Lecture 1: tensor network states
(MPS, PEPS & iPEPS, Tree TN, MERA, 2D MERA)

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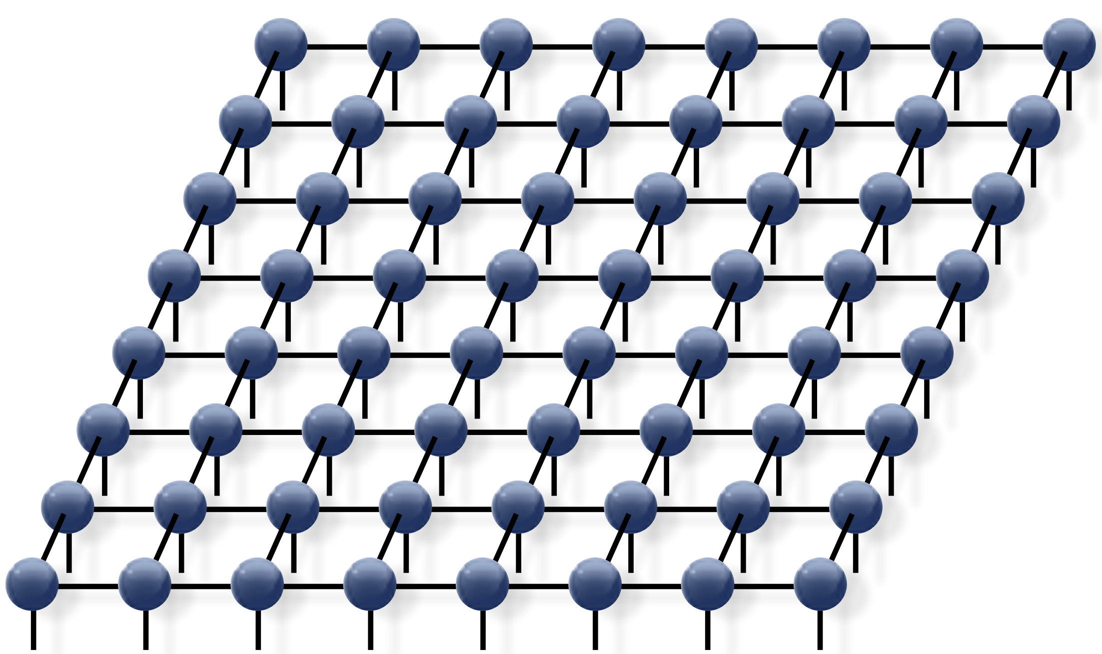
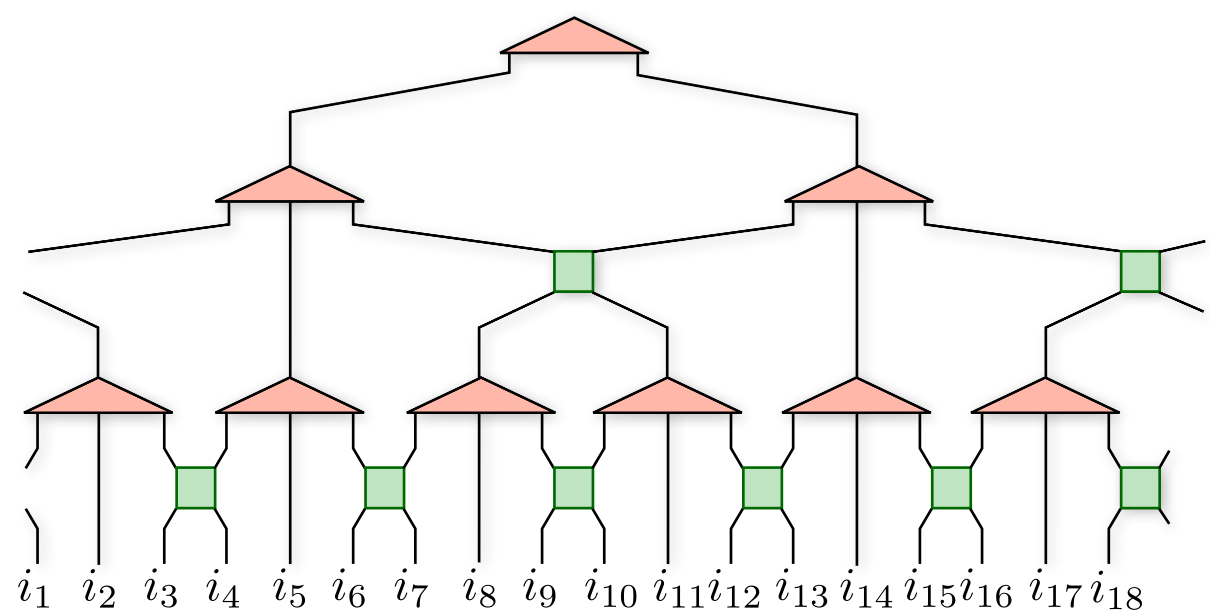




