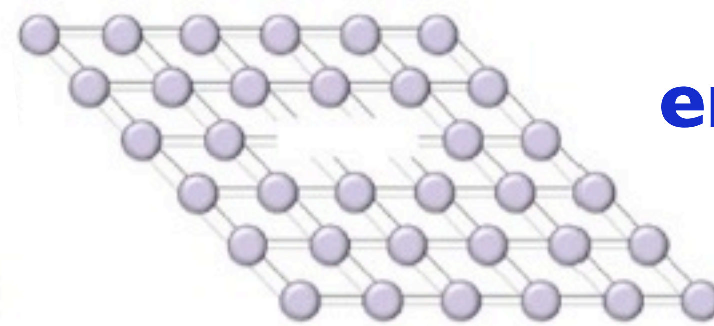
proceed...

★ We can do this from several directions

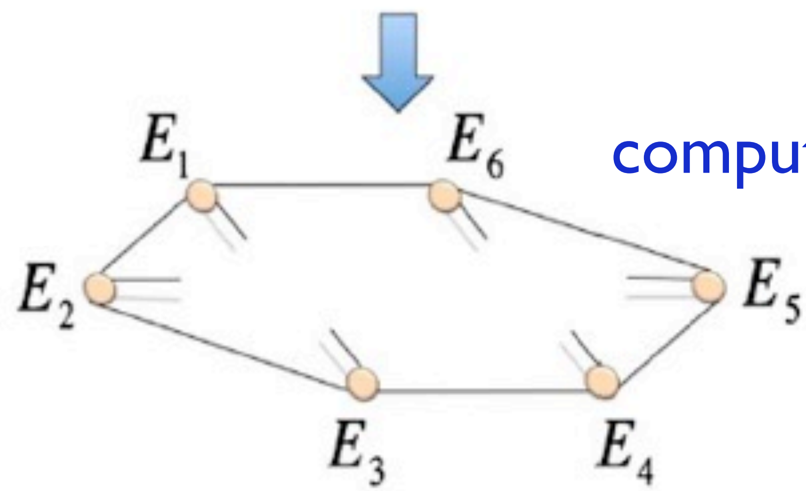
★ Similar procedure when computing an expectation value

Compute expectation values

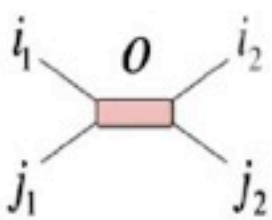


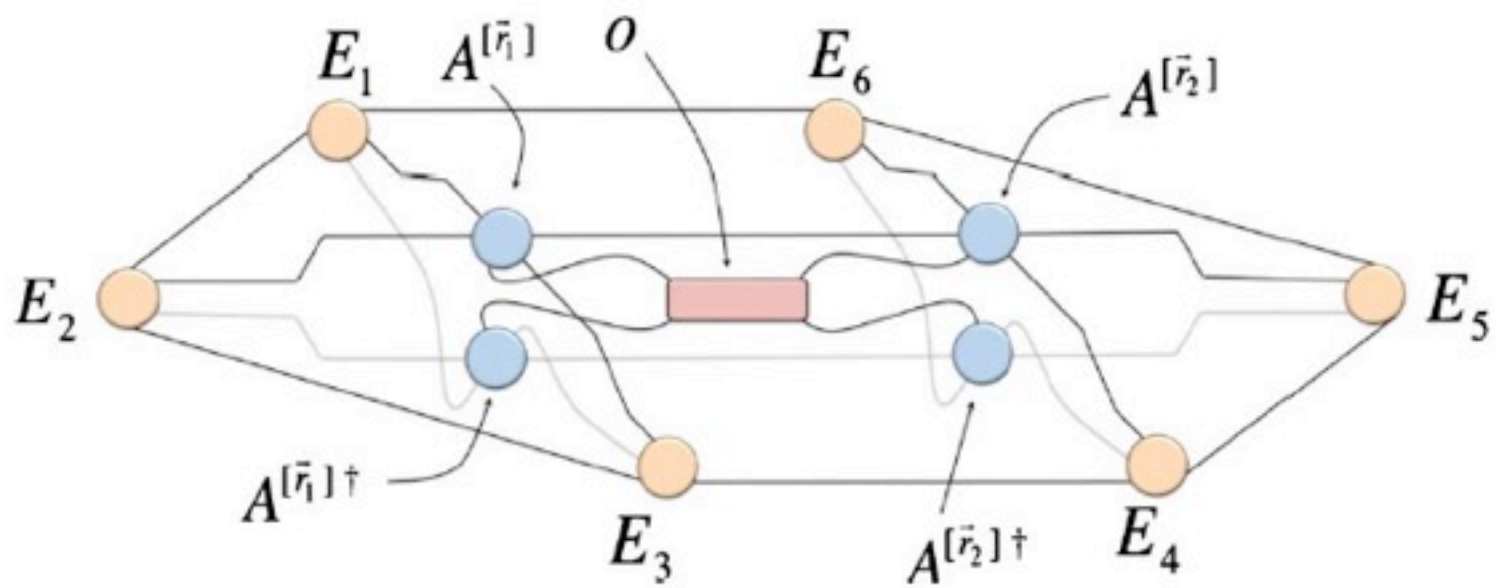


environment



compute environment approximately





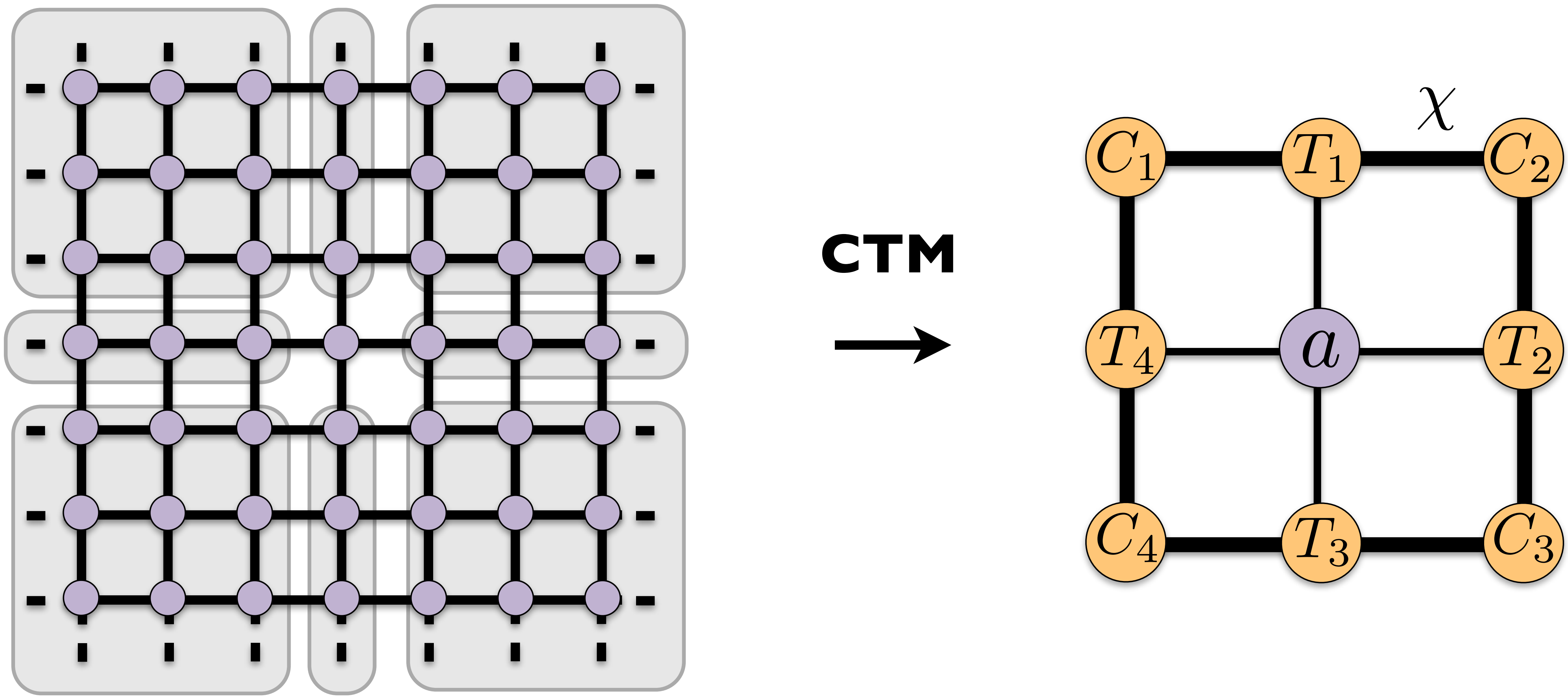
Connect two-body operator

Contract this network!

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

Contracting the iPEPS using the corner transfer matrix 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)

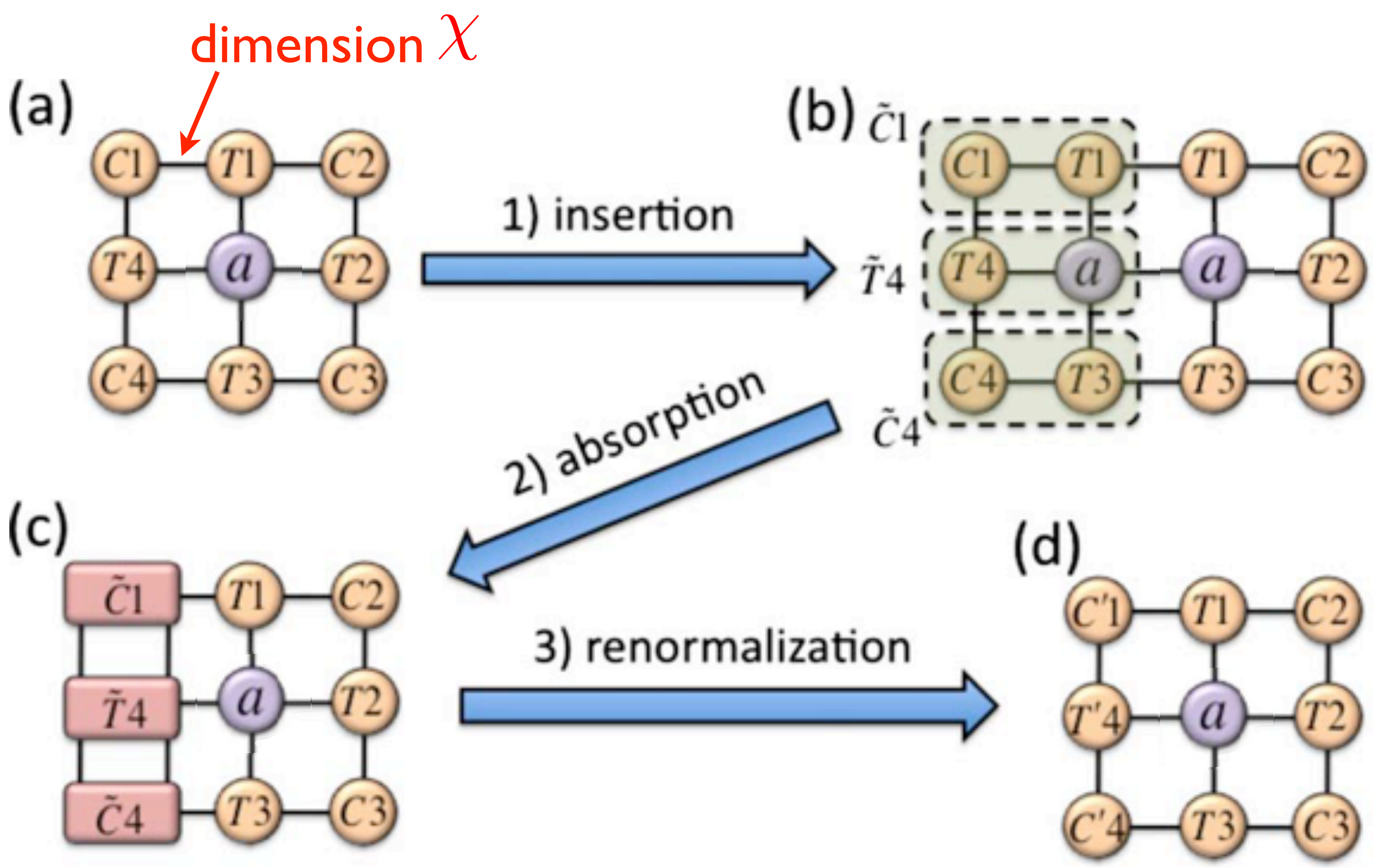
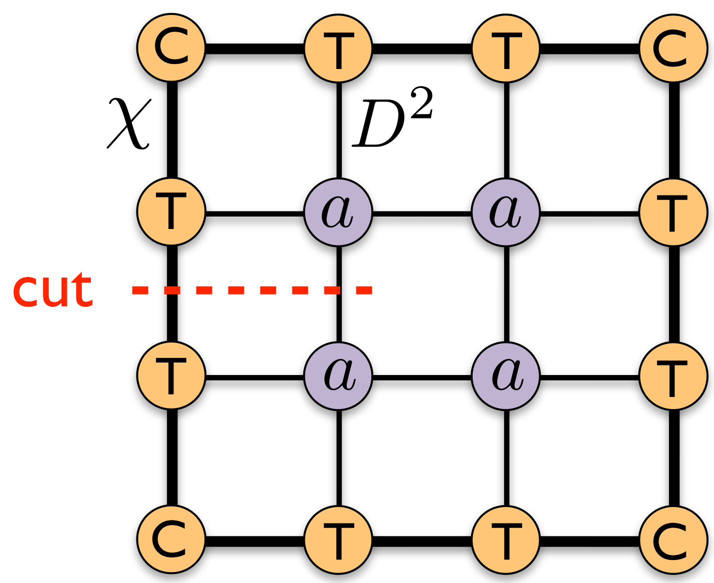


figure taken from Orus, Vidal, PRB 80 (2009)

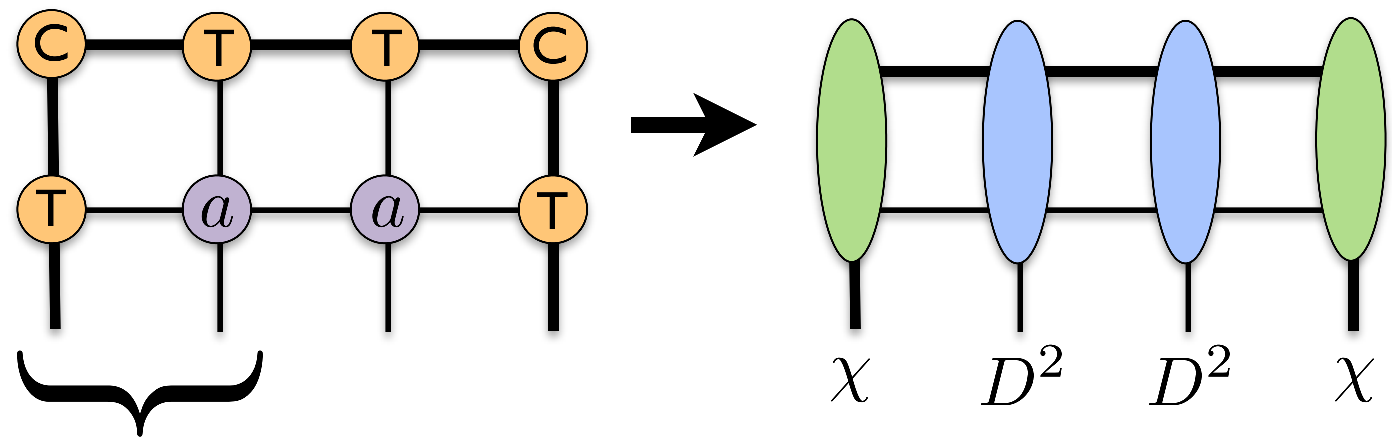
- ★ Let the system grow in all directions.
- ★ Repeat until convergence is reached
- ★ The boundary tensors form the **environment**
- ★ Can be generalized to arbitrary unit cell sizes
  Corboz, et al., PRB 84 (2011)

Simplest case: rotational symmetric tensors

Nishino, Okunishi, JPSJ65 (1996)



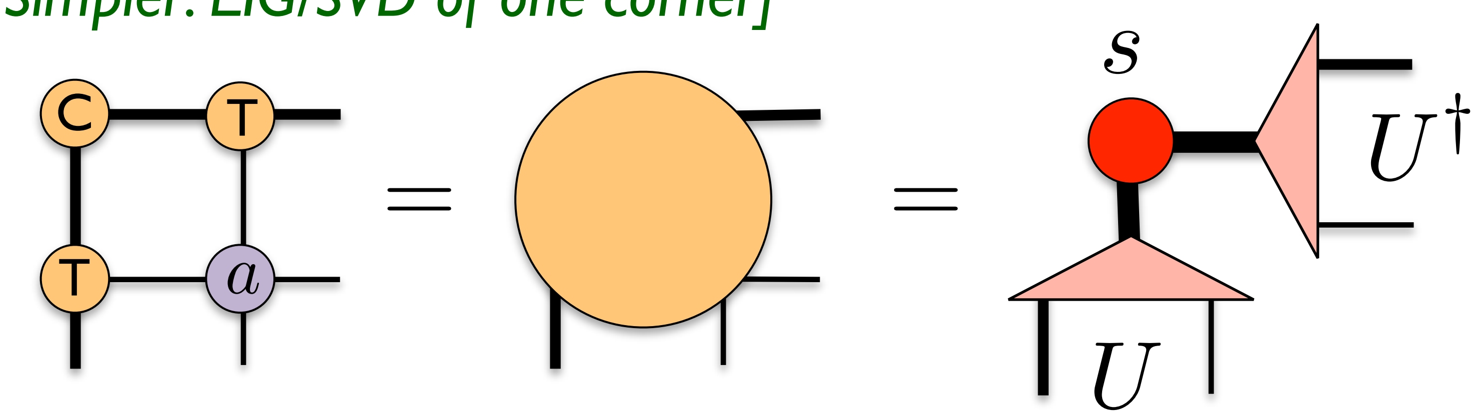
$$"\rho_{left}"$$



Relevant subspace?

DMRG: Eigenvectors with largest eigenvalues of ρ_{left}

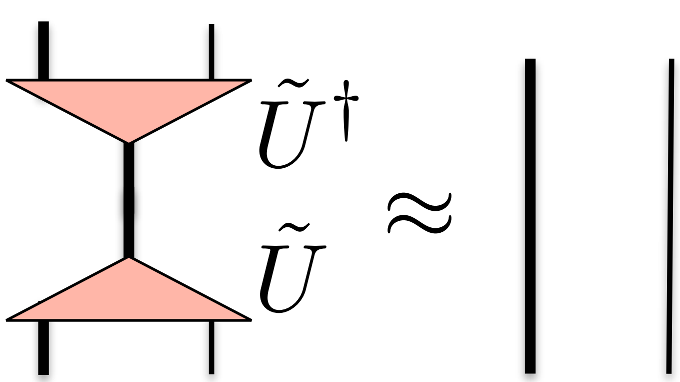
[Simpler: EIG/SVD of one corner]



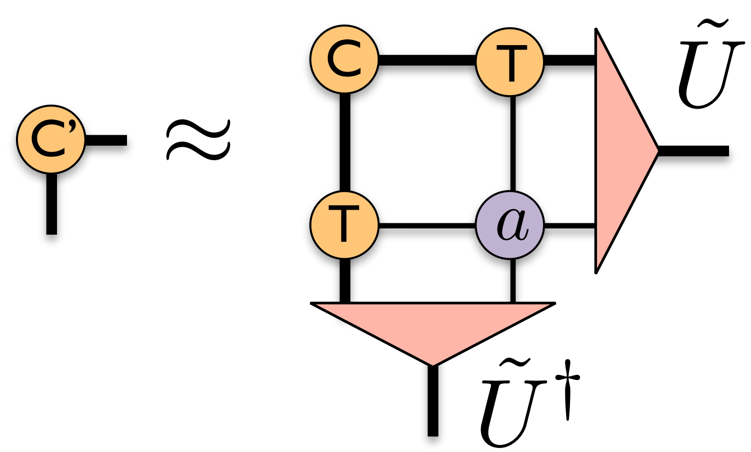
How can we best truncate from

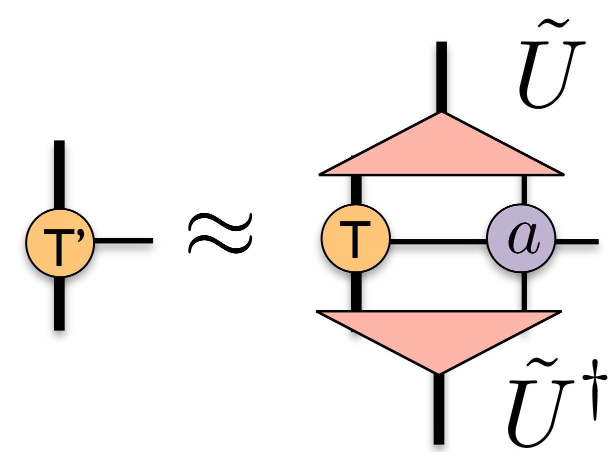
$$\chi D^2 \to \chi$$

Approximate resolution of the identity (in the relevant subspace)

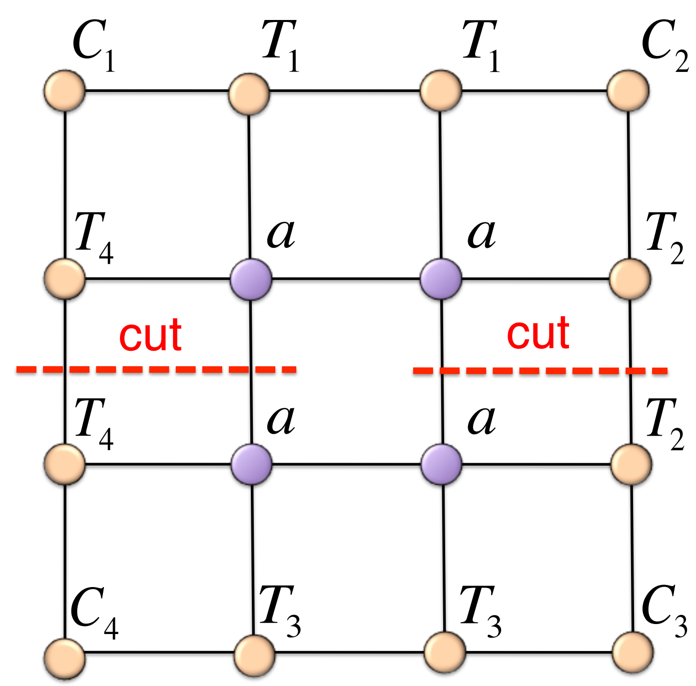


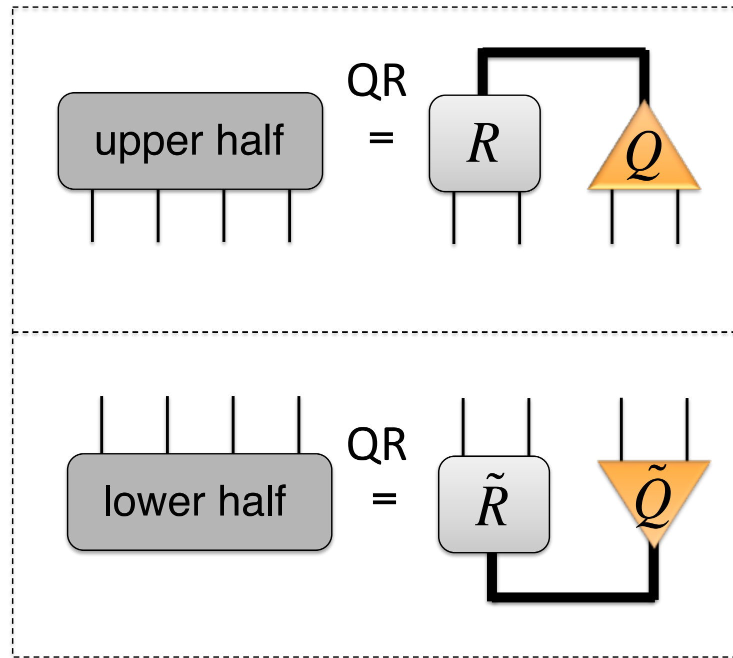
Renormalized tensors: keep only χ states with largest weight

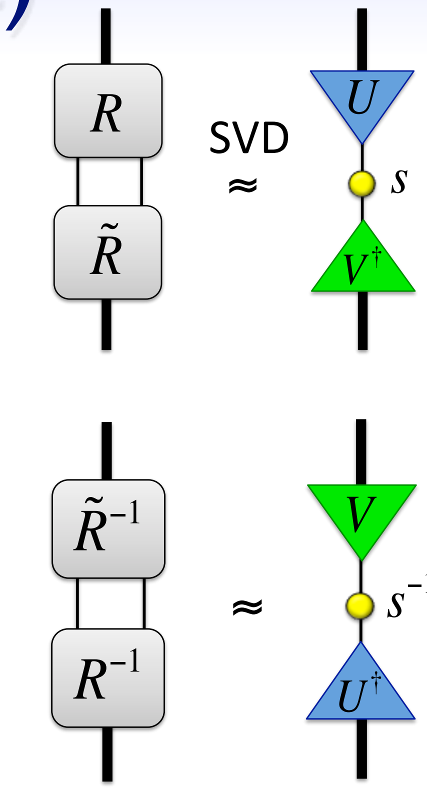


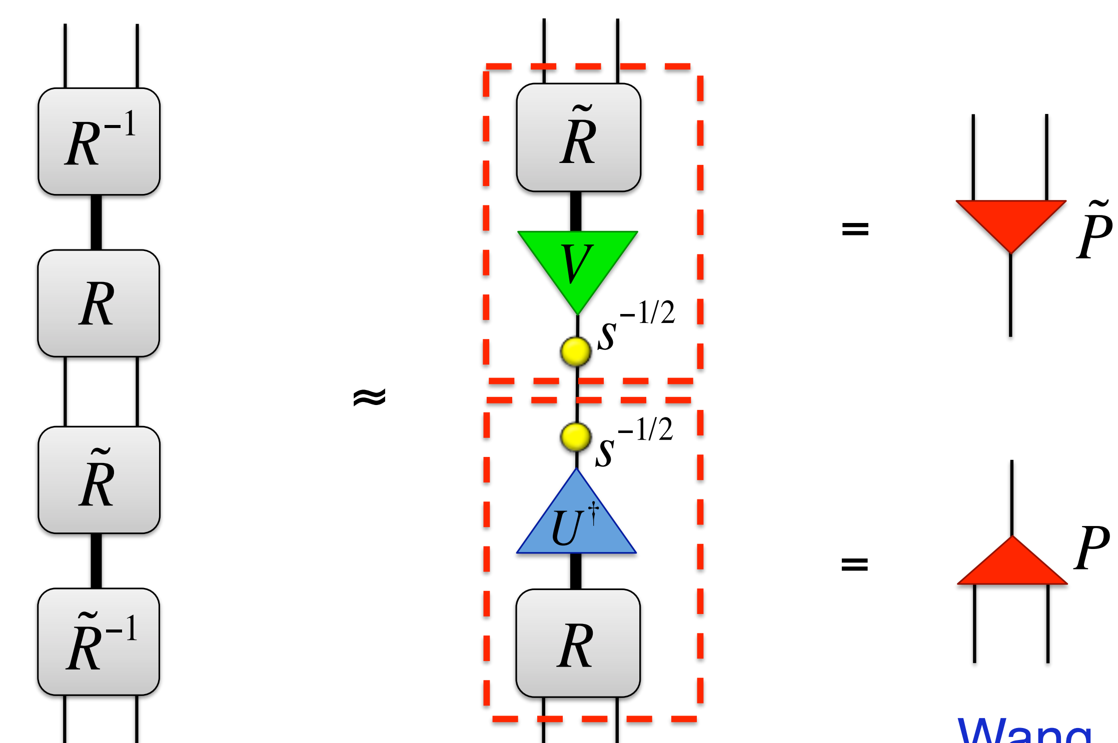


General case: Renormalization step (left move)





