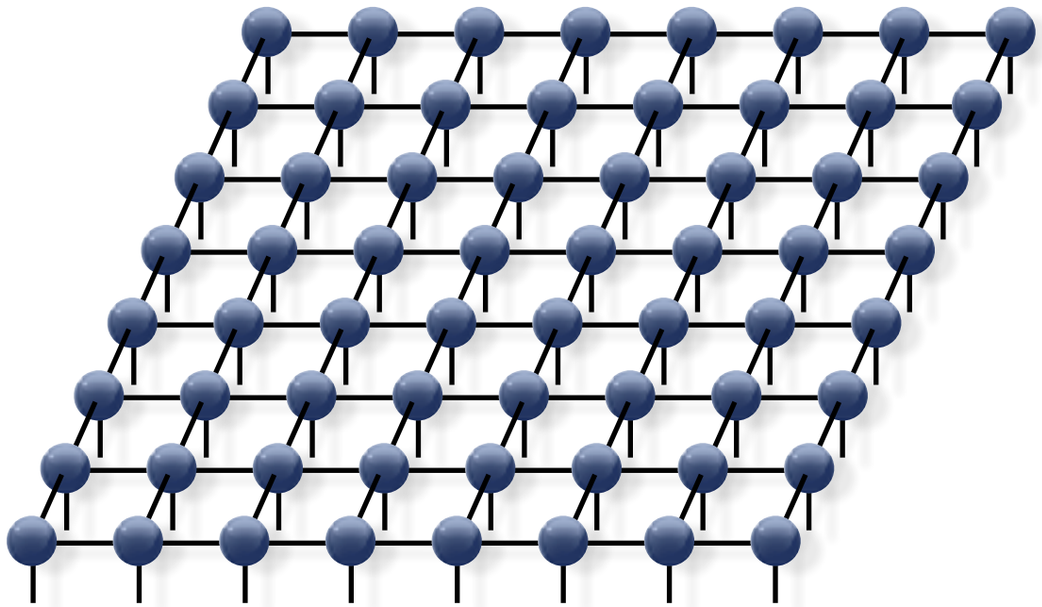
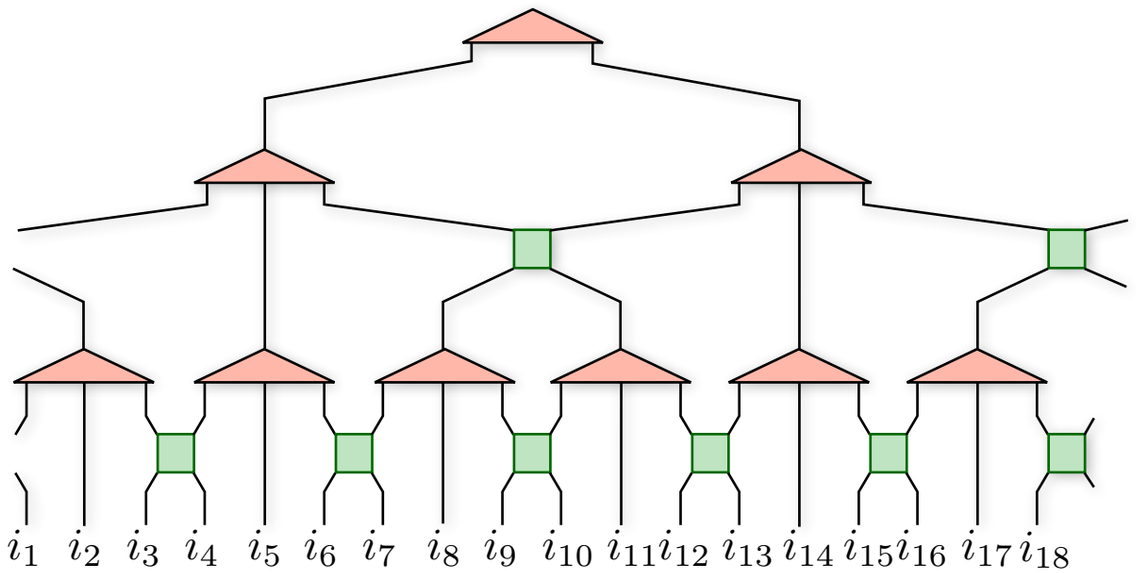
Introduction to (i)PEPS & MERA

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam





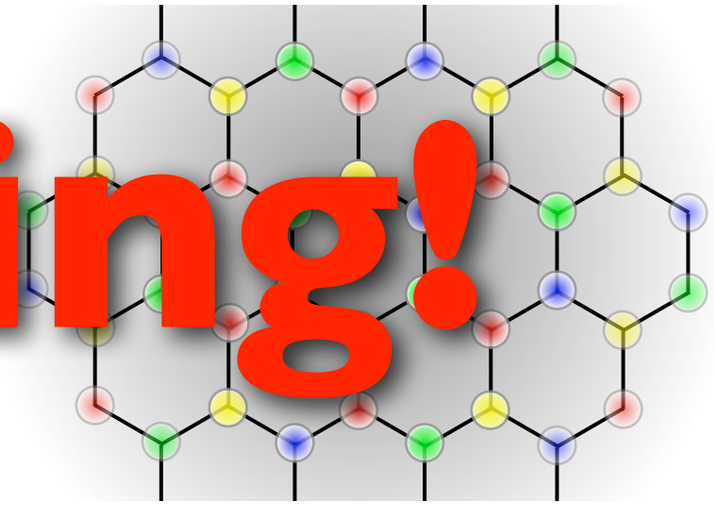
Tensor Network based approaches to Quantum Many-Body Systems
ICCUB School 2021

Motivation: Strongly correlated quantum many-body systems

High-Tc superconductivity

Quantum magnetism / spin liquids

Novel phases with ultra-cold atoms



Challenging!

Typically:

- No exact analytical solution
- Mean-field / perturbation theory fails
- Exact diagonalization: O(exp(N))

Accurate and efficient numerical simulations are essential!

Quantum Monte Carlo

- Main idea: **Statistical sampling** of the exponentially large configuration space
- Computational cost is polynomial in N and not exponential

Very powerful for many spin and bosonic systems

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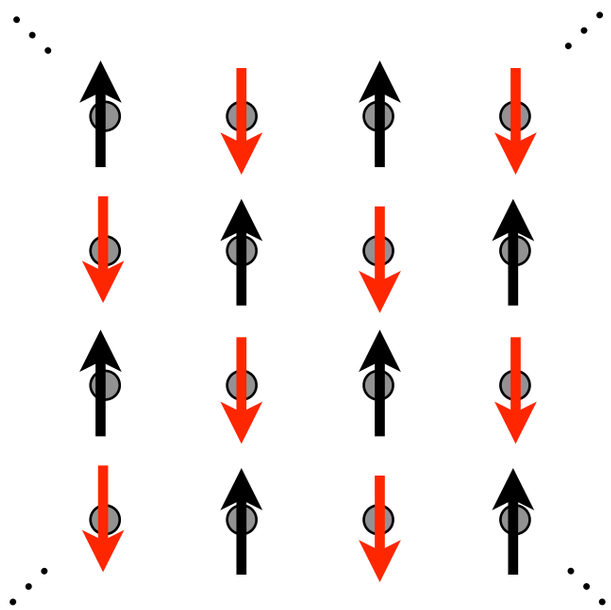
Very powerful for many spin and bosonic systems

Example: The Heisenberg model

$$H = \sum_{\langle i,j \rangle} S_i S_j$$

Ground state has Néel order



Sandvik & Evertz, PRB 82 (2010):
system sizes up to 256x256

Hilbert space: 2^{65536}

sublattice magn. $m = 0.30743(1)$

Quantum Monte Carlo

- Main idea: **Statistical sampling** of the exponentially large configuration space
- Computational cost is polynomial in N and not exponential

Very powerful for many spin and bosonic systems

BUT

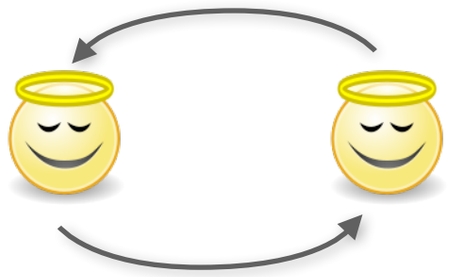
Quantum Monte Carlo & the negative sign problem

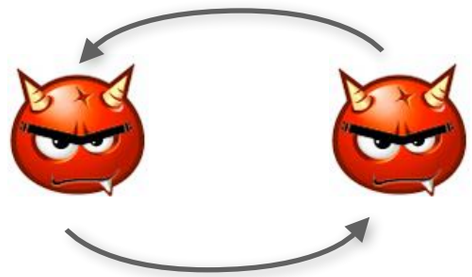
Bosons

(e.g. ^{4}He)

Fermions

(e.g electrons)





$$\Psi_B(x_1, x_2) = \Psi_B(x_2, x_1)$$

symmetric!

✓

$$t_{sim} \sim \mathcal{O}(poly(N/T))$$

$$\Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1)$$

antisymmetric!

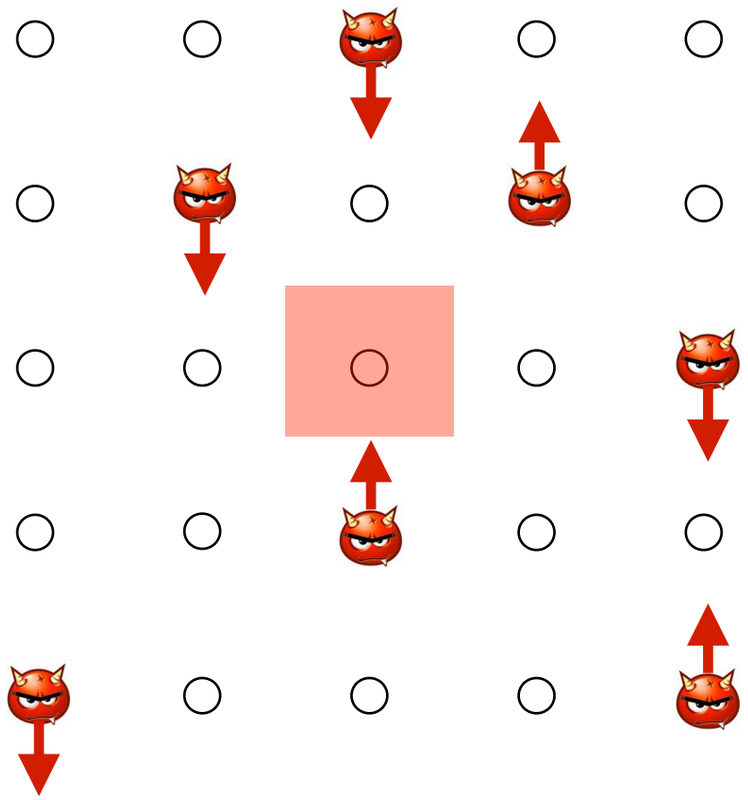
this leads to the infamous negative sign problem

$$t_{sim} \sim \mathcal{O}(\exp(N/T))$$

cannot solve large systems at low temperature!

Strongly correlated fermionic systems

2D Hubbard model



$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

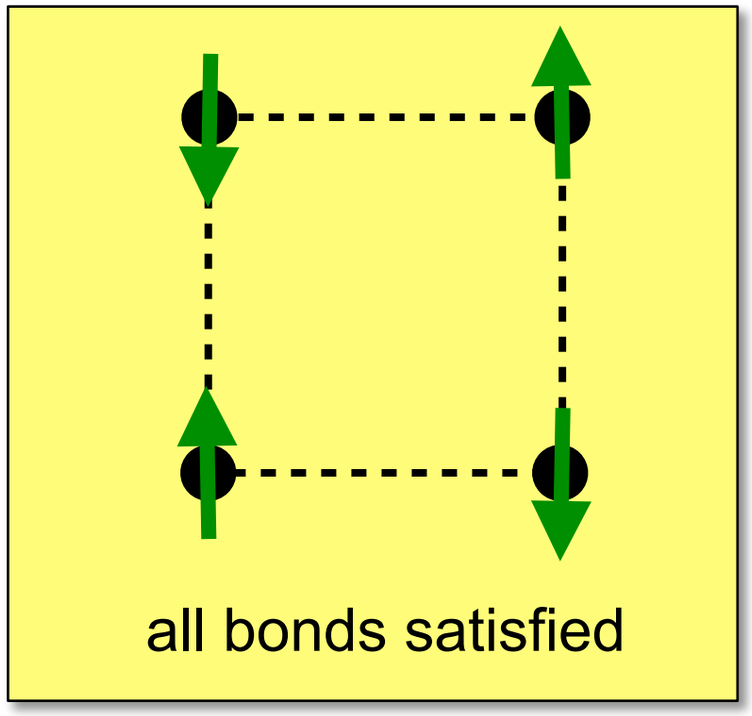
Hopping between nearest-neighbor sites

On-site repulsion between electrons with opposite spin

Is it the relevant model of high-temperature superconductors?

Quantum Monte Carlo & the negative sign problem

Non-frustrated spin systems

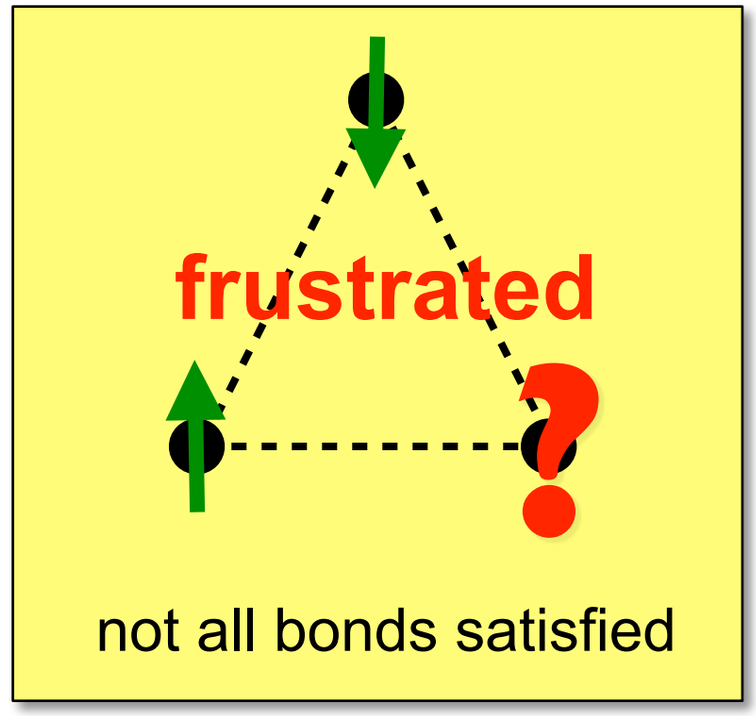


all bonds satisfied

✓

$t_{sim} \sim \mathcal{O}(poly(N/T))$

Frustrated spin systems



not all bonds satisfied

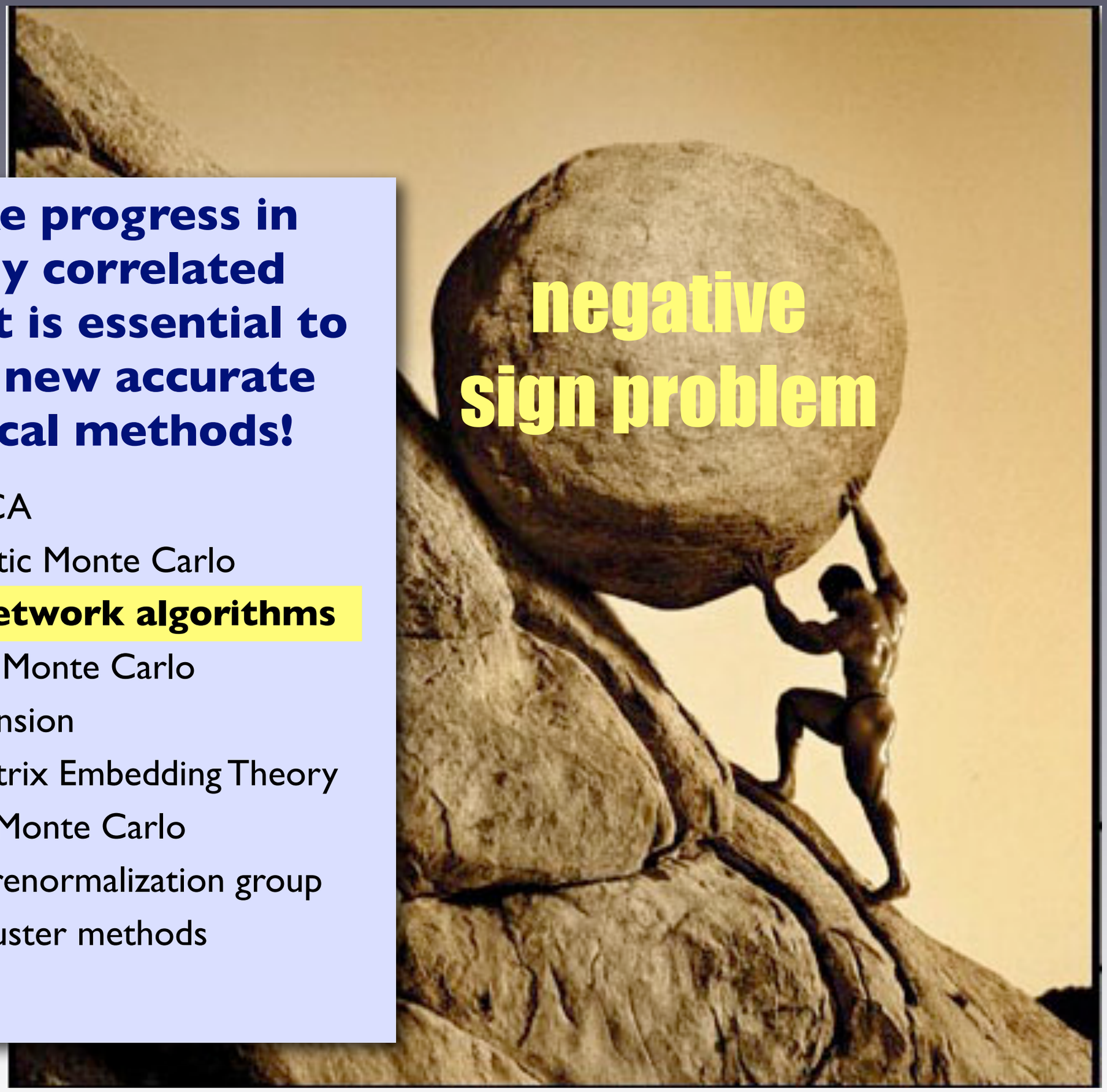
this leads to the infamous negative sign problem

$t_{sim} \sim \mathcal{O}(\exp(N/T))$

cannot solve large systems at low temperature!

To make progress in strongly correlated systems it is essential to develop new accurate numerical methods!

- DMFT / DCA
- Diagrammatic Monte Carlo
- **Tensor network algorithms**
- Fixed-node Monte Carlo
- Series expansion
- Density Matrix Embedding Theory
- Variational Monte Carlo
- Functional renormalization group
- Coupled-cluster methods
- ...

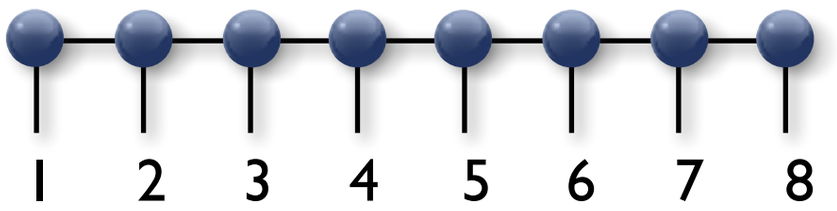


Overview: tensor networks in 1D and 2D

1D

MPS

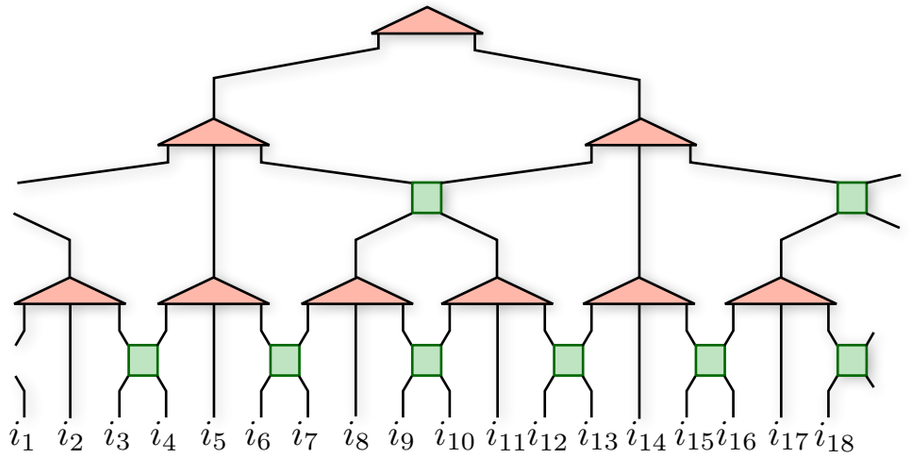
Matrix-product state



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

1D MERA

Multi-scale entanglement renormalization ansatz



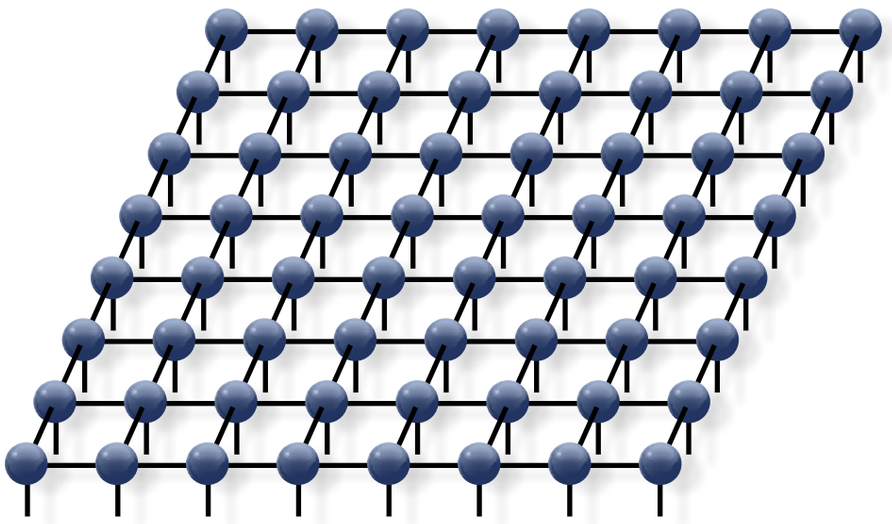
and more

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

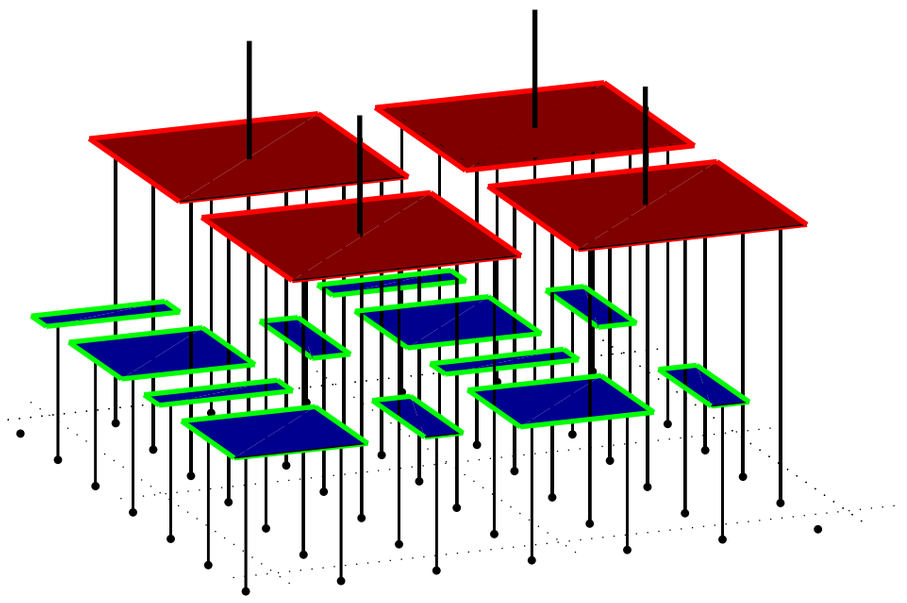
2D

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)*

- Part III: Optimization
- Part IV: iPEPS application example
- Part V: Fermionic 2D tensor networks
- Part VI: Selected recent developments

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: $\{|\uparrow\rangle, |\downarrow\rangle\}$

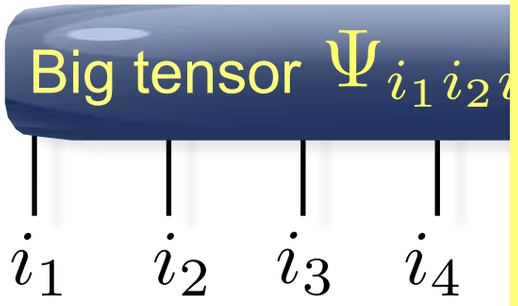
2^6 basis states

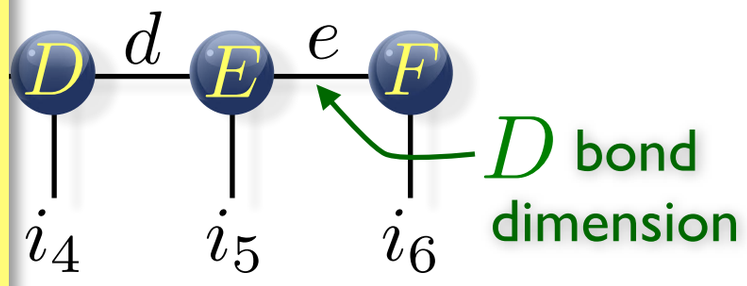
2^6 coefficients

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/multidimensi… …atrix product state (**MPS**)

Why is this possible??



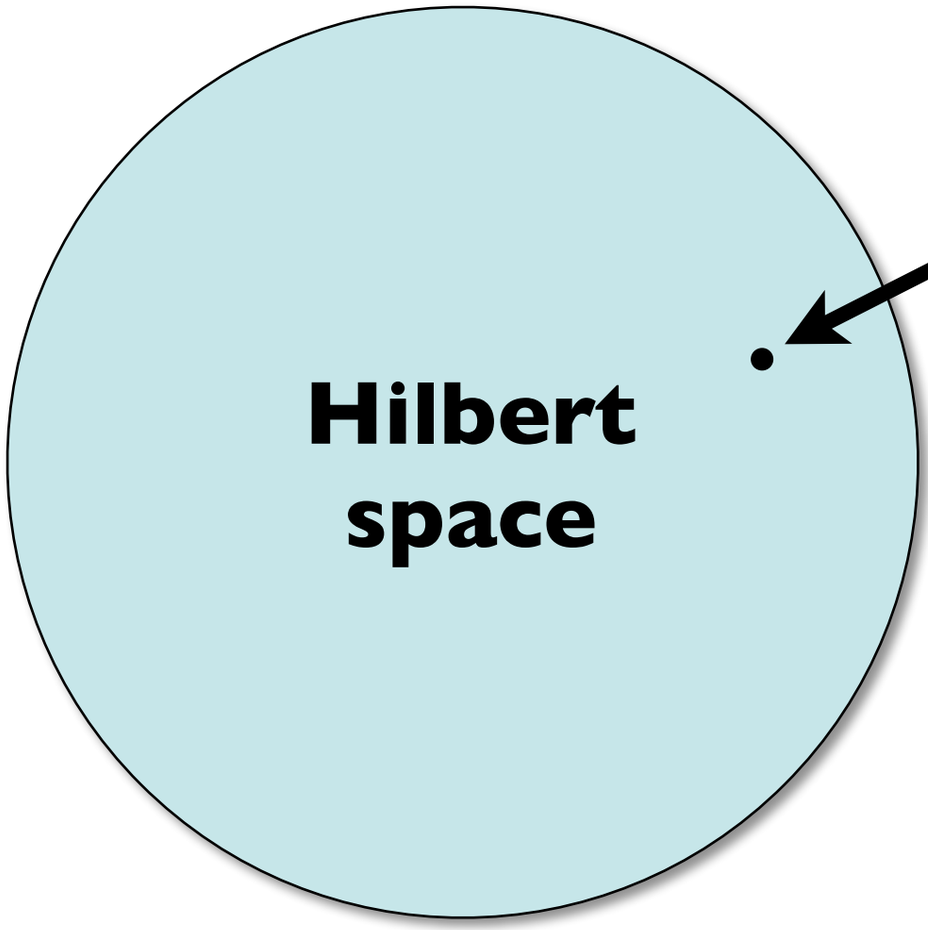


$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6} \approx \sum_{abcde} A^a_{i_1} B^{ab}_{i_2} C^{bc}_{i_3} D^{cd}_{i_4} E^{de}_{i_5} F^e_{i_6} = \tilde{\Psi}_{i_1 i_2 i_3 i_4 i_5 i_6}$$

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

Efficient representation!

“Corner” of the Hilbert space



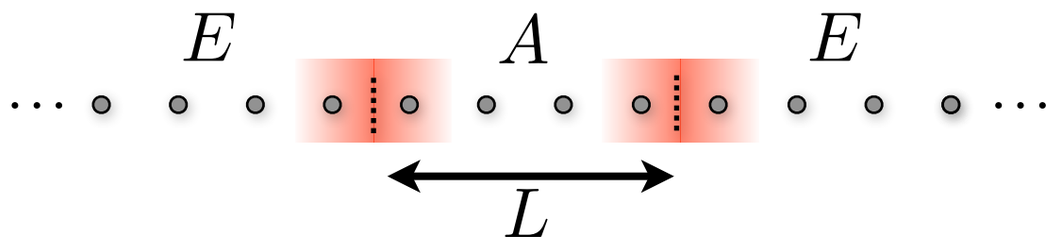
Ground states (local H)

★ GS of local H’s are less entangled than a random state in the Hilbert space

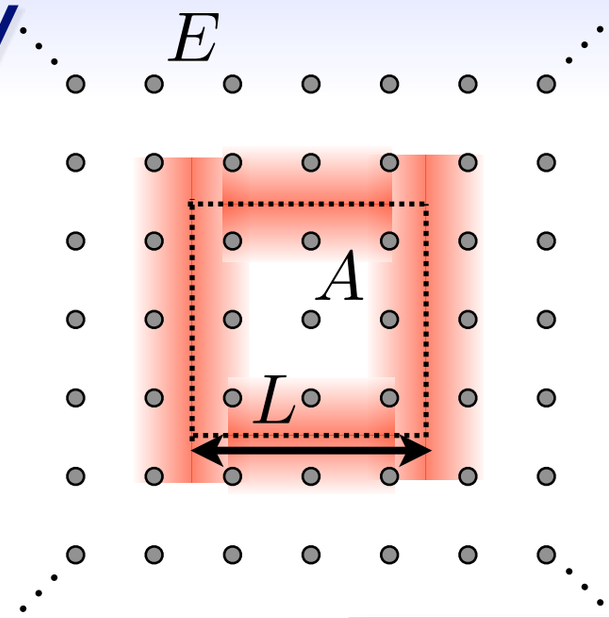
★ *Area law of the entanglement entropy*

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

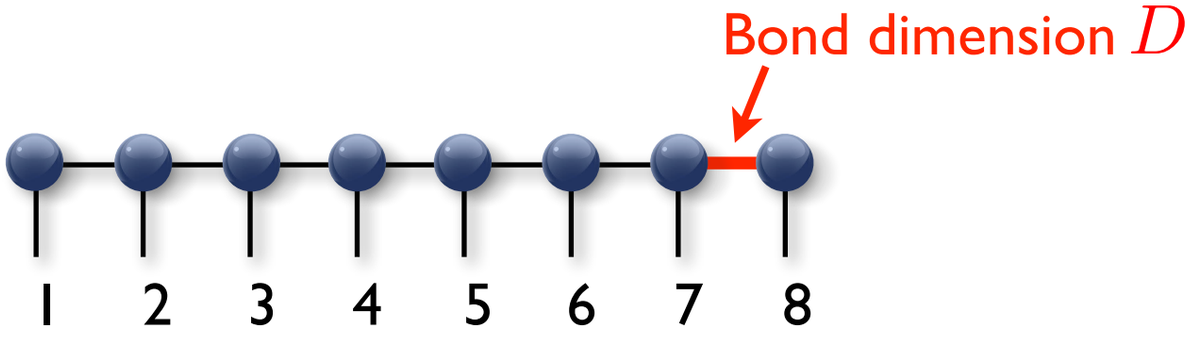
1D	$S(L) = const$	$\chi = const$
2D	$S(L) \sim \alpha L$	$\chi \sim \exp(\alpha L)$

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

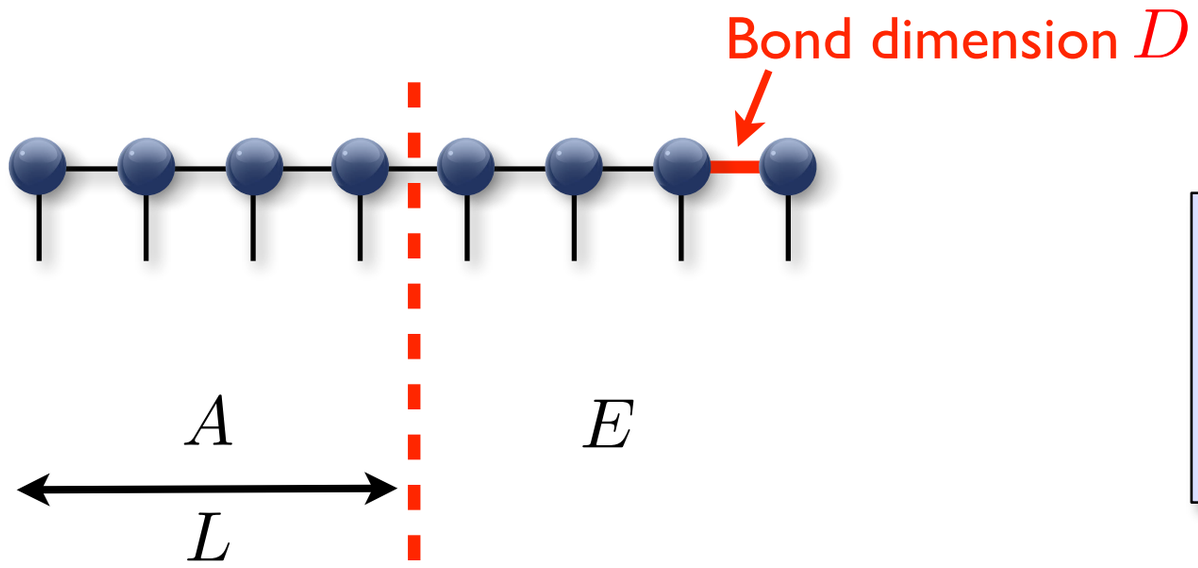
$$S(L) = const$$

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

$$S(L) = const$$

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

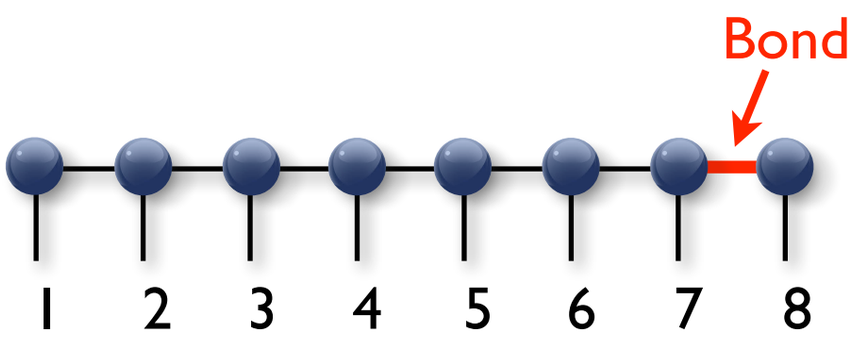
$$\lambda_i = \frac{1}{D} \rightarrow \; S(A) = -\sum_i^D \frac{1}{D} \log \frac{1}{D} = \log(D)$$

MPS & PEPS

1D

MPS

Matrix-product state



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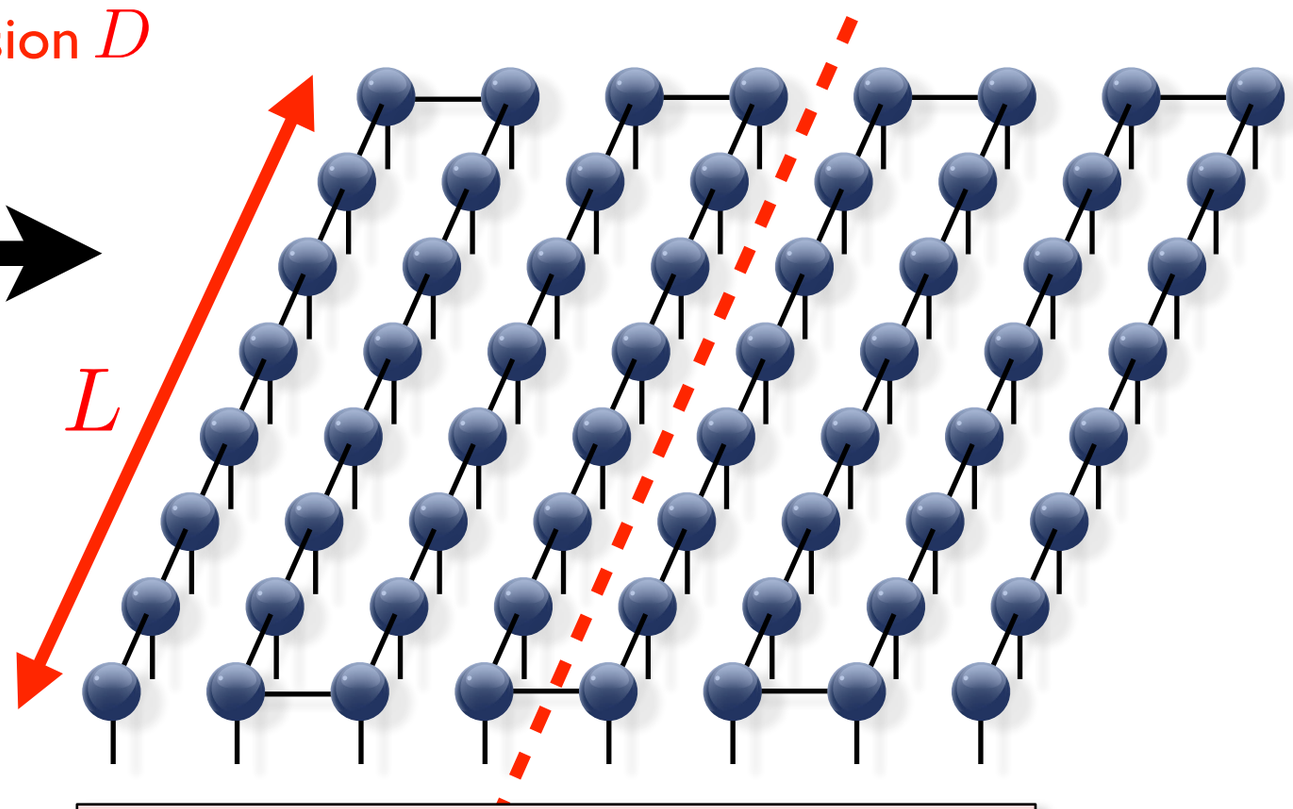
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

can we use an MPS?



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

$$S(L) \sim L$$

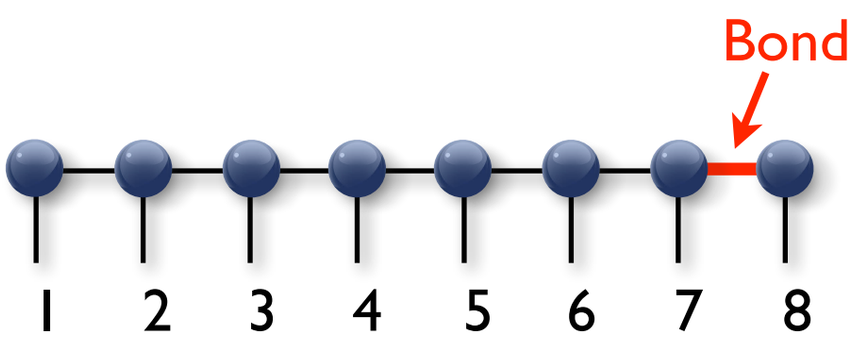
$$\rightarrow D \sim exp(L)$$

MPS & PEPS

1D

MPS

Matrix-product state



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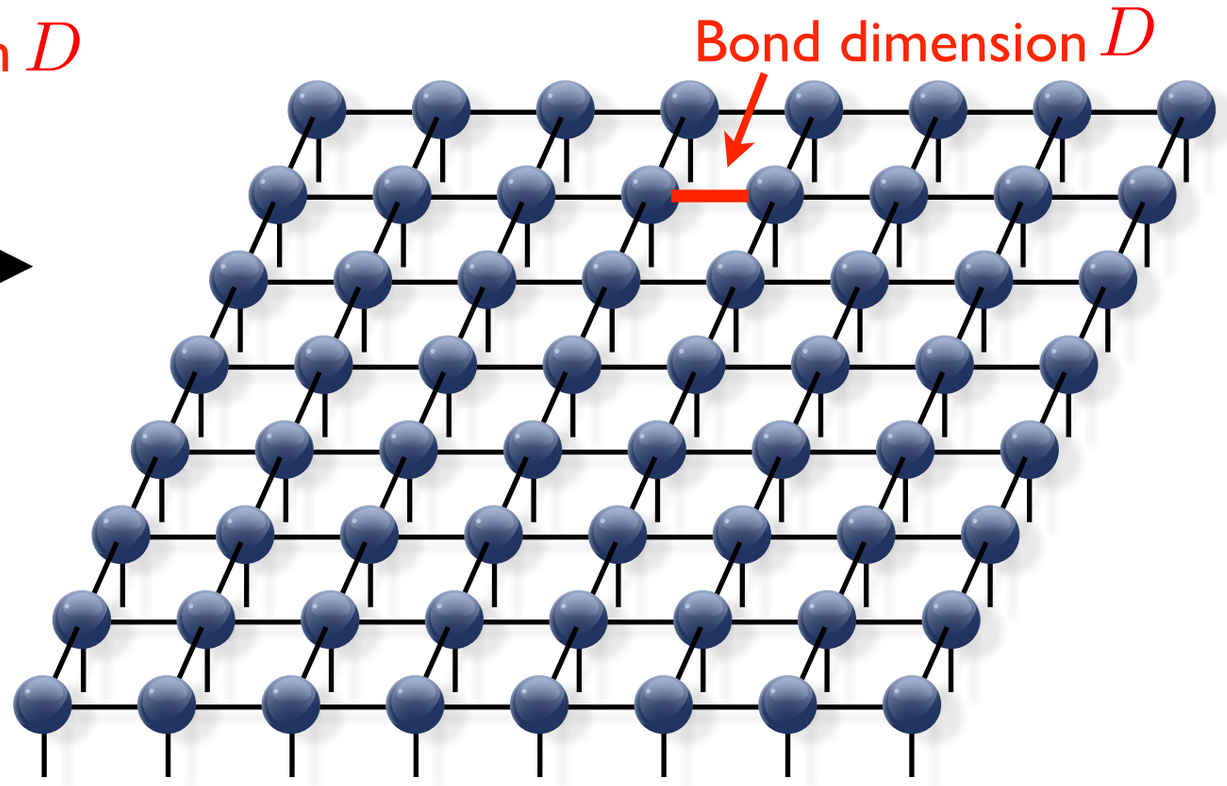
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)

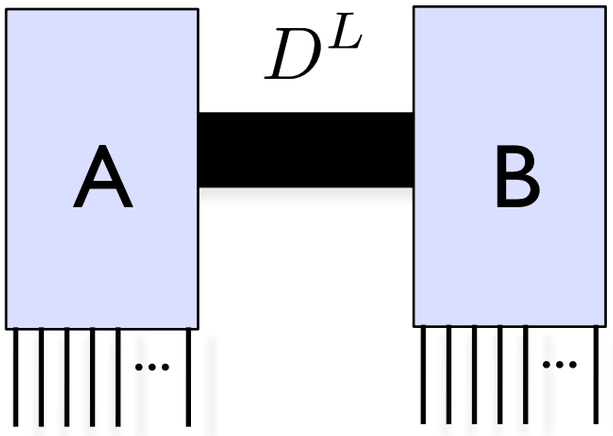


F. Verstraete, J. I. Cirac, cond-mat/0407066
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

✓ Reproduces area-law in 2D

$$S(L) \sim L$$

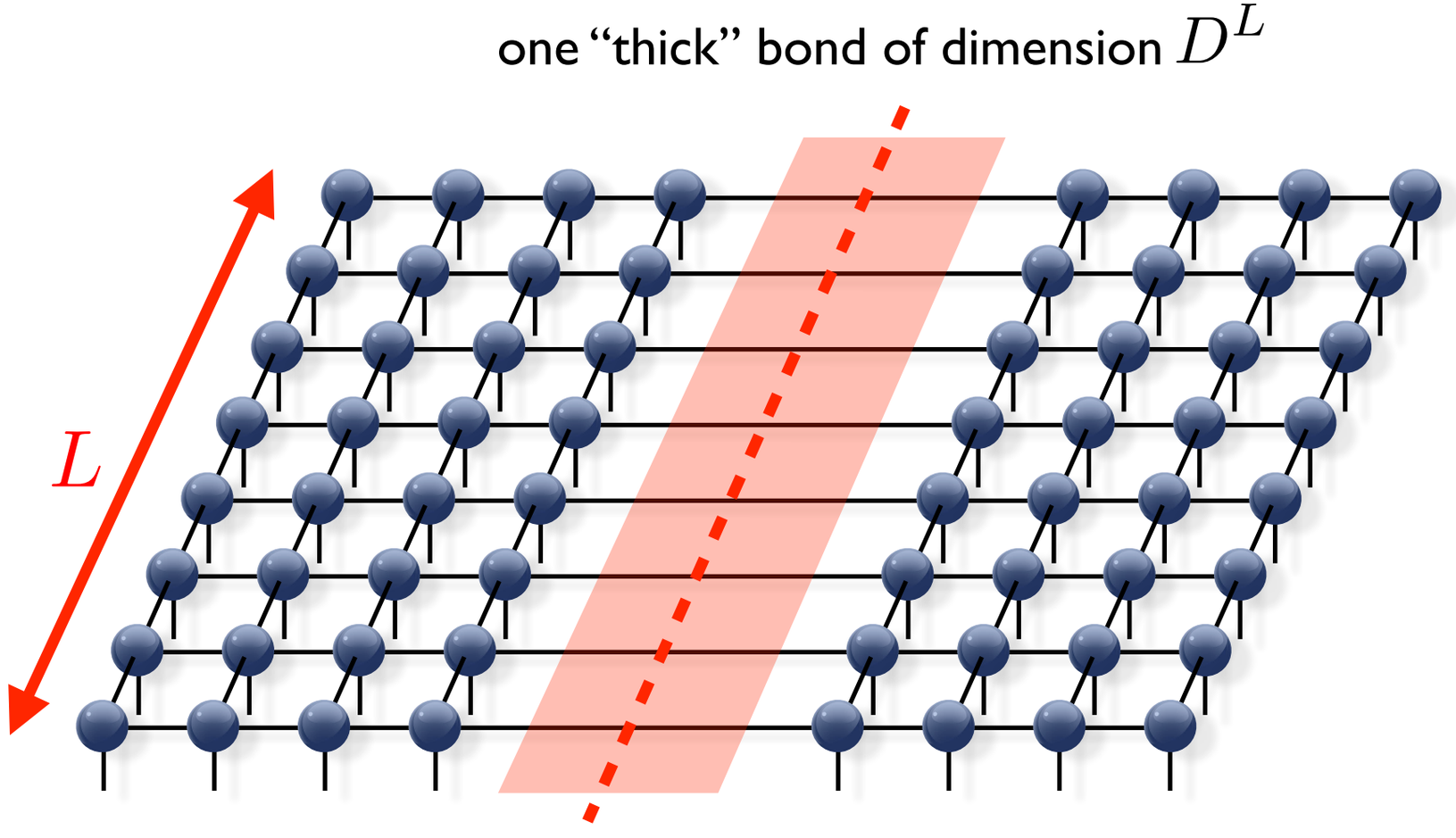
PEPS: Area law



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

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

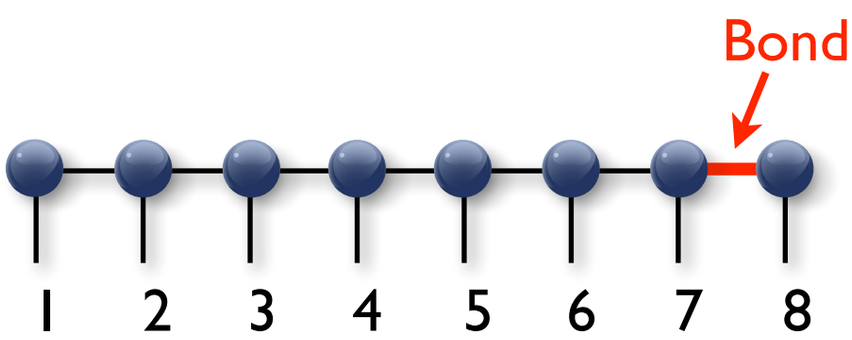
$$S(L) \sim L$$

MPS & PEPS

1D

MPS

Matrix-product state



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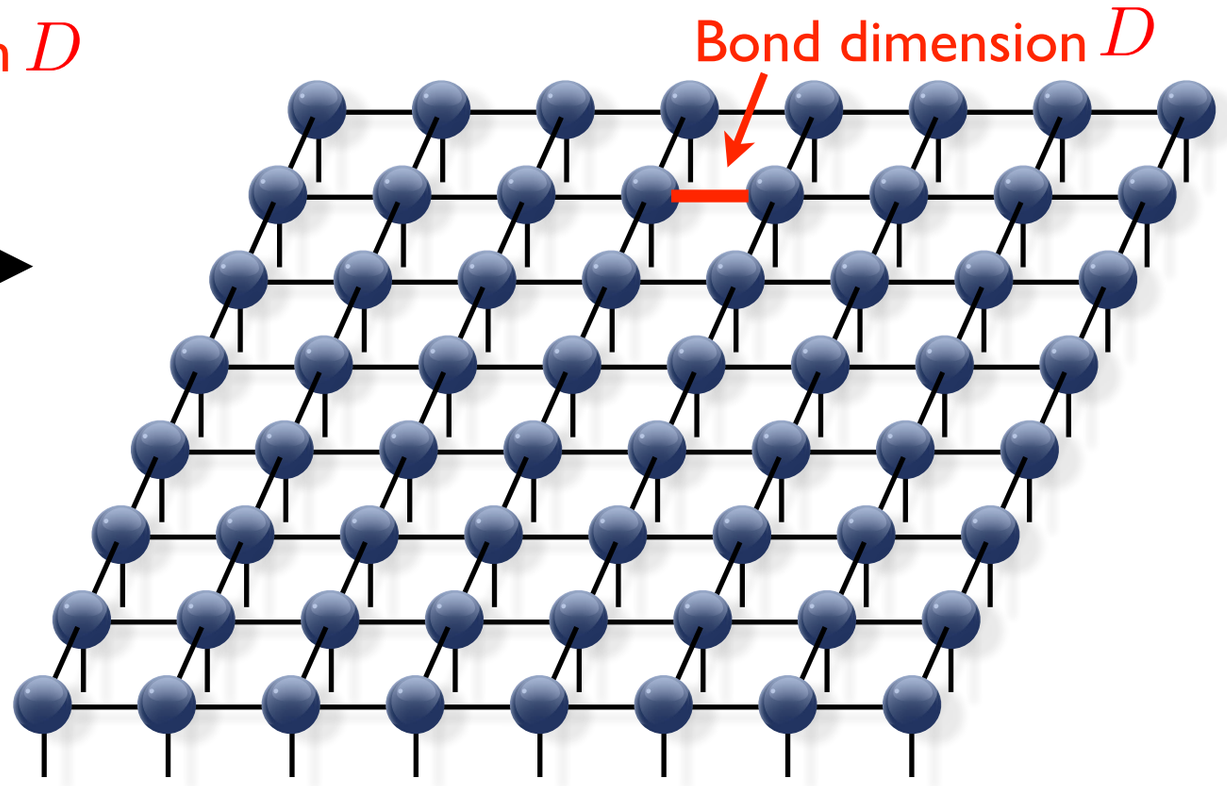
$$S(L) = const$$

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



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✓ Reproduces area-law in 2D

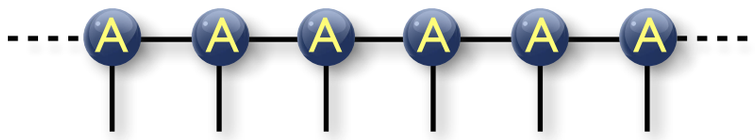
$$S(L) \sim L$$

Infinite PEPS (iPEPS)

1D

iMPS

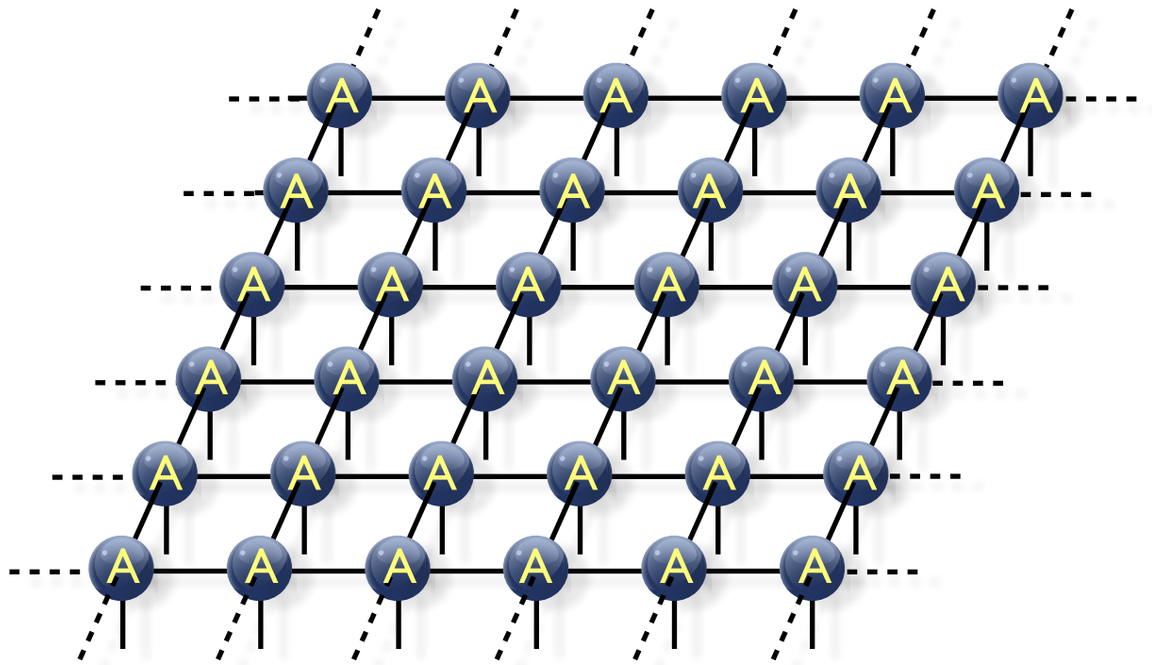
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

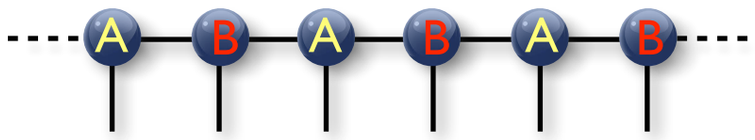
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

Infinite PEPS (iPEPS)

1D

iMPS

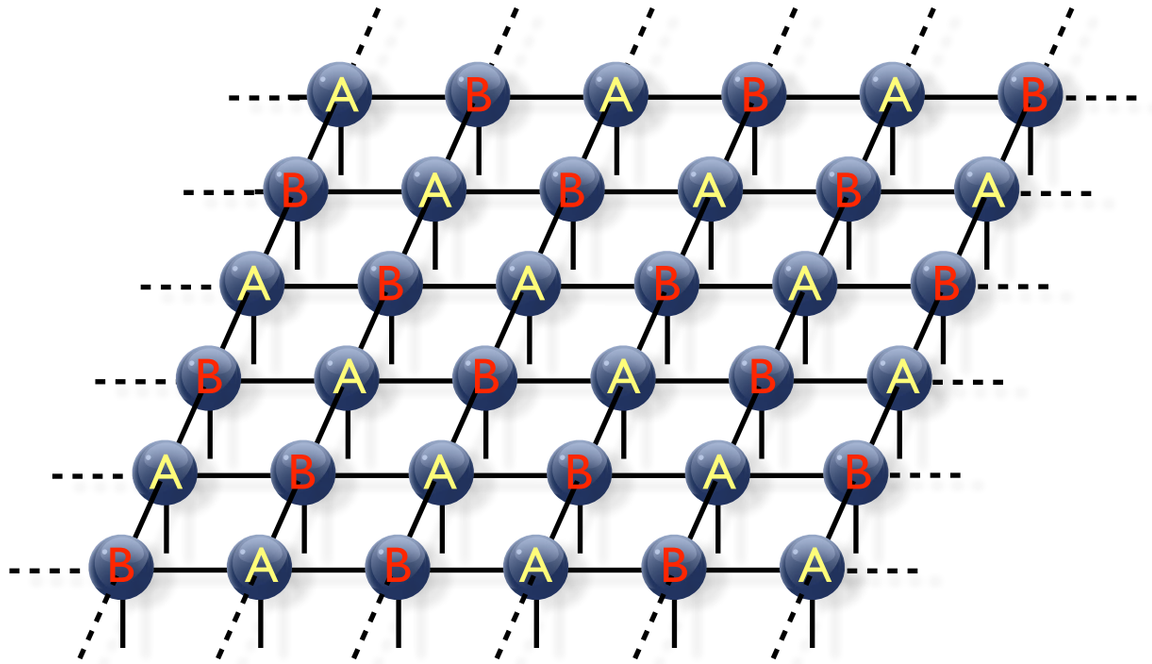
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

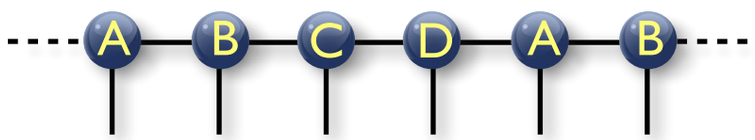
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

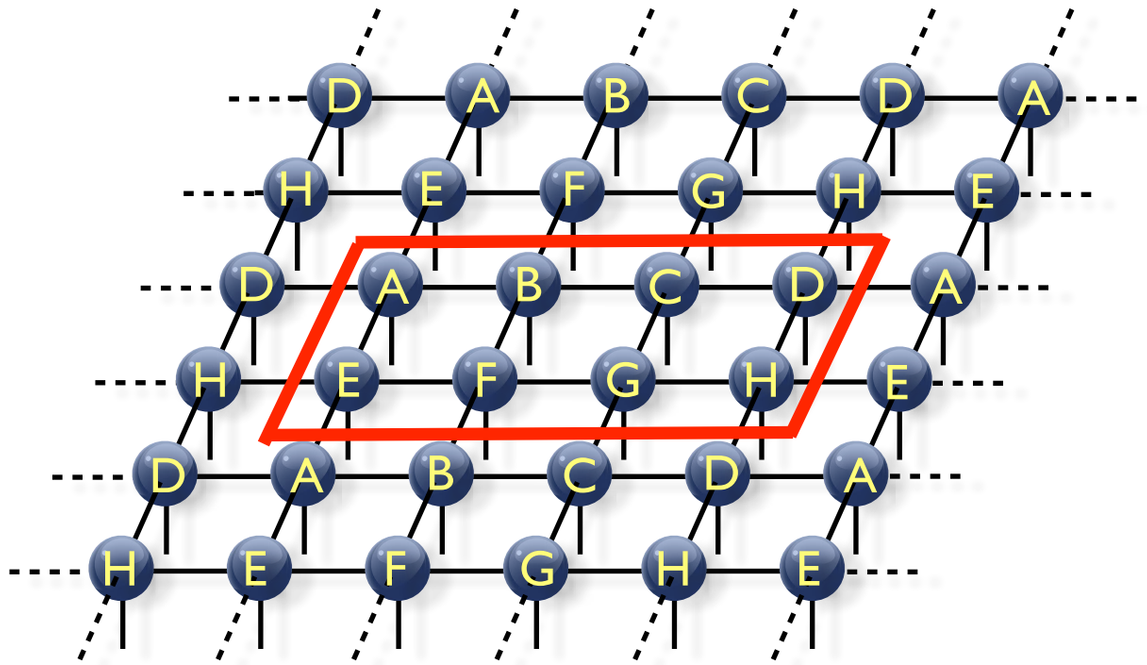
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



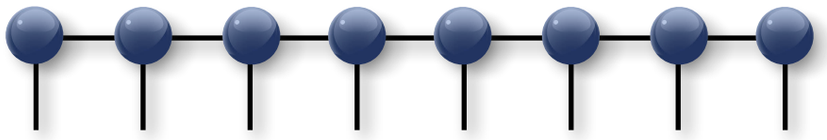
here: 4x2 unit cell

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

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

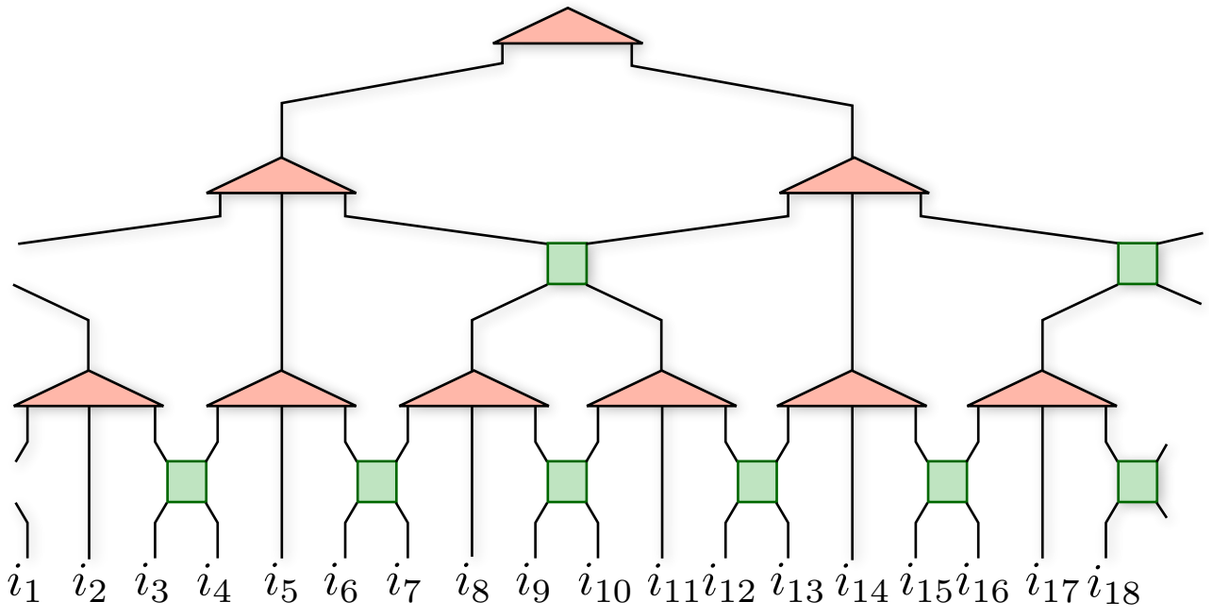
Hierarchical tensor networks (TTN/MERA)

MPS



"flat"

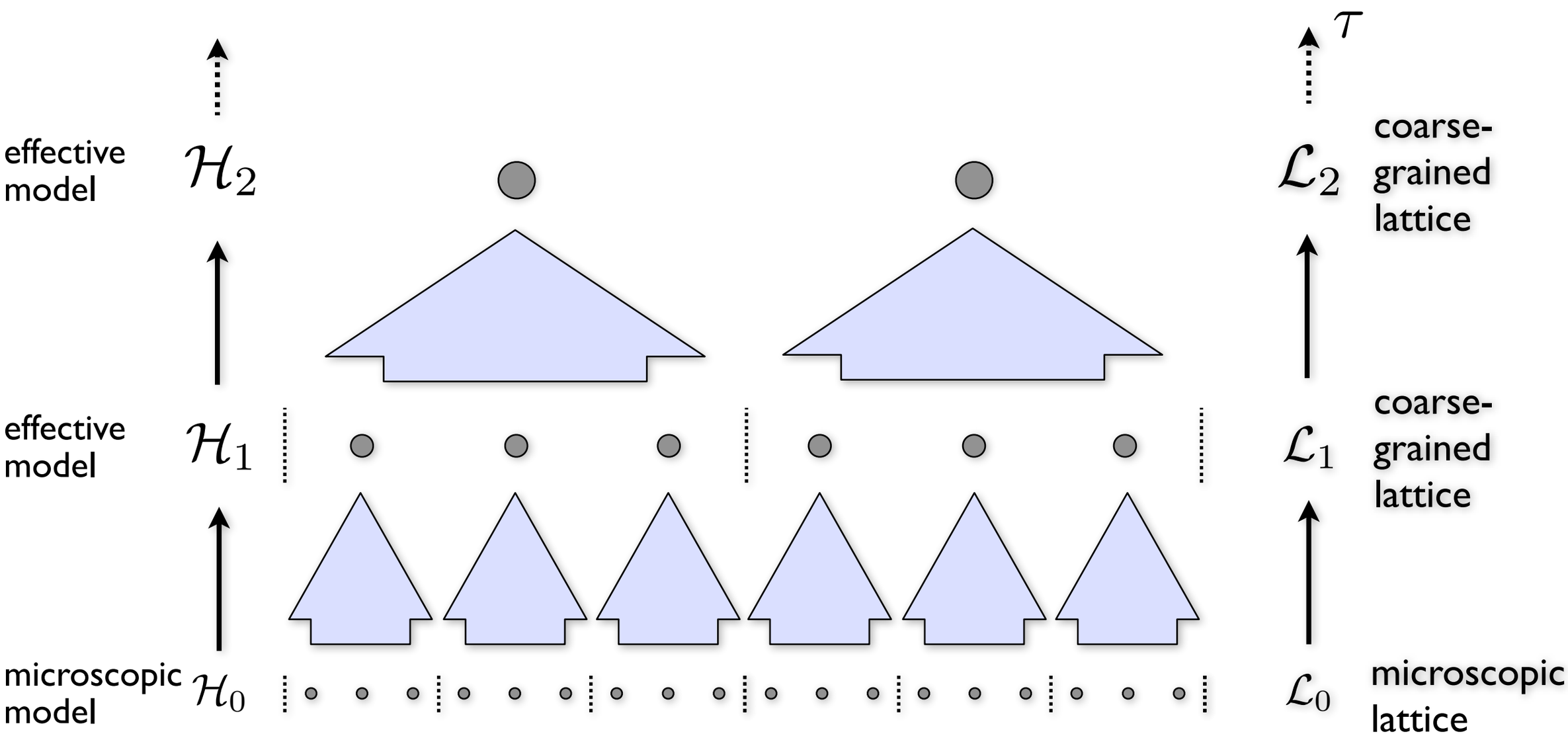
MERA



tensors at different length scales

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

Real-space renormalization group transformation

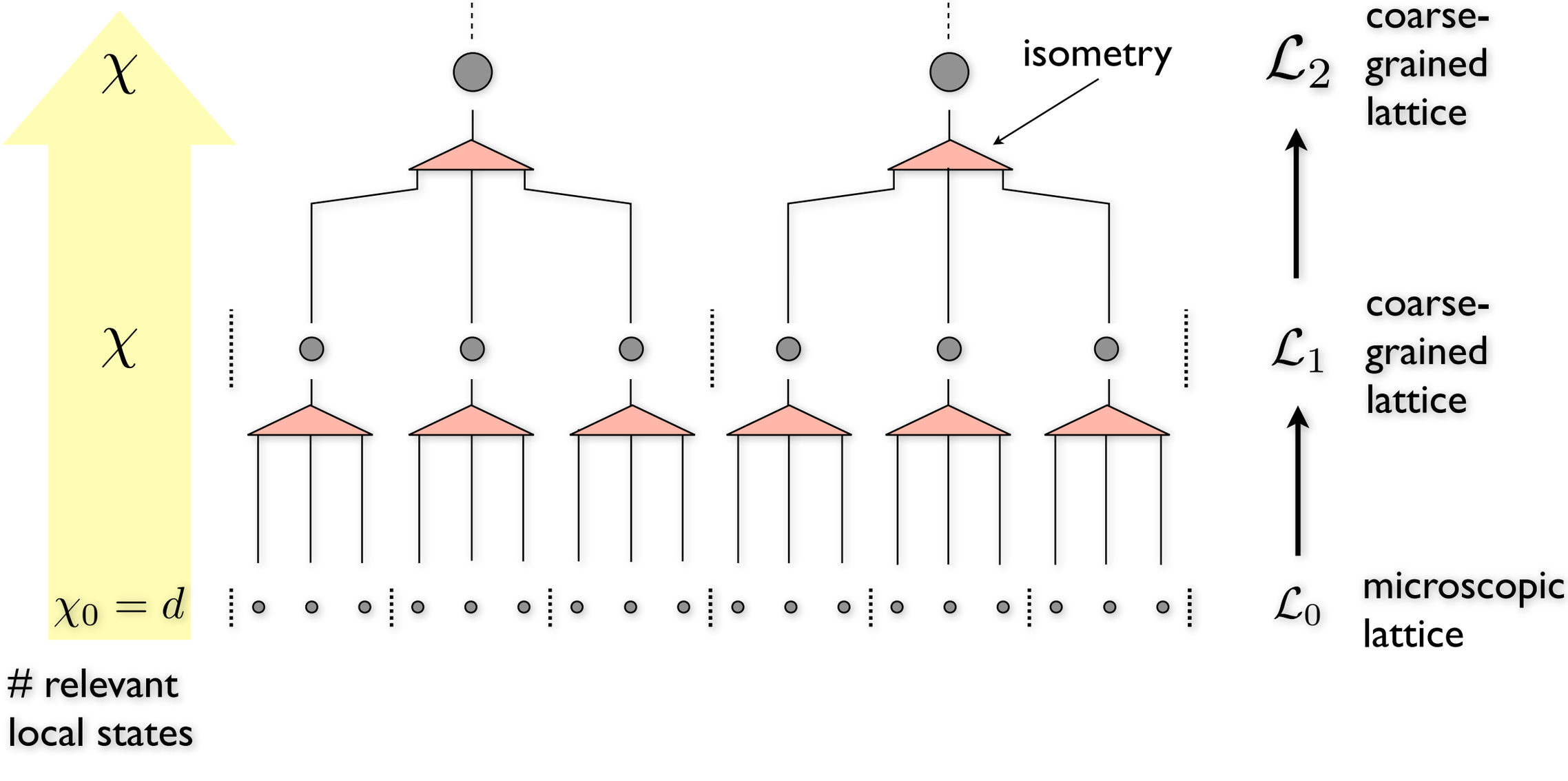


Tree Tensor Network (1D)

1D systems (non-critical)

$$S(L) = const$$

$$\chi_\tau = const$$

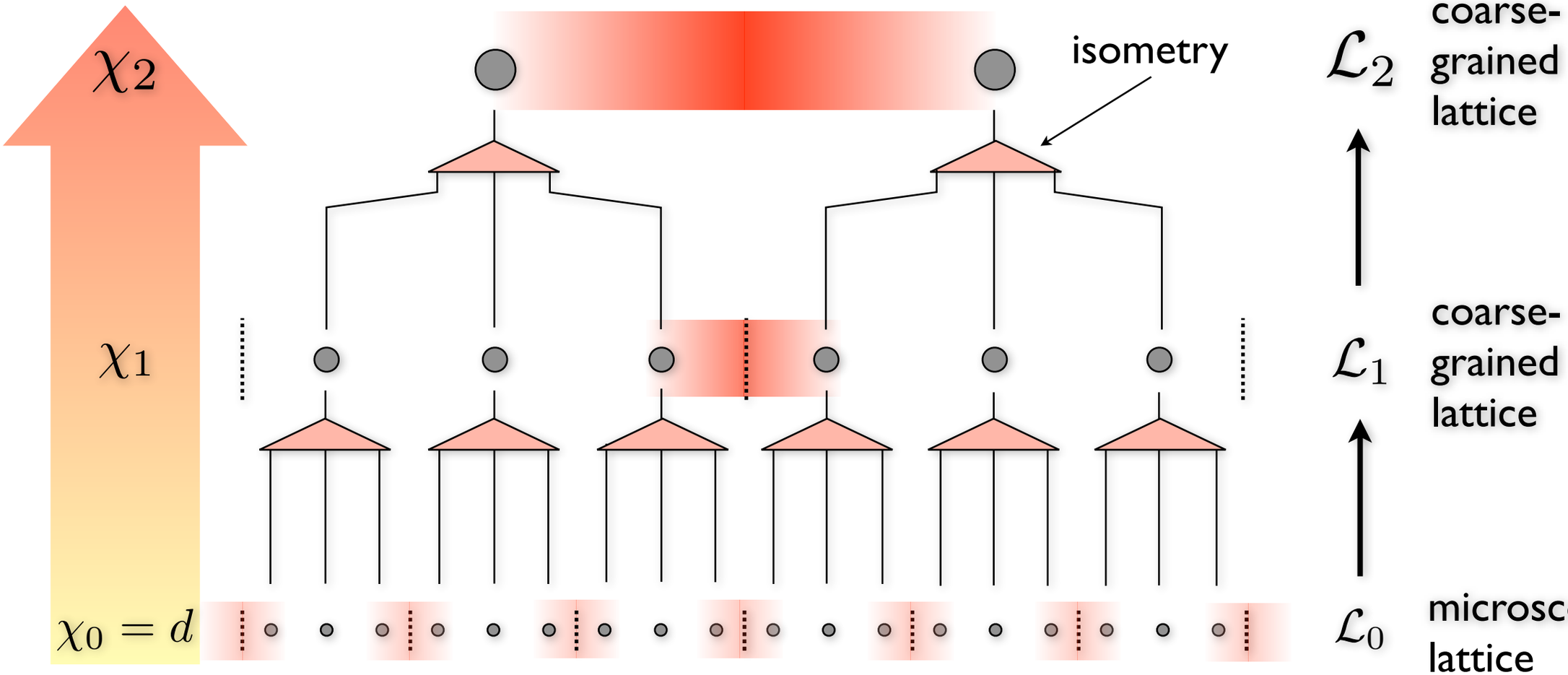


Tree Tensor Network (1D)

1D critical systems

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

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



relevant local states

The MERA (The multi-scale entanglement renormalization ansatz)

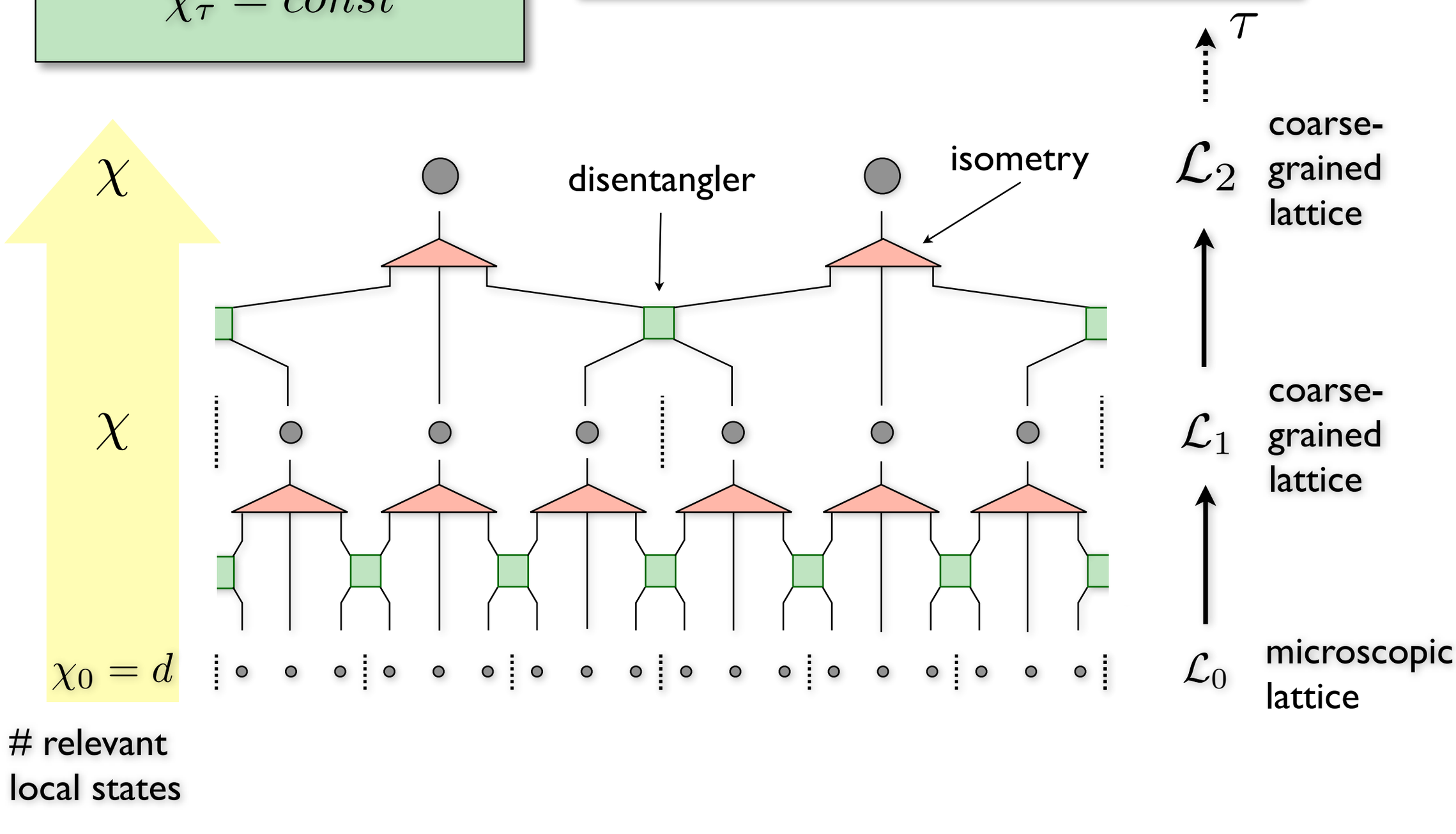
G. Vidal, PRL 99, 220405 (2007)
G. Vidal, PRL 101, 110501 (2008)

1D systems (critical)

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

$$\chi_\tau = const$$

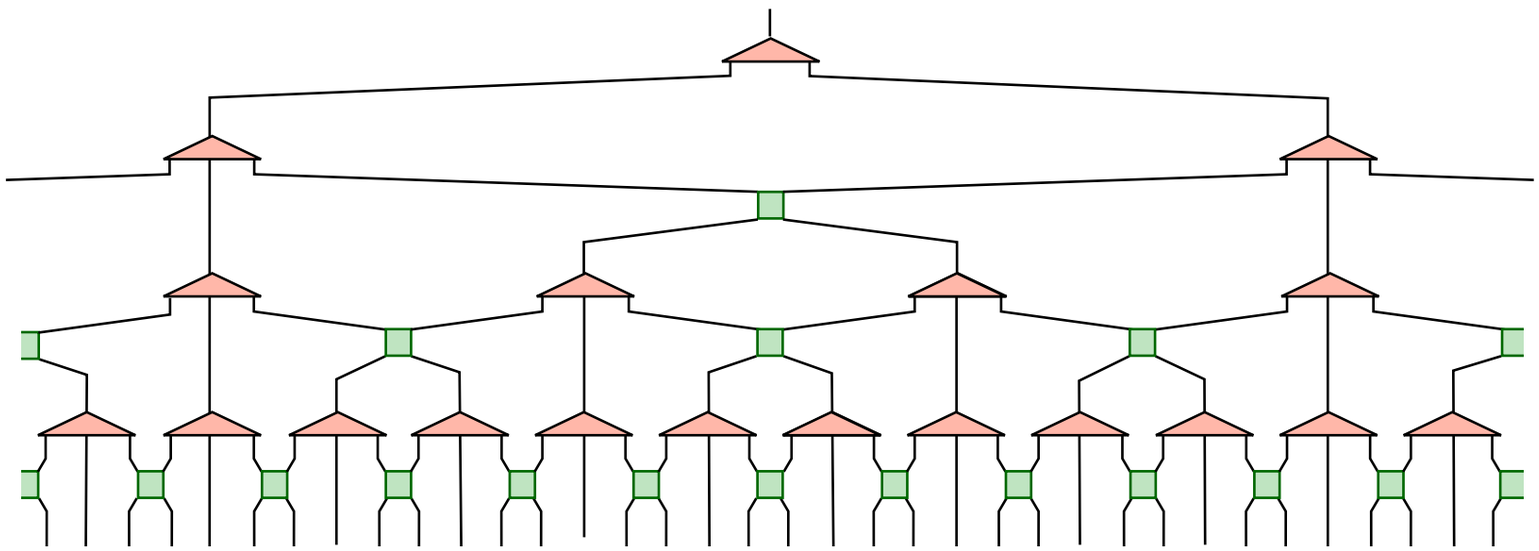
KEY: disentanglers reduce the amount of short-range entanglement