Outline

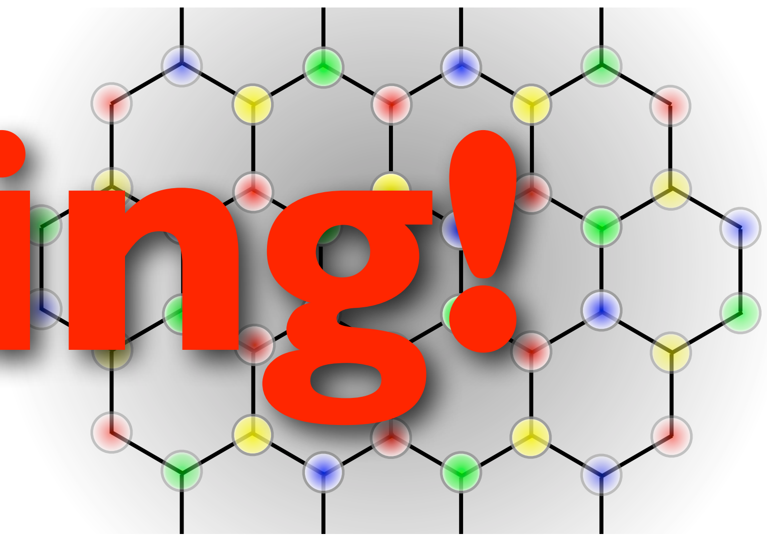
- Lecture I: tensor network states
  - *Main idea of a tensor network ansatz & area law of the entanglement entropy*
  - *MPS, PEPS & iPEPS, Tree tensor networks, MERA & 2D MERA*
  - *Classify tensor network ansatz according to its entanglement scaling*
- Lecture II: tensor network algorithms (iPEPS)
  - *Contraction & Optimization*
- Lecture III: Fermionic tensor networks
  - *Formalism & applications to the 2D Hubbard model*
  - *Other recent progress*

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))

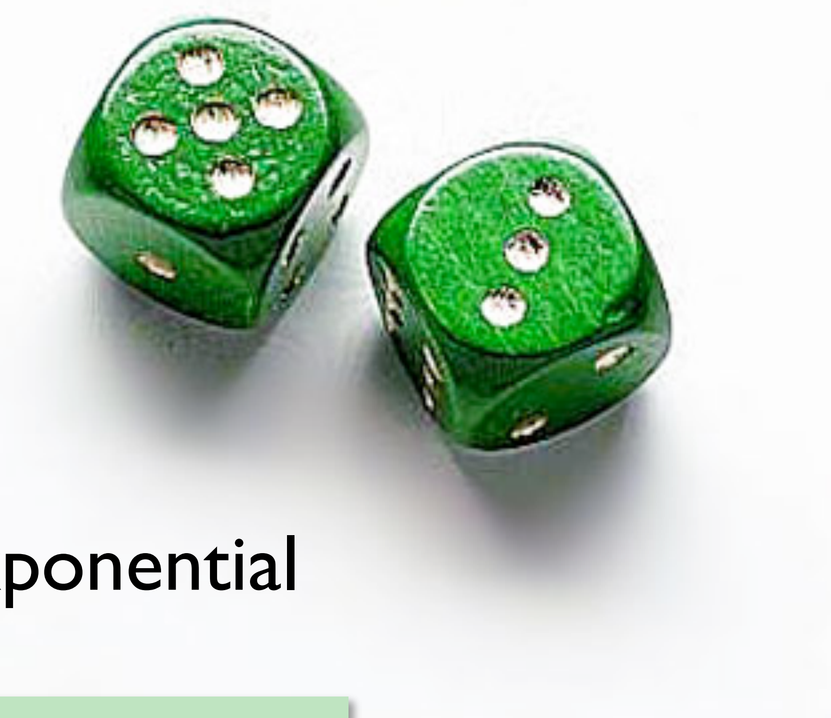
Accurate and efficient numerical simulations are essential!