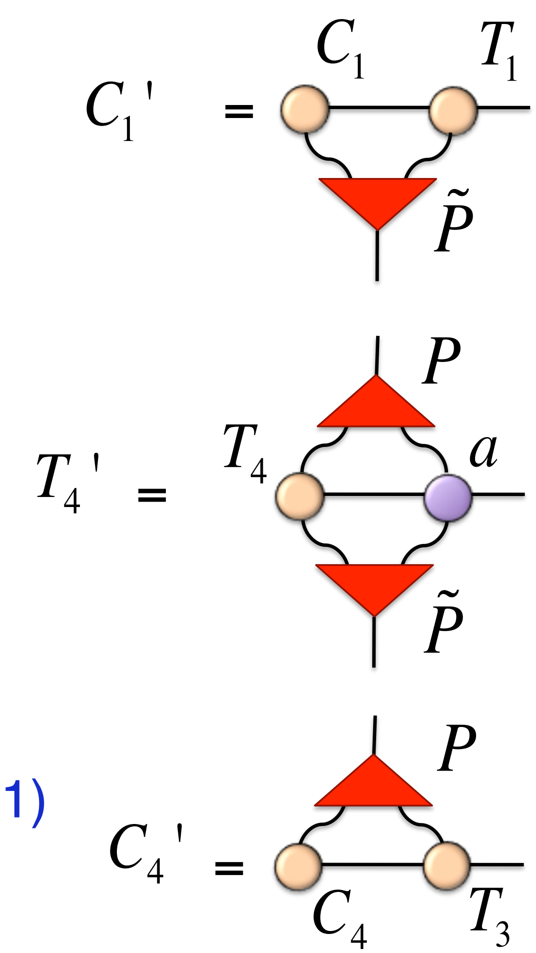




identity

approx. identity

projectors onto relevant subspace

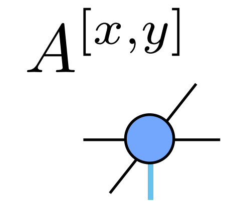


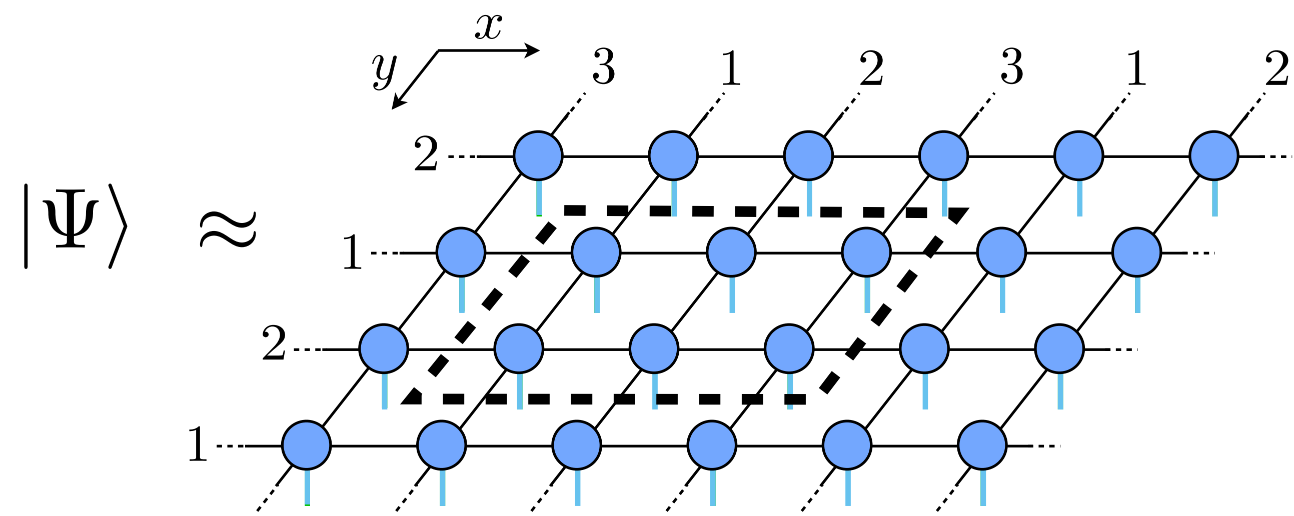
Wang, Pižorn & Verstraete, PRB 83 (2011)
Huang, Chen & Kao, PRB 86 (2012)
PC, Rice, Troyer, PRL 113 (2014)

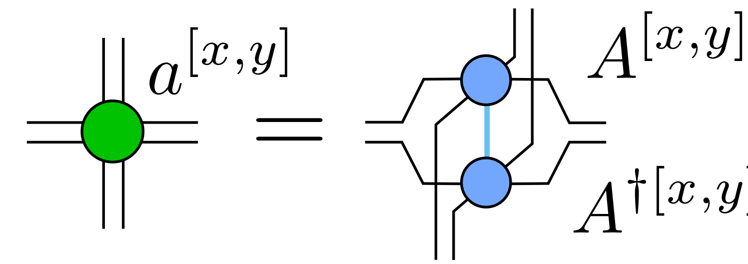
CTM with larger unit cells

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

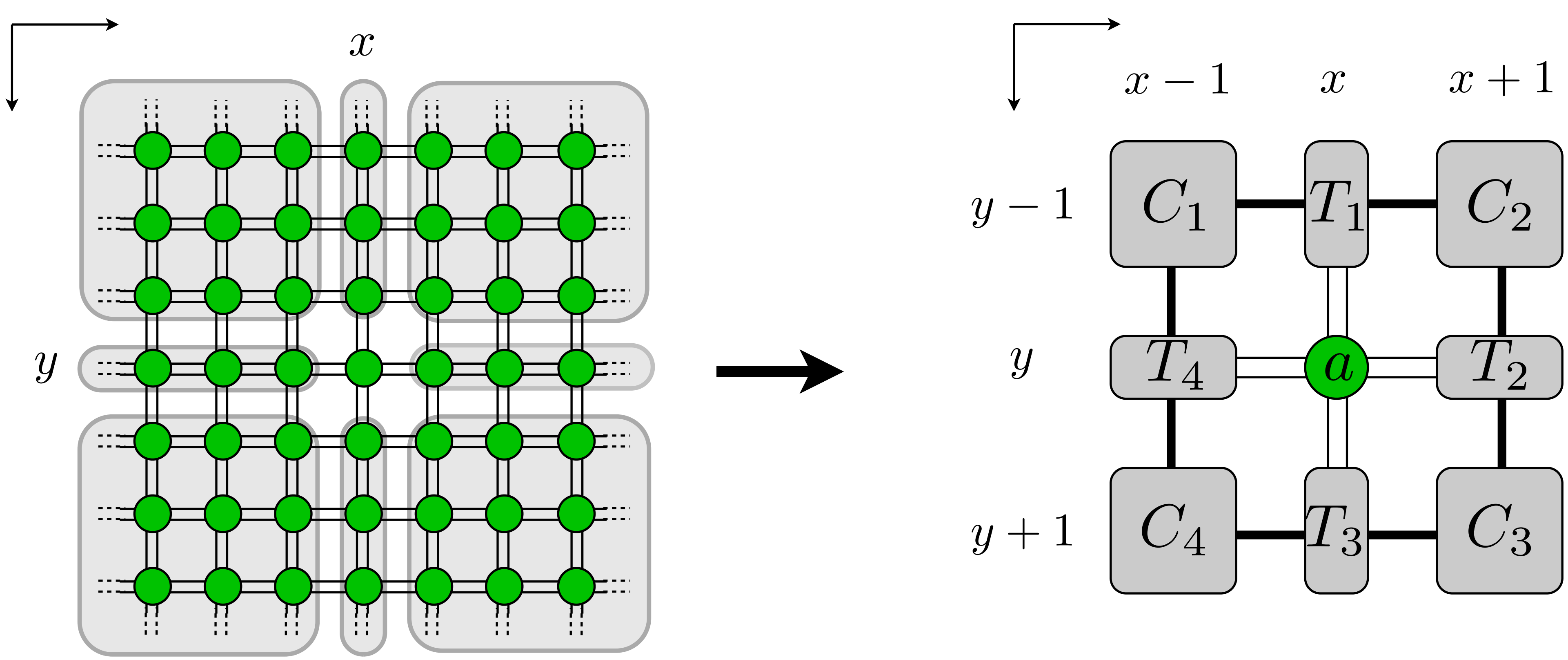
★ Each tensor has coordinates with respect to the unit cell:





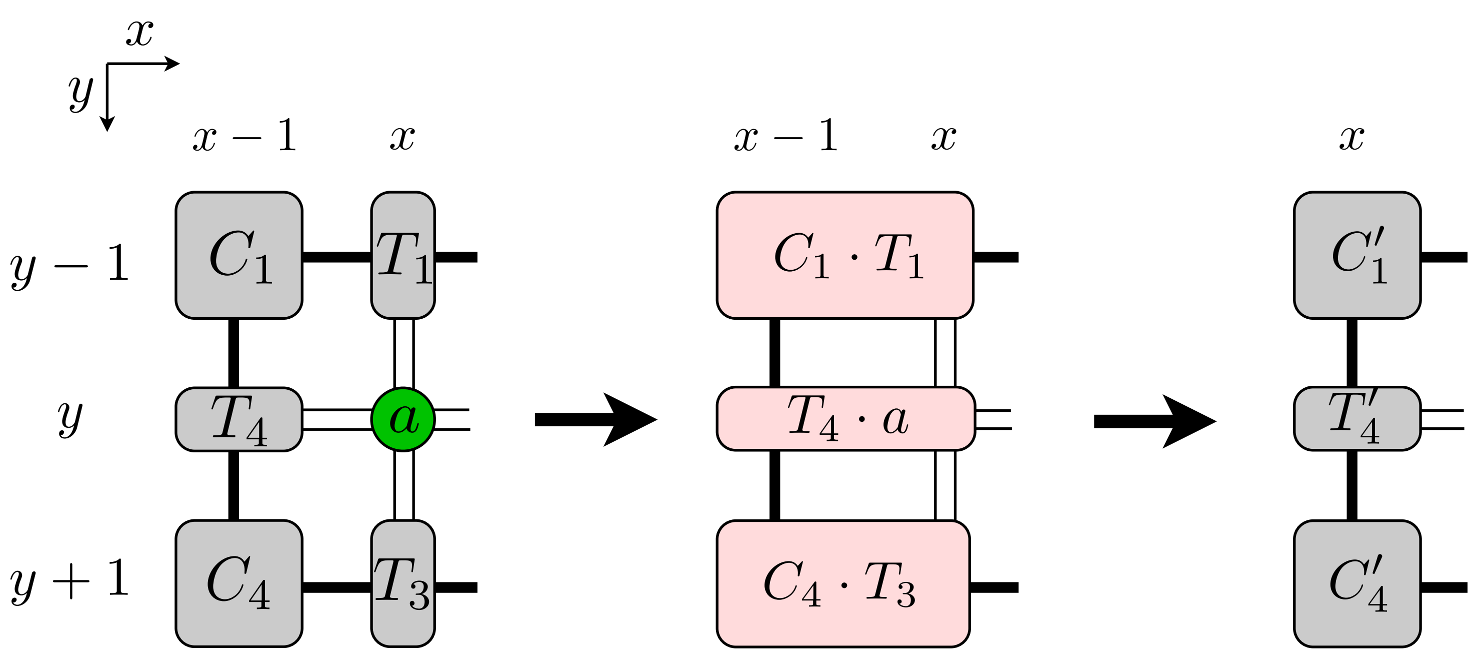


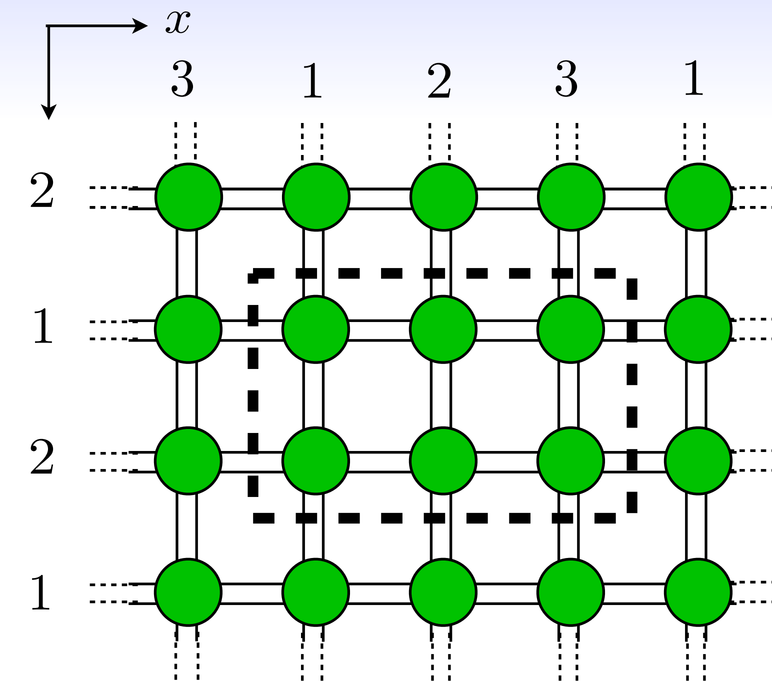
★ Keep a copy of every environment tensors C1, ... C4, T1, ..., T4 for each coordinate



CTM with larger unit cells

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

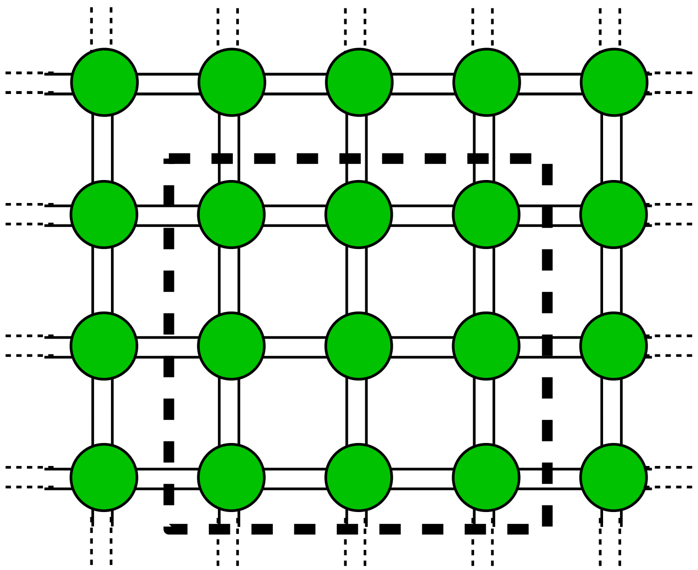




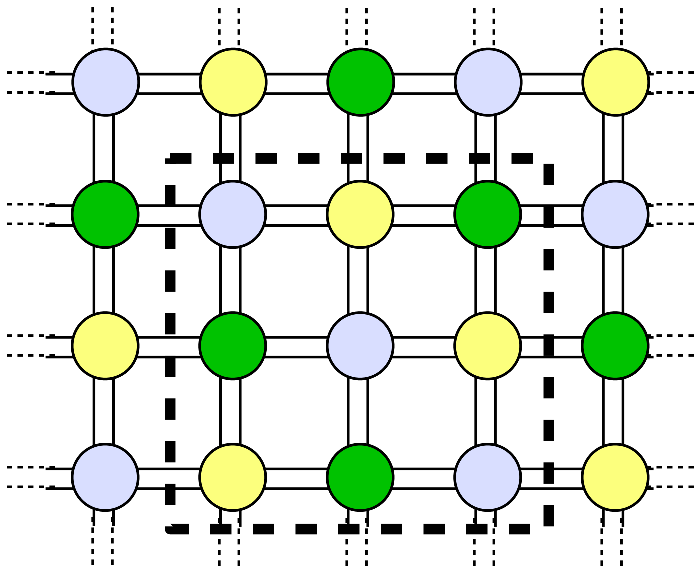
CTM with larger unit cells

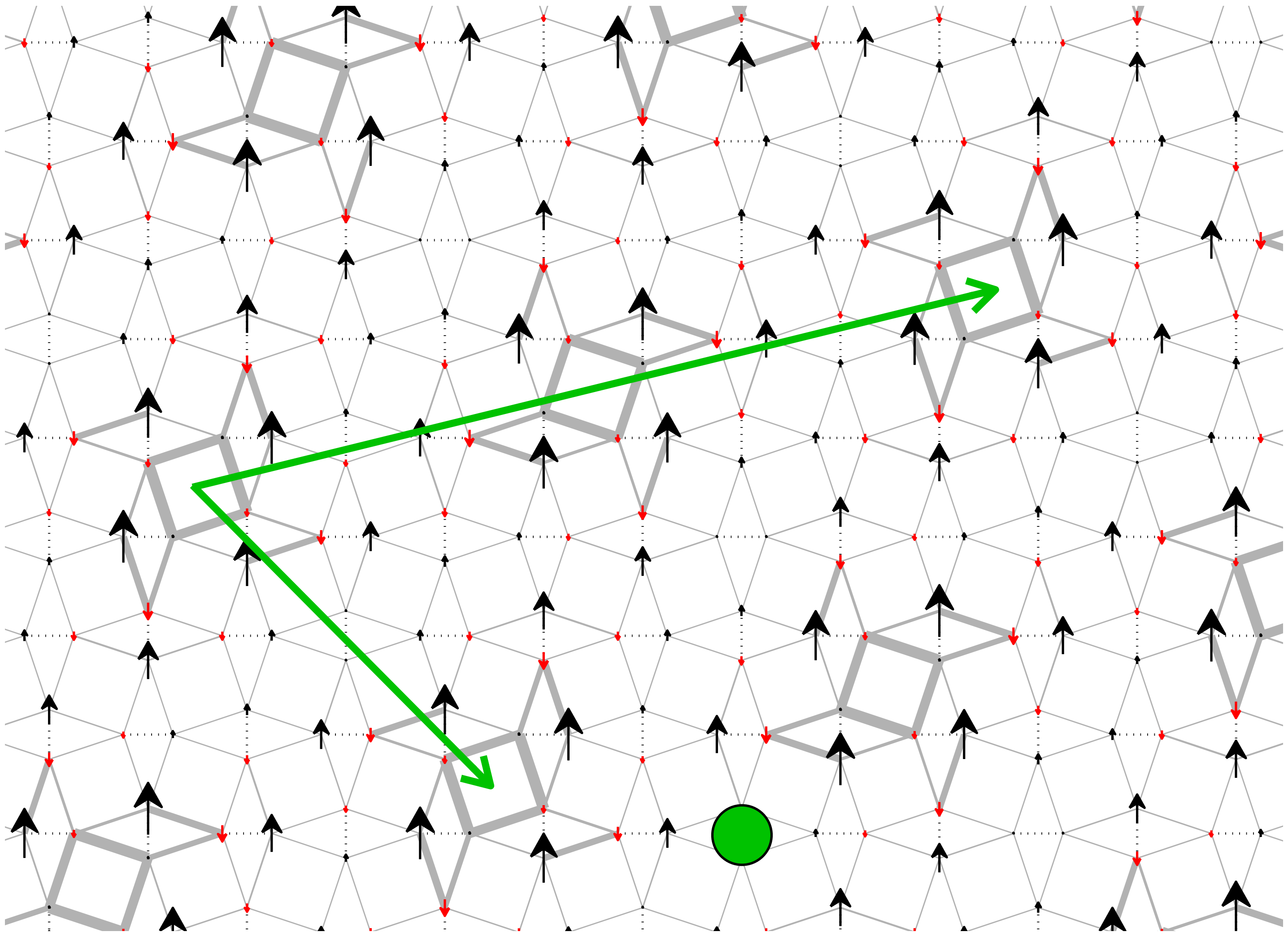
Other shapes than rectangular cell possible:

All 9 tensors different:



Only 3 different tensors:





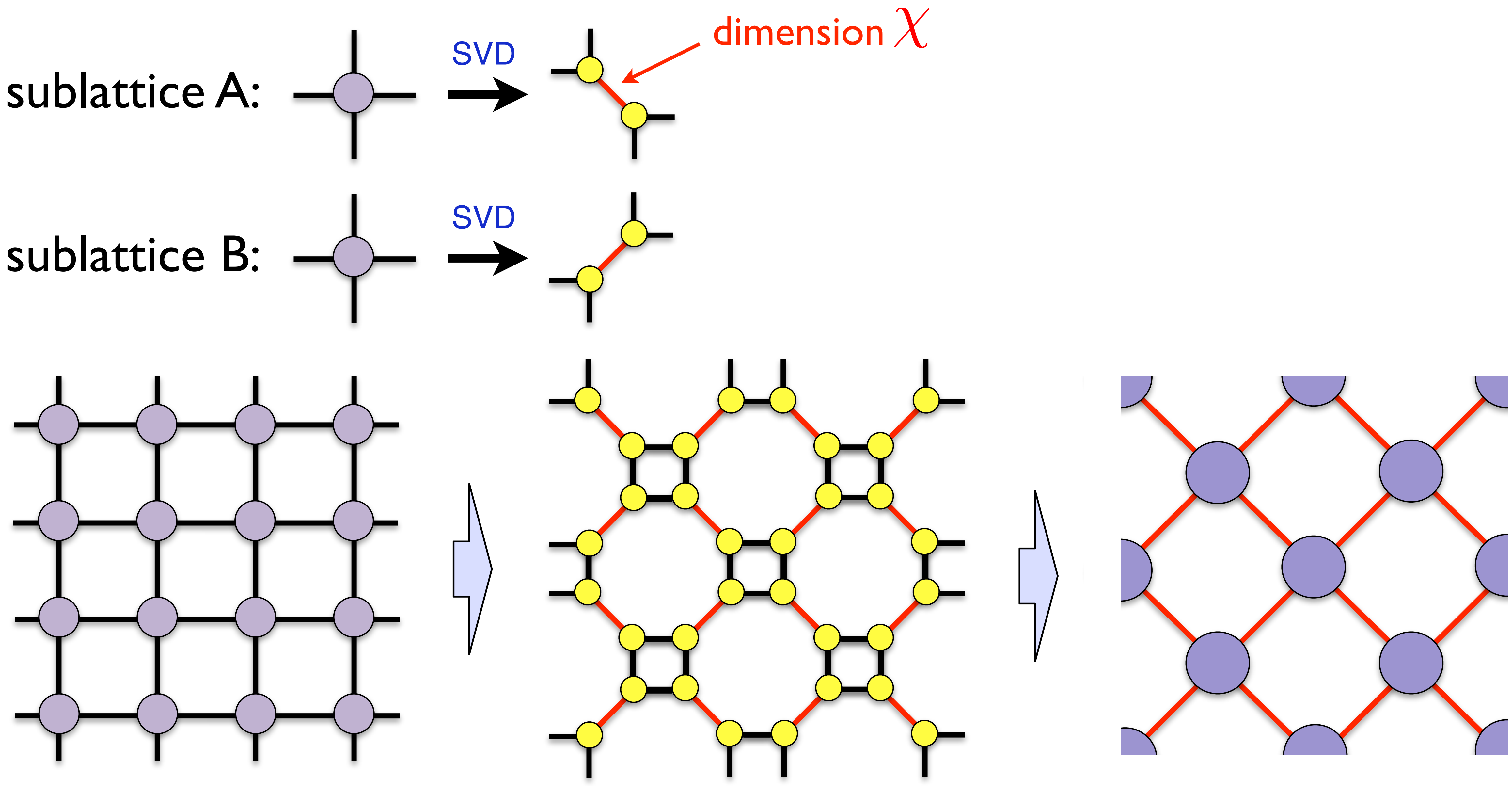
Unit cell with 30 tensors (60 sites)

(example: Shastry-Sutherland model)

Contracting the PEPS/iPEPS using TRG

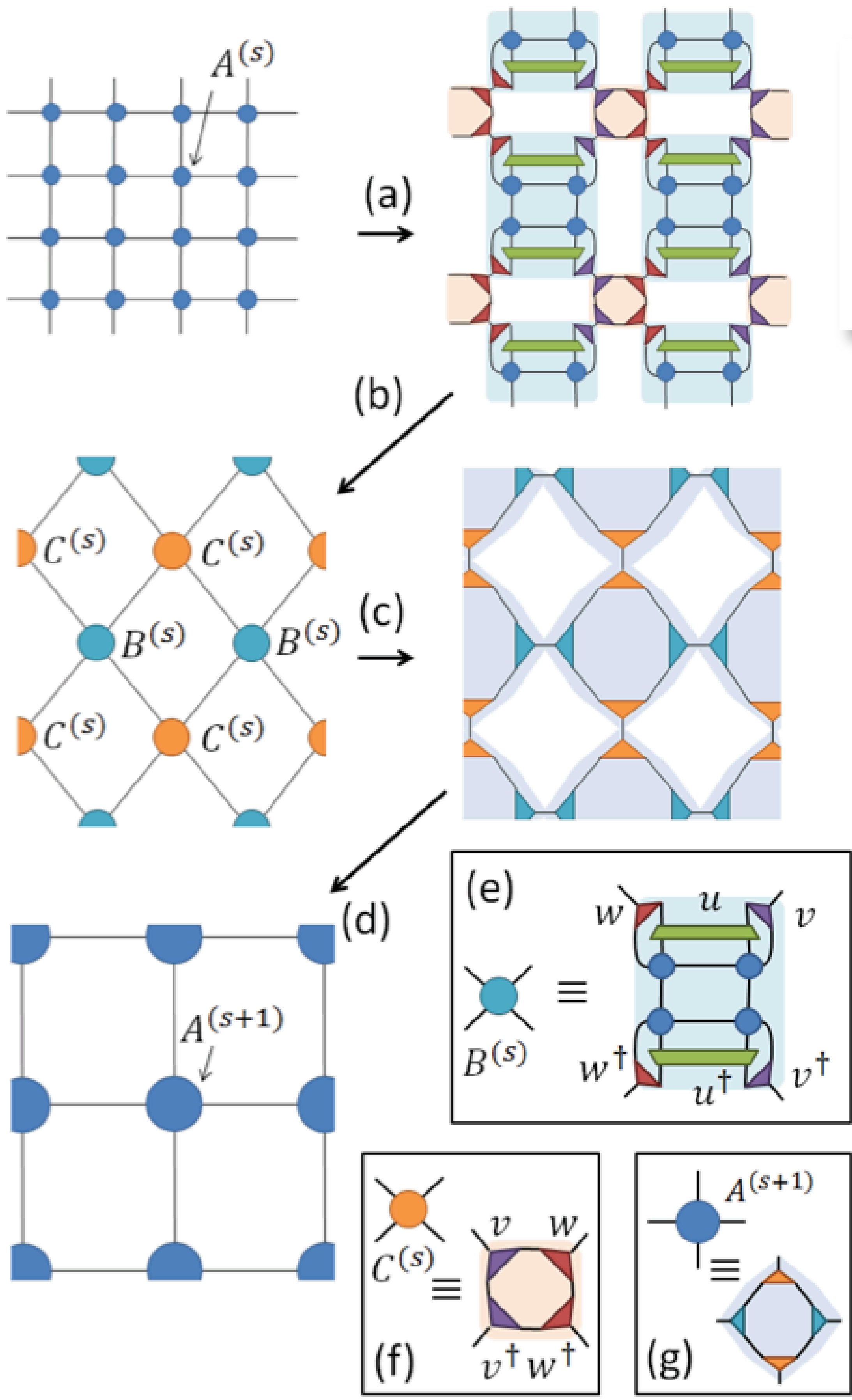
Tensor Renormalization Group

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, ...