MERA: Properties

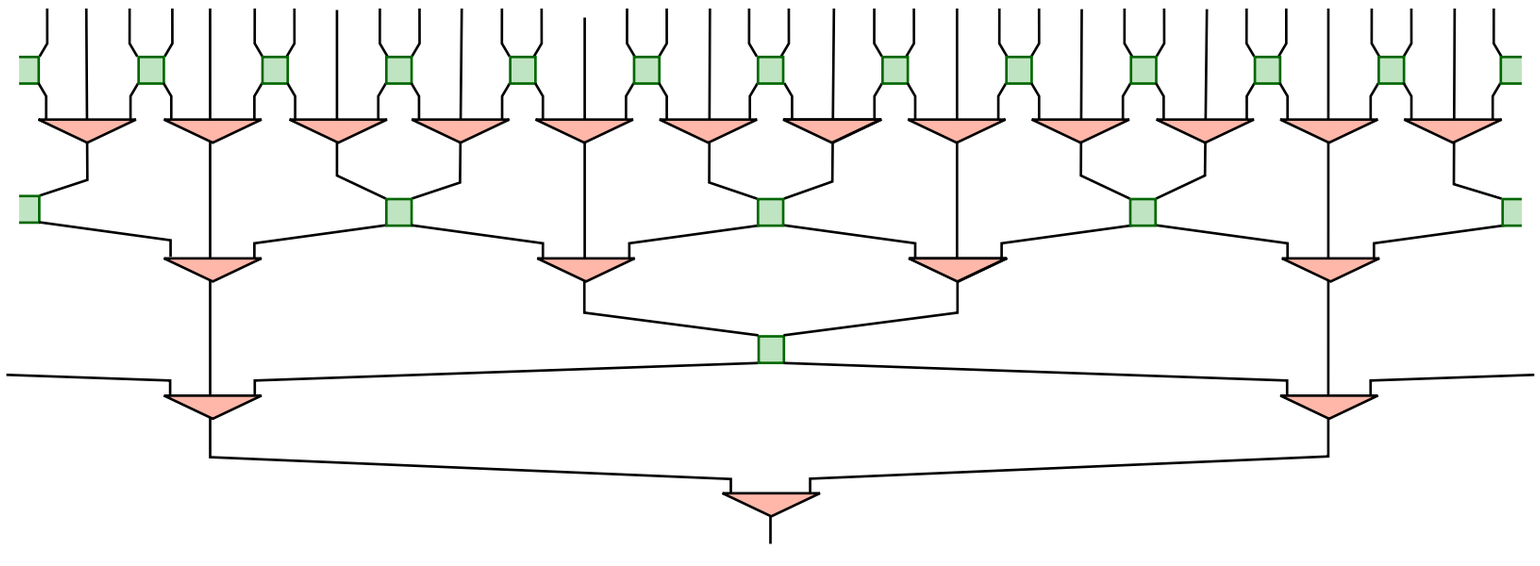
Let's compute $\langle\Psi|O|\Psi\rangle$ O: two-site operator

$|\Psi\rangle$

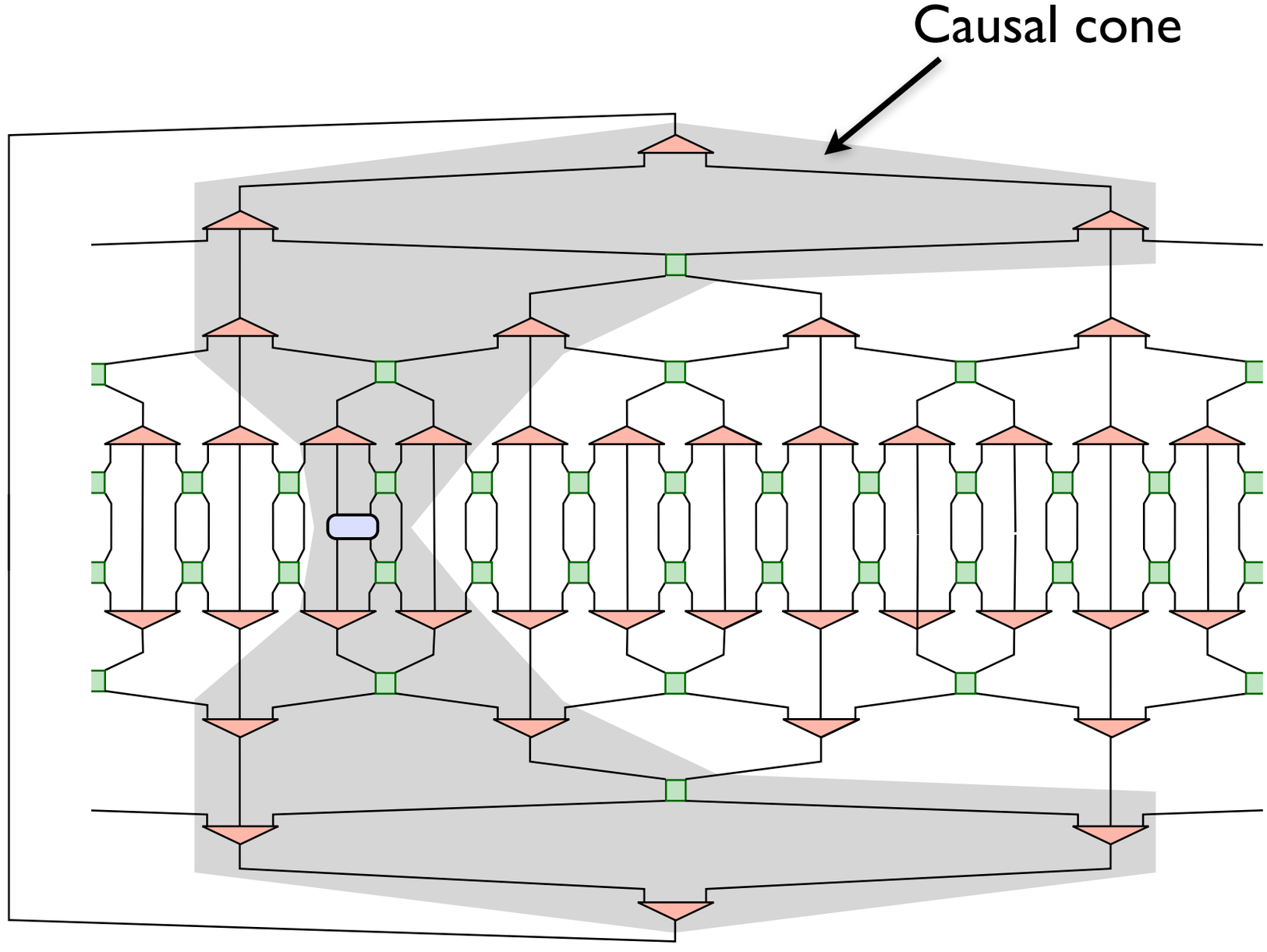


O

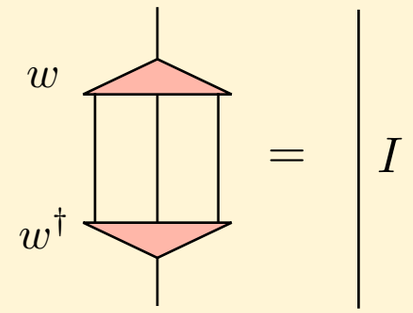
$\langle\Psi|$



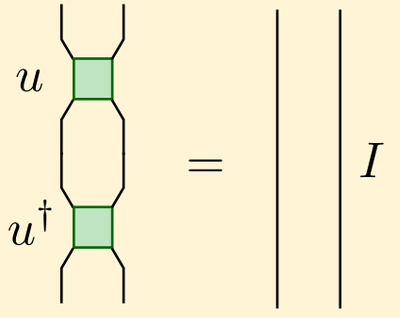
MERA: Properties



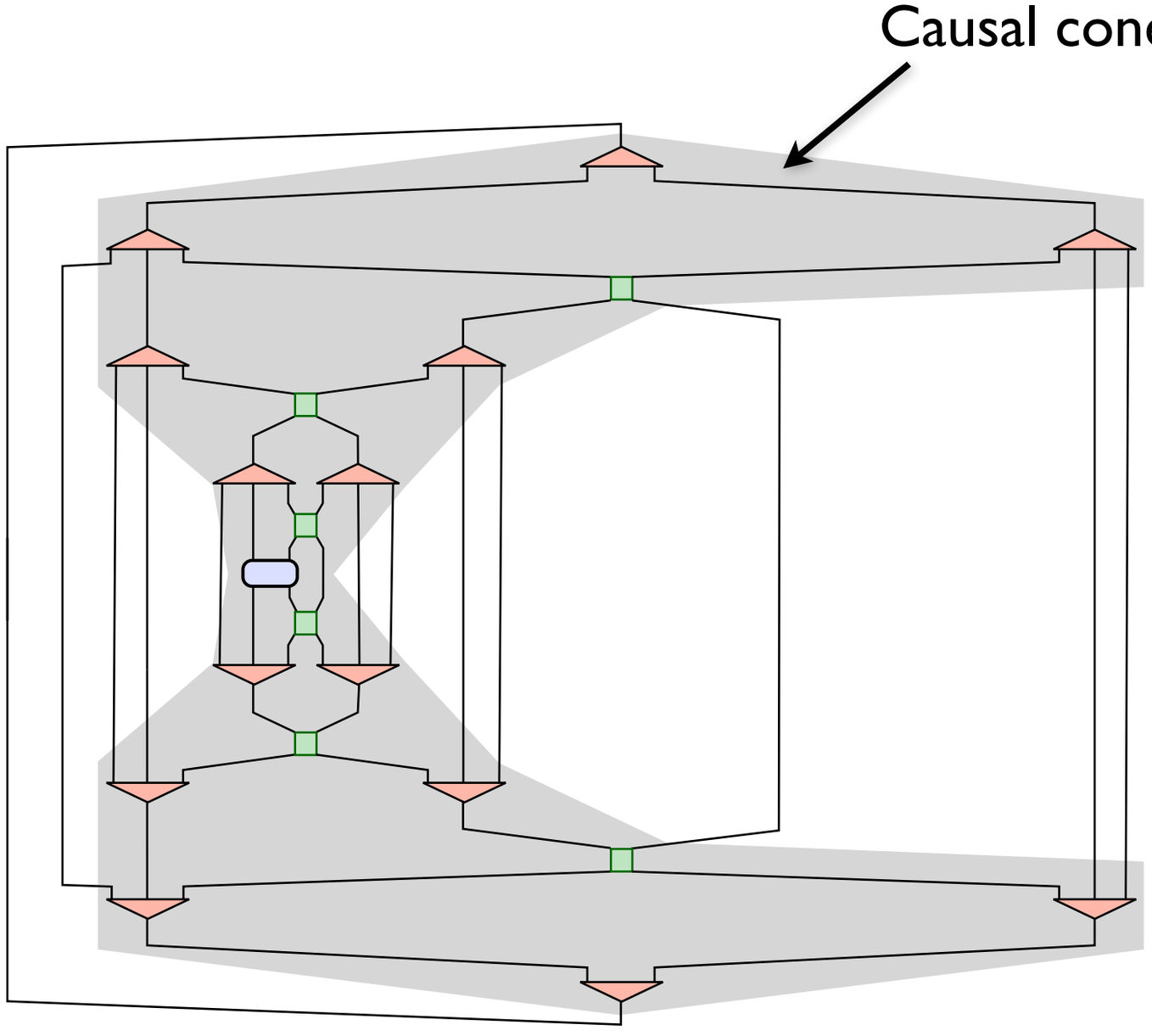
Isometries are *isometric*



Disentanglers are *unitary*

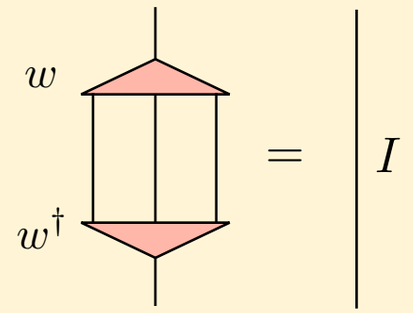


MERA: Properties

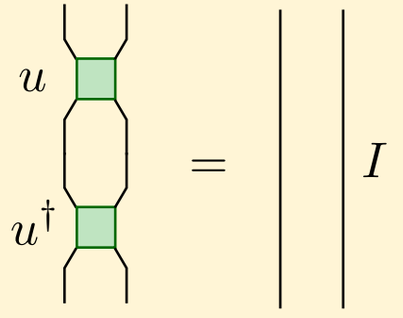


$\langle\Psi|O|\Psi\rangle$

Isometries are *isometric*



Disentanglers are *unitary*

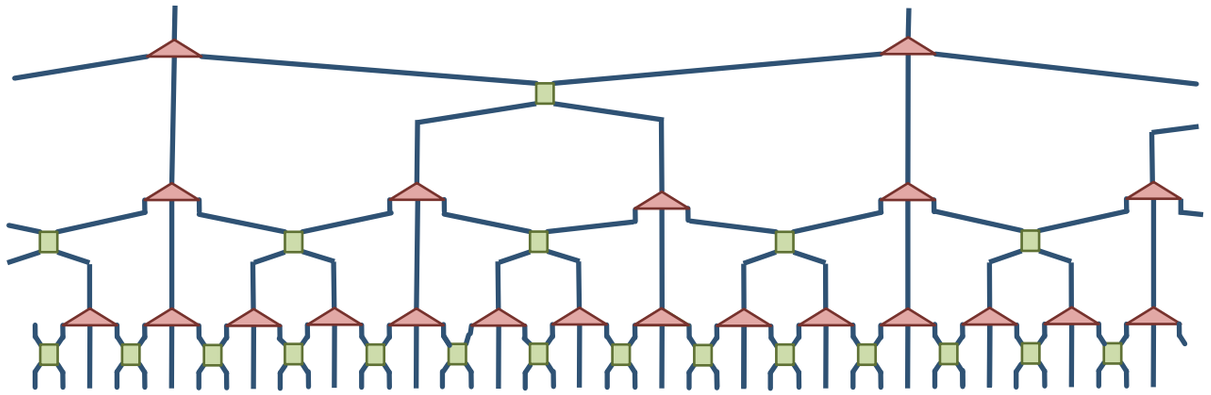


Efficient computation of expectation values of observables!

Different types of MERA's

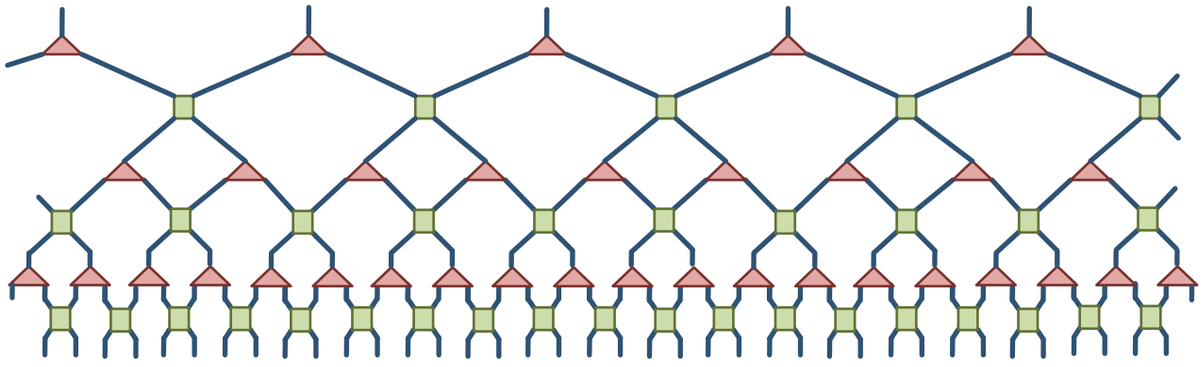
Figures by G. Evenbly

Ternary MERA:
3-to-1 blocking



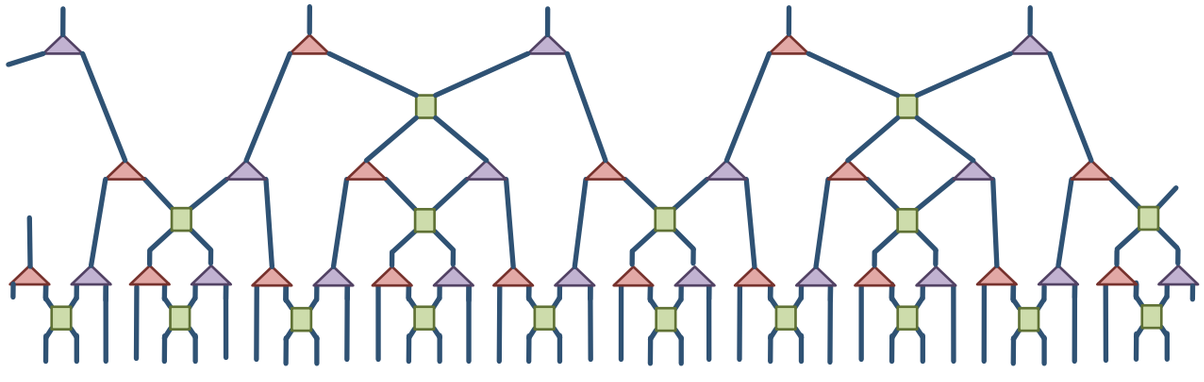
$O(\chi^8)$

Binary MERA:
2-to-1 blocking



$O(\chi^9)$

Modified
binary MERA:
2-to-1 blocking



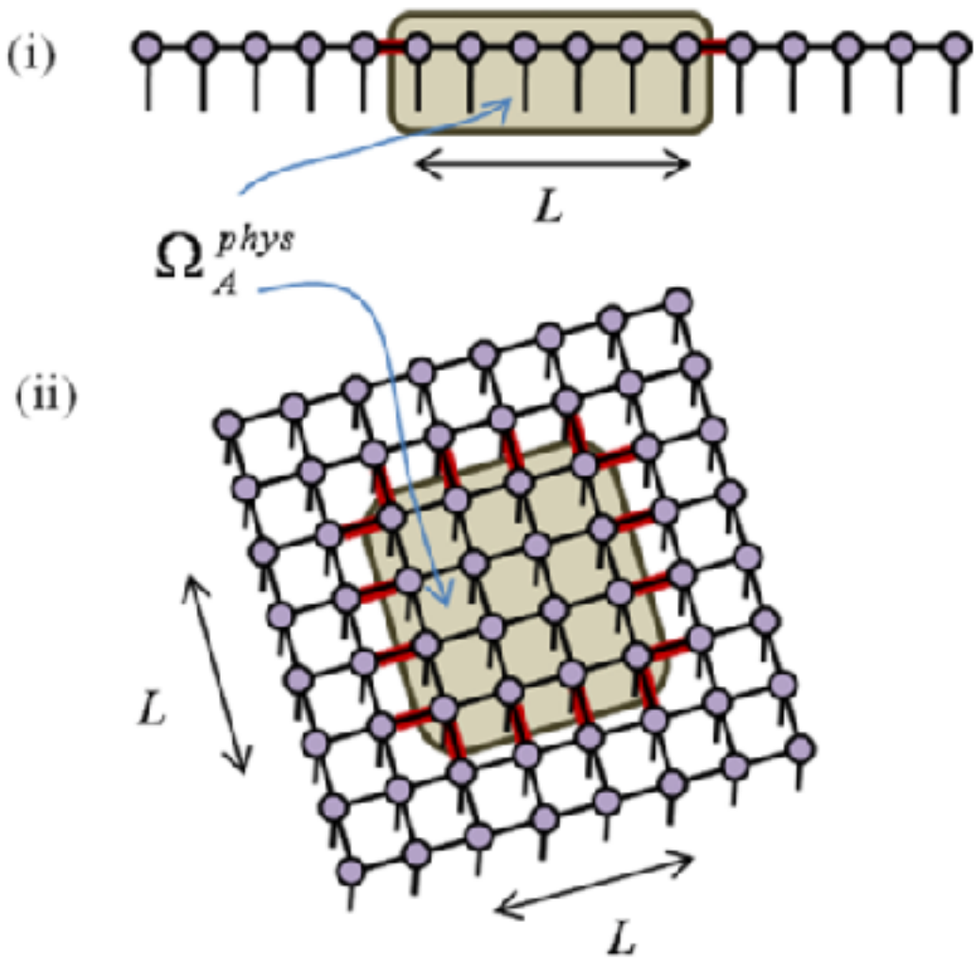
$O(\chi^7)$

TRADEOFF: computational cost vs efficiency of coarse-graining

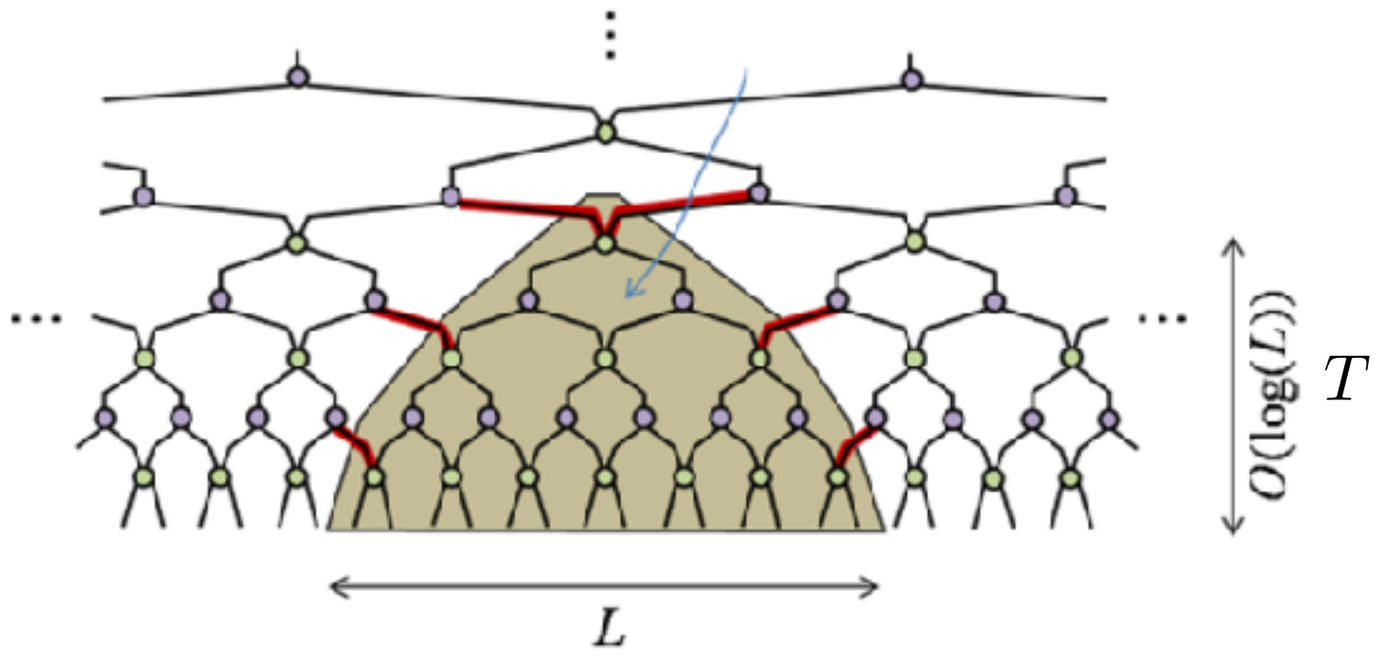
MERA: Entanglement entropy

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

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



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



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

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

Reproduces log(L) scaling of 1D critical systems

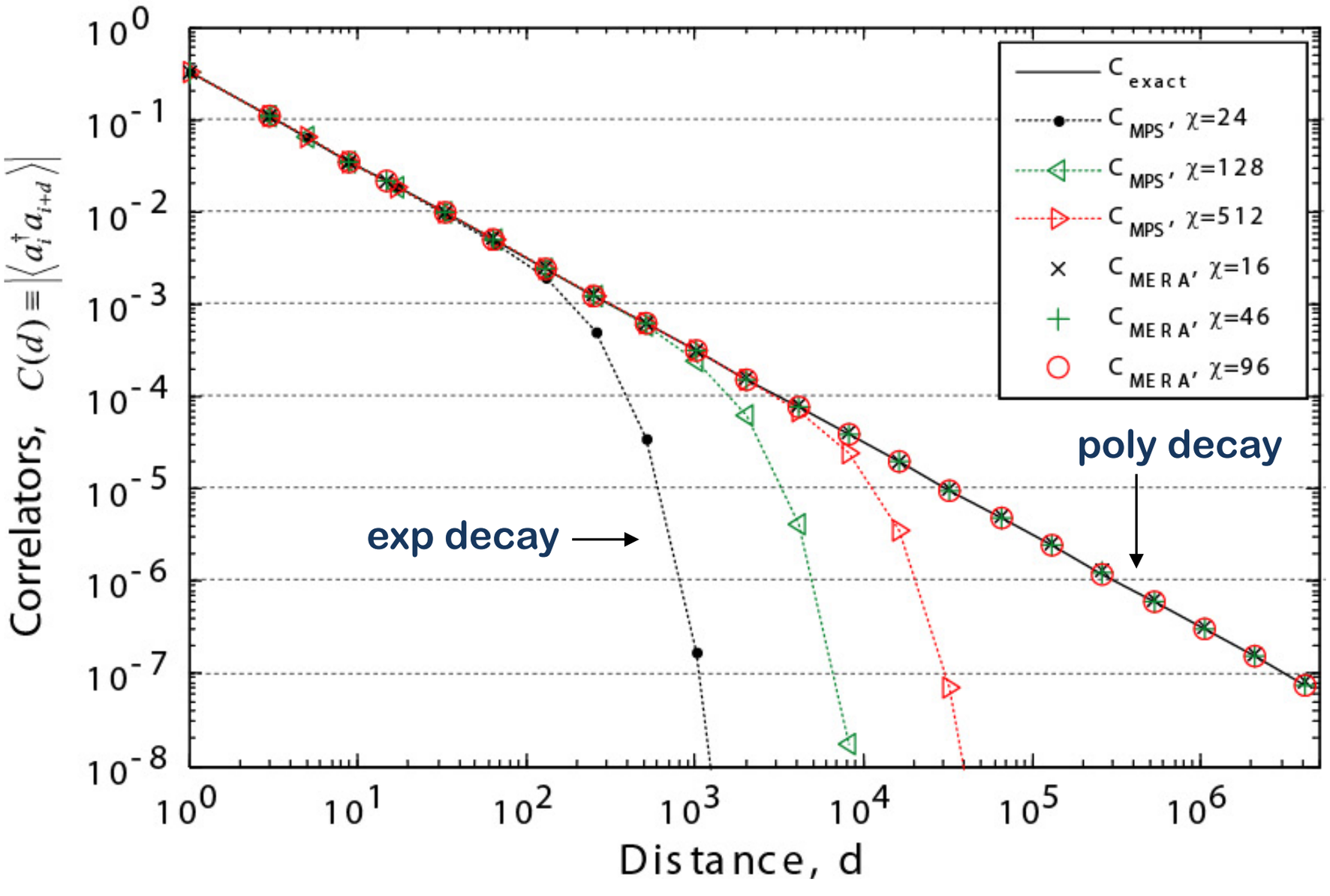
figures from Evenbly & Vidal, J Stat Phys **145** (2011)

Power-law decaying correlations

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

quantum XX model: (critical, c=1)

$$H_{\mathrm{XX}} = \sum_r \left(\sigma_r^X \sigma_{r+1}^X + \sigma_r^Y \sigma_{r+1}^Y \right)$$



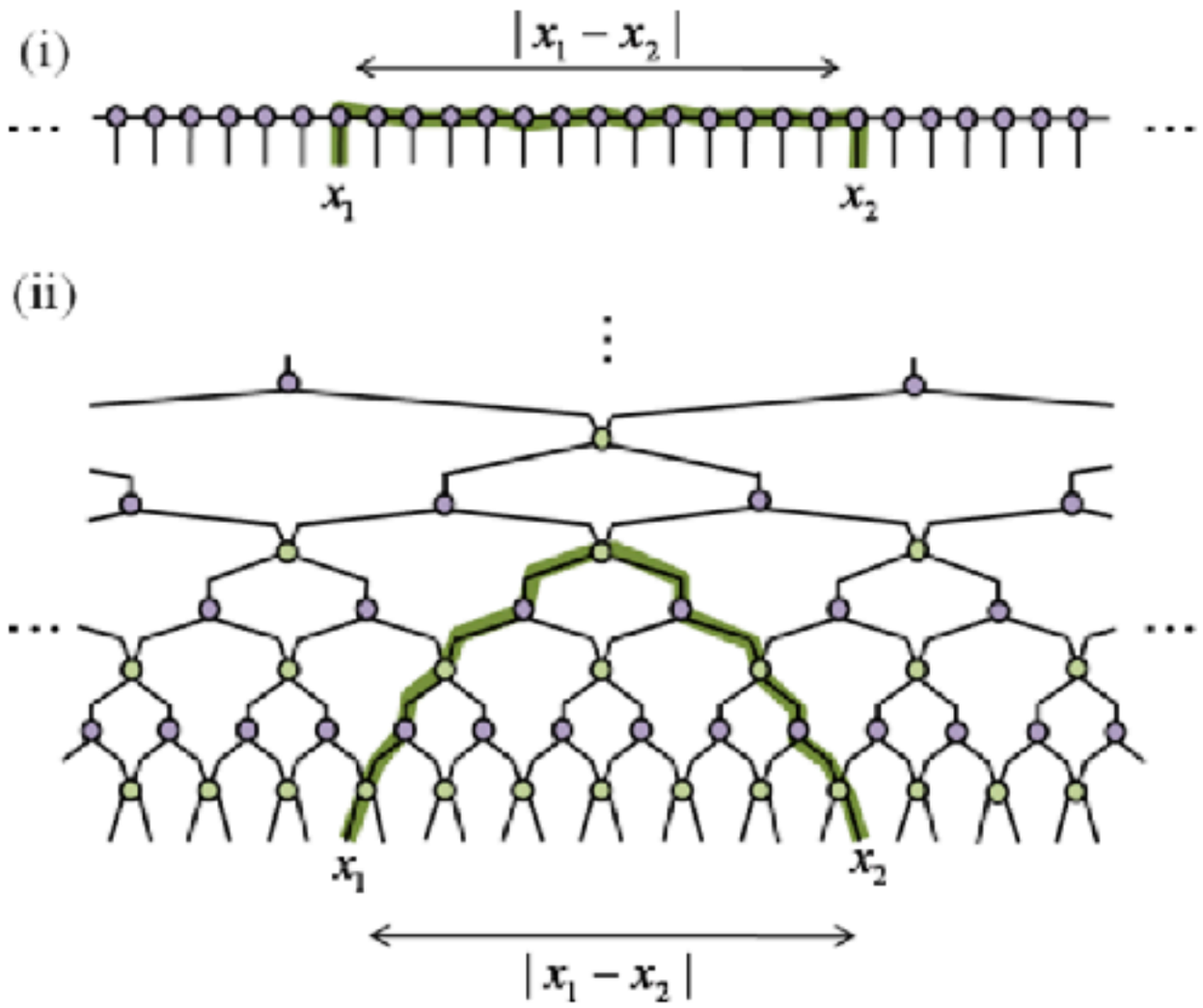
However, critical systems can still be studied with MPS!

slide from Glen Evenbly

Correlations

Correlations decay exponentially:

$$C(x_1, x_2) \approx e^{-\alpha D(x_1, x_2)}$$



$$D_{\text{phys}}(x_1, x_2) \approx |x_1 - x_2|$$

$$C_{\text{MPS}}(x_1, x_2) \approx e^{-\alpha D_{\text{phys}}(x_1, x_2)} \approx e^{-|x_1 - x_2|/\xi}$$

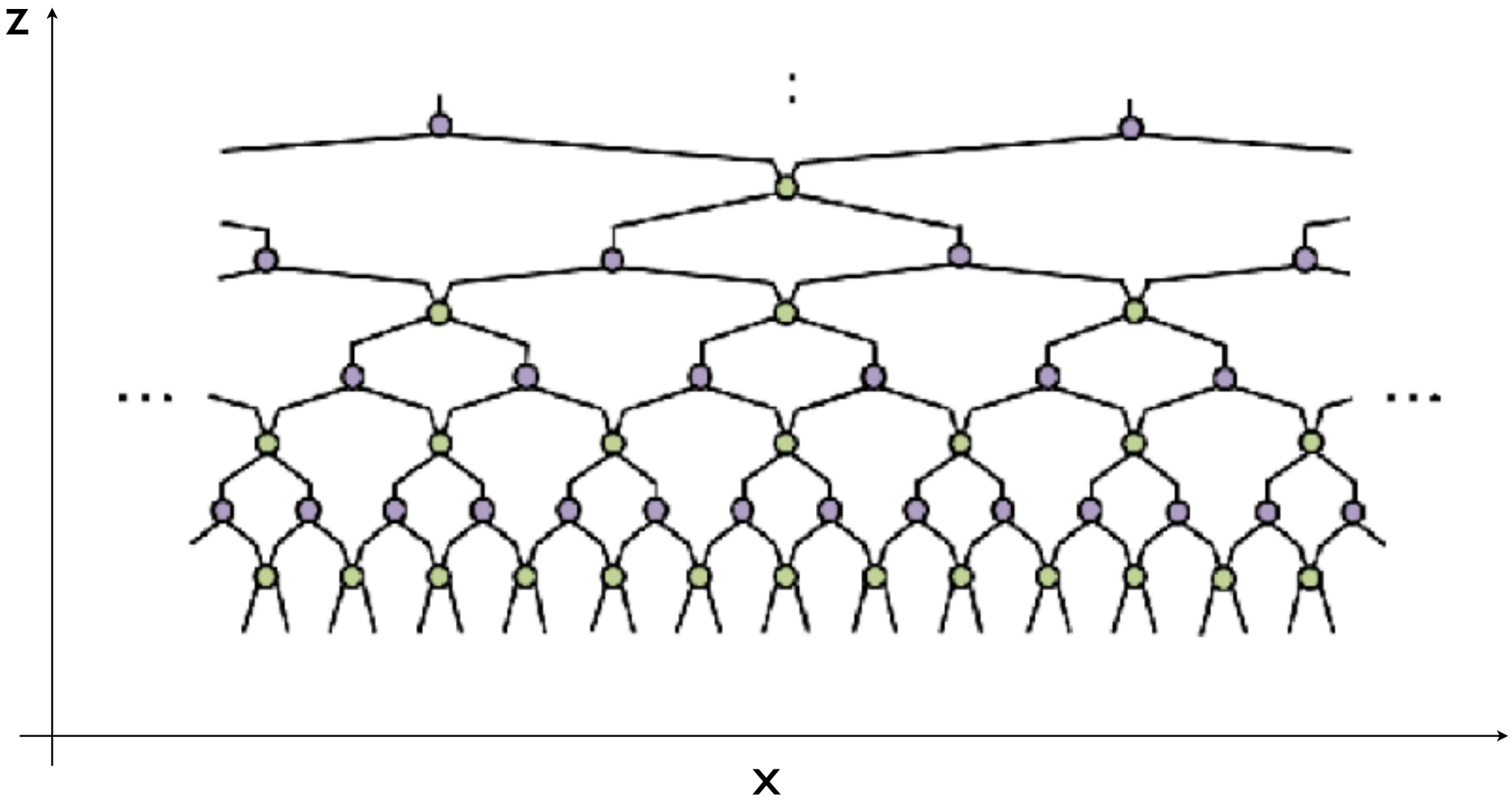
$$D_{\text{hol}}(x_1, x_2) \approx \log_2(|x_1 - x_2|)$$

$$C_{\text{MERA}}(x_1, x_2) \approx e^{-\alpha D_{\text{hol}}(x_1, x_2)}$$

$$\approx e^{-q \log_2(|x_1 - x_2|)} = |x_1 - x_2|^{-q}$$

Evenbly and G. Vidal, J Stat Phys **145**, 891(2011).

Scale invariant MERA



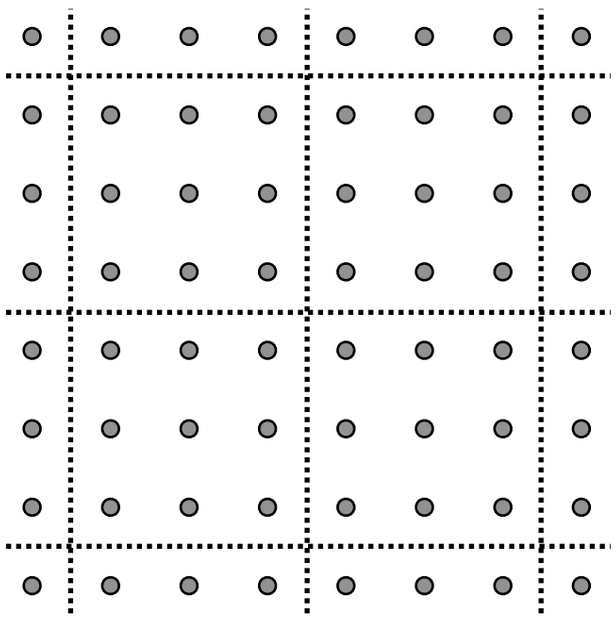
Translational invariance: *same tensors along x*

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

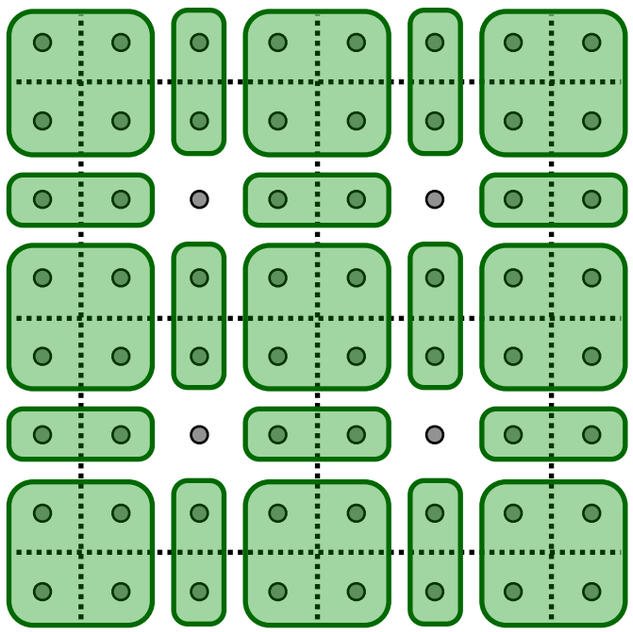
2D MERA (top view)

Evenbly, Vidal. PRL 102, 180406 (2009)

Original lattice



Apply disentanglers

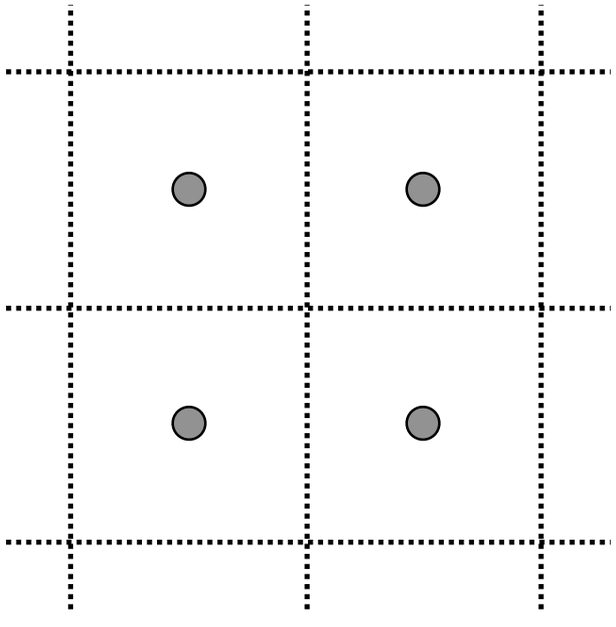


✓ Accounts for area-law in 2D systems

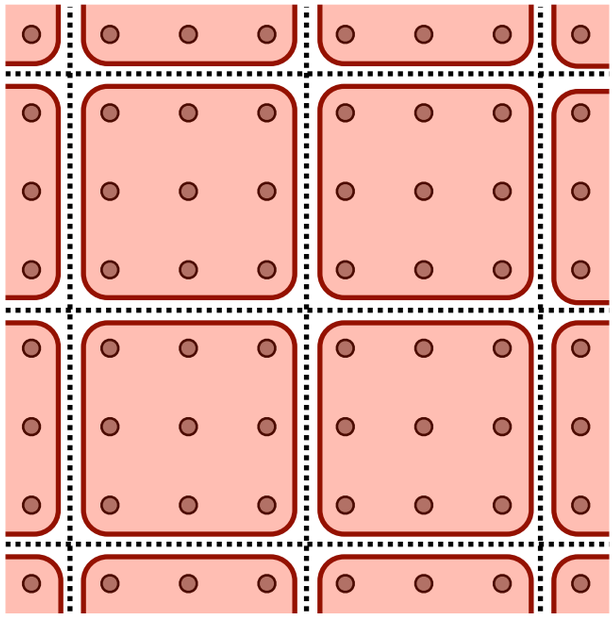
$$S(L) \sim L$$

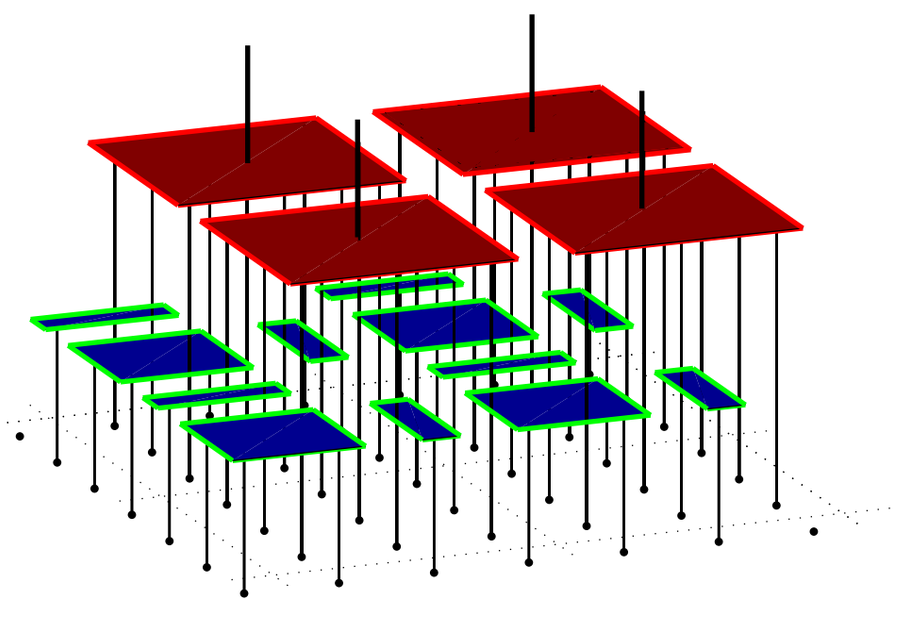
$$\chi_\tau = const$$

Coarse-grained lattice

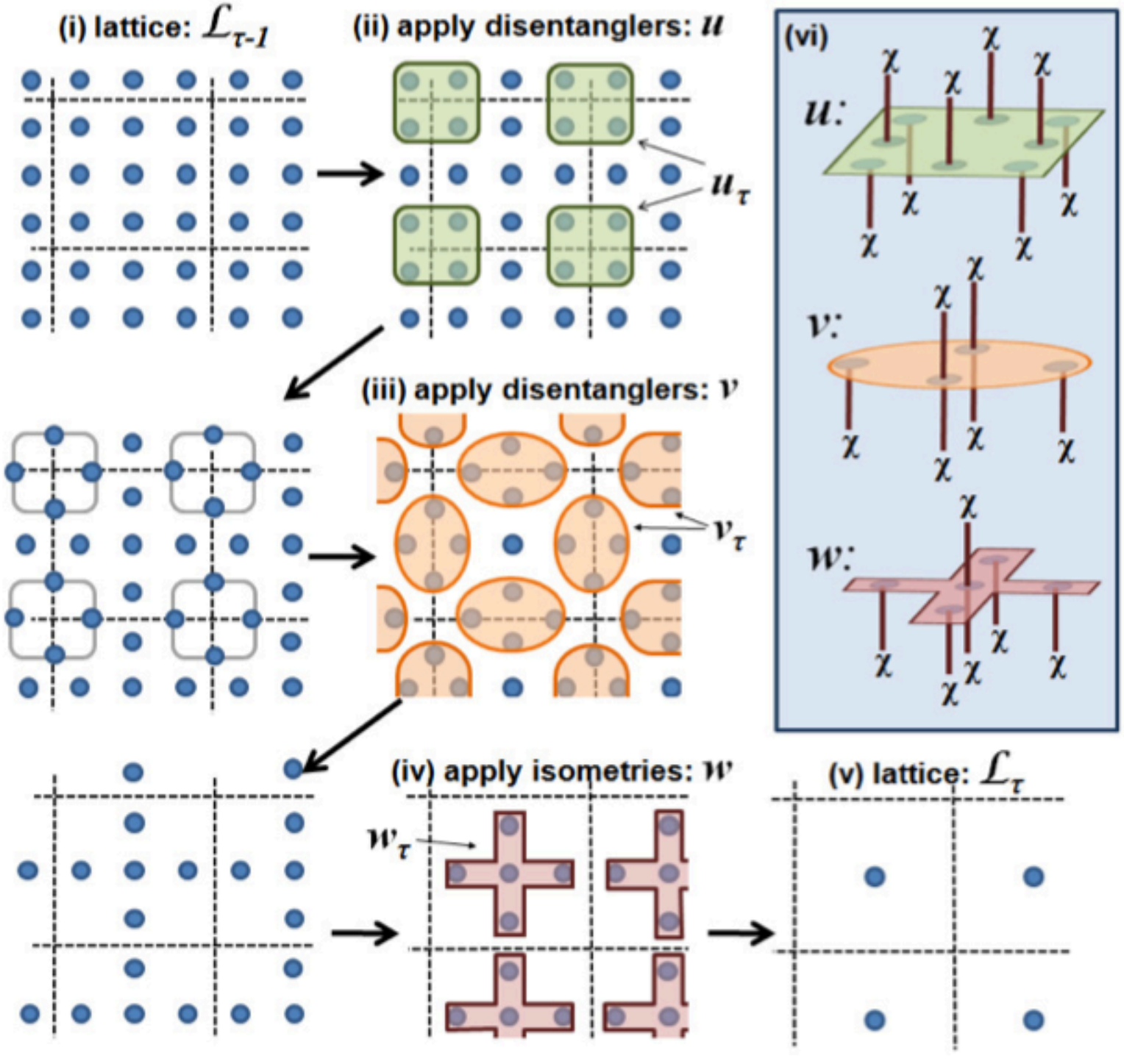


Apply isometries



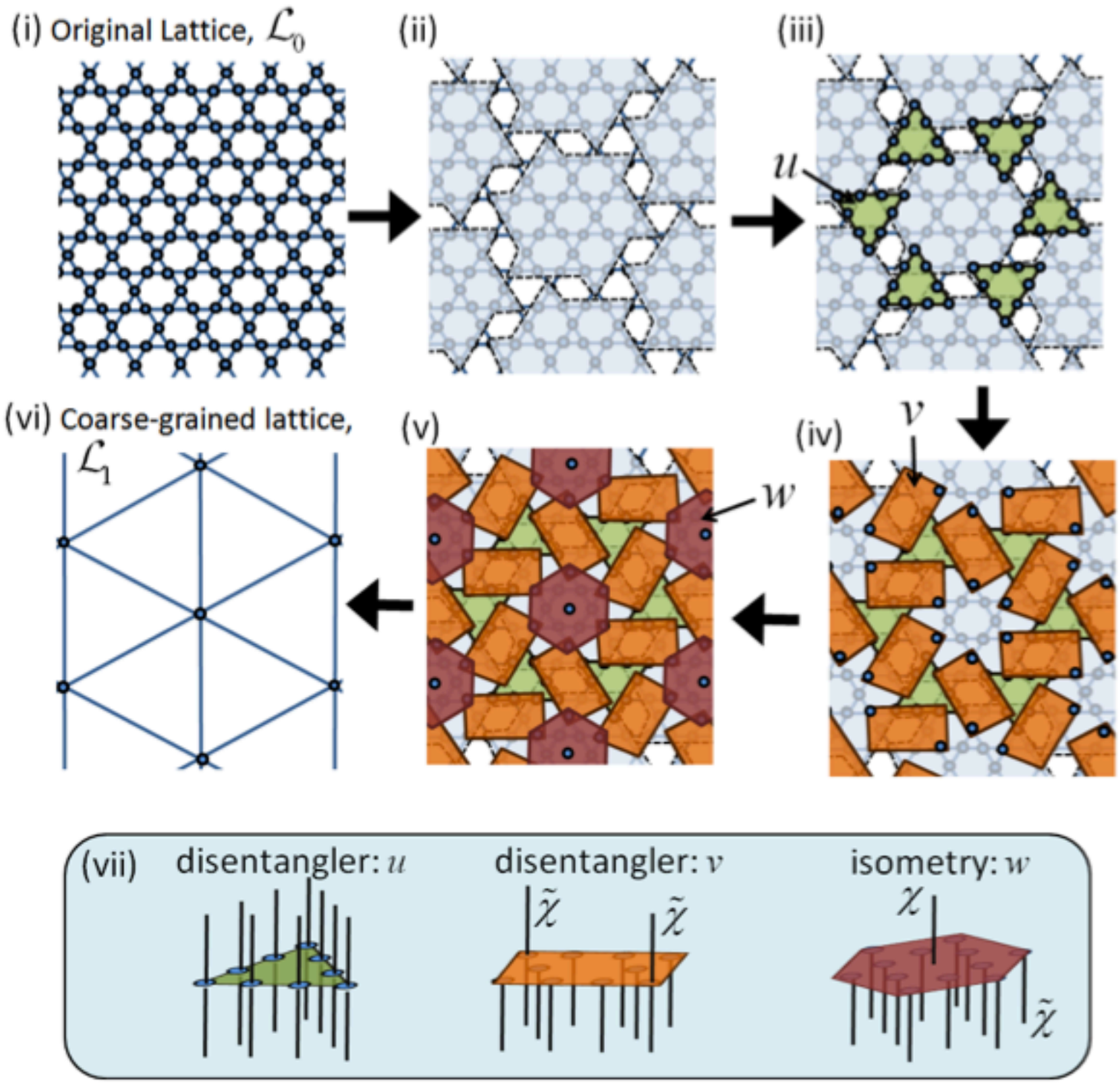


Different structures of the 2D MERA...



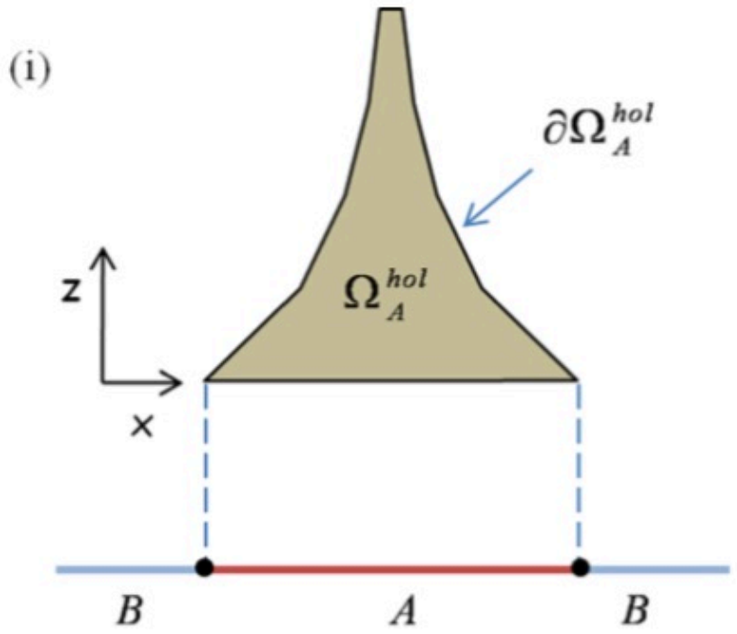
Evenbly & Vidal, PRL **102**, 180406 (2009)

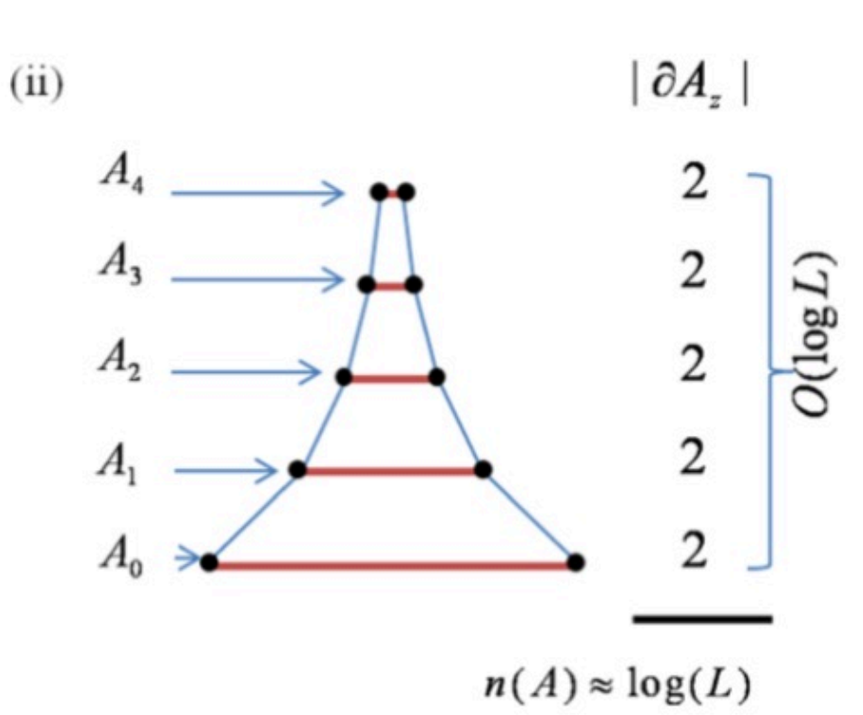
2D MERA on the Kagome lattice



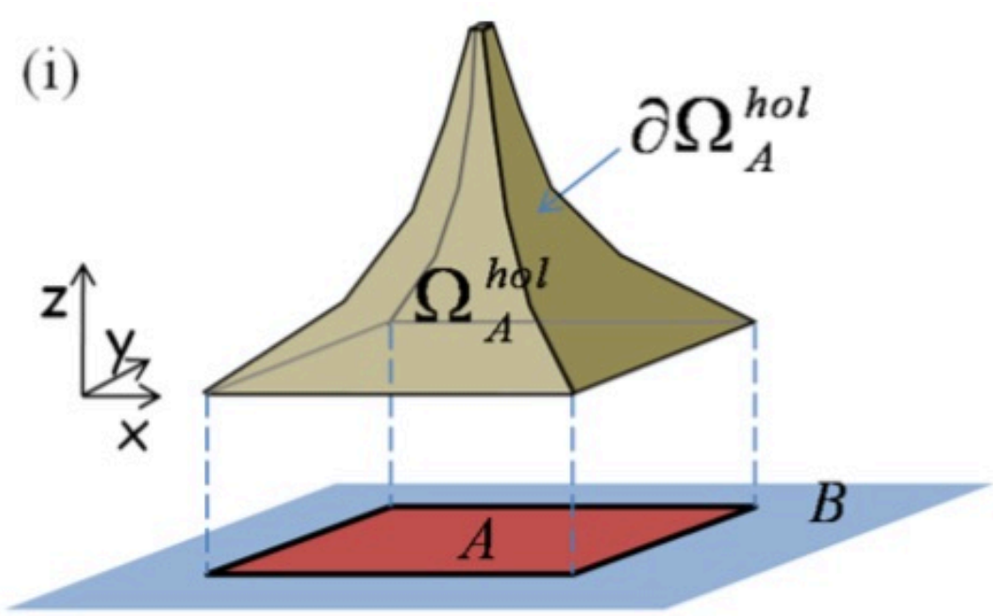
Evenbly & Vidal, PRL 104, 187203 (2010)

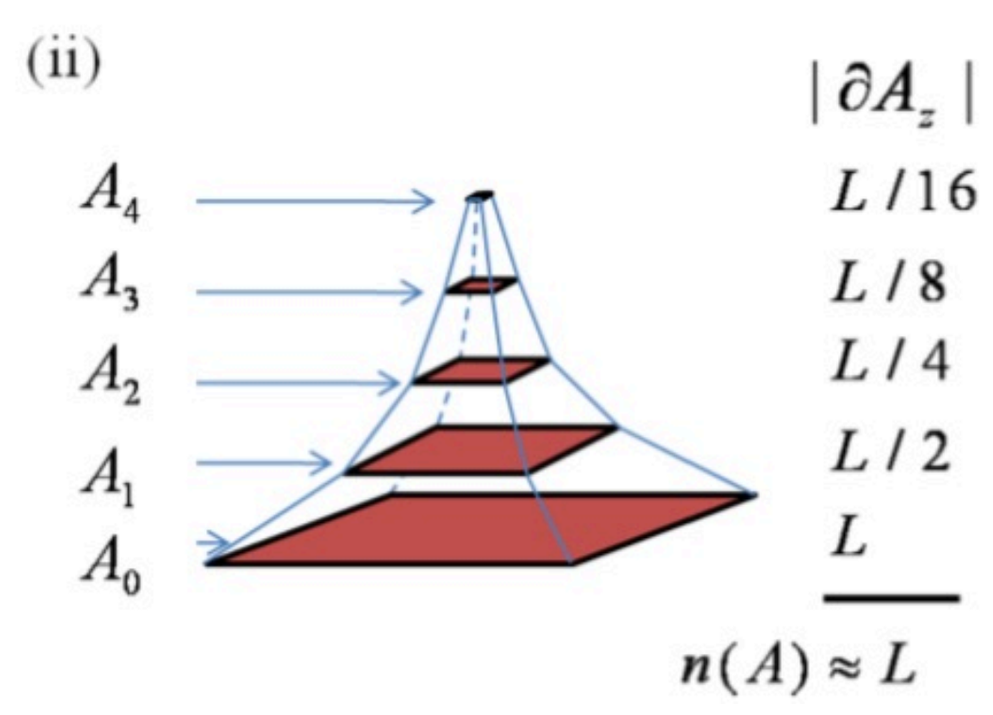
1D vs 2D MERA





same number of
connections in each layer

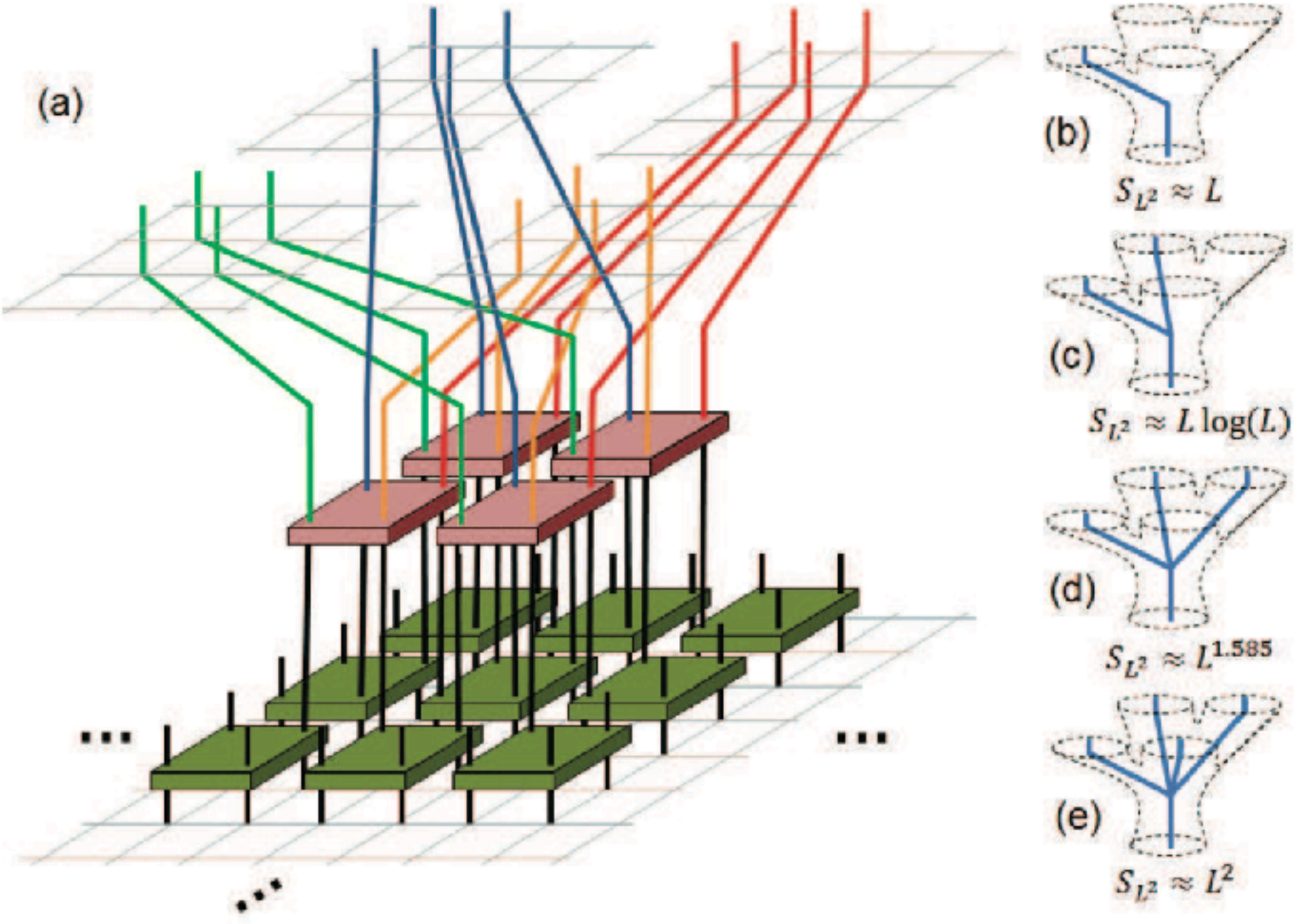




decreasing number
of connections

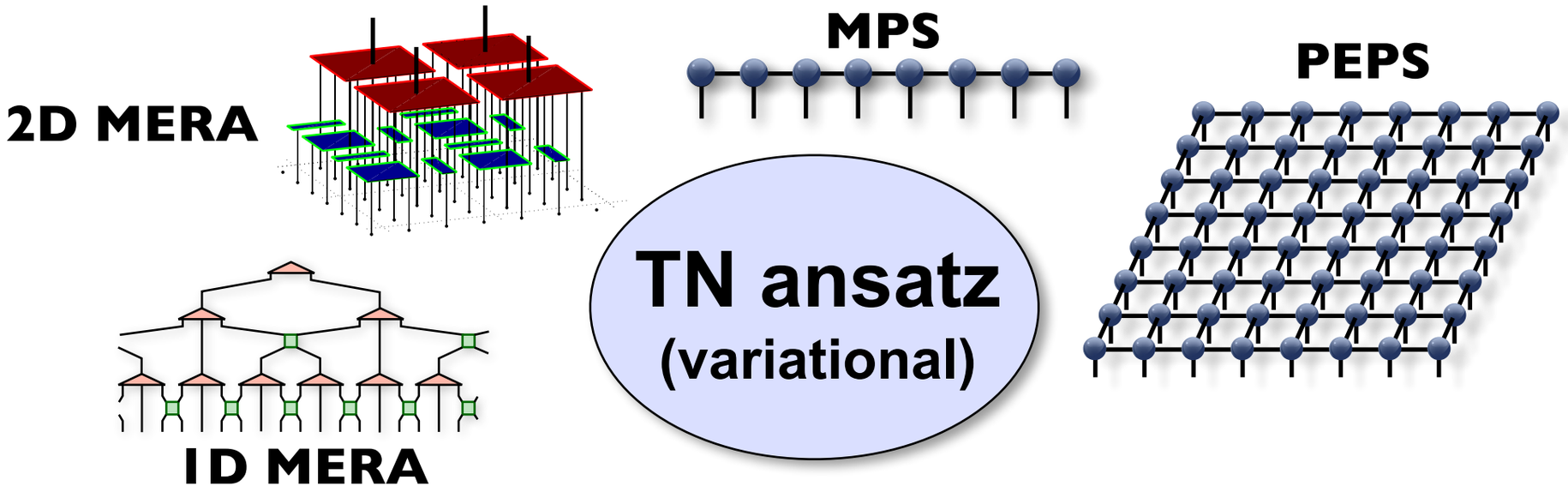
Evenbly and G. Vidal, J Stat Phys **145**, 891(2011).

Branching MERA: beyond area law scaling in 2D



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

PART I summary: Tensor network ansätze



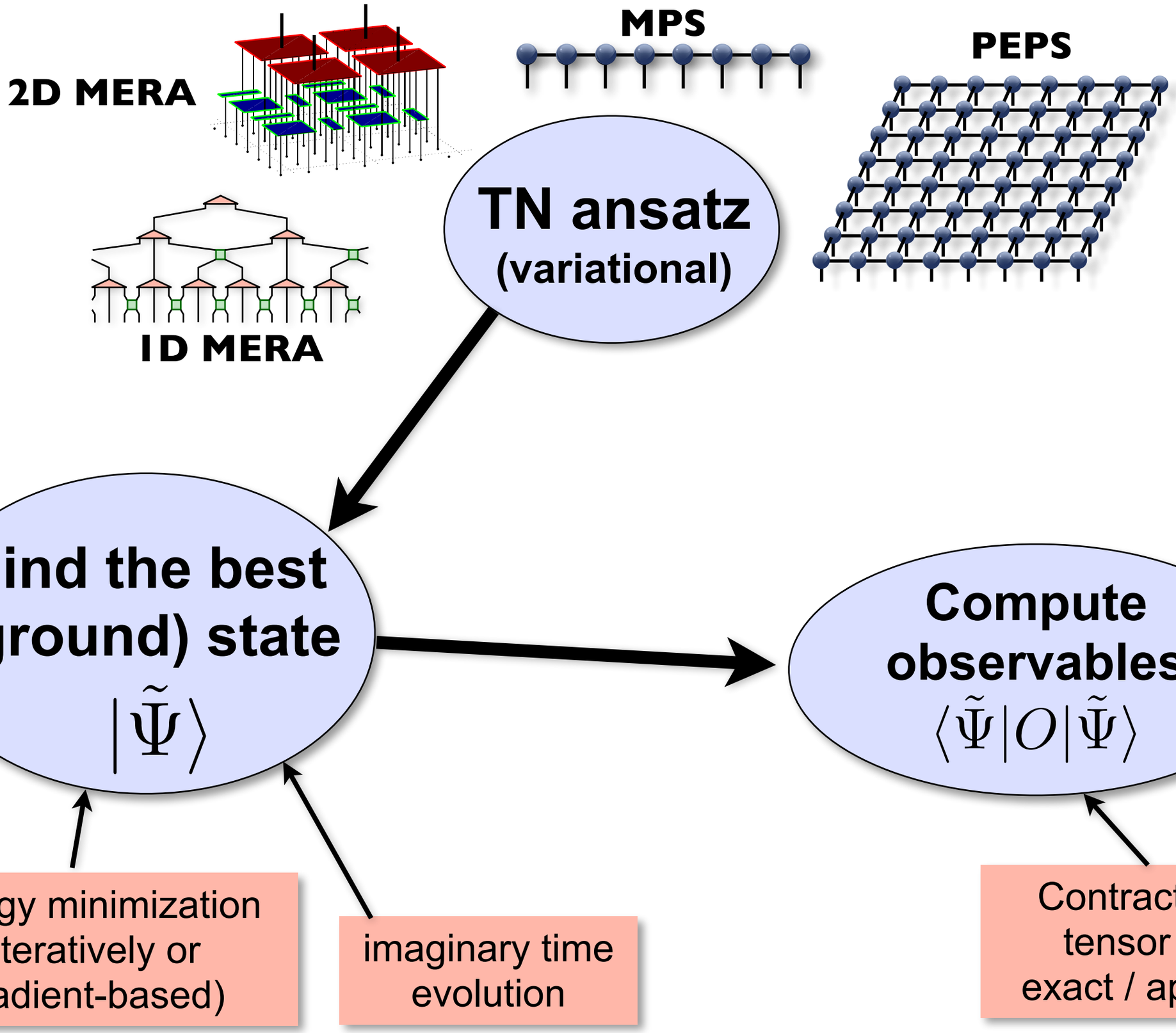
➡ A tensor network ansatz is an efficient variational ansatz for ground states of local H where the accuracy can be systematically controlled

➡ 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)

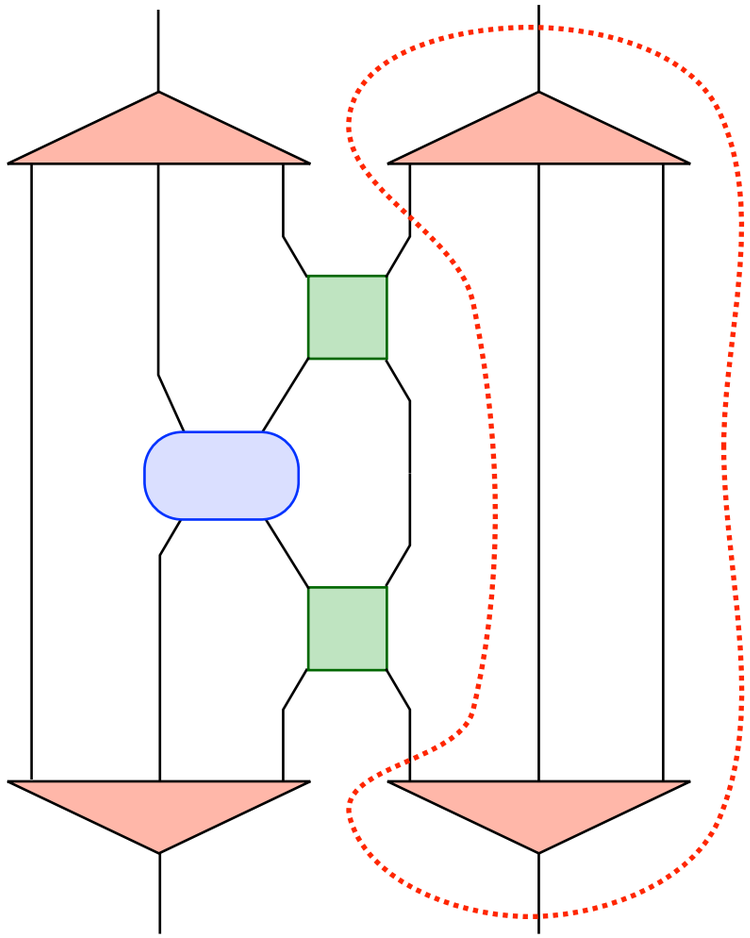
➡ But nevertheless, MPS may still be used to study critical or finite 2D systems

Overview: Tensor network algorithms (ground state)

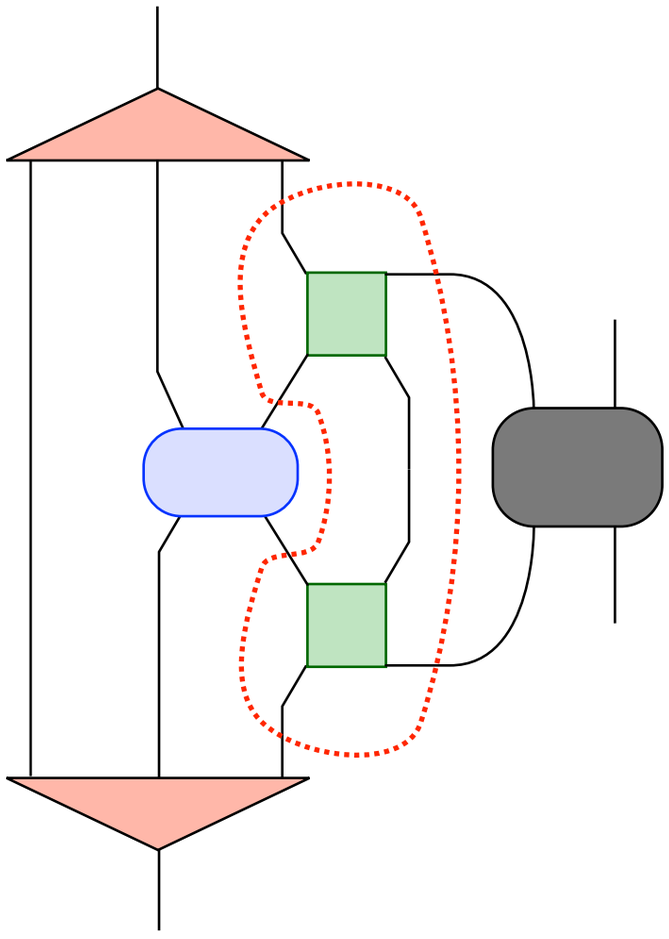


PART II: Contraction

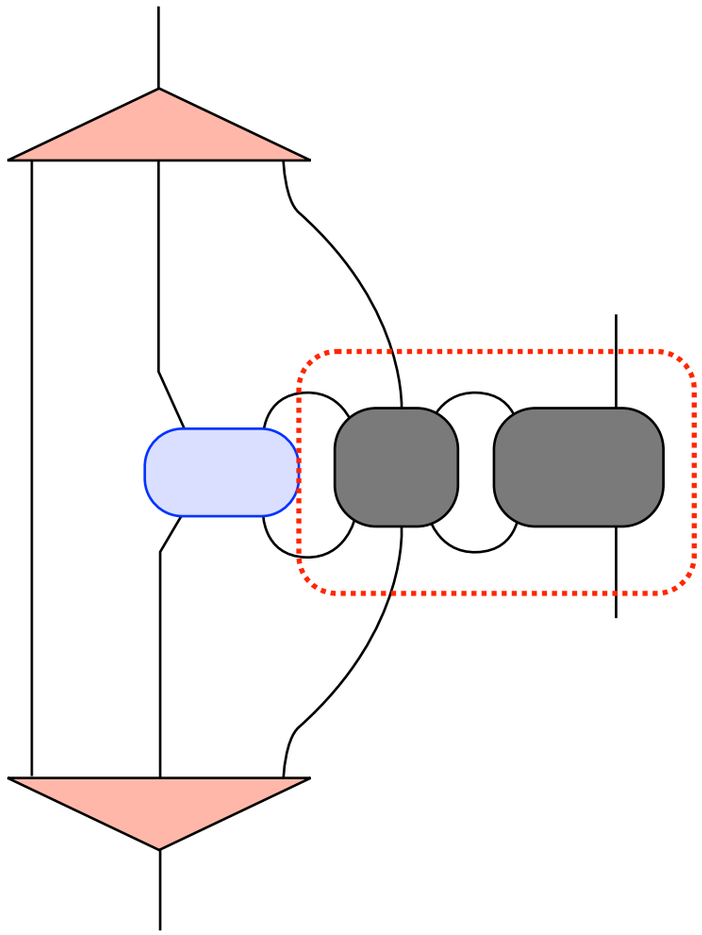
Contracting a tensor network (repetition)



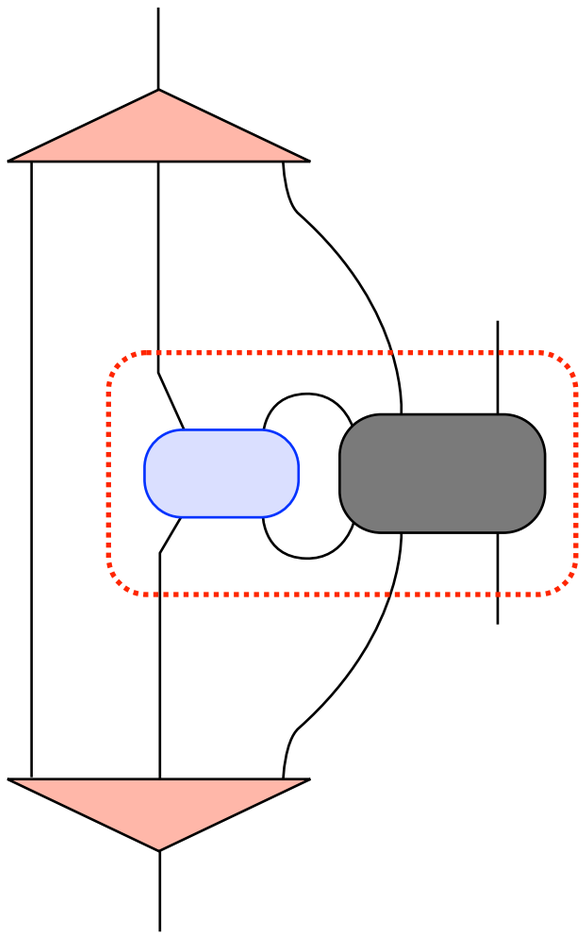
Pairwise contractions...



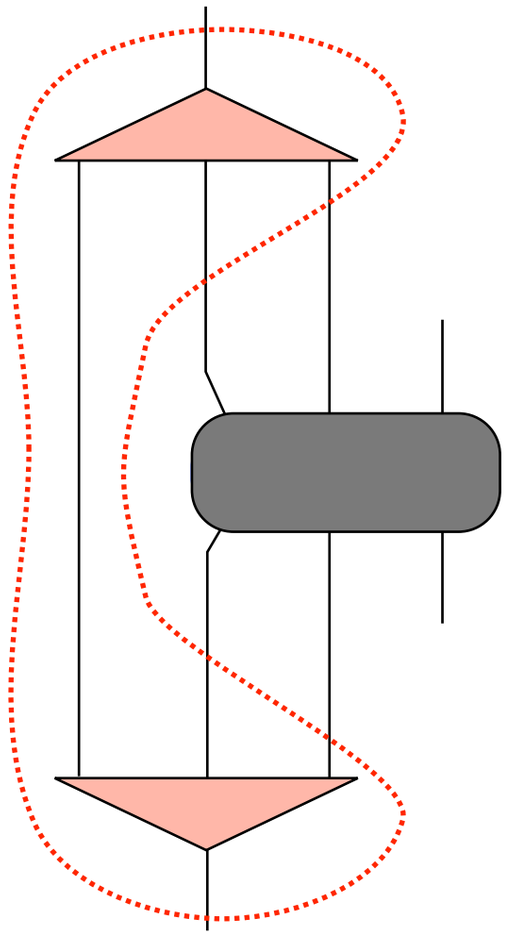
Pairwise contractions...



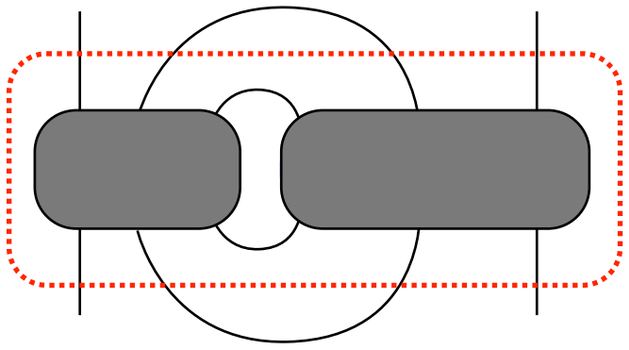
Pairwise contractions...



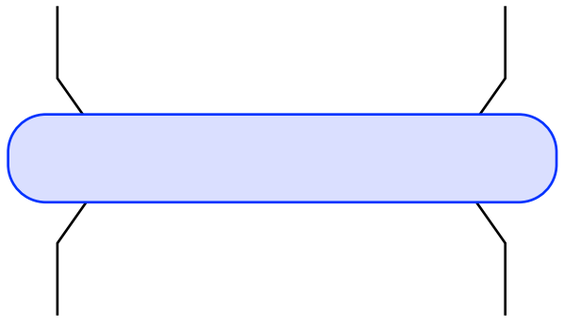
Pairwise contractions...



Pairwise contractions...



Pairwise contractions...