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

Quantum Monte Carlo



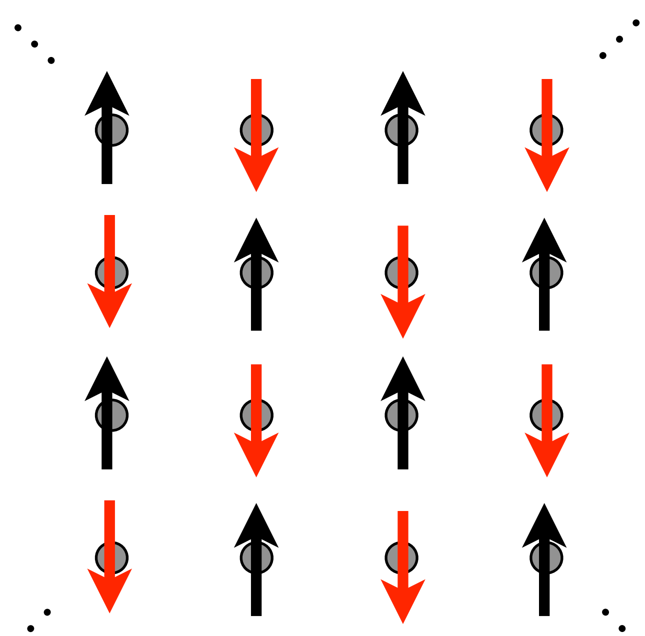
- Main idea: **Statistical sampling** of the exponentially large configuration space
- Computational cost is polynomial in N and not exponential

Very powerful for many spin and bosonic systems

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

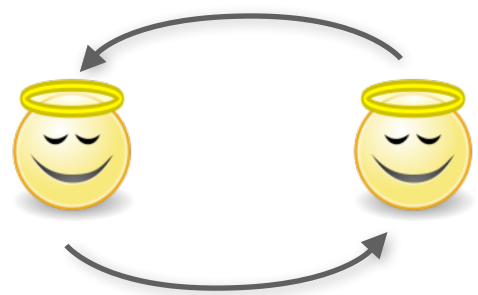
Quantum Monte Carlo & the negative sign problem

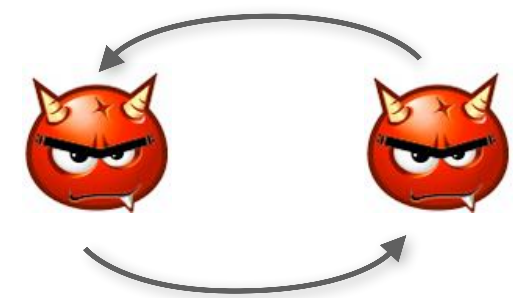
Bosons

(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!