New: 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, arXiv:1512.04938

Contracting the PEPS

★ Exact contraction of an PEPS is exponentially hard!

→ *use controlled approximate contraction scheme*

MPS-MPO-based approach

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

Corner transfer matrix method

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

TRG

Tensor Renormalization Group
(+HOTRG, SRG, HOSRG)

Levin, Nave, PRL99 (2007)
Xie et al. PRL 103, (2009)

TNR

Tensor Network Renormalization

Evenbly & Vidal, PRL 115 (2015

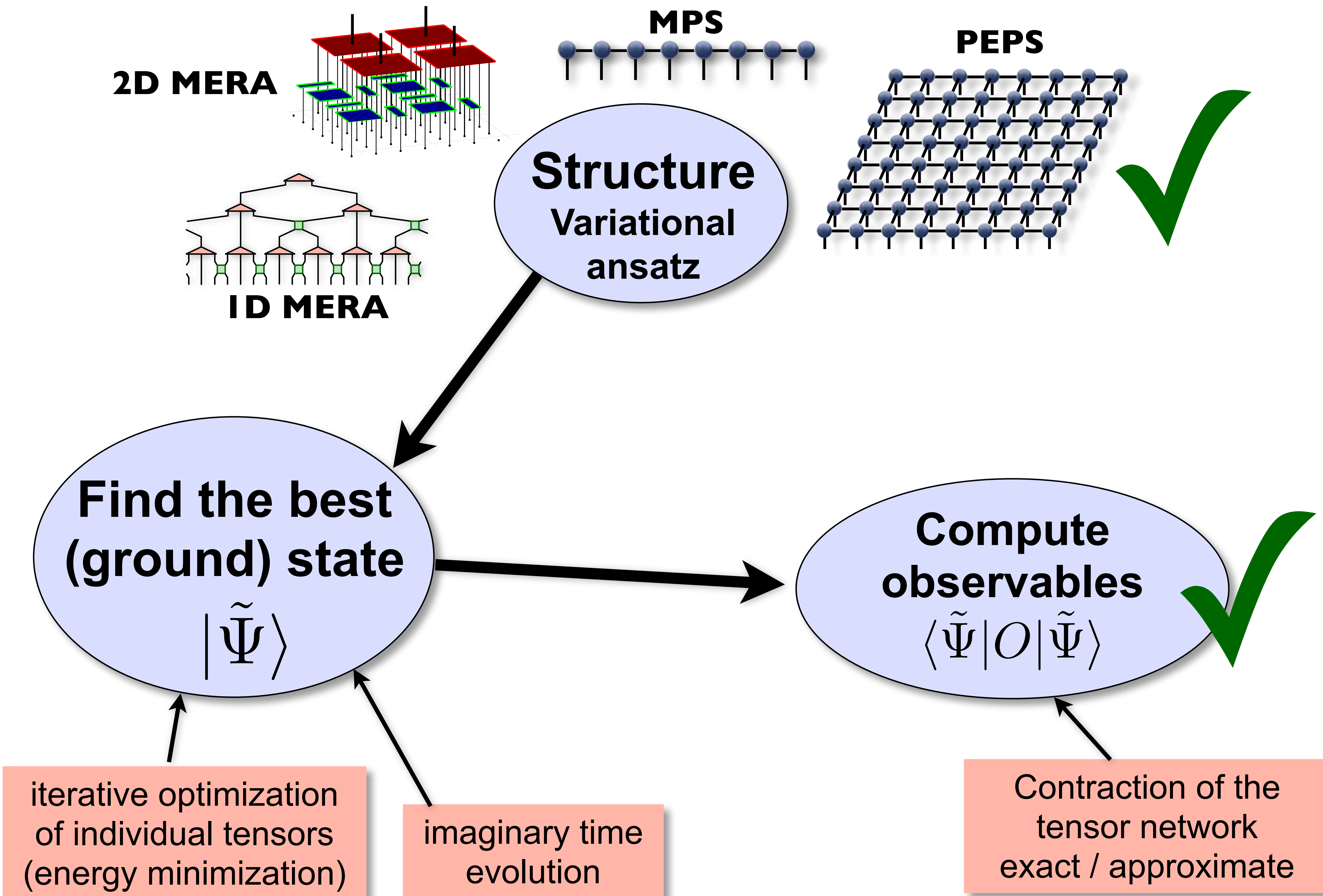
Loop-TNR:
Yang, Gu & Wen, arXiv:1512.04938

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

★ Convergence in χ needs to be carefully checked

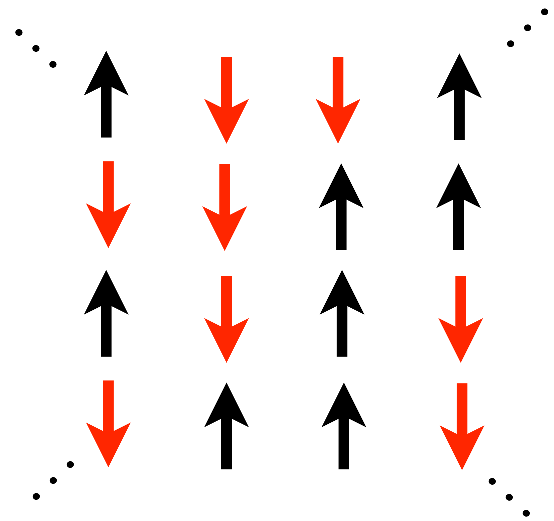
★ Overall cost: $\mathcal{O}(D^{10\ldots14})$ with $\chi \sim D^2$

Summary: Tensor network algorithm for ground state

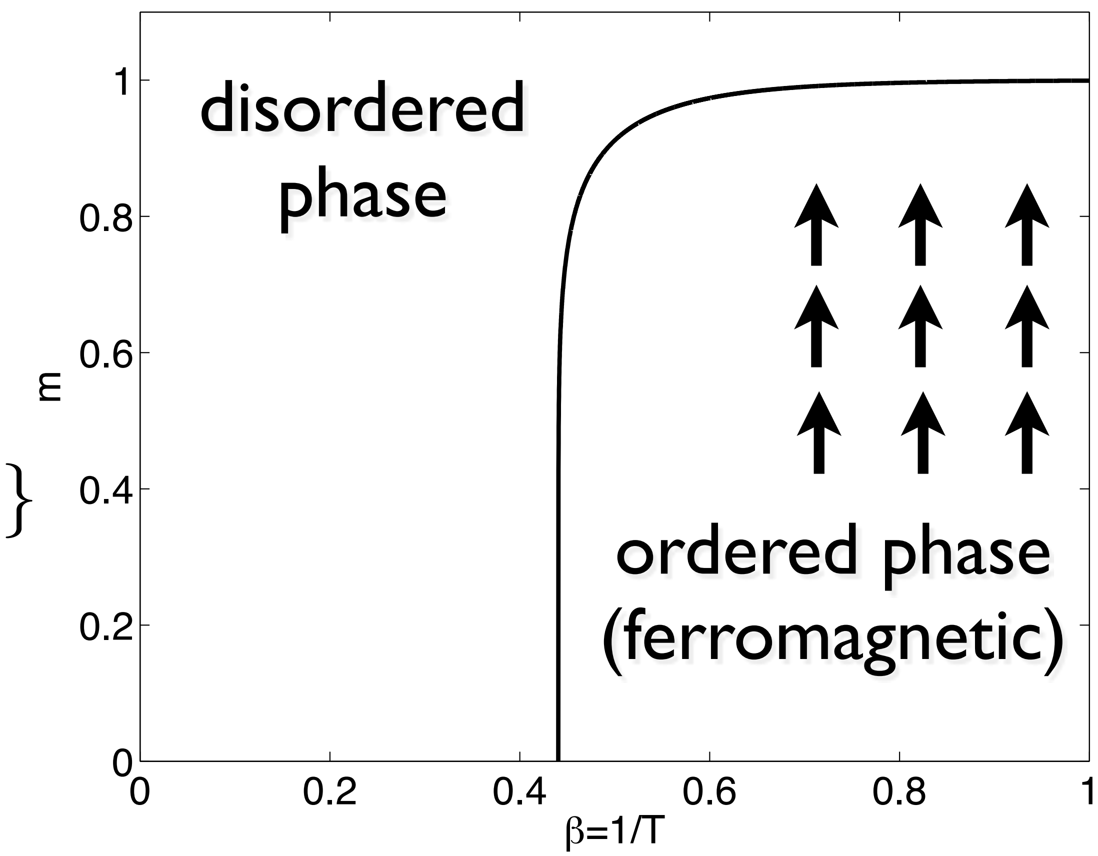


Simple example / exercise

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

$$Q_{s_i s_j} = \exp(-\beta H_b(s_i, s_j))$$

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

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

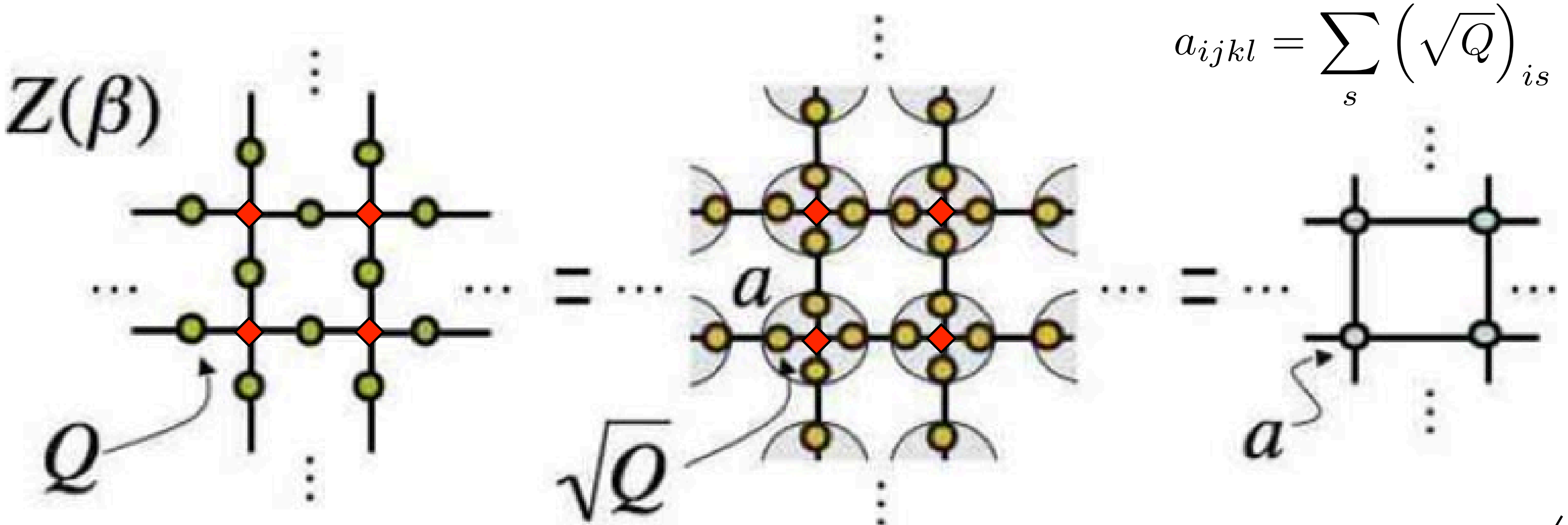
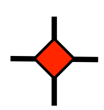
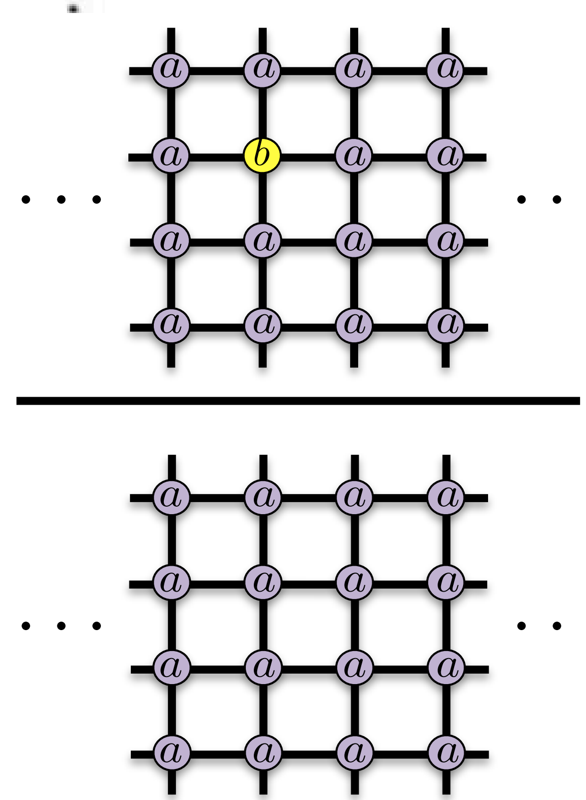


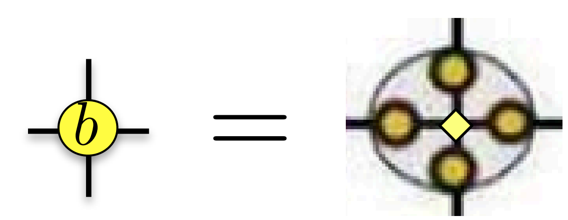
Figure taken from Orús & Vidal, PRB 78, 155117 (2008).

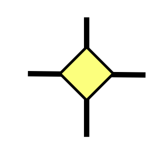
 $g_{ijkl} = \delta_{ijkl}$

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

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

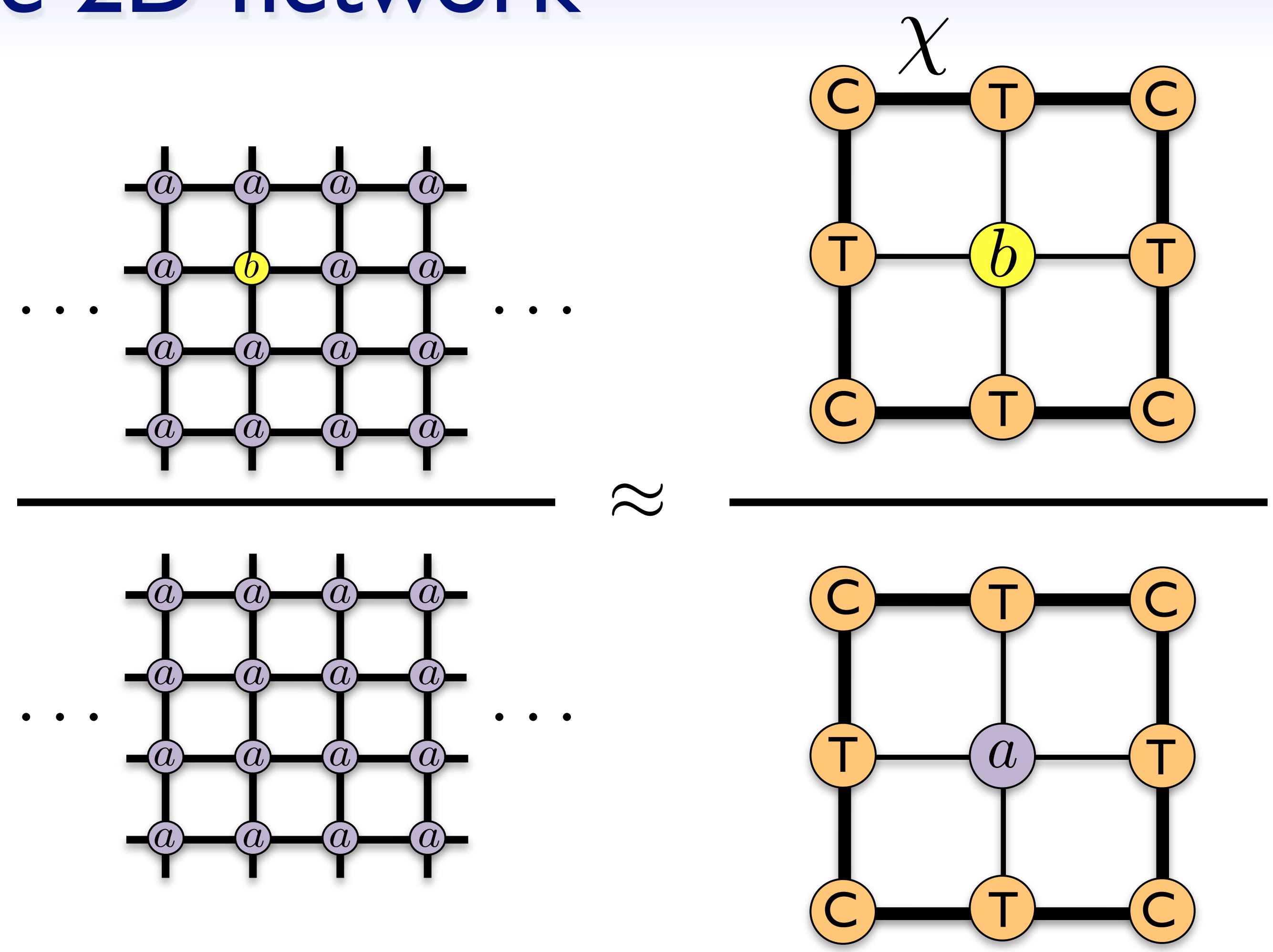




 $g'_{ijkl} = s_i \delta_{ijkl}$

Use CTM to contract the 2D network

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



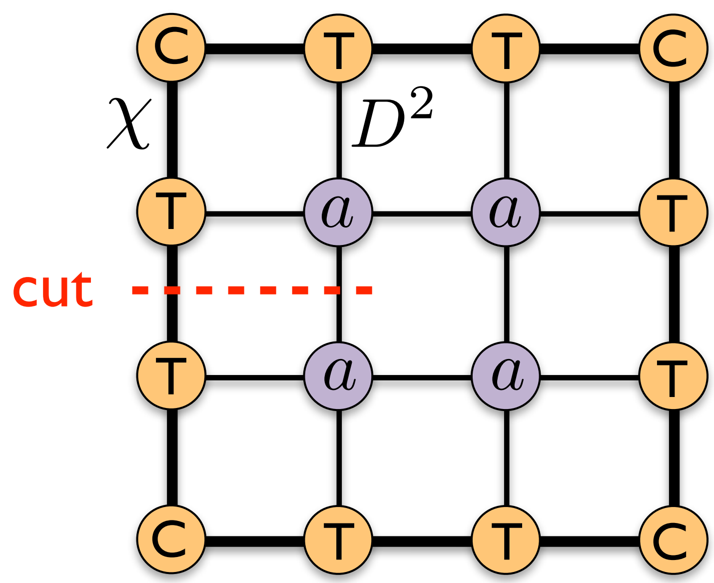
- Compute environment tensors C and T iteratively (CTM)
- Here: symmetric case: all corner/edge tensors the same and

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

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

Simplest case: rotational symmetric tensors

Nishino, Okunishi, JPSJ65 (1996)

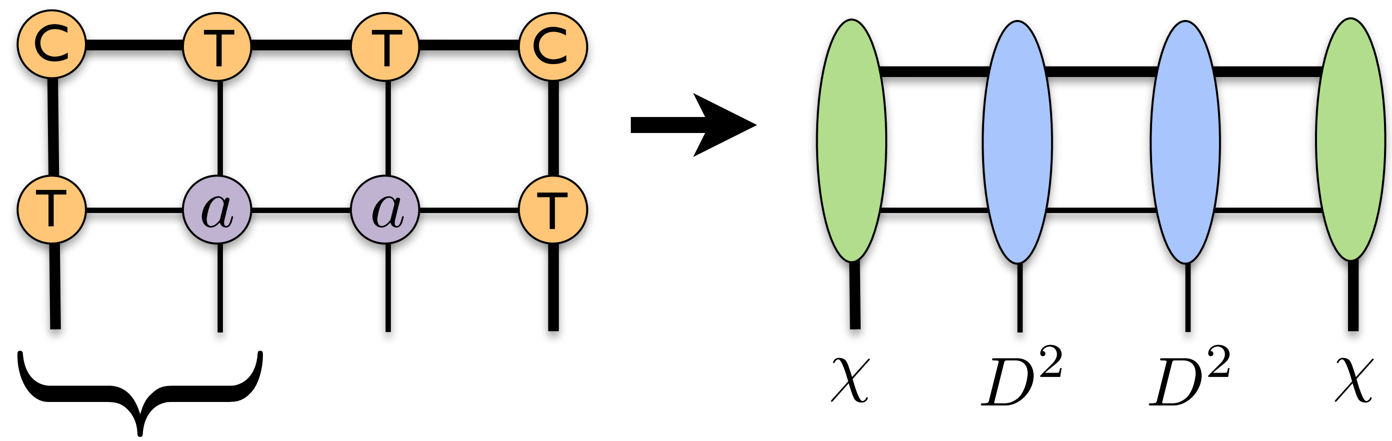


$$"\rho_{left}"$$

How can we best truncate from

$$\chi D^2 \rightarrow \chi$$

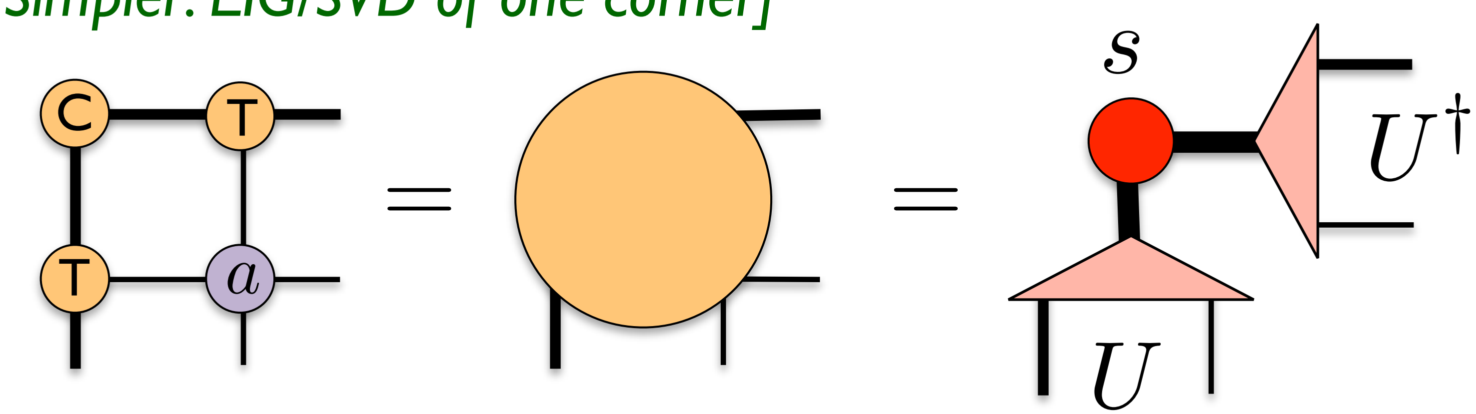
Keep numbers bounded:
e.g. divide each tensor by its largest element



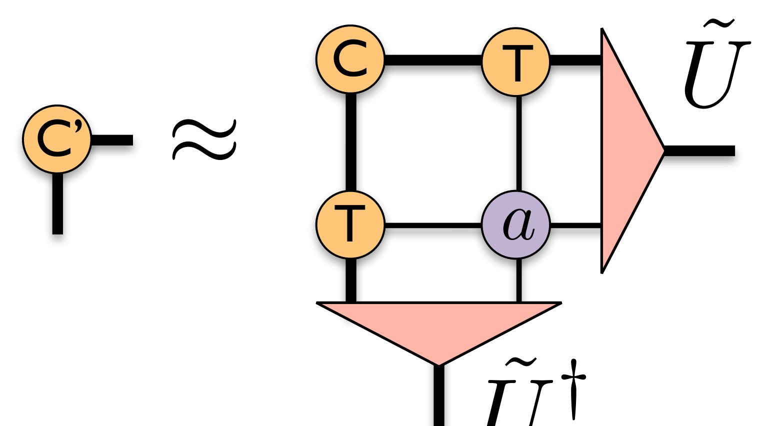
Relevant subspace?