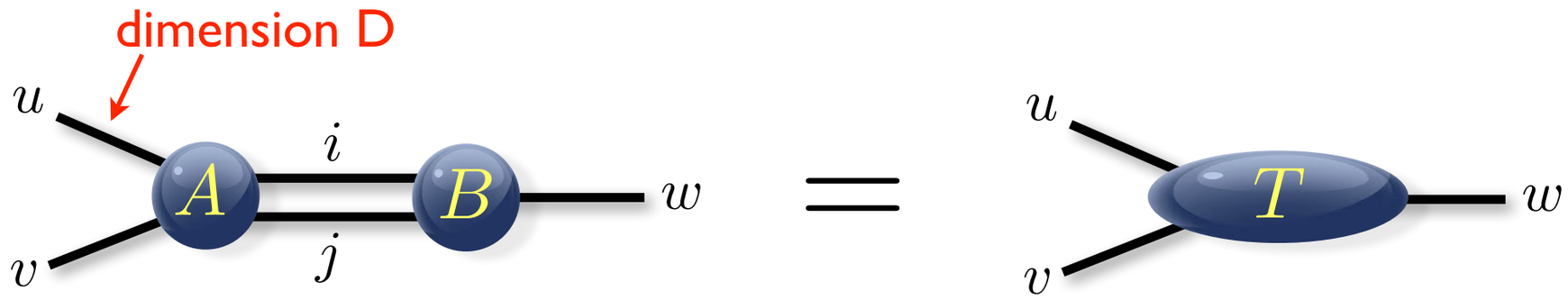


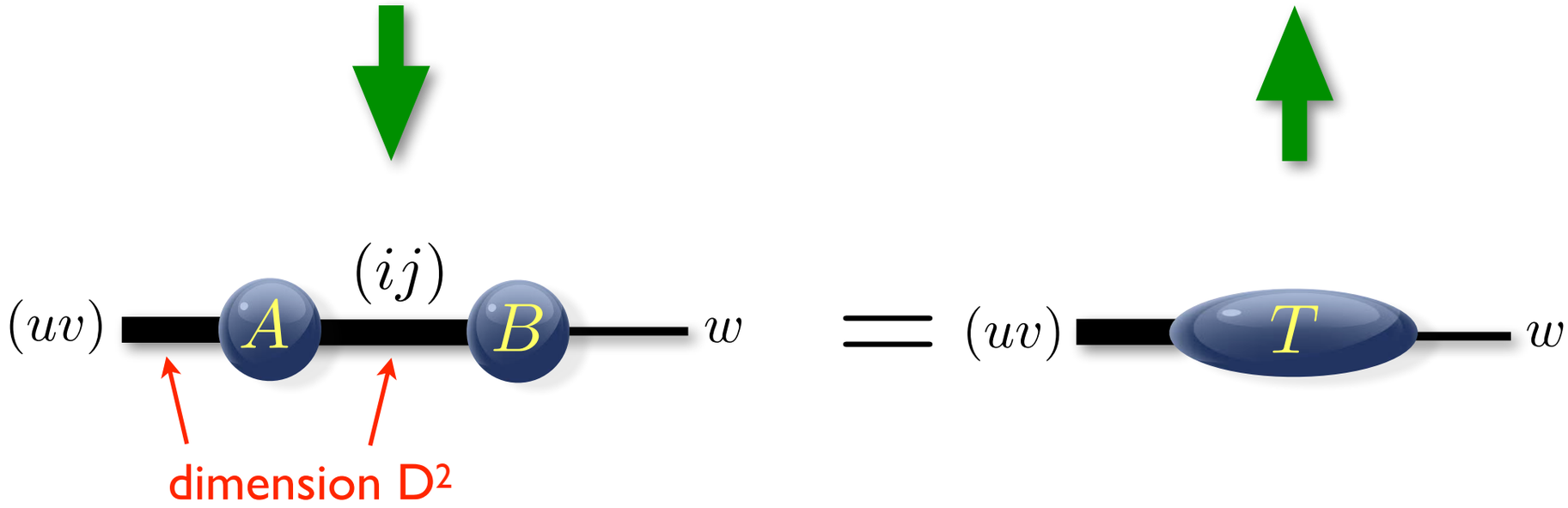
done!

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

Contracting a tensor network

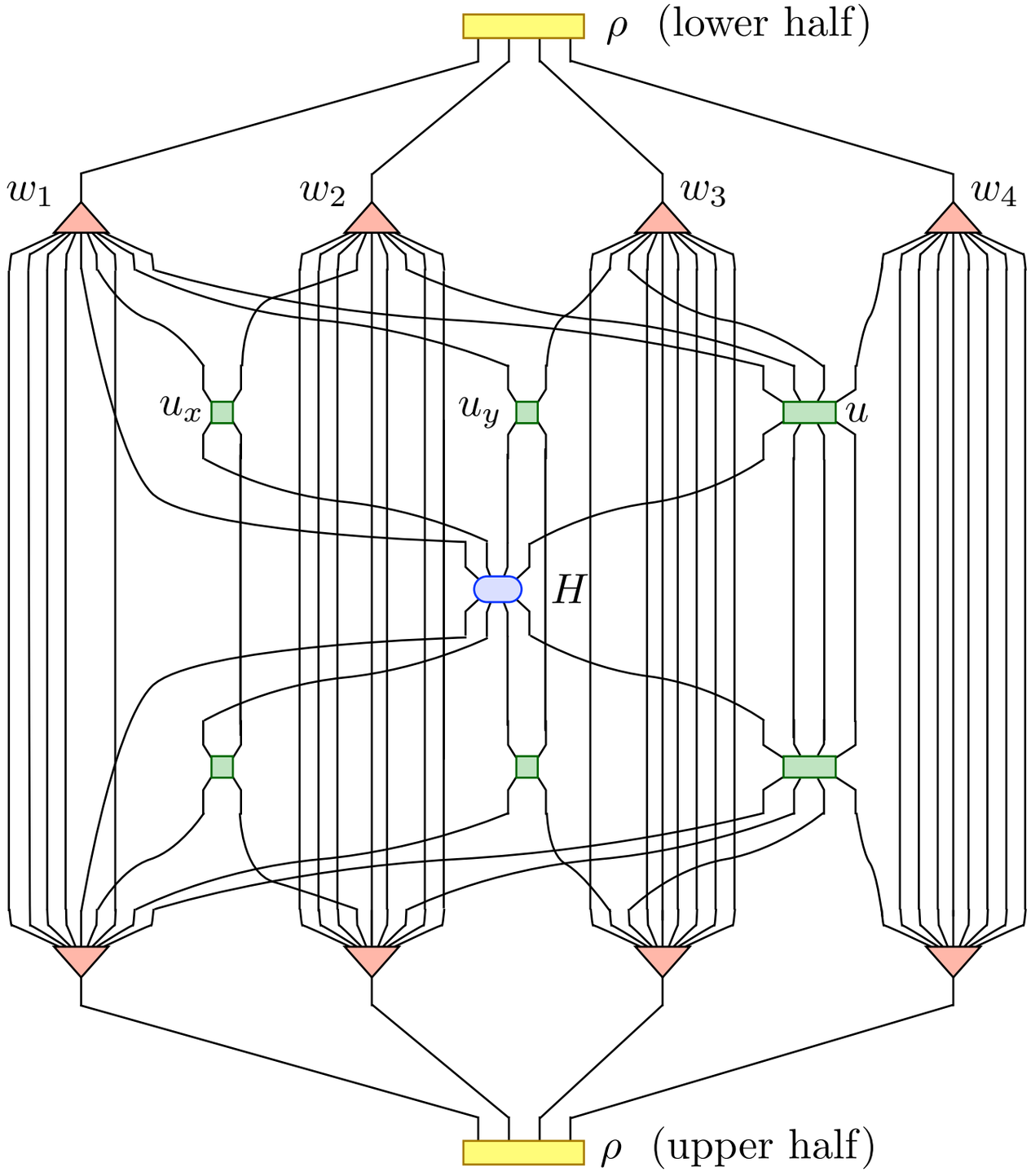
★ Reshape tensors into matrices and multiply them with optimized routines (BLAS)





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

Contraction: Example from the 2D MERA



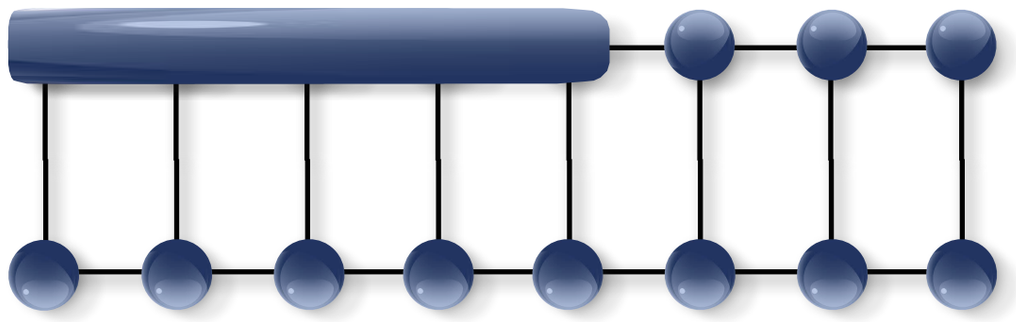
What is the optimal contraction order?

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

Pfeifer, Haegeman, Verstraete, PRE 90 (2014)

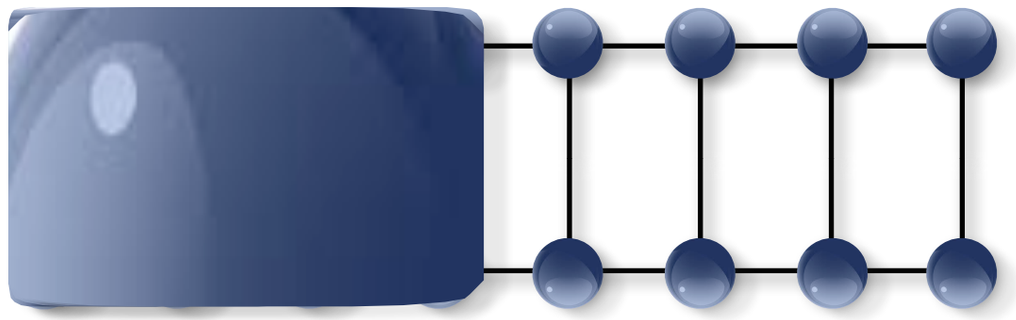
Contracting an MPS

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



BAD!

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

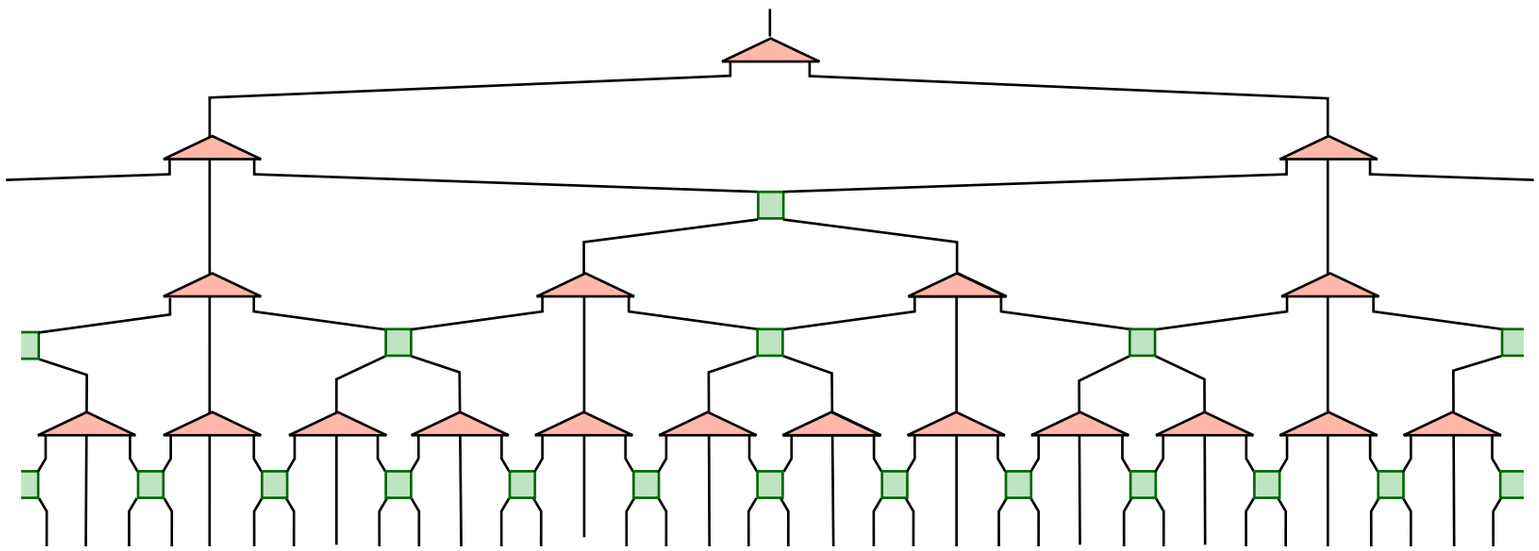


Good!

MERA: Contraction

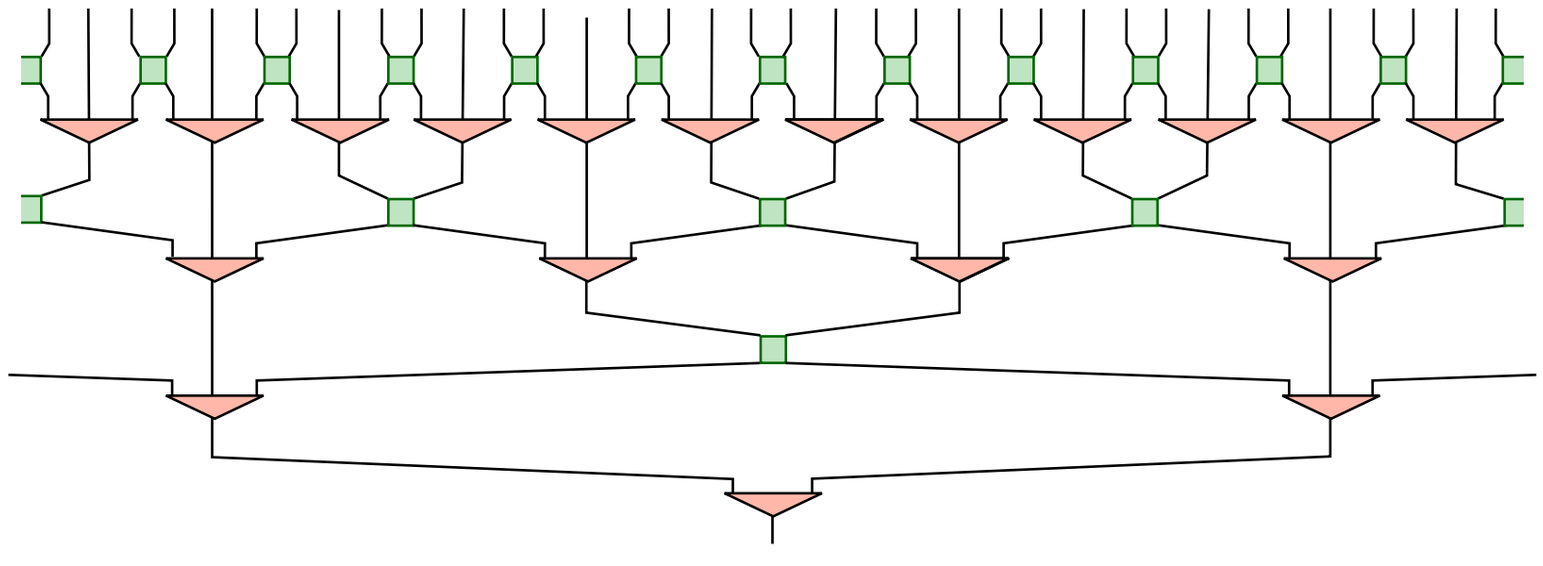
Let's compute $\langle\Psi|O|\Psi\rangle$ O: two-site operator

$|\Psi\rangle$

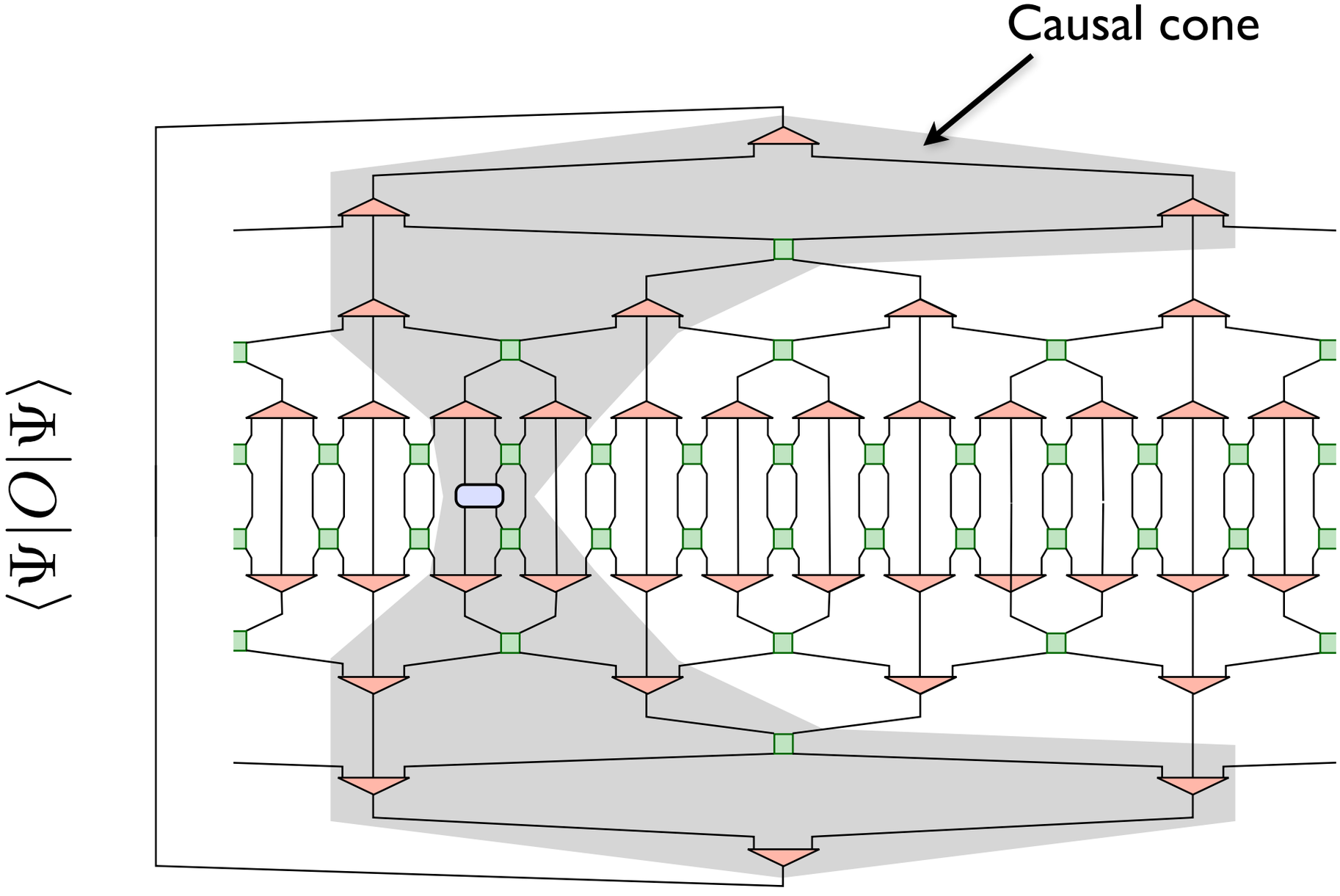


O

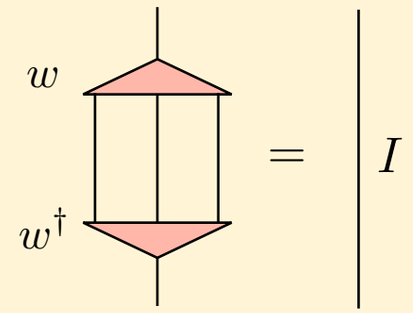
$\langle\Psi|$



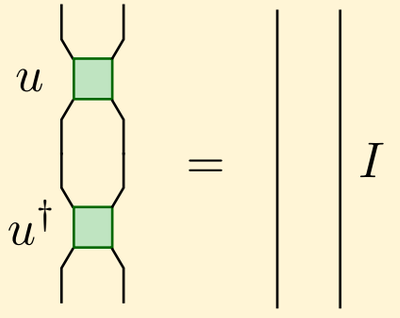
MERA: Contraction



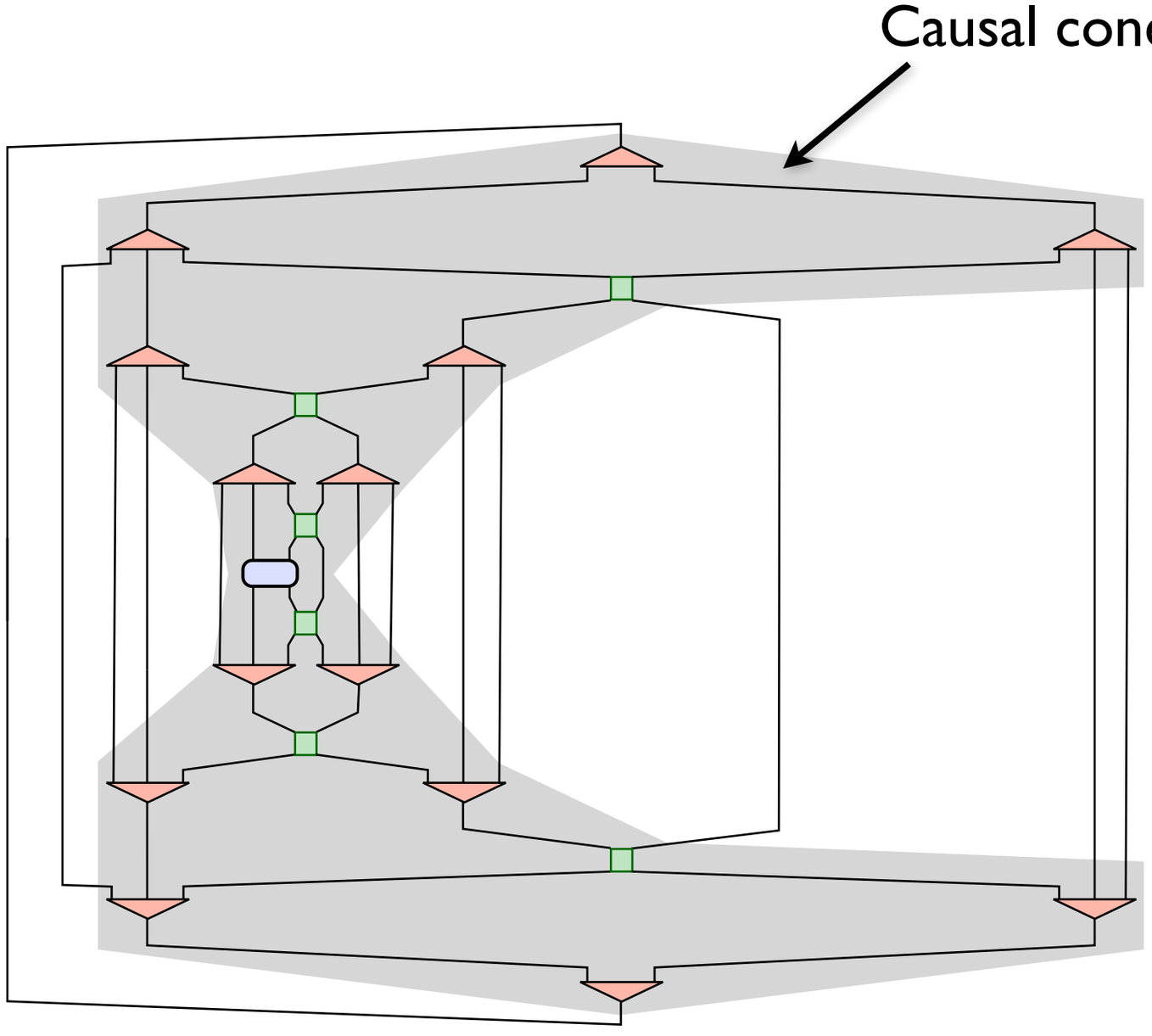
Isometries are *isometric*



Disentanglers are *unitary*

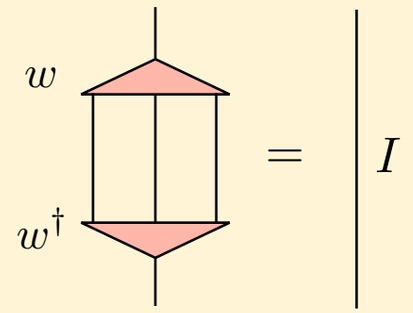


MERA: Contraction

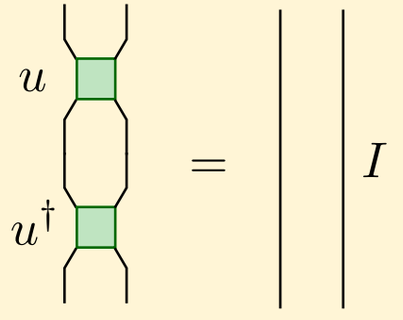


$\langle\Psi|O|\Psi\rangle$

Isometries are *isometric*



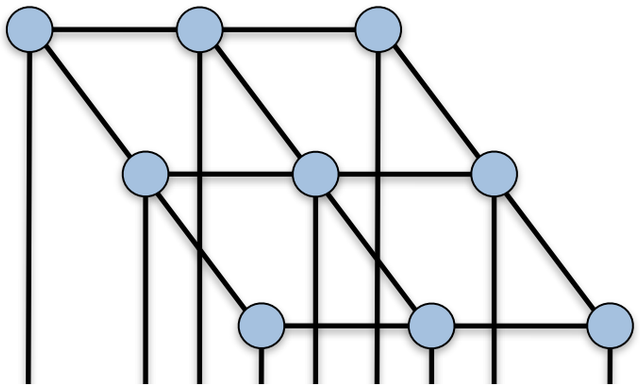
Disentanglers are *unitary*

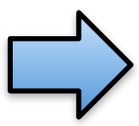


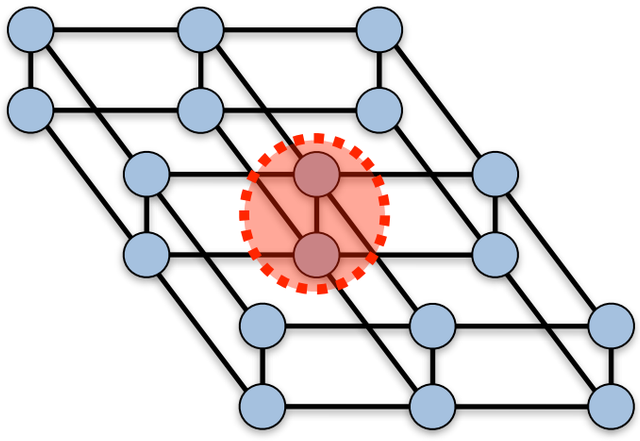
Efficient computation of expectation values of observables!

Contracting the PEPS

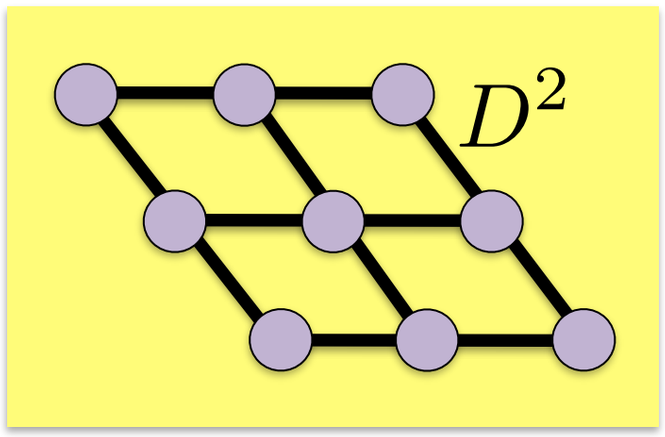
$\langle \Psi | \Psi \rangle$

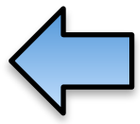


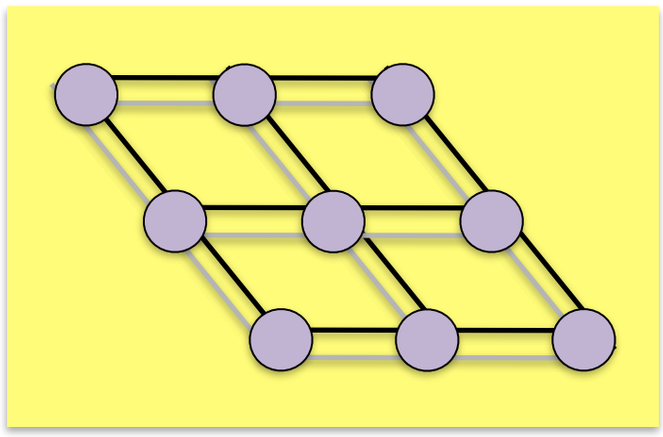




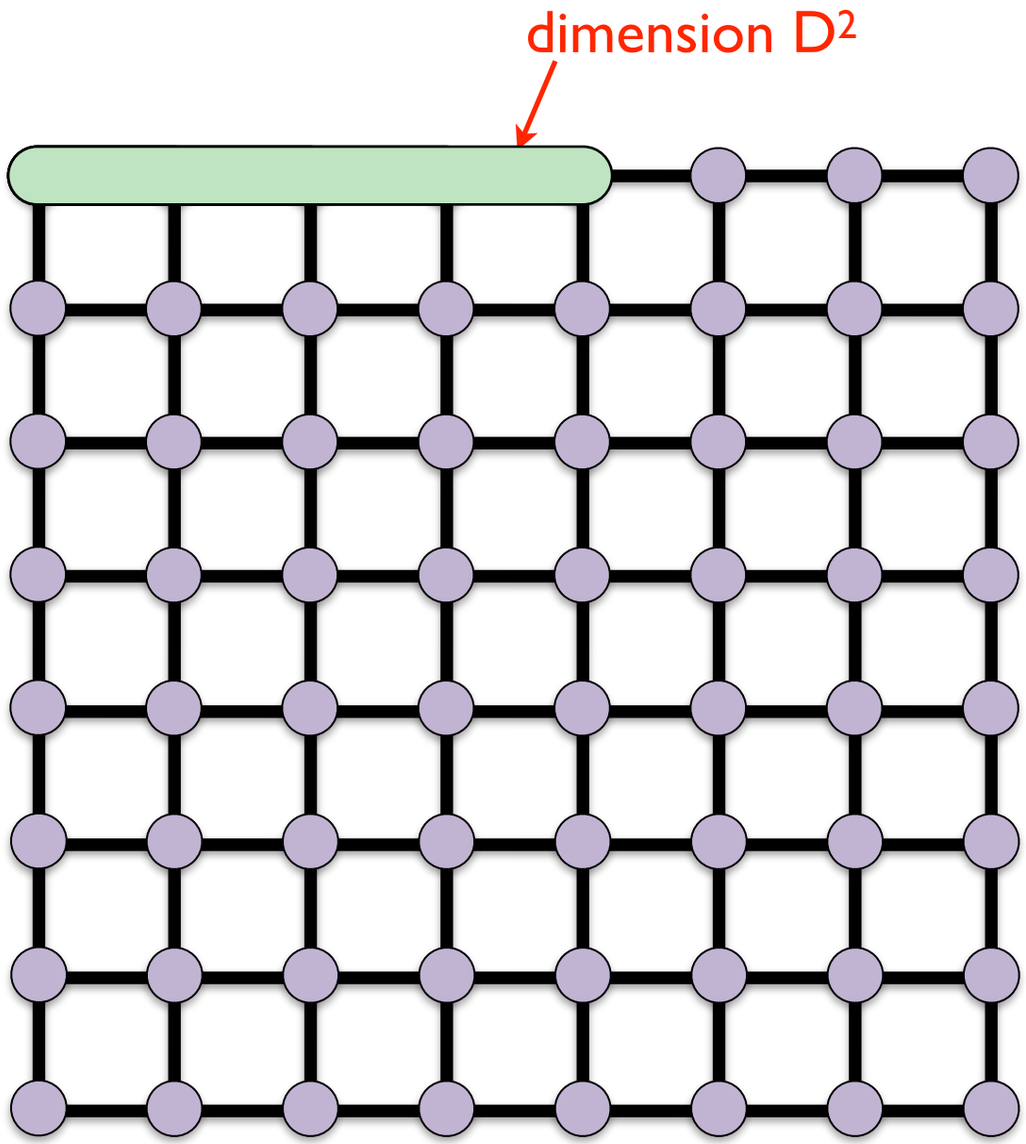
reduced tensors







Contracting the PEPS



Problem:

exact contraction ~ D^{2L}

O(exp(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, PRB 98 (2018)
…

TRG

Tensor Renormalization Group

(variants: HOTRG, SRG, HOSRG)

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

★ 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 $\chi \sim D^2$

TNR

Tensor Network Renormalization

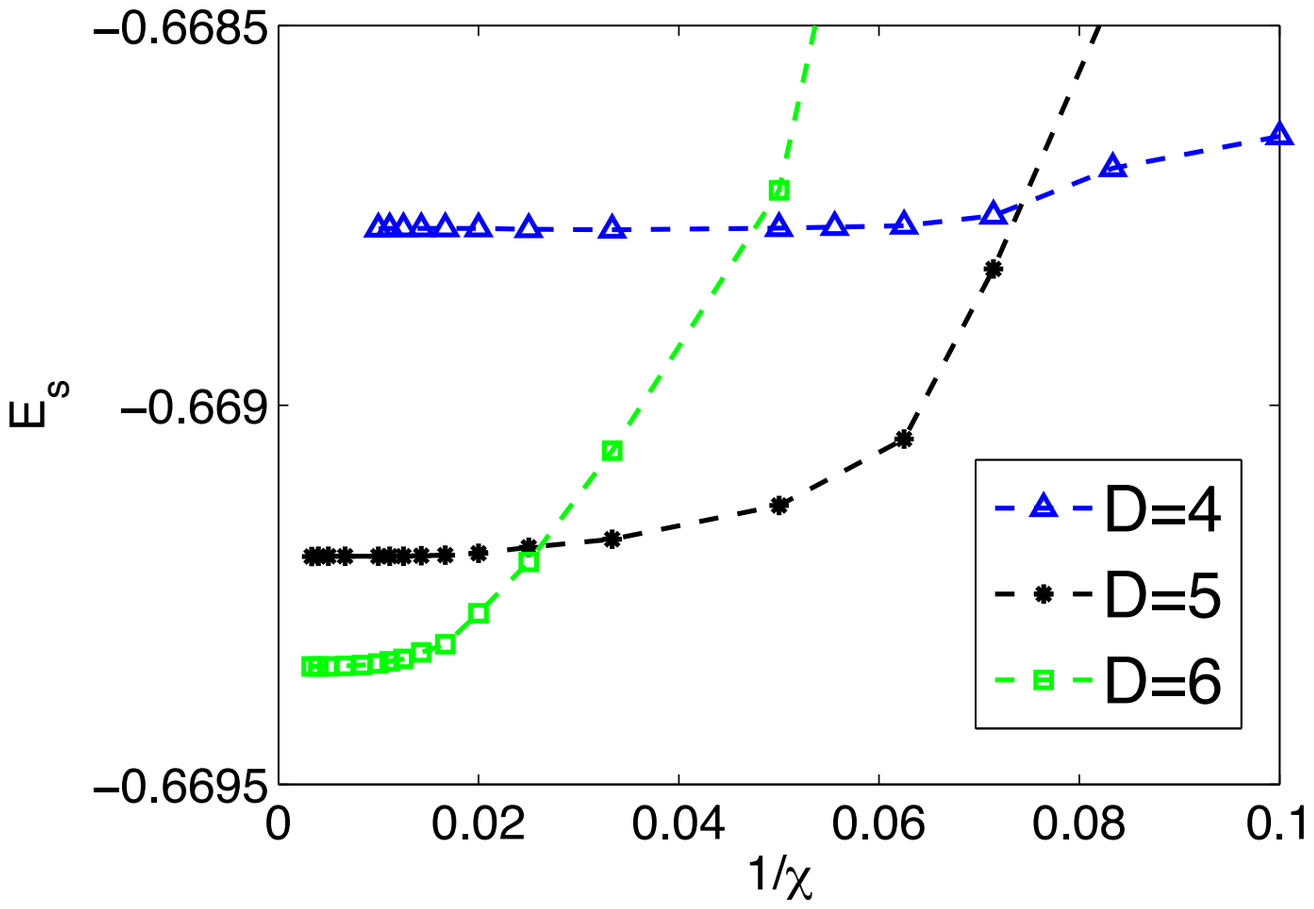
Evenbly & Vidal, PRL 115 (2015)

Loop-TNR:

Yang, Gu & Wen, PRL 118 (2017)

Contracting the PEPS

Example: 2D Heisenberg model (CTM)



★ 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

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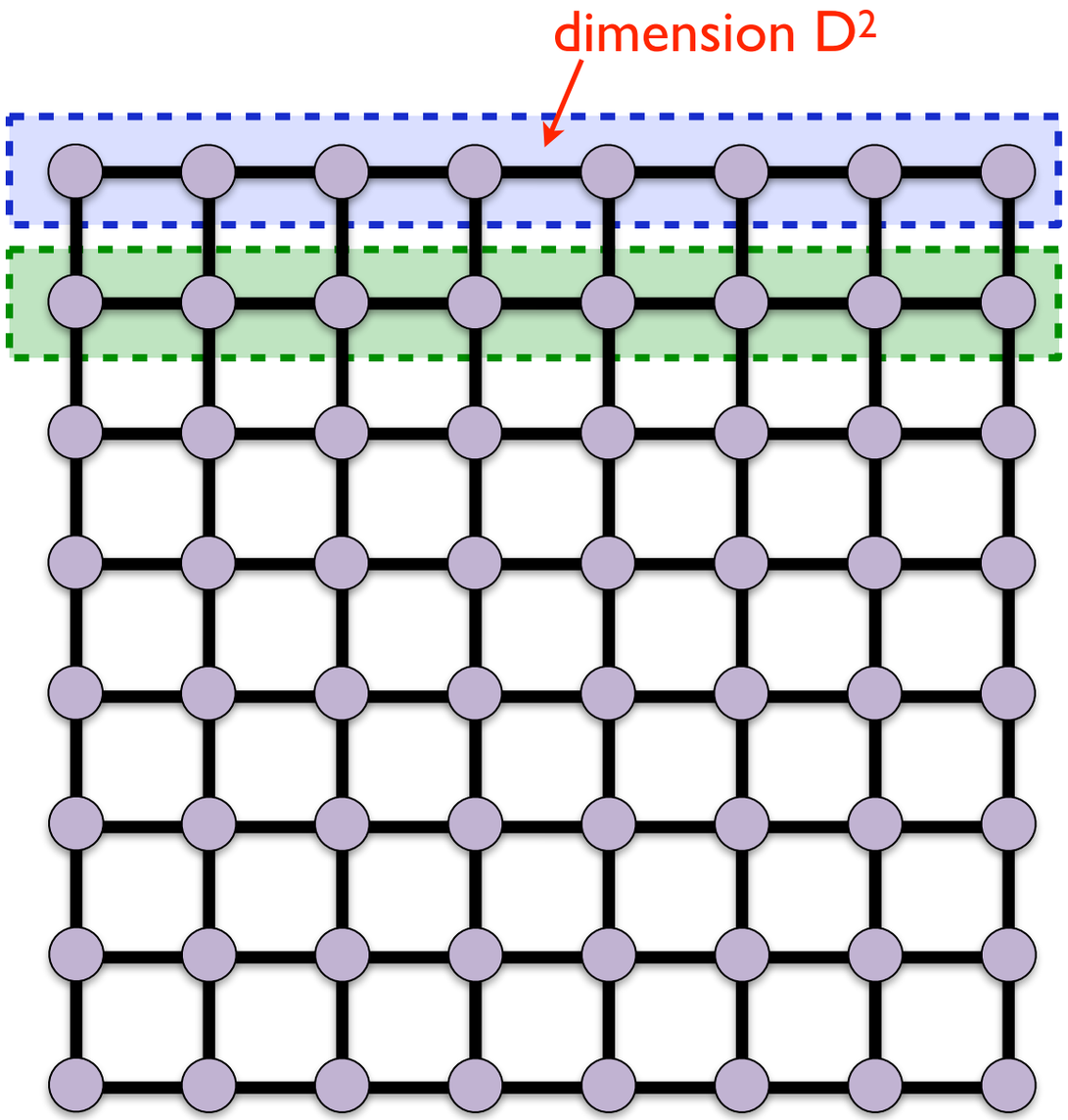
Contracting the PEPS using an MPS

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

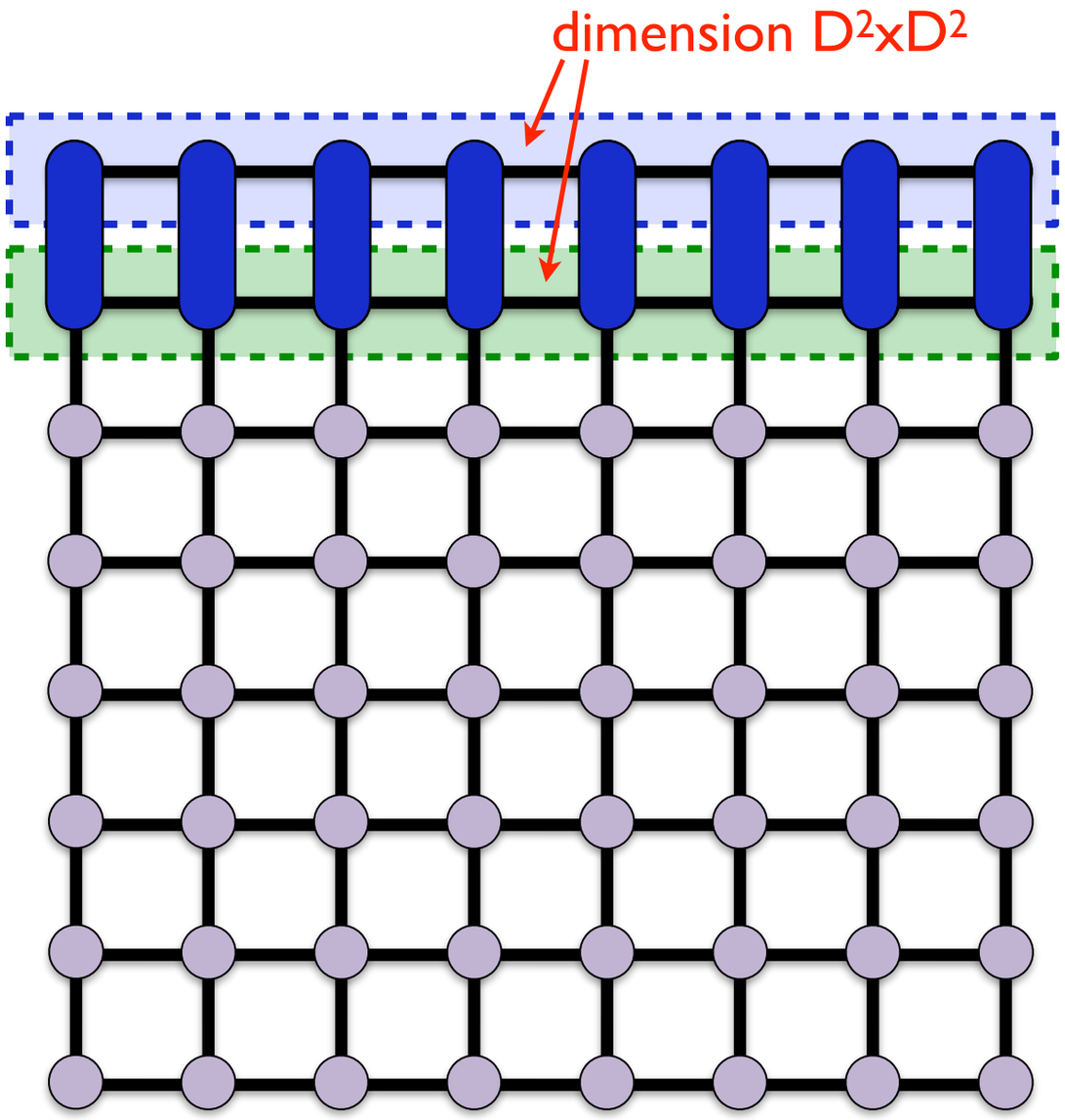


this is an MPS

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 $D^2 \times D^2$

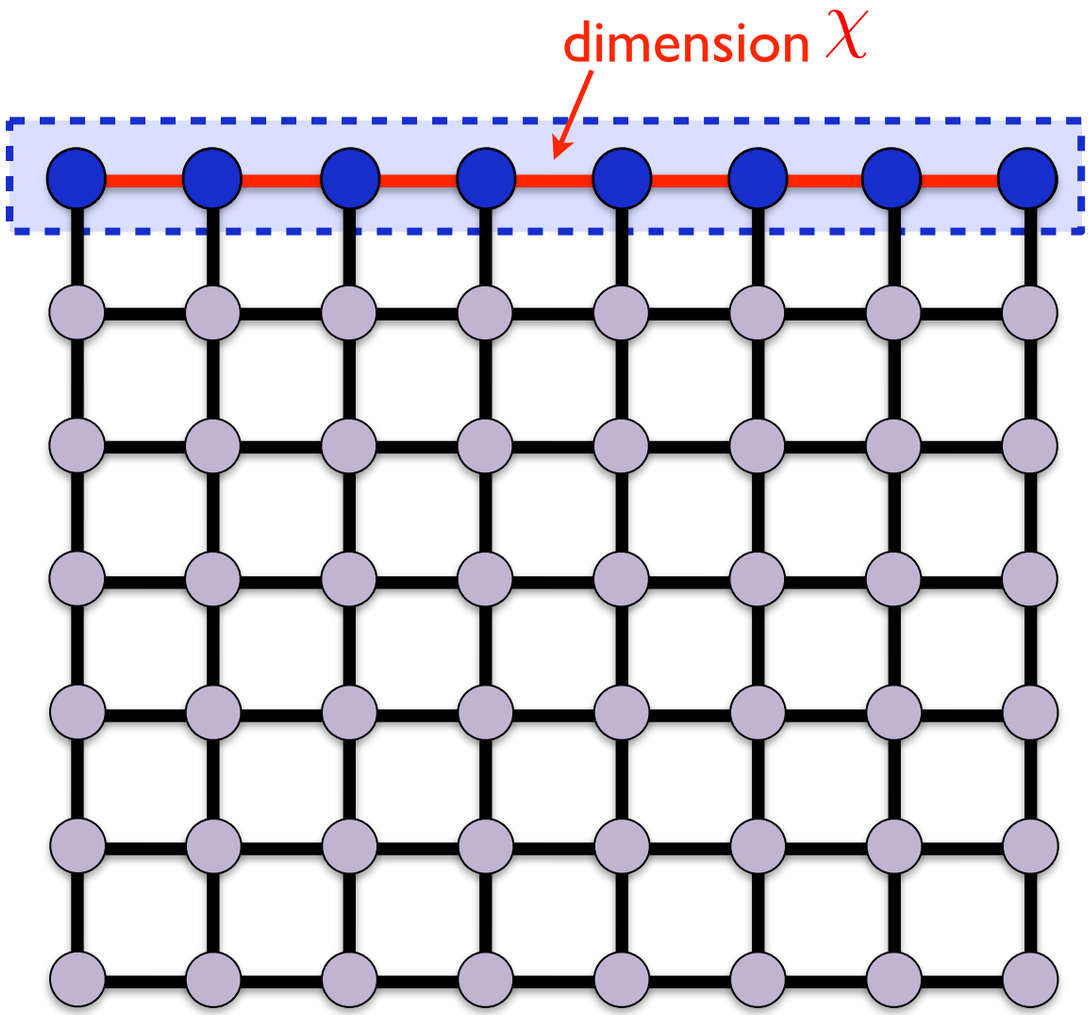
truncate the bonds to χ

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)

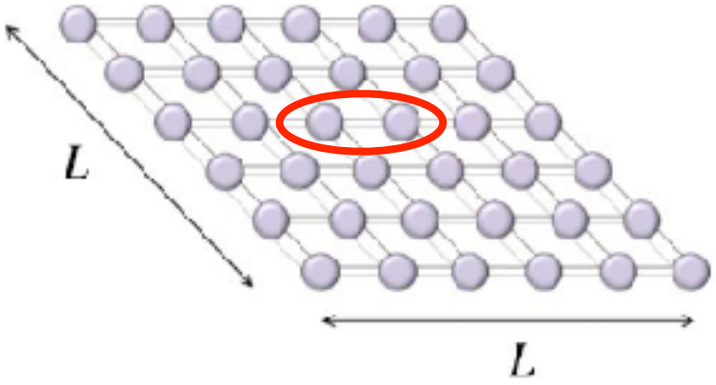


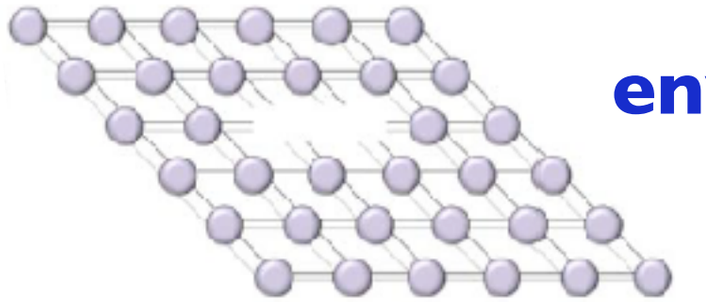
proceed...

★ We can do this from several directions

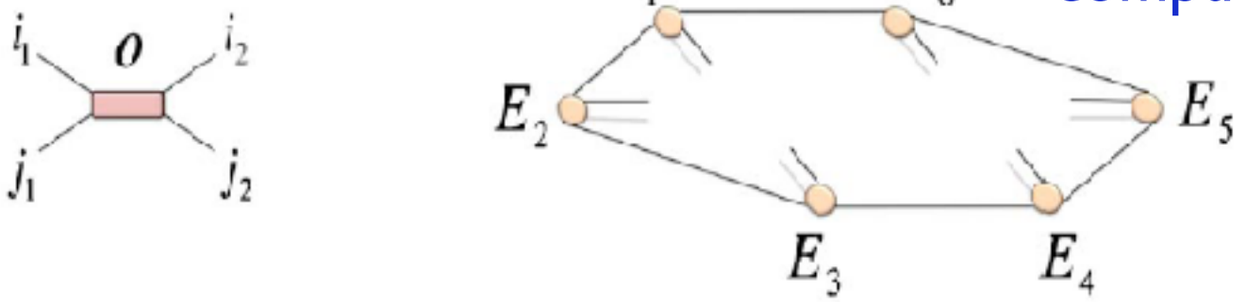
★ Similar procedure when computing an expectation value

Compute expectation values

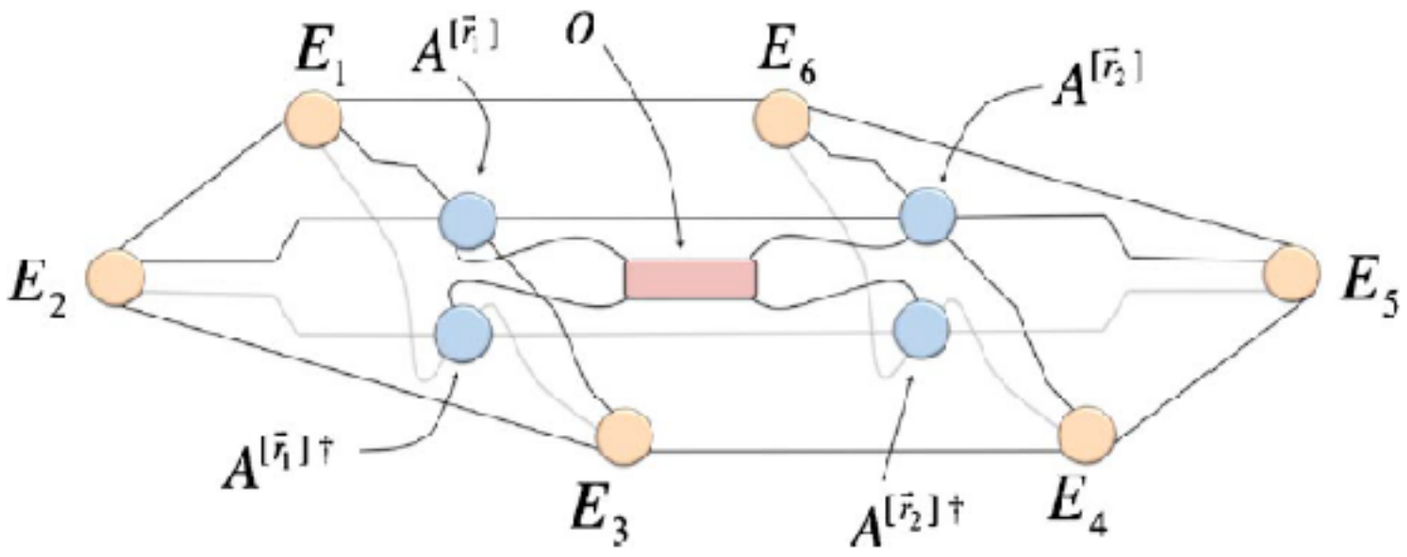




environment



compute environment approximately



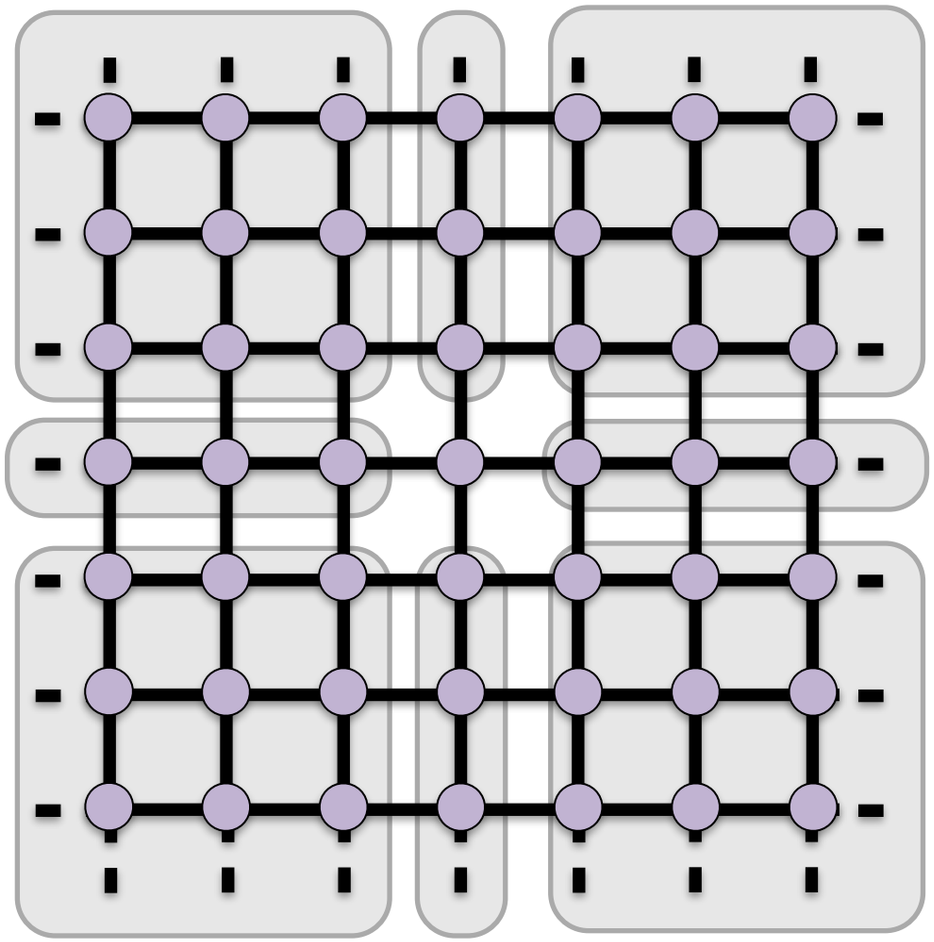
Connect two-body operator

Contract this network!

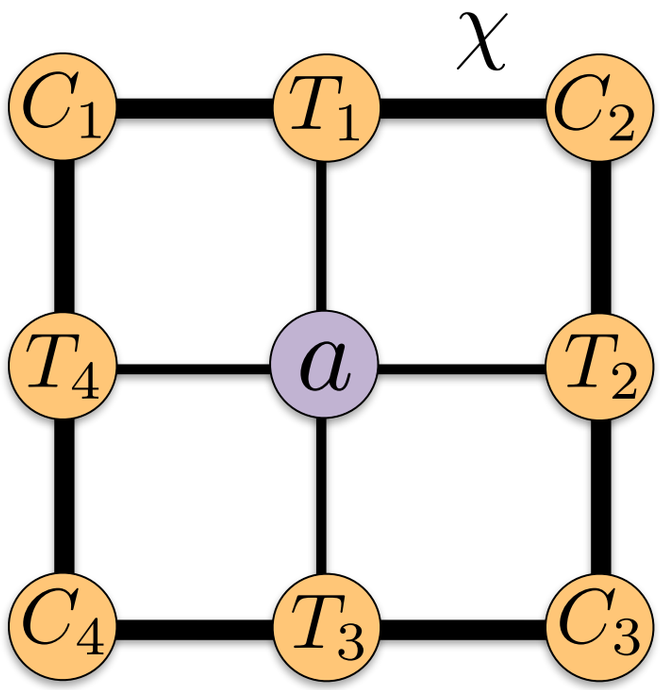
Figure taken from Corboz, Orús, Bauer, Vidal, PRB 81, 165104 (2010)

Contracting the iPEPS using the corner transfer matrix method

Nishino, Okunishi, JPSJ65 (1996)



CTM



- 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)

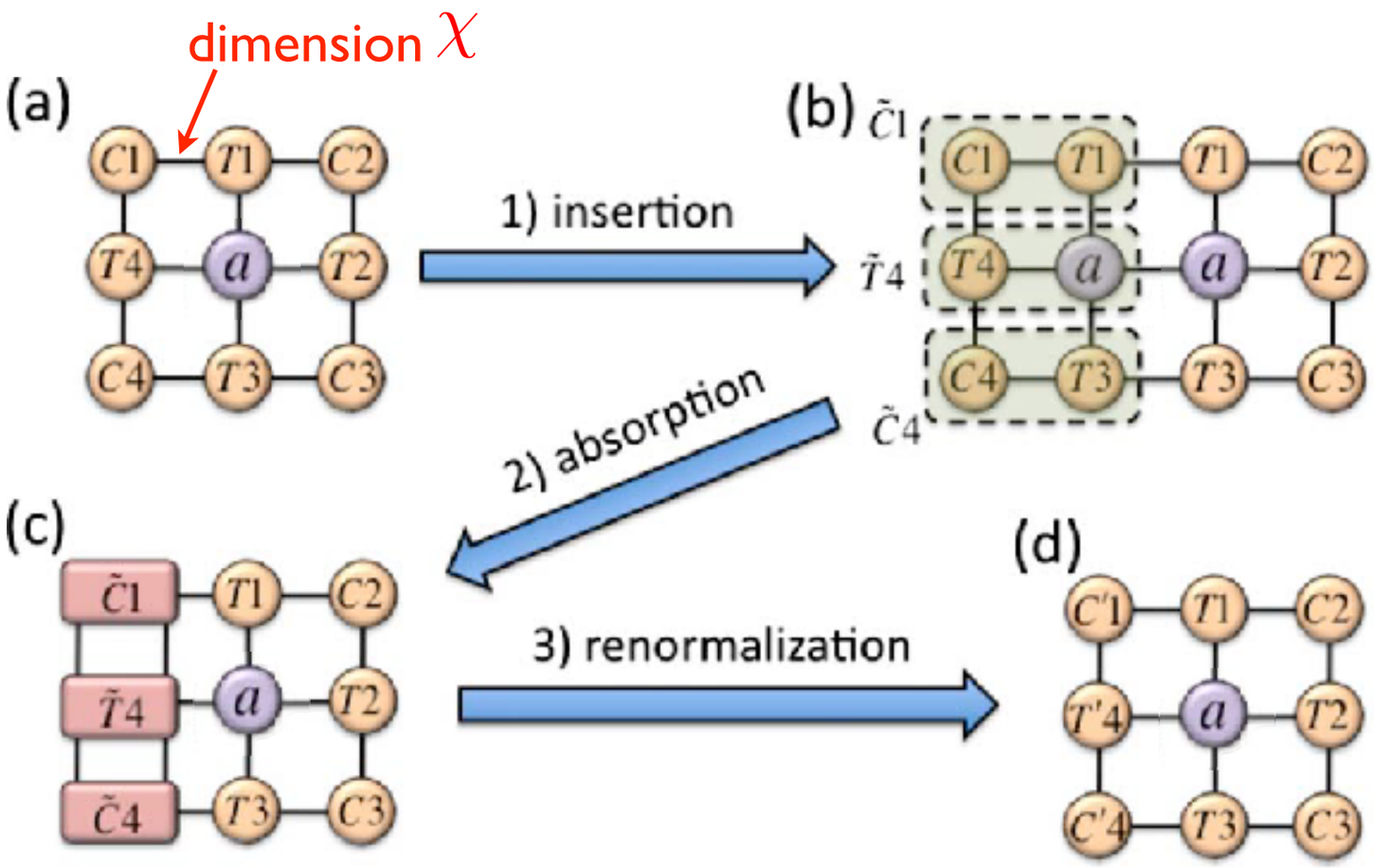


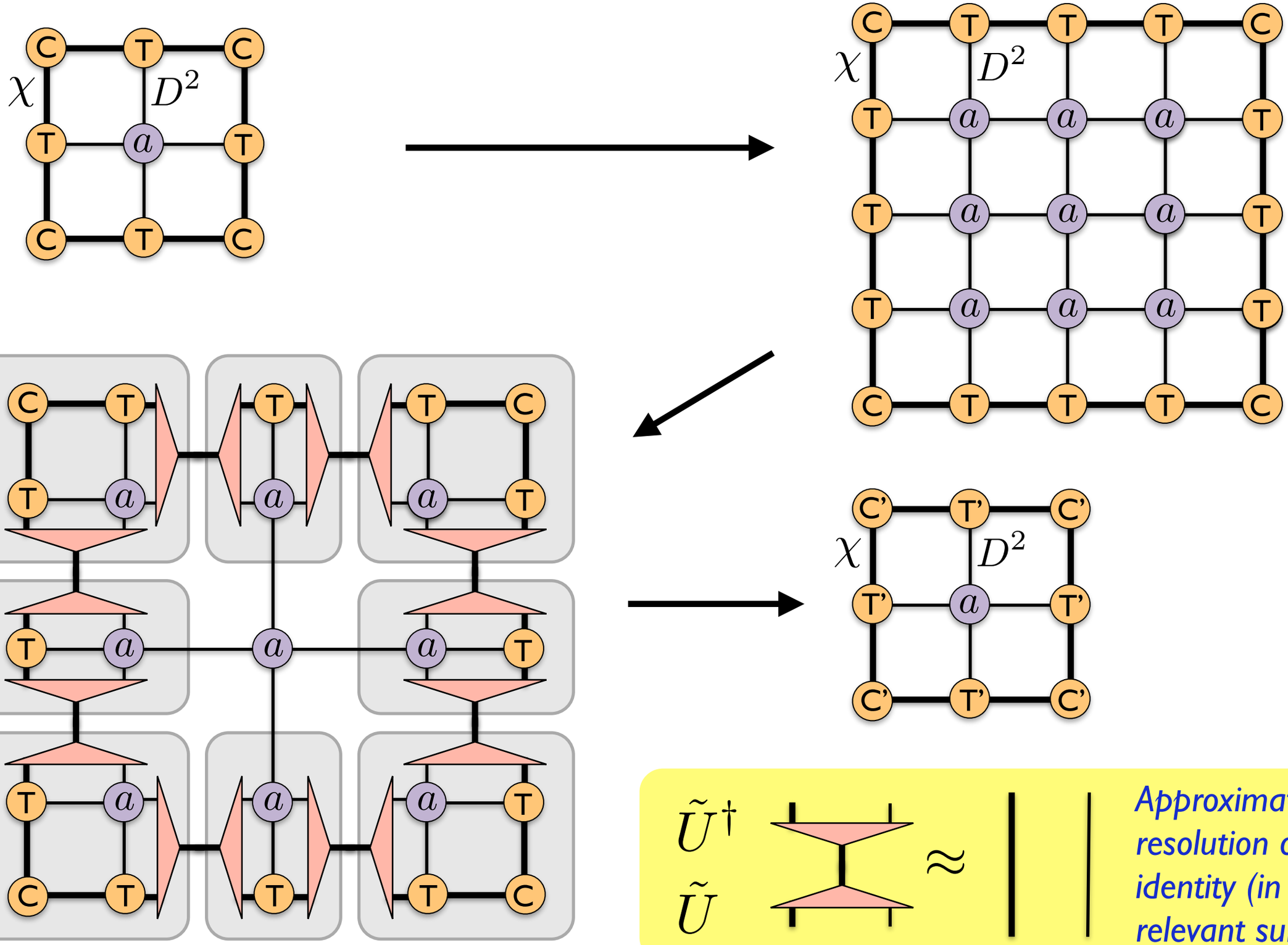
figure taken from Orus, Vidal, PRB 80 (2009)

- ★ 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

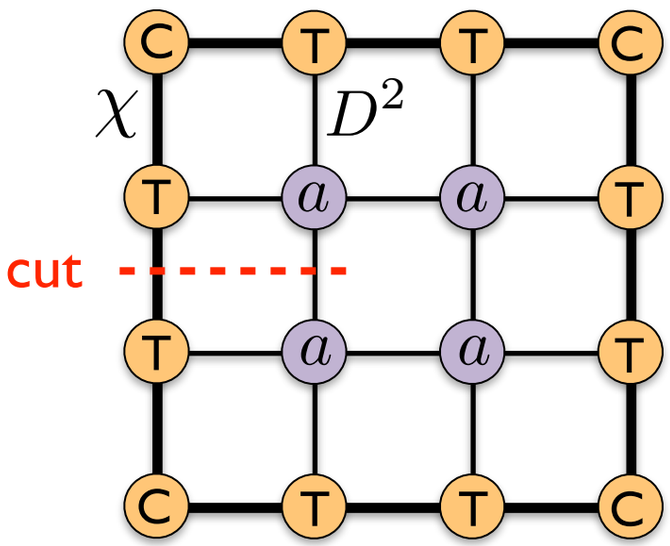
Nishino, Okunishi, JPSJ65 (1996)



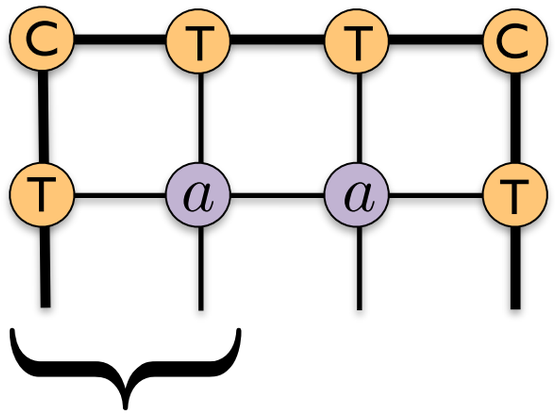
Approximate resolution of the identity (in the relevant subspace)

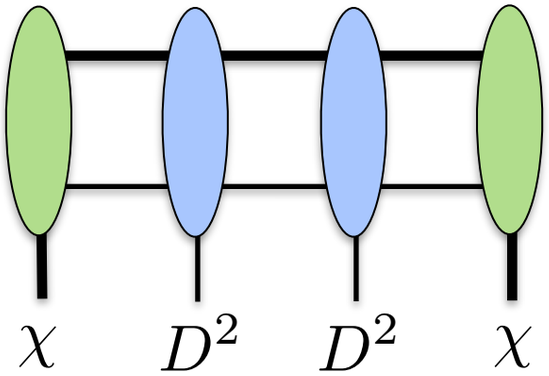
Simplest case: rotational symmetric tensors

Nishino, Okunishi, JPSJ65 (1996)



"ρ_{left}"



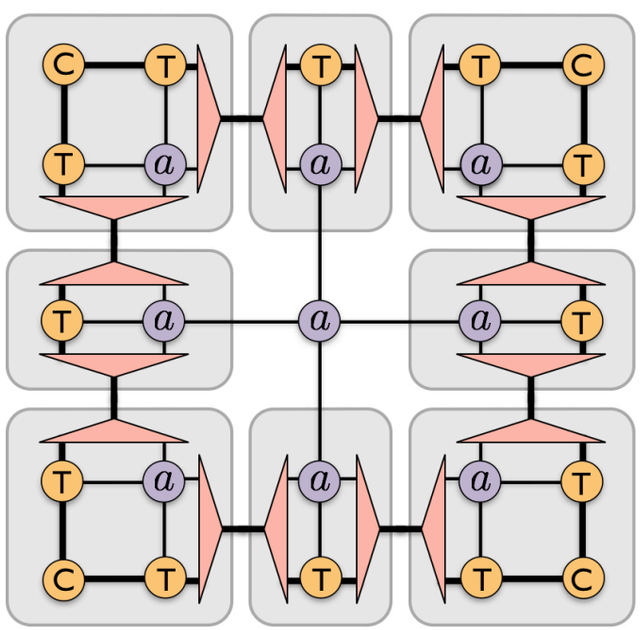


Relevant subspace?

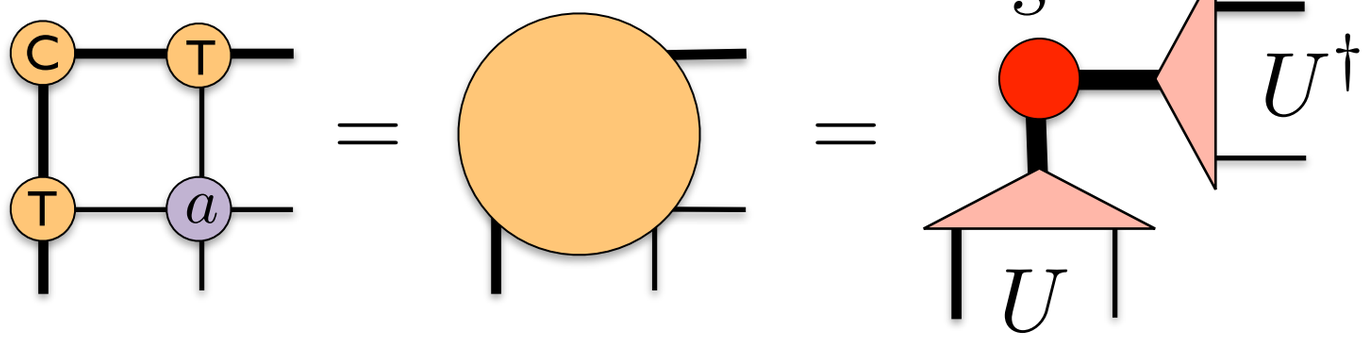
→ DMRG: Eigenvectors with largest eigenvalues of ρ_{left}

How can we best truncate from

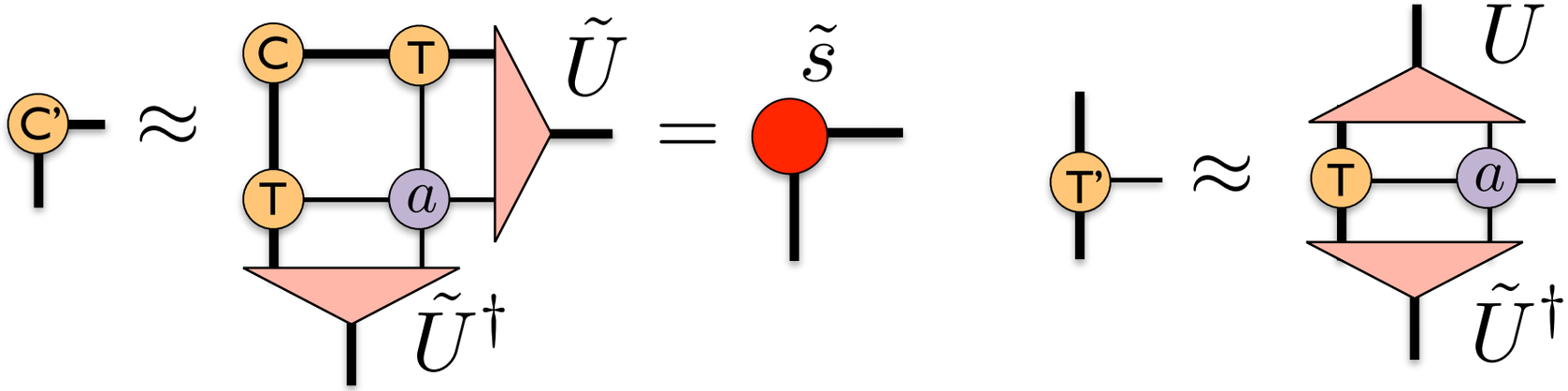
$\chi D^2 \to \chi$



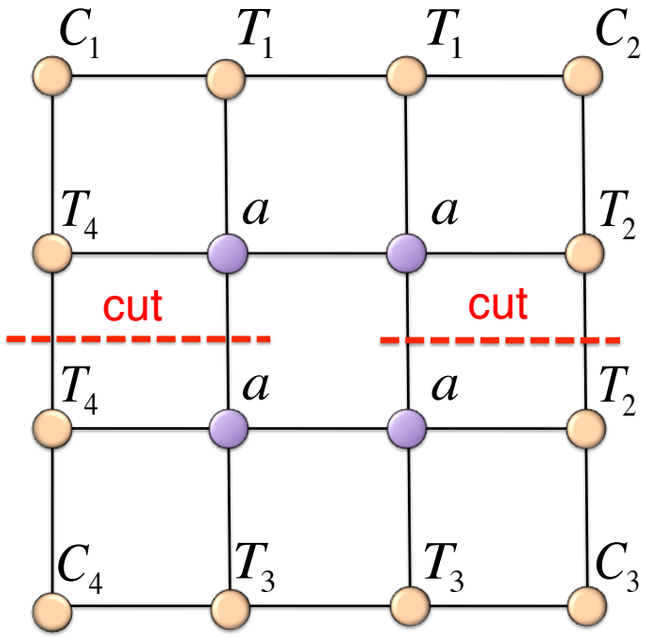
[Simpler: EIG/SVD of one corner]

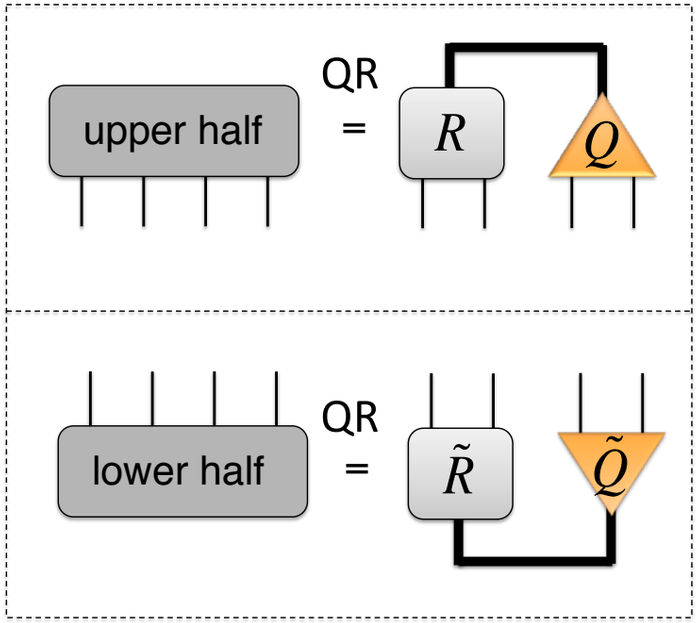


Renormalized tensors: keep only χ states with largest weight

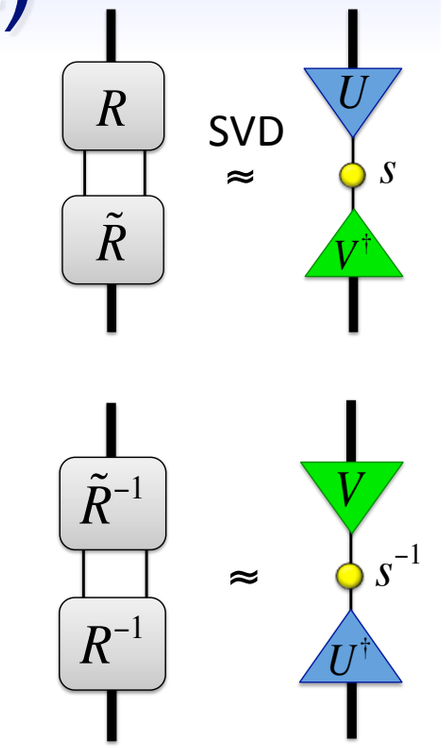


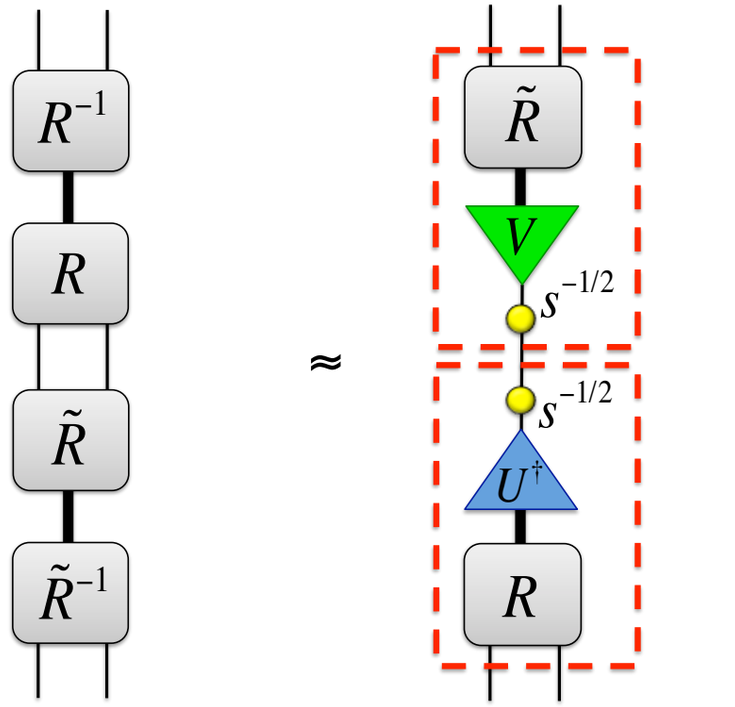
General case: Renormalization step (left move)

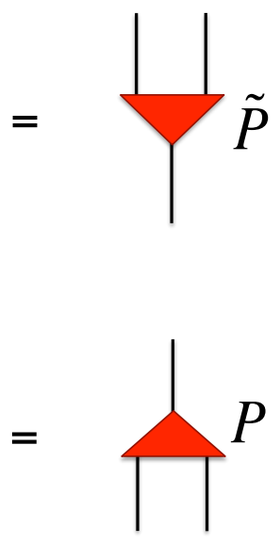




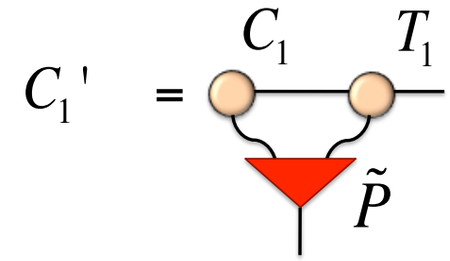
alternatively: only use upper left and lower left corners

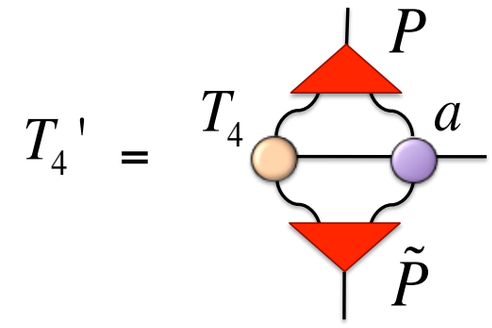


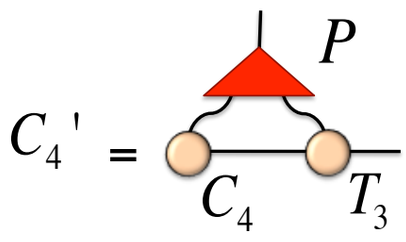




projectors onto relevant subspace

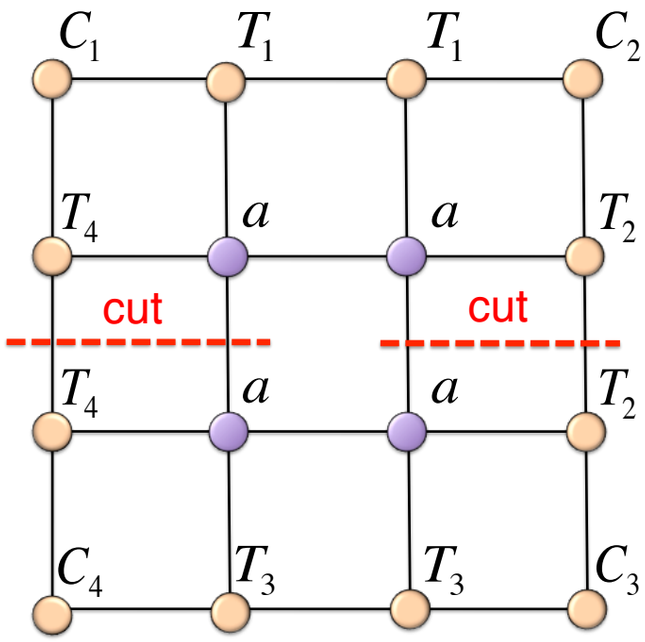




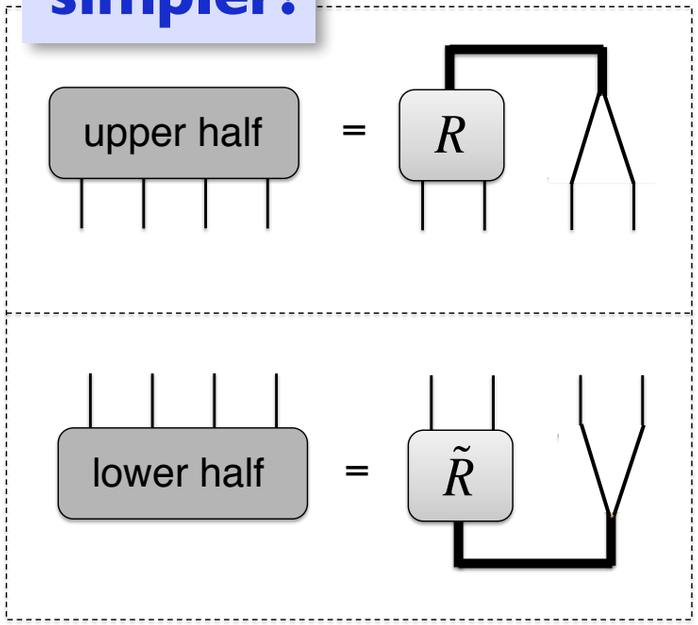


Wang, Pižorn & Verstraete, PRB 83 (2011)
Huang, Chen & Kao, PRB 86 (2012)
PC, Rice, Troyer, PRL 113 (2014)

General case: Renormalization step (left move)

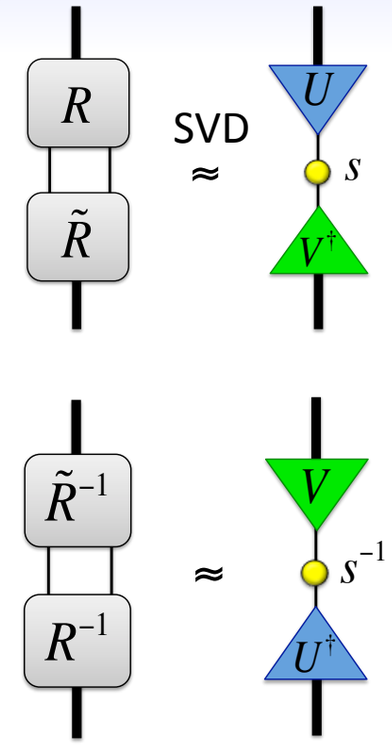


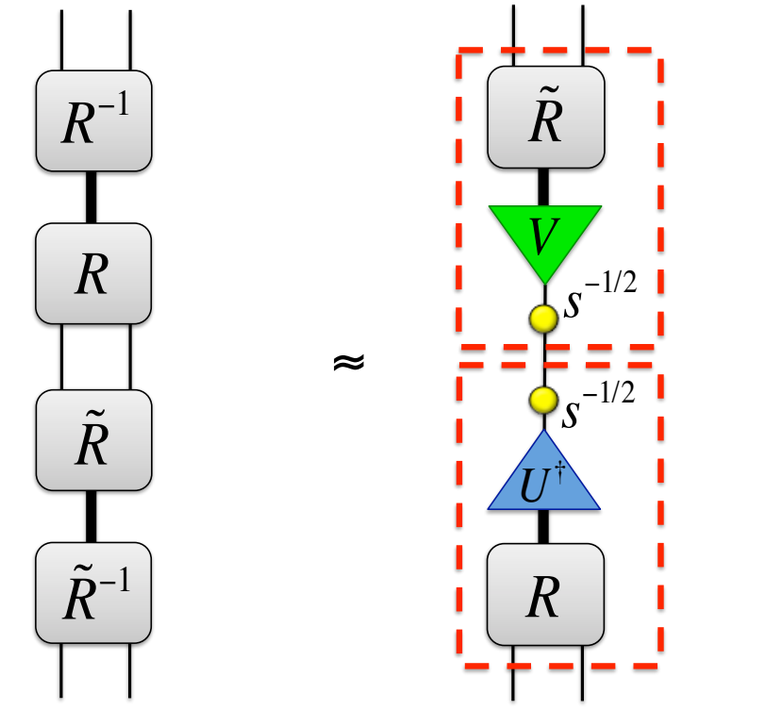
simpler!