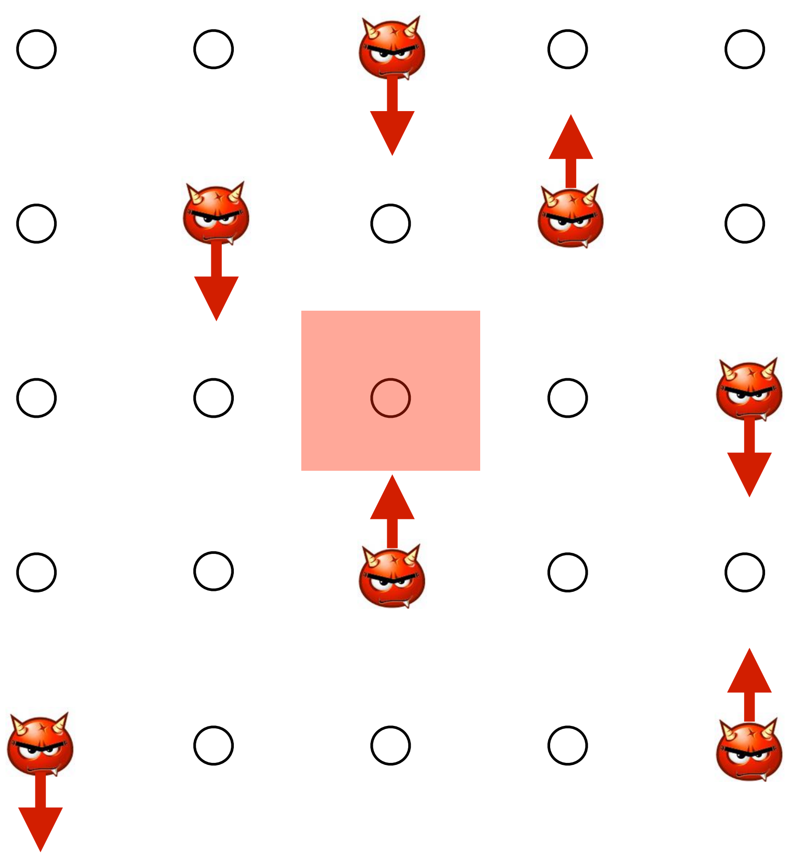
this leads to the infamous negative sign problem

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

cannot solve large systems at low temperature!

Strongly correlated fermionic systems

2D Hubbard model



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

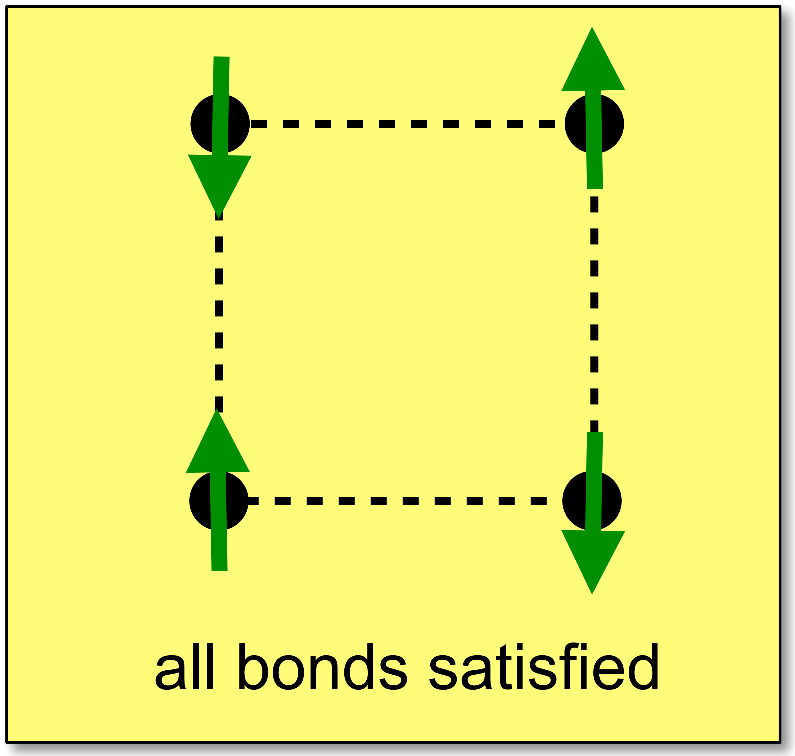
Hopping between nearest-neighbor sites

On-site repulsion between electrons with opposite spin

Is it the relevant model of high-temperature superconductors?