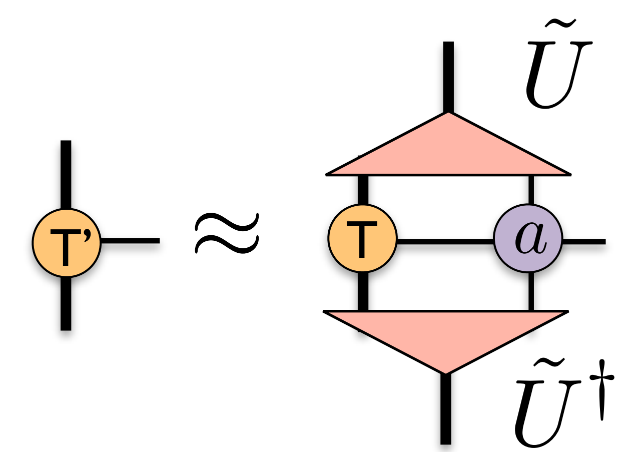
DMRG: Eigenvectors with largest eigenvalues of ρ_{left}

[Simpler: EIG/SVD of one corner]



Renormalized tensors: keep only χ states with largest weight





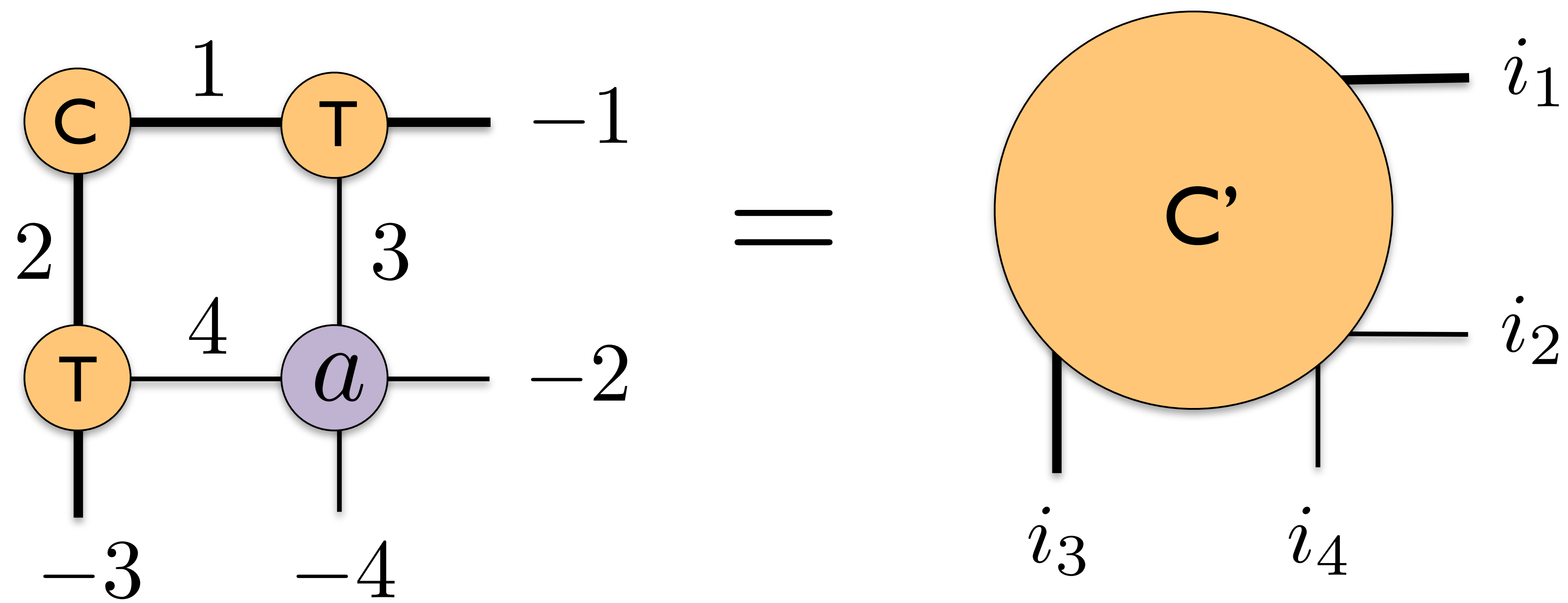
CTM algorithm summary

- 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!**
- **Example MATLAB code:** http://tinyurl.com/yaykmdrz

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:



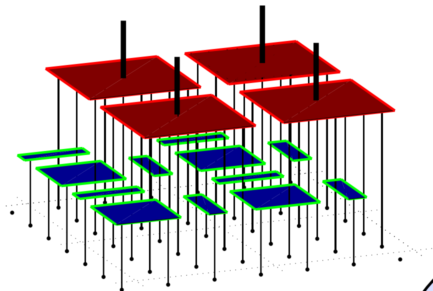
- Code: `Cp = ncon({C, T, T, a},{[1 2], [-1 1 3], [2 -3 4], [-2 3 4 -4]});`

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

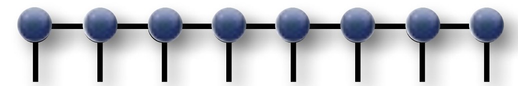
PART III: Optimization

Summary: Tensor network algorithm for ground state

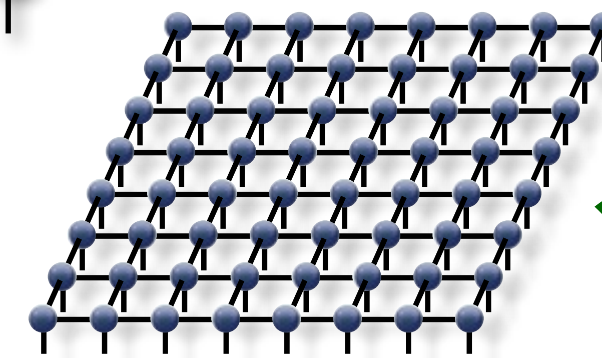
2D MERA

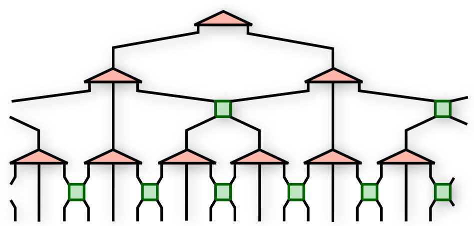


MPS



PEPS





1D MERA

Structure
Variational ansatz

Find the best (ground) state
$|\tilde{\Psi}\rangle$

Compute observables
$\langle\tilde{\Psi}|O|\tilde{\Psi}\rangle$

iterative optimization of individual tensors (energy minimization)

imaginary time evolution

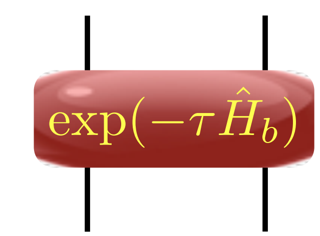
Contraction of the tensor network exact / approximate

Optimization via imaginary time evolution

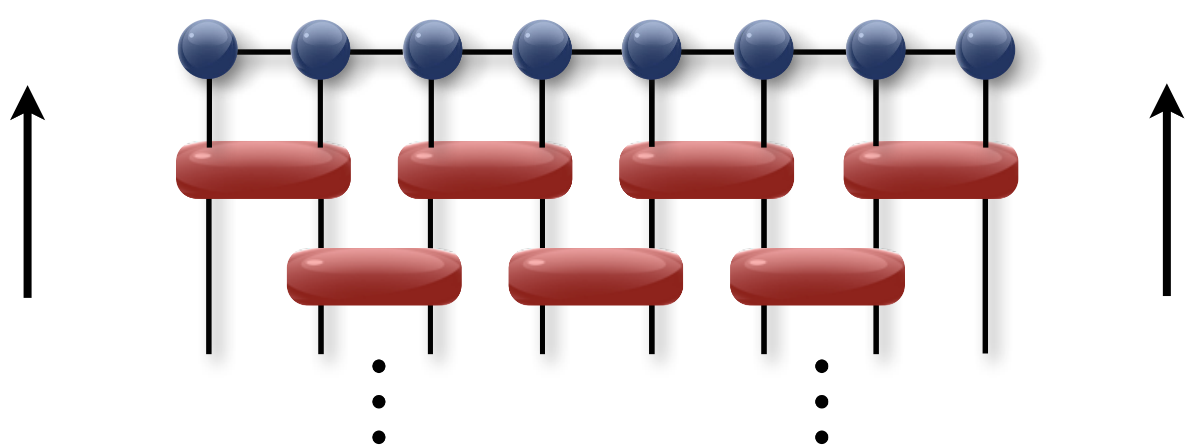
- Idea: $\exp(-\beta\hat{H})|\Psi_i\rangle \xrightarrow{\beta\to\infty} |\Psi_{GS}\rangle$

Trotter-Suzuki decomposition:

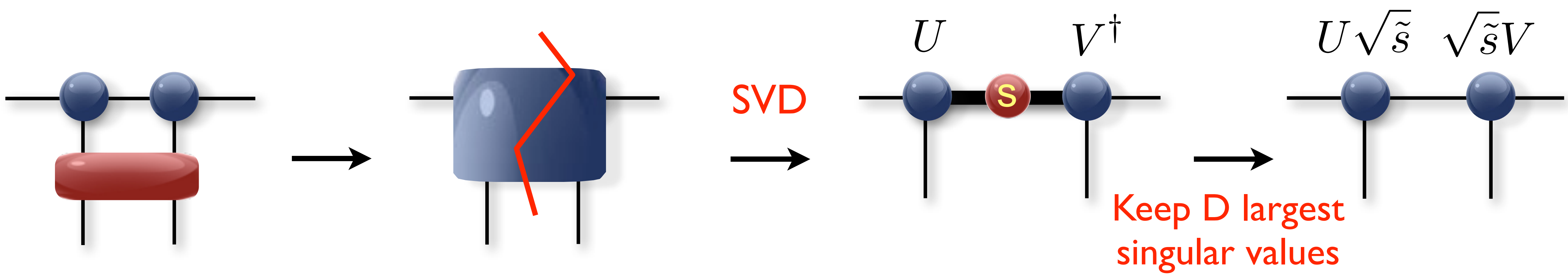
$$\exp(-\beta\hat{H}) = \exp(-\beta\sum_b \hat{H}_b) = \left(\exp(-\tau\sum_b \hat{H}_b)\right)^n \approx \left(\prod_b \exp(-\tau\hat{H}_b)\right)^n \qquad \tau = \beta/n$$



- 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

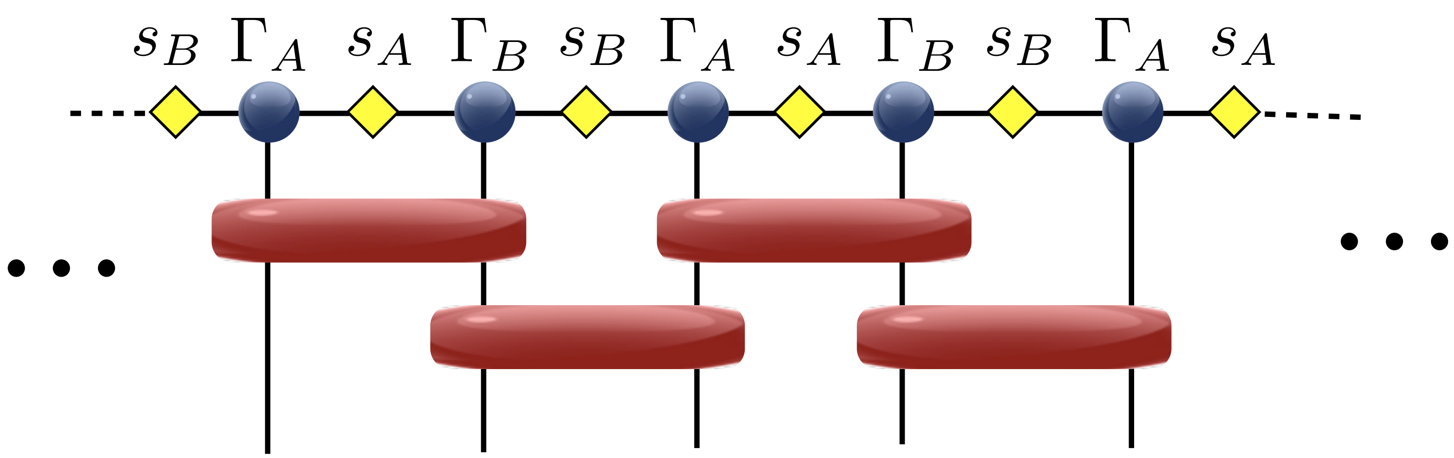
Optimization via imaginary time evolution

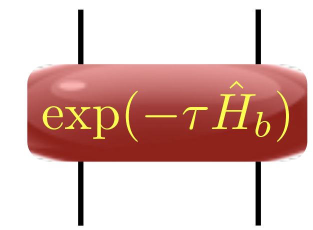
- Idea: $\exp(-\beta\hat{H})|\Psi_i\rangle \xrightarrow{\beta\to\infty} |\Psi_{GS}\rangle$

Trotter-Suzuki decomposition:

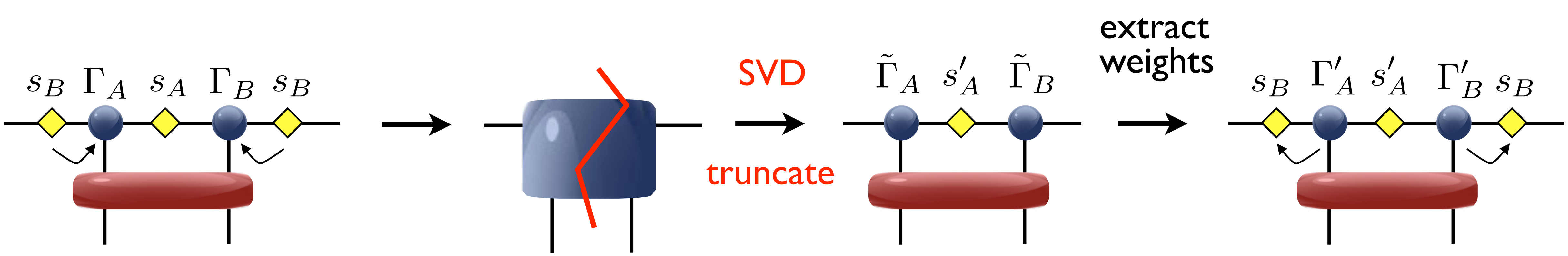
$$\exp(-\beta\hat{H}) = \exp(-\beta\sum_b \hat{H}_b) = \left(\exp(-\tau\sum_b \hat{H}_b)\right)^n \approx \left(\prod_b \exp(-\tau\hat{H}_b)\right)^n \qquad \tau=\beta/n$$

- 1D:



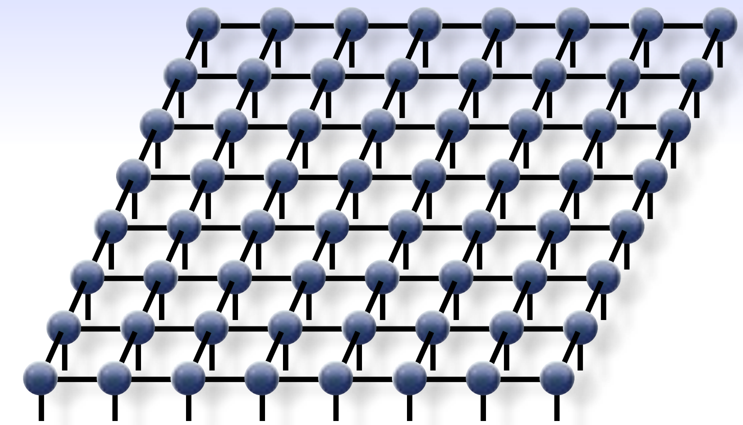


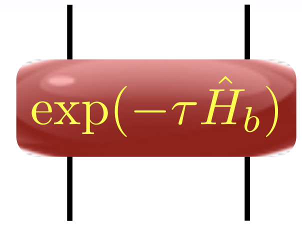
- At each step: apply a two-site operator to a bond and truncate bond back to *D*



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

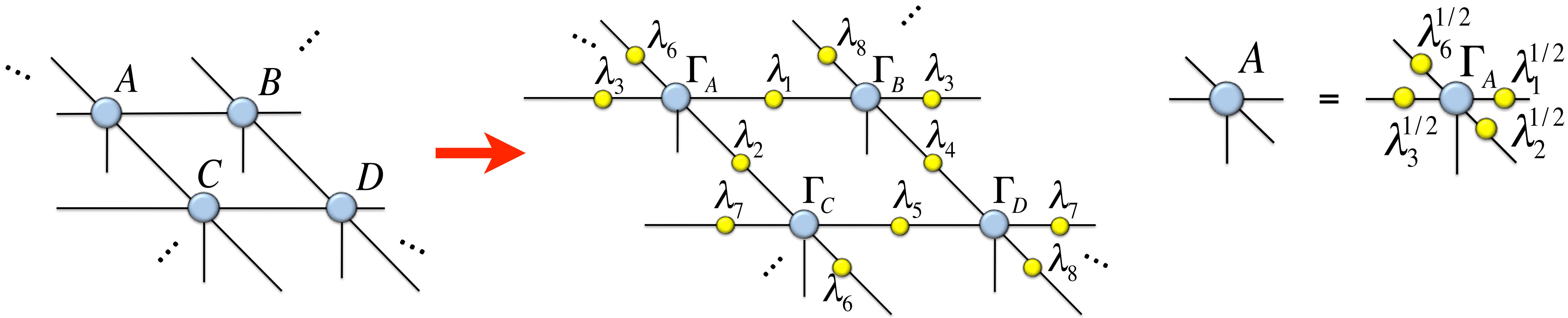
★ Fast-full update [Phien et al, PRB 92 (2015)]

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

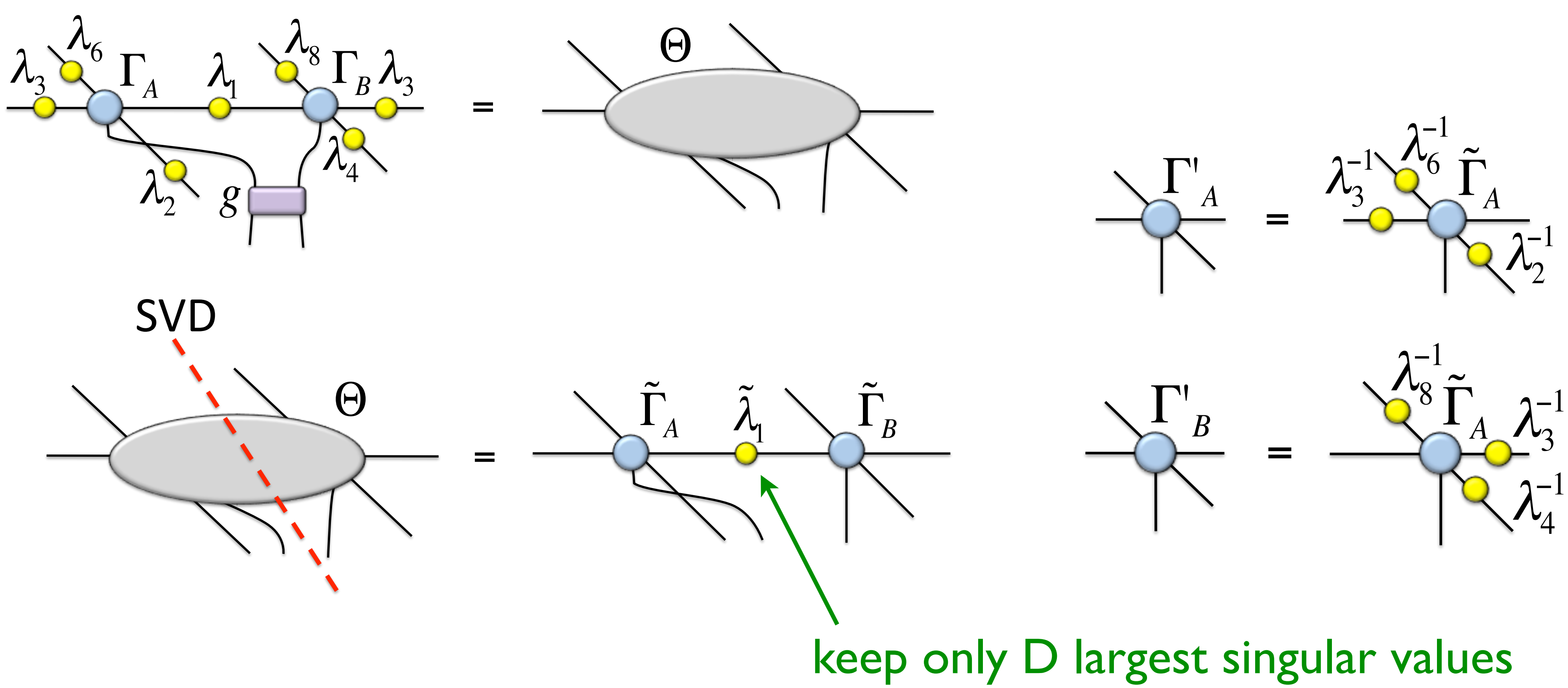
Optimization: simple update

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

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

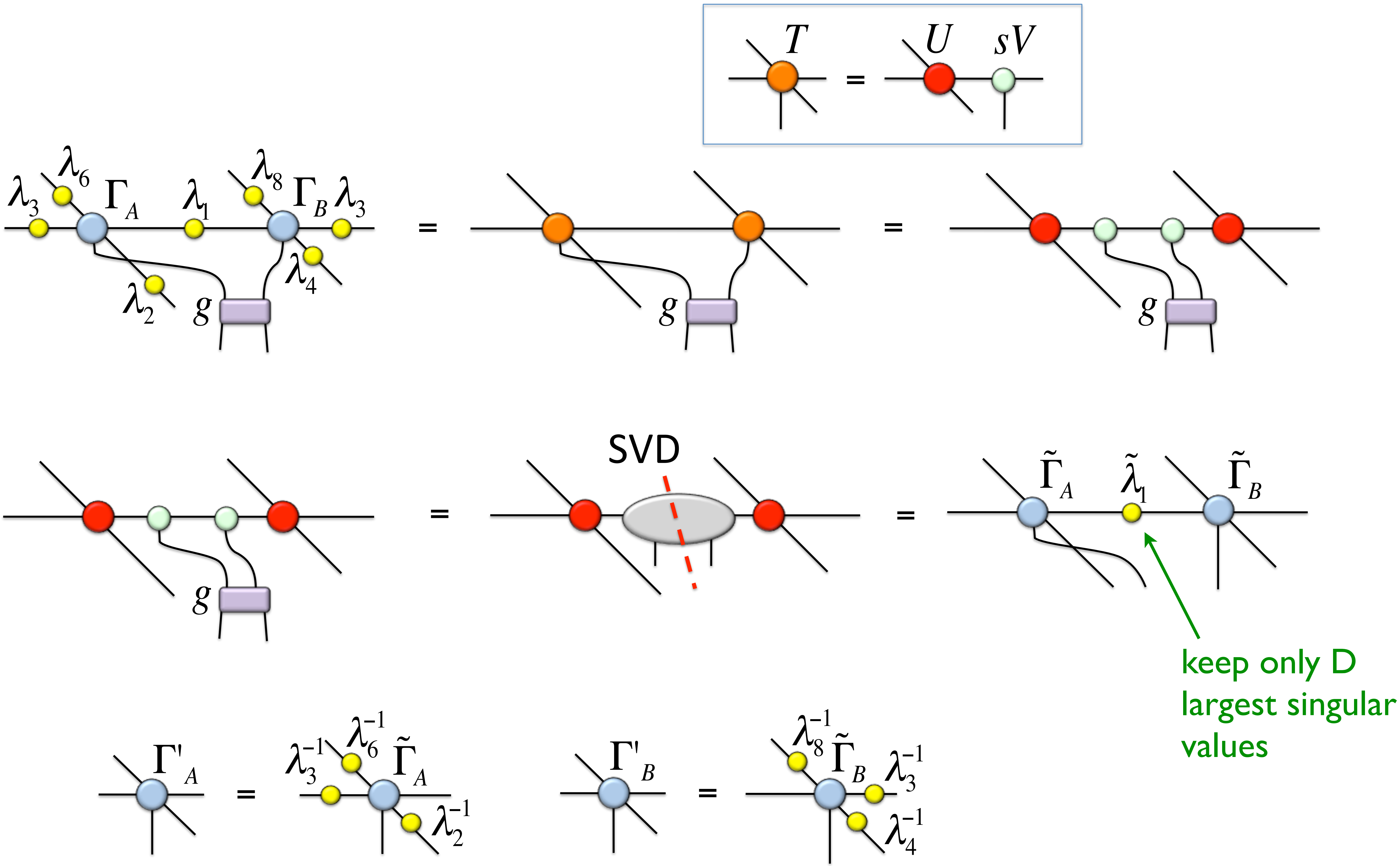


- Update works like in 1D with iTEBD



Trick to make it cheaper

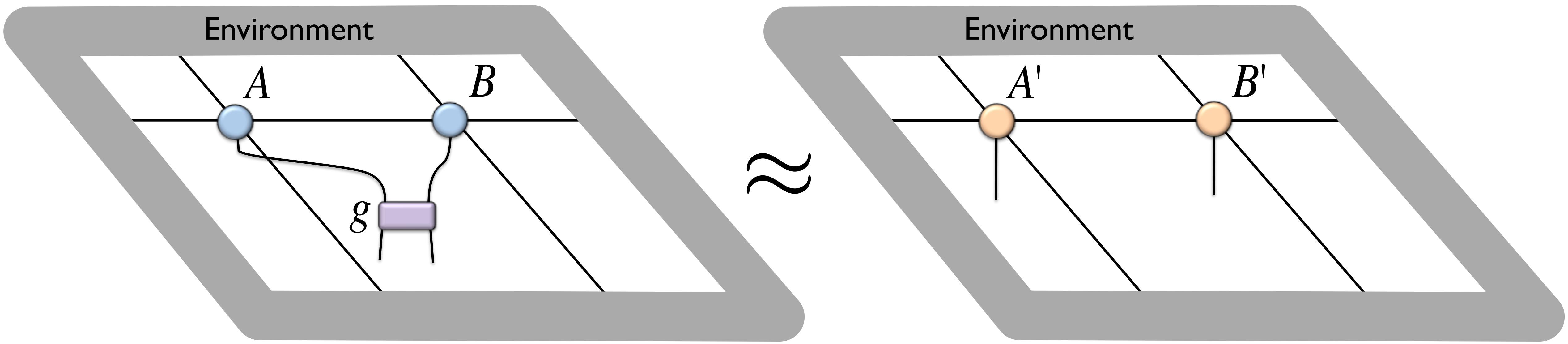
- Idea: Split off the part of the tensor which is updated



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

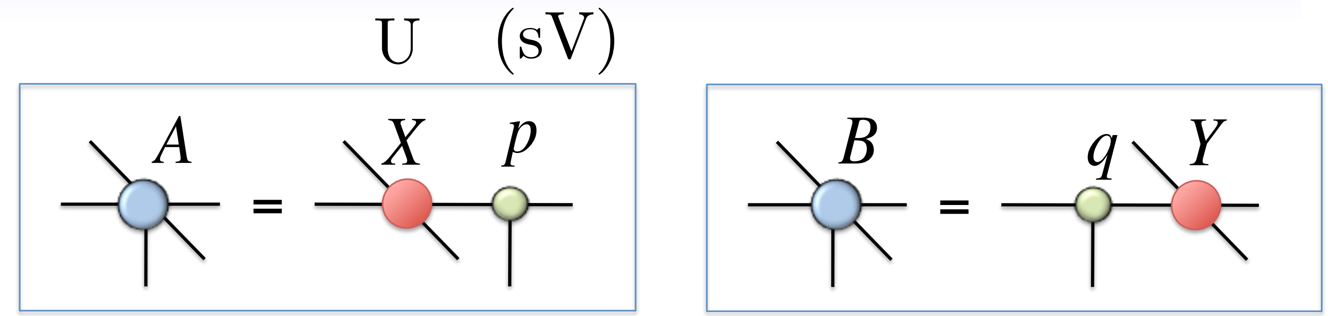


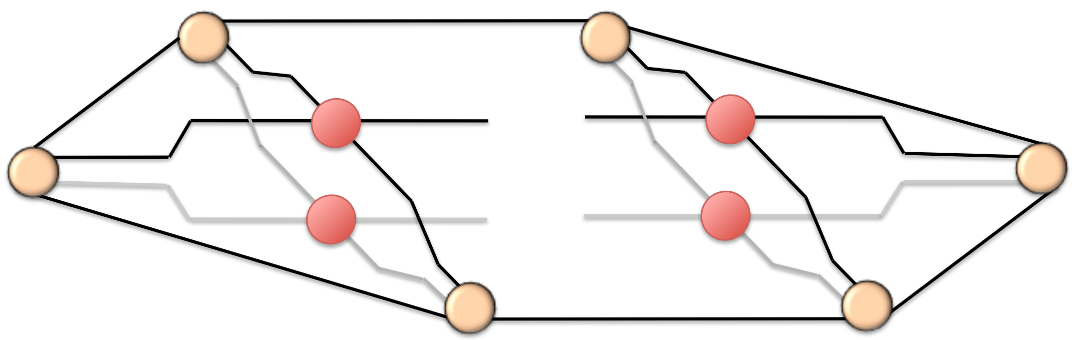
$$|\tilde{\Psi}\rangle = g|\Psi\rangle \qquad \approx \qquad |\Psi'\rangle$$

- 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 / ...
- The full wave function is taken into account for the truncation!
- At each step the environment has to be computed! expensive... but optimal!