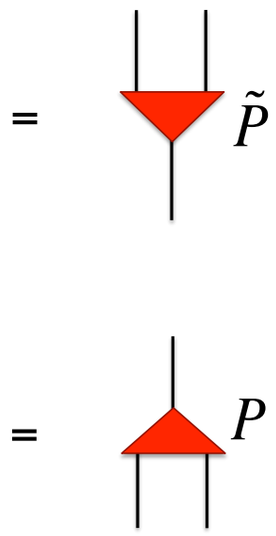


QR is actually not required!

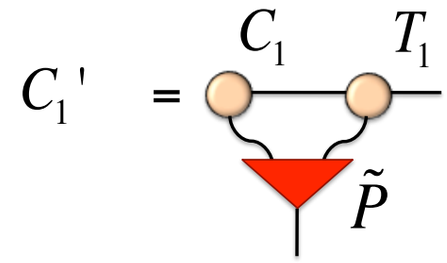
T. Okubo, private comm.

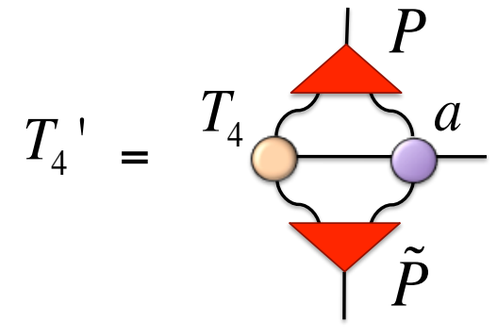


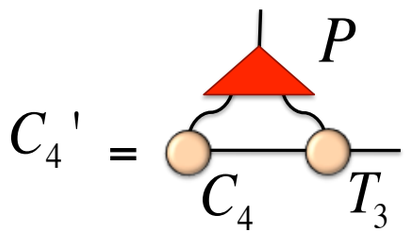




projectors onto relevant subspace





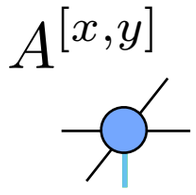


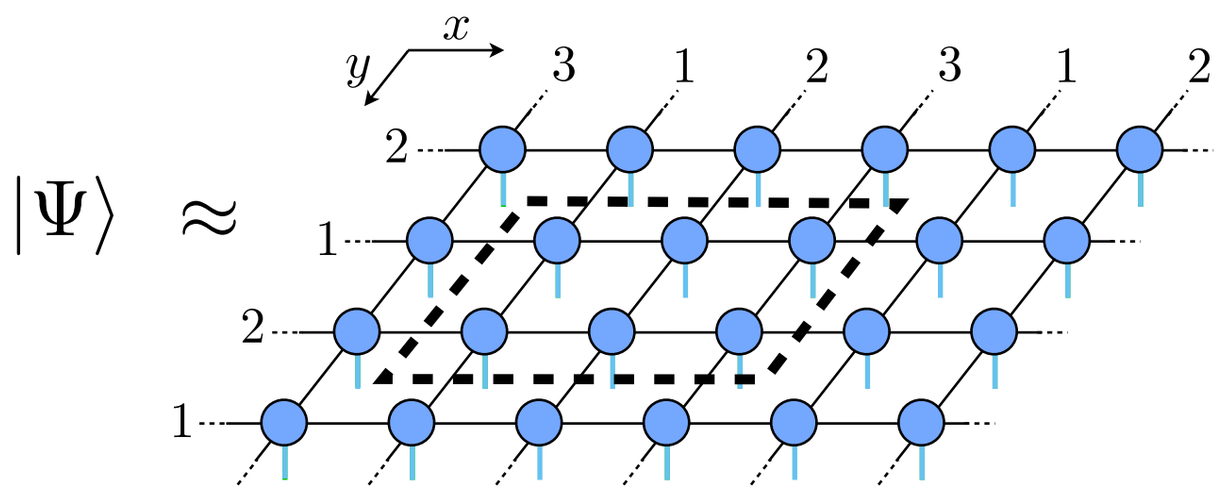
Wang, Pižorn & Verstraete, PRB 83 (2011)
Huang, Chen & Kao, PRB 86 (2012)
PC, Rice, Troyer, PRL 113 (2014)

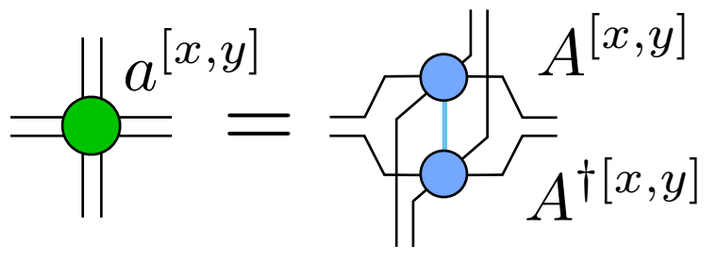
CTM with larger unit cells

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

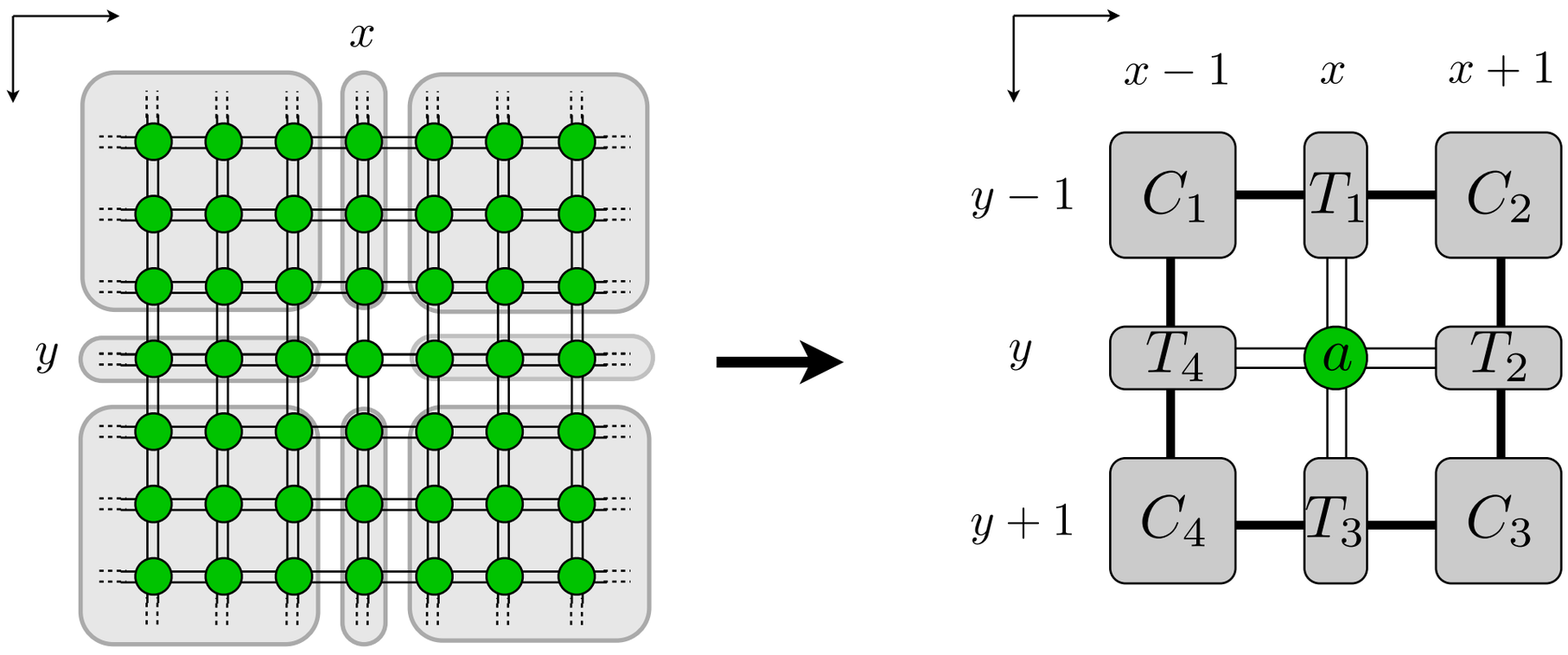
★ Each tensor has coordinates with respect to the unit cell:





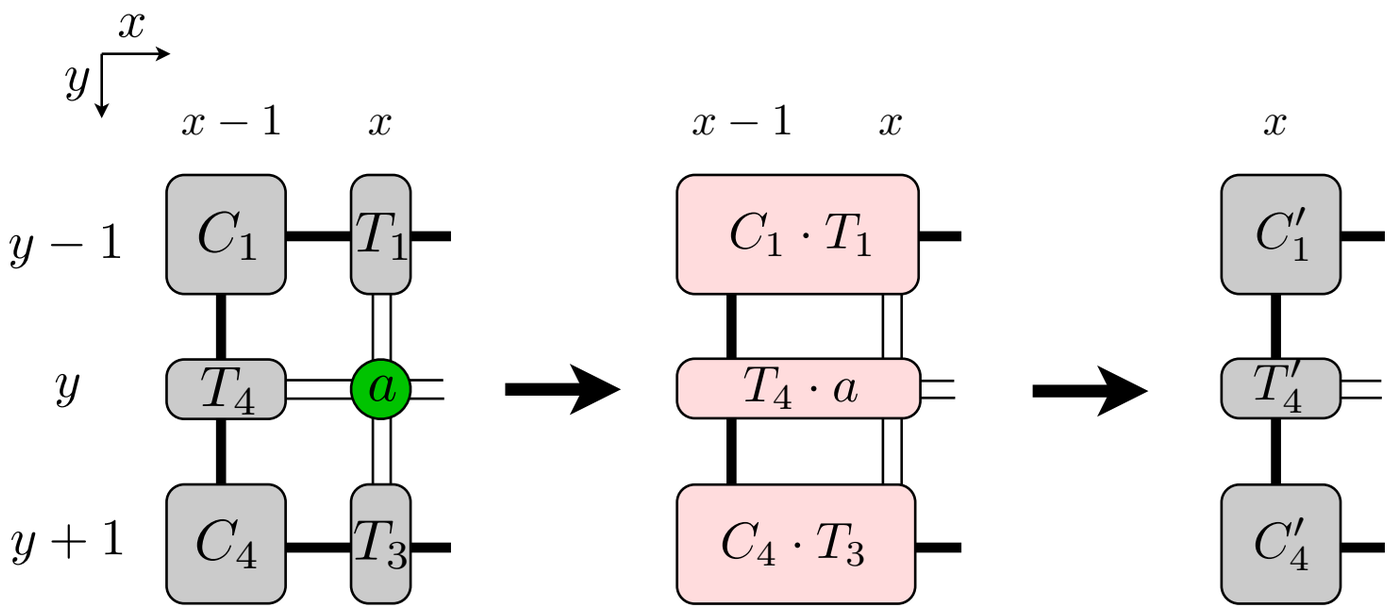


★ Keep a copy of every environment tensors $C_1, \ldots C_4, T_1, \ldots, T_4$ for each coordinate

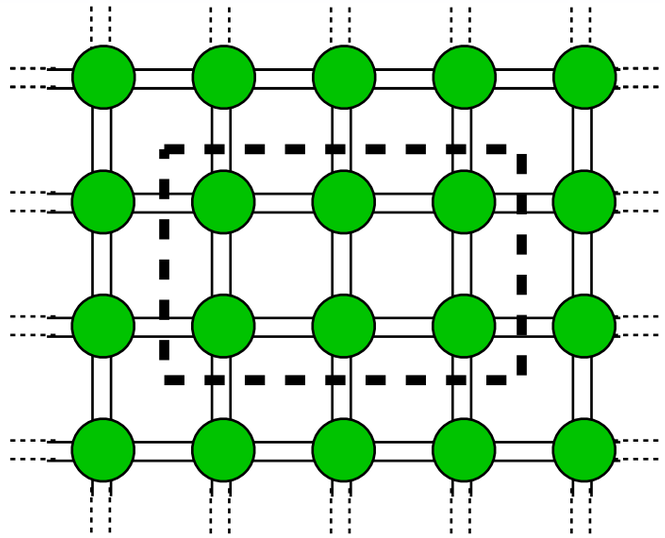


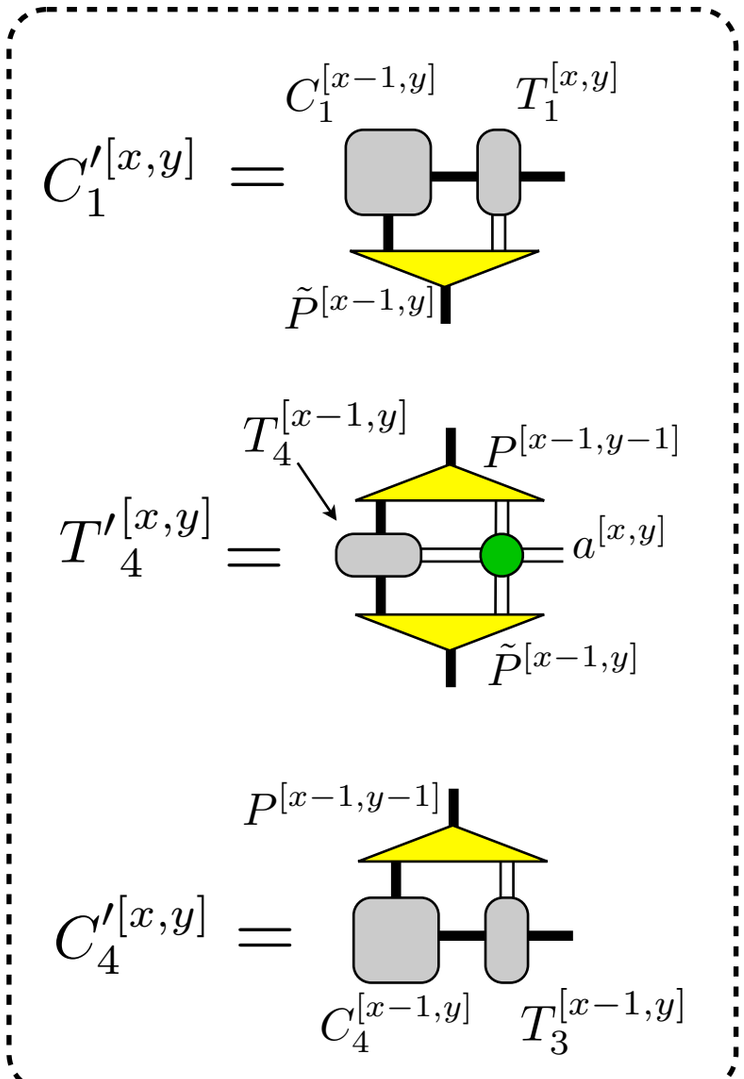
CTM with larger unit cells

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



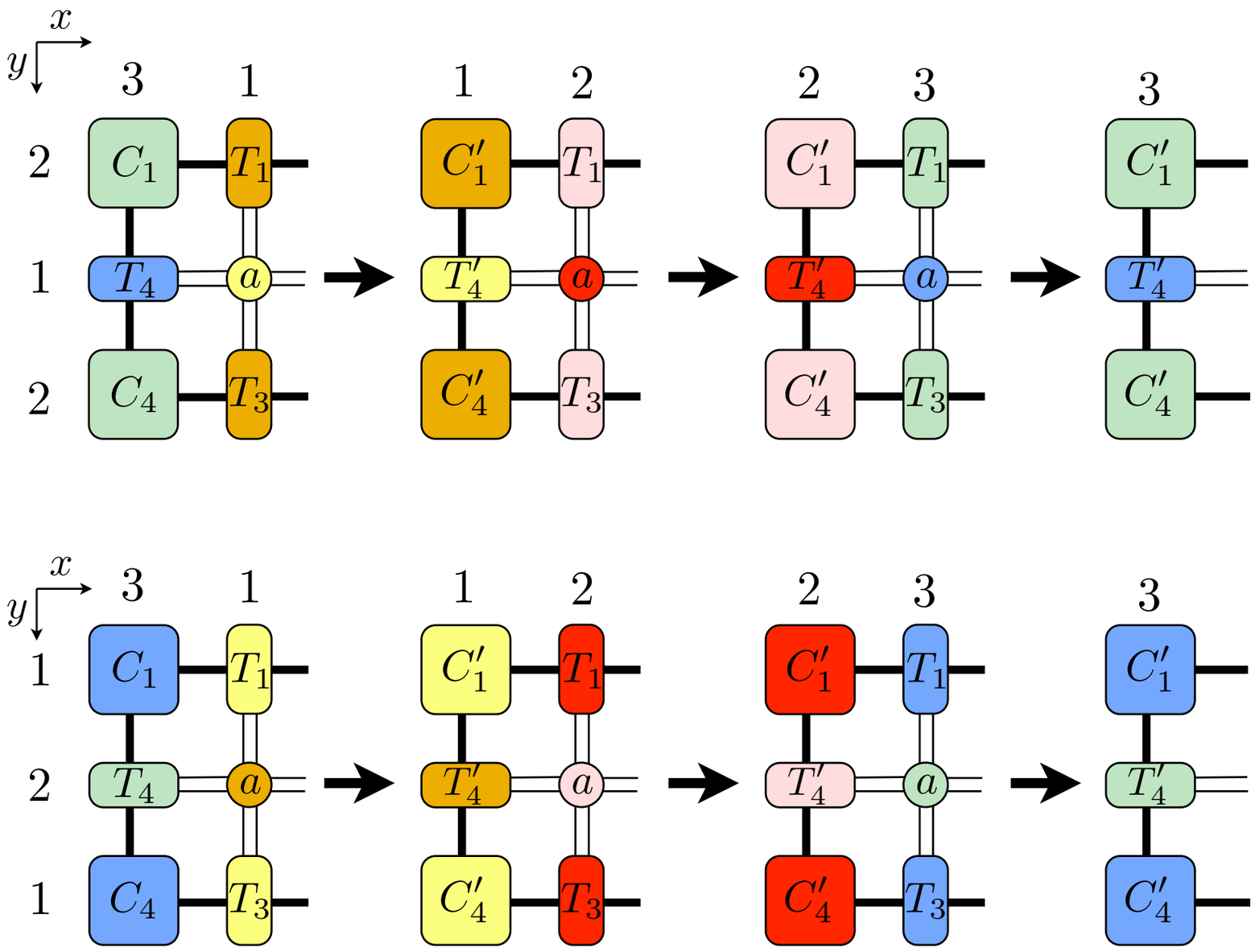
- Do for all $x \in [1, L_x]$
  - Do for all $y \in [1, L_y]$
    - Compute projectors $P^{[x-1,y]}$, $\tilde{P}^{[x-1,y]}$
  - Do for all $y \in [1, L_y]$
    - Compute updated environment tensors: $C_1'^{[x,y]}$, $C_4'^{[x,y]}$, $T_4'^{[x,y]}$

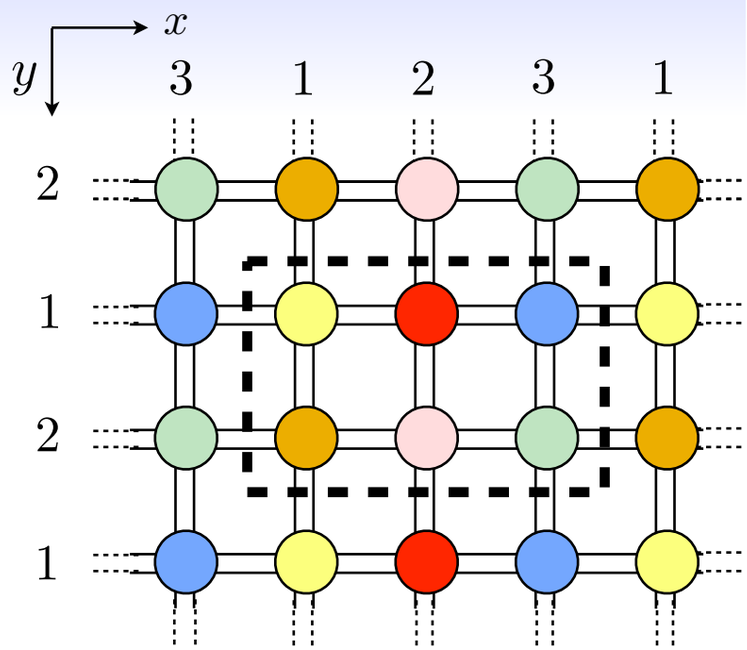




CTM with larger unit cells

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



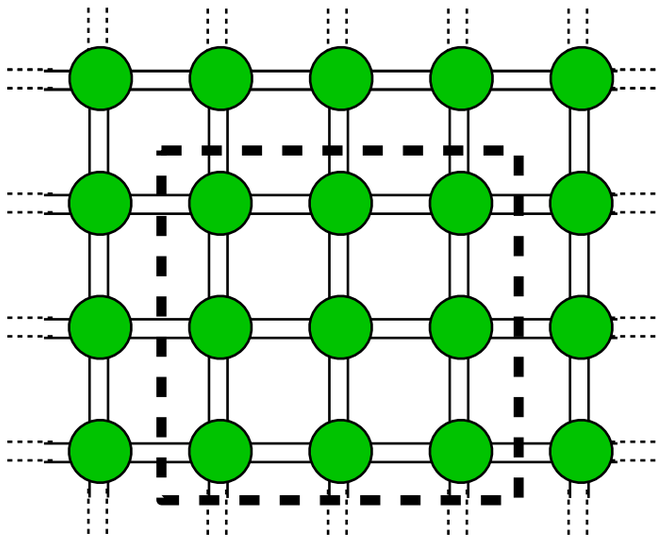


Completed left move of entire unit cell!

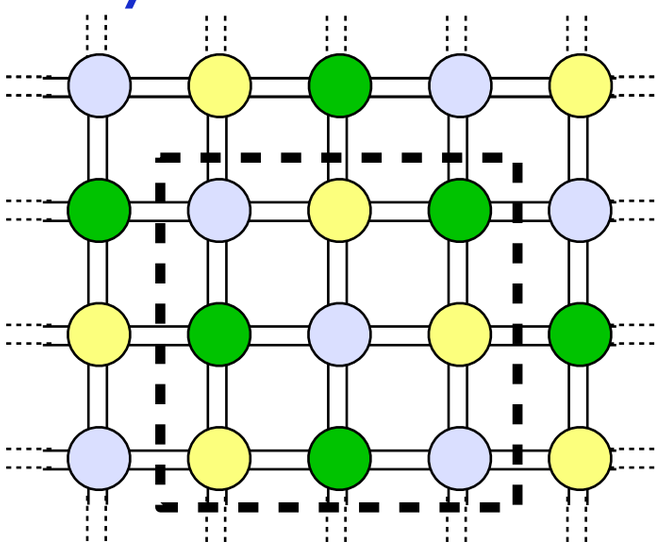
CTM with larger unit cells

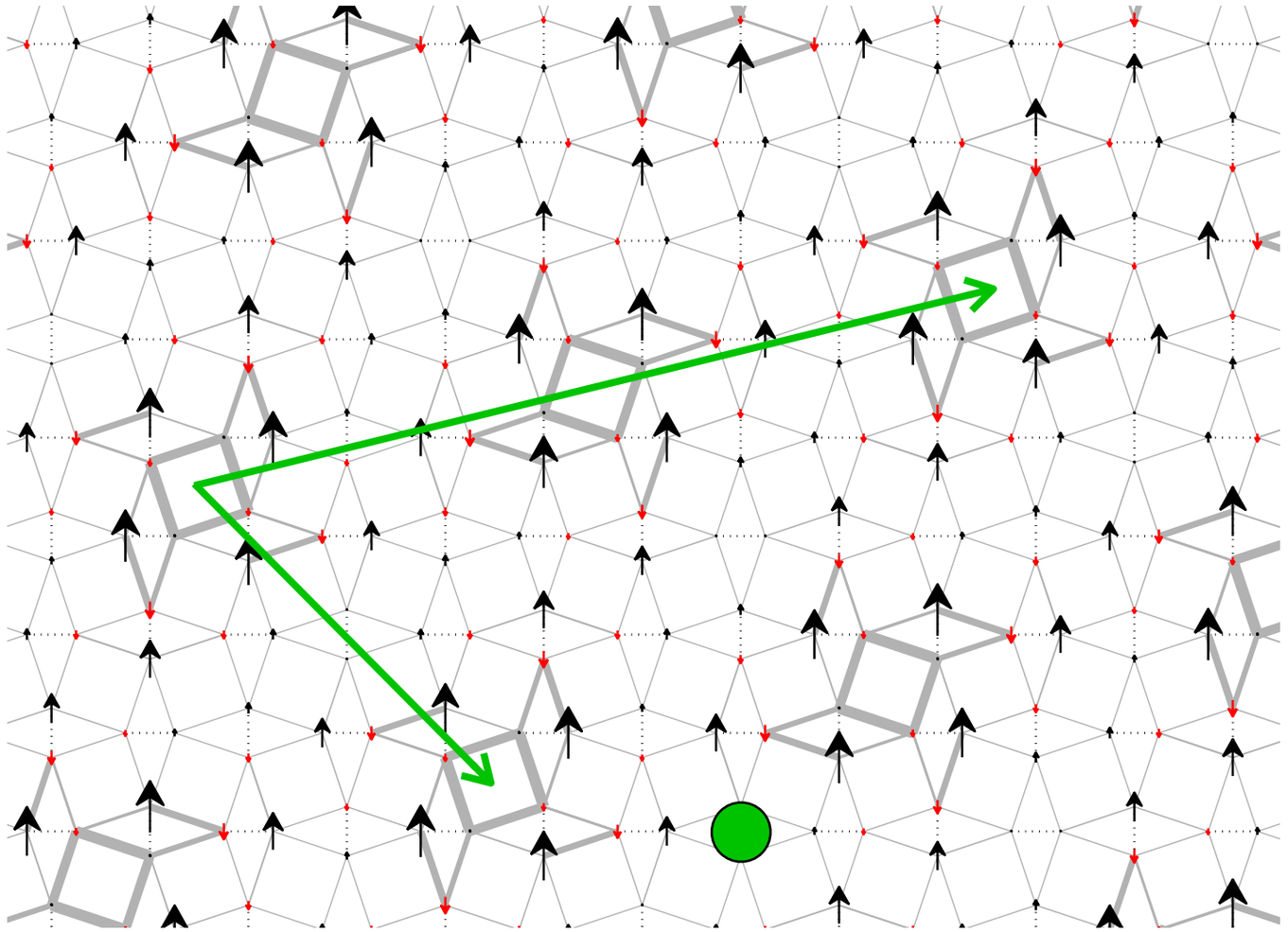
Other shapes than rectangular cell possible:

All 9 tensors different:



Only 3 different tensors:





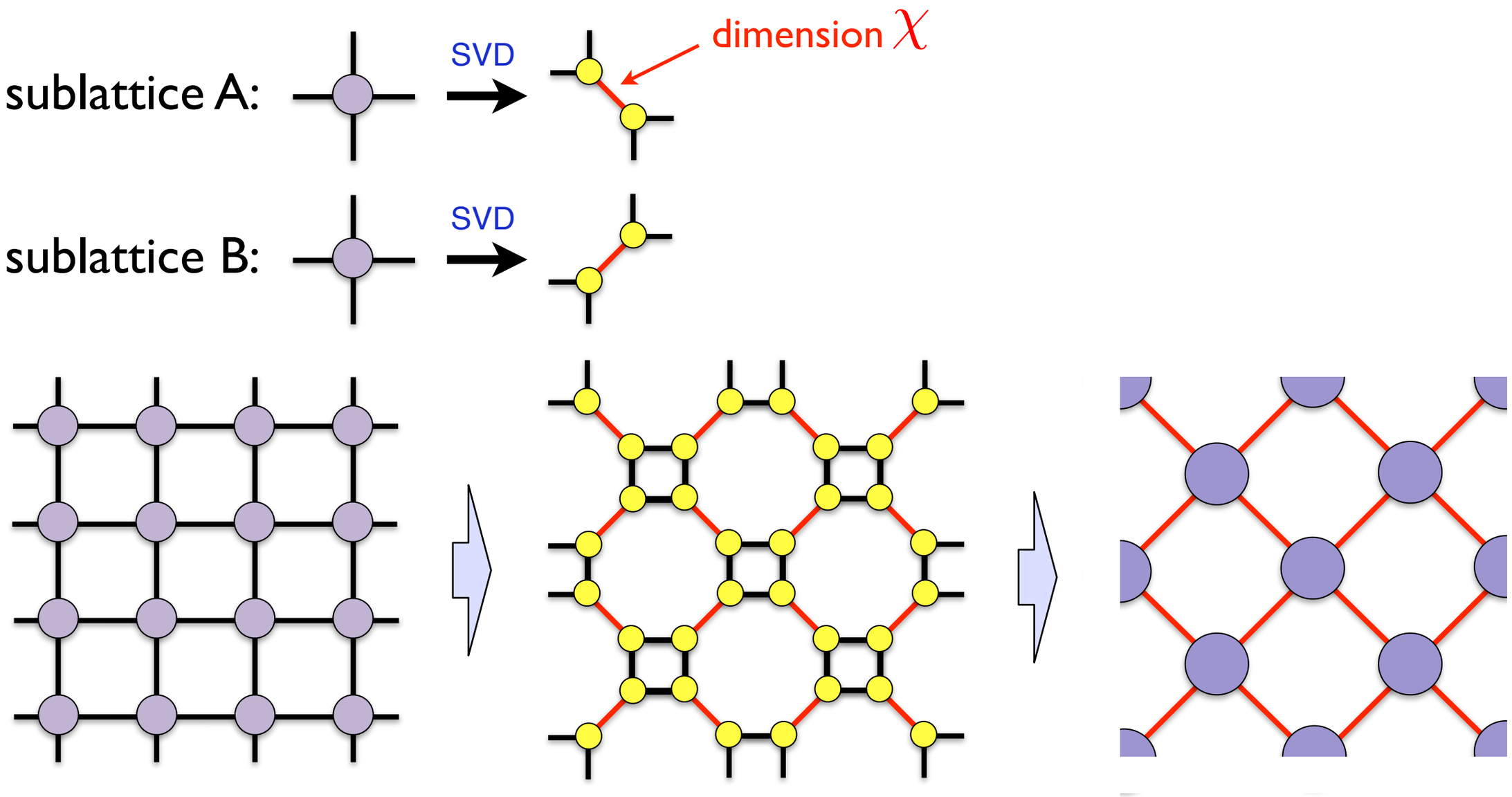
Unit cell with 30 tensors (60 sites)

(example: Shastry-Sutherland model)

Contracting the PEPS/iPEPS using TRG

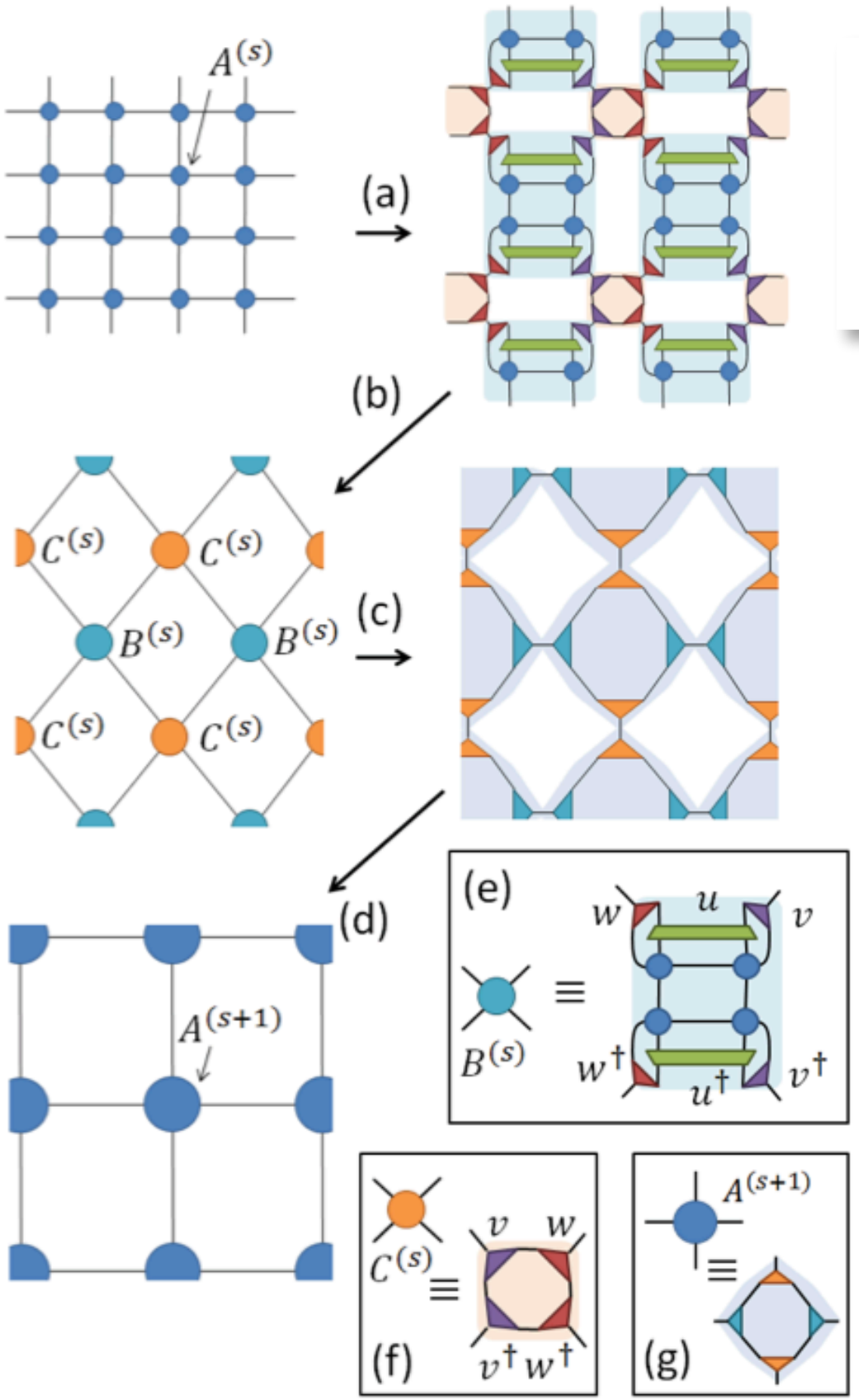
Tensor **R**enormalization **G**roup

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, PRB 98 (2018)
…

TRG

Tensor Renormalization Group

(variants: HOTRG, SRG, HOSRG)

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

★ 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 $\chi \sim D^2$

TNR

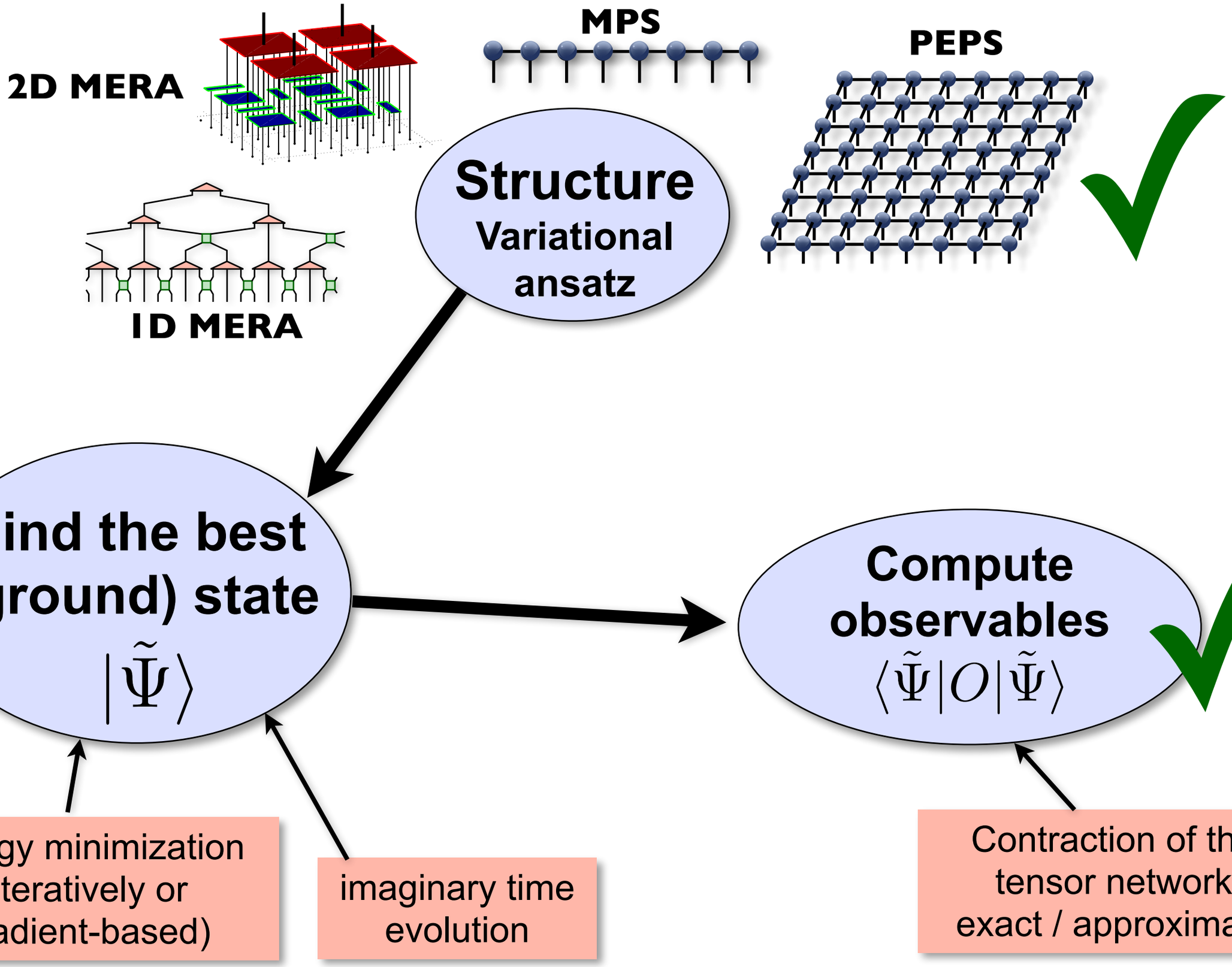
Tensor Network Renormalization

Evenbly & Vidal, PRL 115 (2015)

Loop-TNR:

Yang, Gu & Wen, PRL 118 (2017)

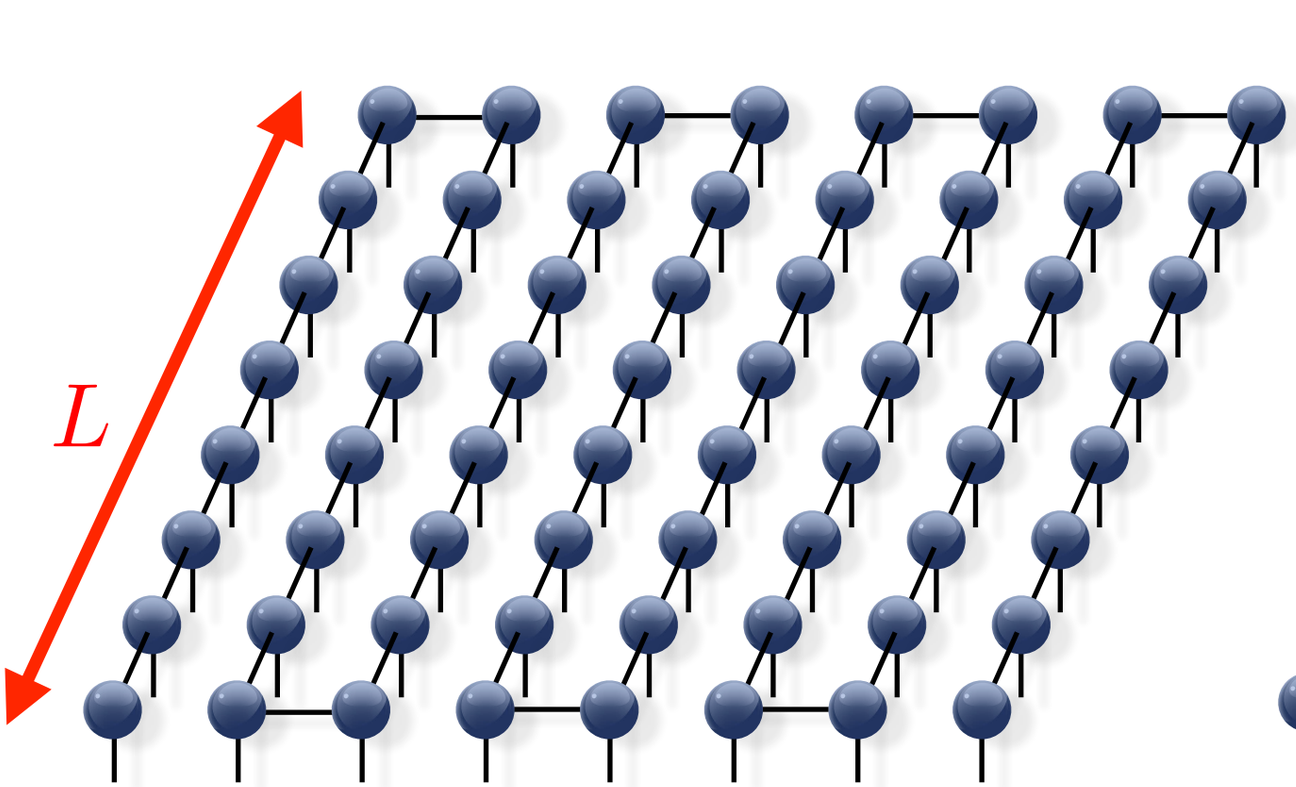
Summary: Tensor network algorithm for ground state

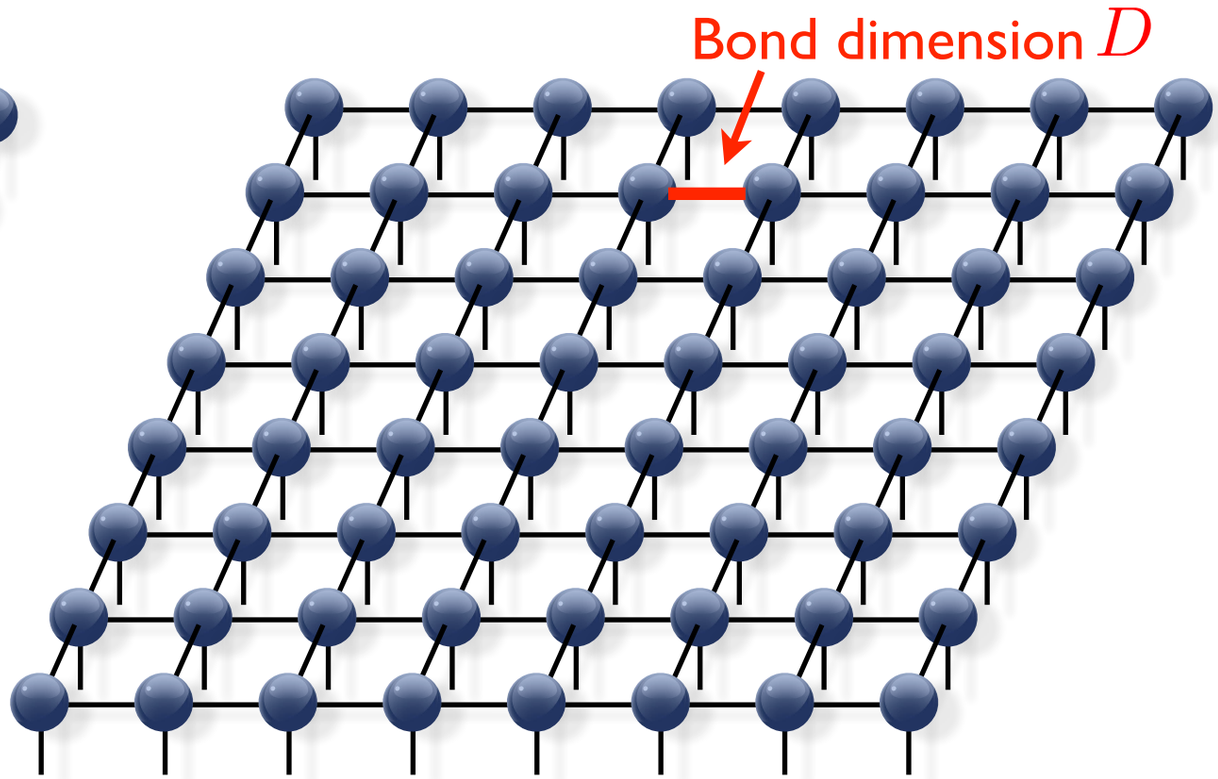


Comparison MPS vs PEPS

Comparison: MPS in 2D vs iPEPS

Snake MPS vs **(i)PEPS**





★ Scaling of algorithm: D^3

★ Simpler algorithms & implementation

★ Very accurate results for "small" L

- inaccurate beyond certain L
  because $D \sim exp(L)$

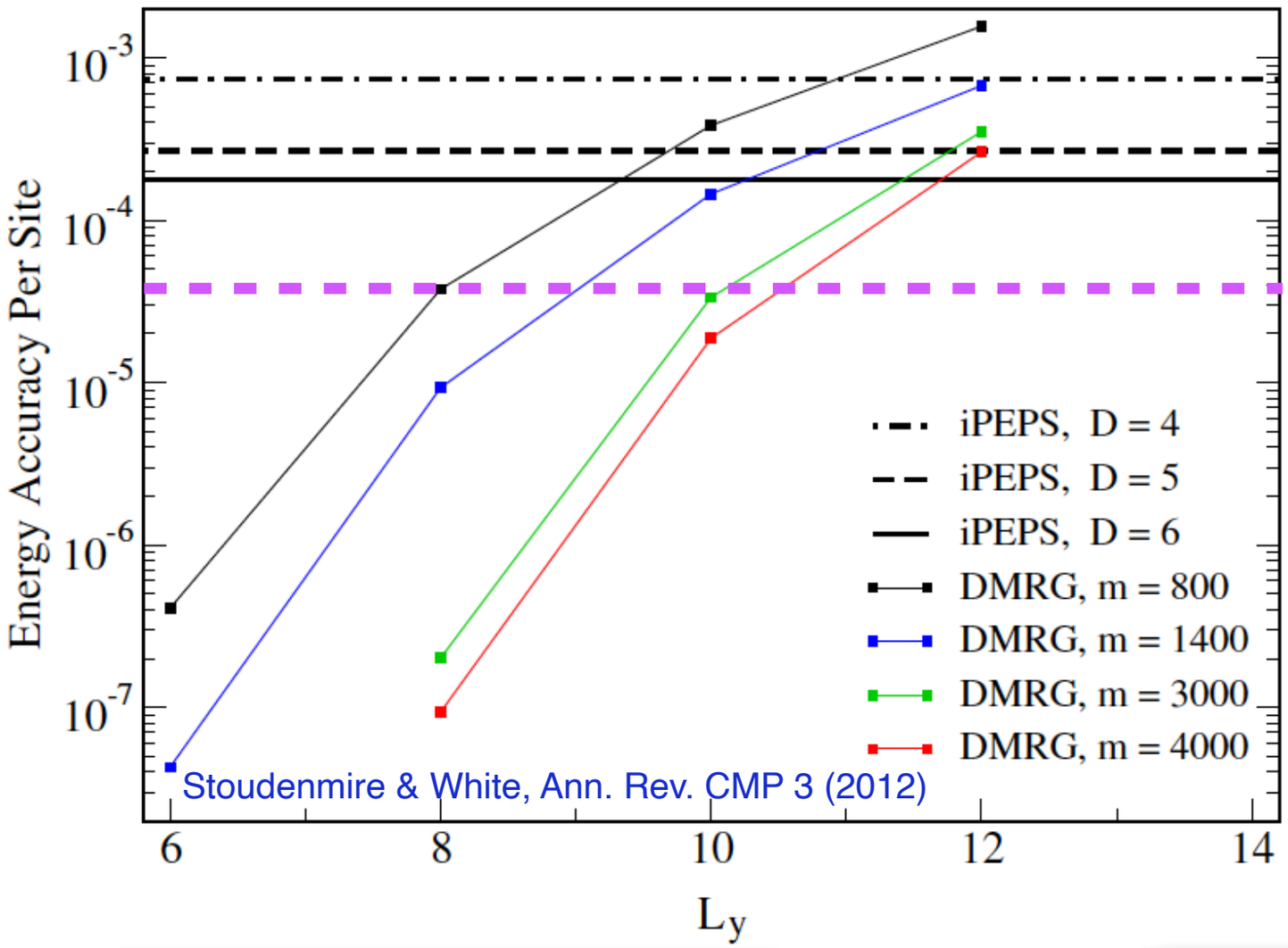
★ Large / infinite systems (scalable)!

★ Much fewer variational parameters
  because much more natural 2D ansatz

- Algorithms more complicated

- Large cost of roughly D^{10}

Comparison MPS & iPEPS: 2D Heisenberg model



← iPEPS D=6
(variational optimization)

iPEPS D=6 in the thermodynamic limit

~ 2'600 variational pars.

similar accuracy ~

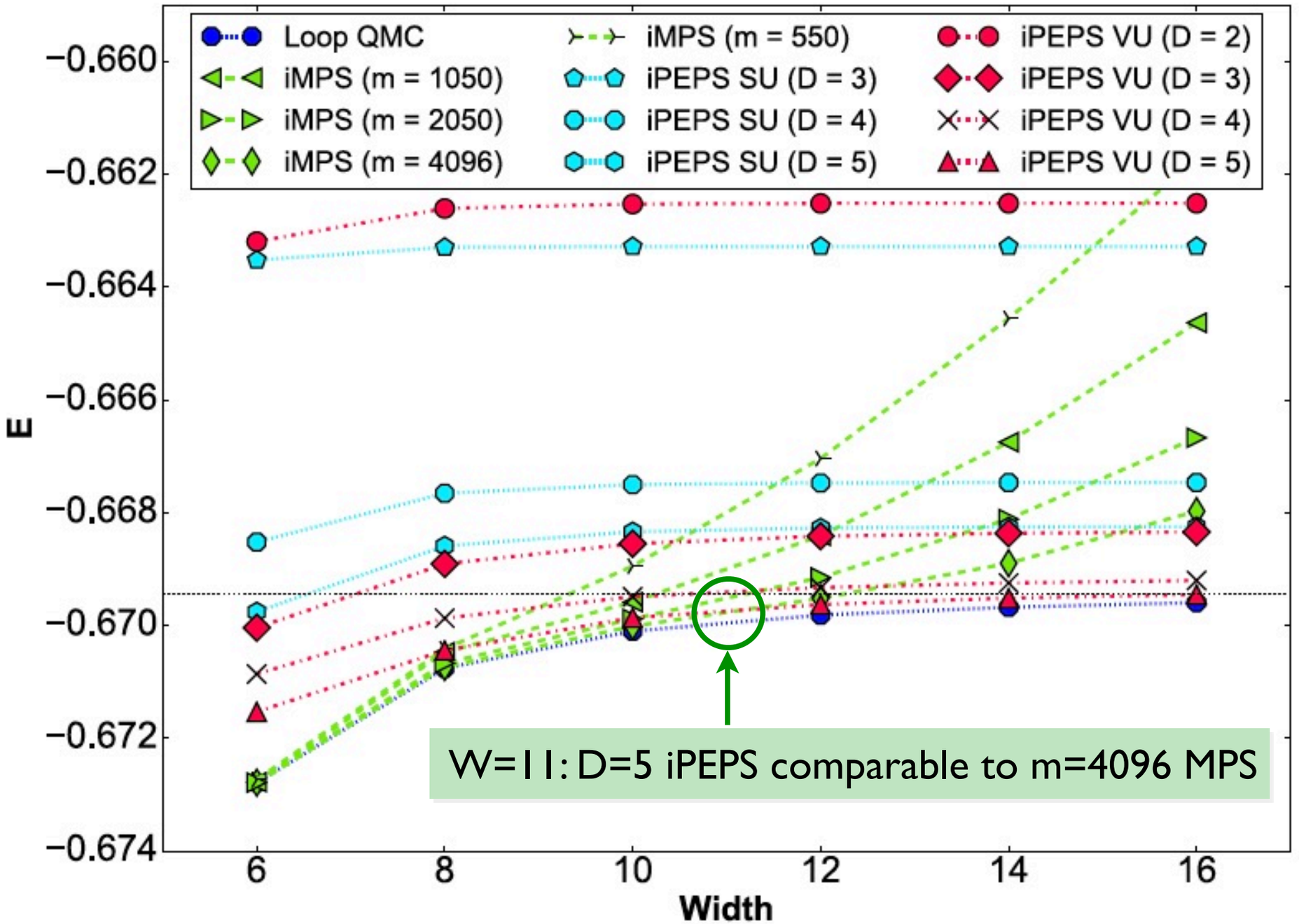
MPS D=3000 on finite Ly=10 cylinder

~ 18'000'000

4 orders of magnitude fewer parameters (per tensor)

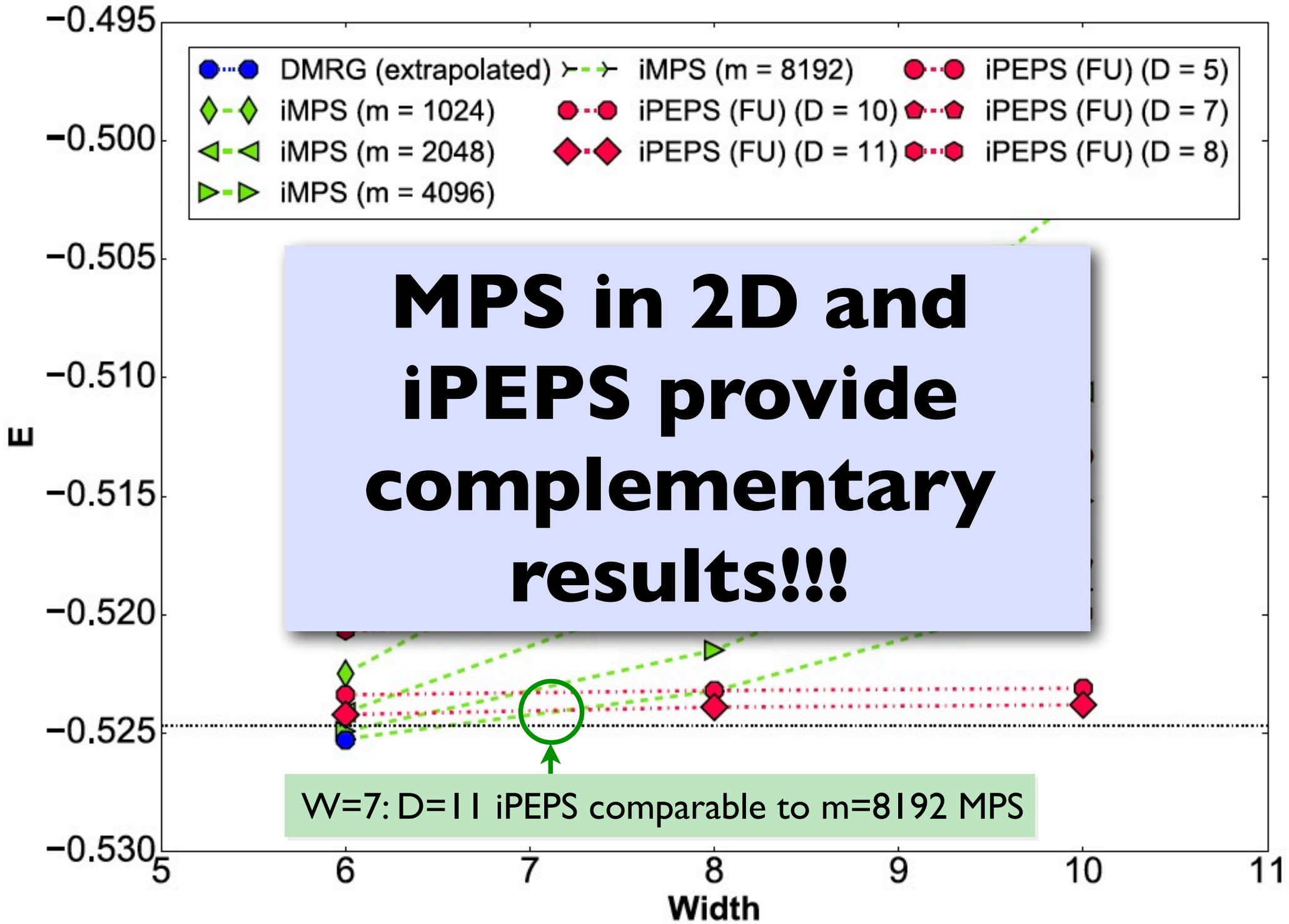
iMPS vs iPEPS on infinite cylinders: Heisenberg model

J. Osorio Iregui, M. Troyer & PC, PRB 96 (2017)



iMPS vs iPEPS on infinite cylinders: Hubbard model (n=1)

J. Osorio Iregui, M. Troyer & PC, PRB 96 (2017)

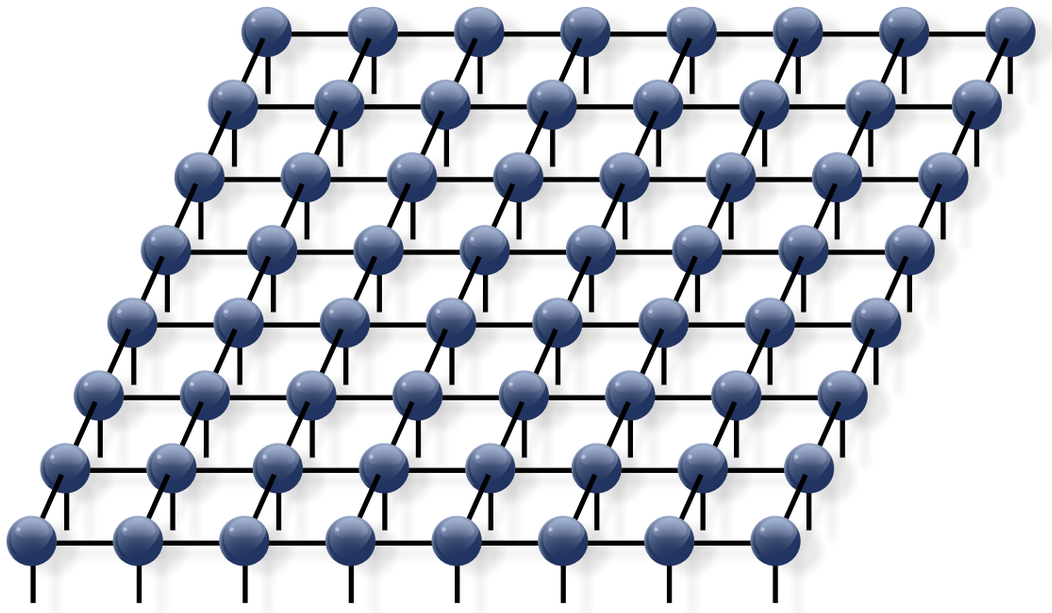


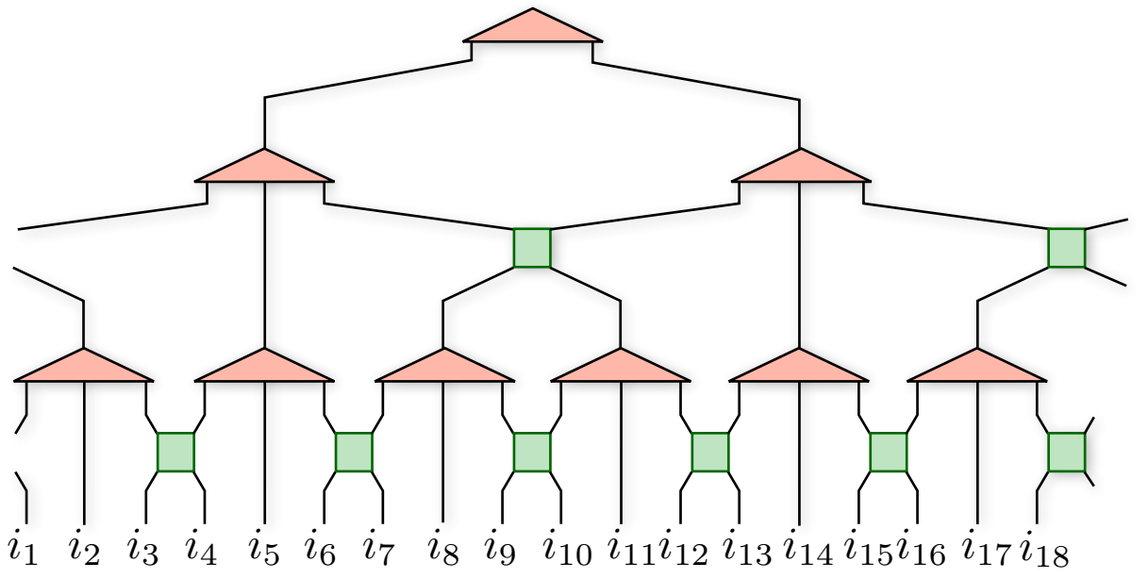
MPS in 2D and iPEPS provide complementary results!!!

Introduction to (i)PEPS & MERA

Lecture II

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam





Tensor Network based approaches to Quantum Many-Body Systems

ICCUB School 2021

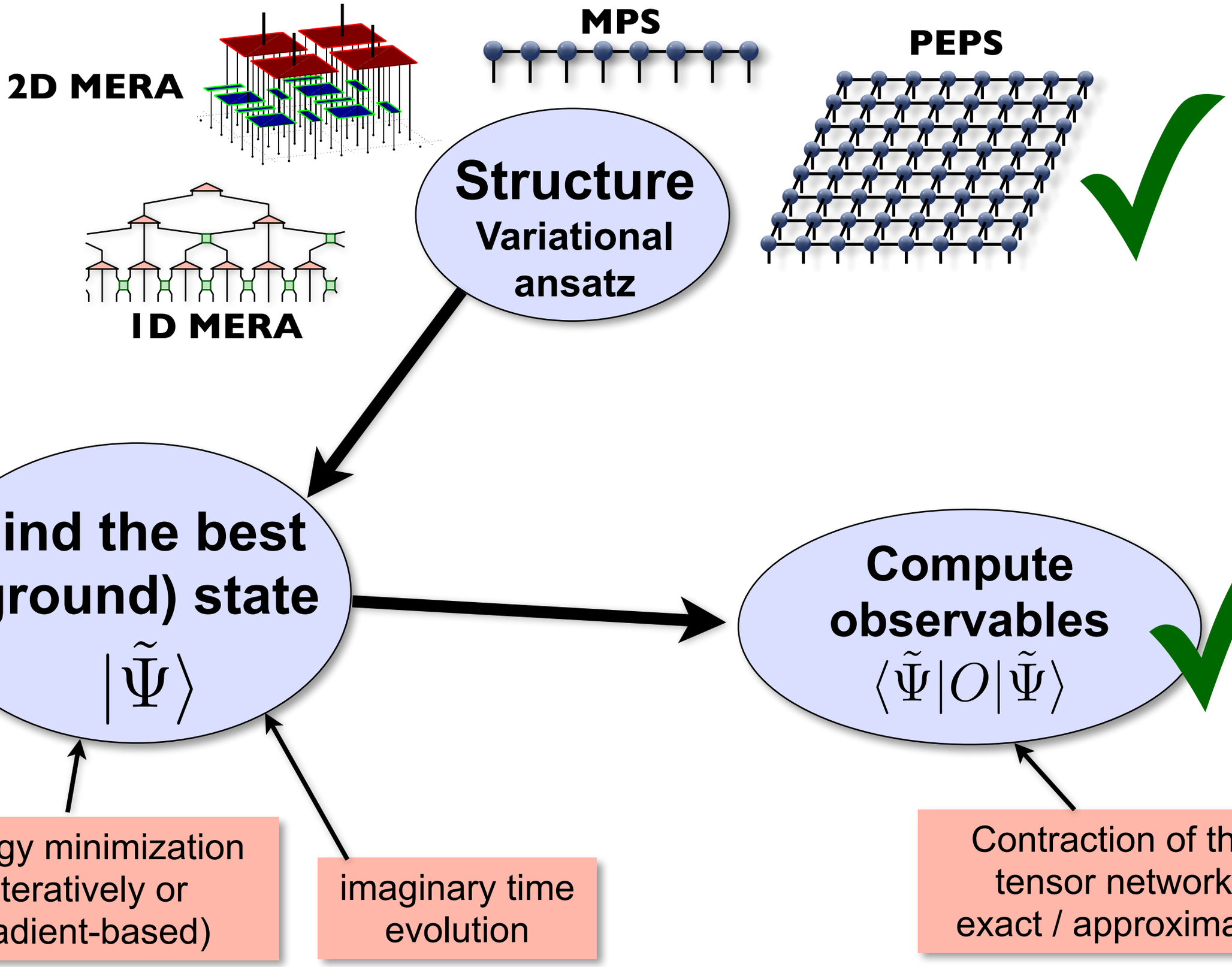
Outline

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

- Part III: Optimization (PEPS + iPEPS)
  - ✦ *Imaginary time evolution: simple vs full optimization*
  - ✦ *Variational optimization & automatic differentiation (energy minimization)*
- Part IV: iPEPS application example
  - ✦ *Magnetization plateaus in the Shastry-Sutherland model*
- Part V: Fermionic 2D tensor networks
- Part VI: Selected recent developments (iPEPS)
  - ✦ *Finite temperature simulations*
  - ✦ *iPEPS excitation ansatz*
  - ✦ *iPEPS in 3D*
  - ✦ *Finite correlation length scaling*

PART III: Optimization

Summary: Tensor network algorithm for ground state



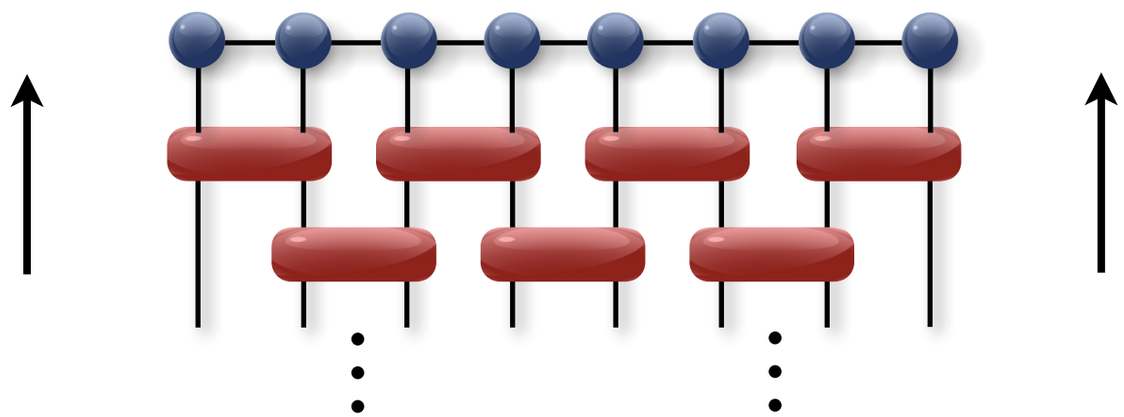
Optimization via imaginary time evolution

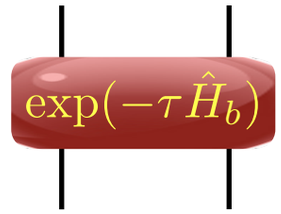
- Idea: $\exp(-\beta\hat{H})|\Psi_i\rangle \xrightarrow{\beta\to\infty} |\Psi_{GS}\rangle$

Trotter-Suzuki decomposition:

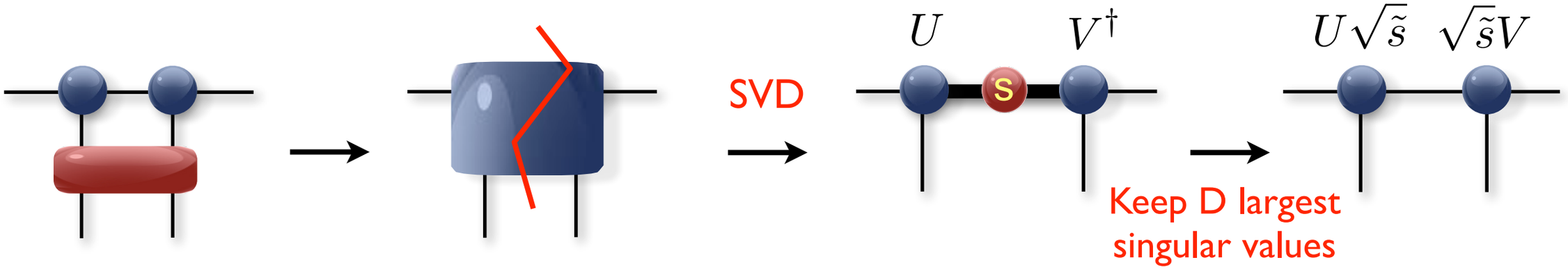
$$\exp(-\beta\hat{H}) = \exp(-\beta\sum_b \hat{H}_b) = \left(\exp(-\tau\sum_b \hat{H}_b)\right)^n \approx \left(\prod_b \exp(-\tau\hat{H}_b)\right)^n \qquad \tau = \beta/n$$

- 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

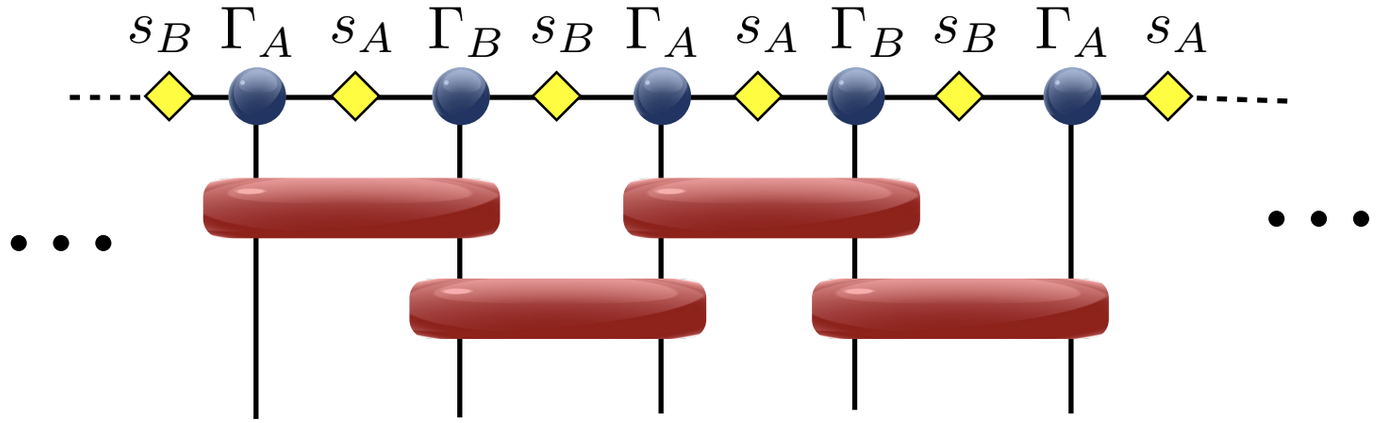
Note: MPS needs to be in canonical form

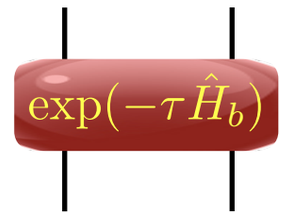
Optimization via imaginary time evolution

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

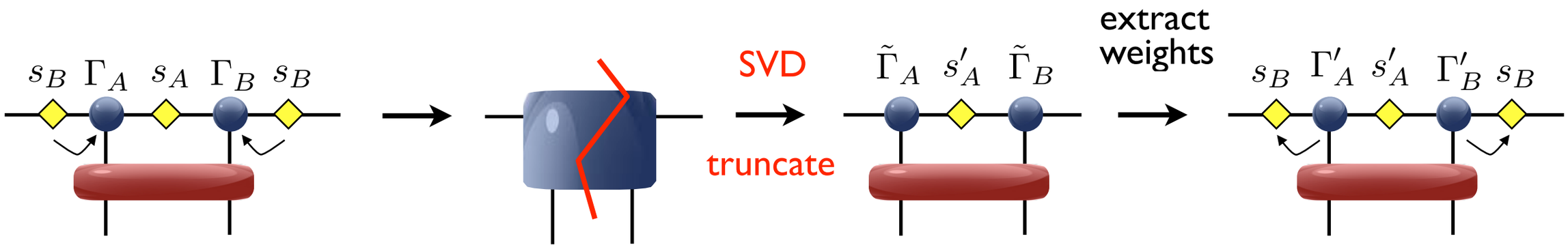
Trotter-Suzuki decomposition: $\exp(-\beta\hat{H}) = \exp(-\beta\sum_b \hat{H}_b) = \left(\exp(-\tau\sum_b \hat{H}_b)\right)^n \approx \left(\prod_b \exp(-\tau\hat{H}_b)\right)^n$, $\tau = \beta/n$

- 1D:



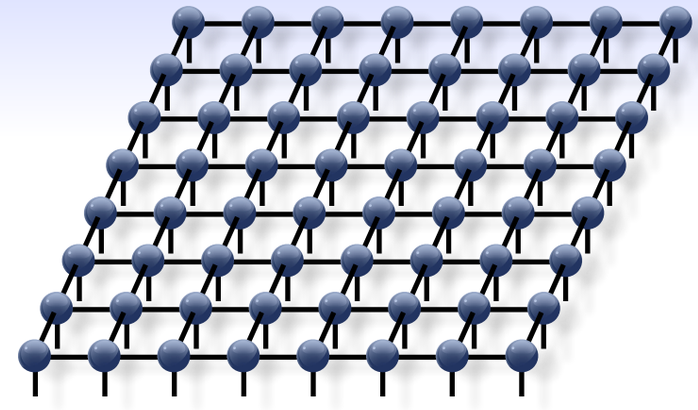


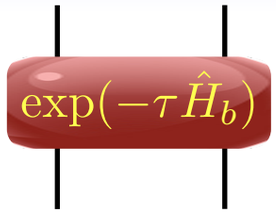
- At each step: apply a two-site operator to a bond and truncate bond back to *D*



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

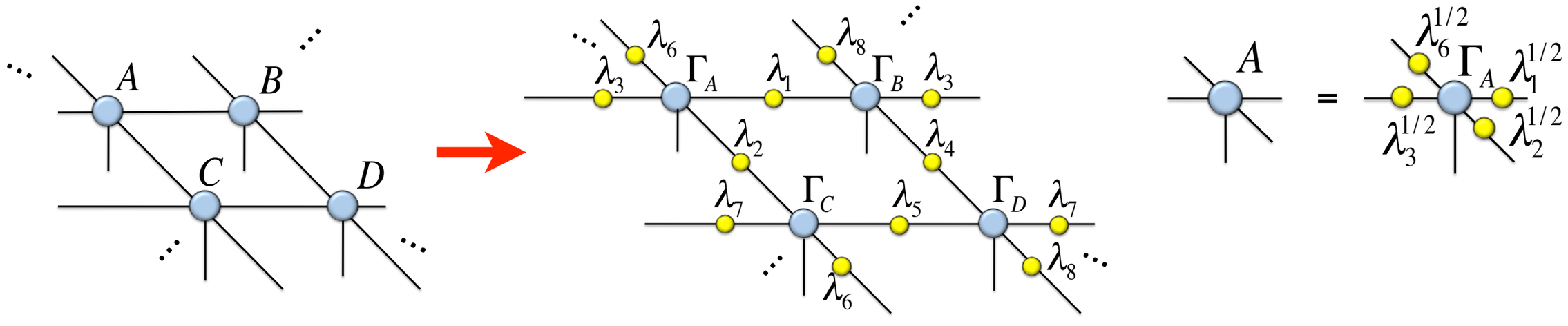
★ Fast-full update [Phien et al, PRB 92 (2015)]

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

Optimization: simple update

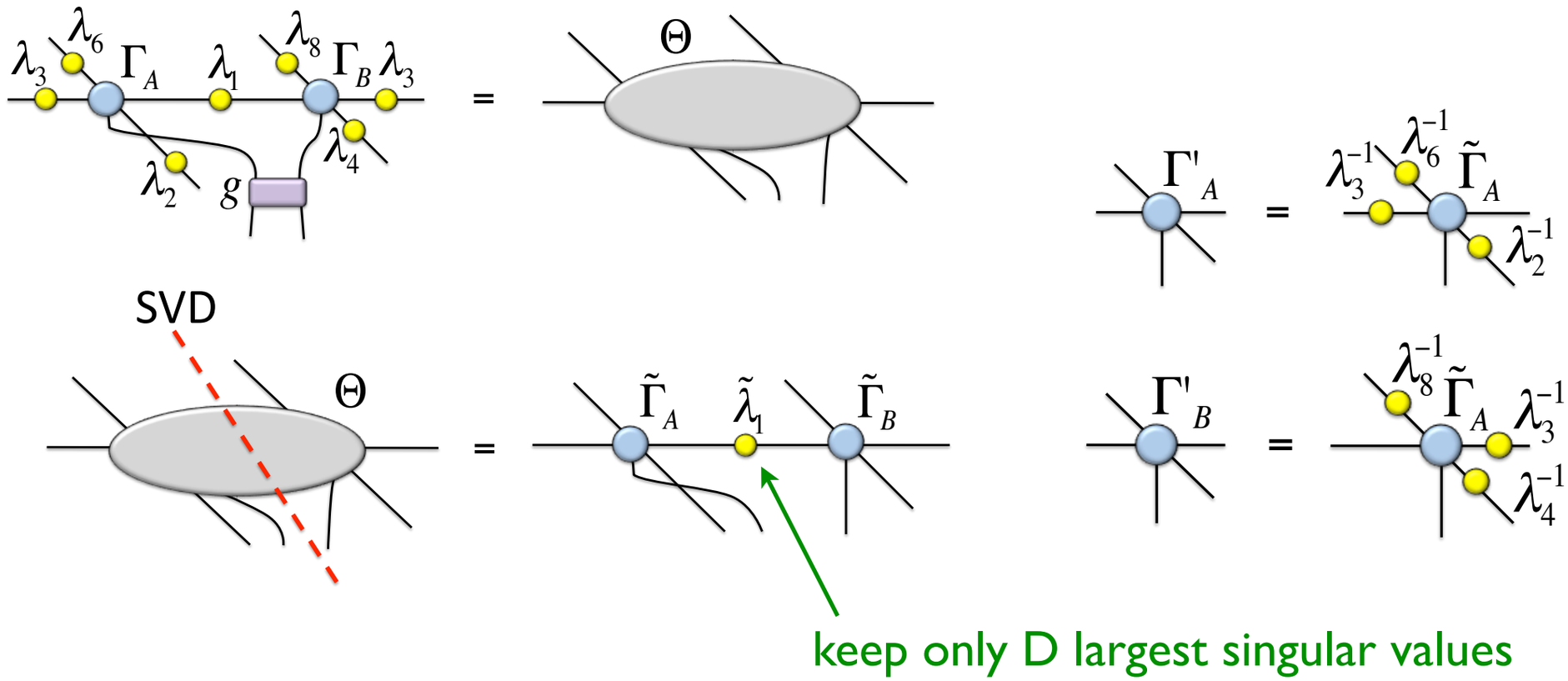
Jiang, et al., PRL 101, 090603 (2008)

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



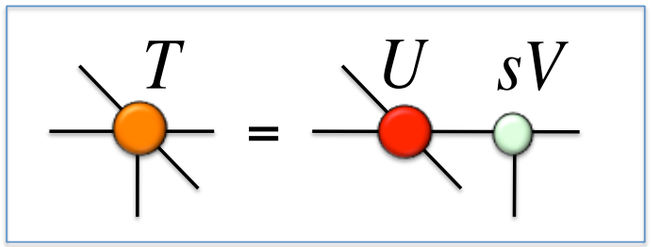
- Update works like in 1D with iTEBD (infinite time-evolving block decimation)

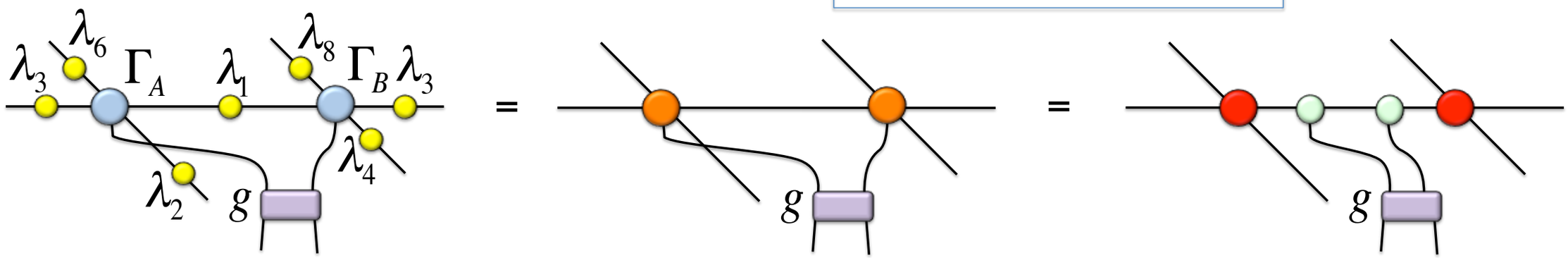
G. Vidal, PRL 91, 147902 (2003)

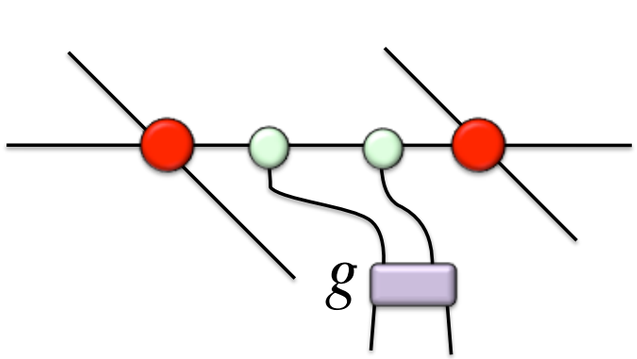


Trick to make it cheaper

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







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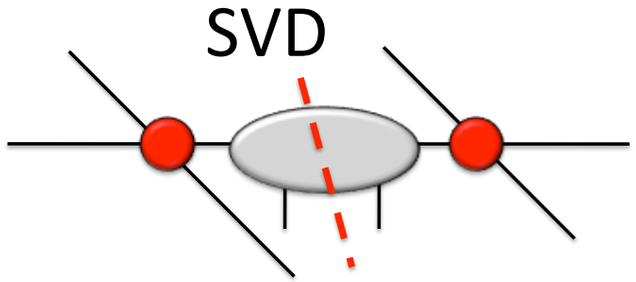

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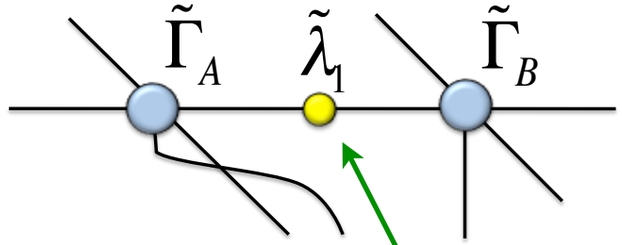
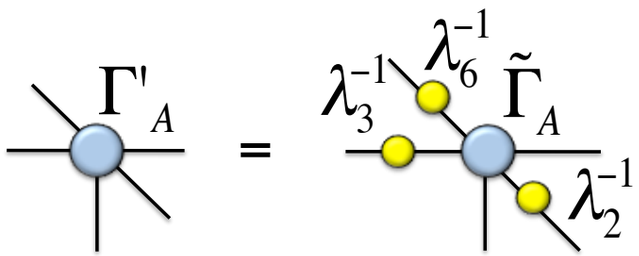
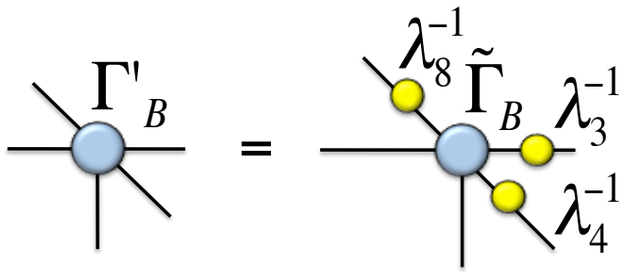


keep only D largest singular values

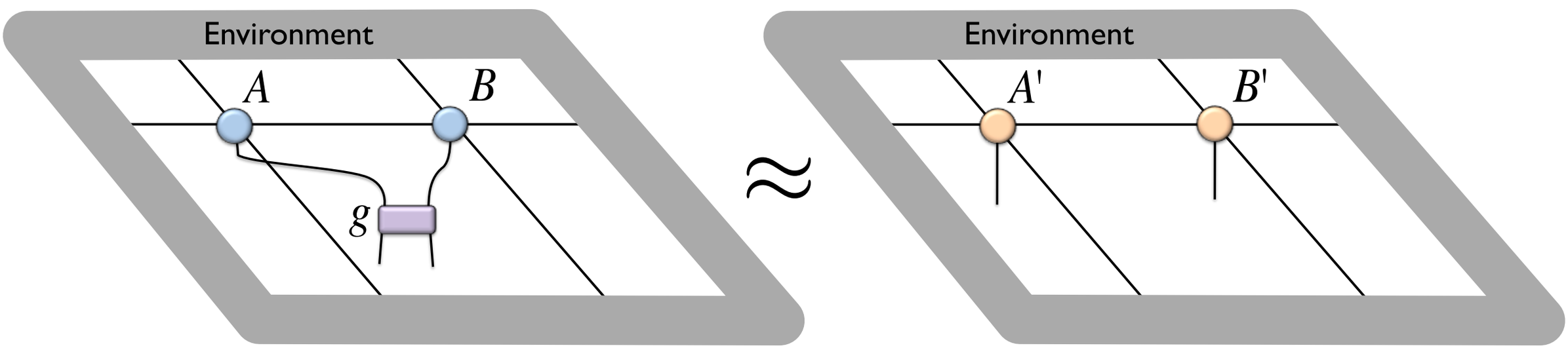




Optimization: full update

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

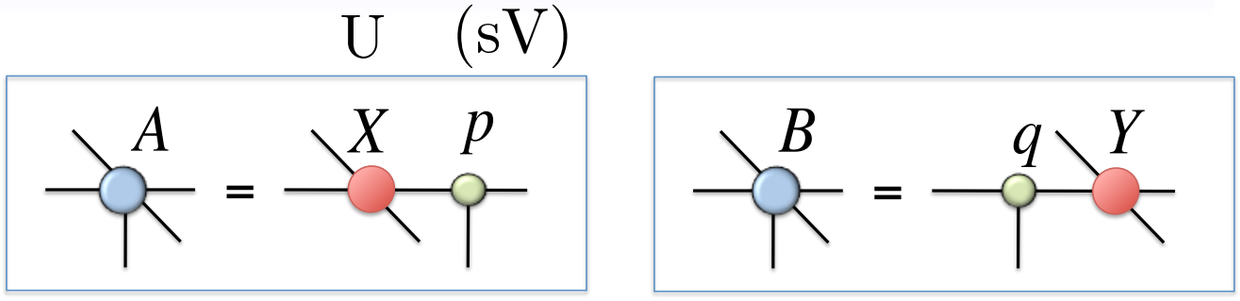


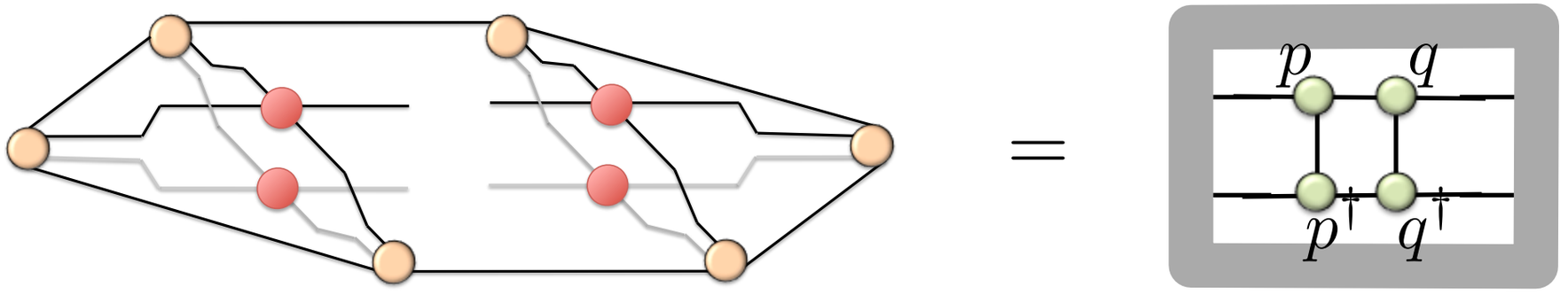
$$|\tilde{\Psi}\rangle = g|\Psi\rangle \qquad \approx \qquad |\Psi'\rangle$$

- Minimize $|| \, |\tilde{\Psi}\rangle - |\Psi'\rangle \, ||^2 = \langle\tilde{\Psi}|\tilde{\Psi}\rangle + \langle\Psi'|\Psi'\rangle - \langle\tilde{\Psi}|\Psi'\rangle - \langle\Psi'|\tilde{\Psi}\rangle$
- Iteratively / CG / Newton / ...