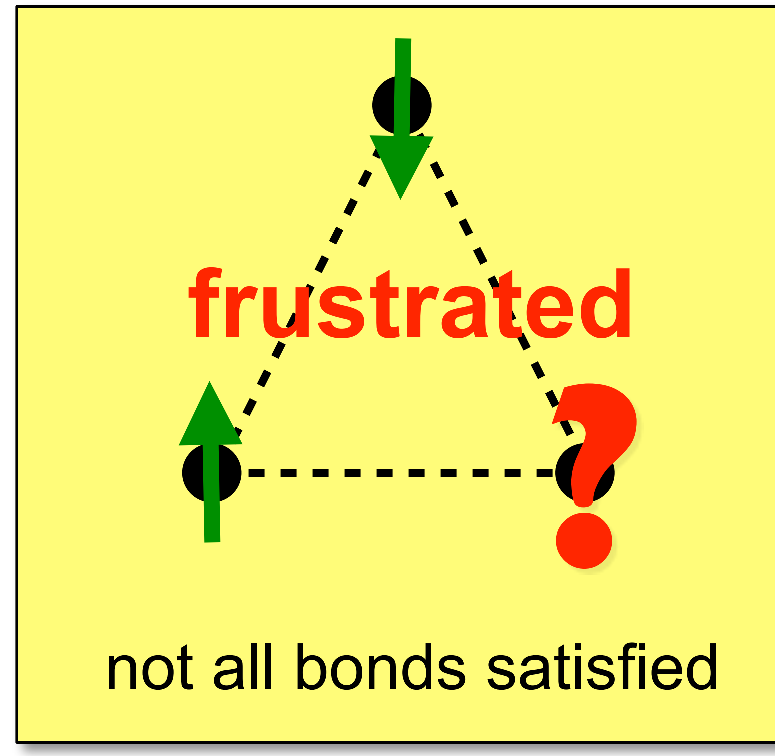
Quantum Monte Carlo & the negative sign problem

Non-frustrated spin systems



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

Frustrated spin systems



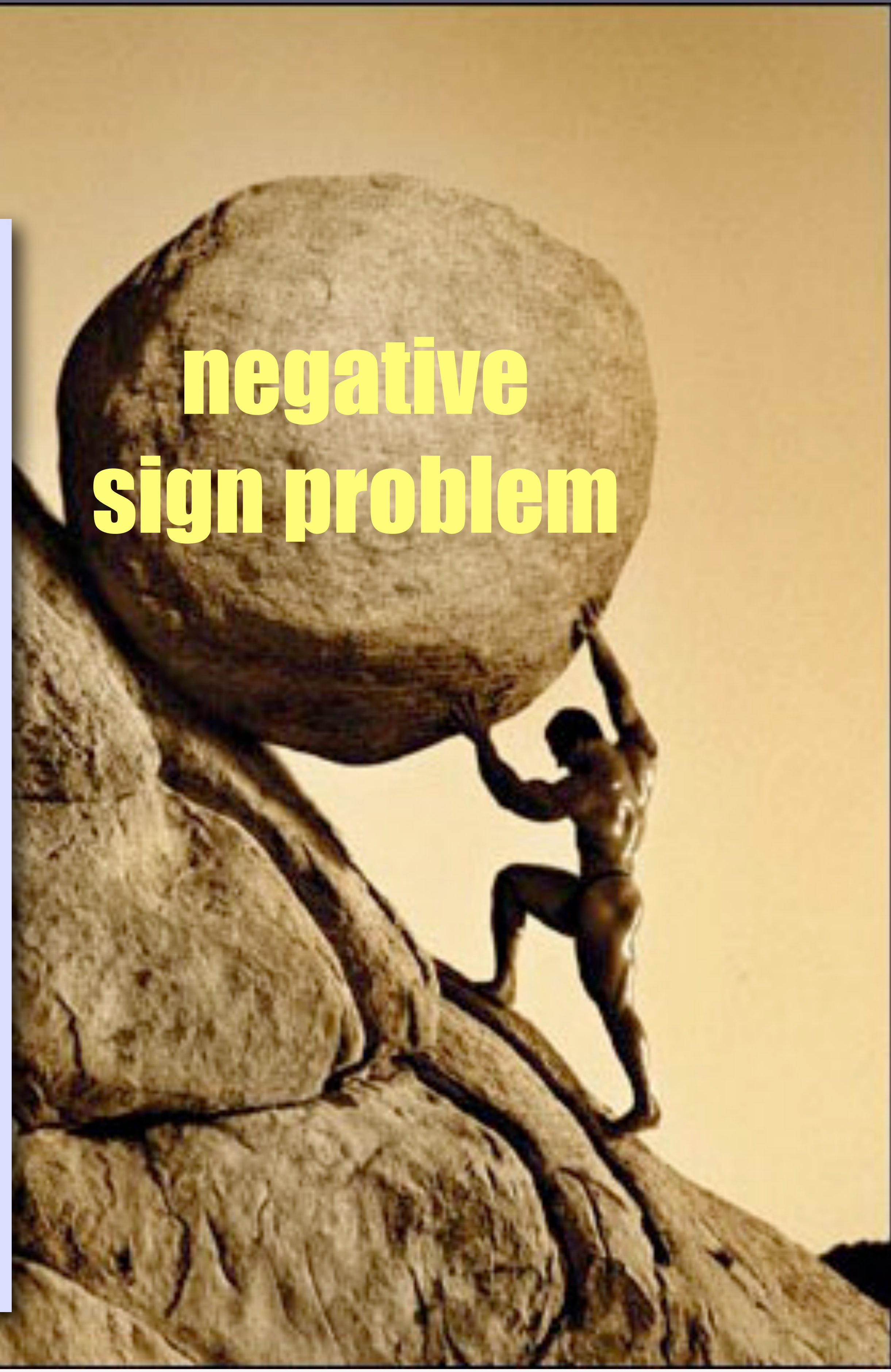
this leads to the infamous negative sign problem