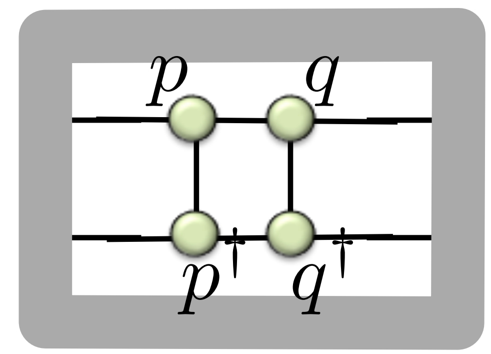
Full-update: details

- Split off the part of the tensor which is updated





$=$

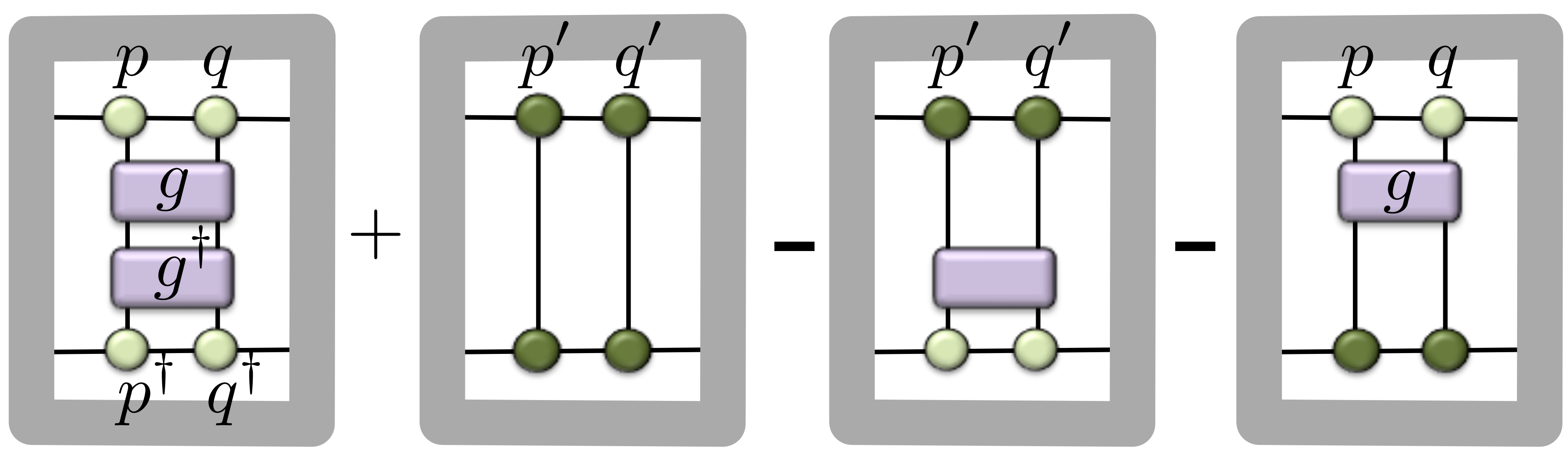


Environment of p and q tensors

$$|\tilde{\Psi}\rangle = g|\Psi(p,q)\rangle \approx |\Psi'(p',q')\rangle$$ find new p', and q' to minimize: $|| \, |\tilde{\Psi}\rangle - |\Psi'\rangle \, ||^2$

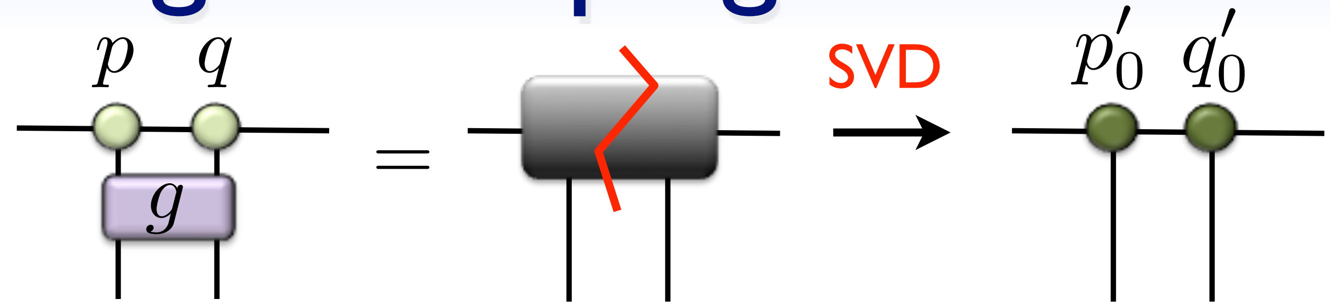
$$d(p',q') = \langle\tilde{\Psi}|\tilde{\Psi}\rangle + \langle\Psi'|\Psi'\rangle - \langle\tilde{\Psi}|\Psi'\rangle - \langle\Psi'|\tilde{\Psi}\rangle$$

"Cost-function"

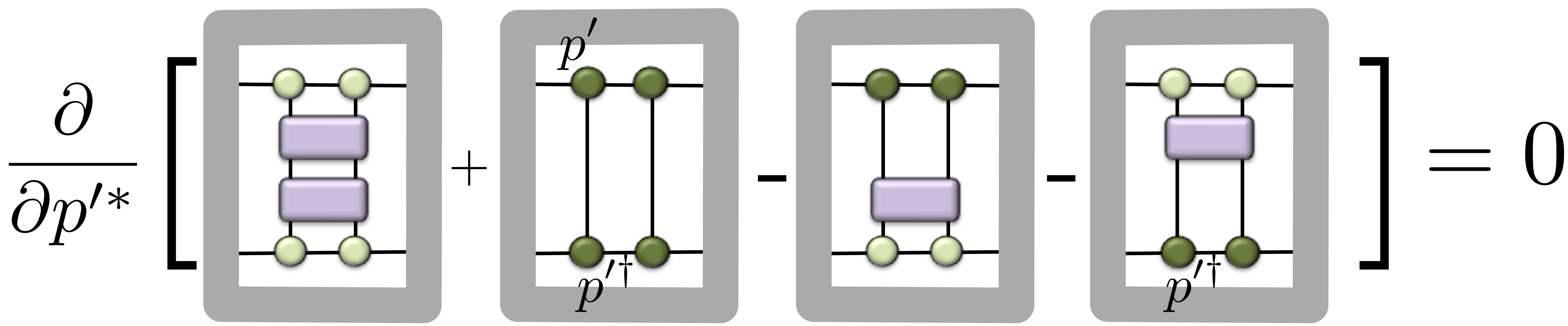


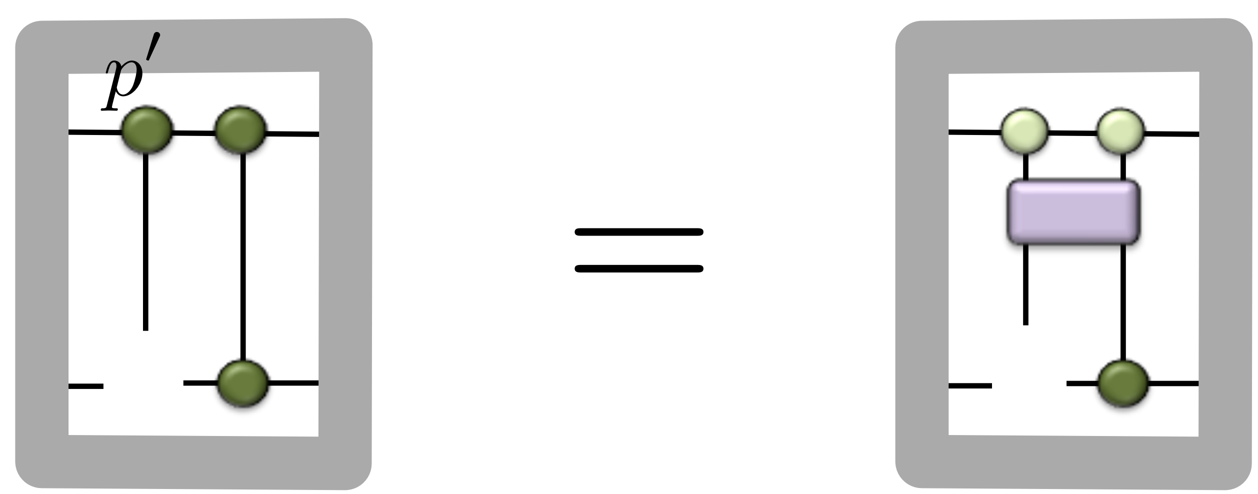
Finding p’ and q’ through sweeping

- Initial guess with SVD:



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

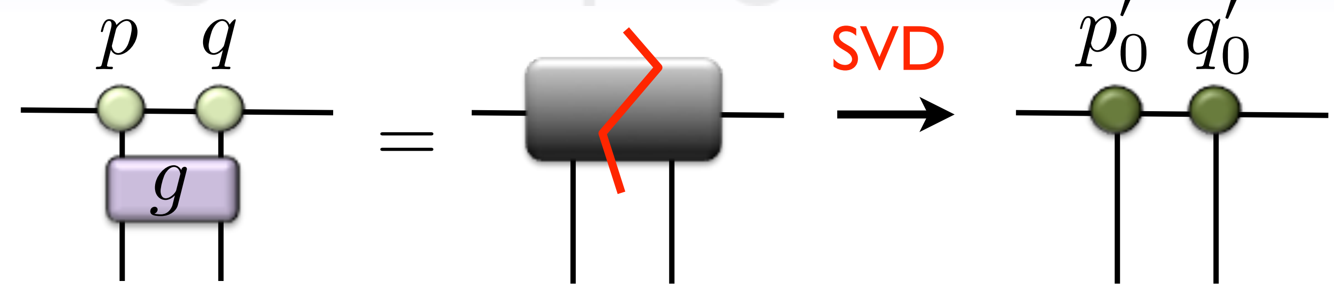




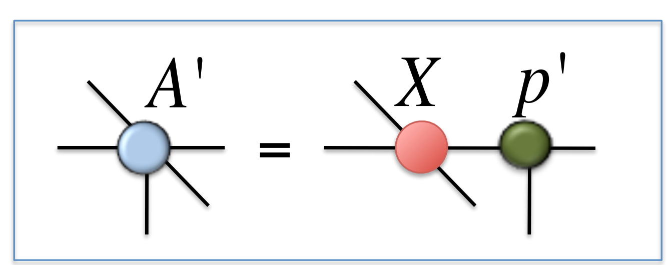
- Solve linear system: $\quad Mp' = b \quad \rightarrow$ **new p’**

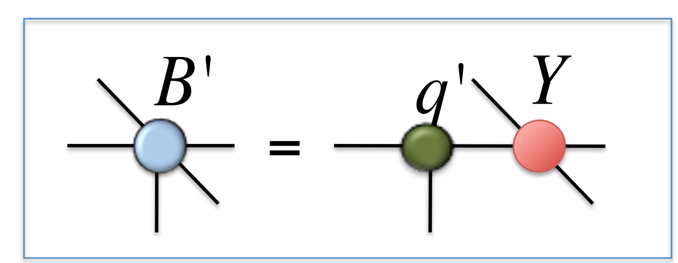
Finding p' and q' through sweeping

- Initial guess with SVD:



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





Optimization: full update

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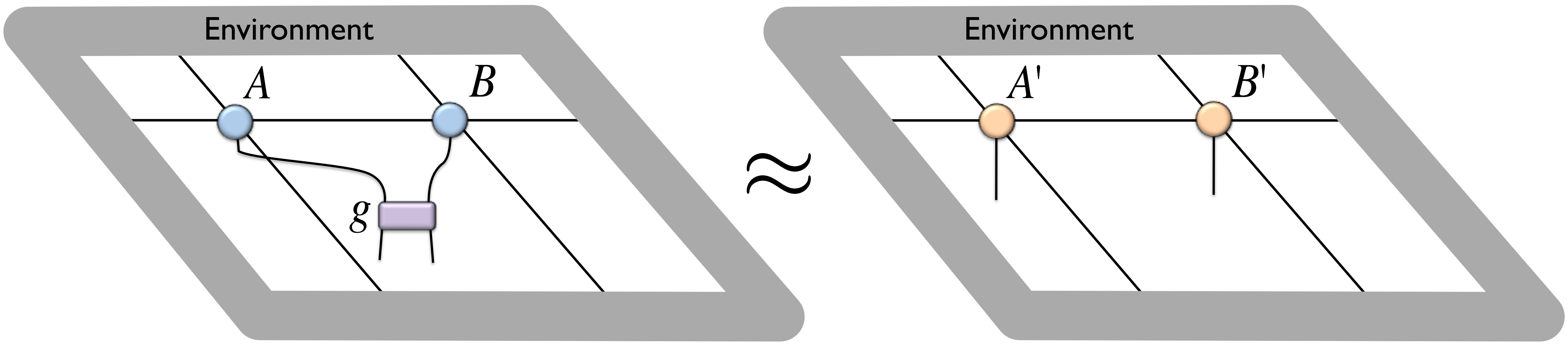

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- Iteratively / CG / Newton / ...
- The full wave function is taken into account for the truncation!
- At each step the environment has to be computed! expensive... but optimal!

Optimization: simple vs full update

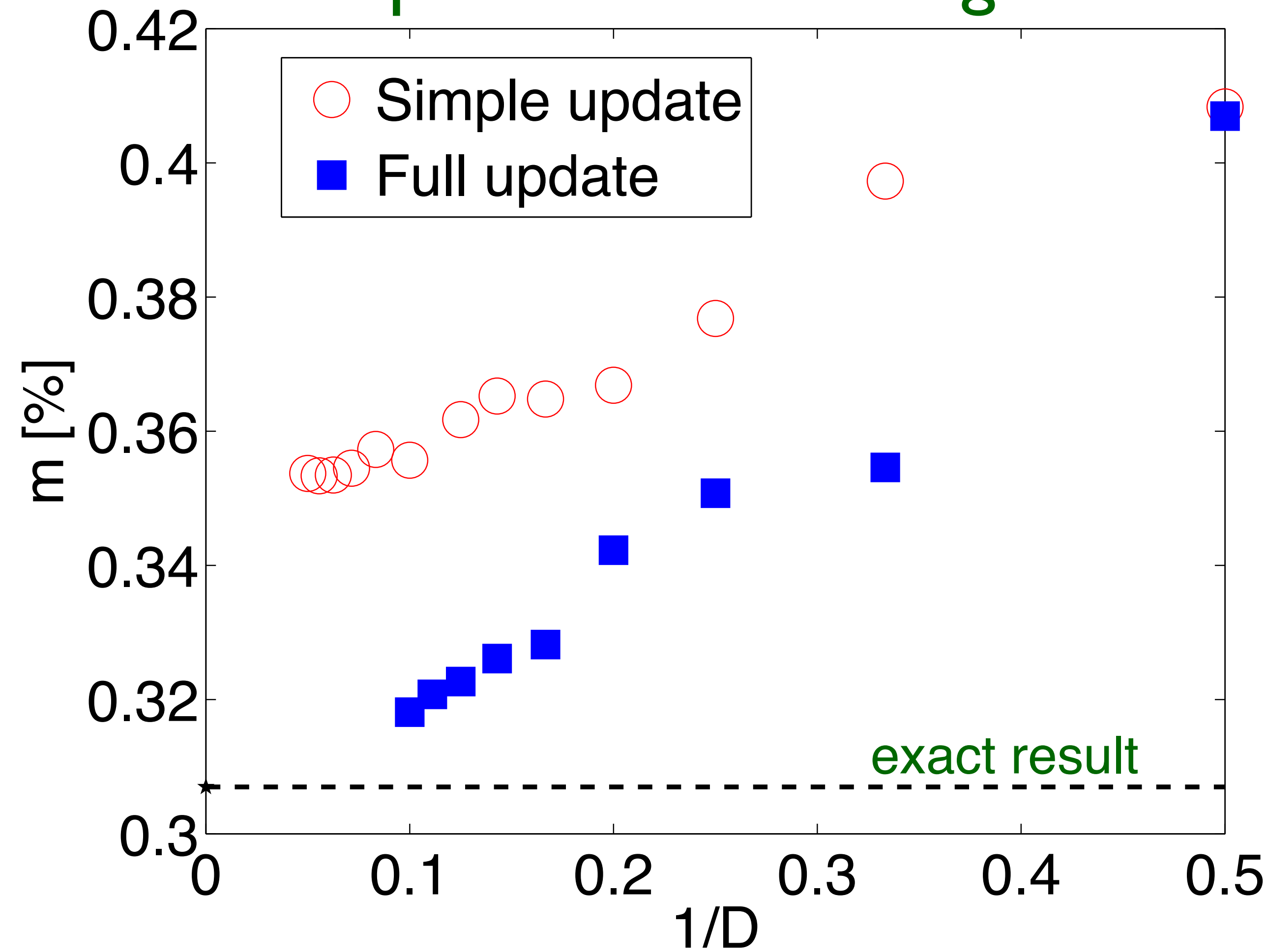
simple update

- ★ "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

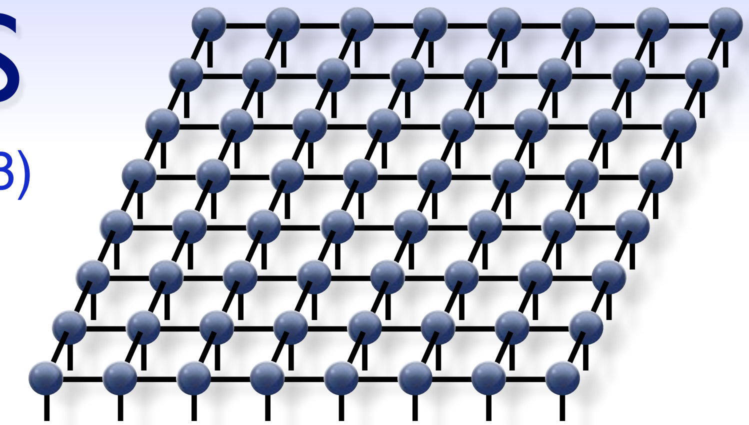


- Combine the two: Use simple update to get an initial state for the full update

- 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

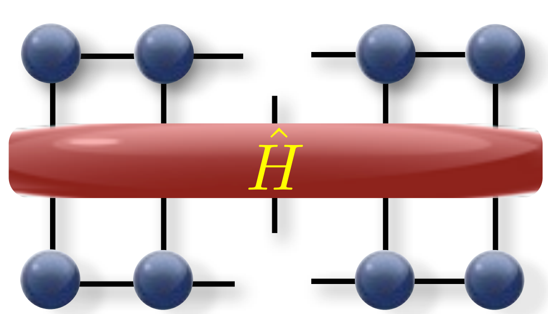
tensor A reshaped as a vector

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

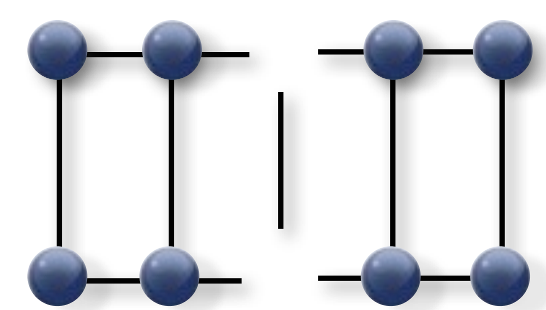
solve generalized eigenvalue problem

$\mathbf{H} =$

in 1D:

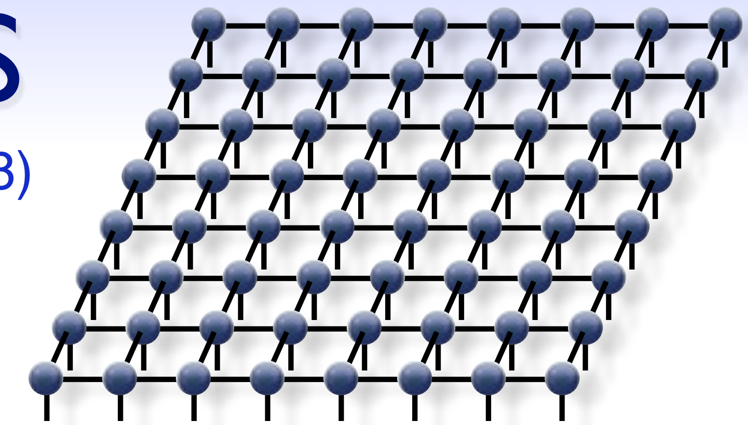


$\mathbf{N} =$



Variational optimization for PEPS

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



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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

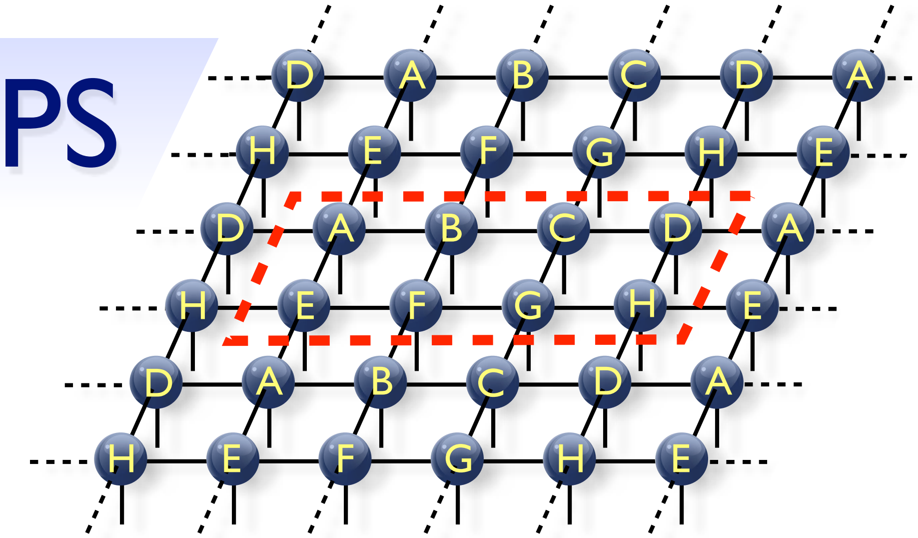
$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \xrightarrow{\text{minimize}} \mathbf{H}\, x = E\, \mathbf{N}\, x$$

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)]