Full-update: details

- Split off the part of the tensor which is updated



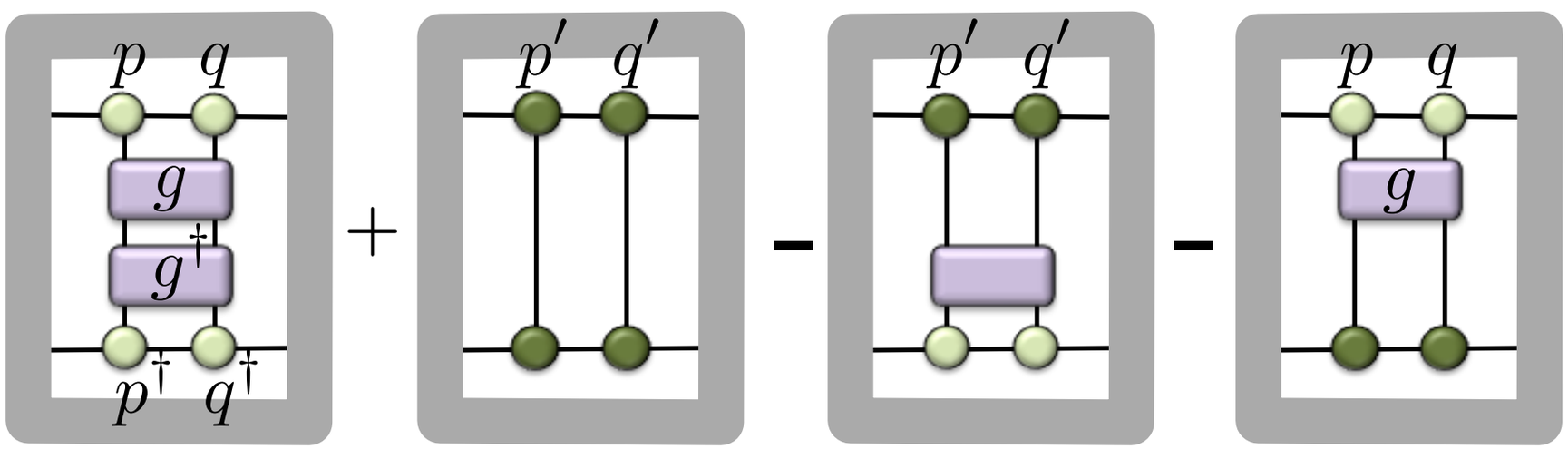


Environment of p and q tensors

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

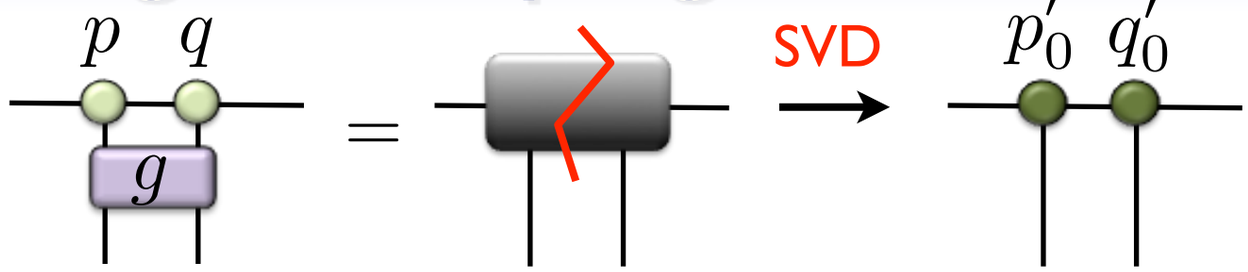
$$d(p',q') = \langle\tilde{\Psi}|\tilde{\Psi}\rangle + \langle\Psi'|\Psi'\rangle - \langle\tilde{\Psi}|\Psi'\rangle - \langle\Psi'|\tilde{\Psi}\rangle$$

"Cost-function"



Finding p' and q' through sweeping

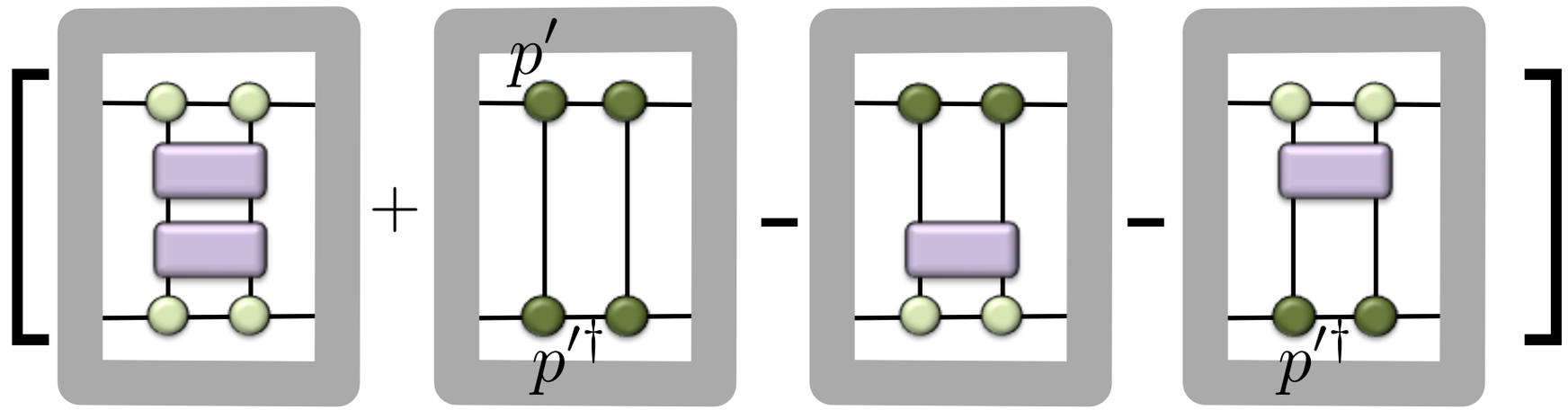
- Initial guess with SVD:



- Keep q' fixed and optimize with respect to p'

$$\frac{\partial}{\partial p'^*} d(p', q') = 0$$

$$\frac{\partial}{\partial p'^*}$$

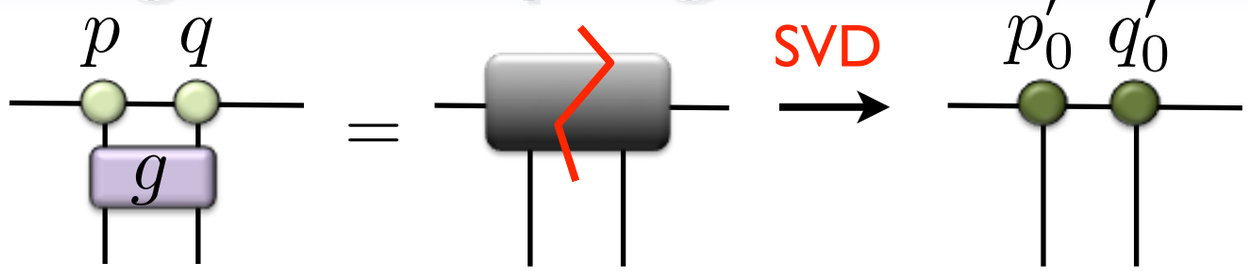


$$= 0$$

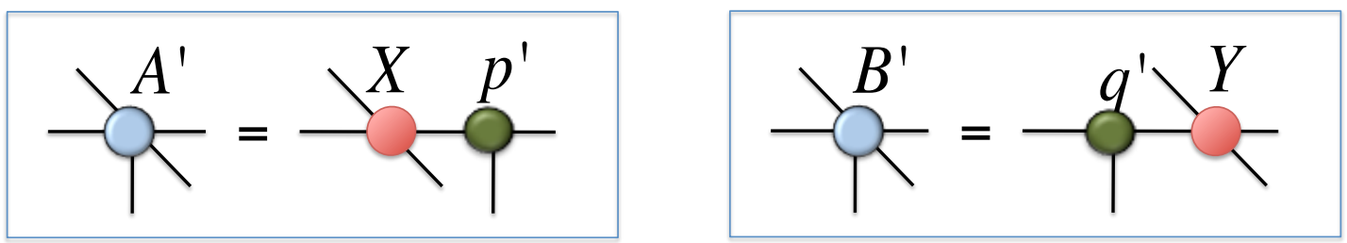
- Solve linear system: $Mp' = b$ → **new p'**

Finding p' and q' through sweeping

- Initial guess with SVD:



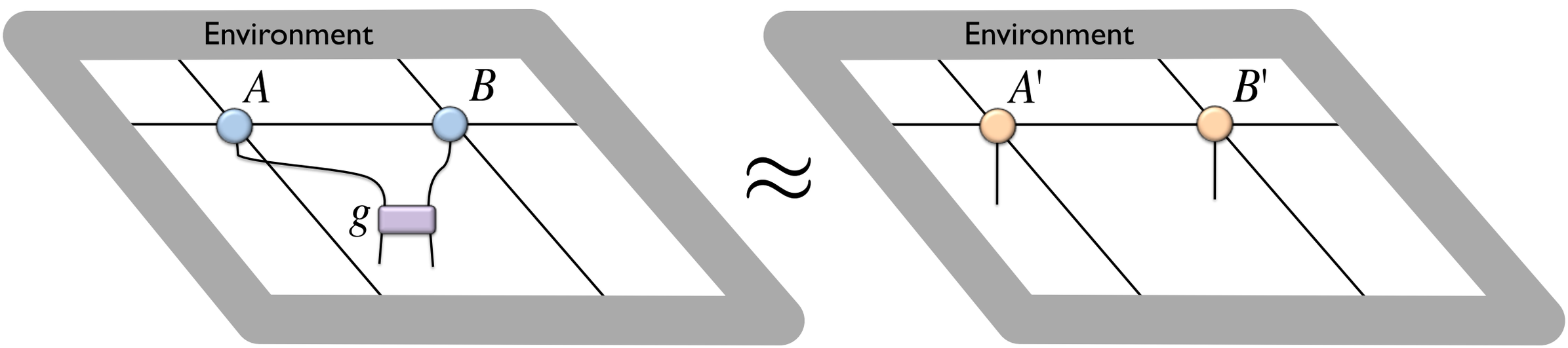
- Keep q' fixed and optimize with respect to p': $\frac{\partial}{\partial p'^*} d(p', q') = 0$
- Solve linear system: $Mp' = b$ → **new p'**
- Keep p' fixed and optimize with respect to q': $\frac{\partial}{\partial q'^*} d(p', q') = 0$
- Solve linear system: $\tilde{M}q' = \tilde{b}$ → **new q'**
- 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



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

- 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

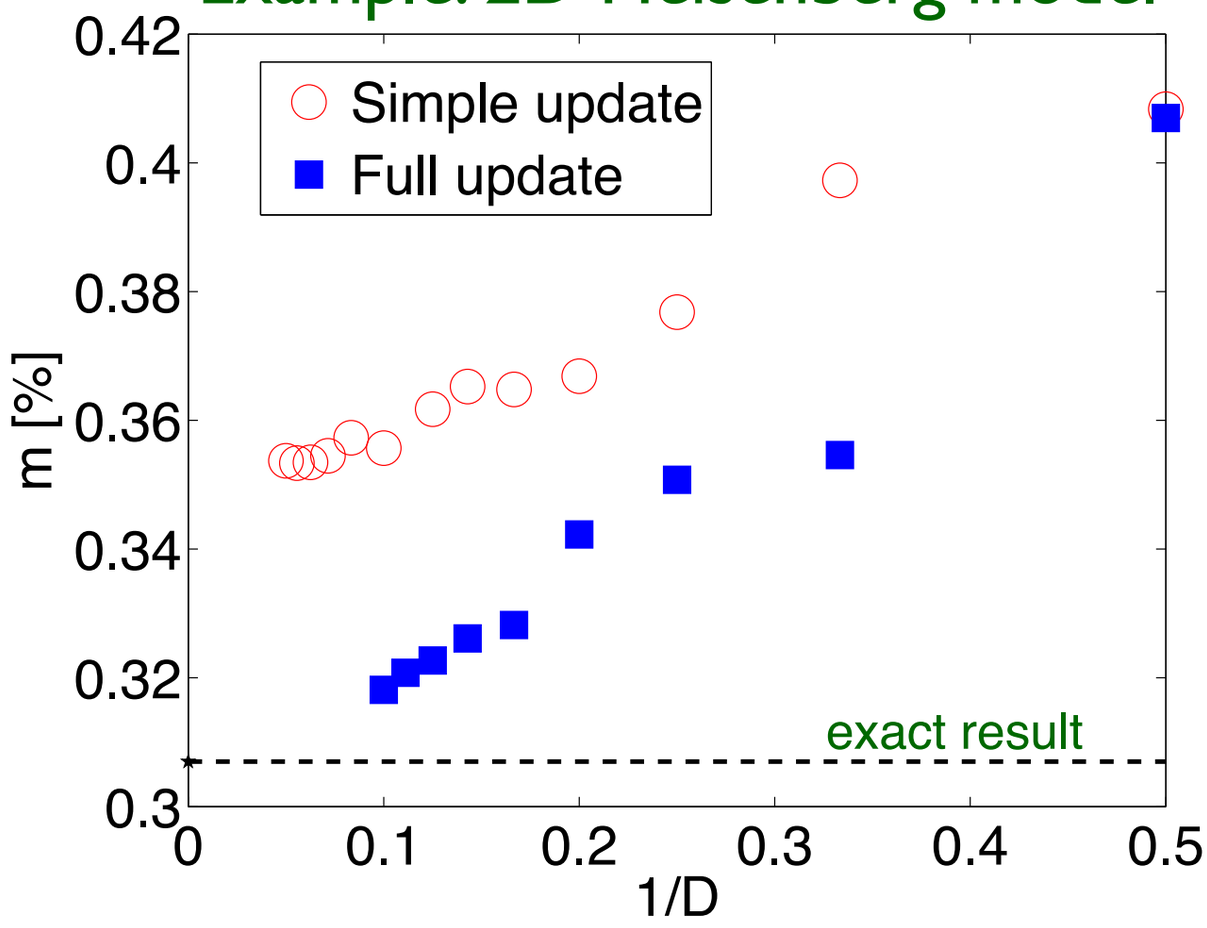
★ Cheap, but not optimal
(e.g. overestimates magnetization
in S=1/2 Heisenberg model)

full update

★ Take the full wave function into account for truncation

★ optimal, but computationally more expensive

Example: 2D Heisenberg model



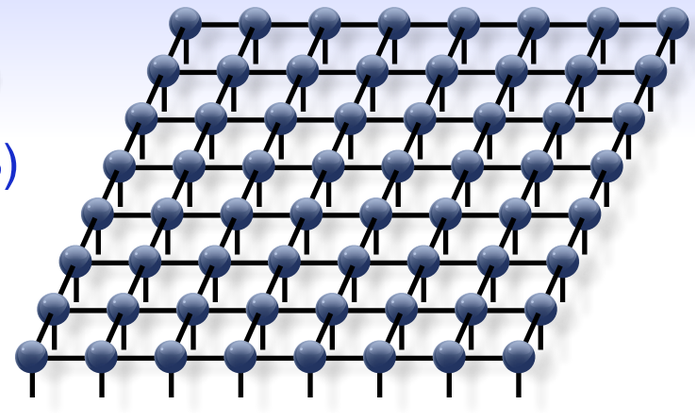
- Combine the two: Use simple update to get an initial state for the full update

- 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:

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

tensor network including all Hamiltonian terms

tensor network from norm term

tensor A reshaped as a vector

solve generalized eigenvalue problem

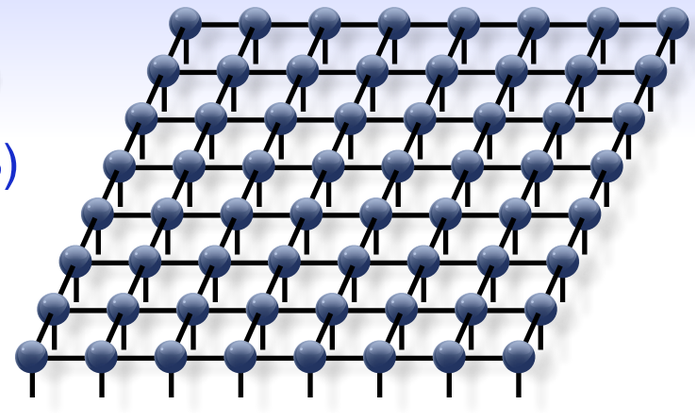
$\mathbf{H} =$

$\mathbf{N} =$

in 1D:

Variational optimization for PEPS

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



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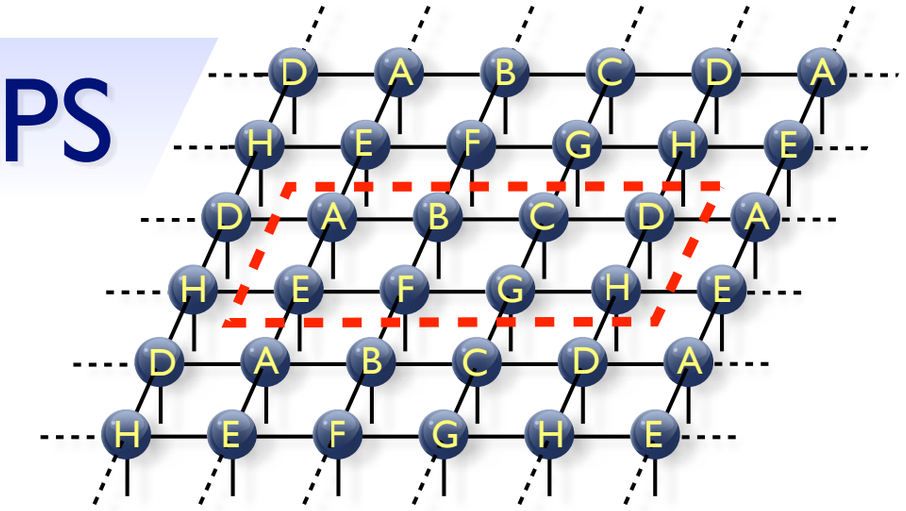
tensor A reshaped as a vector

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

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

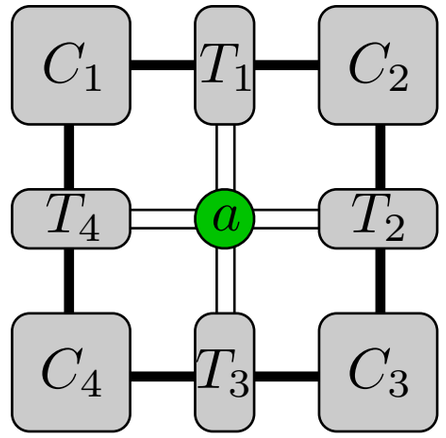
tensor A reshaped as a vector

H-environment

tensor network including
all Hamiltonian terms

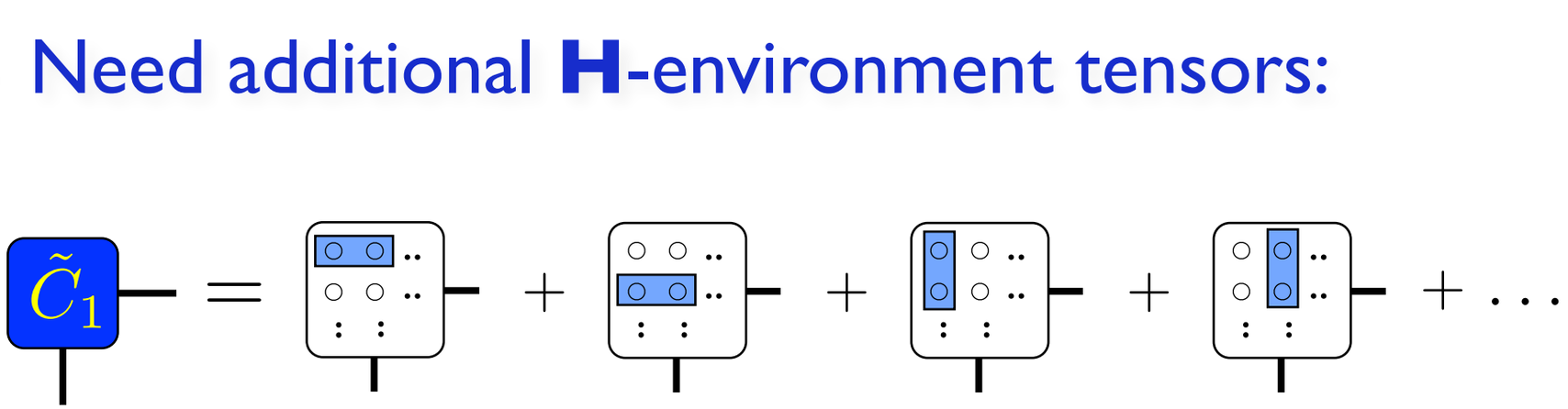
tensor network from norm

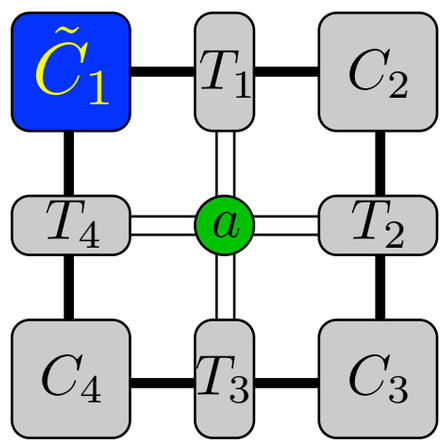
$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \xrightarrow{\text{minimize}} \mathbf{H}\,x = E\,\mathbf{N}\,x$$



But how about H ??

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

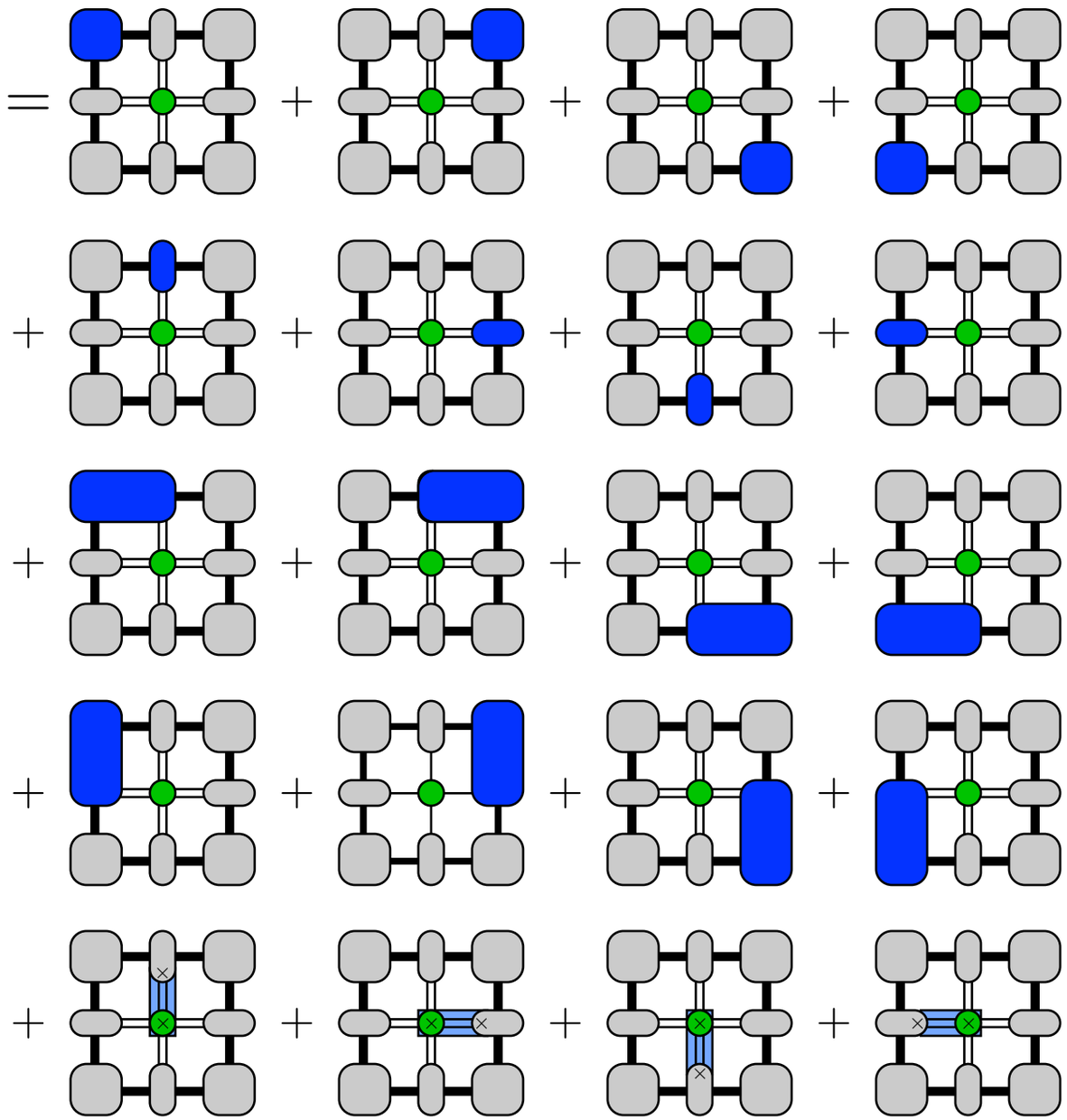




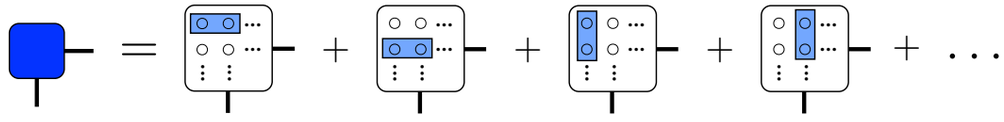
➡ taking into account all Hamiltonian contributions in the infinite upper left corner

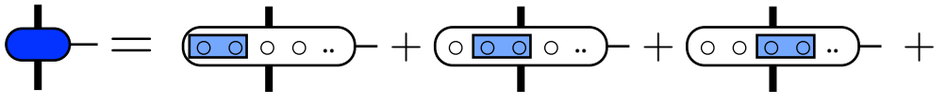
H-environment

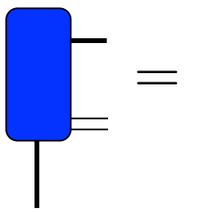
$$\langle \Psi | \hat{H} | \Psi \rangle =$$



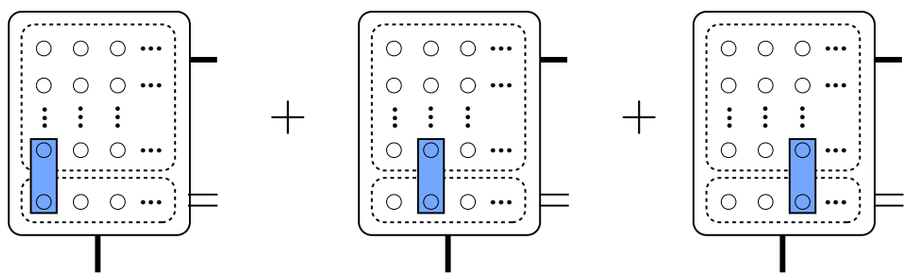
Corner terms







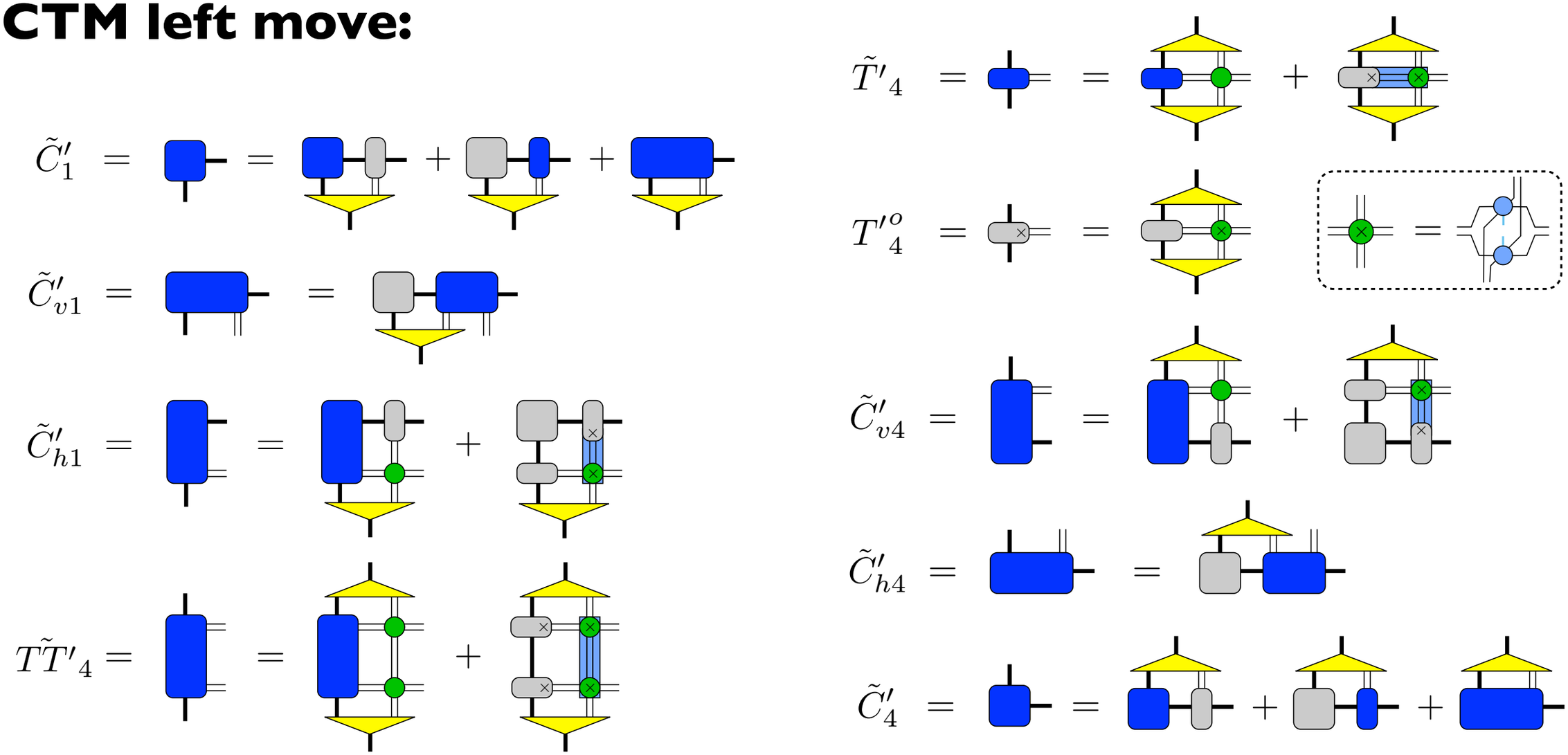
Terms between a corner and an edge tensor



Local terms

H-environment: bookkeeping

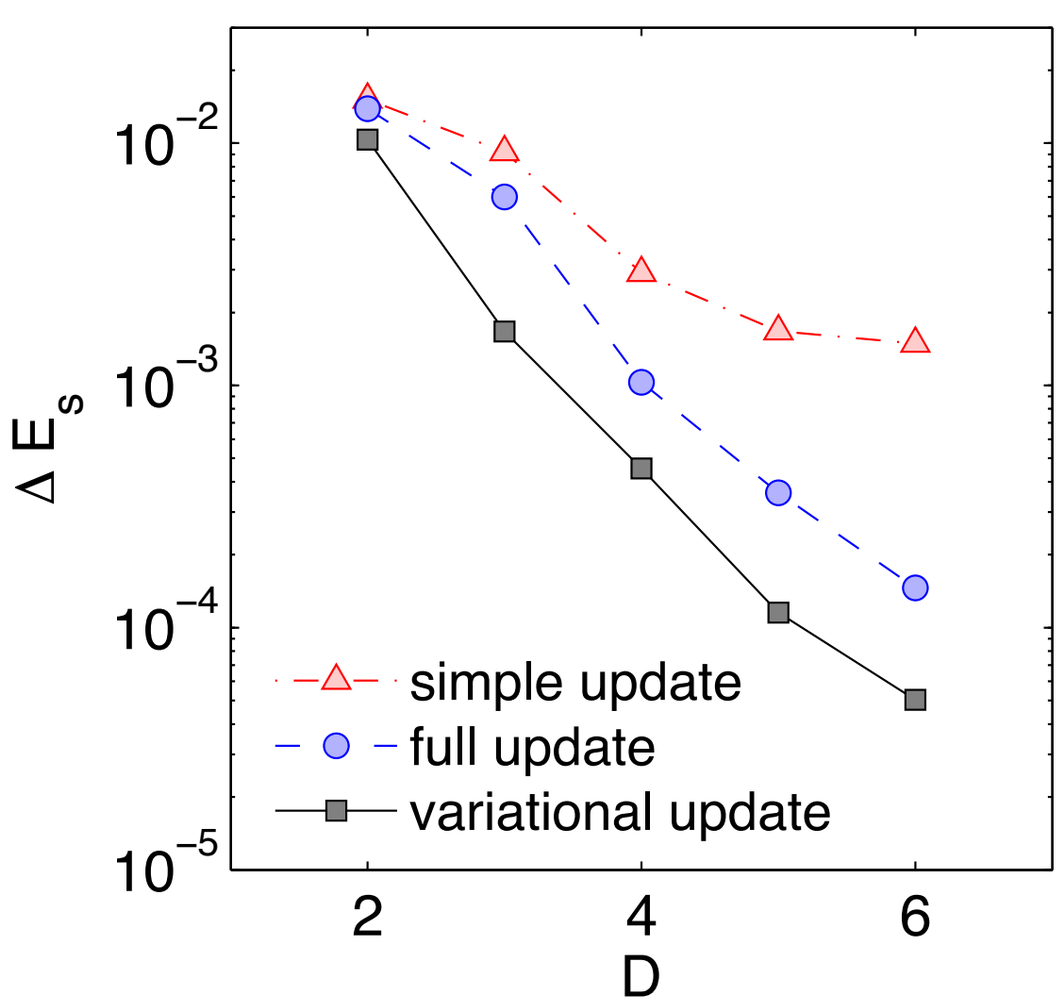
CTM left move:

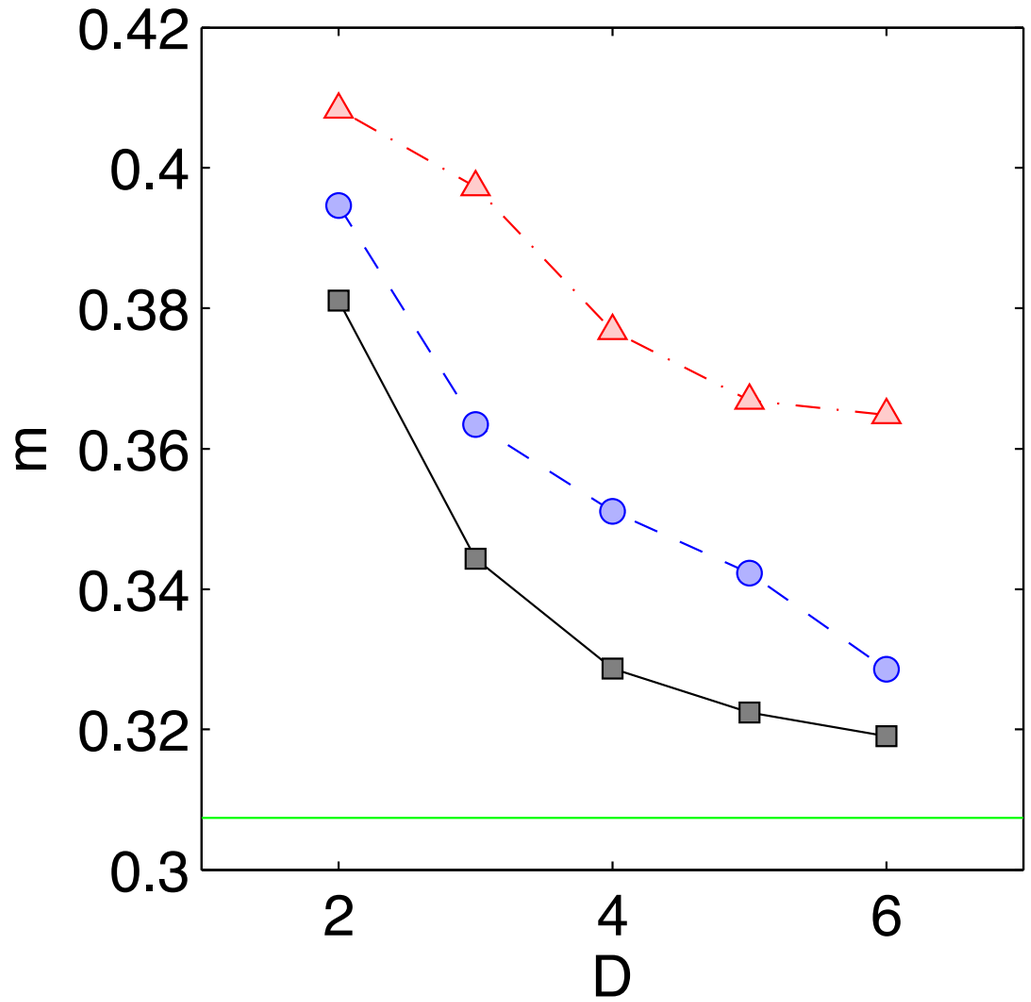


... and similarly for right-, top-, bottom-move

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

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]

Automatic differentiation

PHYSICAL REVIEW X **9,** 031041 (2019)

Differentiable Programming Tensor Networks

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[3]*Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China*
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(Received 2 April 2019; published 5 September 2019)

Differentiable programming is a fresh programming paradigm which composes parameterized algorithmic components and optimizes them using gradient search. The concept emerges from deep learning but is rogramming tensor netwo orithm as a computation l efficiently using automa or networks contraction a nd efficient backpropaga heat of the Ising model the tensor renormalizati of infinite projected ent in state-of-the-art variatio ng removes laborious human efforts in deriving and implementing analytical gradients for tensor network programs, which opens the door to more innovations in tensor network algorithms and applications.

Computing gradients in an automatized fashion!
Simplifies codes substantially!
Implemented in machine learning frameworks (TensorFlow, PyTorch, …)

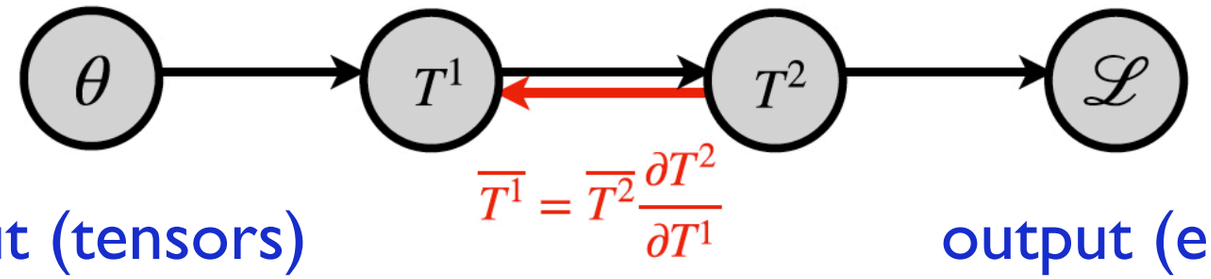
DOI: 10.1103/PhysRevX.9.031041

Subject Areas: Computational Physics, Condensed Matter Physics

Automatic differentiation

Liao, Liu, Wang, Xiang, PRX (2019)

computation graph:



input (tensors) output (e.g. energy)

Compute the gradient via chain rule:

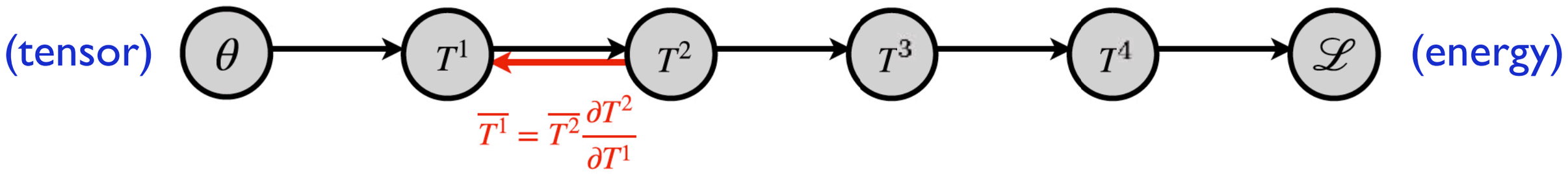
$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{\partial \mathcal{L}}{\partial T^n}\frac{\partial T^n}{\partial T^{n-1}}\cdots\frac{\partial T^2}{\partial T^1}\frac{\partial T^1}{\partial \theta}$$

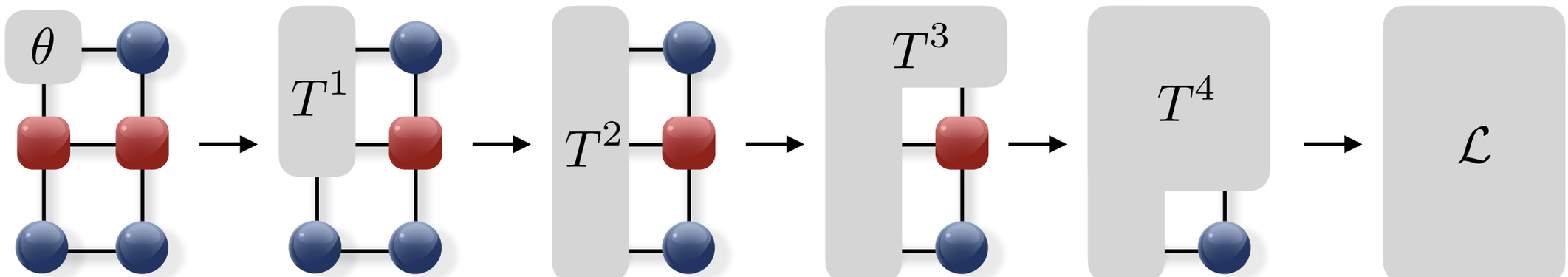
from left to right
(back propagation algorithm)

Define forward and backward function of each elementary operation (primitives), e.g. addition, multiplication, math functions, matrix-matrix multiplications, eigenvalue decompositions, etc.

→ Gradient can be computed in an automatized fashion

Simple example

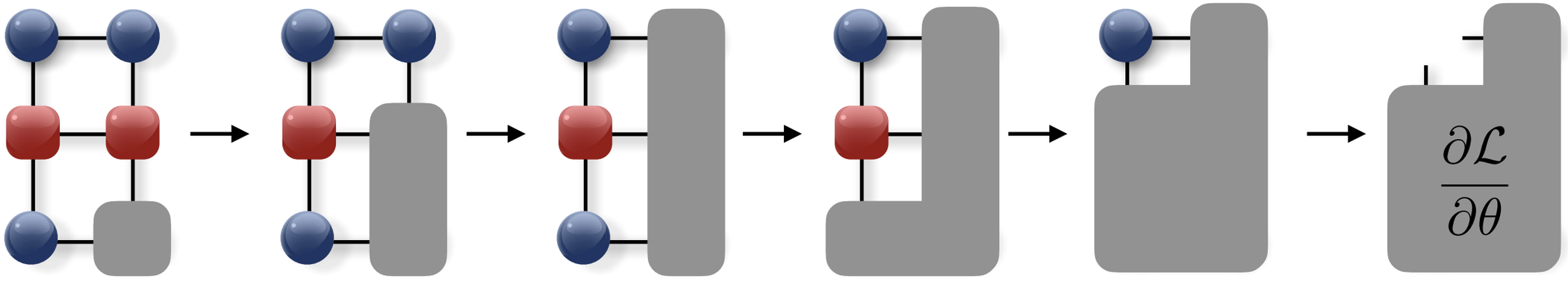




Compute the gradient via chain rule:

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{\partial \mathcal{L}}{\partial T^4}\frac{\partial T^4}{\partial T^3}\frac{\partial T^3}{\partial T^2}\frac{\partial T^2}{\partial T^1}\frac{\partial T^1}{\partial \theta}$$

from left to right
(back propagation algorithm)



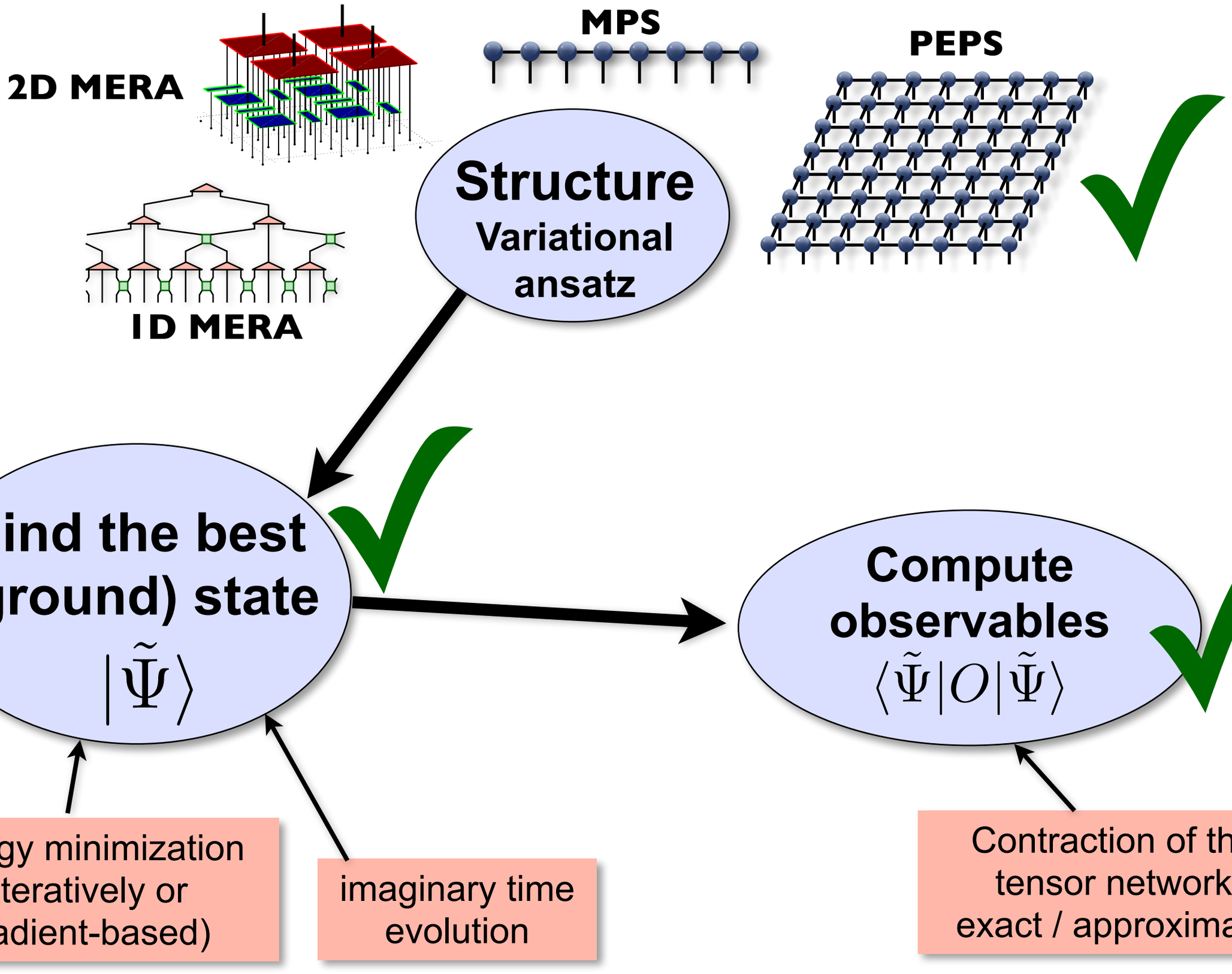
Summary: optimization in iPEPS

- 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
  - ✦ 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)
  - ✦ Automatic differentiation: higher accuracy, similar cost and **simpler!**
    Nishino et al. Prog. Theor. Phys 105 (2001), Gendiar et al. Prog. Theor. Phys 110 (2003)
  - ✦ … and more …

Summary: Tensor network algorithms (ground state)



Part IV: iPEPS application example

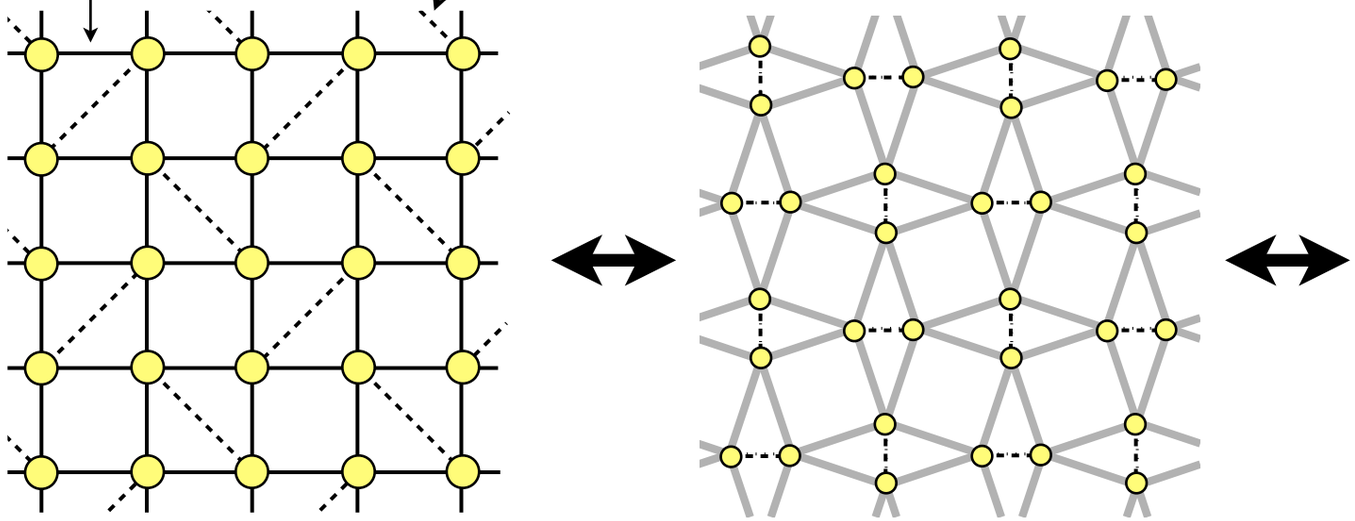
iPEPS ground state simulations

- Many applications to challenging problems, including frustrated spin, SU(N), and bosonic systems, t-J / Hubbard models, and more, see e.g.:

P. Corboz, A. M. Läuchli, K. Penc, M. Troyer and F. Mila, PRL 107 (2011)
S. Dusuel, M. Kamfor, R. Orús, K. P. Schmidt, and J. Vidal, PRL 106, 107203 (2011)
H. H. Zhao, C. Xu, Q. N. Chen, Z. C. Wei, M. P. Qin, G. M. Zhang and T. Xiang, PRB 85 (2012)
P. Corboz, M. Lajkó, A. M. Läuchli, K. Penc and F. Mila, PRX 2 (2012)
P. Corboz and F. Mila, PRB 87 (2013); PRL 112 (2014)
Z.-C. Gu, H.-C. Jiang, D. N. Sheng, H. Yao, L. Balents and X.-G. Wen, PRB 88 (2013)
J. Osorio Iregui, P. Corboz and M. Troyer, PRB 90 (2014)
P. Corboz, T. Rice and M. Troyer, PRL 113 (2014)
T. Picot and D. Poilblanc, PRB 91 (2015)
T. Picot, M. Ziegler, R. Orús and D. Poilblanc, PRB 93 (2016)
P. Nataf, M. Lajkó, P. Corboz, A. M. Läuchli, K. Penc and F. Mila, PRB 93 (2016)
H. Liao, Z. Xie, J. Chen, Z. Liu, H. Xie, R. Huang, B. Normand and T. Xiang, PRL 118 (2017)
B.-X. Zheng, et al., Science 358, 1155 (2017)
I. Niesen and P. Corboz, PRB 95 (2017); SciPost Physics 3, 030 (2017); Rev. B 97, 245146 (2018)
R. Haghshenas, W.-W. Lan, S.-S. Gong, and D. N. Sheng, PRB 97 (2018)
J.-Y. Chen, L. Vanderstraeten, S. Capponi, and D. Poilblanc, PRB 98 (2018)
S. S. Jahromi and R. Orús, PRB 98 (2018)
H.-Y. Lee and N. Kawashima, PRB 97 (2018)
H. Yamaguchi, Y. Sasaki, T. Okubo, et al.,PRB 98, 094402 (2018)
R. Haghshenas, S.-S. Gong, and D. N. Sheng, PRB 99, 174423 (2019)
S. S. Chung and P. Corboz, PRB 100 (2019)
B. Ponsioen, S. S. Chung, and P. Corboz, PRB 100 (2019)
C. Boos, S. P. G. Crone, I. A. Niesen, P. Corboz, K. P. Schmidt, and F. Mila, PRB 100 (2019)
Z. Shi, et al, Nature Communications 10, 2439 (2019)
A. Kshetrimayum, C. Balz, B. Lake, and J. Eisert, ArXiv:1904.00028 (2019)
H.-Y. Lee, R. Kaneko, T. Okubo, and N. Kawashima, PRL 123, 087203 (2019).
O. Gauthé, S. Capponi, M. Mambrini, and D. Poilblanc, PRB 101, 205144 (2020).
H.-Y. Lee, R. Kaneko, L. E. Chern, T. Okubo, Y. Yamaji, N. Kawashima, and Y. B. Kim, Nature Communications 11 (2020)
W.-Y. Liu, S.-S. Gong, Y.-B. Li, D. Poilblanc, W.-Q. Chen, and Z.-C. Gu, ArXiv:2009.01821 (2020)
J.-Y. Chen, S. Capponi, A. Wietek, M. Mambrini, N. Schuch, and D. Poilblanc, PRL 125, 017201 (2020)
J. Hasik, D. Poilblanc, and F. Becca, SciPost Physics 10, 012 (2021)
… and many more …

The Shastry-Sutherland model and $SrCu_2(BO_3)_2$

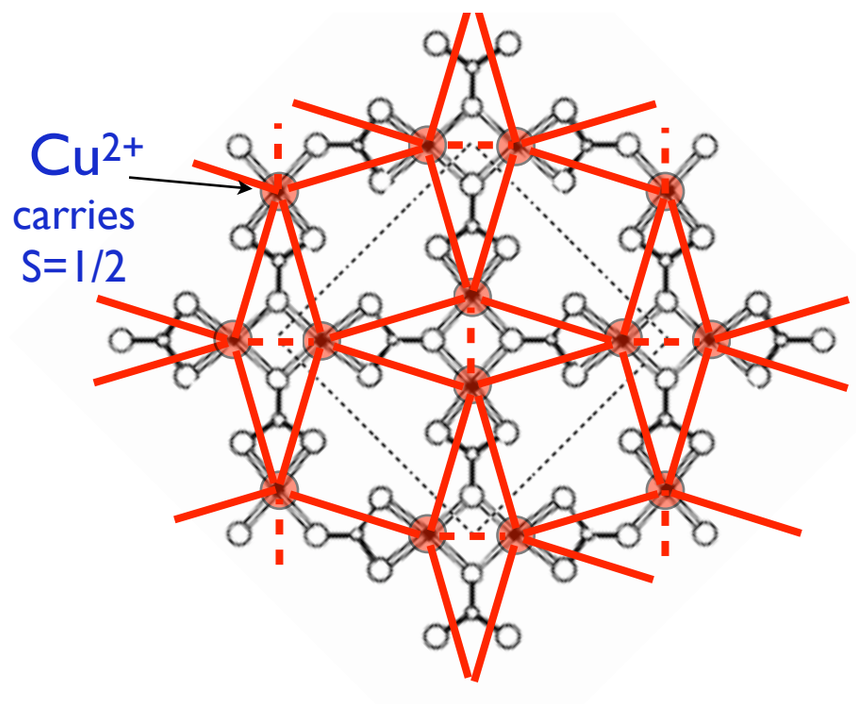
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j$$



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

$SrCu_2(BO_3)_2$

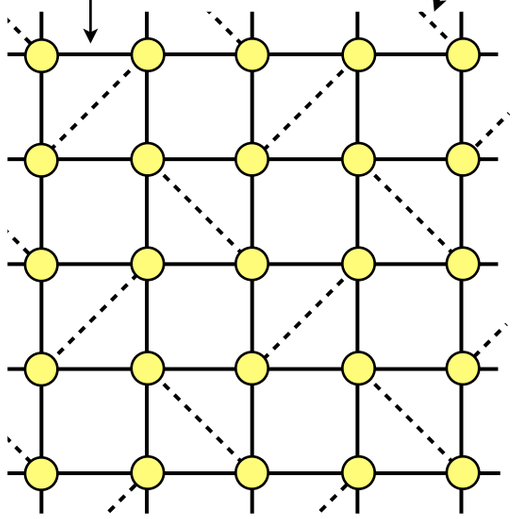
Spin-gap system (~35K)

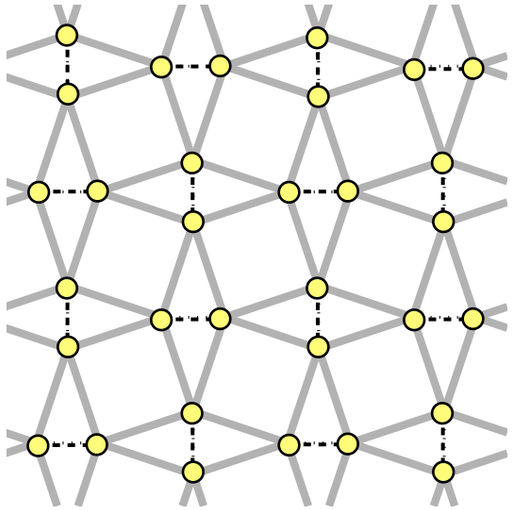


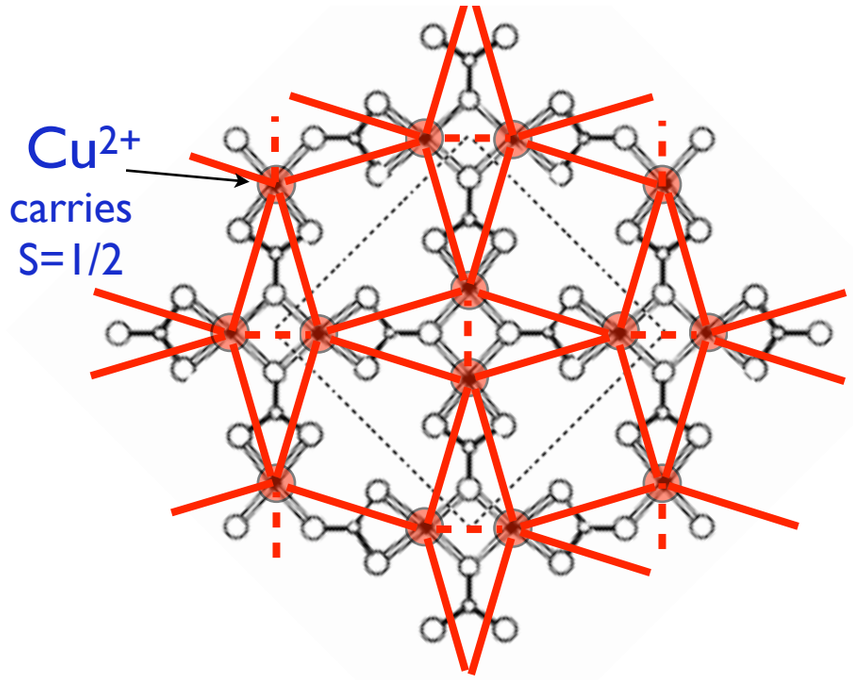
Kageyama et al. PRL **82** (1999)

The Shastry-Sutherland model and $SrCu_2(BO_3)_2$

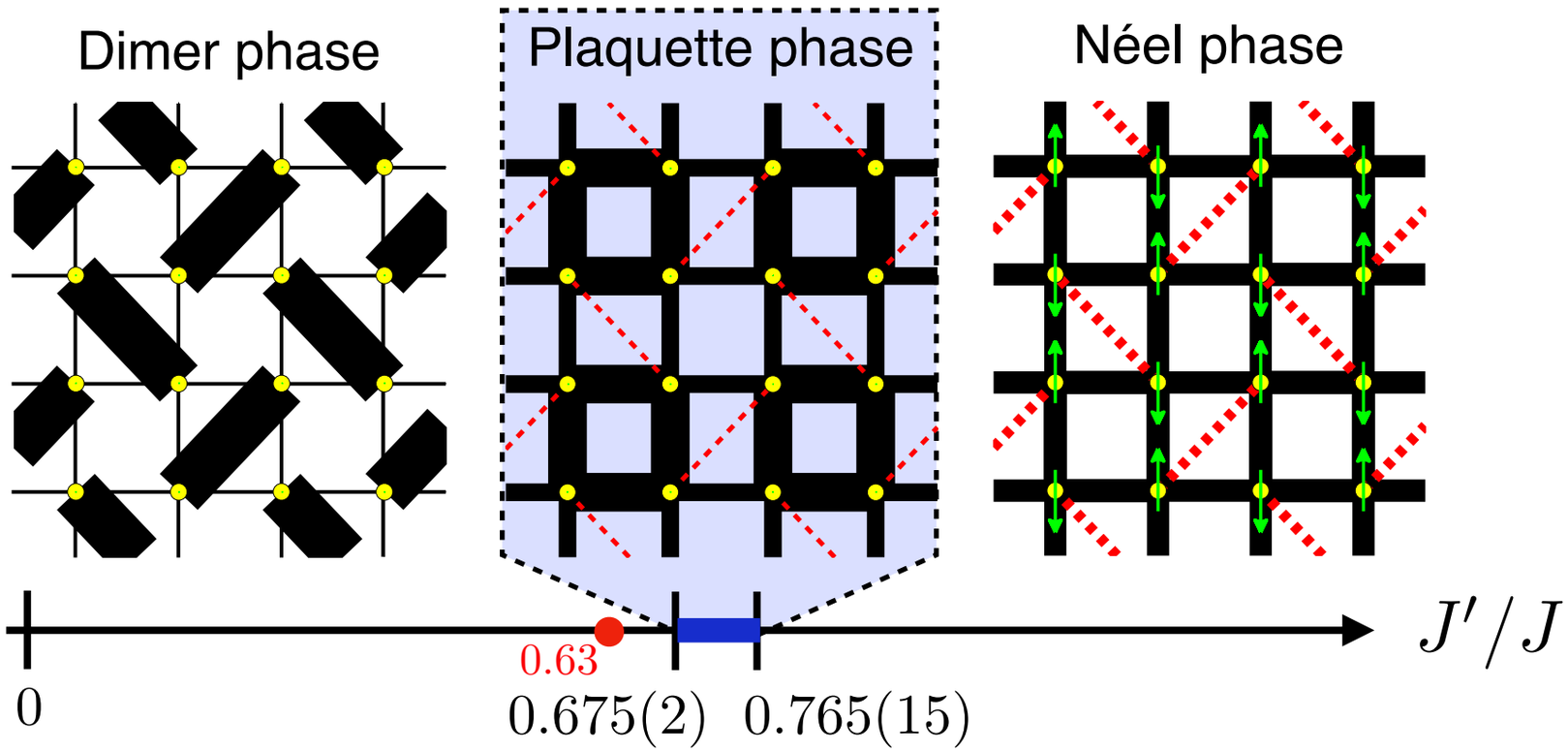
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\text{dimer}}} S_i \cdot S_j$$







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



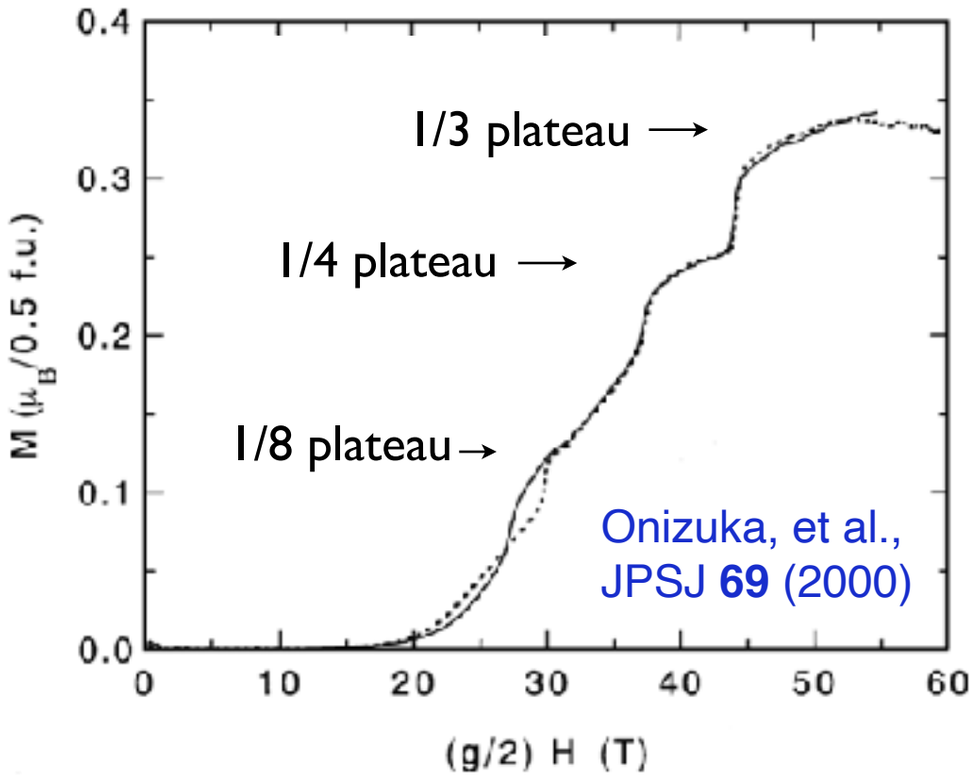
Corboz and Mila, PRB **87** (2013)

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

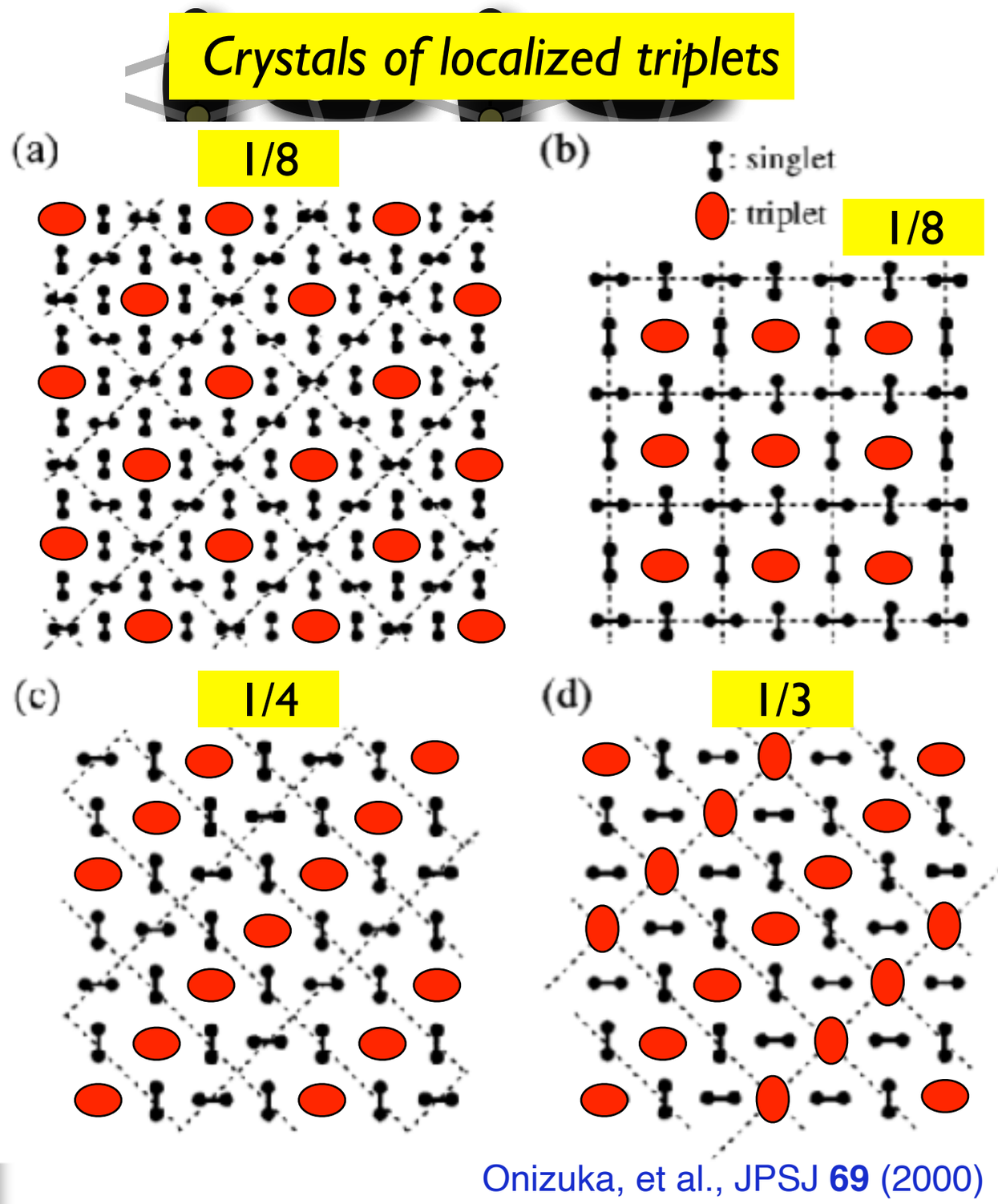
$SrCu_2(BO_3)_2$ in a magnetic field exhibits several magnetization plateaus



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)



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...