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

cannot solve large systems at low temperature!

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

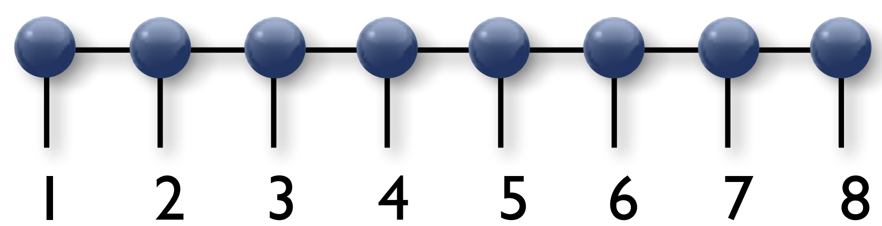
- DMFT / DCA
- Diagrammatic Monte Carlo
- **Tensor network algorithms**
- Fixed-node Monte Carlo
- Series expansion
- Density Matrix Embedding Theory
- Variational Monte Carlo
- Functional renormalization group
- Coupled-cluster methods
- …



Overview: tensor networks in 1D and 2D

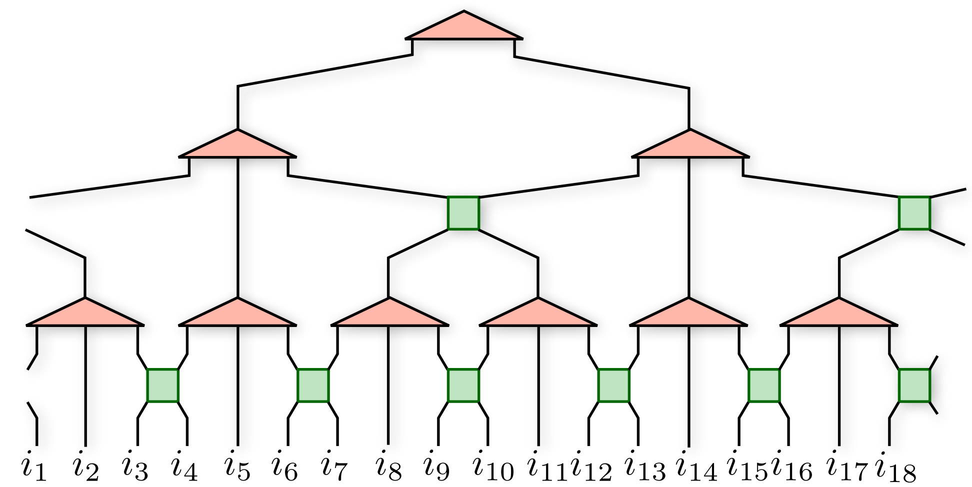
1D

MPS
Matrix-product state



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

1D MERA
Multi-scale entanglement renormalization ansatz

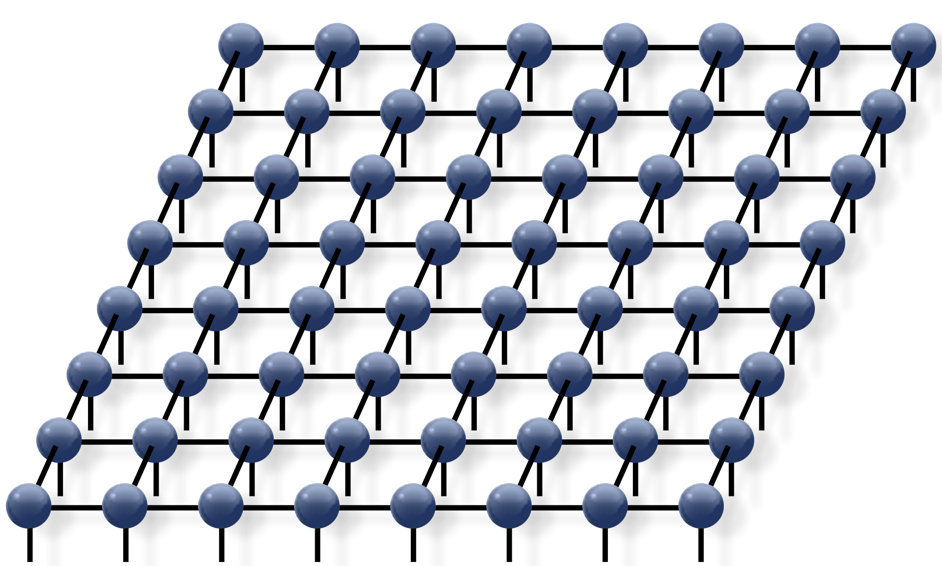


and more

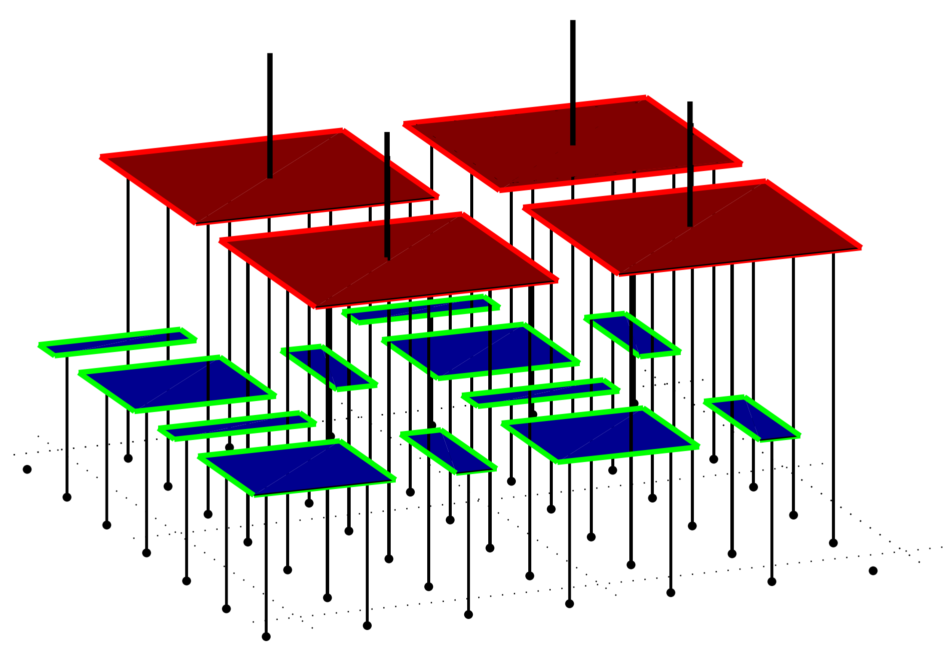
- 1D tree tensor network
- correlator product states
- ...