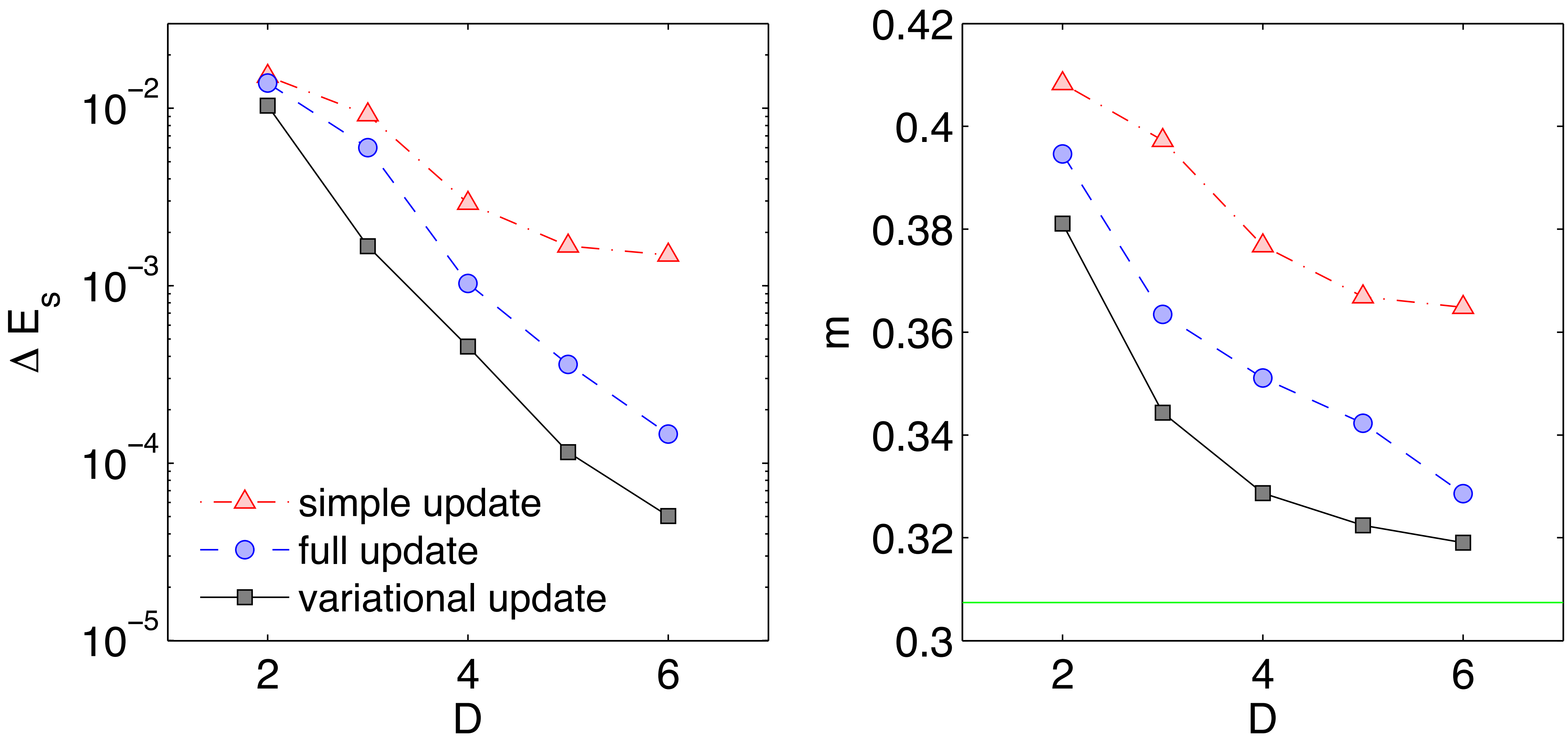
tensor network including all Hamiltonian terms

tensor network from norm term

tensor A reshaped as a vector

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

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]

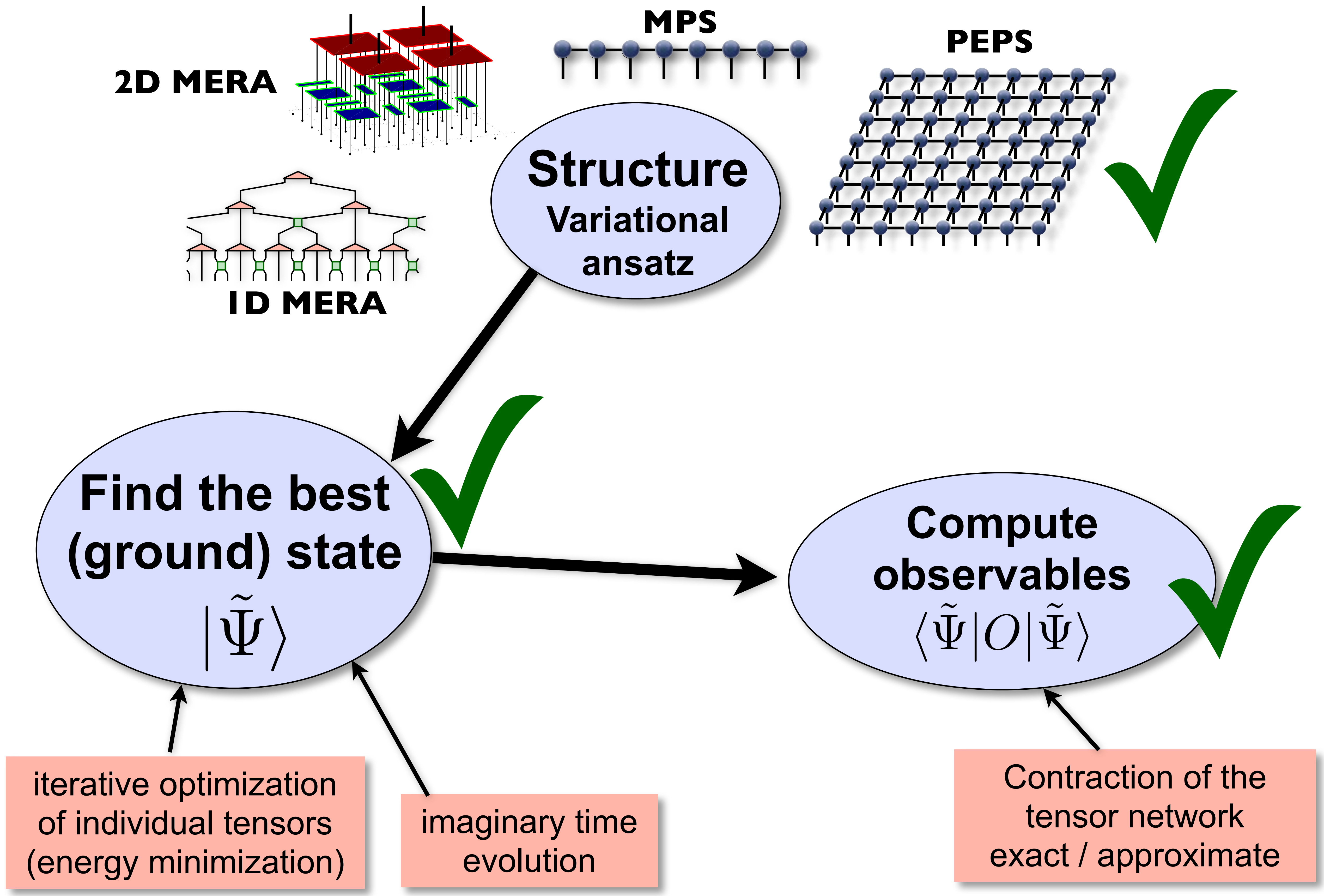
Summary: optimization in iPEPS

- 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: Example application

Overview: iPEPS simulations

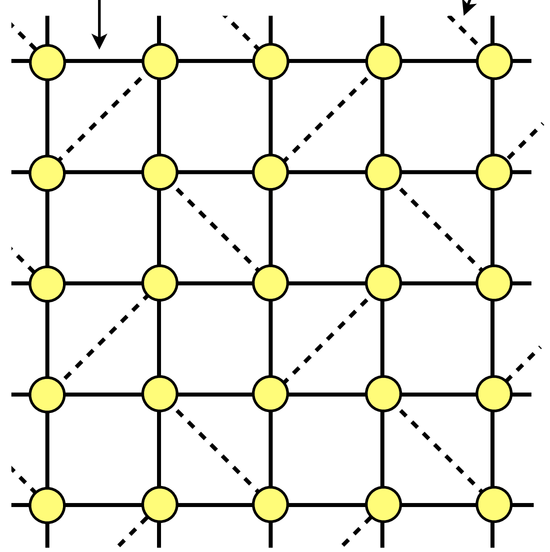
- interacting spinless fermions
  - honeycomb & square lattice
- t-J model & Hubbard model
  - square lattice
- SU(N) Heisenberg models
  - N=3 square, triangular, kagome & honeycomb lattice
  - N=4 square, honeycomb & checkerboard lattice
  - N=5 square lattice
  - N=6 honeycomb lattice
- frustrated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

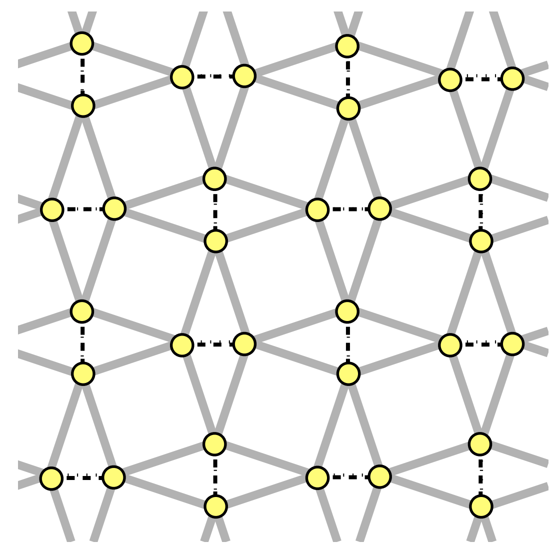
iPEPS is a very **competitive** variational method!

Find new physics thanks to (largely) unbiased simulations

The Shastry-Sutherland model

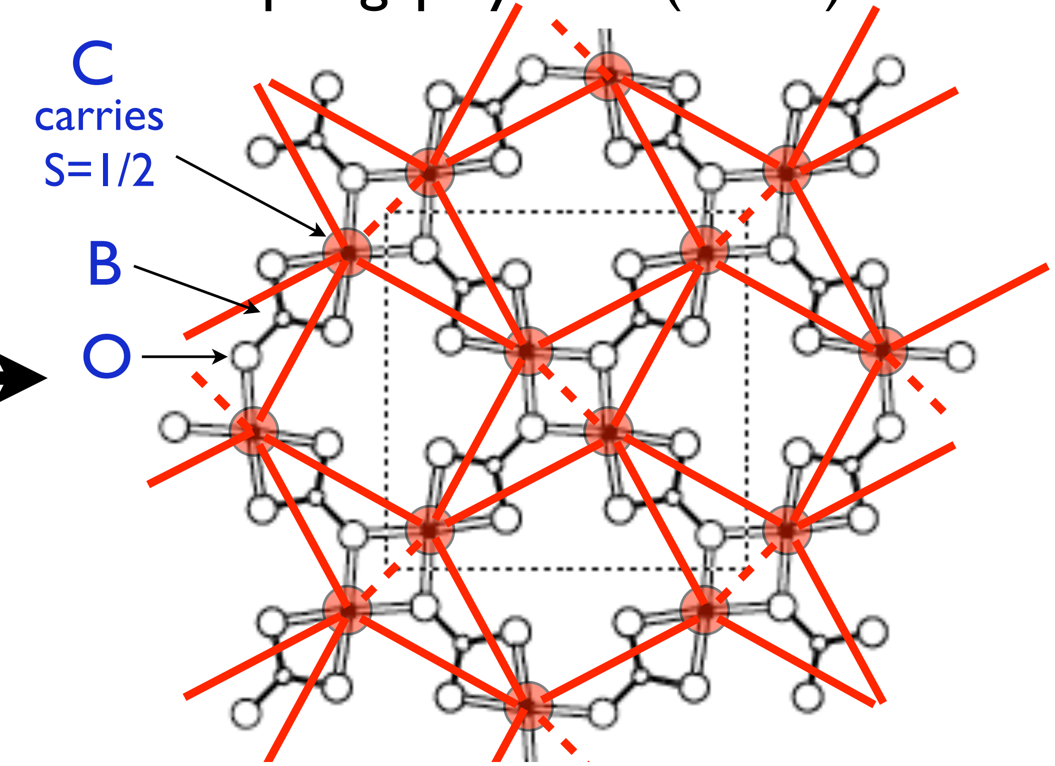
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j$$





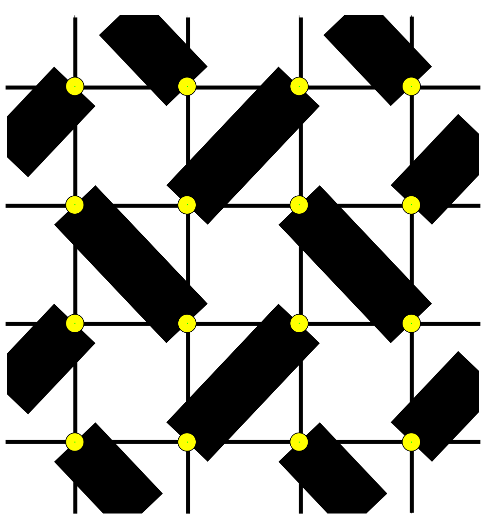
$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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

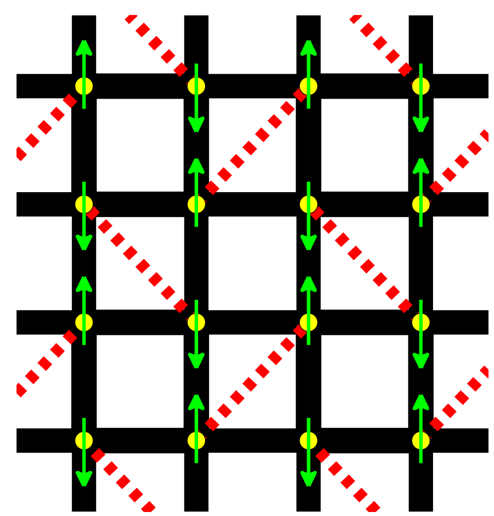
Dimer phase

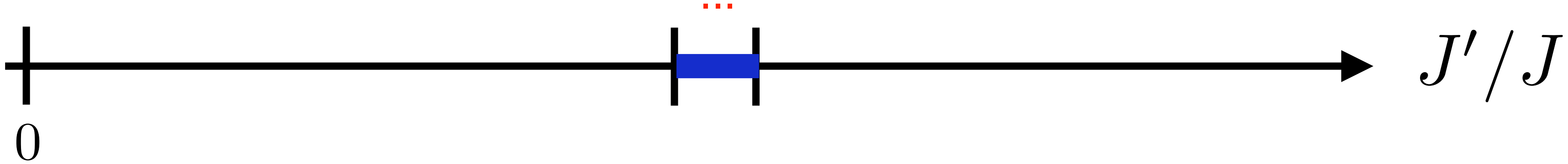


?

helical?
columnar-dimer?
plaquette?
spin-liquid?
...

Néel phase



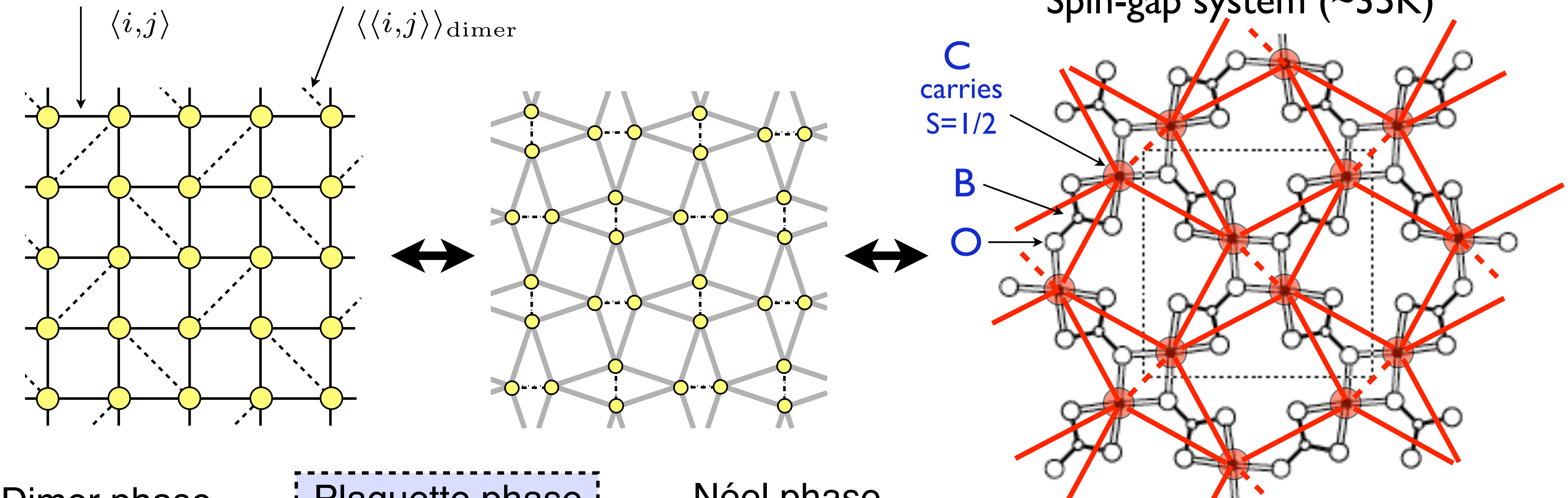


The Shastry-Sutherland model

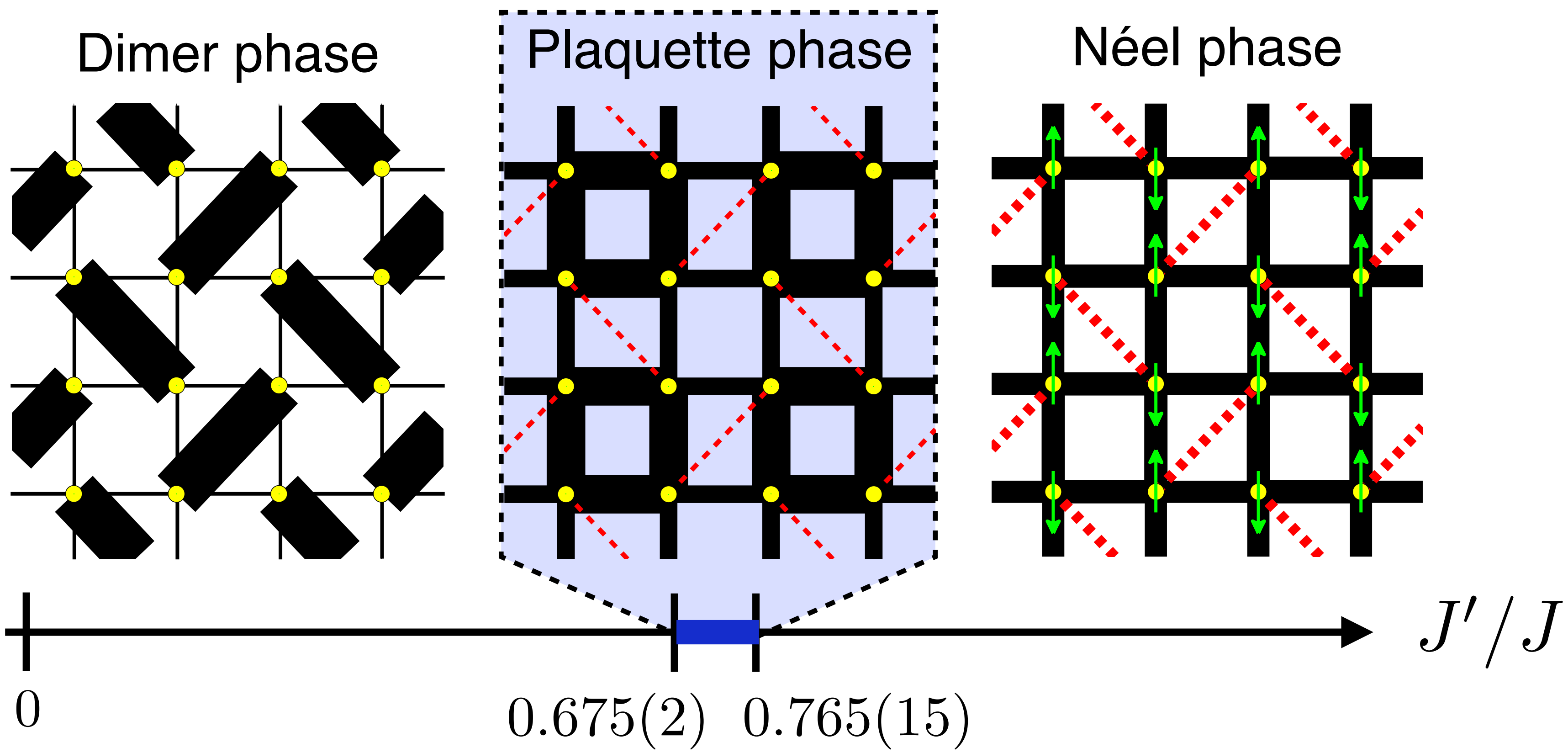
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j$$

$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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



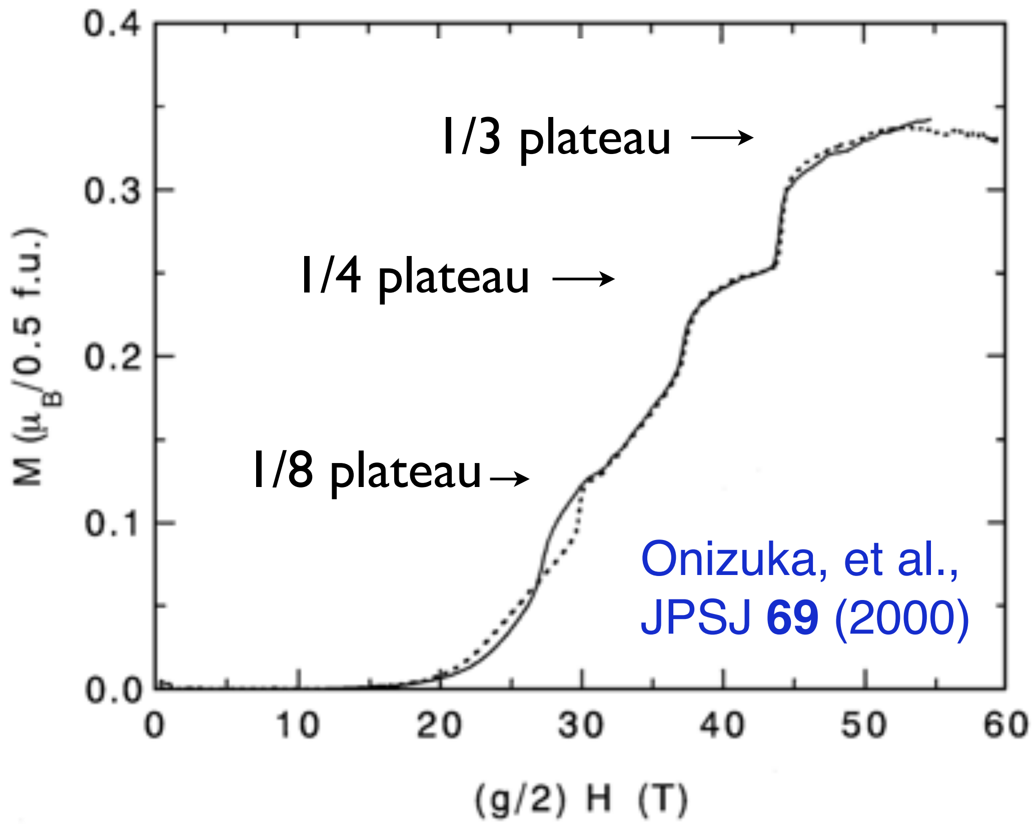
Corboz and Mila, PRB **87** (2013)

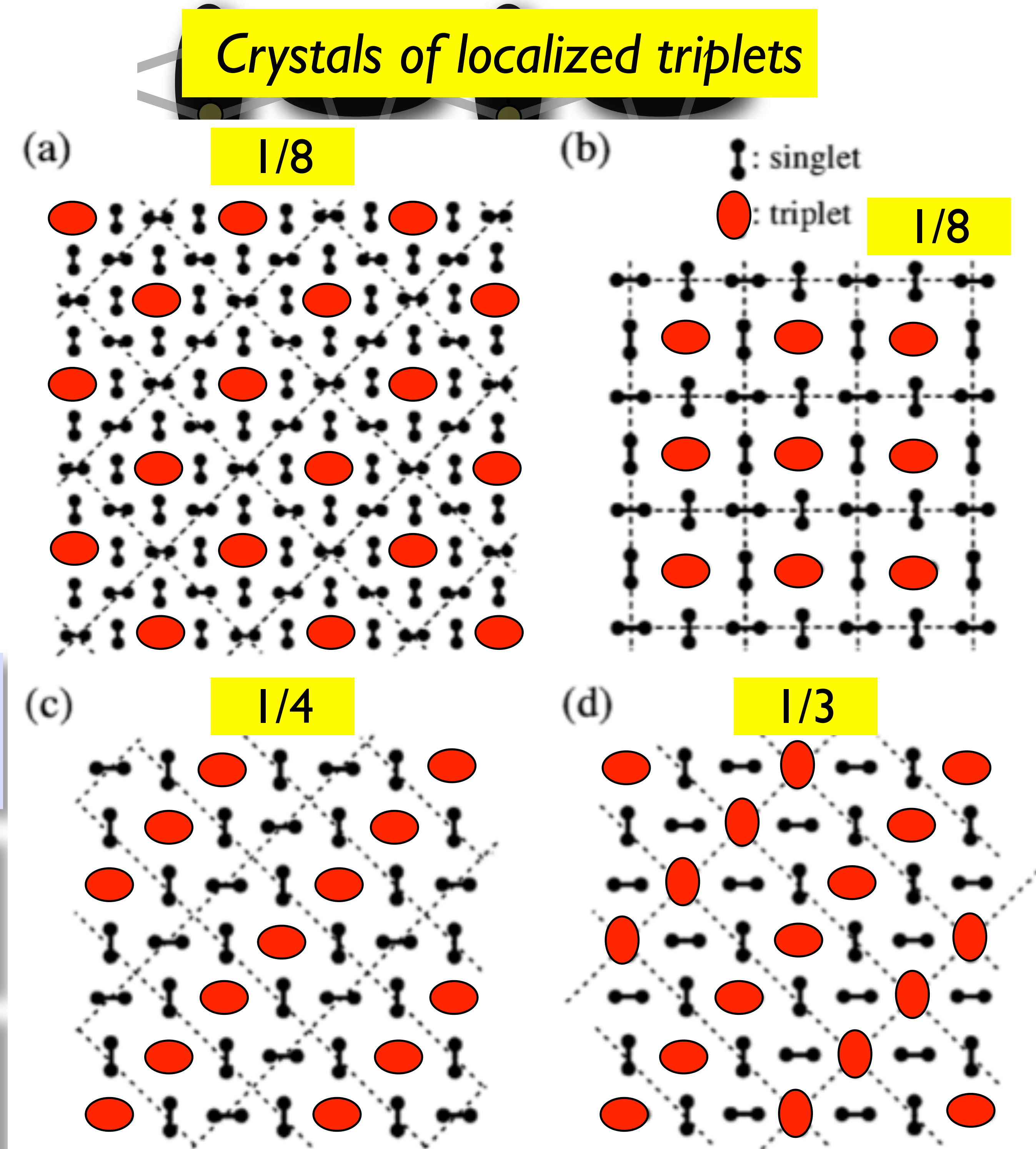
previously found in:

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





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

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

- 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

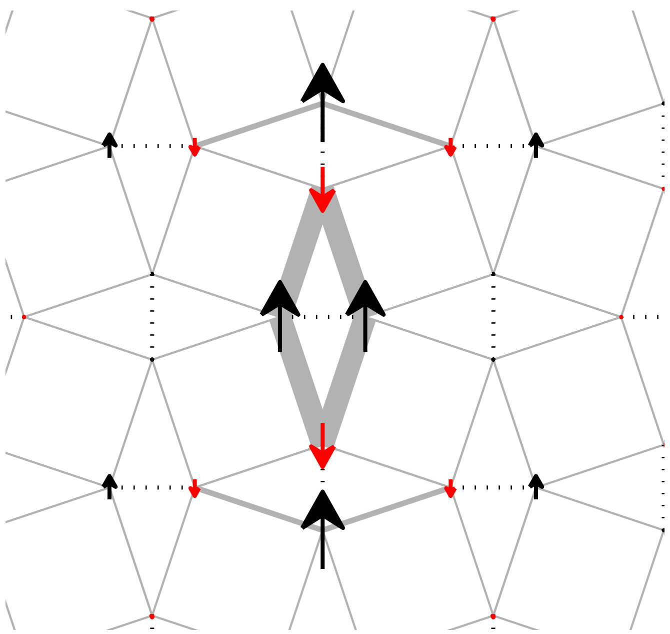
BUT!