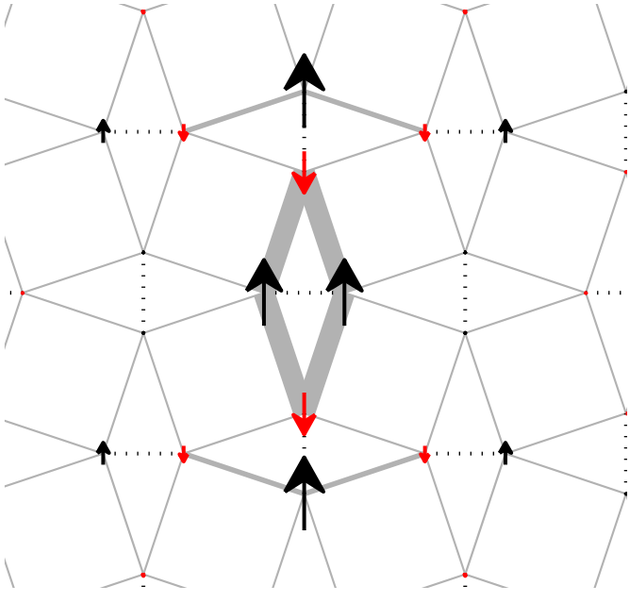
Kageyama et al, PRL **82** (1999)
Onizuka et al, JPSJ **69** (2000)
Kageyama et al, PRL **84** (2000)
Kodama et al, Science **298** (2002)
Takigawa et al, Physica **27** (2004)
Levy et al, EPL **81** (2008)
Sebastian et al, PNAS **105** (2008)
Isaev et al, PRL **103** (2009)
Jaime et al, PNAS **109** (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

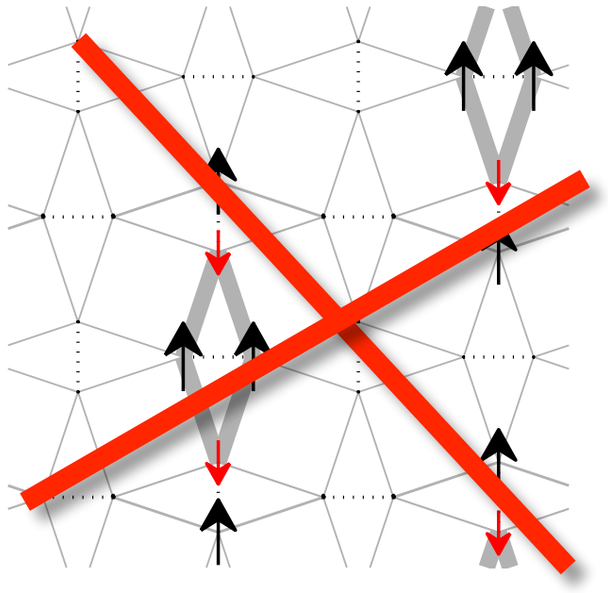
iPEPS simulations of the SSM in a magnetic field

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

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

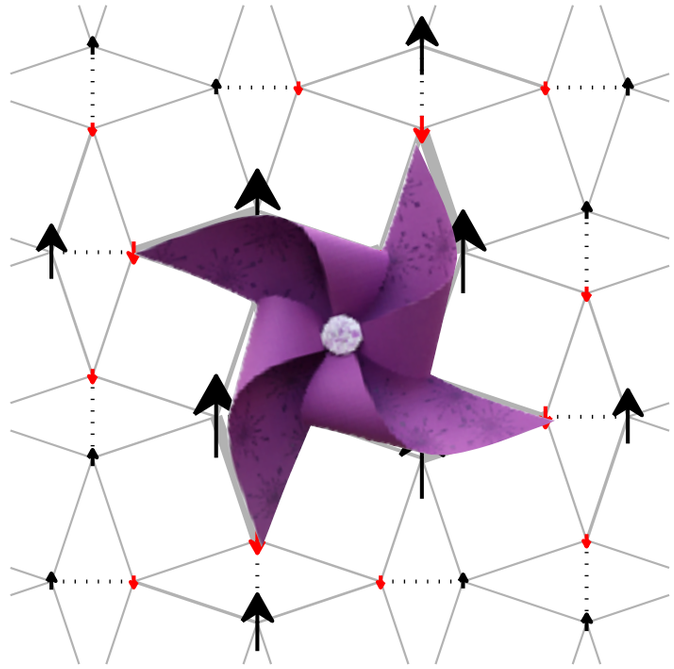


spin structure of 1 localized triplet in a 4x4 cell



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

small D
(mean-field result)



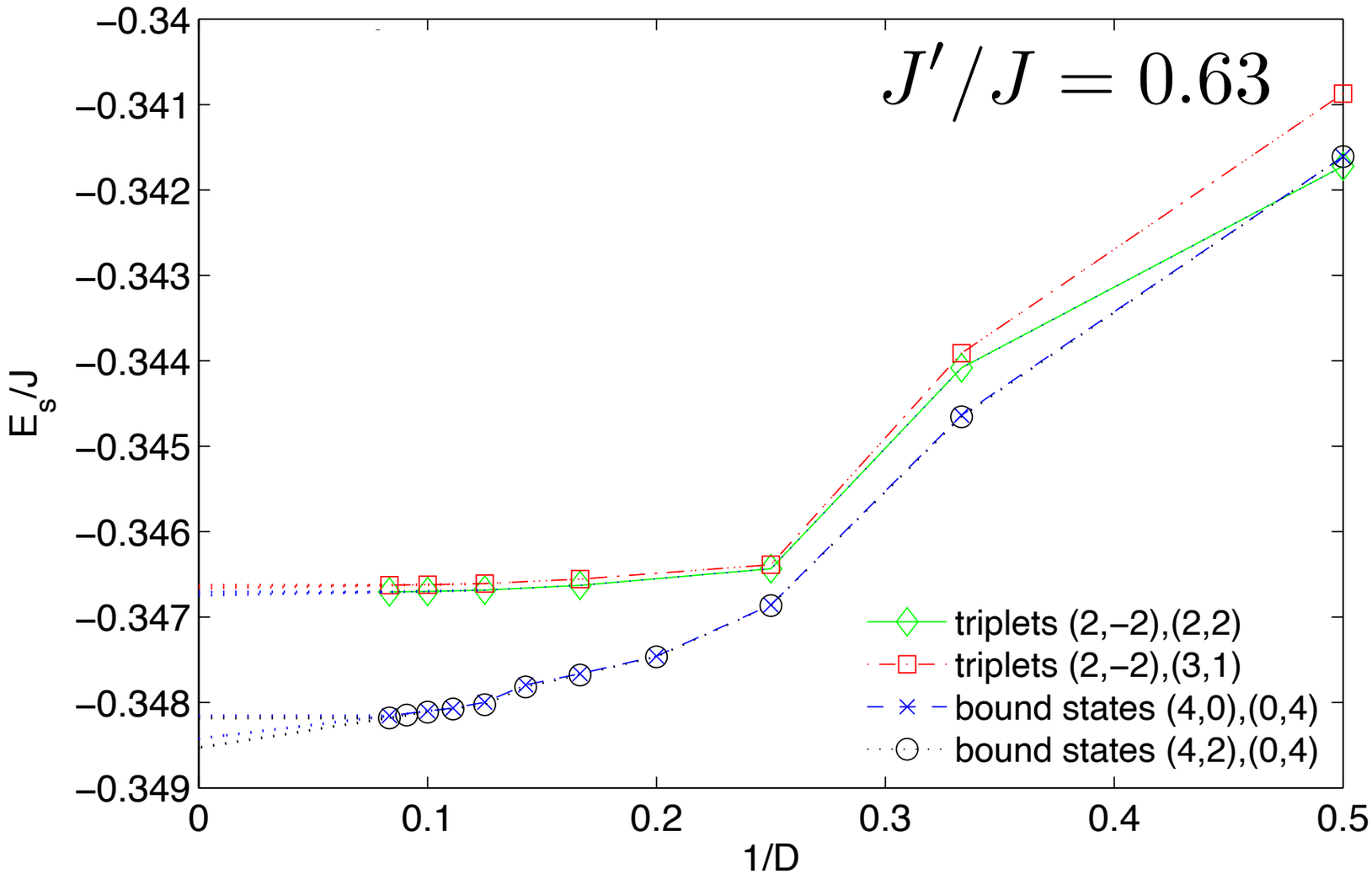
spin structure of a Sz=2 excitation in a 4x4 cell

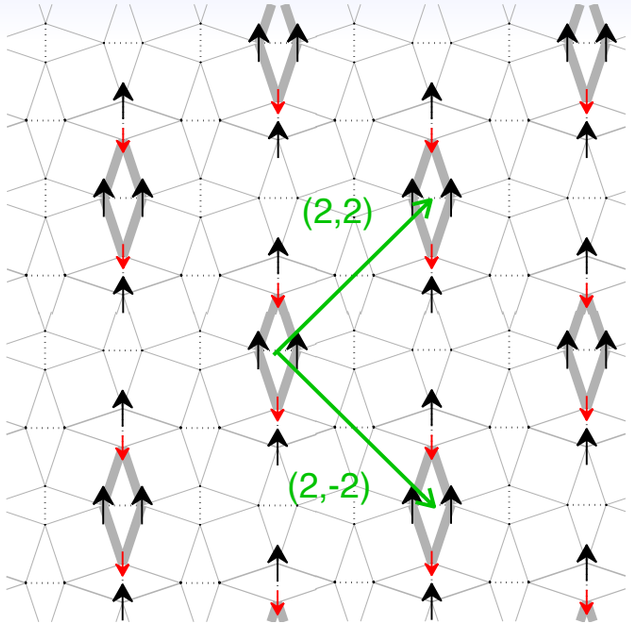
obtained with iPEPS
for D>4

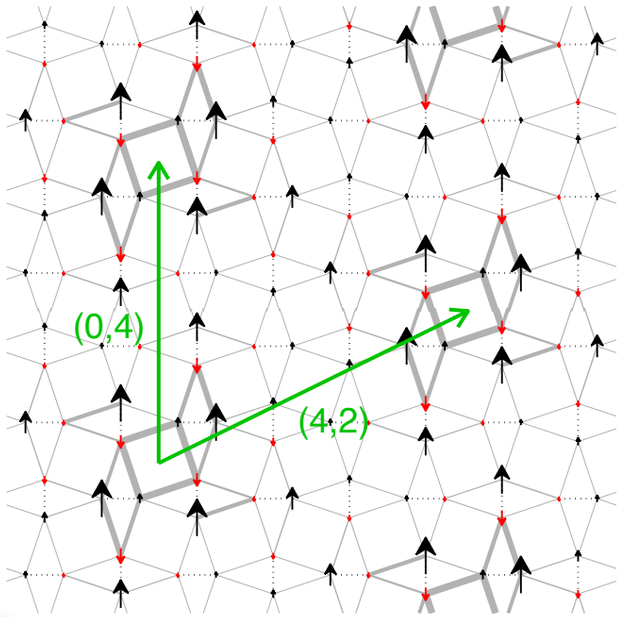
Bound state of two triplets!

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

Example: 1/8 plateau

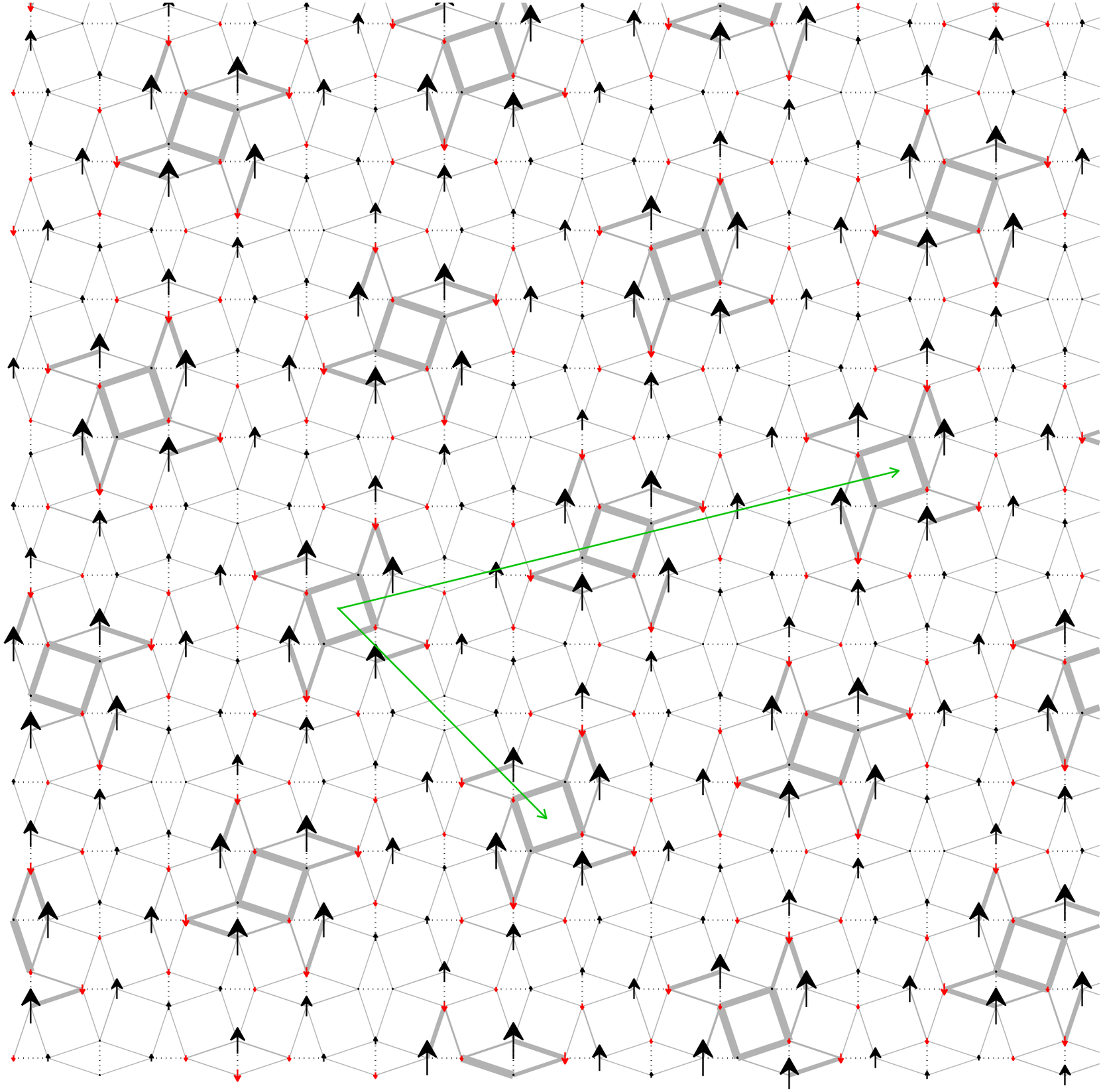






- All the proposed triplet crystals have a higher energy than the crystals made of bound states!
- Similar results found for other plateaus below 1/4

2/15 plateau

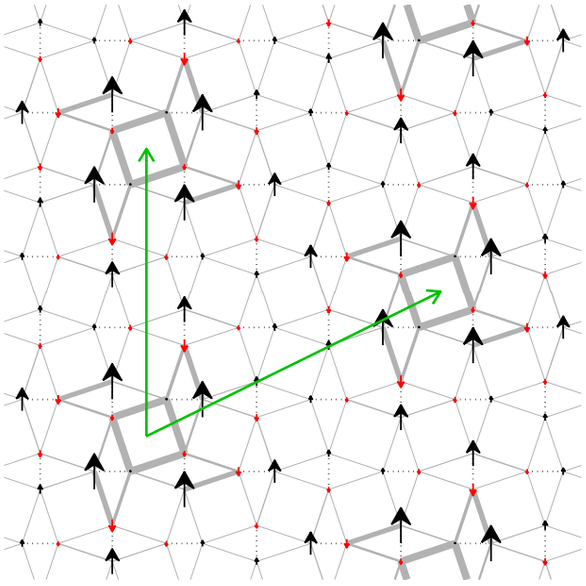


Unit cell with 30 tensors (60 sites)

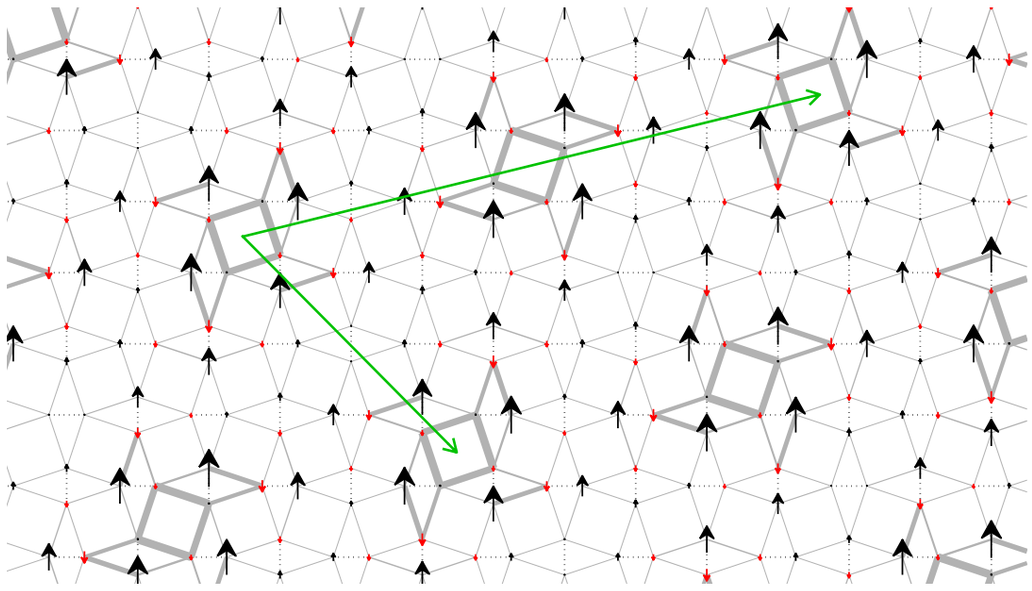
Regular pattern of bound states!

Computing the energies of all possible crystals

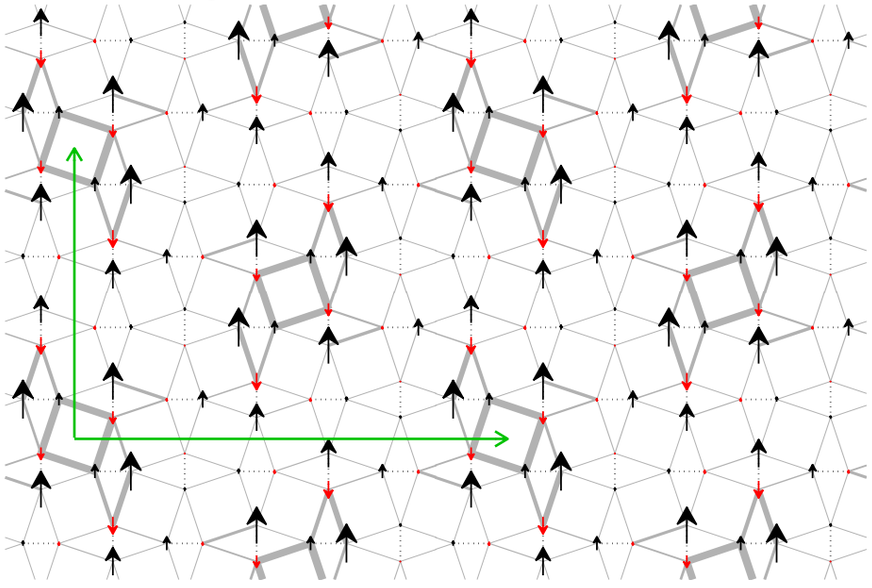
1/8 rhomboid : (4,2),(0,4)



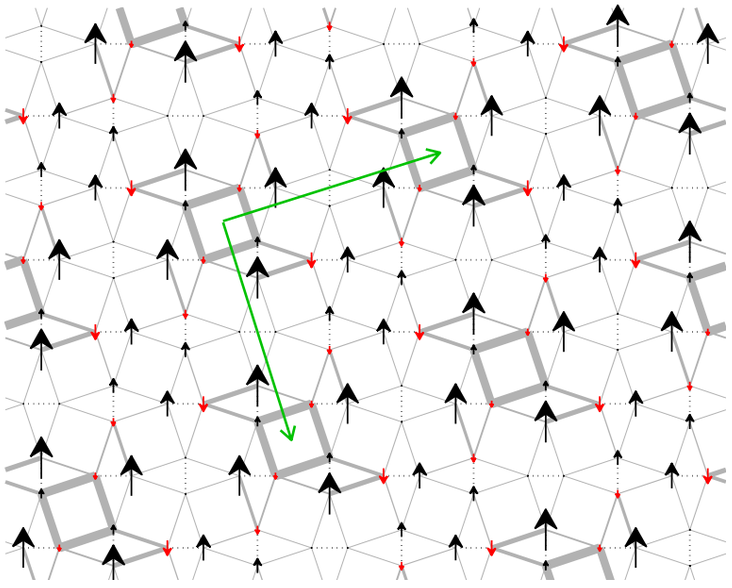
2/15 : (3,-3),(8,2)



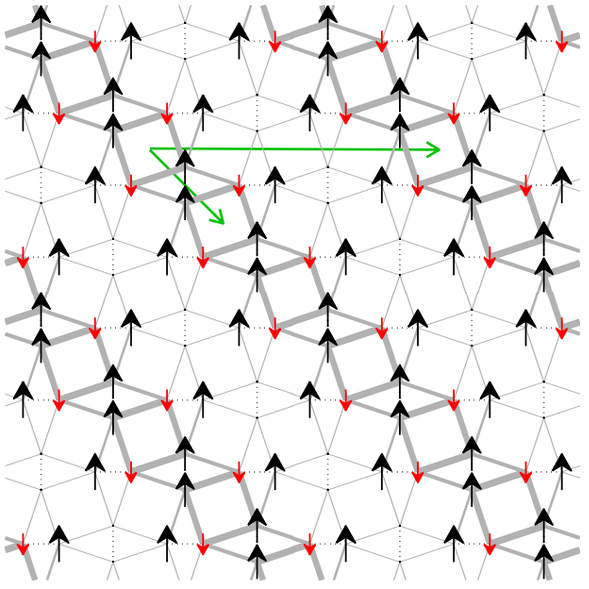
1/6 rectangular : (6,0),(0,4)



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

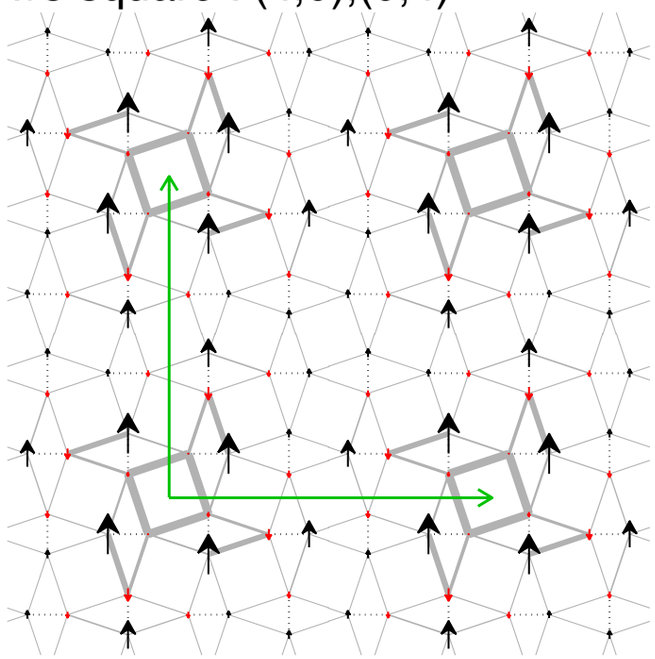


1/4 : (1,-1),(4,0)

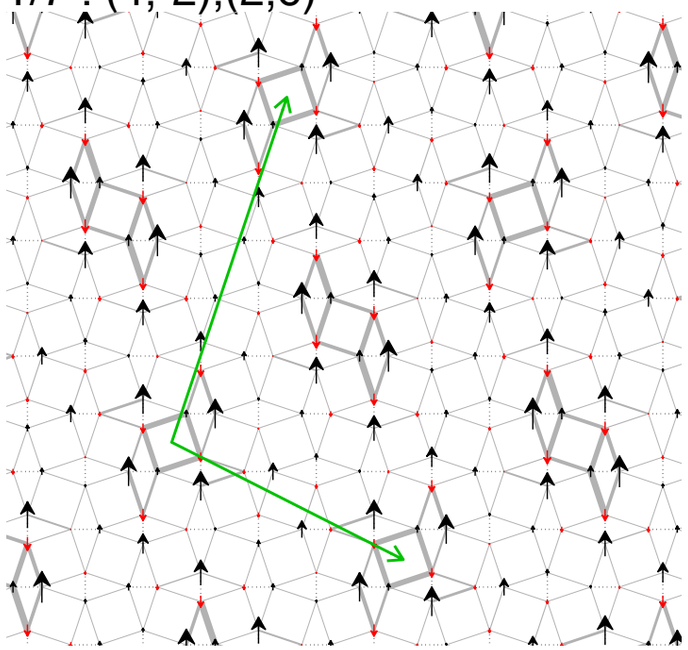


Computing the energies of all possible crystals

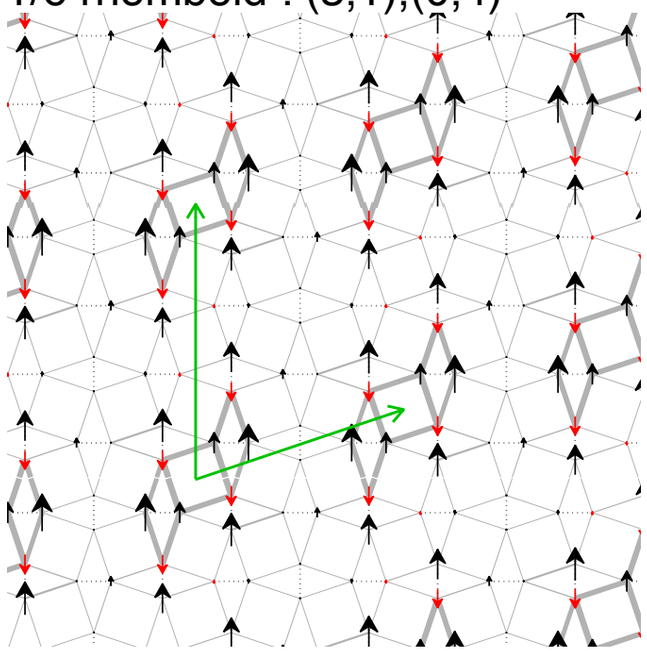
1/8 square : (4,0),(0,4)



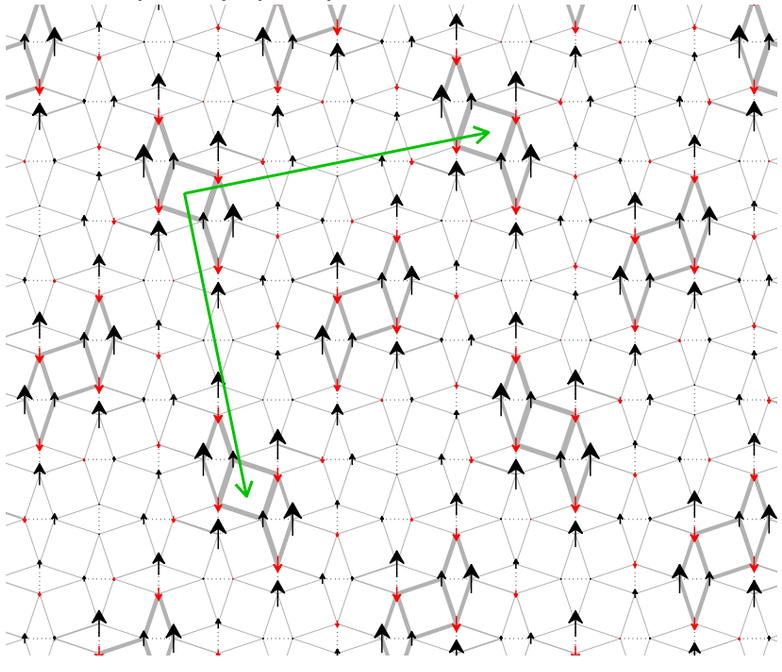
1/7 : (4,-2),(2,6)



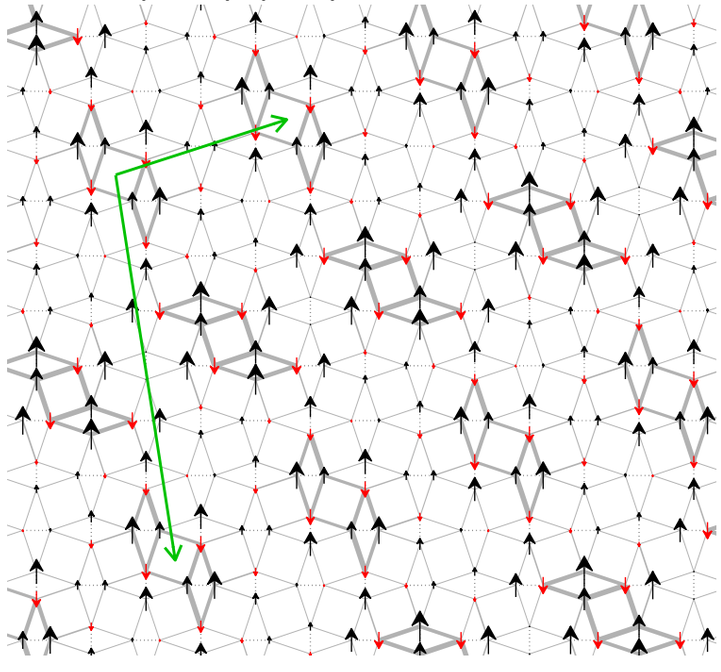
1/6 rhomboid : (3,1),(0,4)



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

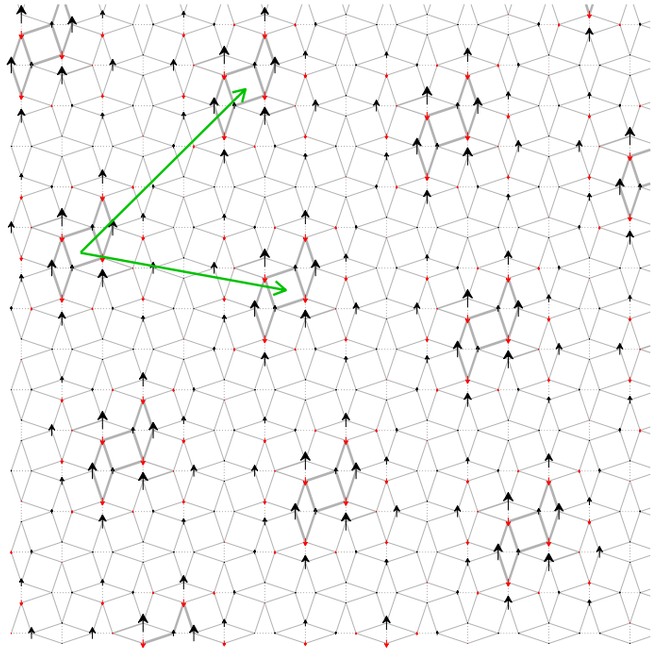


2/11 : (1,-7),(3,1)

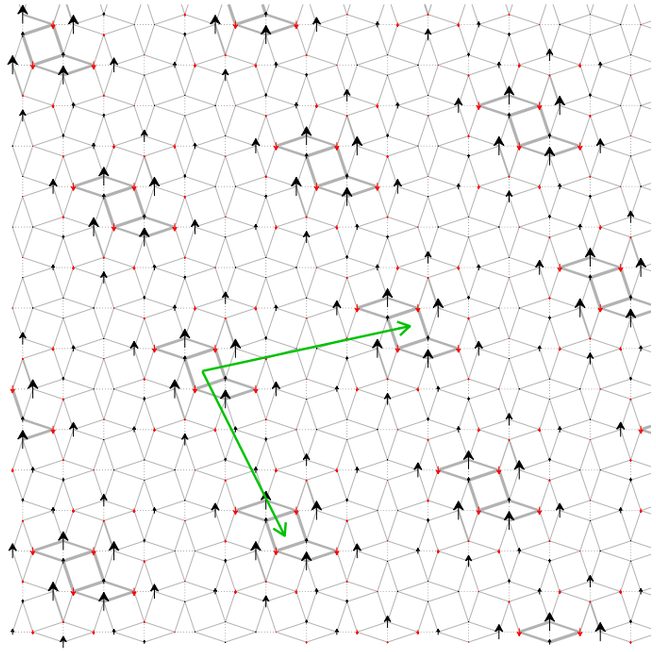


Computing the energies of all possible crystals

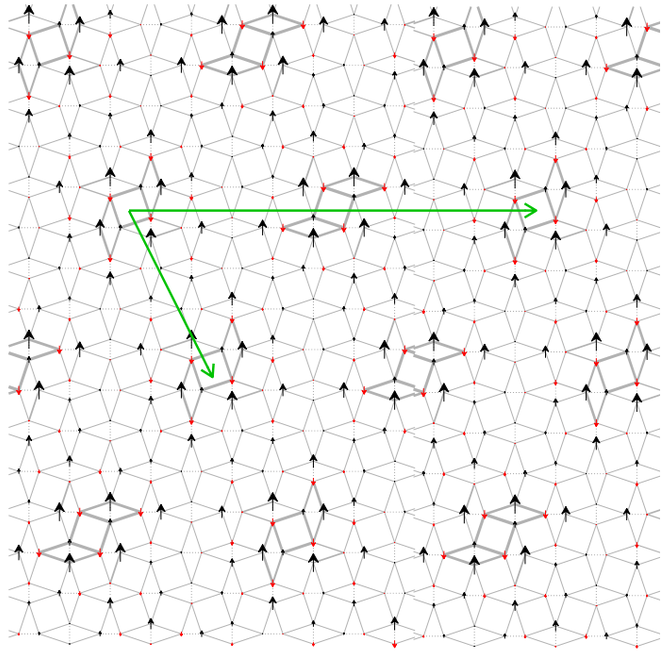
1/12 : (1,-5),(5,-1)



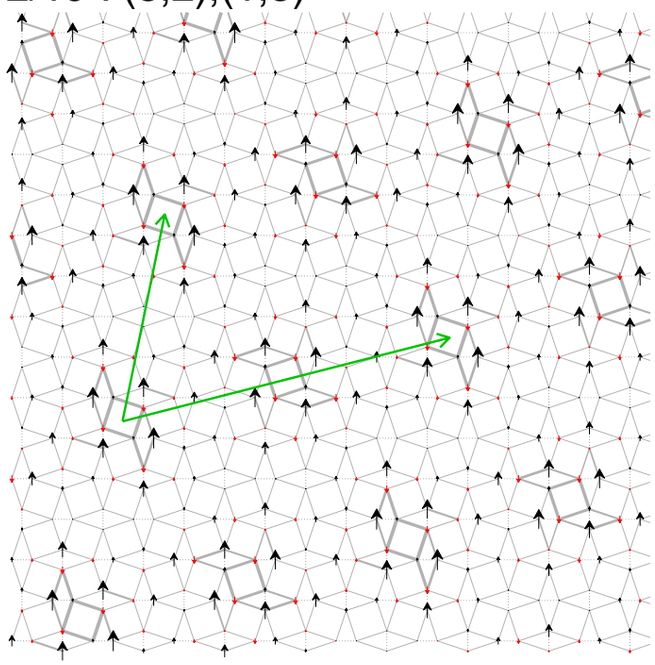
1/11 : (2,-4),(5,1)



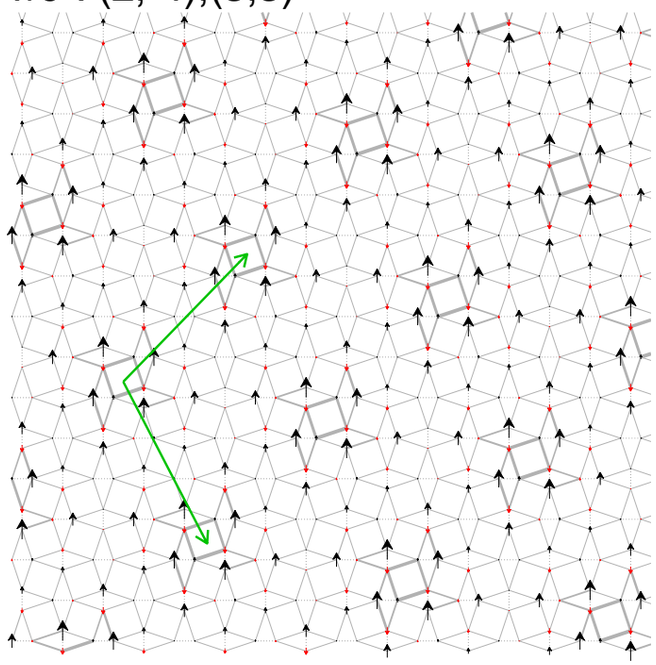
1/10 : (2,-4),(10,0)



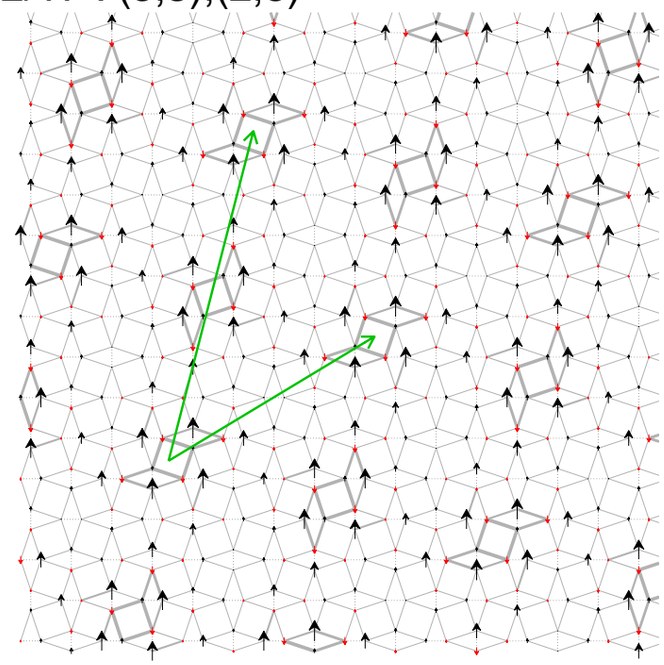
2/19 : (8,2),(1,5)



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

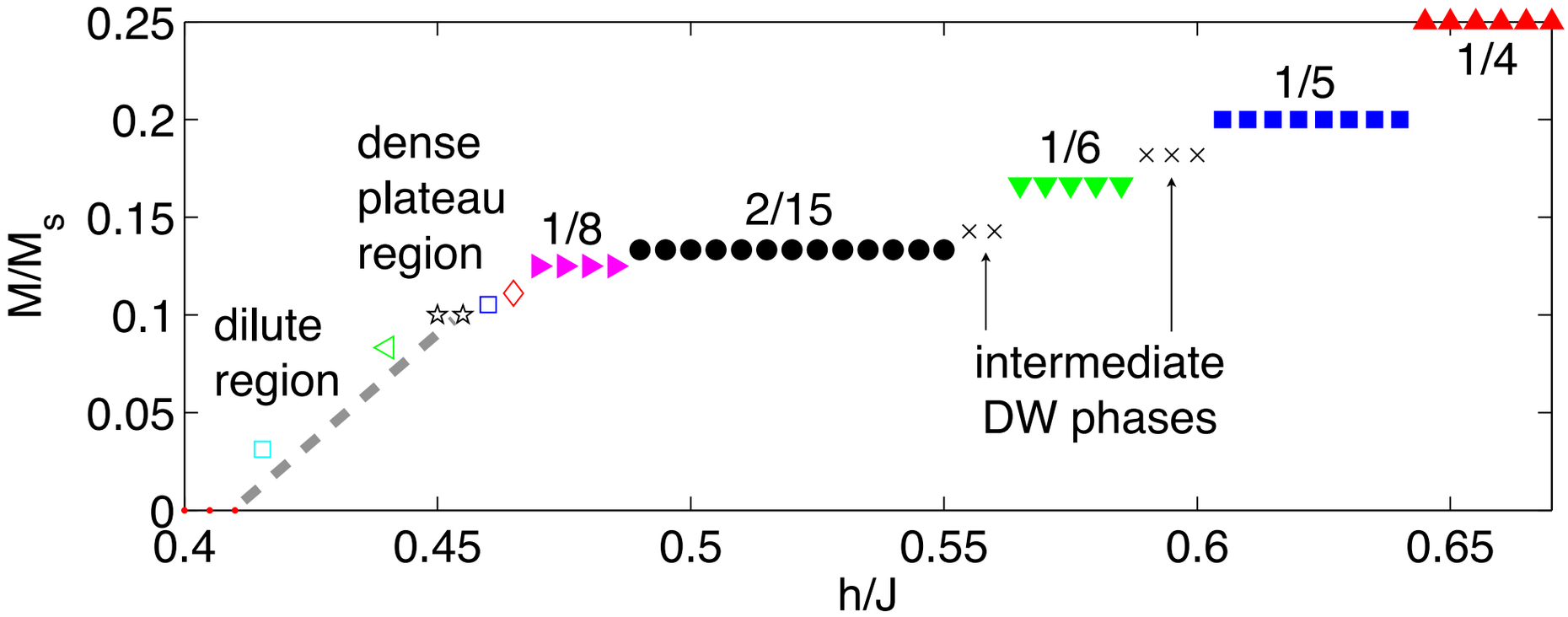


2/17 : (5,3),(2,8)



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)

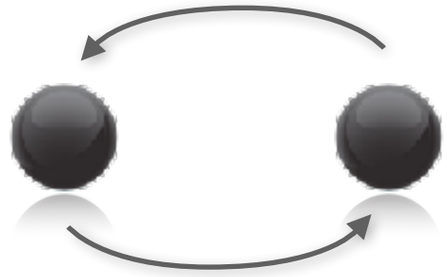
Part V
Fermionic 2D tensor networks

Steve White, 2005: *Perhaps the holy grail, reliable, accurate, and unbiased simulations of large 2D fermion clusters, is becoming within reach!*
(Journal Club for Condensed Matter Physics 2005)

BUT how can we simulate fermions with tensor networks in 2D???

Fermions with 2D tensor networks

How to take fermionic statistics into account?



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

fermionic operators *anti*commute

Different formulations (but same fermionic ansatz):

PC, Evenbly, Verstraete, Vidal (2009)

Kraus, Schuch, Verstraete, Cirac (2009)

Pineda, Barthel, Eisert (2009)

PC & Vidal (2009)

Barthel, Pineda, Eisert (2009)

Shi, Li, Zhao, Zhou (2009)

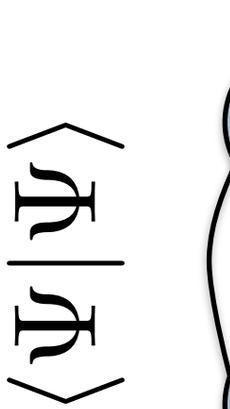
PC, Orus, Bauer, Vidal (2009)

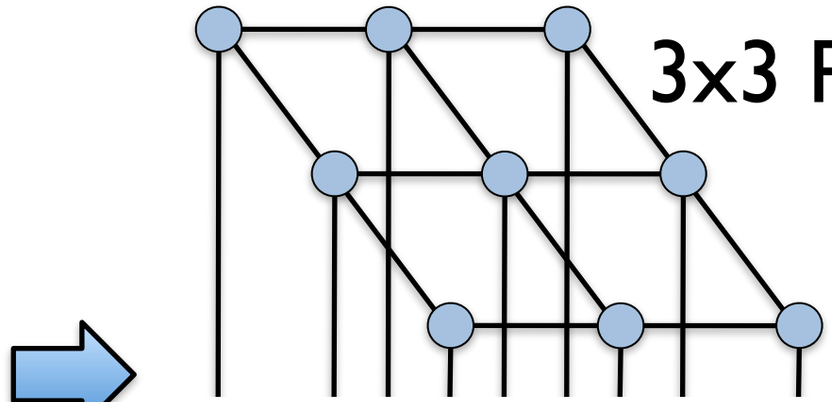
Pizorn, Verstraete (2010)

Gu, Verstraete, Wen (2010)

...

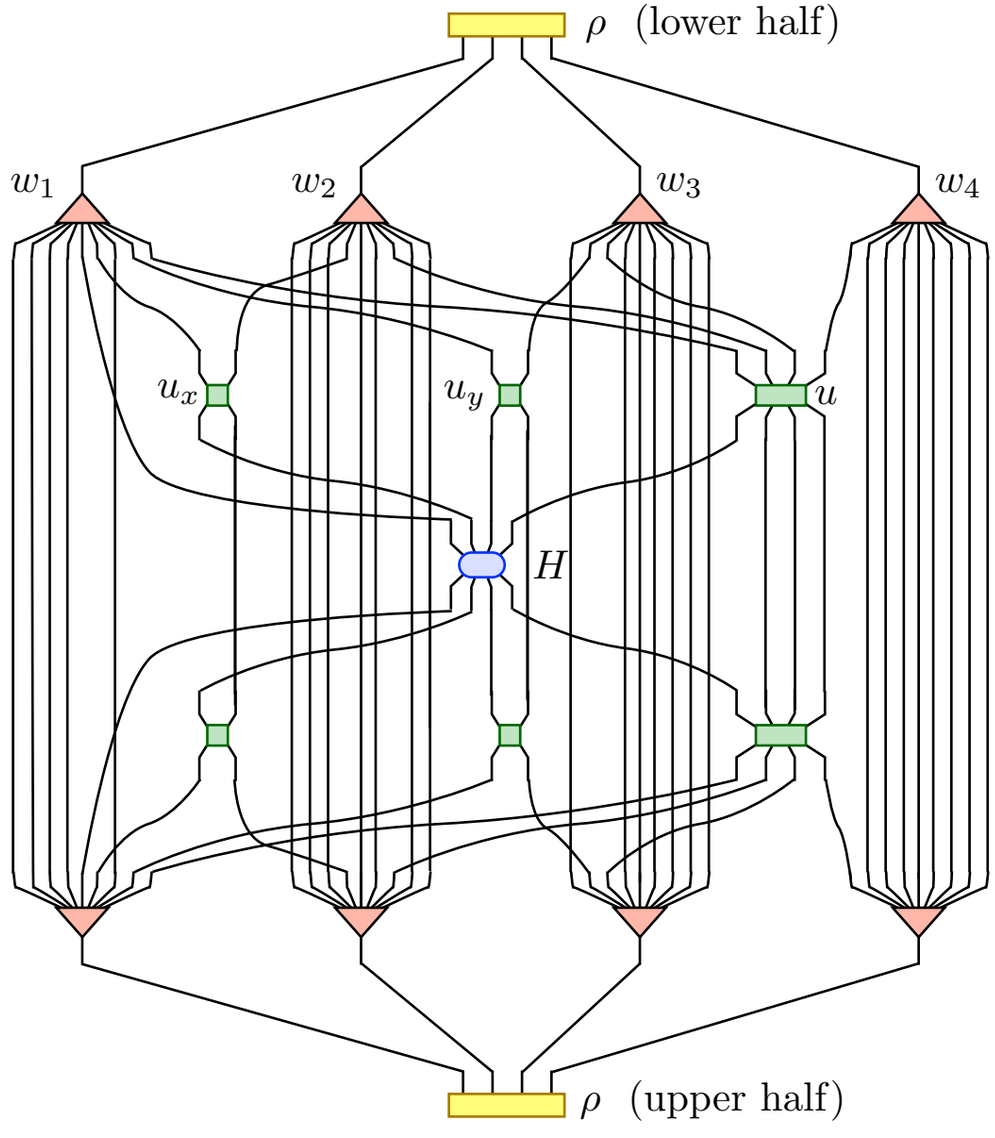
Crossings in 2D tensor networks



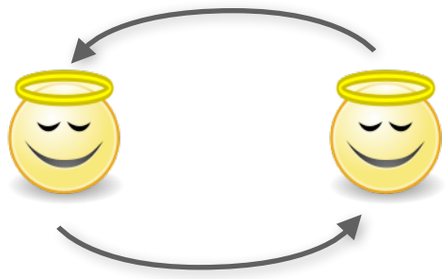


Crossings appear when projecting the 3D network onto 2D!

Example network of the 2D MERA

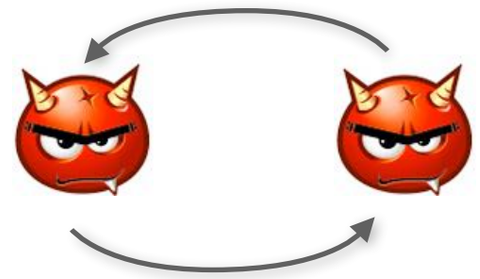


Bosons vs Fermions



$$\Psi_B(x_1, x_2) = \Psi_B(x_2, x_1)$$

symmetric!



$$\Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1)$$

antisymmetric!

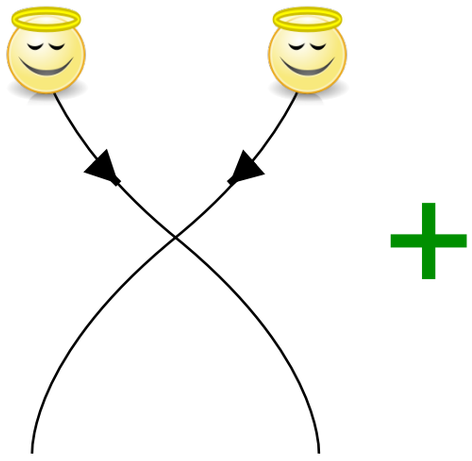
$$\hat{b}_i \hat{b}_j = \hat{b}_j \hat{b}_i$$

operators commute

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

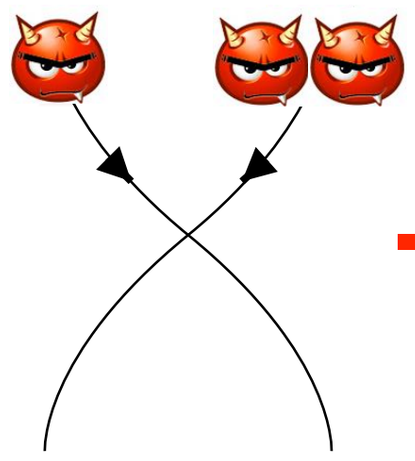
operators *anti*commute

Crossings in a tensor network



+

ignore crossings

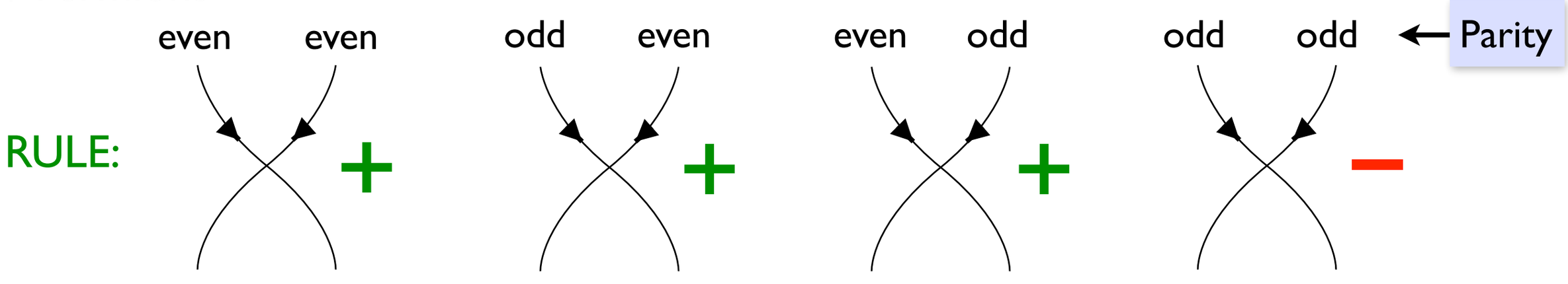


− − = +

take care!

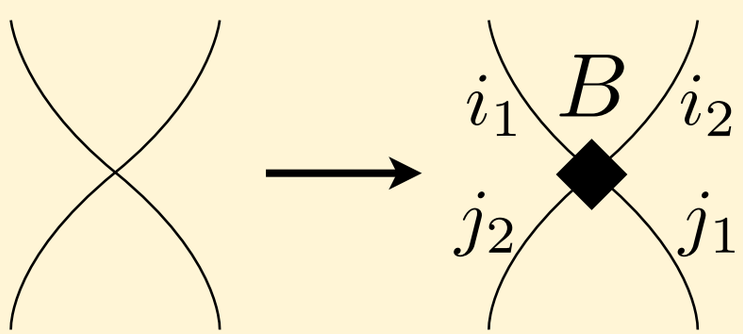
The swap tensor

Fermions



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

Replace crossing by **swap tensor**



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

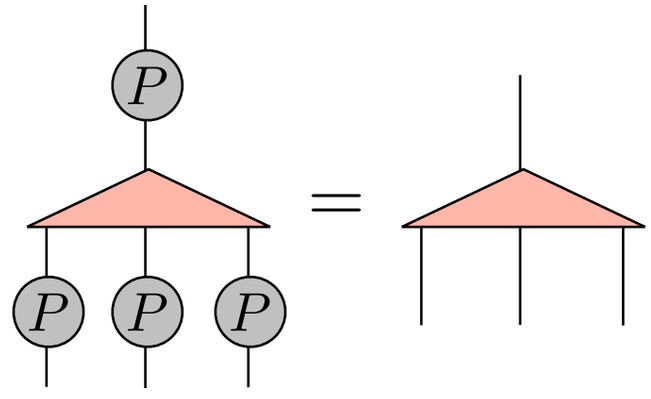
$$S(P(i_1), P(i_2)) = \begin{cases} -1 & \text{if } P(i_1) = P(i_2) = -1 \\ +1 & \text{otherwise} \end{cases}$$

Parity symmetry

- Fermionic systems exhibit **parity symmetry**! $[\hat{H}, \hat{P}] = 0$

- Choose all tensors to be **parity preserving**!

$$T_{i_1 i_2 \ldots i_M} = 0 \quad \text{if } P(i_1)P(i_2)\ldots P(i_M) \neq 1$$



- Decomposing local Hilbert spaces into even and odd parity sectors

$$\mathbb{V} = \mathbb{V}^{(+)} \oplus \mathbb{V}^{(-)}$$

even odd

- Label state by a composite index

parity sector

enumerate states in parity sector p

$$i = (p, \alpha_p)$$

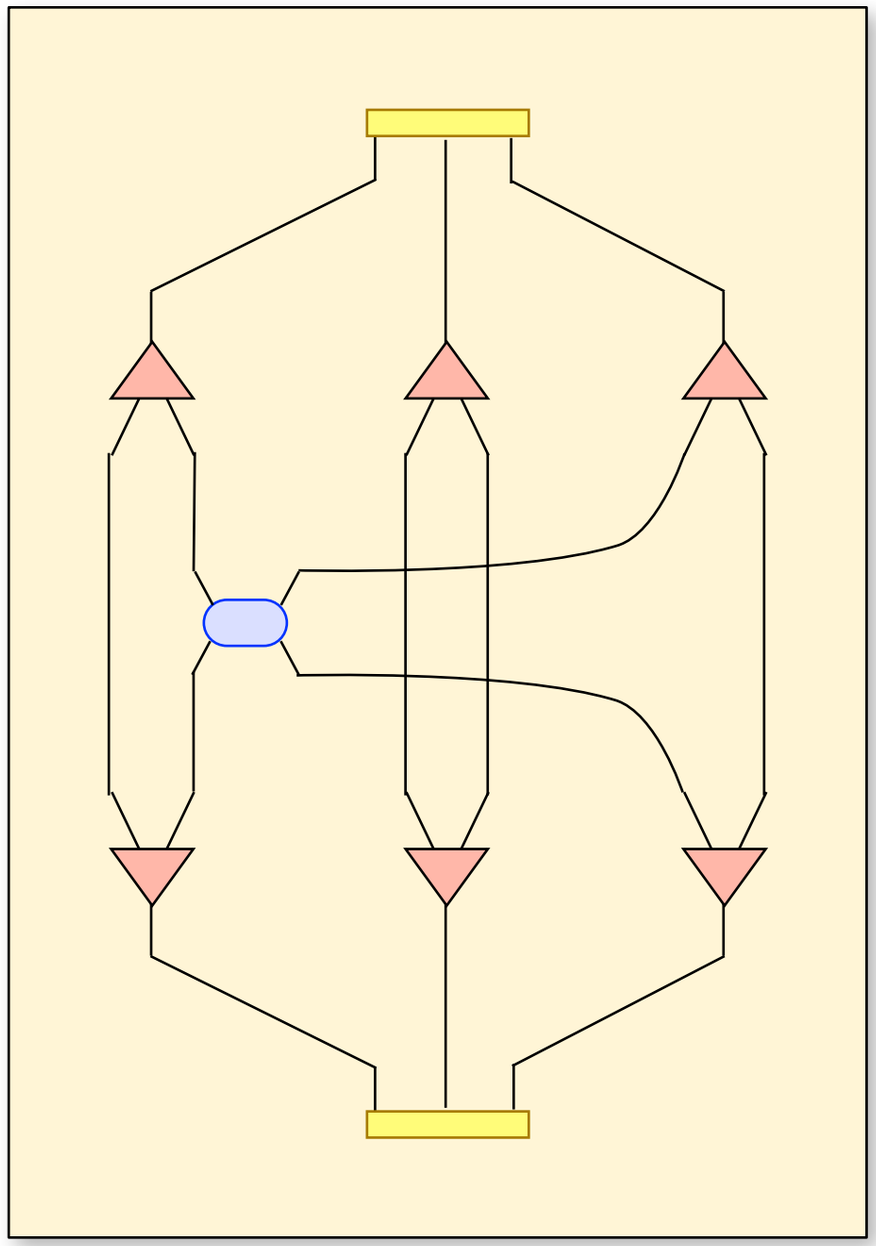
➡ tensor with a block structure (similar to a block diagonal matrix)

➡ Easy identification of the parity of a state!

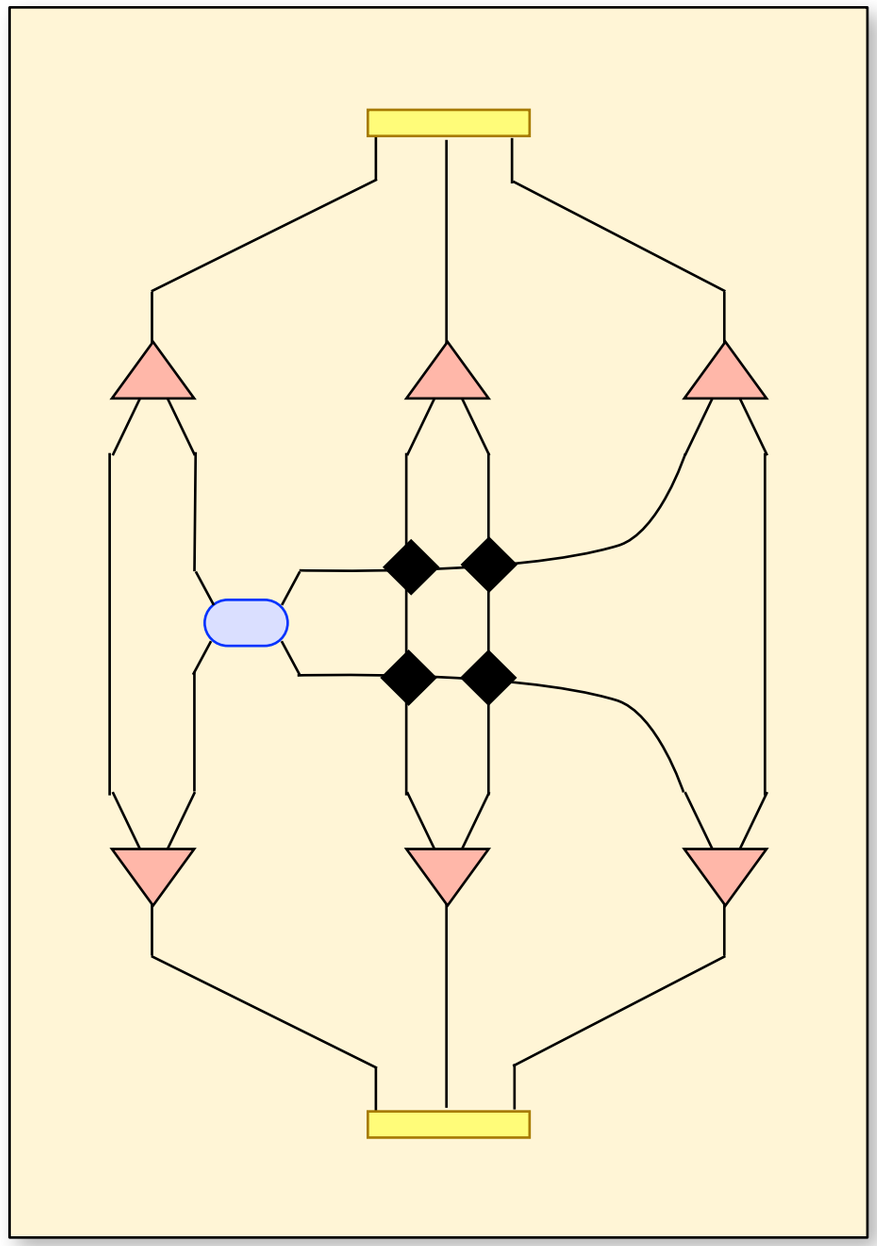
➡ Important for efficiency

Example

Bosonic tensor network



Fermionic tensor network



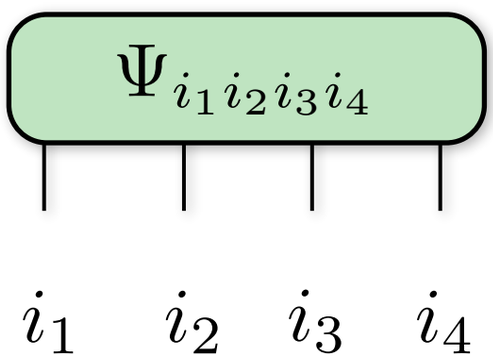
Fermionic "operator networks"

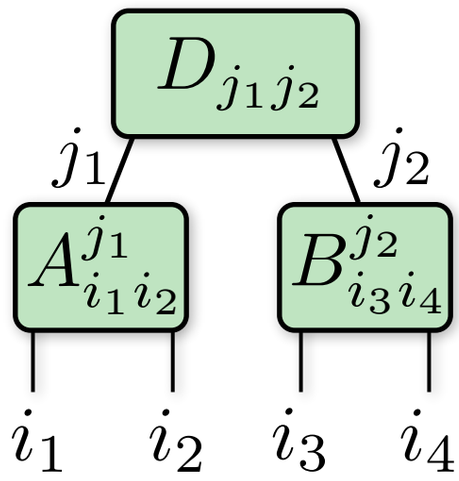
State of 4 site system $|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4} \Psi_{i_1 i_2 i_3 i_4} |i_1 i_2 i_3 i_4\rangle$

$\{|0\rangle, |1\rangle\}$

Bosons

Tensor



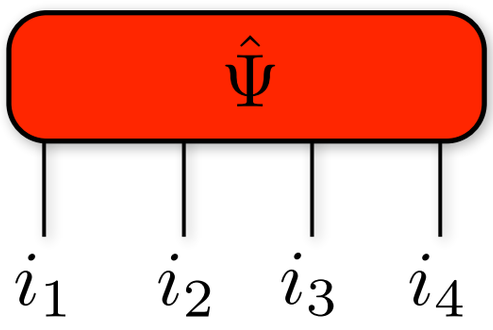


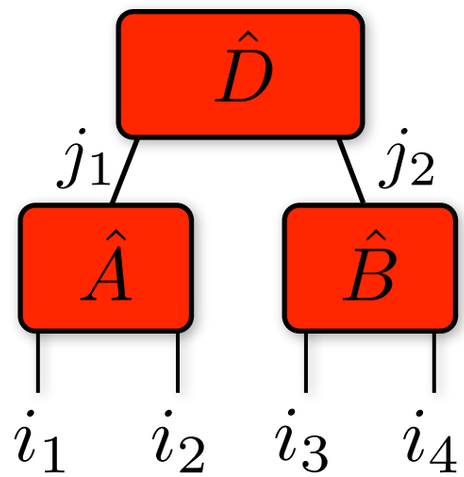
bosonic tensor network

Contract

Fermions

Tensor + fermionic ops





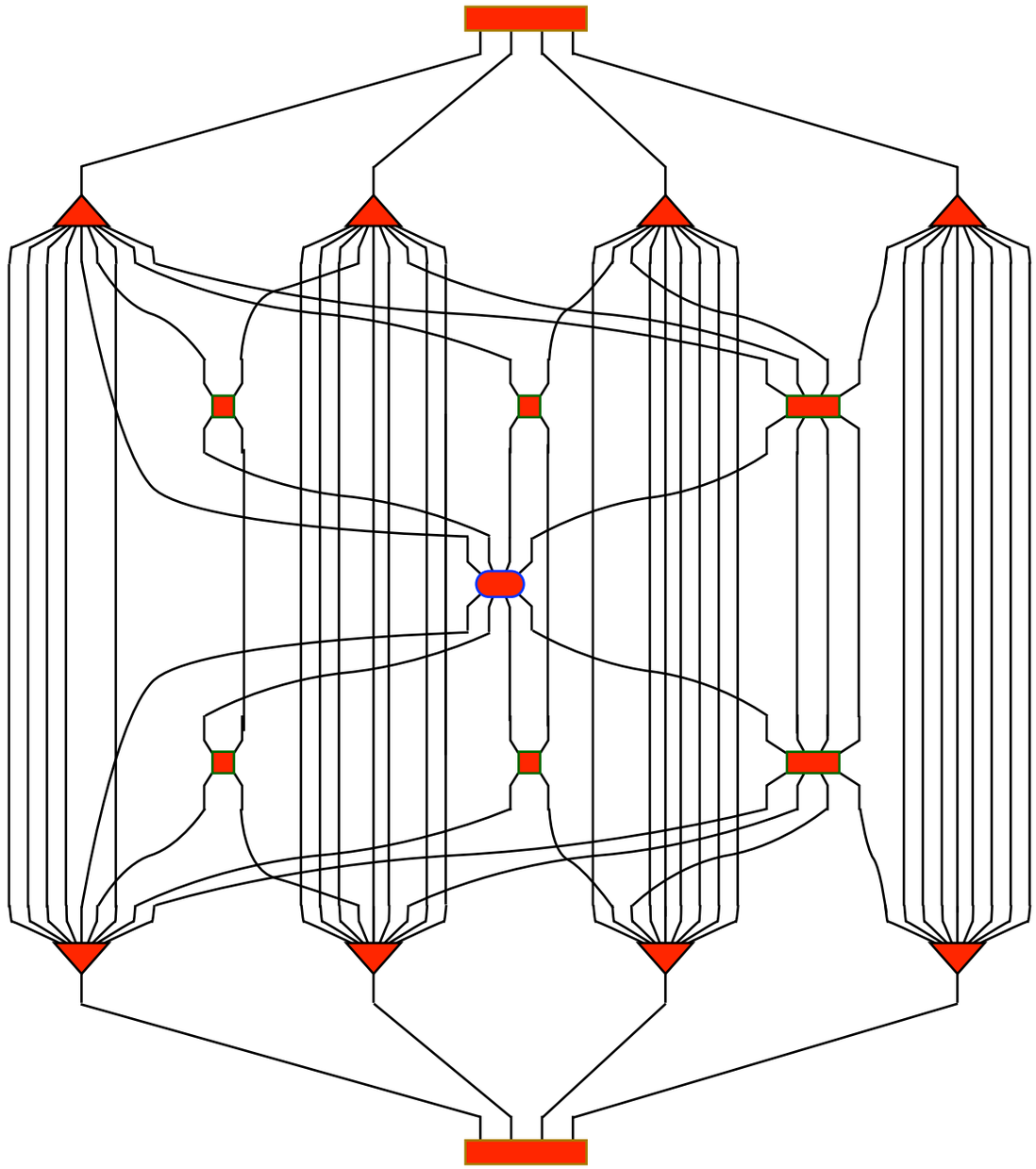
fermionic operator network

Contract + operator calculus

$$\hat{A} = A^{j_1}_{i_1 i_2} |i_1 i_2\rangle\langle j_1| = A^{j_1}_{i_1 i_2} \hat{c}_1^{\dagger i_1} \hat{c}_2^{\dagger i_2} |0\rangle\langle 0| \hat{c}_1^{j_1}$$

Fermionic "operator network"

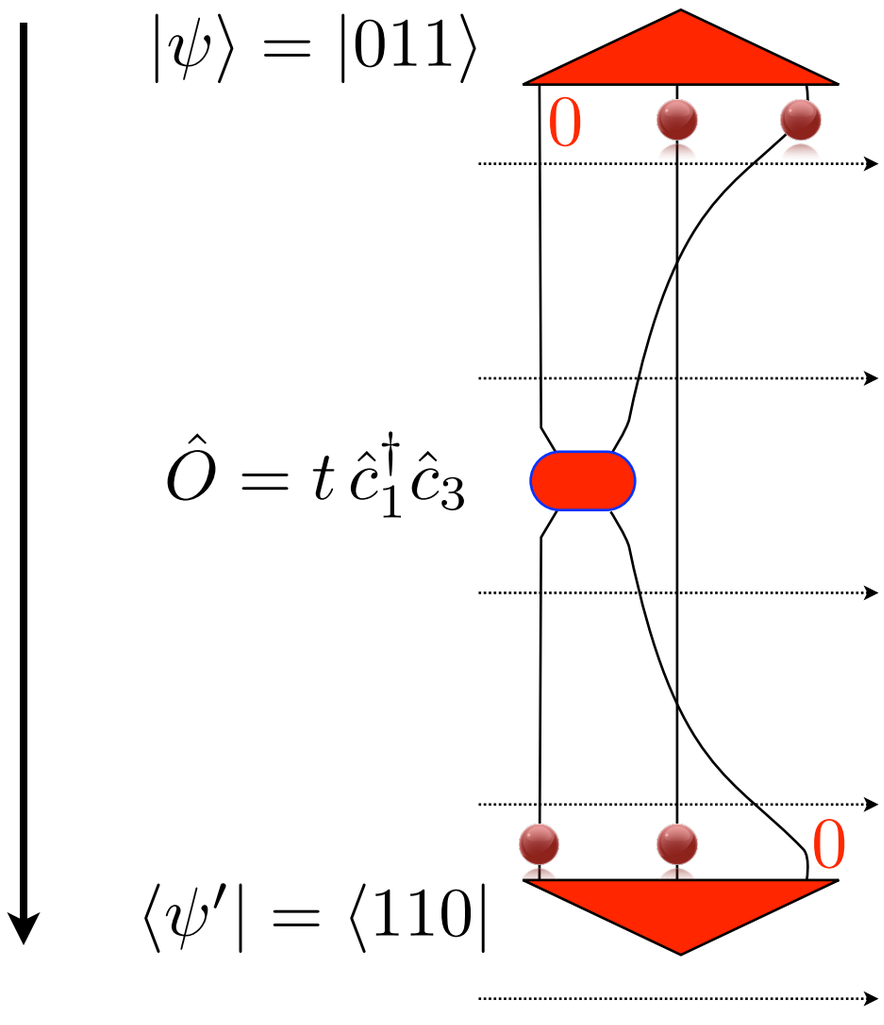
Use anticommutation rules to evaluate fermionic operator network:



Solution:
Map it to a tensor network by replacing crossings by swap tensors

Example

A simple example: $\langle\psi'|\hat{O}|\psi\rangle\,, \quad \hat{O} = t\,\hat{c}_1^\dagger \hat{c}_3$



$$\hat{c}_2^\dagger \hat{c}_3^\dagger |0\rangle$$

$$-\hat{c}_3^\dagger \hat{c}_2^\dagger |0\rangle$$

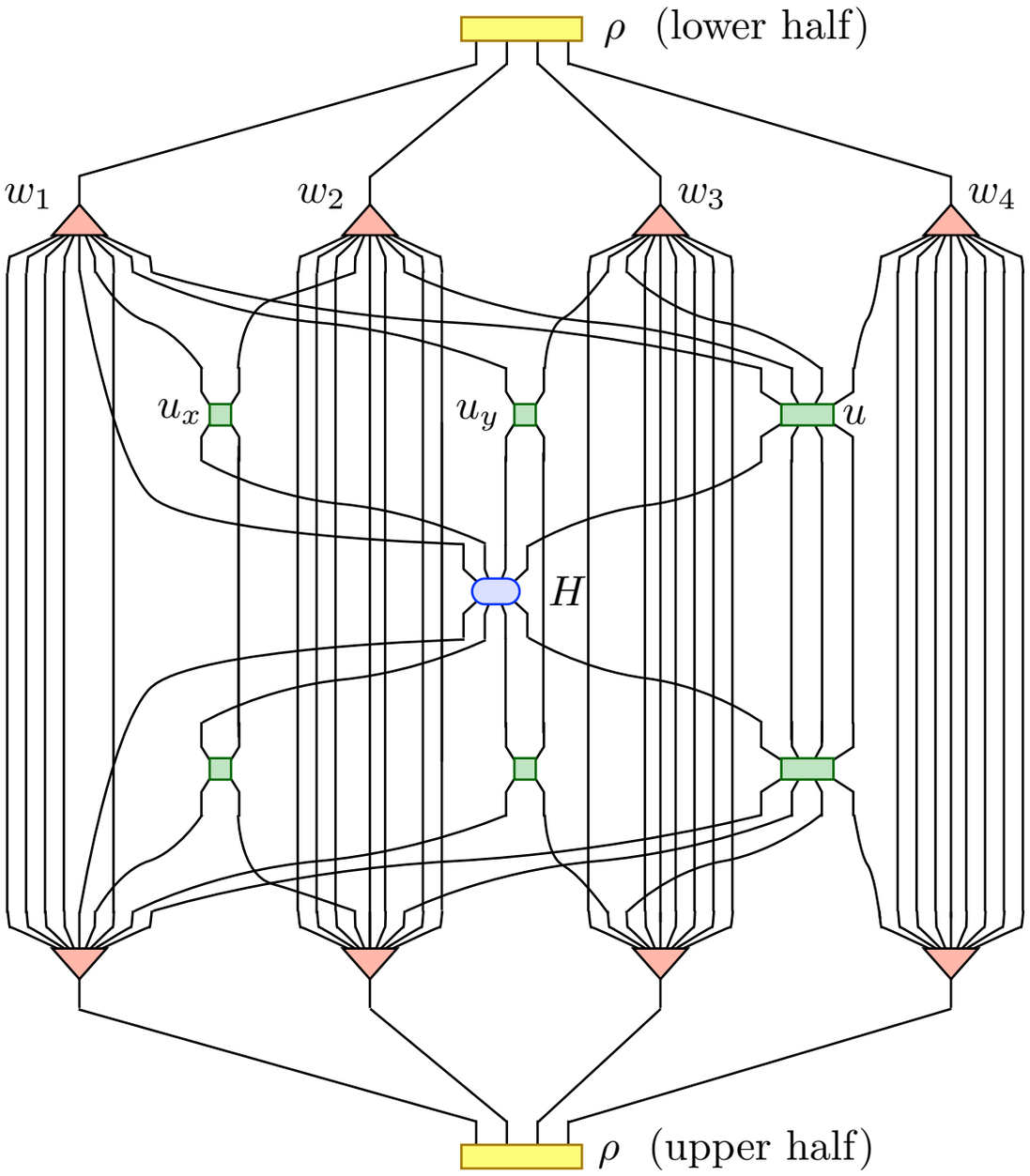
$$\begin{cases} -t\hat{c}_1^\dagger \hat{c}_3 \hat{c}_3^\dagger \hat{c}_2^\dagger |0\rangle = \\ = -t\hat{c}_1^\dagger \mathbb{I}_3 \hat{c}_2^\dagger |0\rangle \end{cases}$$

$$-t\hat{c}_1^\dagger \hat{c}_2^\dagger \mathbb{I}_3 |0\rangle = (-t)|110\rangle$$

$$\langle 110|(-t)|110\rangle = -t$$

➡ All involved anticommutations to evaluate a fermionic operator network are represented by a crossing

Cost of fermionic tensor networks??



First thought:

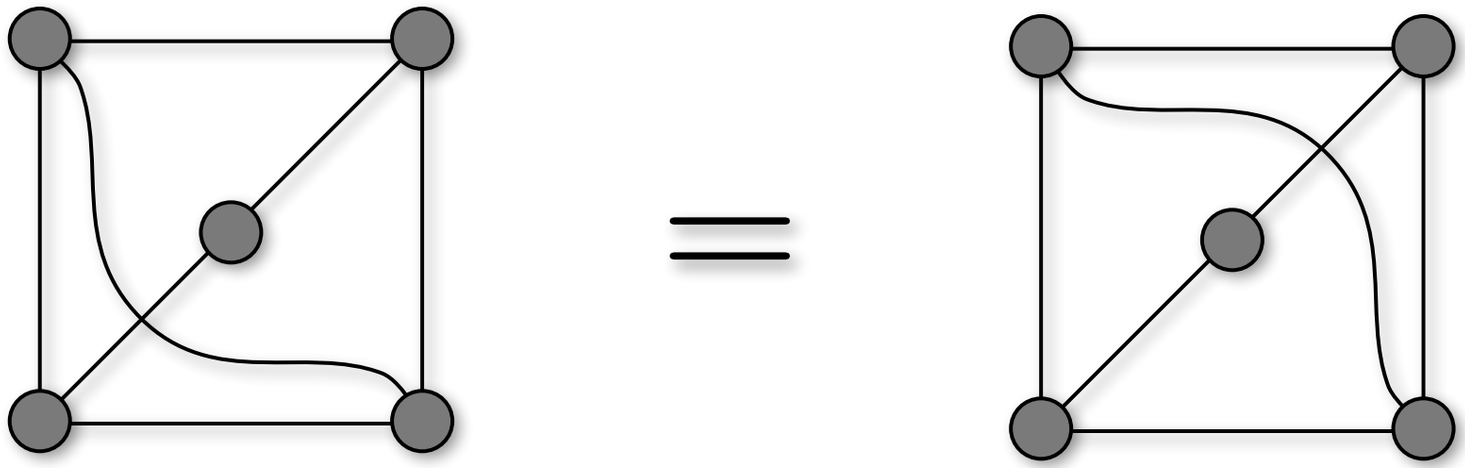
Many crossings → many more tensors

→ **larger computational cost??**

NO!