SURPRISE!

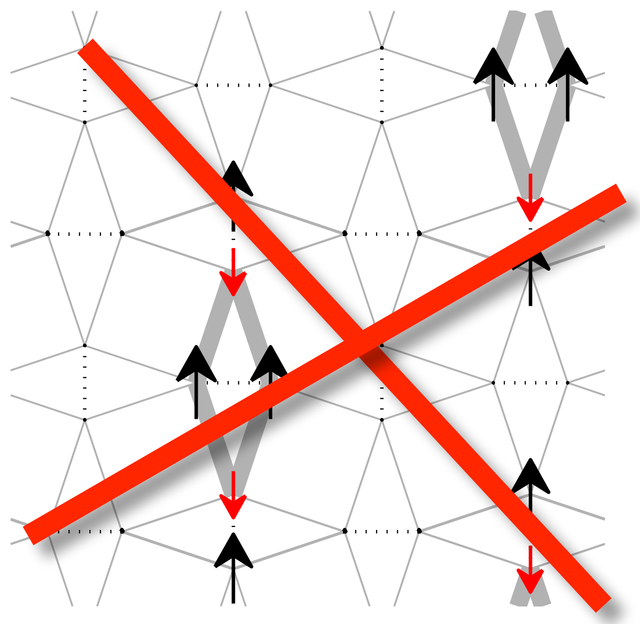
iPEPS simulations of the SSM in a magnetic field

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

- The assumption that plateaus correspond to crystals of triplets is wrong!
  (for the plateaus below 1/4)

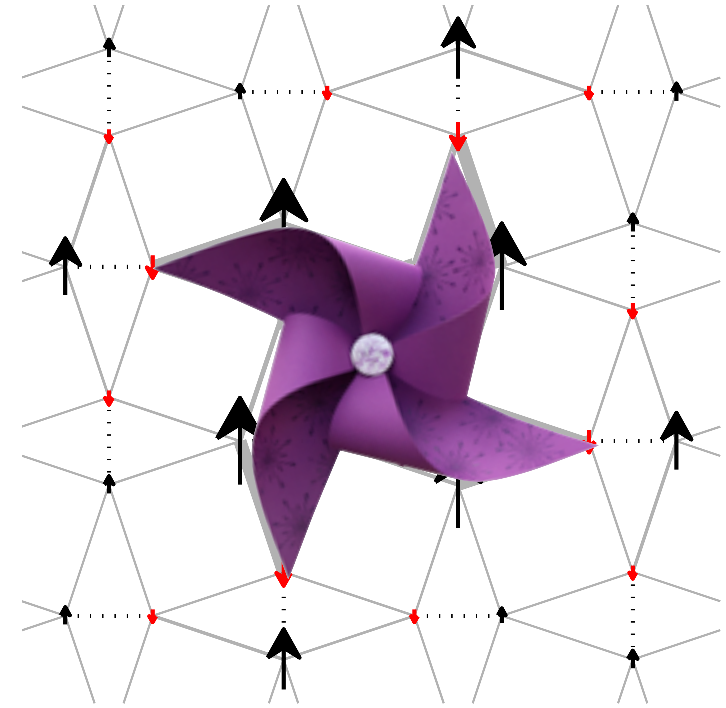


spin structure of 1 localized triplet in a 4x4 cell



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

small D (mean-field result)



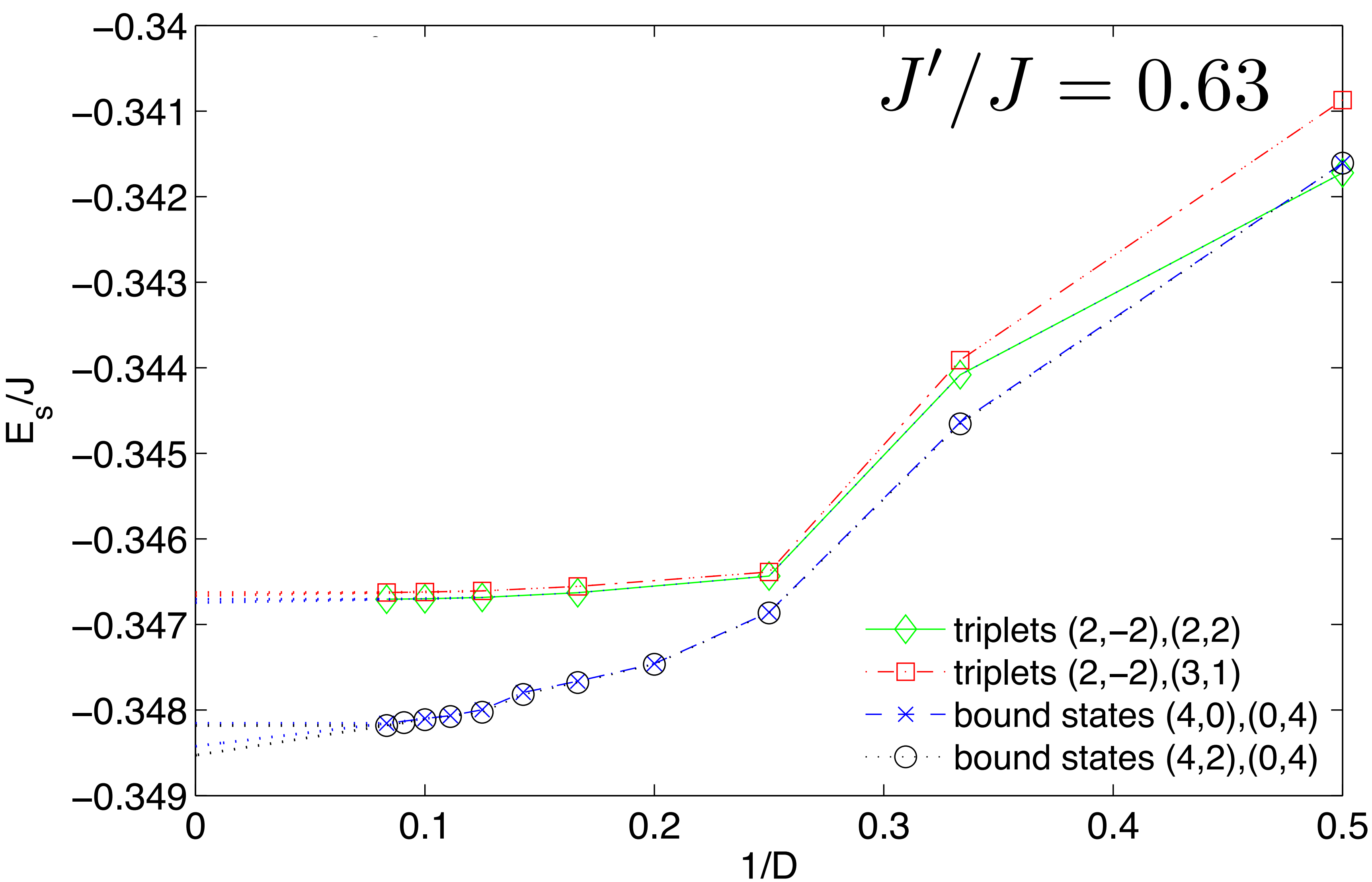
spin structure of a Sz=2 excitation in a 4x4 cell

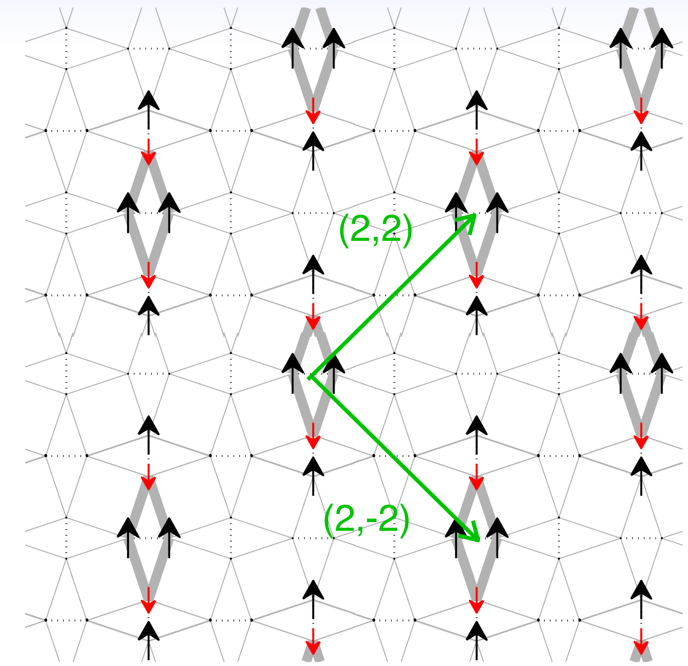
obtained with iPEPS for D>4

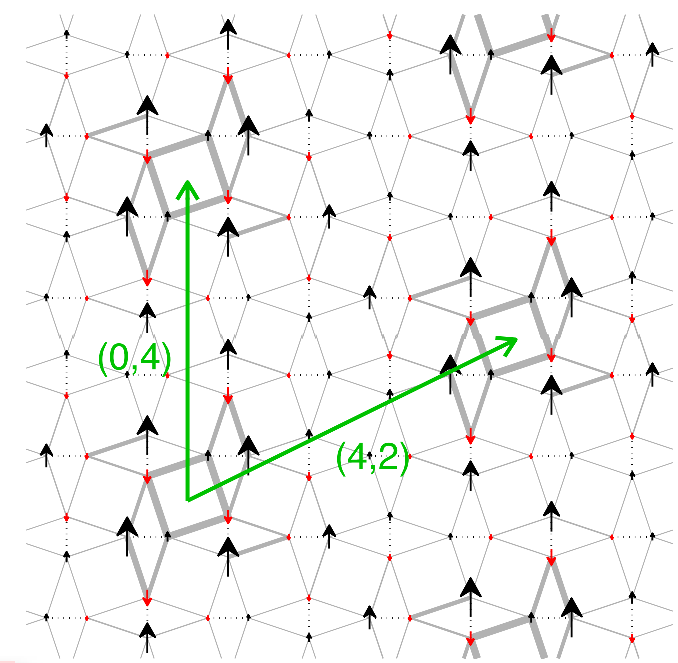
Bound state of two triplets!

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

Example: 1/8 plateau

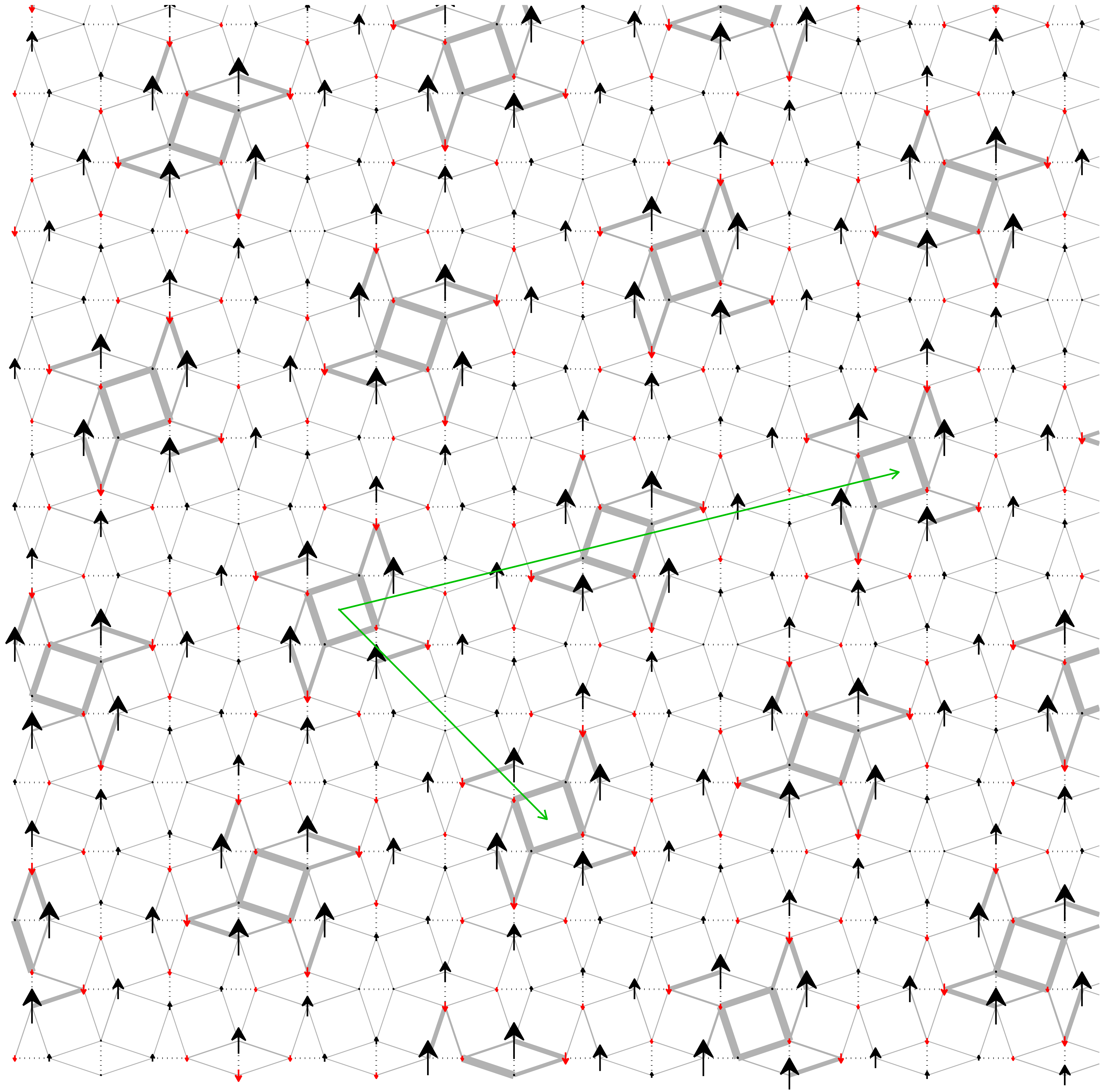






- All the proposed triplet crystals have a higher energy than the crystals made of bound states!
- Similar results found for other plateaus below 1/4

2/15 plateau

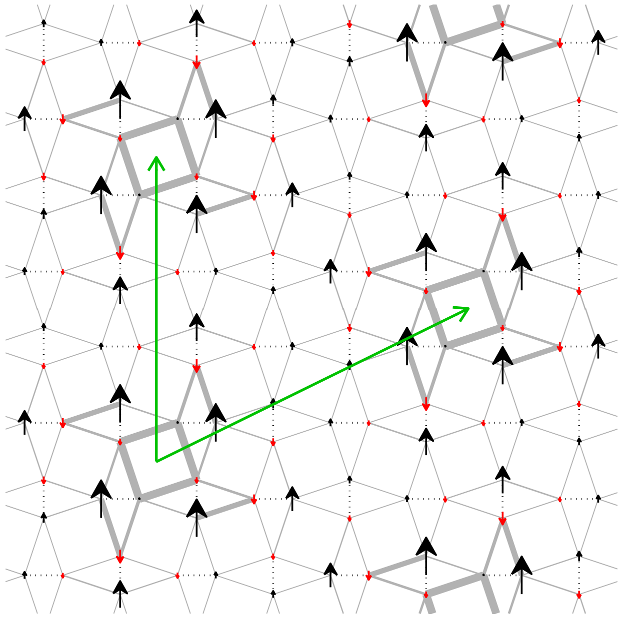


Unit cell with 30 tensors (60 sites)

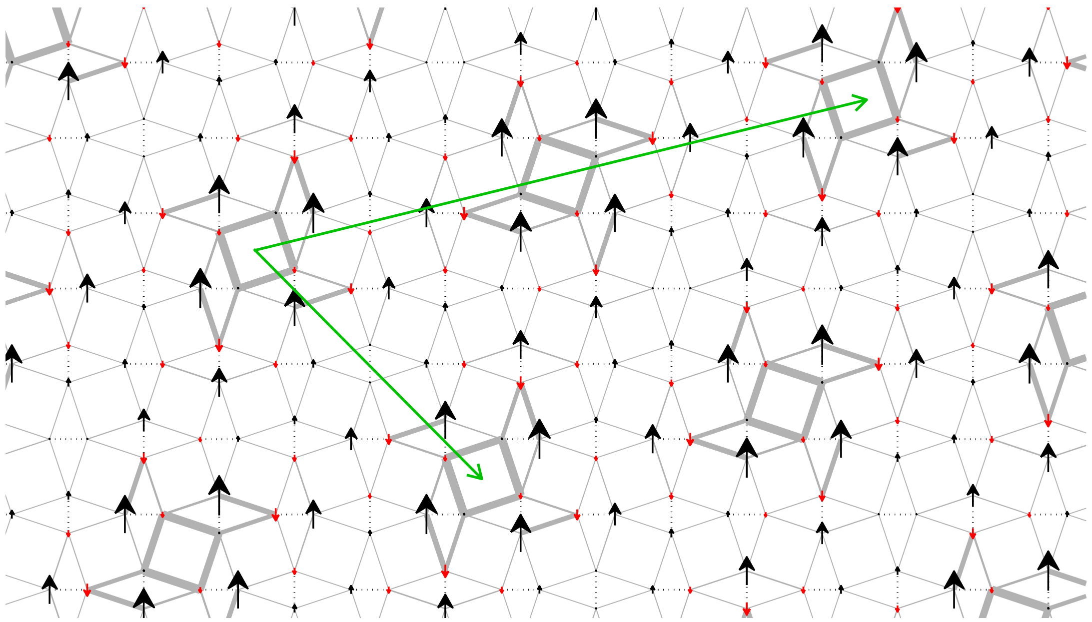
Regular pattern of bound states!

Computing the energies of all possible crystals

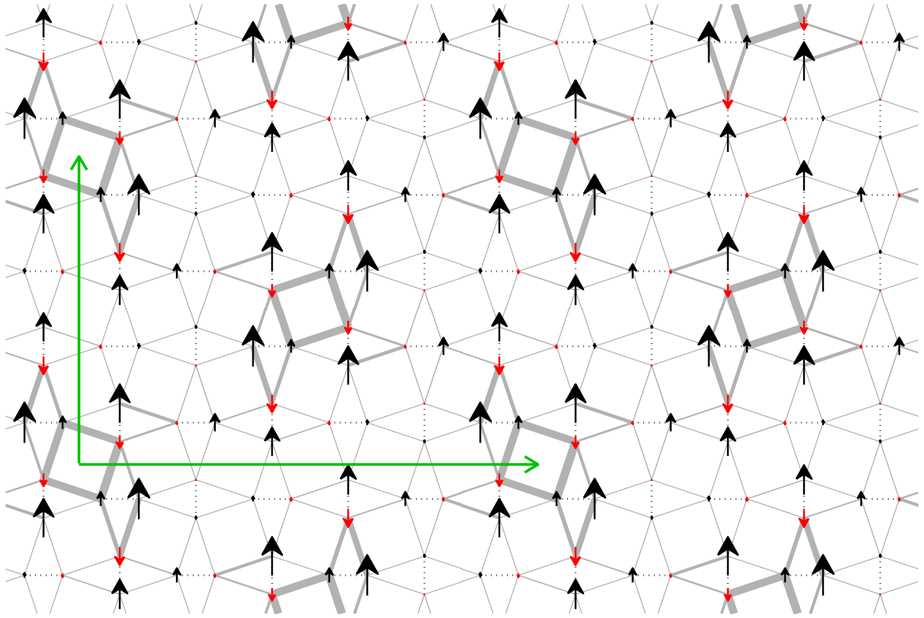
1/8 rhomboid : (4,2),(0,4)



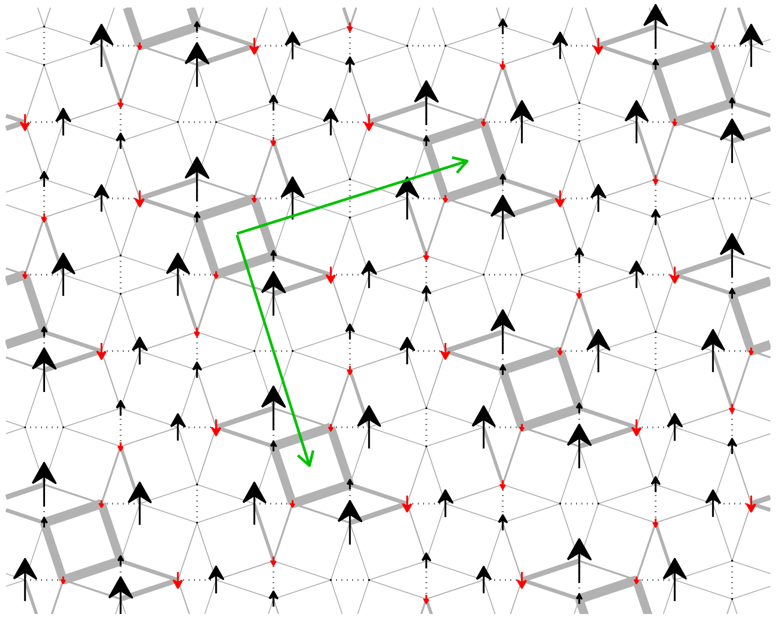
2/15 : (3,-3),(8,2)



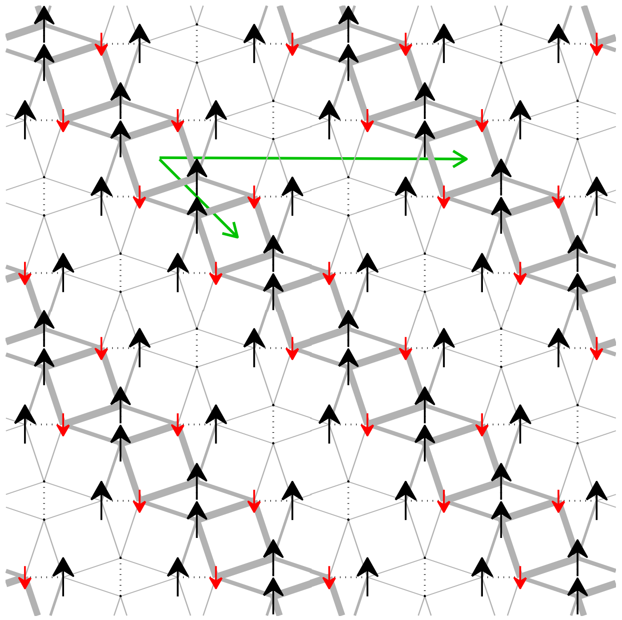
1/6 rectangular : (6,0),(0,4)



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

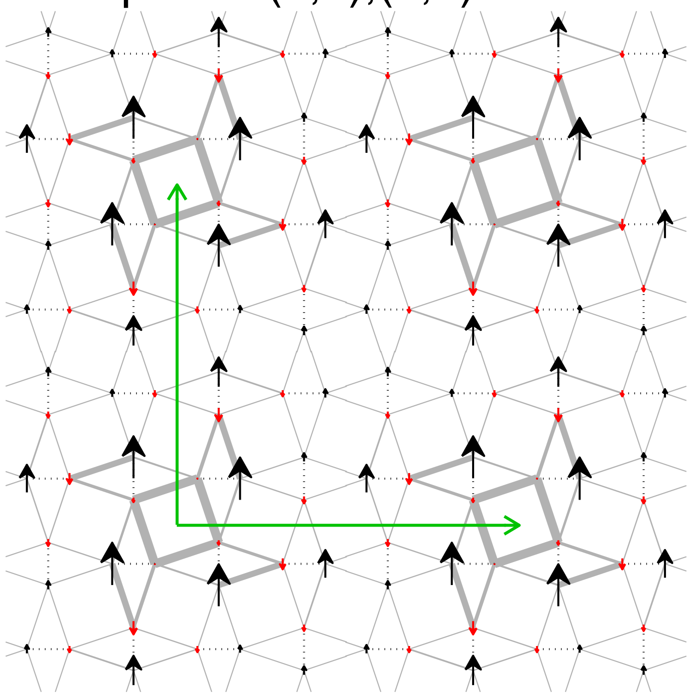


1/4 : (1,-1),(4,0)