Same computational cost

The "jump" move

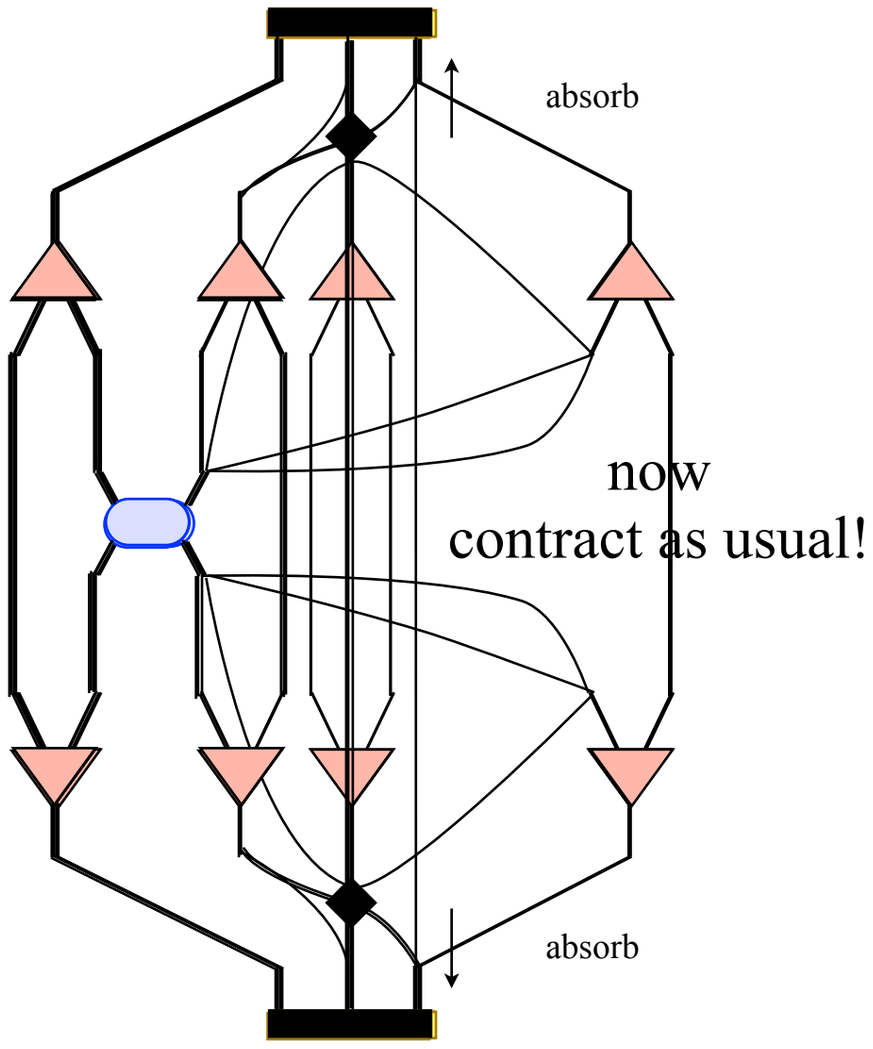


- Jumps over tensors leave the tensor network **invariant**
- Follows form parity preserving tensors

$$[\hat{T}, \hat{c}_k] = 0, \quad \text{if } k \notin \sup[\hat{T}]$$

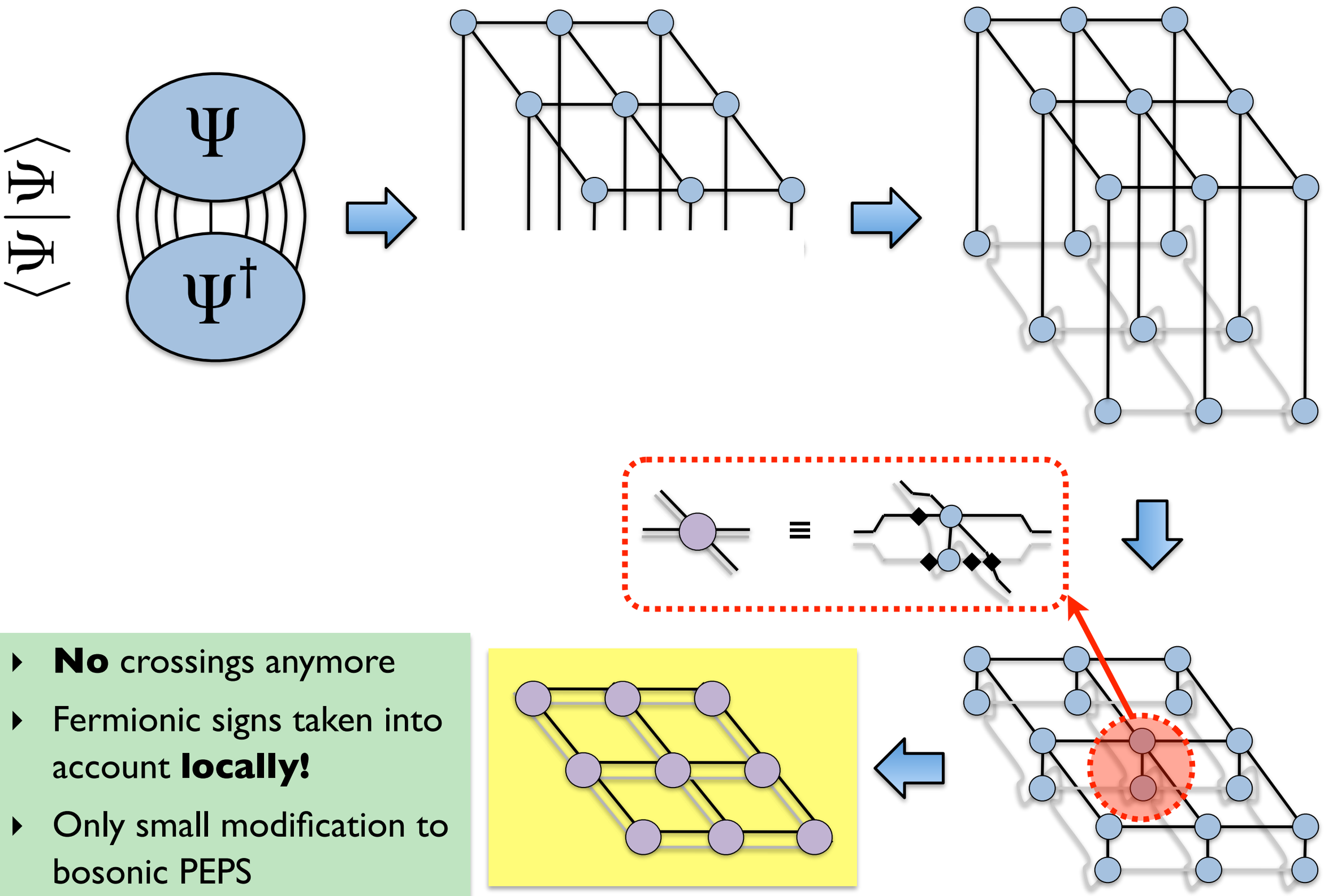
- Allows us to simplify the tensor network
- Final cost of contraction is the same as in a bosonic tensor network

Example of the "jump" move



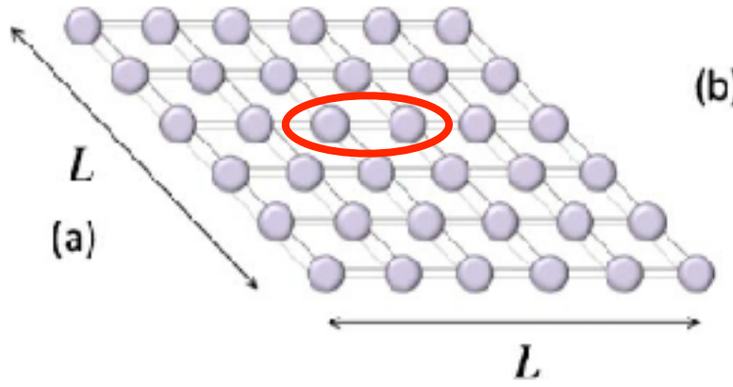
- **Possible to automatize: add swap whenever legs of tensors are permuted**

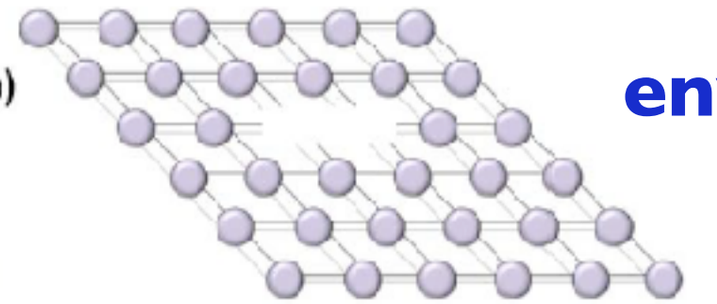
Fermionic (i)PEPS



- **No** crossings anymore
- Fermionic signs taken into account **locally!**
- Only small modification to bosonic PEPS

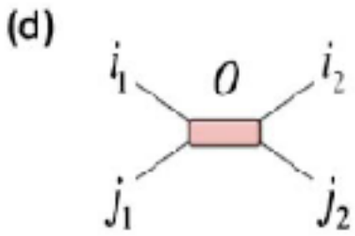
Fermionic (i)PEPS: expectation values

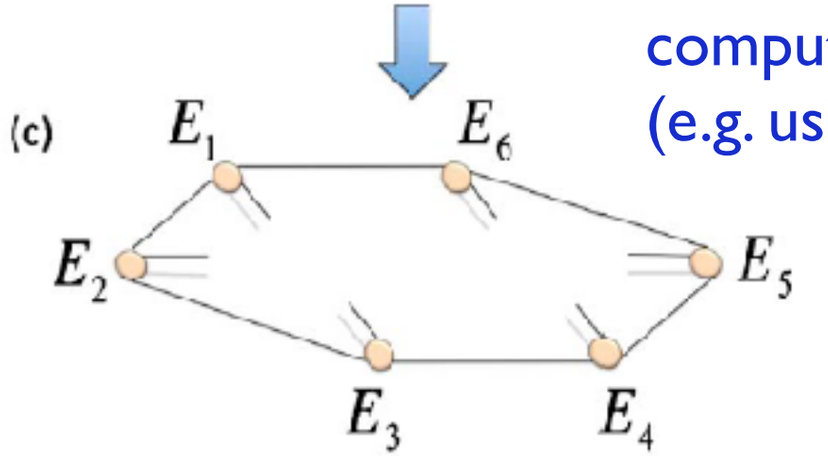


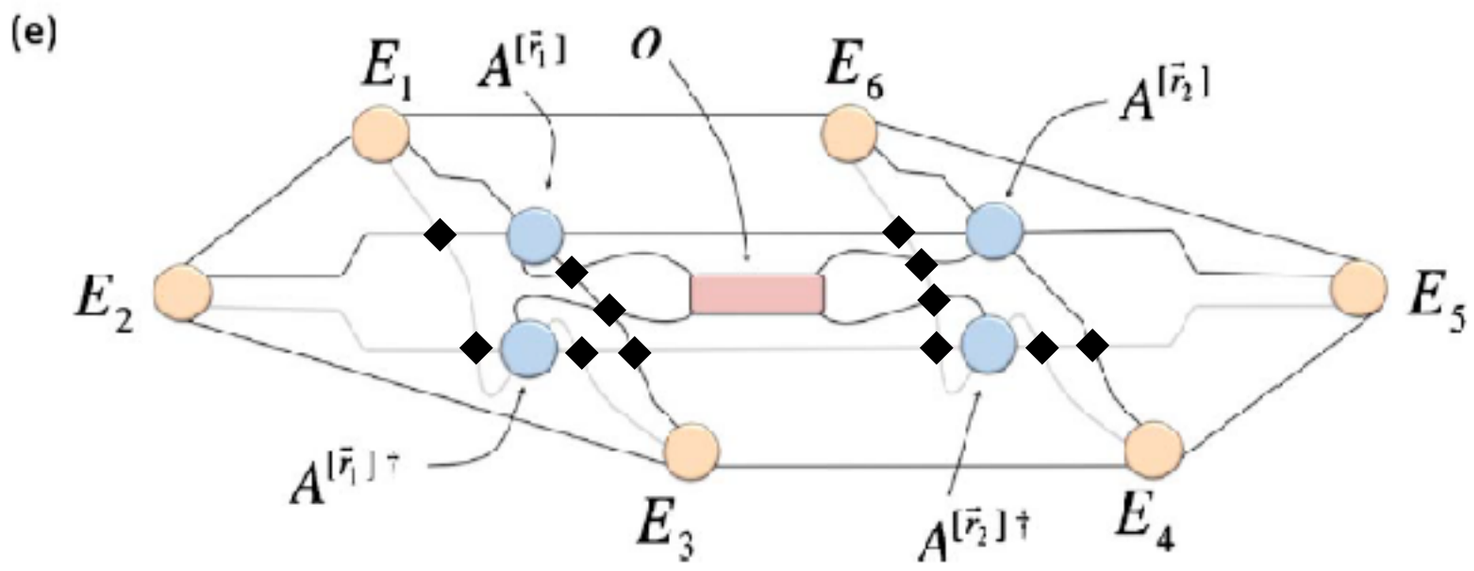


environment

compute environment approximately (e.g. using MPS)







Connect two-body operator

insert swap tensors

Contract this network!

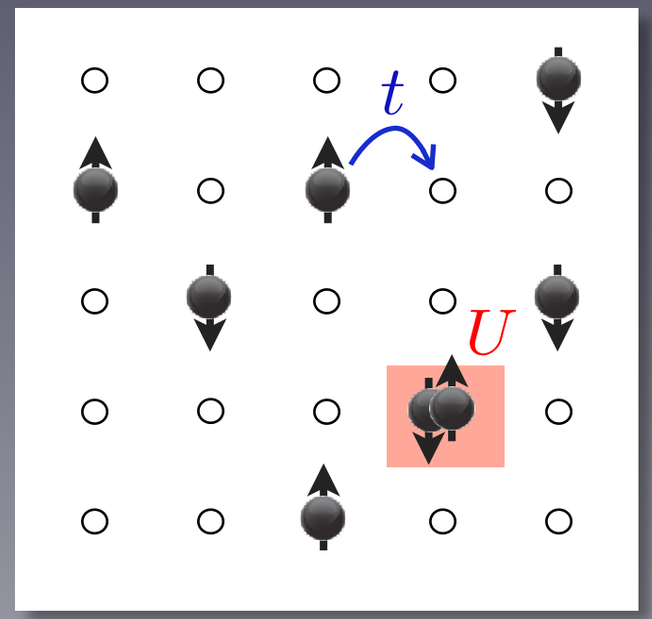
Summary: Fermionic TN

- ➡ Simulate fermionic systems with 2D tensor networks
  - ➡ Replace crossings by swap tensors & use parity preserving tensors
- ➡ Same leading computational cost in D

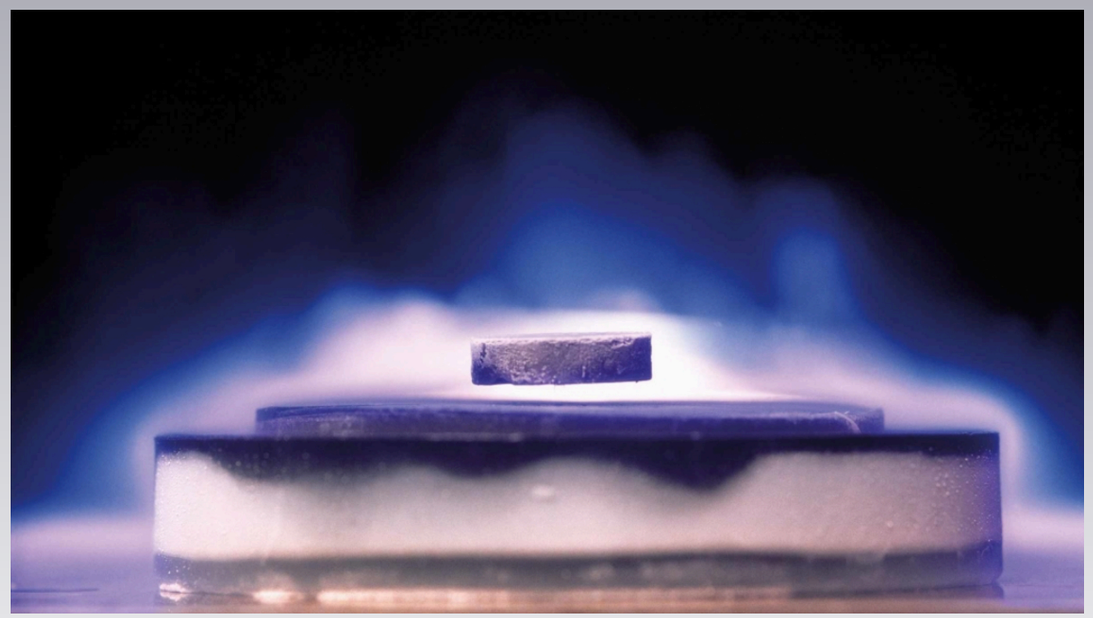
The 2D Hubbard model

★ *The most basic model of strongly correlated electrons*

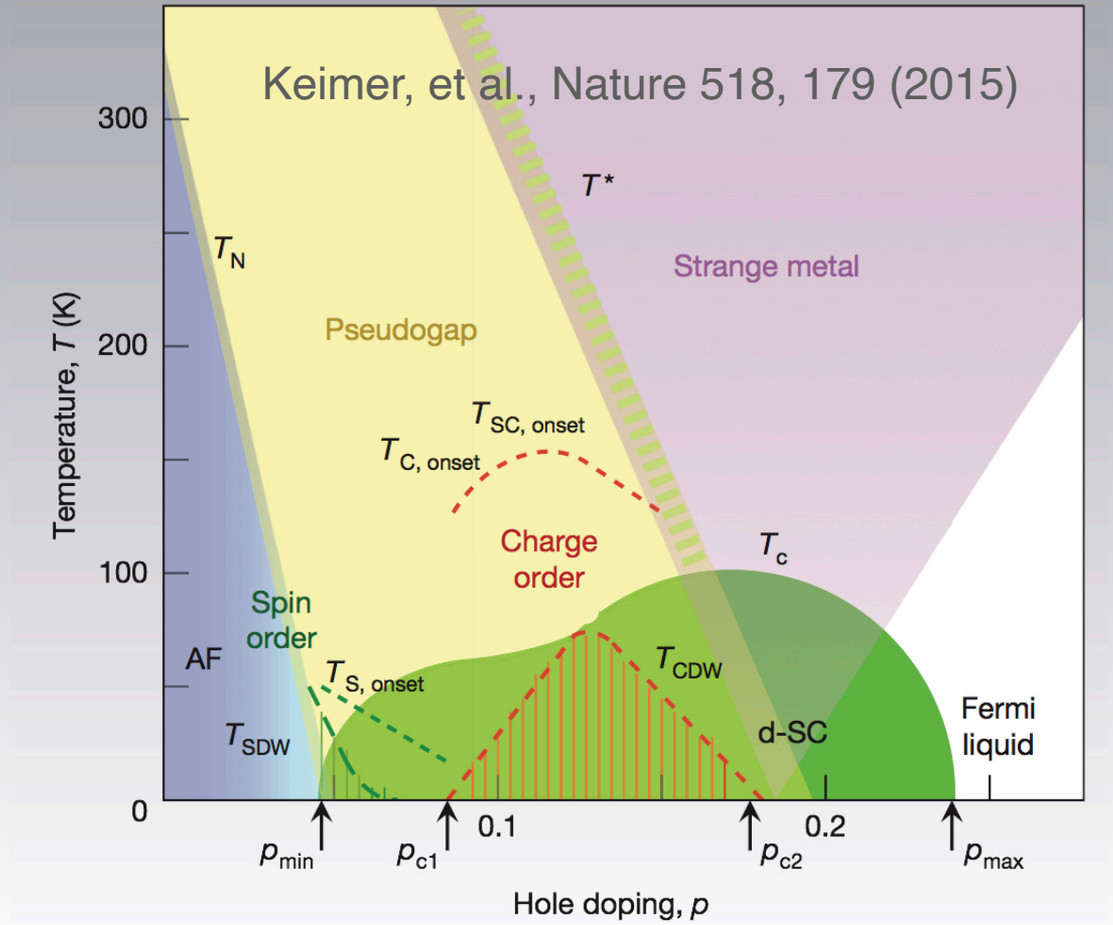
$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + h.c. + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



★ *Is it the relevant model for high-T_c superconductivity (cuprates)? Phase diagram?*



Physics World, Oct 2018

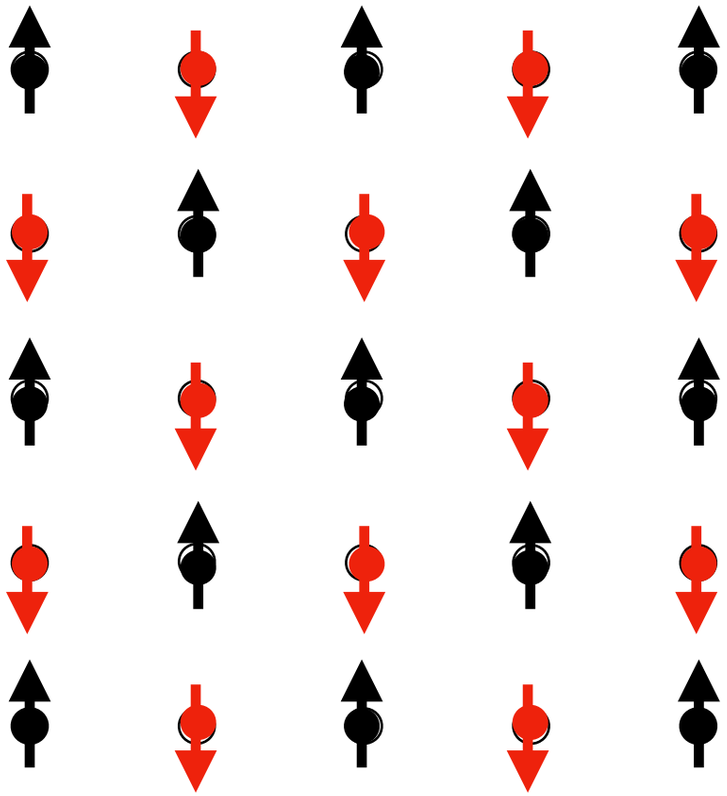


Hubbard model: Main candidates for U/t~8, δ~1/8

or in the *t-J* model (effective model)

Hubbard model: Main candidates for U/t~8, δ~1/8

or in the *t-J* model (effective model)



δ = 0: Antiferromagnet

δ > 0: finite density of holes

What do the holes do??

Hubbard model: Main candidates for U/t~8, δ~1/8

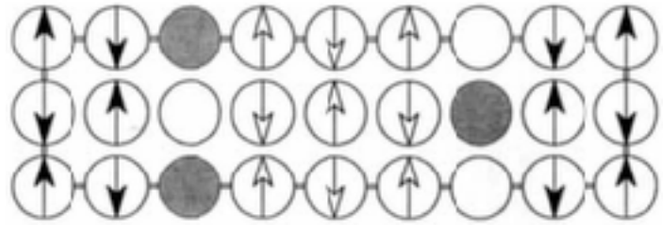
or in the *t-J* model (effective model)

Uniform d-wave superconducting state

Yokoyama & Shiba, JPSJ 57 (1988)
Gros, PRB 38 (1988)
Dagotto et al, PRB 49 (1994)
S. Sorella, et al., PRL 88 (2002)
Maier et al., PRL 95 (2005)
Senechal et al. PRL 94 (2005)
Capone & Kotliar, PRB 74 (2006)
Aichhorn et al., PRB 74 (2006)
Lugas, et al. PRB 74 (2006)
Aimi & Imada, JPSJ 76 (2007)
Yokoyama, Ogata & Tanaka: JPSJ 75 (2006)
Yokoyama, et al. JPSJ 73 (2004)
Eichenberger & Baeriswyl, PRB 76 (2007)
Macridin, Jarrell, Maier, PRB 74 (2006)
Hu, Becca & Sorella, PRB 85 (2012)
Gull, Parcollet, Millis, PRL 110 (2013)
Misawa & Imada, PRB 90 (2014)
... and many more ...

VS

Stripe state
modulated spin/charge
w. or w/o coexisting SC



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Theory:

Zaanen & Gunnarsson, PRB **40** (1989)
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Machida, Physica **158C** (1989)
Schulz, J. Phys. **50** (1989)
Emery, Kivelson & Tranquada PNAS **96** (1999)
White & Scalapino, PRL **80** (1998)
White & Scalapino, PRB **60** (1999)
Himeda, Kato & Ogata, PRL **88** (2002)
Kivelson, Bindloss, Fradkin, Oganesyan,
Tranquada, Kapitulnik & Howald, RMP **75** (’03)
Berg, Fradkin, Kim, Kivelson, Oganesyan,
Tranquada & Zhang PRL **99** (2007)
Chou, Fukushima & Lee, PRB **78** (2008)
Yang, Chen, Rice, Sigrist & Zhang, NJP **11** (2009)
Berg, Fradkin, Kivelson & Tranquada, NJP **11** (‘09)
Berg, Fradkin & Kivelson, PRB **79** (2009)
Vojta, Adv. Phys. **58** (2009)
Fradkin & Kivelson, Nature Physics **8** (2012)
... and many more ...

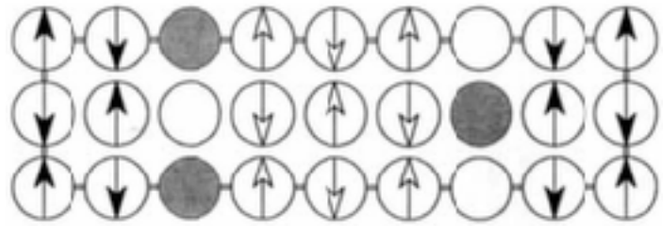
Hubbard model: Main candidates for U/t~8, δ~1/8

or in the *t-J* model (effective model)

Uniform d-wave superconducting state

VS

Stripe state
modulated spin/charge
w. or w/o coexisting SC



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Yokoyama & Shiba; JPS J 57 (1988)
Gros, PR
Dagotto e
S. Sorella
Maier et a
Senechal
Capone &
Aichhorn
Lugas, et
Aimi & Im
Yokoyam
Yokoyam
Eichenbe
Macridin,
Hu, Becc
Gull, Parc
Misawa & Imada, PRB 90 (2014)
... and ma

Schulz, J. Phys. 50 (1989)

? Which is the true ground state ?

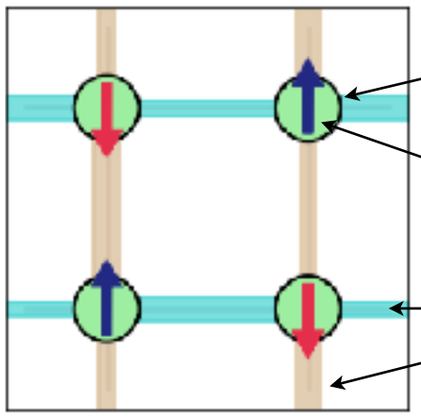
Goal: get conclusive answer
for U/t=8, δ=1/8 using
iPEPS, DMRG, AFQMC, DMET

Zheng, Chung, PC, Ehlers, Qin, Noack, Shi,
White, Zhang, Chan, Science 358, 1155 (2017)

Ground state: **stripe state**

iPEPS: main competing states (U/t=8, δ=1/8)

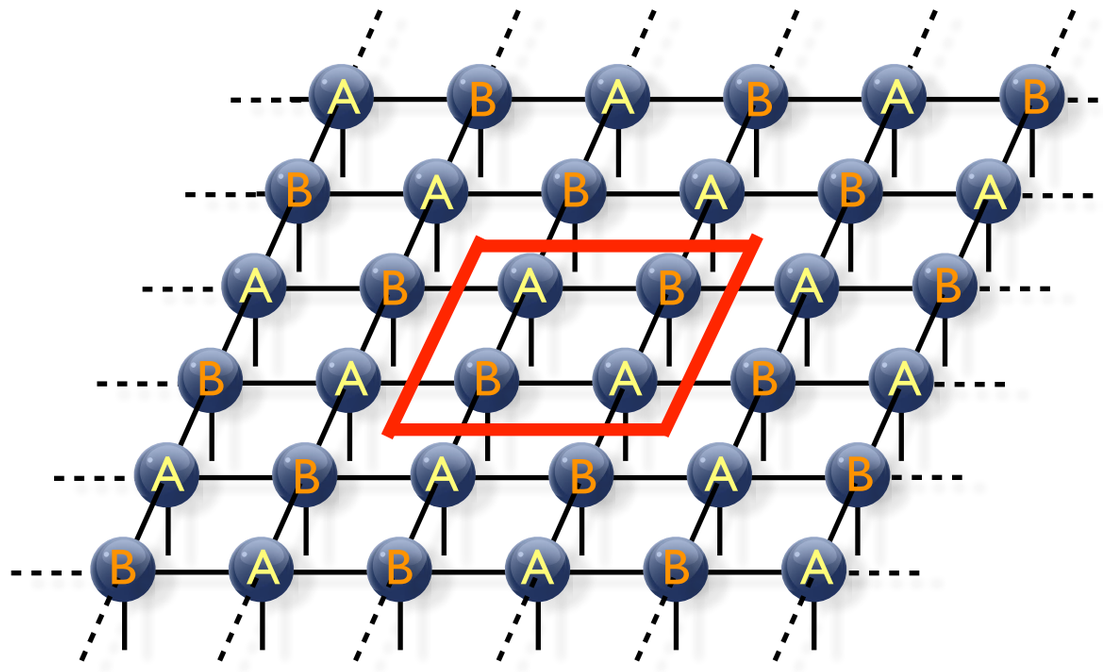
Uniform d-wave SC state (+ AF order)



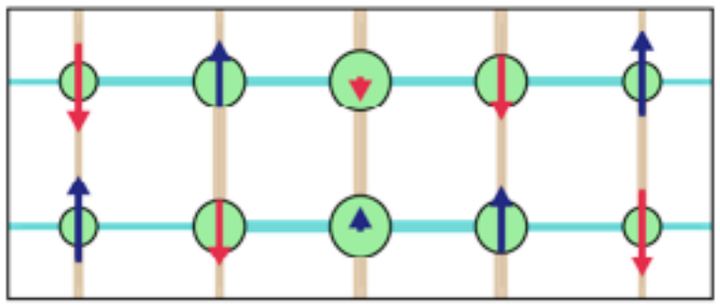
δ_i hole density

m_i magnetic moment

Δ_{ij} nearest-neighbor singlet pairing amplitude



Period λ=5 (W5 stripe)



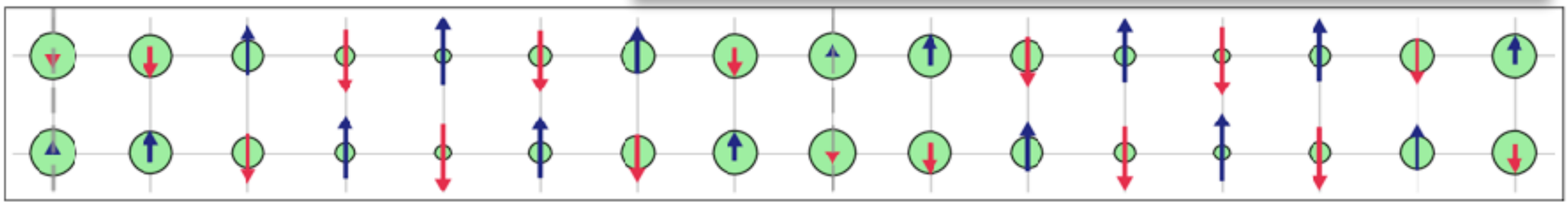
★ Modulation in the charge, AF, and SC order

★ "Site-centered" stripe

★ π-phase shift in the AF order

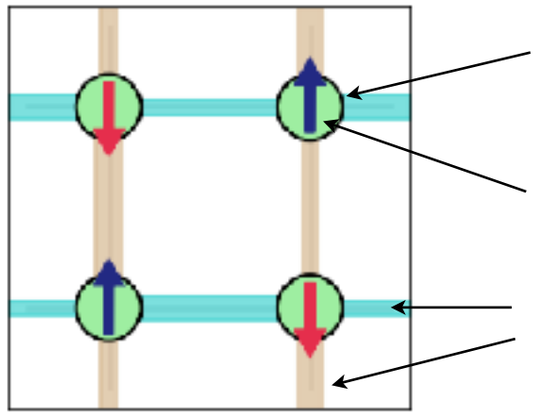
Period λ=8 (W8 stripe)

★ Superconductivity suppressed (1 hole per unit length)



iPEPS: main competing states (U/t=8, δ=1/8)

Uniform d-wave SC state (+ AF order)

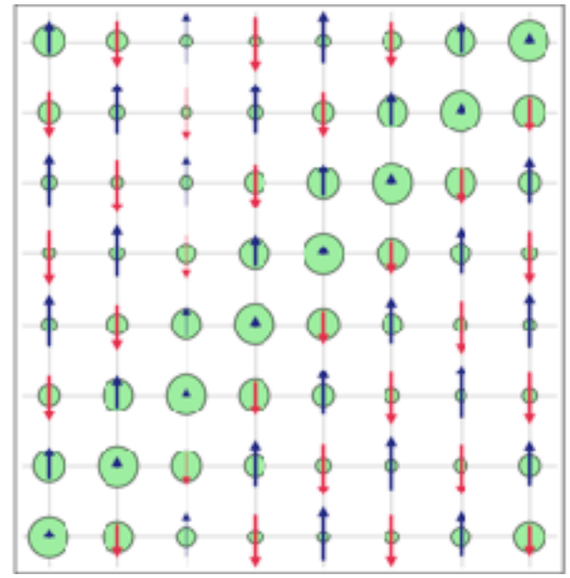


δ_i hole density

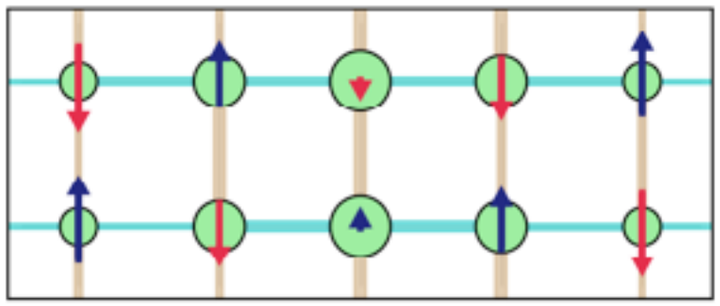
m_i magnetic moment

Δ_{ij} nearest-neighbor singlet pairing amplitude

Diagonal stripe (16x16 cell)



Period λ=5 (W5 stripe)



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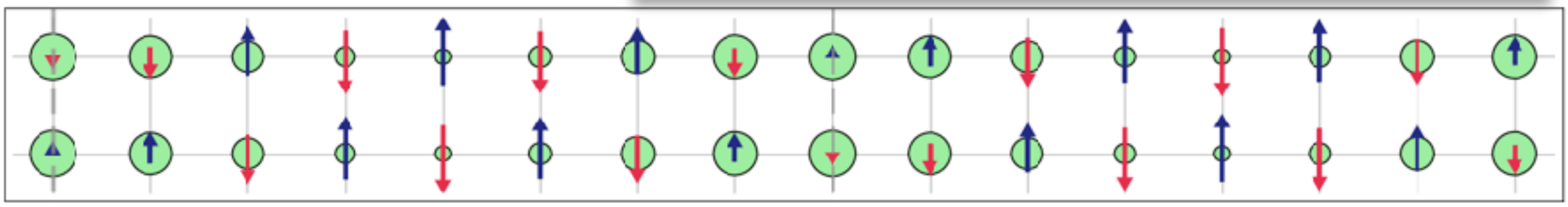
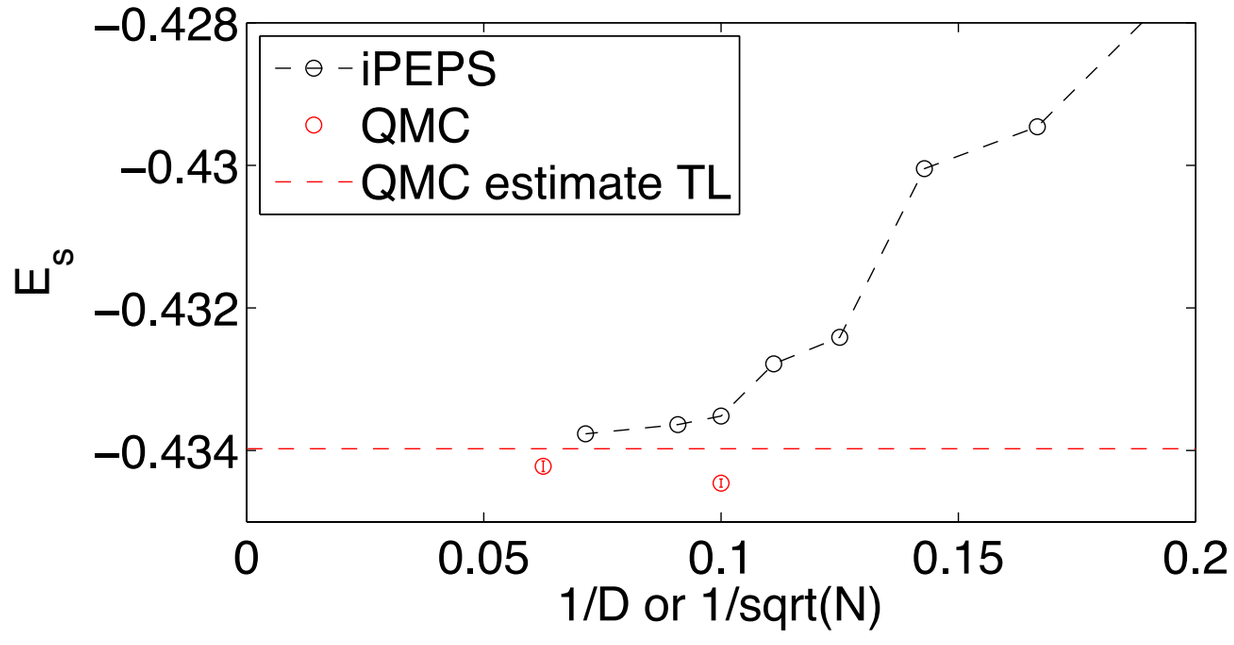


iPEPS: previous benchmarks (here: U/t=10)

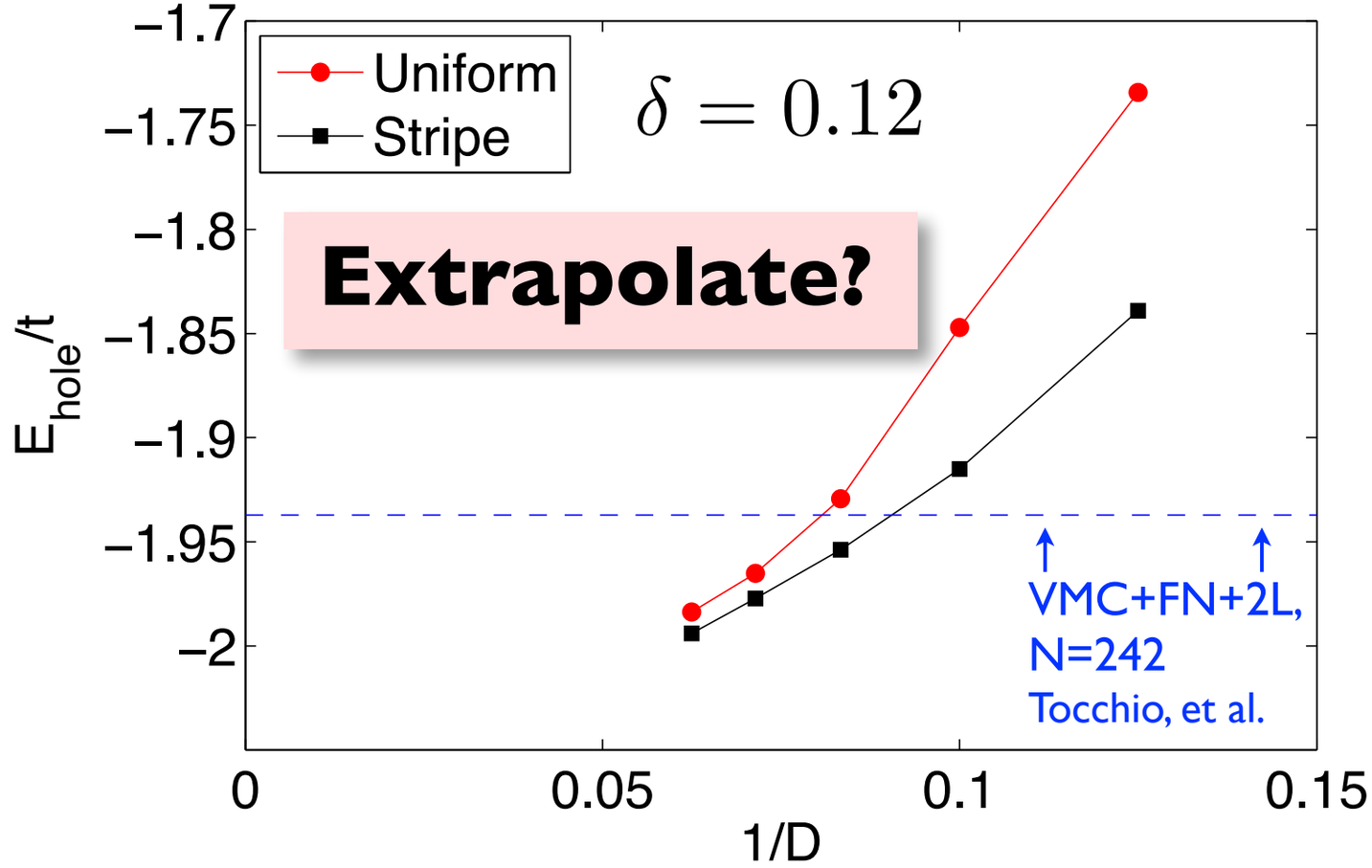
Half-filled case (n=1):

- Relative error in the TL: O(**0.05%**)
  (D=14 without extrapolation!)
- QMC estimate by S. Sorella (unpublished)



Doped case (n=0.88):

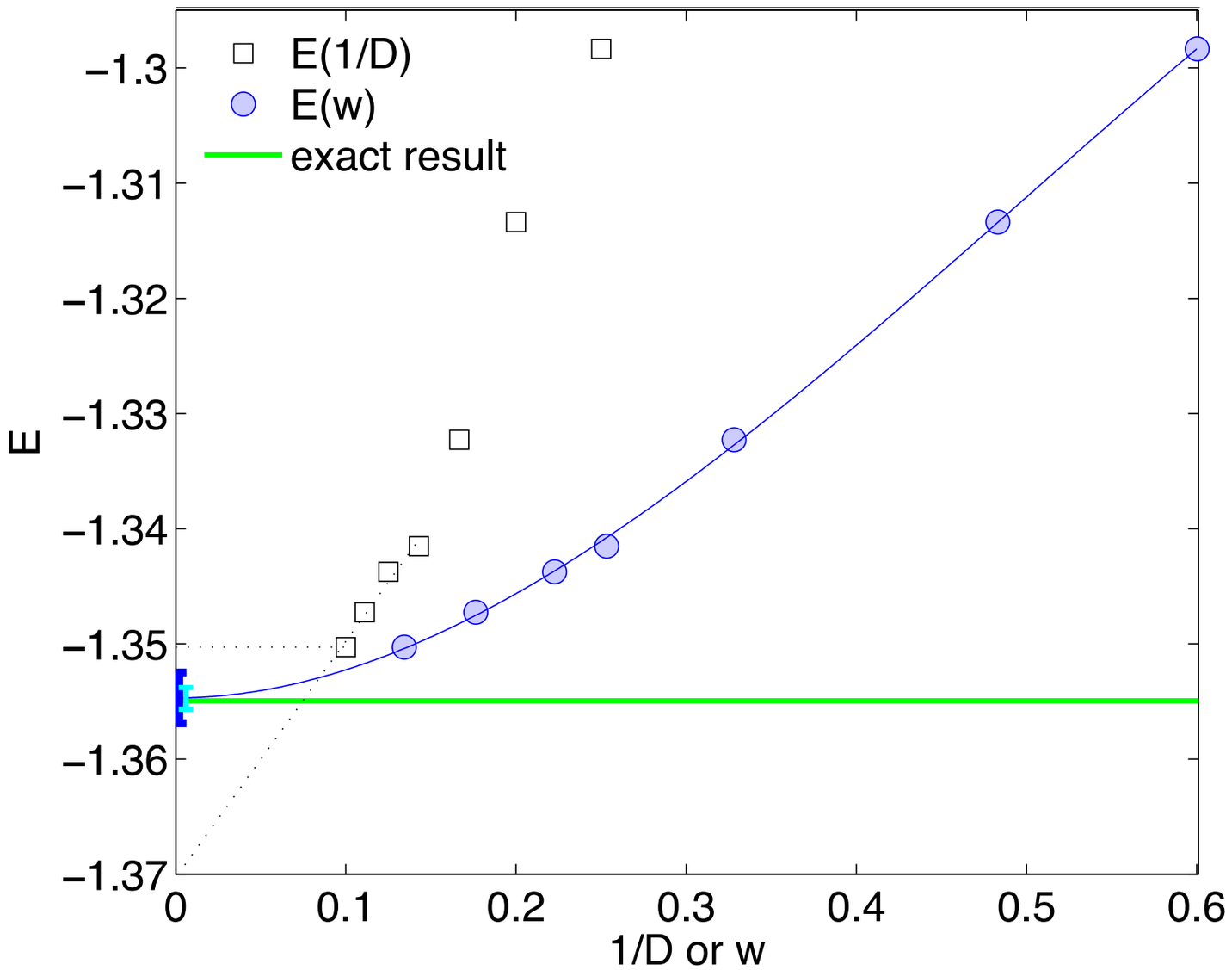
- Lower variational energy than best data from VMC+FN+2L
  [Tocchio, Becca, Sorella, unpublished]



Improving energy extrapolations

PC, PRB **93** (2016)

Motivation: Need accurate energy extrapolation to determine the true ground state

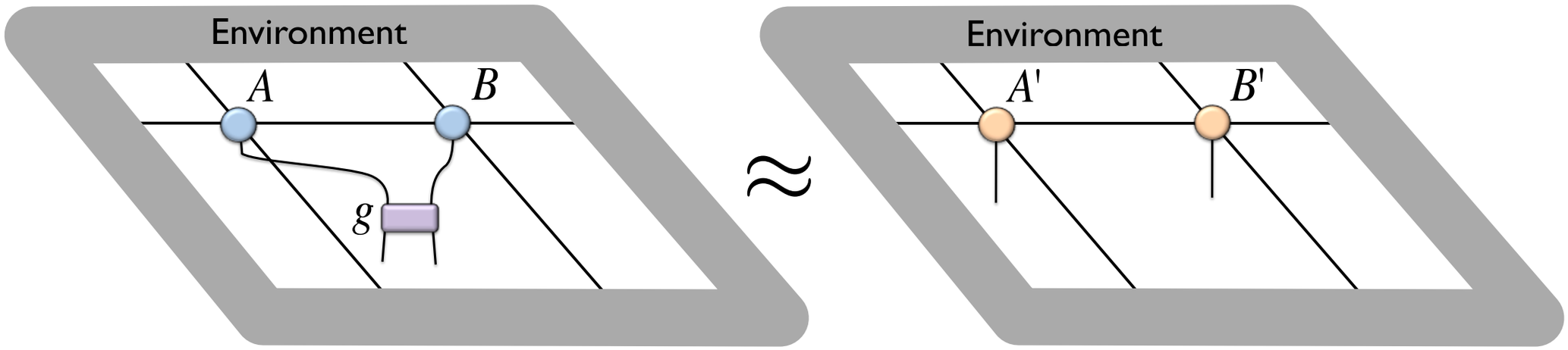


Bad estimate based on 1/D data!

Extrapolate in ***truncation error*** instead!

$$\hat{H} = -t \sum_{\langle i,j,\sigma \rangle} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + H.c. \right) + \sum_{\langle i,j \rangle} \gamma_{ij} \left(\hat{c}^{\dagger}_{i\uparrow} \hat{c}^{\dagger}_{j\downarrow} - \hat{c}^{\dagger}_{i\downarrow} \hat{c}^{\dagger}_{j\uparrow} + H.c. \right)$$

Truncation error in the full update algorithm

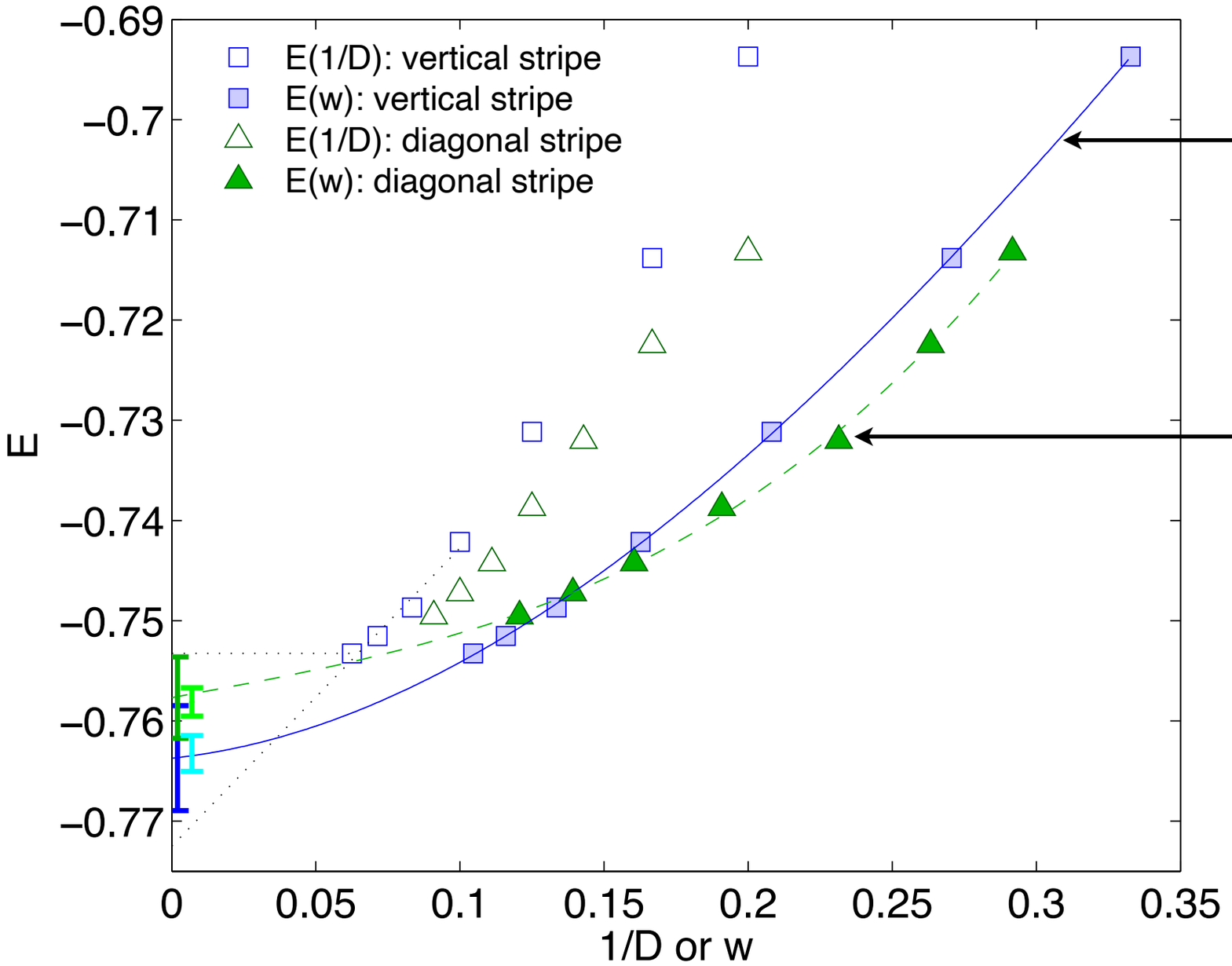


$$|\tilde{\Psi}\rangle = g|\Psi\rangle \qquad \approx \qquad |\Psi'\rangle$$

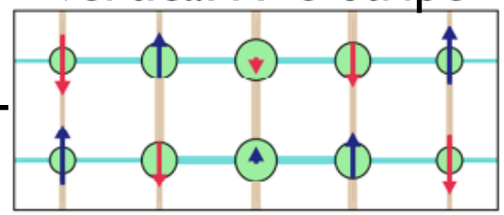
- Cost function: $C = || \, |\tilde{\Psi}\rangle - |\Psi'\rangle \, ||$

- Truncation error: $w(D) = C(D, \beta \to \infty)/\tau$

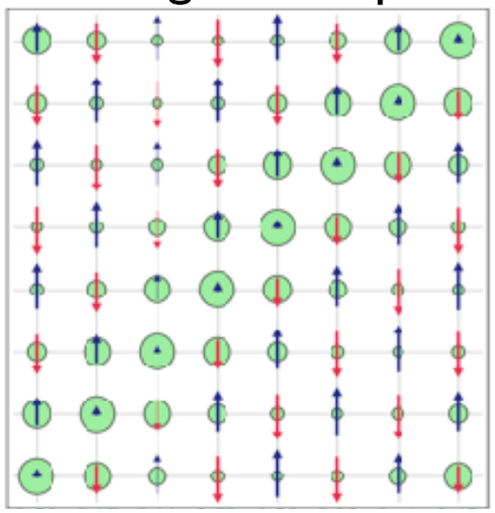
Example: vertical vs diagonal stripe, U/t=8, δ=1/8



Vertical λ=5 stripe

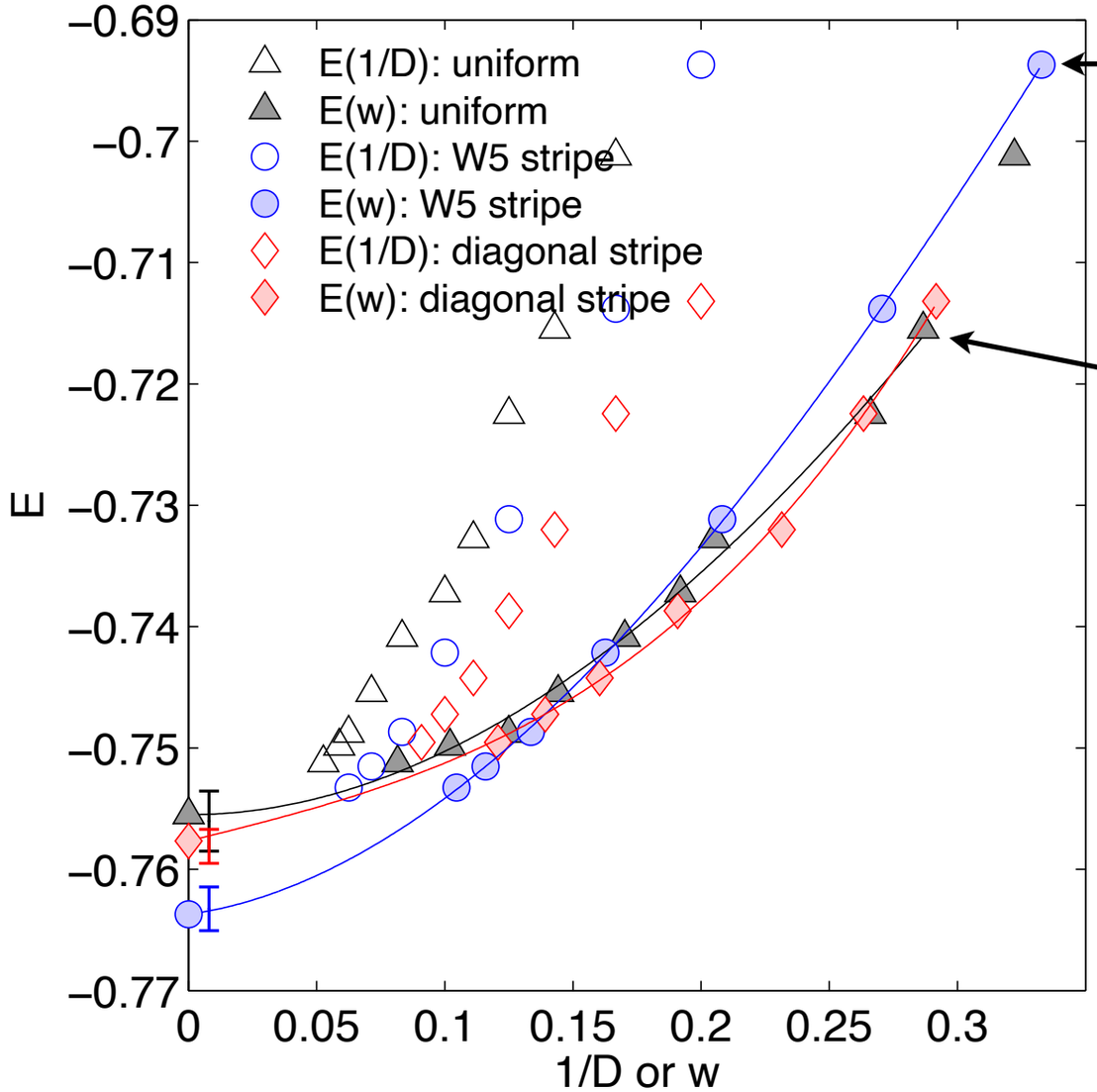


Diagonal stripe

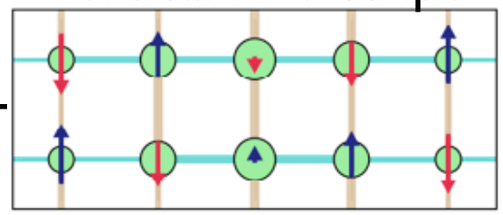


Vertical λ=5 stripe is **lower** than diagonal stripe

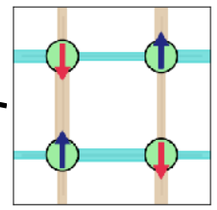
iPEPS: extrapolated energies



Vertical λ=5 stripe



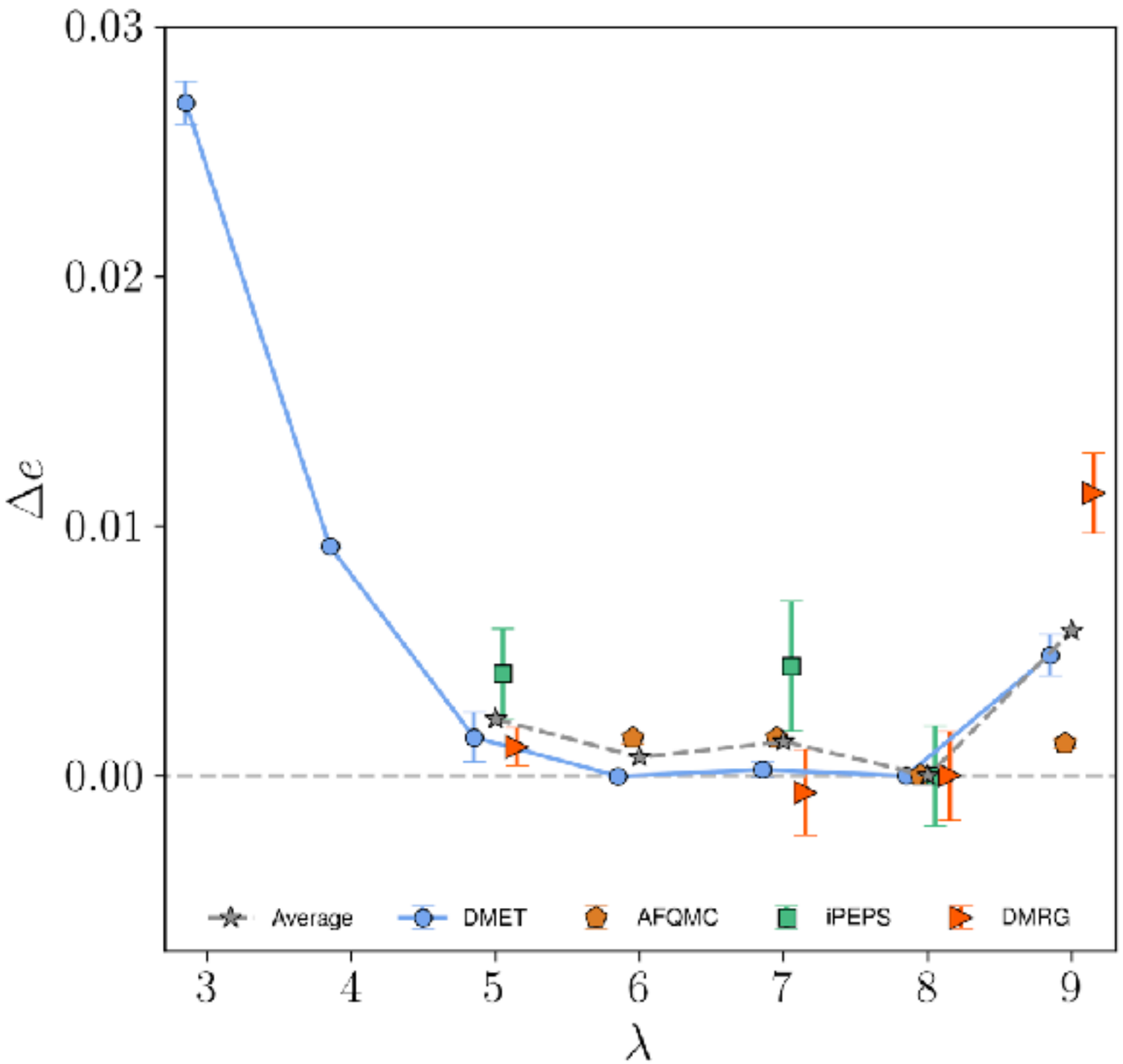
Uniform d-wave

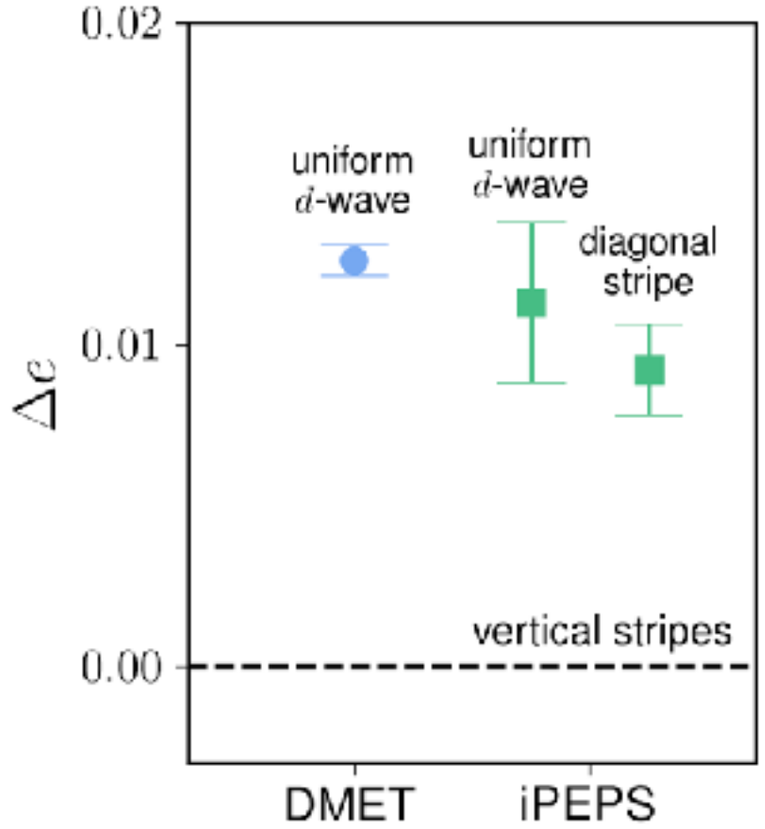


Stripe is lower than uniform state!

λ=8 stripe has lowest energy

Comparison with other methods





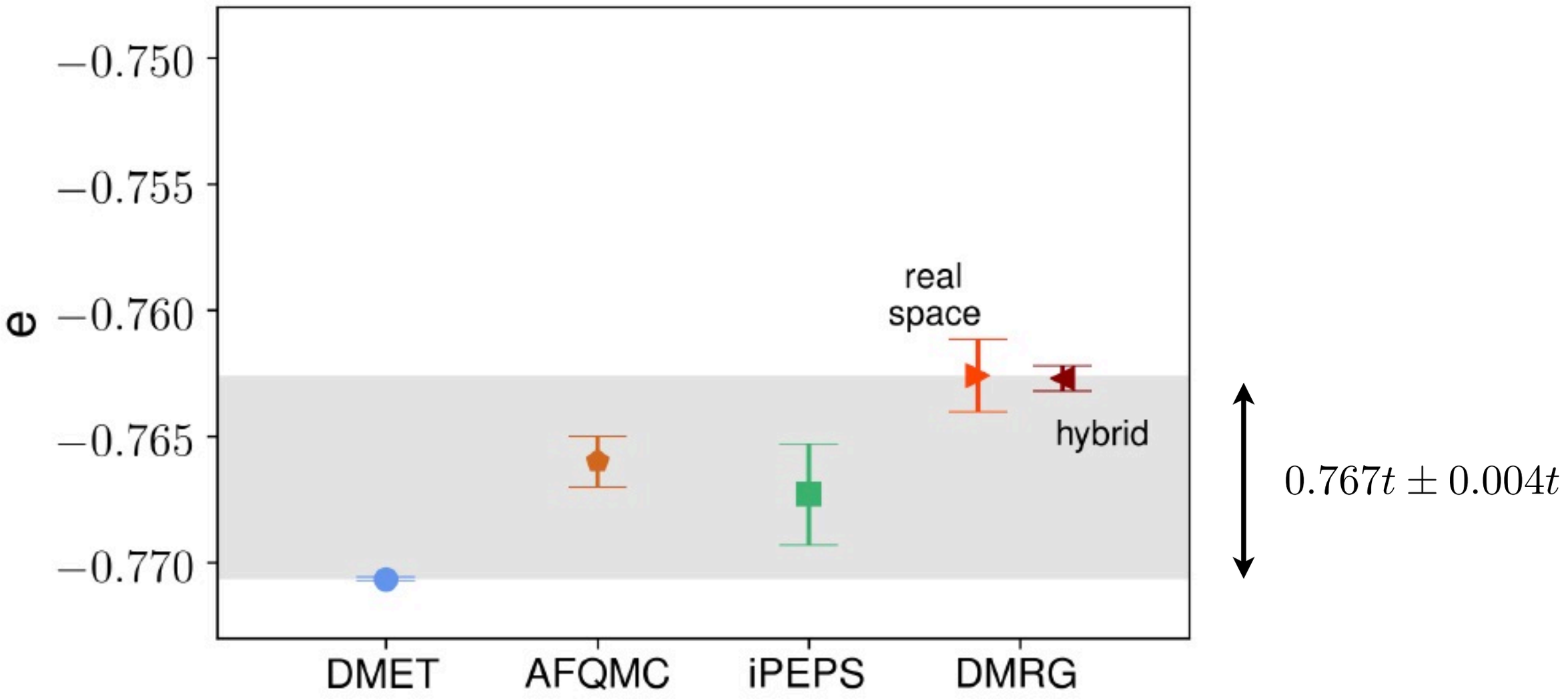
★ Uniform state: higher energy

★ λ=5...8: close in energy

★ λ=8 stripe: slightly lower

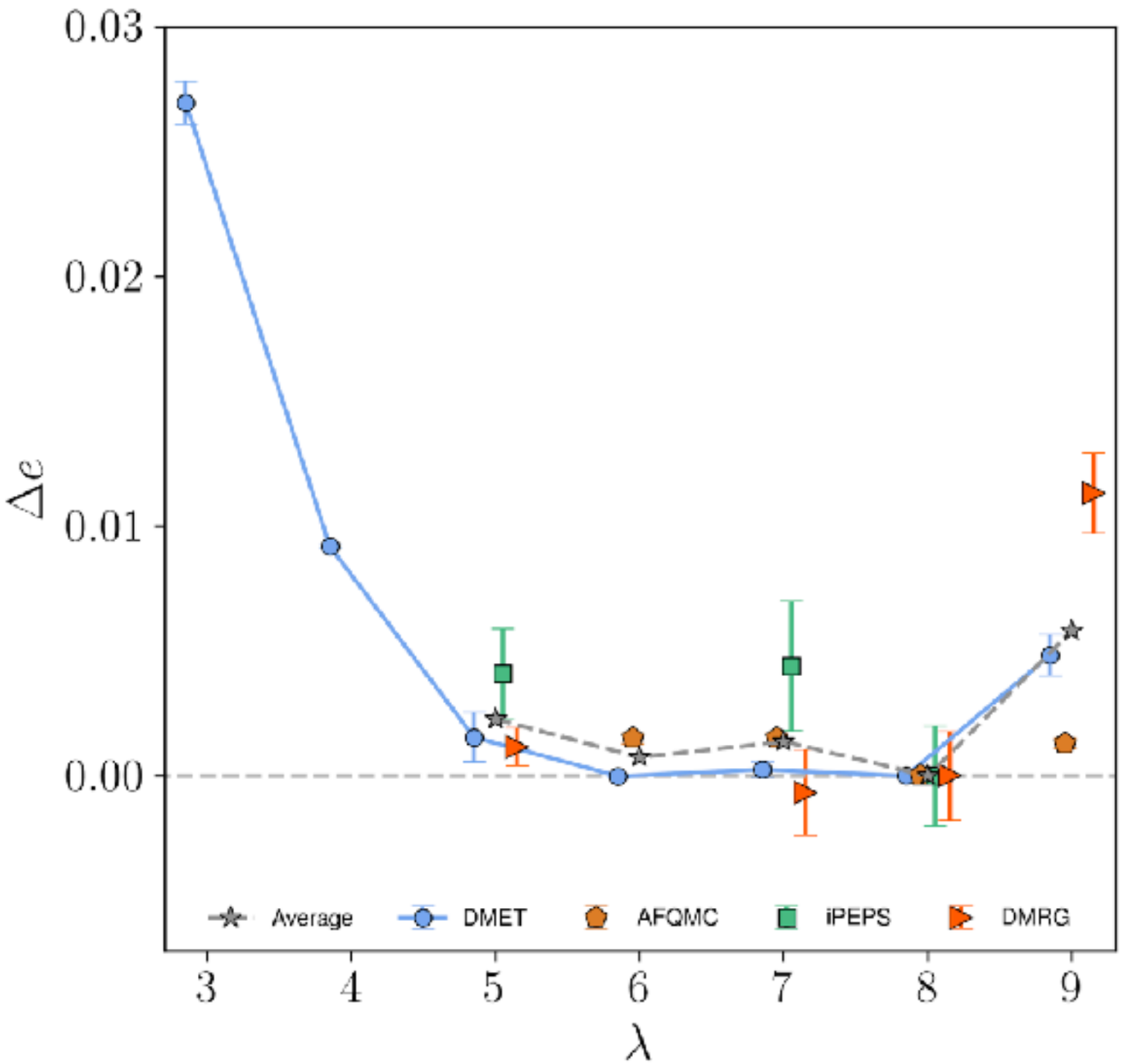
★ also compatible with fluctuating stripes

Energy of λ=8 stripe

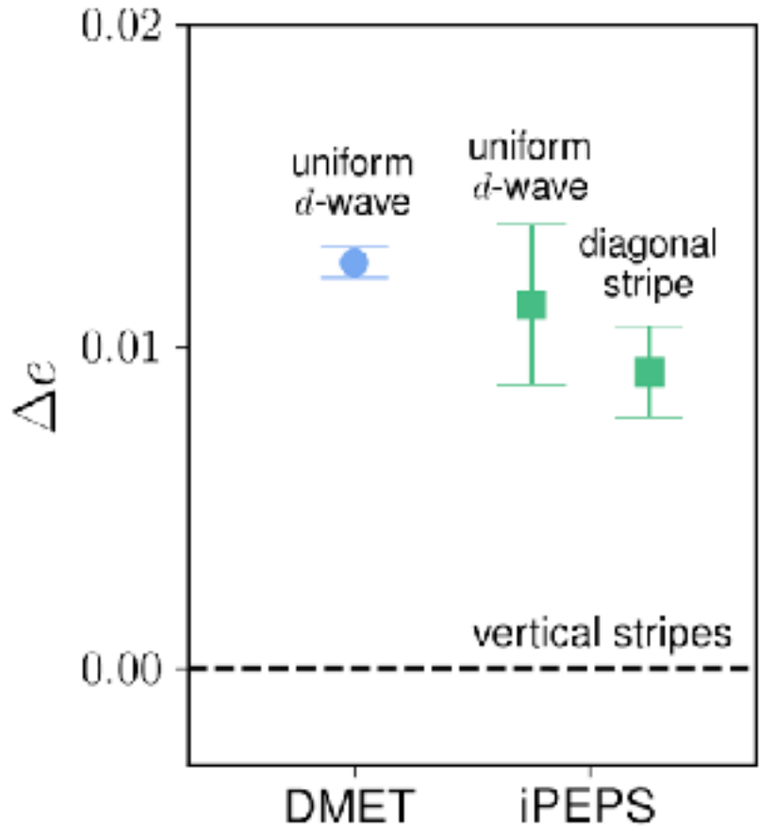


★ Close agreement between methods!

Comparison with other methods



★ Experiments: λ~4, but here higher in energy!



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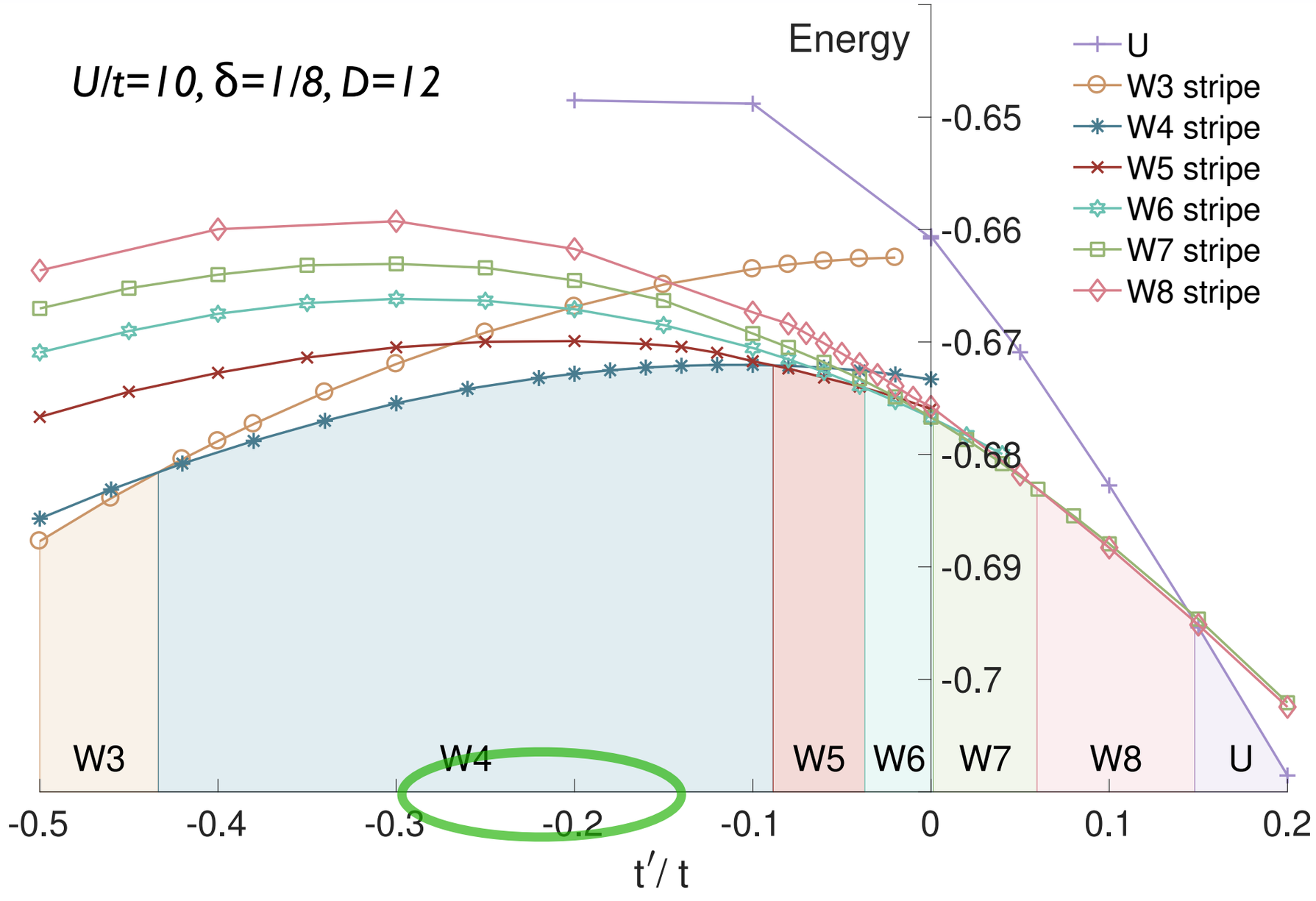
★ λ=8 stripe: slightly lower

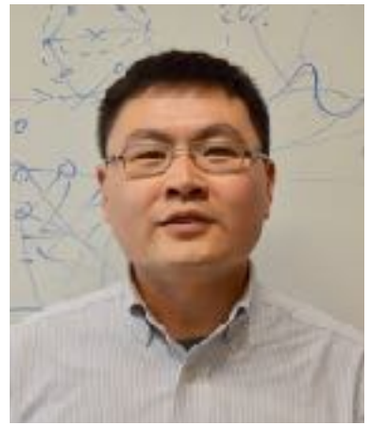
★ also compatible with fluctuating stripes

Extended 2D Hubbard model (+ next-nearest neighbor hopping)



Ponsioen, Chung, PC, PRB 100 (2019)

Boris Ponsioen



Sangwoo Chung

★ Period-4 stripes are stabilized by including a realistic t'/t ~ -0.15…-0.3
[see also: Ido, Ohgoe & Imada, PRB **97** (2018), Jiang & Devereaux, Science 365 (2019)]

★ Competition is weaker in this region than for t'/t=0

★ Superconductivity is suppressed in the period-4 stripe

Summary: 2D Hubbard model, δ=1/8, U/t=8 (U/t=10)

- Doped 2D Hubbard model exhibits many competing low energy states
- Stripe has lower energy than uniform d-wave state (δ=1/8)
- λ=8 stripe lowest energy (U/t=8), with λ=5-7 stripes very close in energy
- Realistic t'/t = -0.2…-0.3: period 4 stripe (with suppressed SC)

★ Next step: more realistic models of the cuprates (multi-band models)

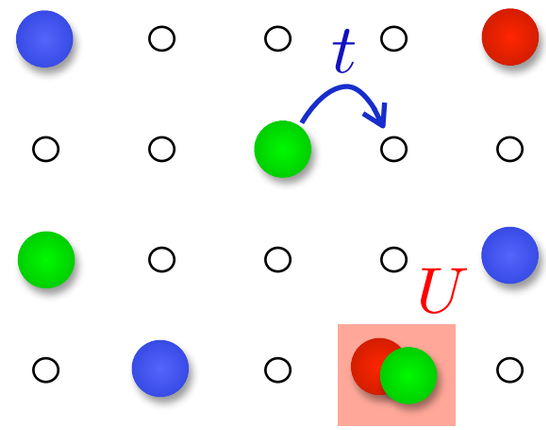
★ Systematic study will help to get a better understanding of the various competing phases in the cuprates!

SU(N) Hubbard models

- Generalization to N species ("colors") of fermions

$$\hat{H} = -t \sum_{\langle i,j \rangle, \alpha} \hat{c}^{\dagger}_{i\alpha} \hat{c}_{j\alpha} + H.c. + U \sum_{i, \alpha<\beta} \hat{n}_{i\alpha} \hat{n}_{i\beta}$$

sum over all colors:  ...