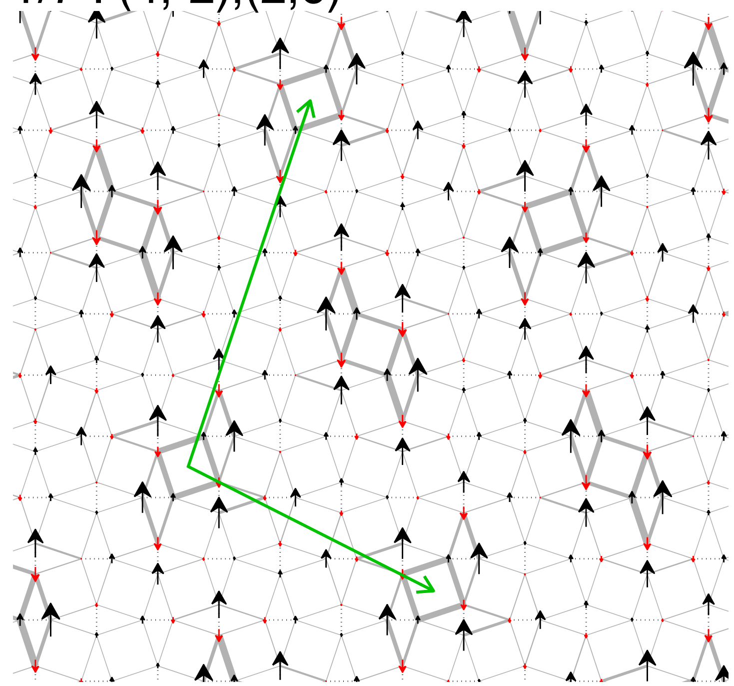


Computing the energies of all possible crystals

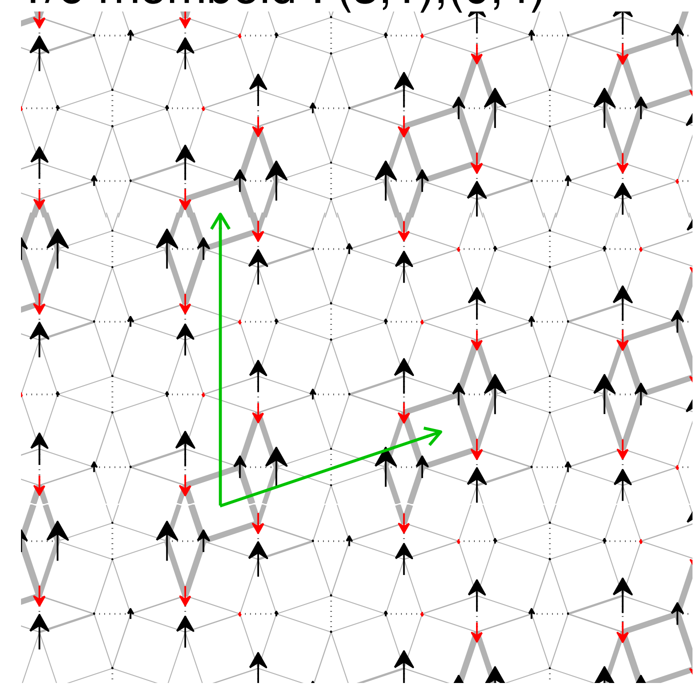
1/8 square : (4,0),(0,4)



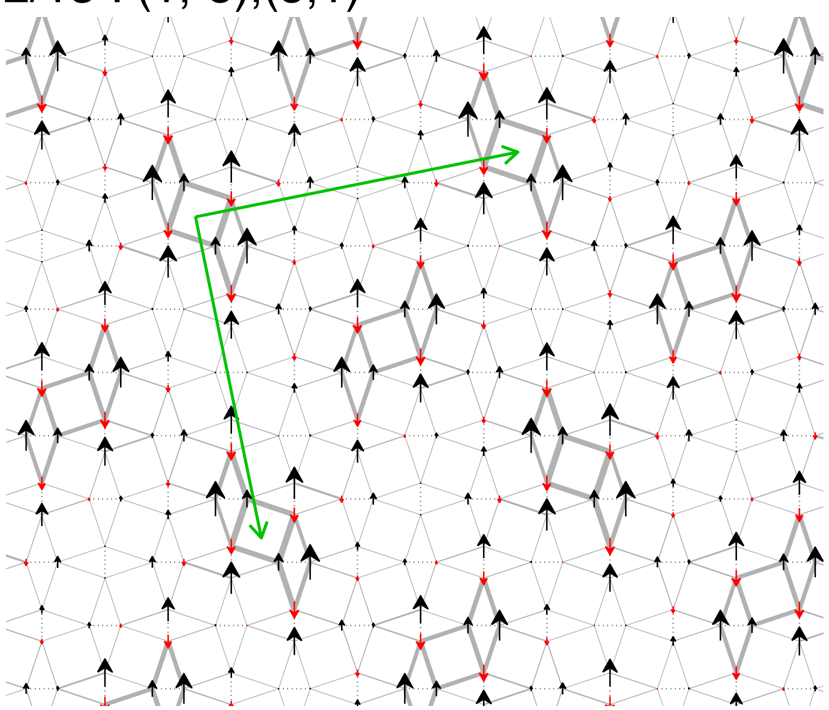
1/7 : (4,-2),(2,6)



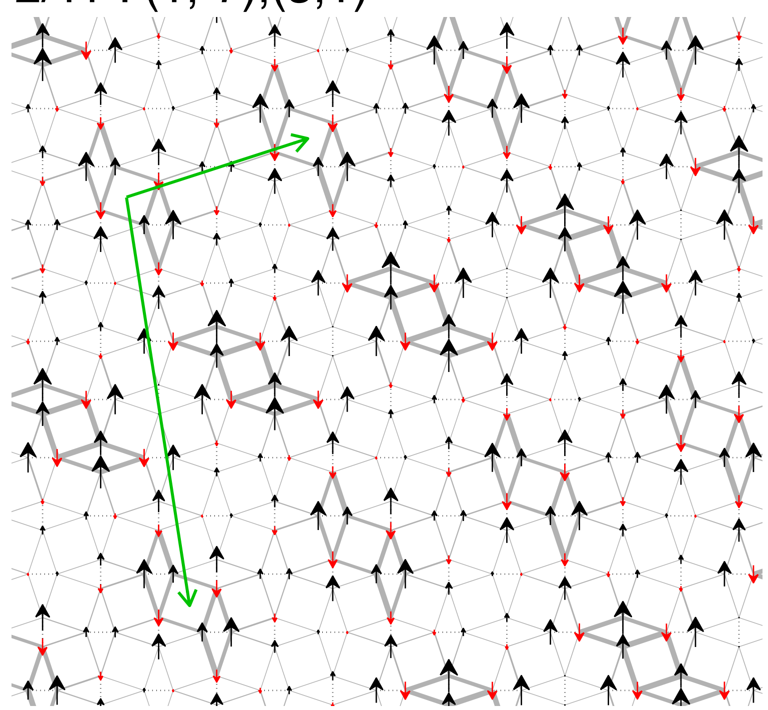
1/6 rhomboid : (3,1),(0,4)



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

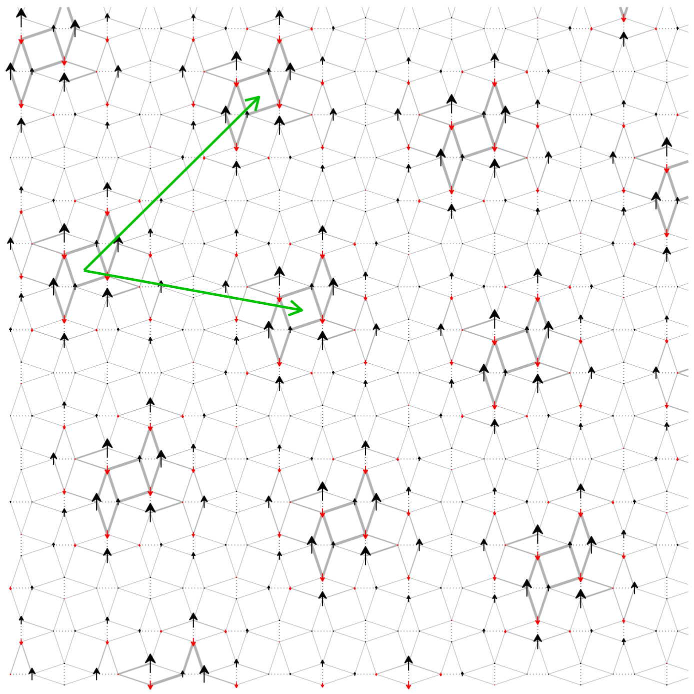


2/11 : (1,-7),(3,1)

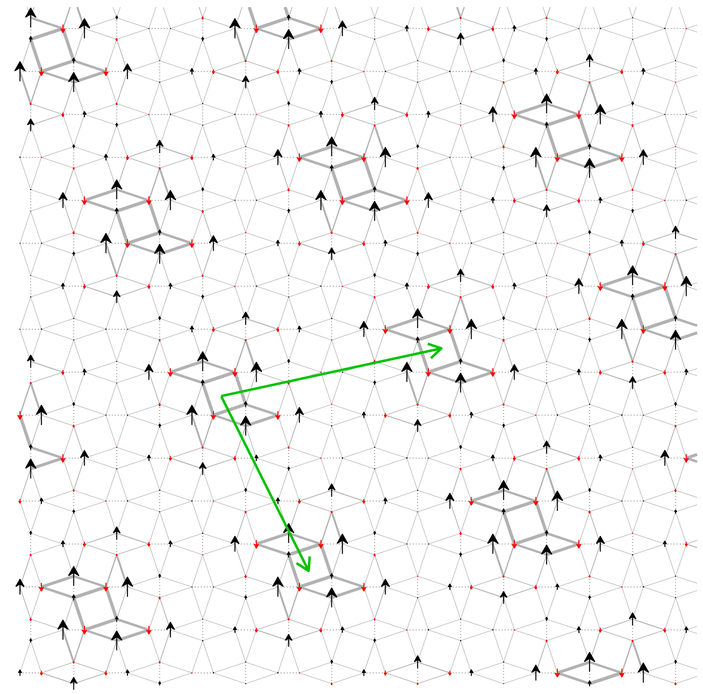


Computing the energies of all possible crystals

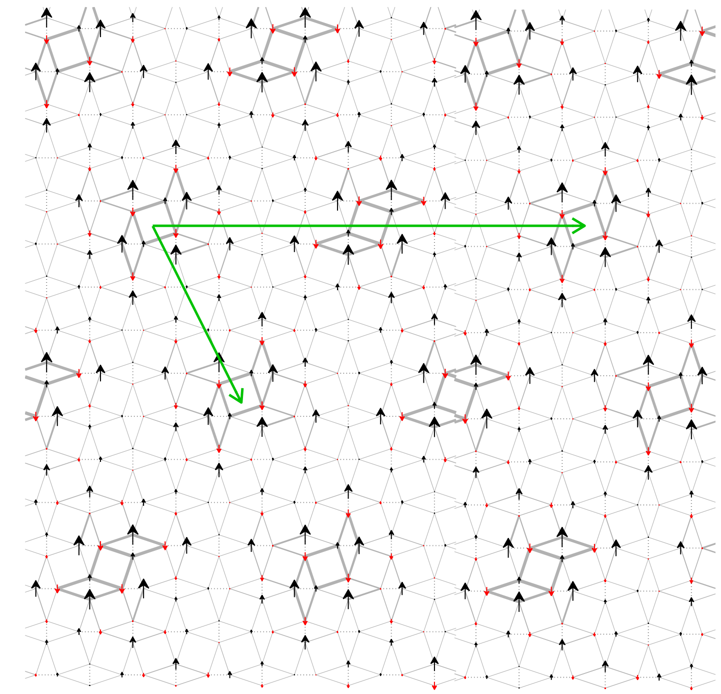
1/12 : (1,-5),(5,-1)



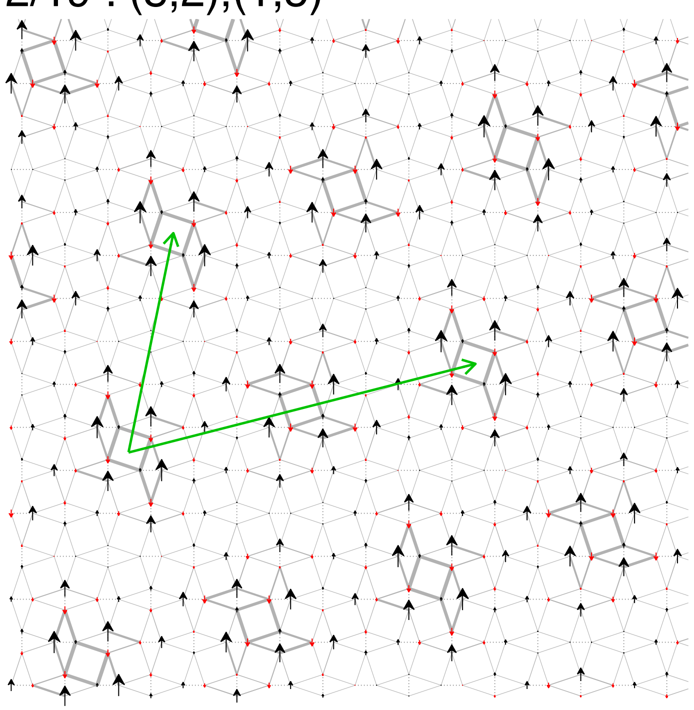
1/11 : (2,-4),(5,1)



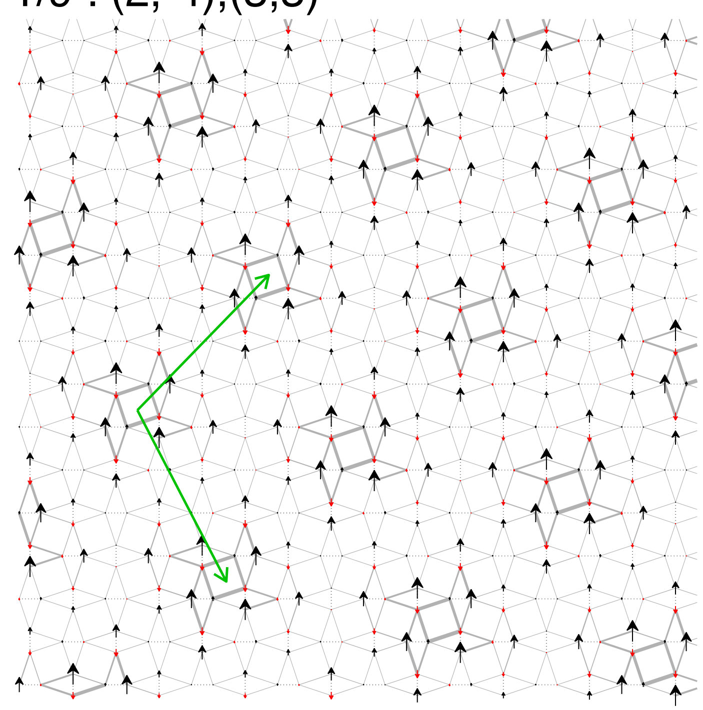
1/10 : (2,-4),(10,0)



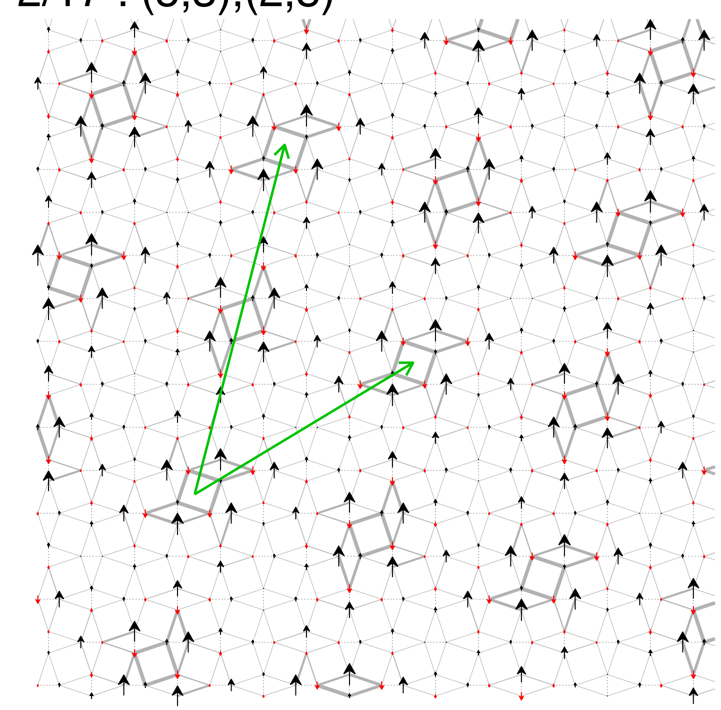
2/19 : (8,2),(1,5)



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

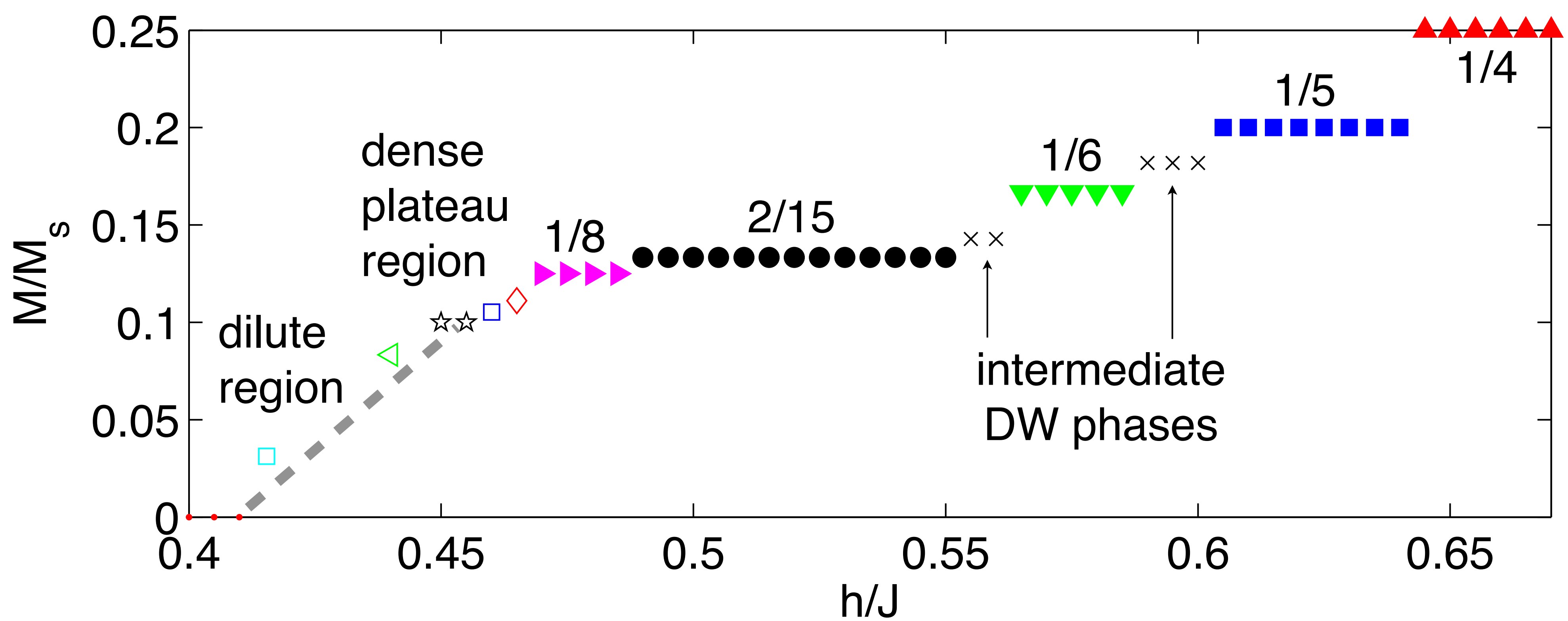


2/17 : (5,3),(2,8)



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]

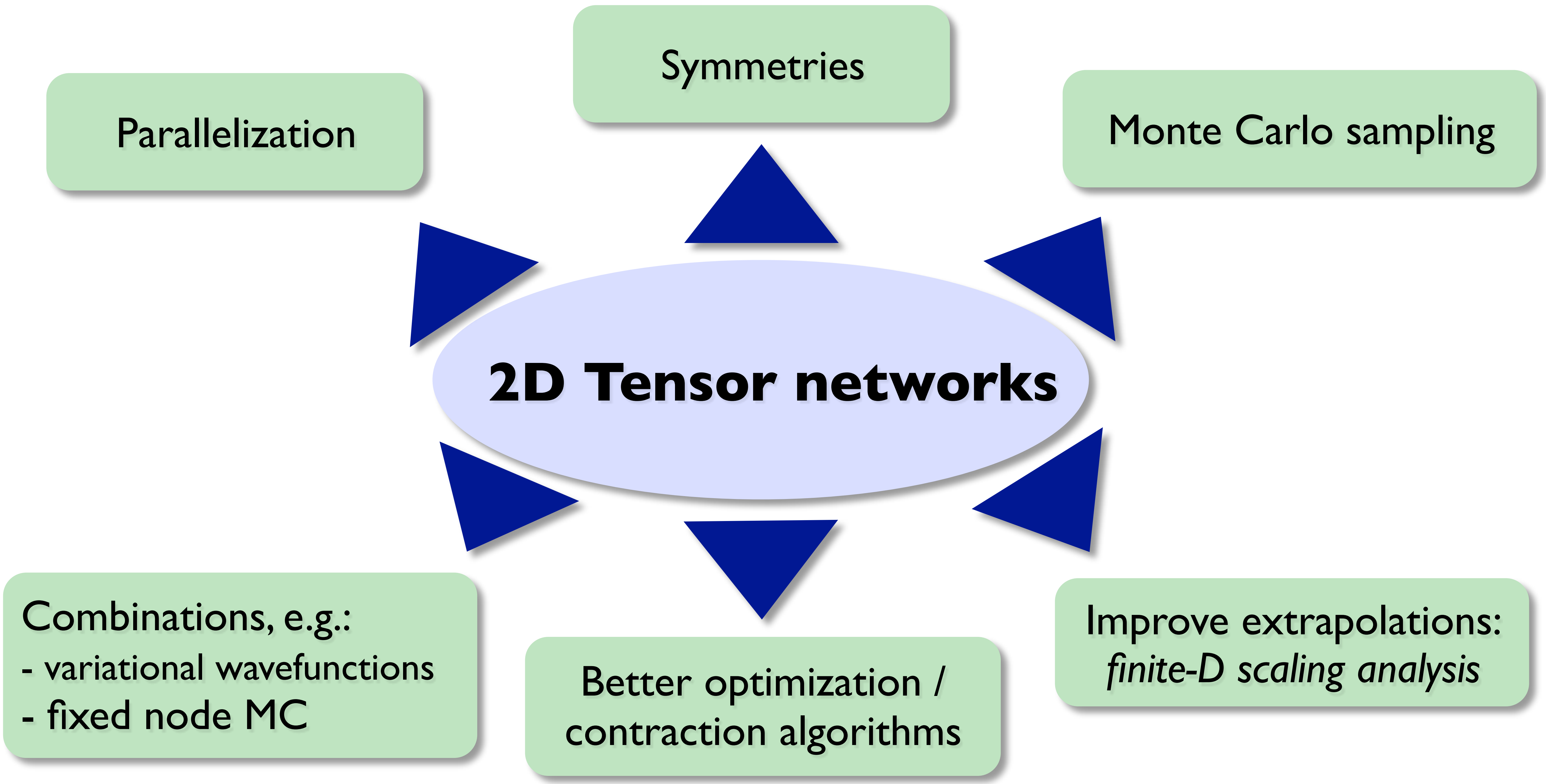
★ **Sequence in agreement with experiments**

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

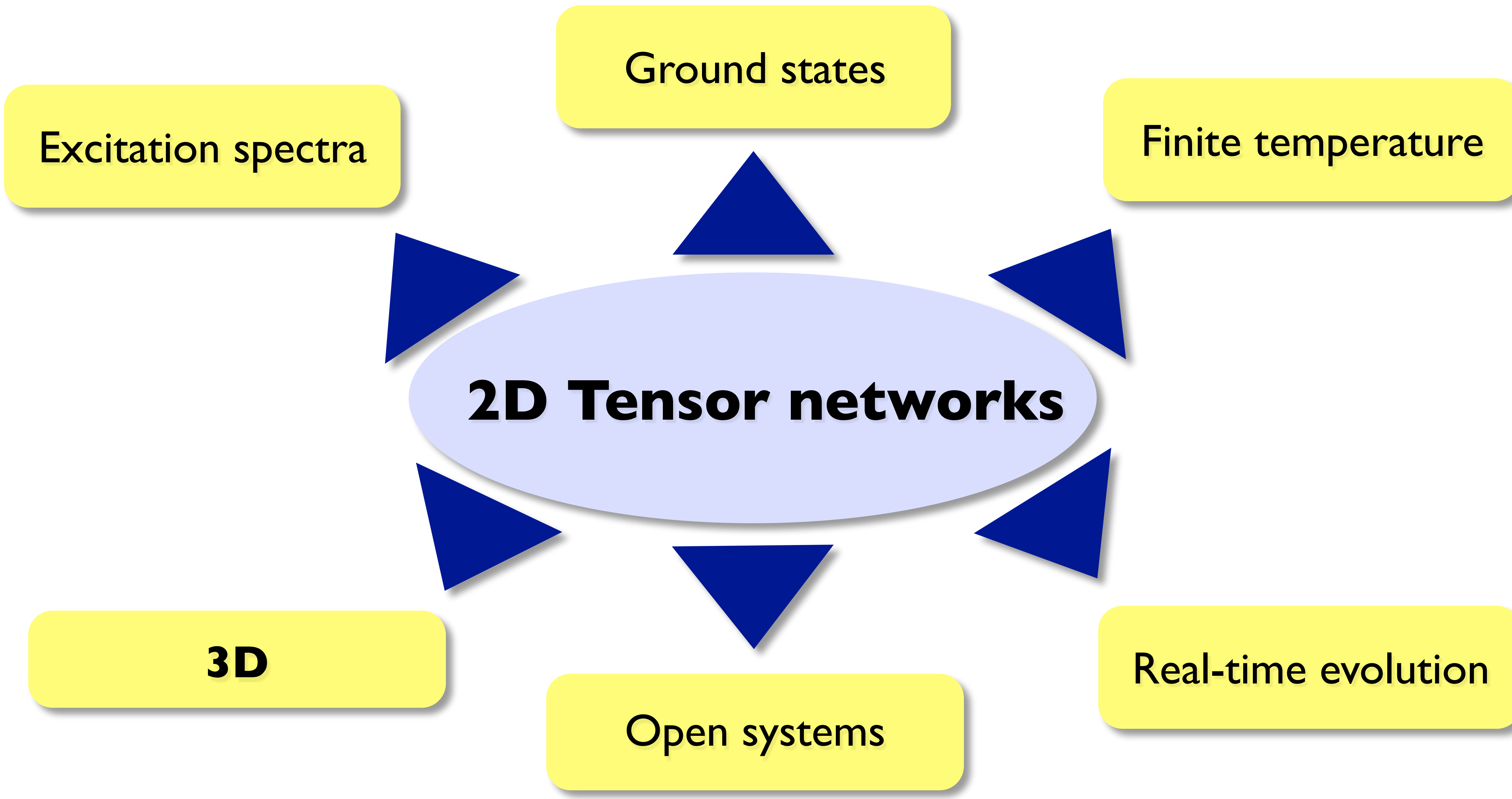
- see also related work: SSM in high fields: Matsuda et al. PRL **111** (2013)

Outlook & summary

Improvements of 2D TN methods



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 & competitive tool to study challenging problems:
- ★ Novel phases in SU(N) Heisenberg models
- ★ Competing phases in the *t-J* & Hubbard model
- ★ Frustrated spin systems (e.g. Shastry-Sutherland mode), and more ...

✓ Big room for improvement. Many possible extensions.

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

Thank you for your attention!