- Realizable in quantum simulators using alkaline-earth atoms in optical lattices

Nuclear spin

^{87}Sr: $I = 9/2 \longrightarrow N_{max} = 2I + 1 = 10$

$$|I_z = 3/2\rangle \leftrightarrow |\bullet\rangle$$
$$|I_z = 1/2\rangle \leftrightarrow |\bullet\rangle$$
$$|I_z = -1/2\rangle \leftrightarrow |\bullet\rangle$$
$$|I_z = -3/2\rangle \leftrightarrow |\bullet\rangle$$
$$\vdots \qquad\qquad \vdots$$

Cazalilla, Ho & Ueda, NJP 11(2009)
Gorshkov, et al, Nat. Phys. 6, 289 (2010).
Taie, Yamazaki, Sugawa & Takahashi, Nat. Phys. 8 (2012).
Scazza, et al., Nat. Phys. 10, 779 (2014).
Zhang, et al, Science 345 (2014).
Cazalilla & Rey, Rep. Prog. Phys. 77 (2014).
Hofrichter, et al, PRX 6 (2016).
Ozawa, Taie, Takasu & Takahashi, PRL 121 (2018).
⋮ ⋮ ⋮

SU(N) Hubbard models

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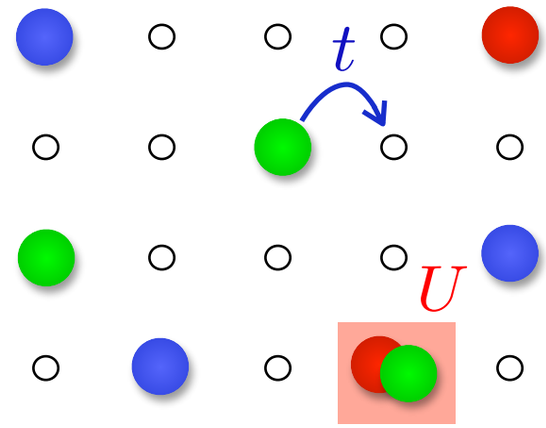
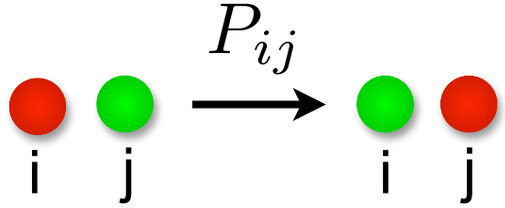


- Strong coupling limit (U>>t), integer filling: *SU(N) Heisenberg model*

$$H = \sum_{\langle i,j \rangle} P_{ij}$$

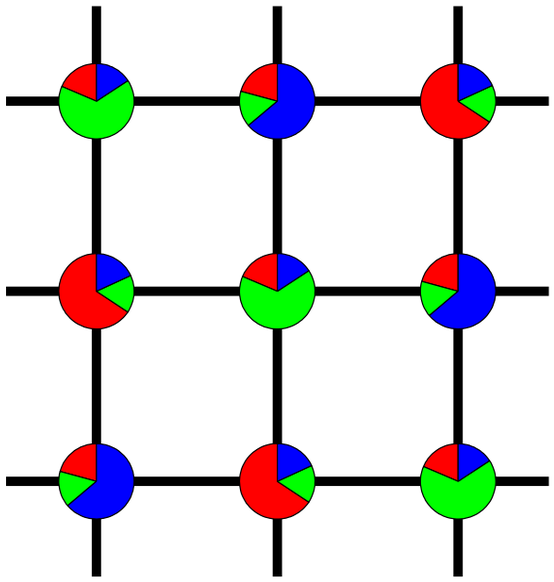
permutation operator



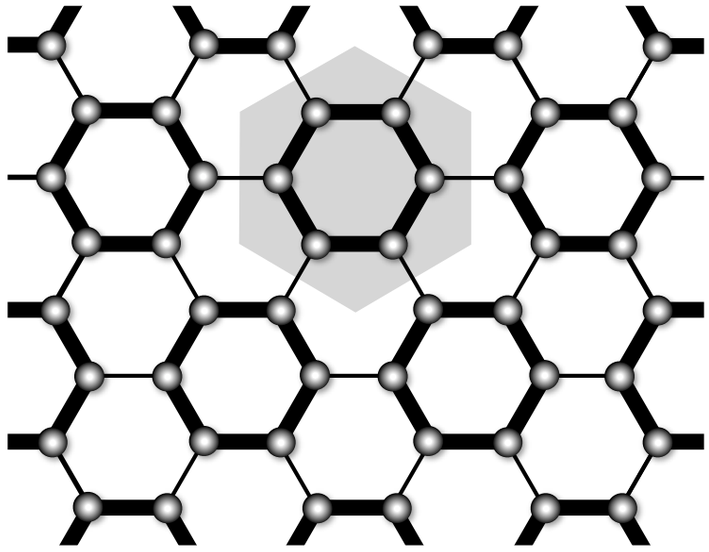
- **In general very challenging to study!**

SU(N) Heisenberg models

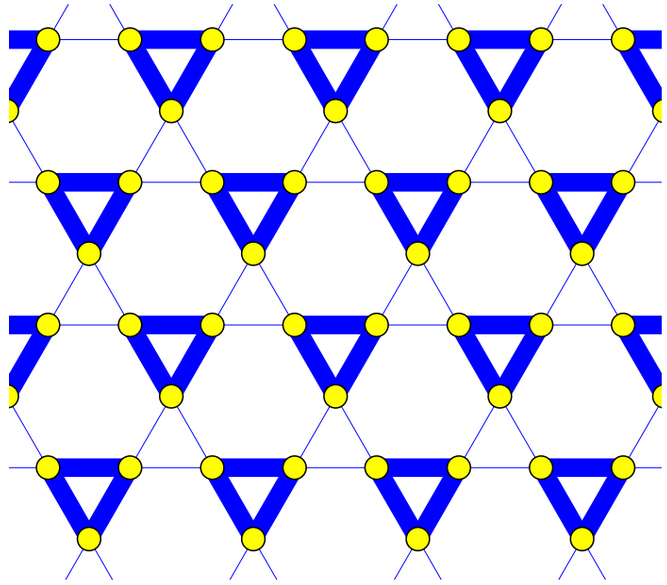
SU(3) square/triangular:
3-sublattice Néel order
Bauer, PC, et al., PRB **85** (2012)



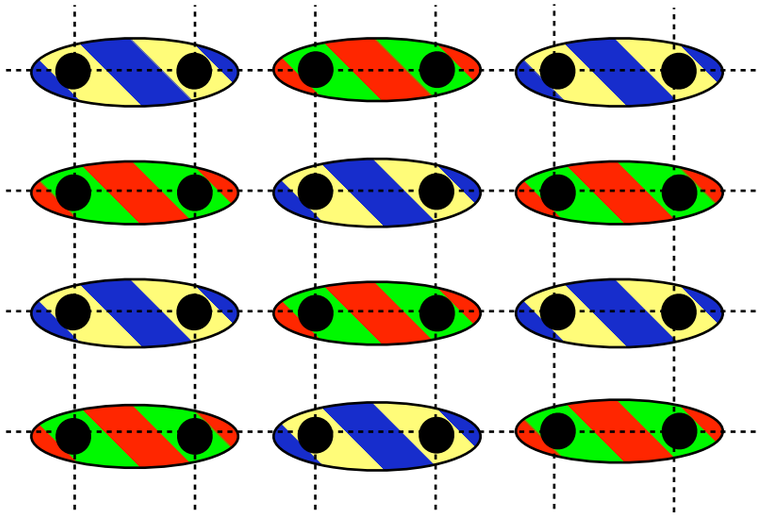
SU(3) honeycomb: *Plaquette state*
Zhao, Xu, Chen, Wei, Qin, Zhang, Xiang, PRB **85** (2012);
PC, Läuchli, Penc, Mila, PRB **87** (2013)



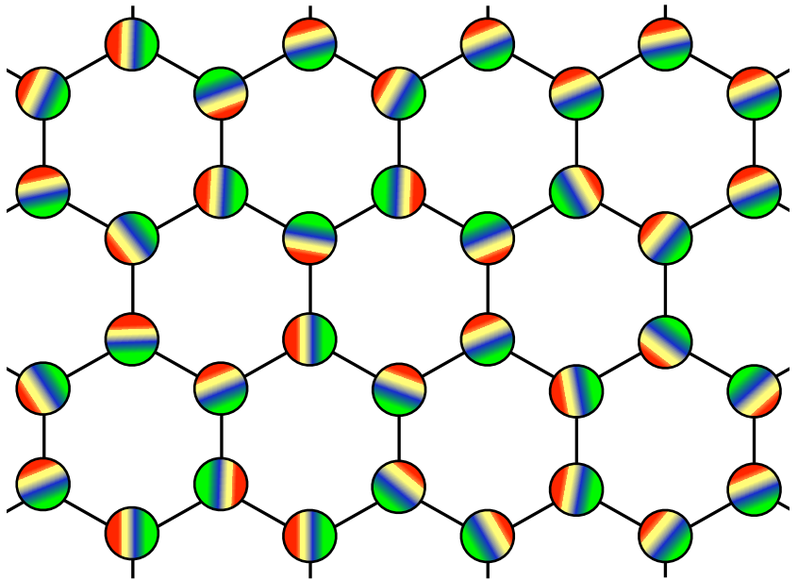
SU(3) kagome:
Simplex solid state
PC, Penc, Mila, Läuchli, PRB **86** (2012)



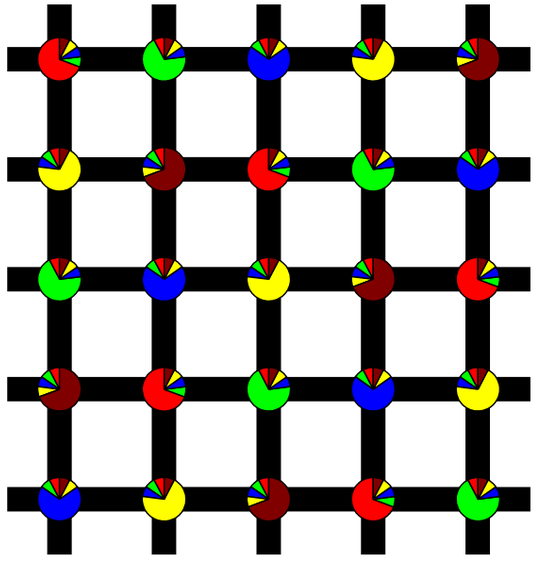
SU(4) square:
Dimer-Néel order
PC, Läuchli, Penc, Troyer, Mila, PRL **107** (2011)



SU(4) honeycomb:
spin-orbital (4-color) liquid
PC, Lajkó, Läuchli, Penc, Mila, PRX **2** ('12)

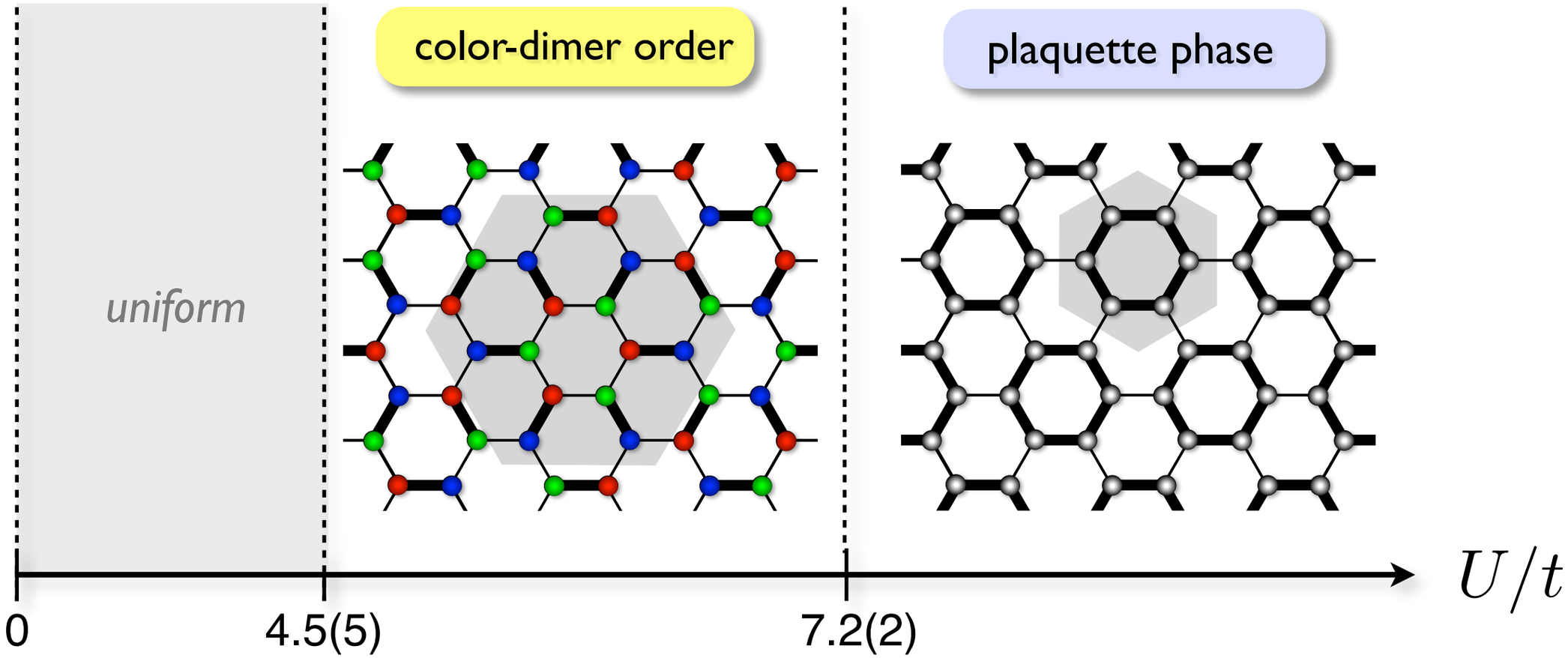


SU(5) square:
color order
PC, Mila, unpublished



SU(3) honeycomb Hubbard model (n=1/3): summary

S. S. Chung, PC, PRB 100, 035134 (2019)



SU(N) Hubbard models: rich physics!

Challenging, but within reach of iPEPS simulations

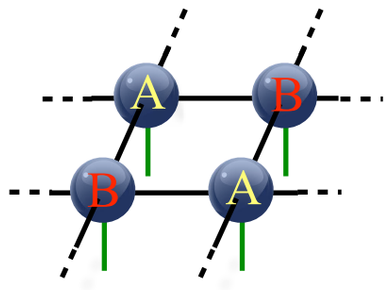
Part VI
Selected recent developments

Finite temperature simulations with iPEPS

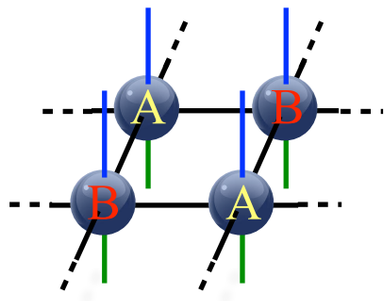
- Methodological developments (2D):

  Li et al. PRL 106 (2011); Czarnik et al. PRB 86 (2012); Czarnik & Dziarmaga PRB 90 (2014); Czarnik & Dziarmaga PRB 92 (2015); Czarnik et al. PRB 94 (2016); Dai et al PRB 95 (2017); Kshetrimayum, Rizzi, Eisert, Orus, PRL 122 (2019), P. Czarnik, J. Dziarmaga, PC, PRB 99 (2019), …

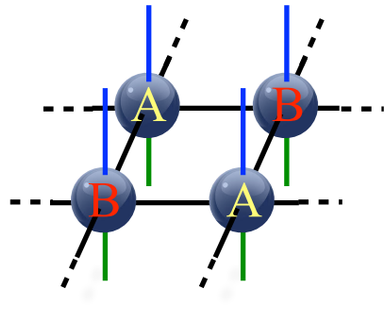
- Wave-function: $|\Psi\rangle \approx$



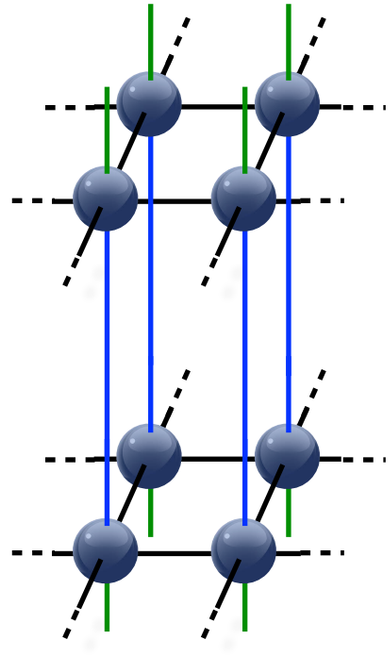
- Density-operator: $\hat{\rho} = e^{-\beta \hat{H}} \approx$



- Symmetric form: $e^{-\beta \hat{H}/2} \approx$



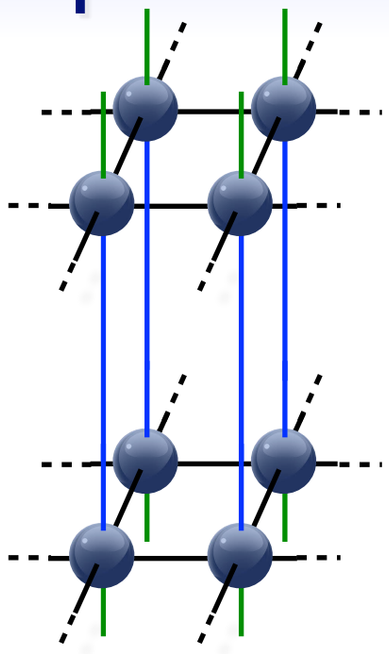
$\hat{\rho}(\beta) \approx$



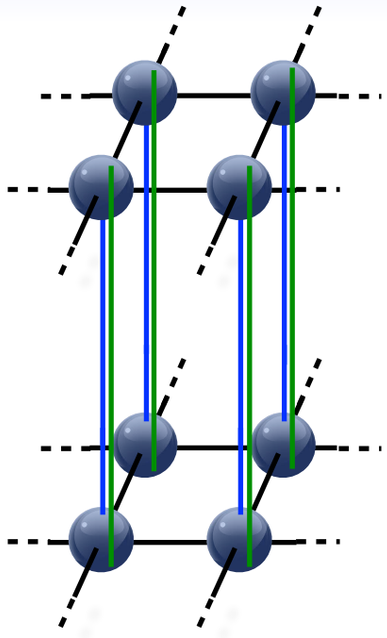
$$\hat{\rho}(\beta) = \hat{\rho}^{\dagger}(\beta)$$ by construction

Finite temperature simulations with iPEPS

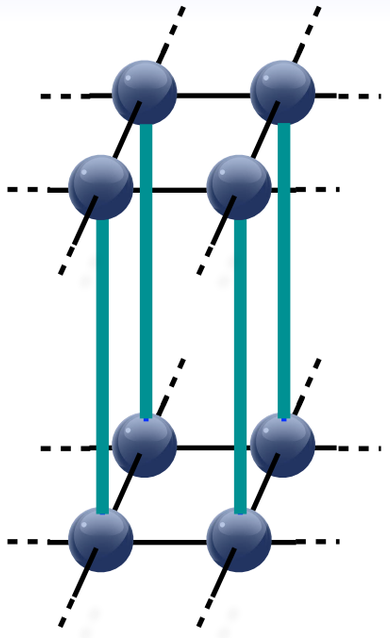
$\hat{\rho}(\beta) \approx$



trace



join legs



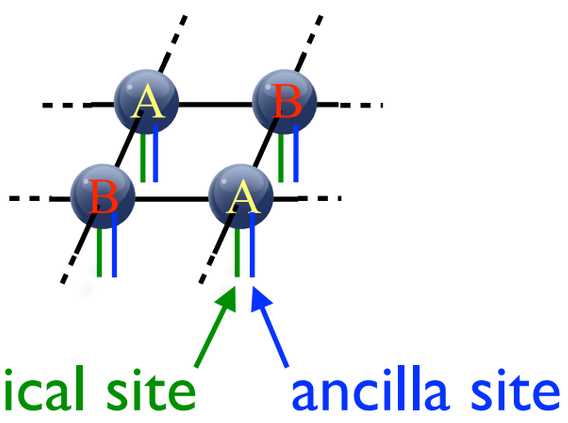
$\langle\Psi|\Psi\rangle$

same structure as
for wave functions

**Recycle algorithms for wave functions!
(CTM + imaginary time evolution)**

Other (equivalent) formulation using purification:

$|\tilde{\Psi}\rangle \approx$



$$\hat{\rho}(\beta) = \mathrm{Tr}_a |\tilde{\Psi}\rangle\langle\tilde{\Psi}|$$

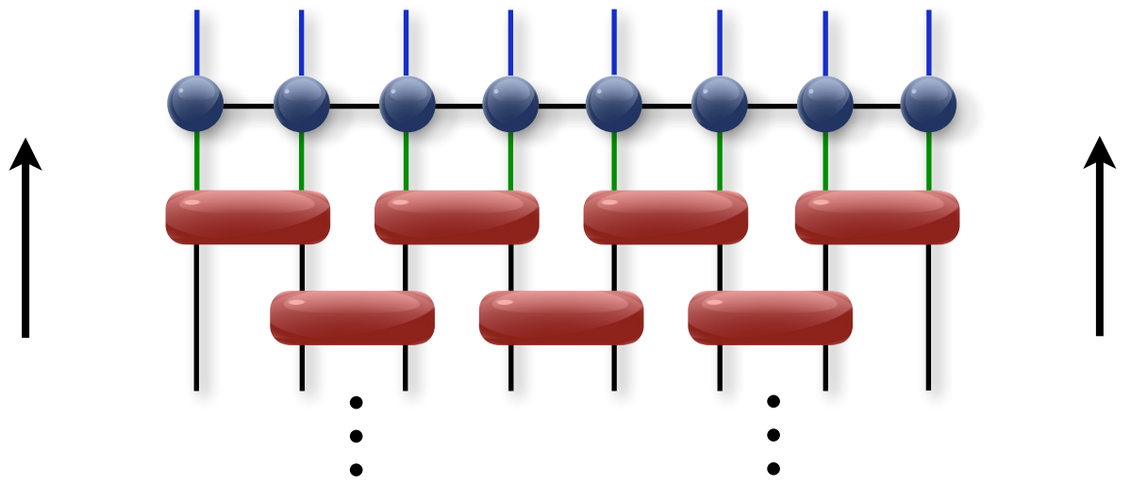
Imaginary time evolution

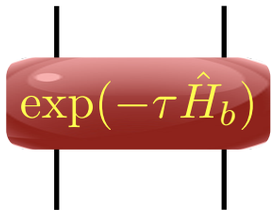
Czarnik, Dziarmaga & PC, PRB 99 (2019)

- Start at infinite temperature: $\hat{\rho}(\beta = 0) = \mathbb{I}$
- Initial state:  exact!
- Evolve in imaginary time: $\hat{\rho}(\beta) = e^{-\beta \hat{H}/2} \hat{\rho}(0) e^{-\beta \hat{H}/2}$

Trotter-Suzuki decomposition:

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



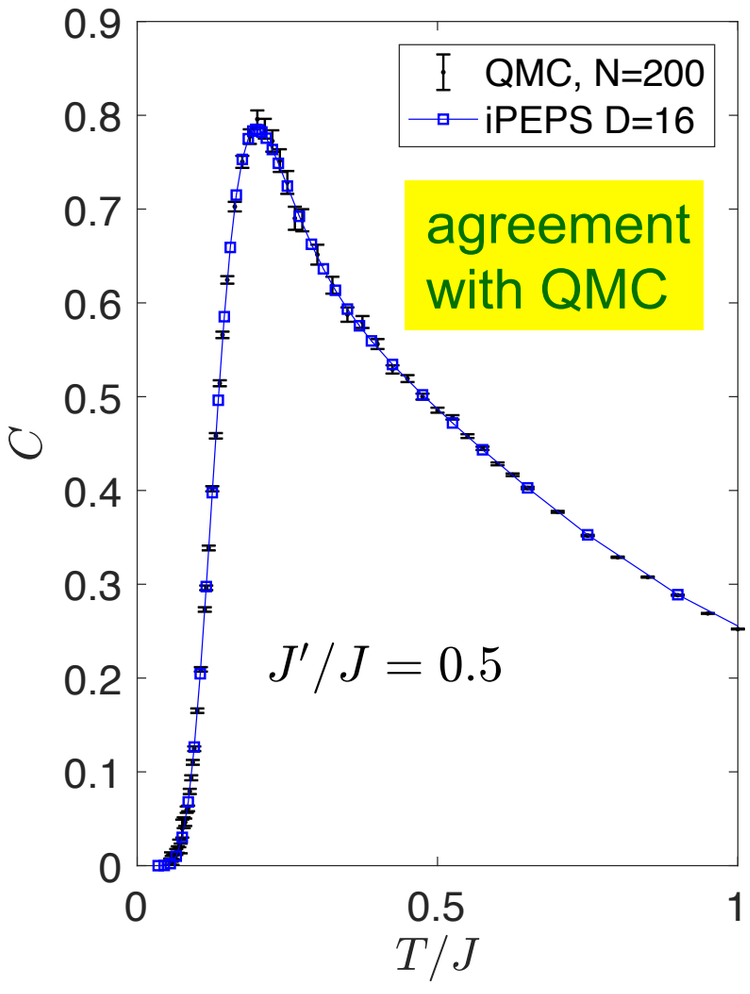


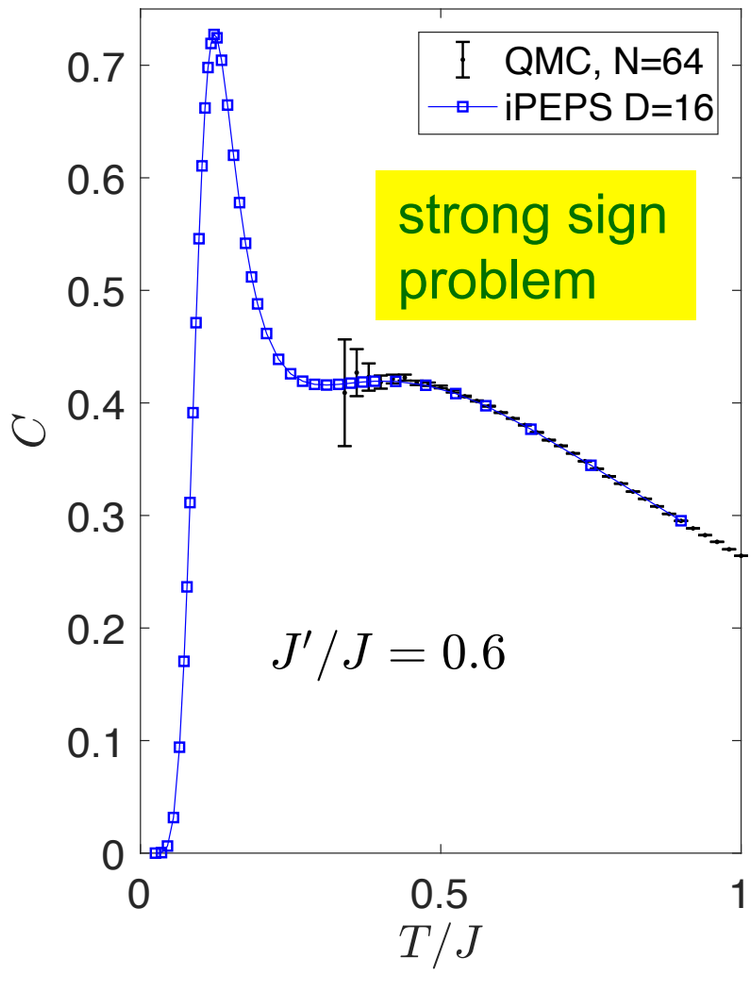
- Truncate after each step using e.g. simple / full update
- Evolve up to target $\beta/2$

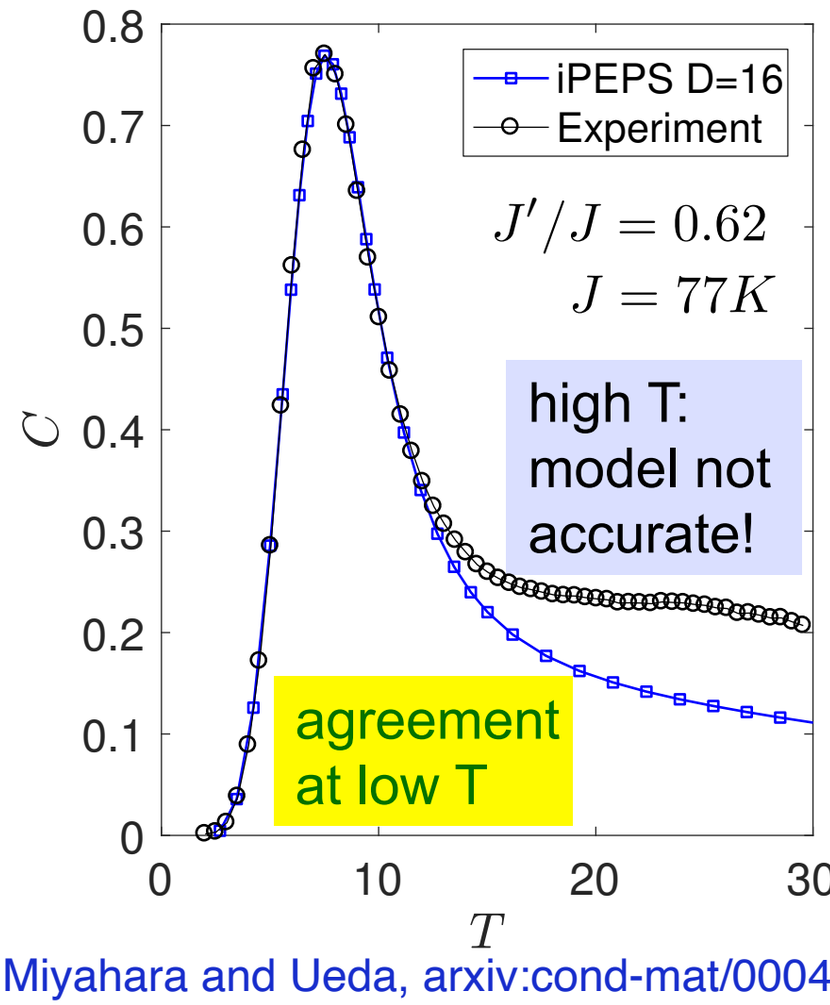
Finite temperature simulation examples

Wietek, PC, Wessel, Normand, Mila, and Honecker, PRR 1 (2019)

- Benchmarks in the dimer phase of the Shastry-Sutherland model
- Comparison between ED, TPQ, QMC, iPEPS

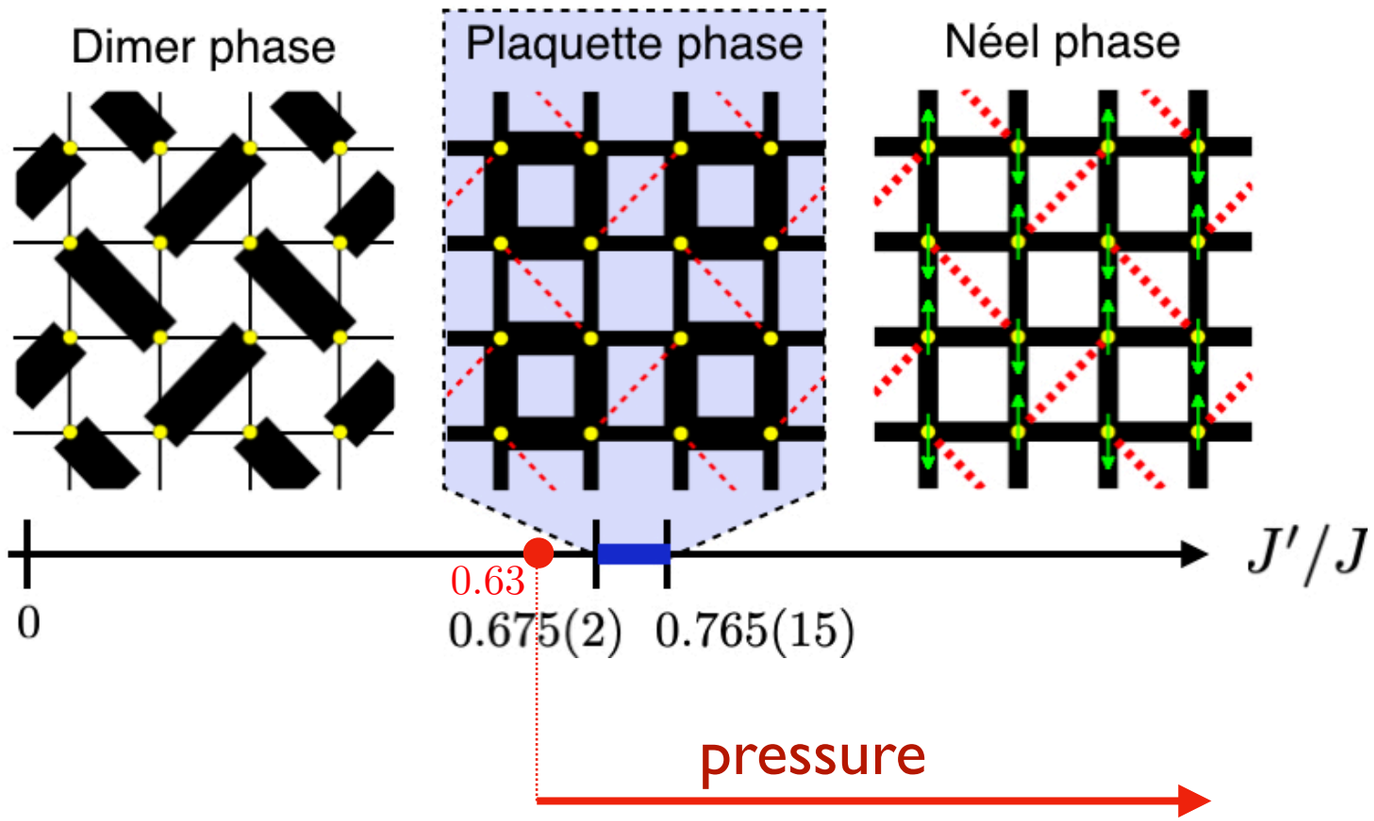






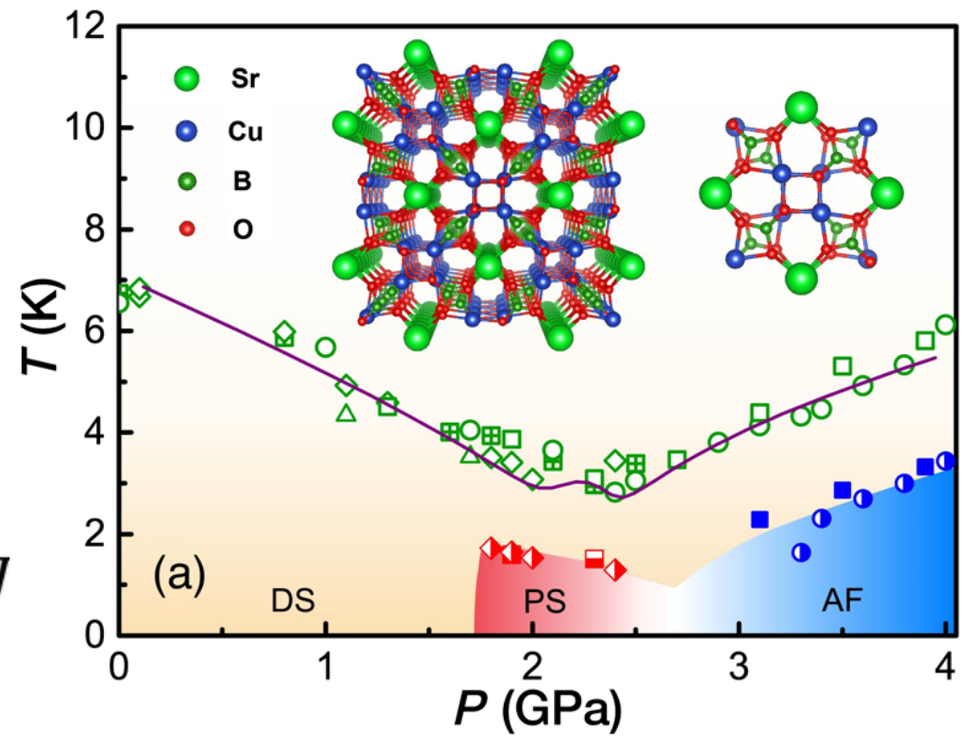
Miyahara and Ueda, arxiv:cond-mat/0004260

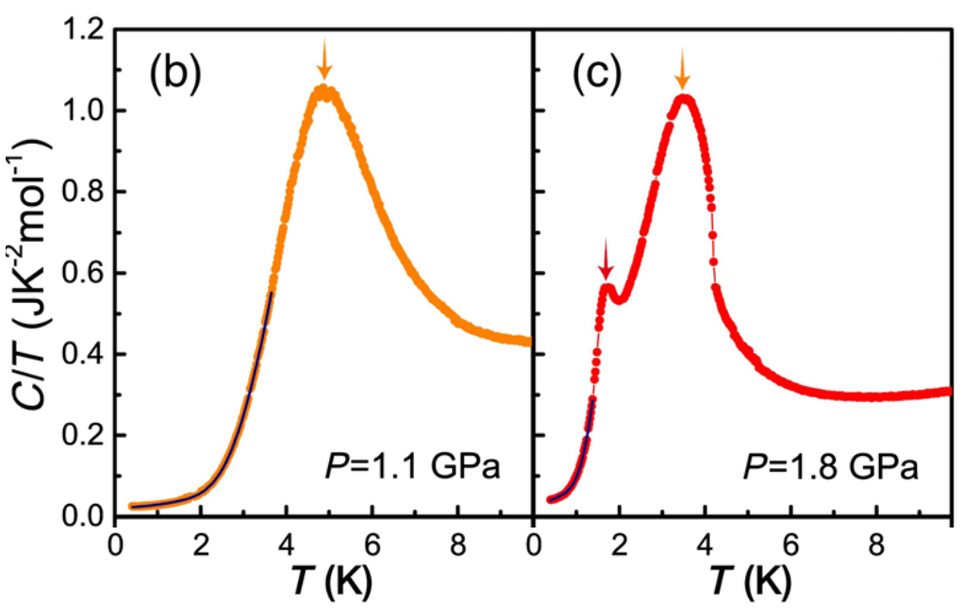
$SrCu_2(BO_3)_2$ under pressure



Drive system across the phase transitions!

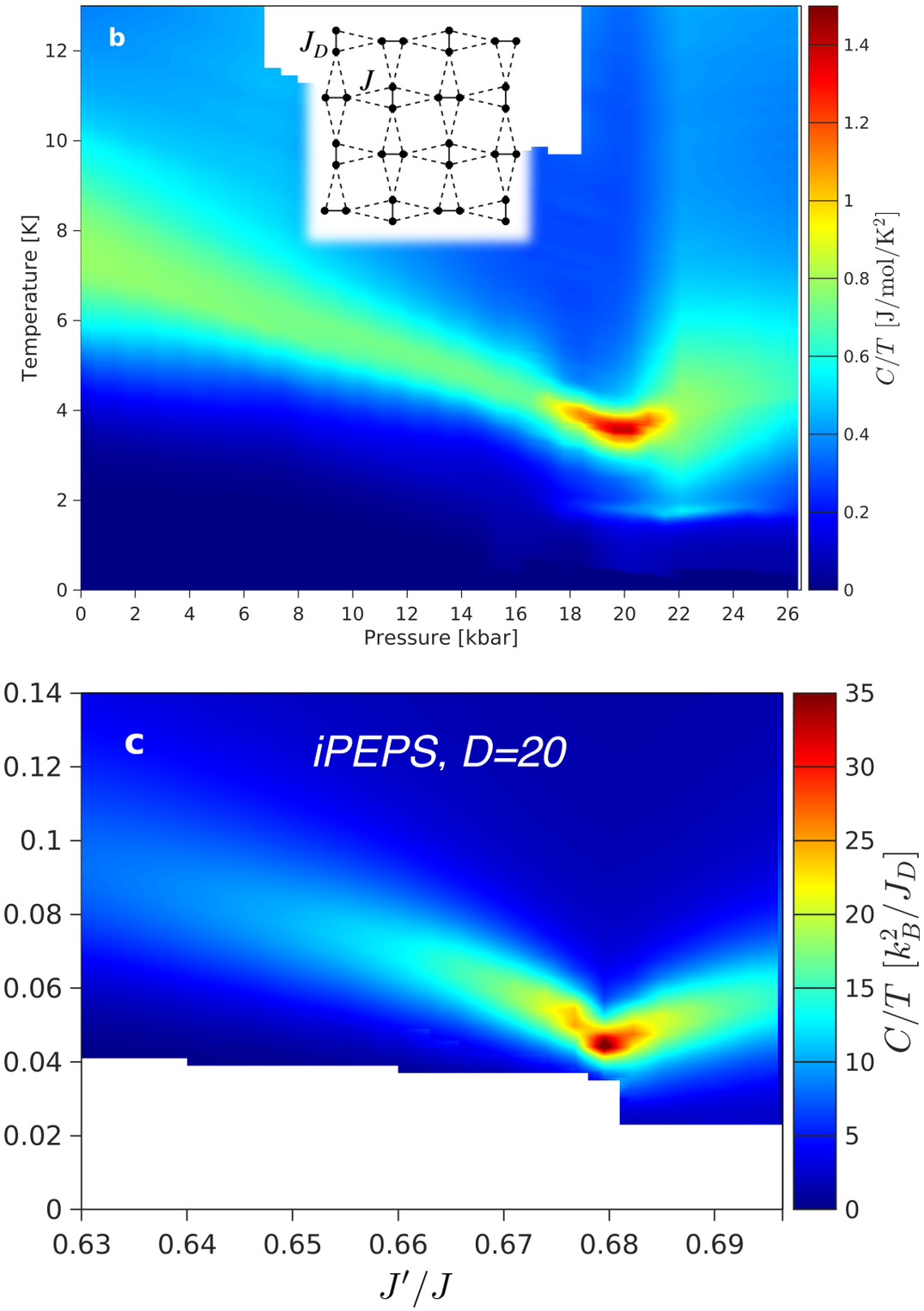
Waki, et al. J. Phys. Soc. Jpn. 76, 073710 (2007)
Haravifard, et al. Nat. Commun. 7, 11956 (2016)
Zayed, et al., Nat. Phys. 13, 962 (2017)
Sakurai, et al., J. Phys. Soc. Jpn. 87, 033701 (2018)
Guo, et al., PRL 124, 206602 (2020)
Bettler, et al,. Phys. Rev. Research 2, 012010 (2020)



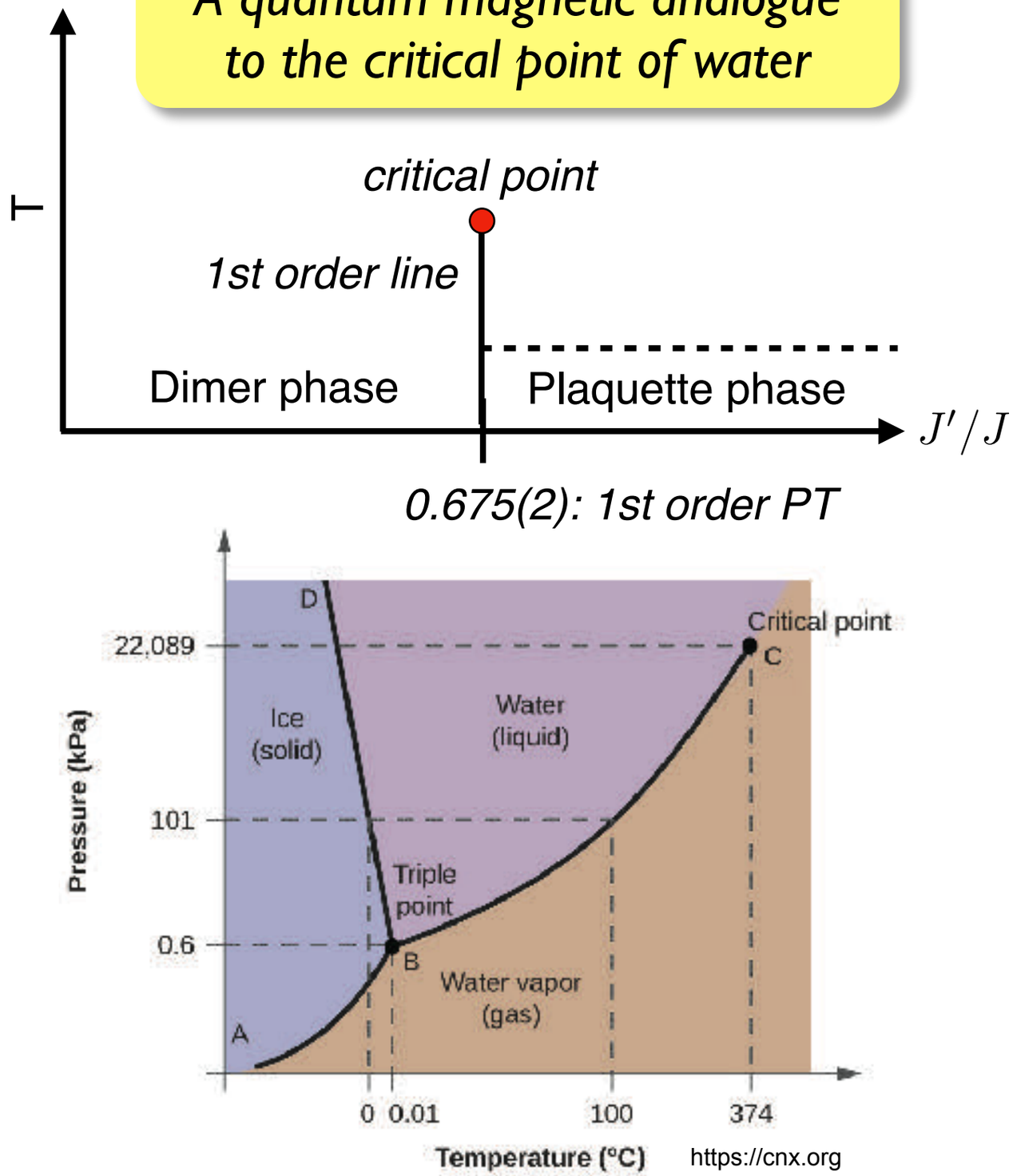


Guo, et al., PRL 124, 206602 (2020)

Specific heat data (group of H. M. Rønnow)



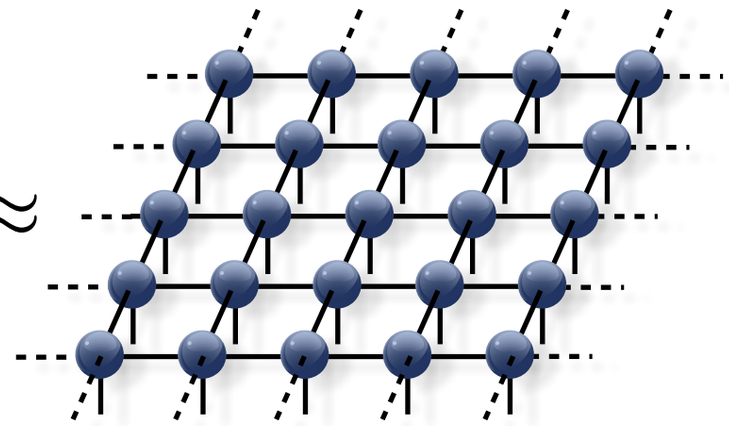
A quantum magnetic analogue to the critical point of water



Jiménez, **Crone**, Fogh, Zayed, Lortz, Pomjakushina, Conder, Läuchli, Weber, Wessel, Honecker, Normand, Rüegg, PC, Rønnow & Mila, Nature 592, 370 (2021)

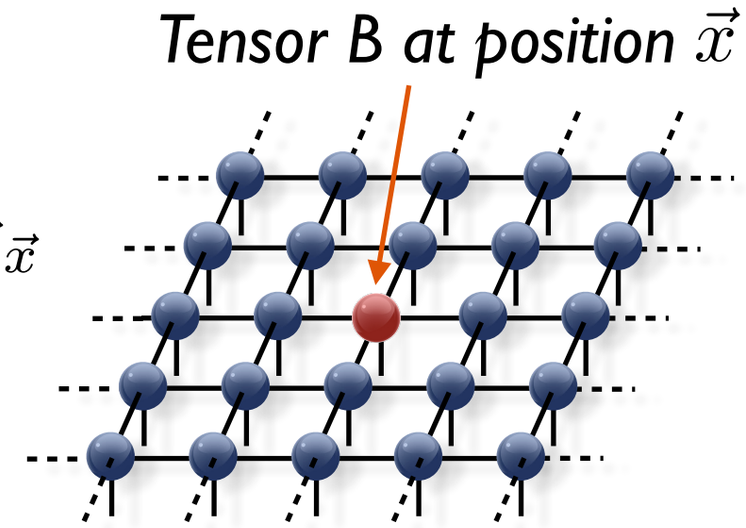
iPEPS excitation ansatz

- Ground state: $|\Psi\rangle \approx$



- Excitation on top of ground state with momentum k

$$|\Phi_{\vec{k}}(B)\rangle \approx \sum_{\vec{x}} e^{i\vec{k}\vec{x}}$$

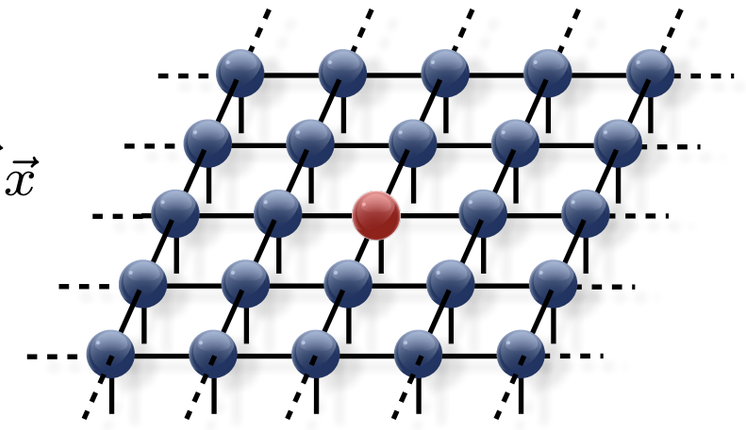


Haegeman, Pirvu, Weir, Cirac, Osborne, Verschelde, and Verstraete, PRB 85, 100408(R) (2012).
Haegeman, Michalakis, Nachtergaele, Osborne, Schuch, and Verstraete, PRL 111, 080401 (2013).
Haegeman, Osborne, and Verstraete, PRB 88, 075133 (2013).
Zauner, Draxler, Vanderstraeten, Degroote, Haegeman, Rams, Stojevic, Schuch, and Verstraete, New J. Phys. 17, 053002 (2015).
Vanderstraeten, Marien, Verstraete, and Haegeman, PRB 92, 201111 (2015)
Vanderstraeten, Haegeman, and Verstraete, PRB 99, 165121 (2019)

iPEPS excitation ansatz: the challenge

- Excitation on top of ground state with momentum k

$$|\Phi_{\vec{k}}(B)\rangle \approx \sum_{\vec{x}} e^{i\vec{k}\vec{x}}$$



Ansatz consists of an infinite sum!

- Minimizing: $\langle\Phi_{\vec{k}}(B)|\hat{H}|\Phi_{\vec{k}}(B)\rangle$

Triple infinite sum!

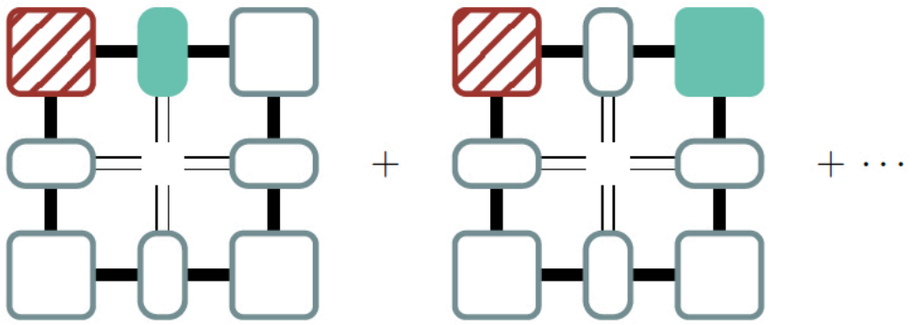
Translational invariance
→ Double infinite sum

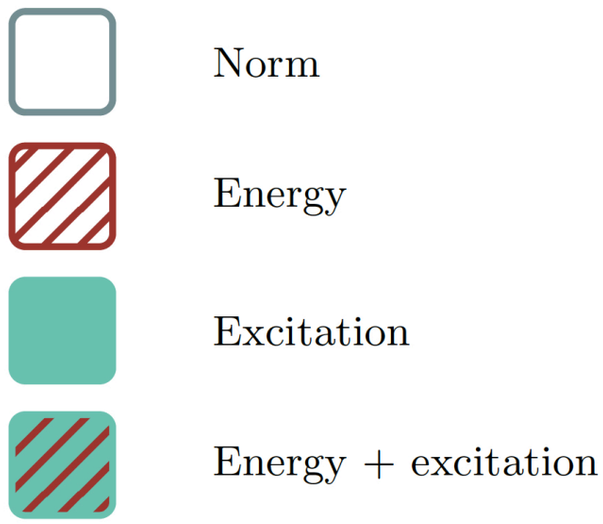
- Use systematic summation:

Channel environments	Vanderstraeten, Marien, Verstraete, and Haegeman, PRB 92 (2015) Vanderstraeten, Haegeman, and Verstraete, PRB 99 (2019)
CTM approach	Ponsioen and PC, PRB 101, 195109 (2020)
CTM + AD approach	Ponsioen, Assaad, PC, arXiv:2107.03399

Systematic summation using CTM

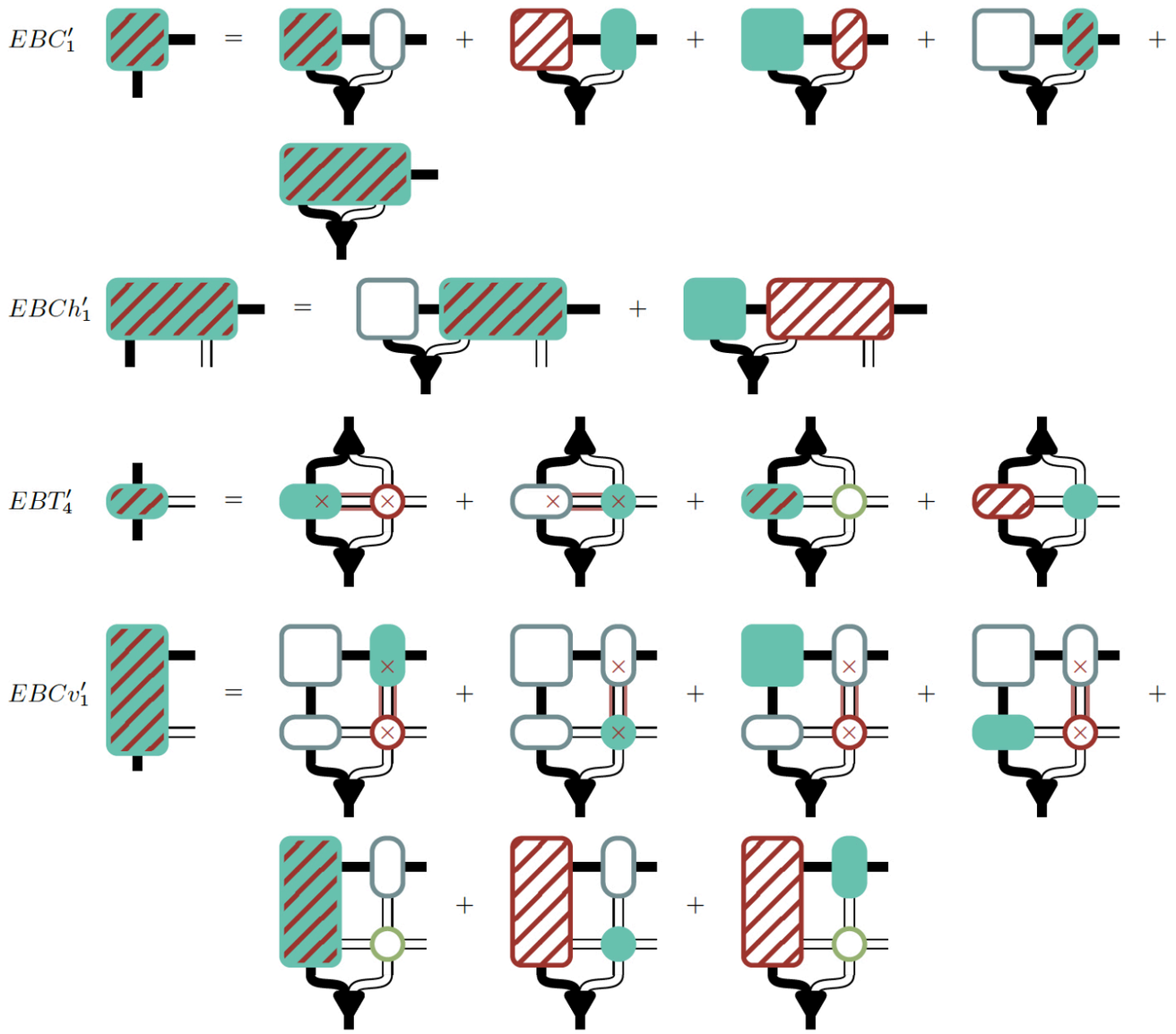
$$\langle \Phi_{\vec{k}}(B) | \hat{H} | \Phi_{\vec{k}}(B) \rangle$$





Ponsioen & PC, PRB 101 (2020)

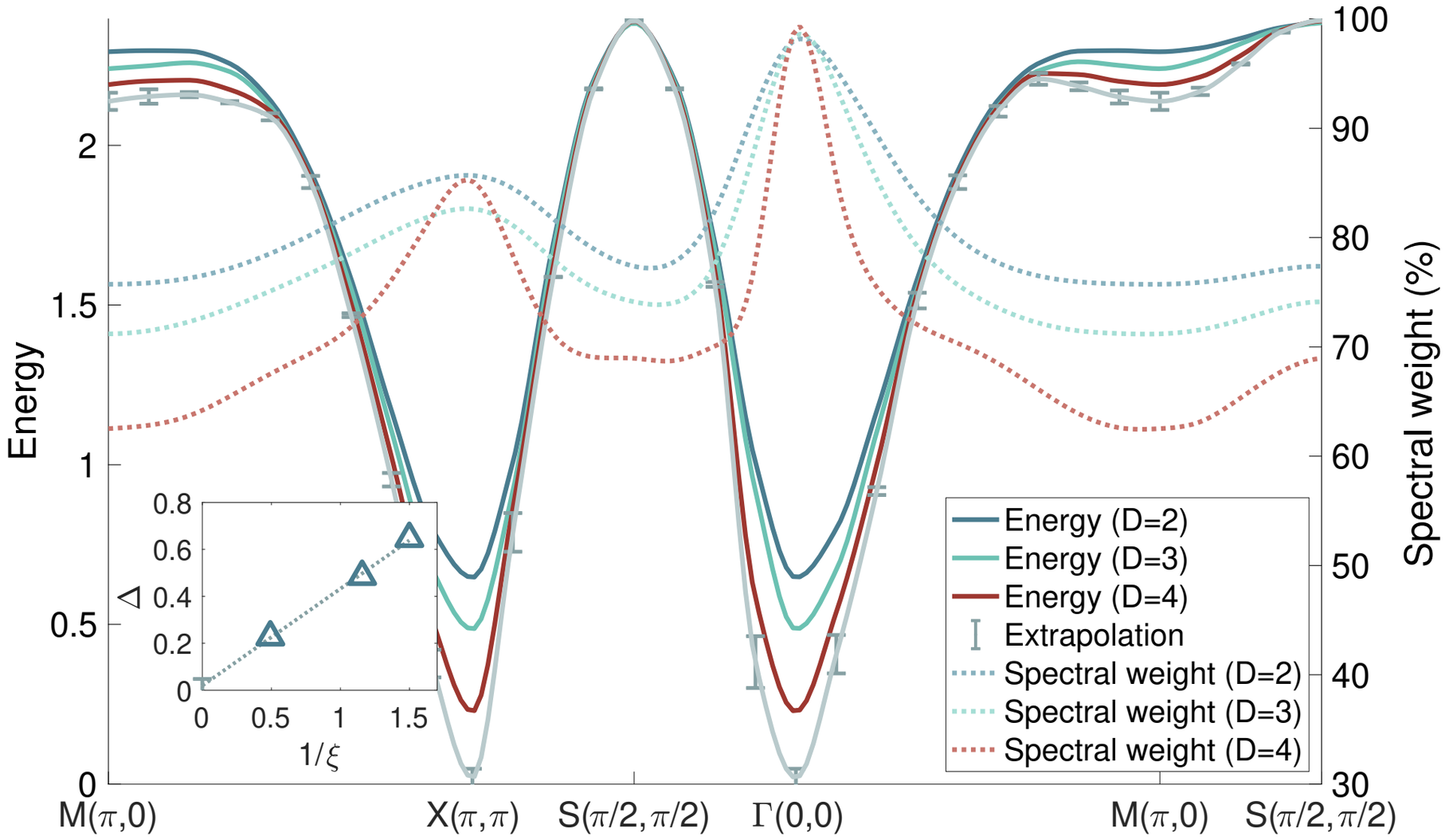
Left move examples:



Simpler: *use AD to avoid the summation of energy terms*

Ponsioen, Assaad, PC, arXiv:2107.03399

Benchmark: 2D Heisenberg model

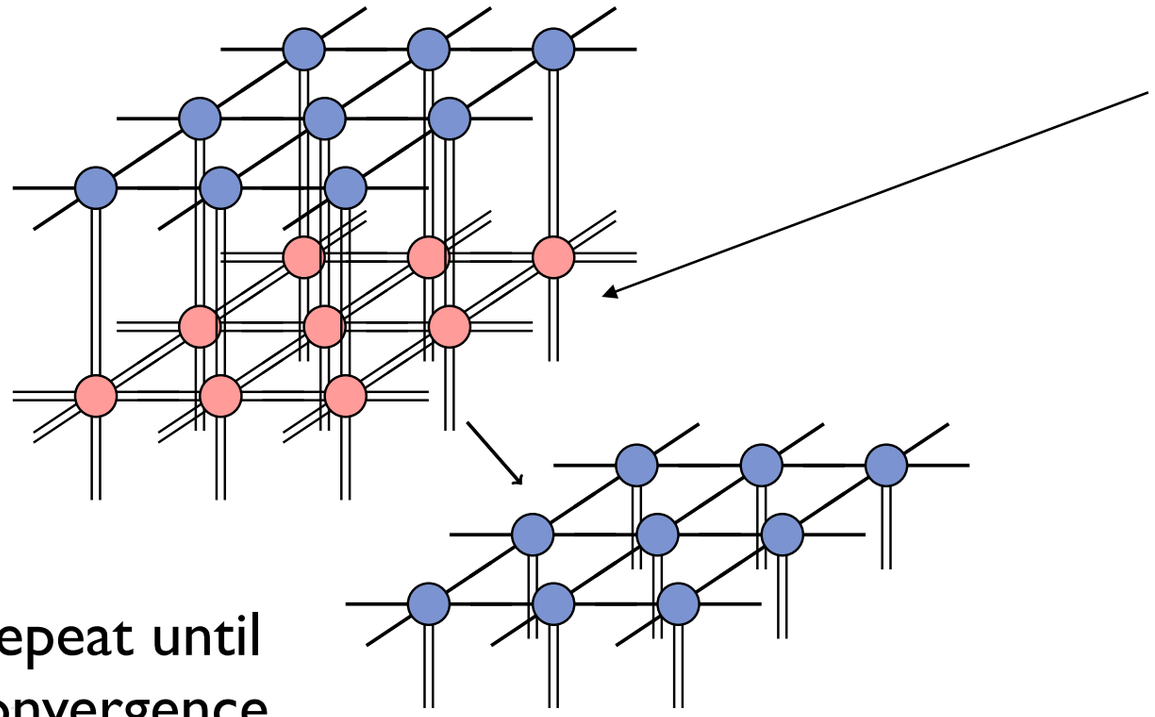


Ponsioen and PC, PRB 101, 195109 (2020)

similar results in:
Vanderstraeten, Haegeman, Verstraete, PRB 99, 165121 (2019)

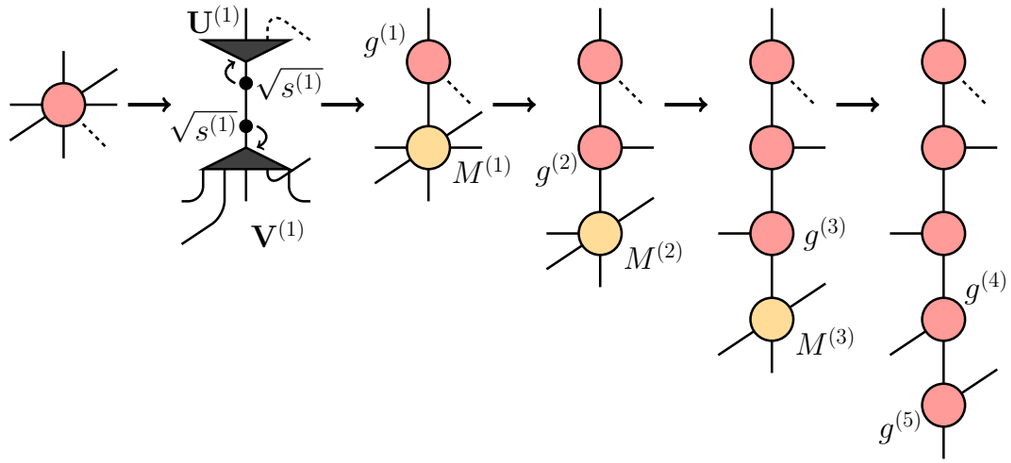
iPEPS in 3D: SU + CTMRG

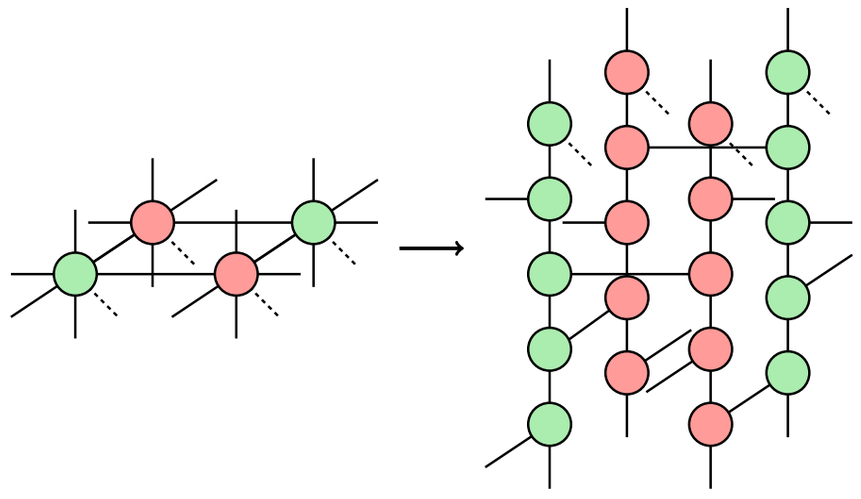
P. C. G. Vlaar, PC, PRB 103, 205137 (2021)



Repeat until convergence

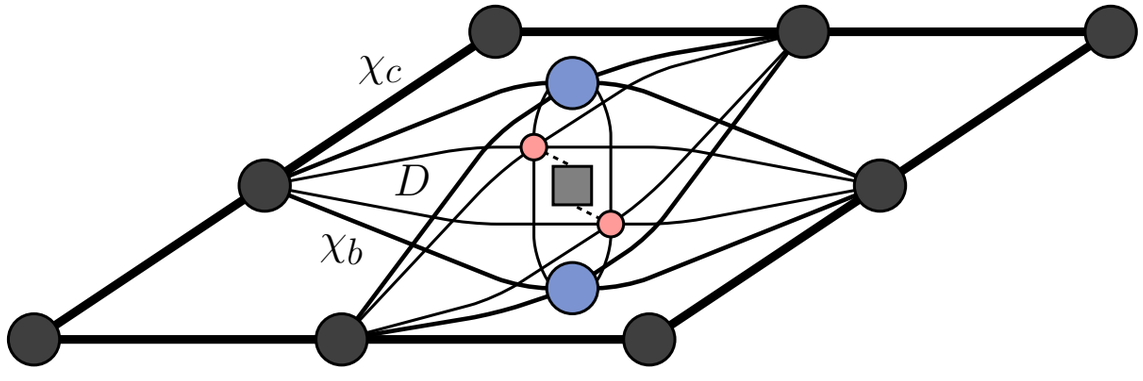
Decompose into series of 2-site operators





use simple update to contract

use CTM to contract resulting 3-layer network



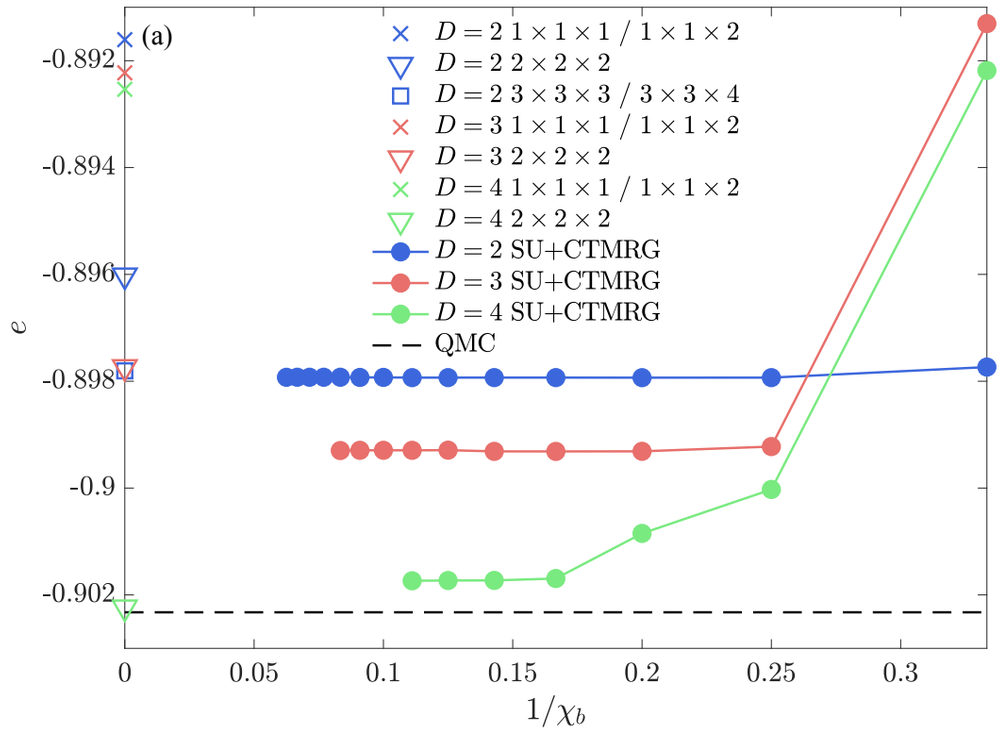
Other boundary PEPS approaches (3D classical):

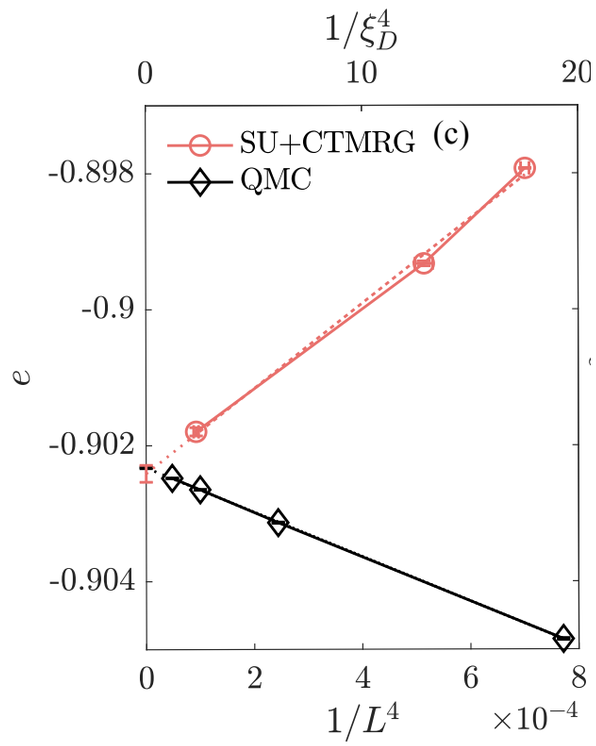
T. Nishino, et al,, Nucl. Phys. B 575, 504 (2000)
T. Nishino, et al, Prog. Theor. Phys. 105, 409 (2001)
A. Gendiar and T. Nishino, Phys. Rev. E 65, 046702 (2002)
A. Gendiar, N. Maeshima, and T. Nishino, Prog. Theor. Phys. 110 (2003)
A. Gendiar and T. Nishino, Phys. Rev. B 71, 024404 (2005)
L. Vanderstraeten, B. Vanhecke, and F. Verstraete, PRE 98 (2018)

iPEPS in 3D examples

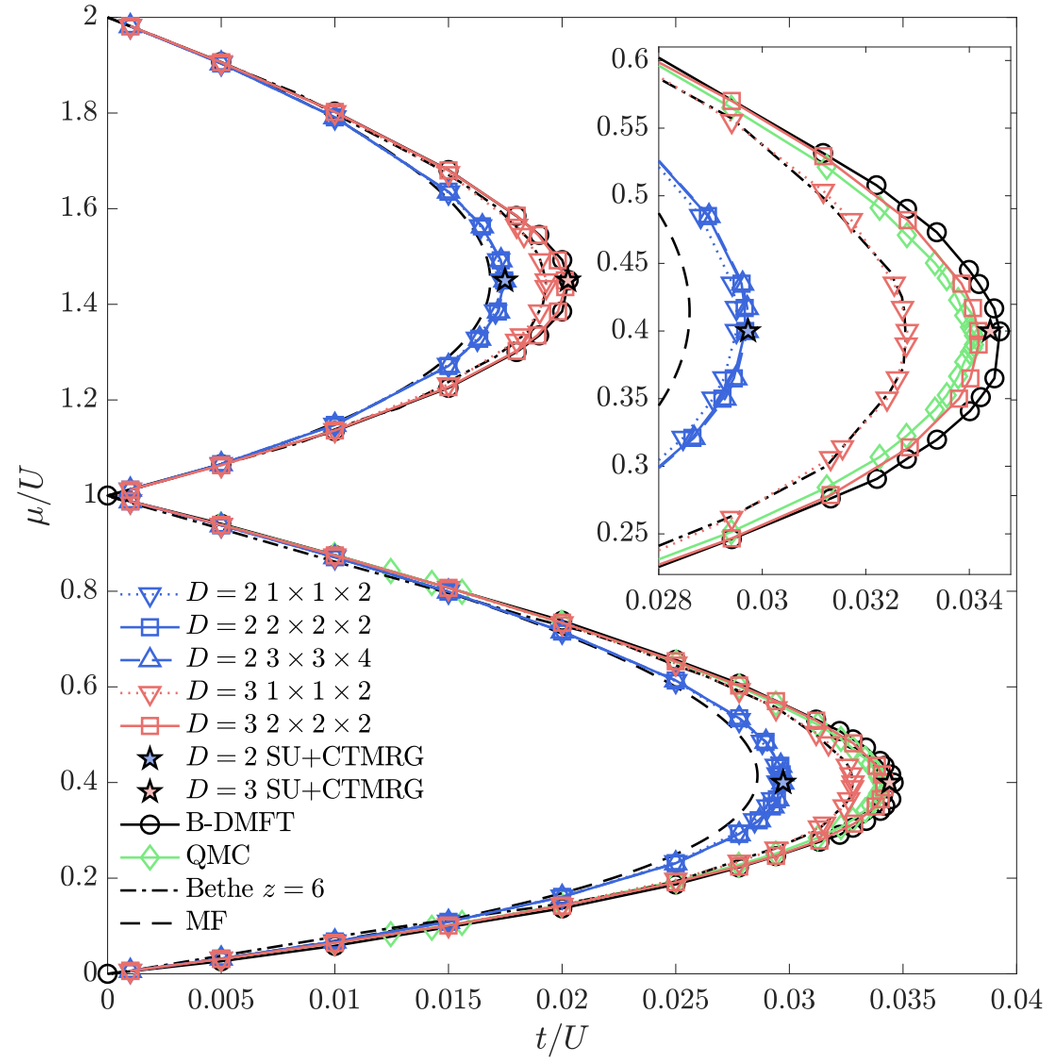
P. C. G. Vlaar, PC, PRB 103, 205137 (2021)

3D Heisenberg model





3D Bose-Hubbard model



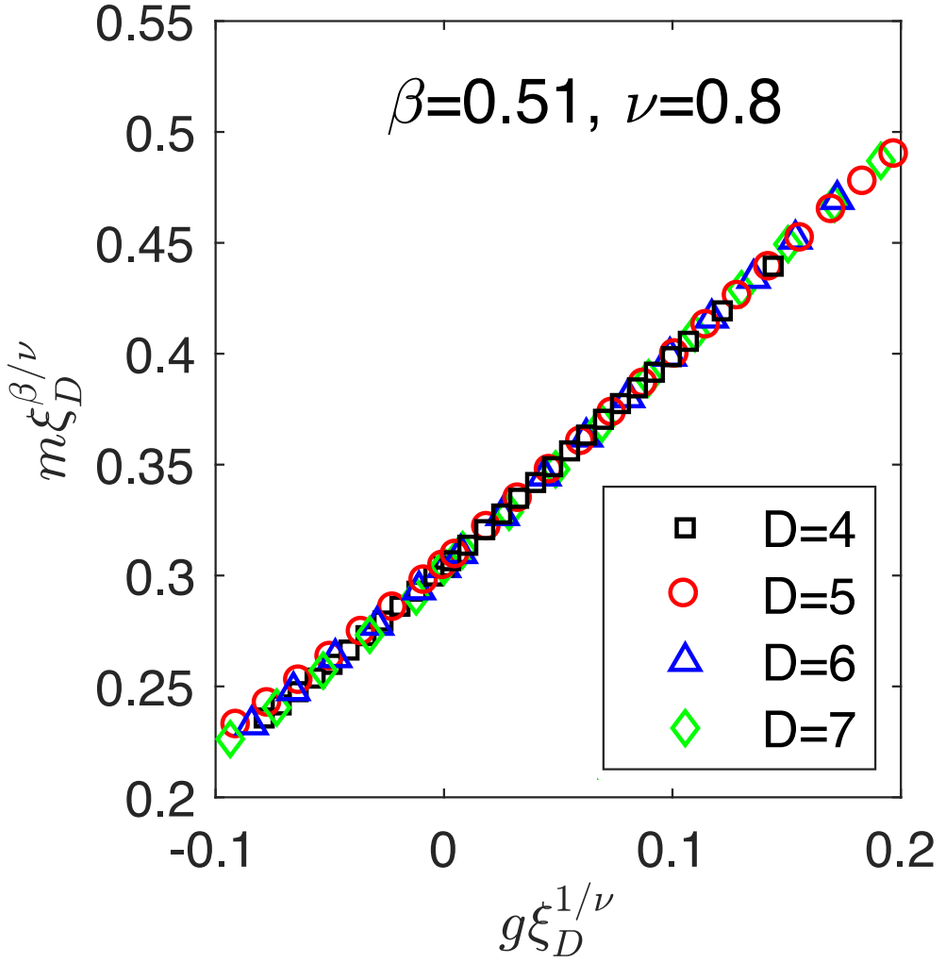
Promising also for challenging problems in 3D!

Finite correlation length scaling with iPEPS

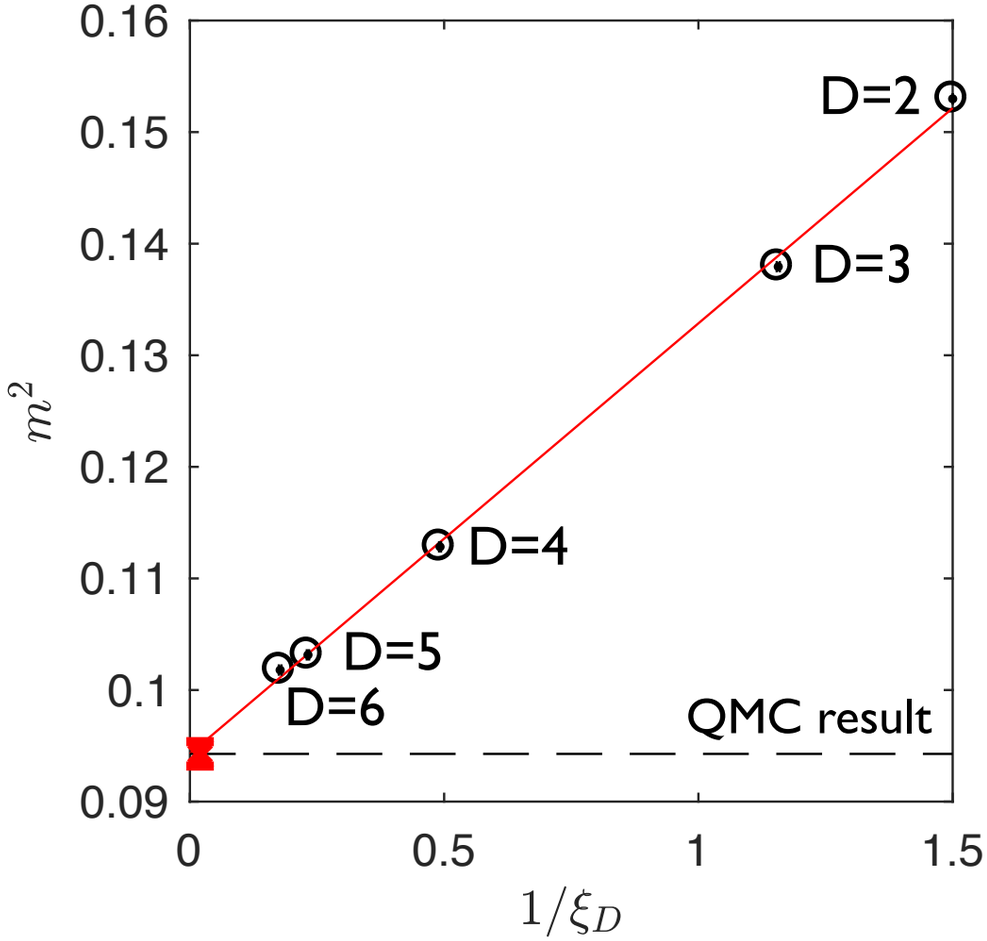
- Similar as standard finite size scaling with $L \to \xi_D$
- Systematic study of continuous quantum phase transitions
  → extract critical couplings and critical exponents

  Tagliacozzo, et al (2008); Pollmann et al (2009); Pirvu et al (2012)
  PC, Czarnik, Kapteijns & Tagliacozzo, PRX 8 (2018); Rader & Läuchli, PRX 8 (2018)

t-V honeycomb model



2D Heisenberg model



Conclusion

- ✓ **1D** tensor networks: State-of-the-art (MPS), MERA: critical systems
- ✓ **2D** tensor networks: A lot of progress in recent years!
  - ★ iPEPS has become a powerful & competitive tool for challenging problems: frustrated spin systems, fermionic systems, SU(N) systems, …
  - ★ New approaches for finite T, time evolution, critical phenomena, excitations, classification of topological order, open systems, 3D systems, …
- ✓ Still big room for improvement & extensions & new applications!

Acknowledgements:

S. Crone, B. Ponsioen, P. Vlaar, N. Chepiga, M. Peschke, J. Arias Espinoza, P. Czarnik, J. Dziarmaga, L. Vanderstraeten, J. Haegeman, F. Verstraete, F. Mila, A. Wietek, S. Wessel, B. Normand, A. Honecker, L. Weber, L. Tagliacozzo, A. Läuchli, F. Assaad