2D

PEPS
projected entangled-pair state



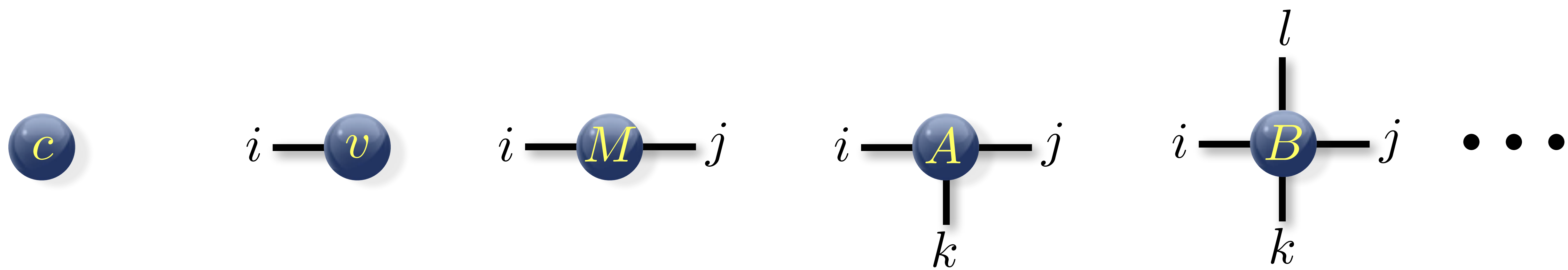
2D MERA



and more

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

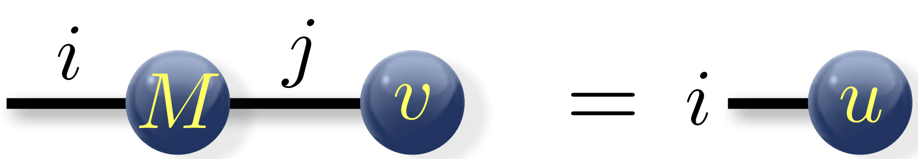
Diagrammatic notation



number	vector v_i	matrix M_{ij}	A_{ijk}	B_{ijkl}
rank-0 tensor	rank-1 tensor	rank-2 tensor	rank-3 tensor	rank-4 tensor

★ We don't need to write down formulas with tensors with many indices!

Example 1:

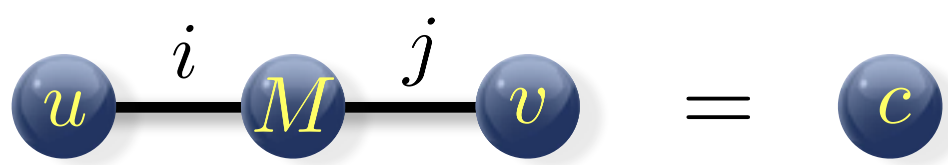


$$\sum_j M_{ij} v_j = u_i$$

★ Connected lines: sum over corresponding indices!

Diagrammatic notation

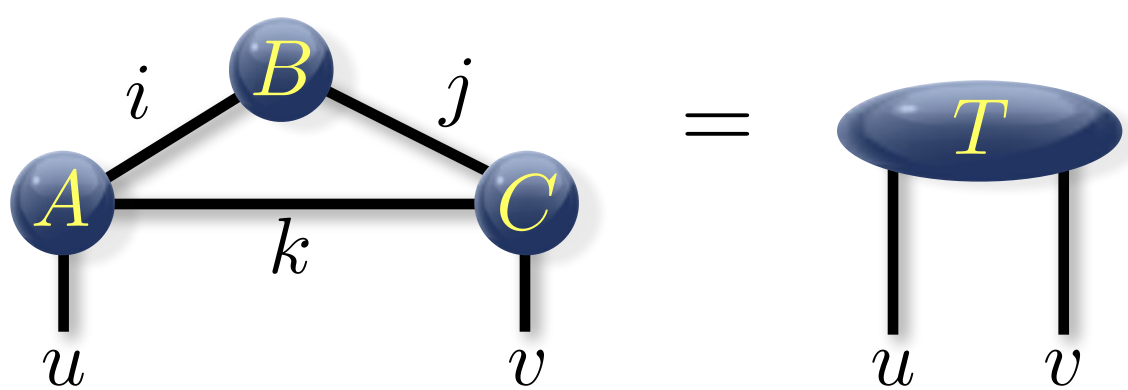
Example 2:



$$\sum_{ij} u_i M_{ij} v_j = c$$

★ sum over all connected indices: **contraction** of a tensor network

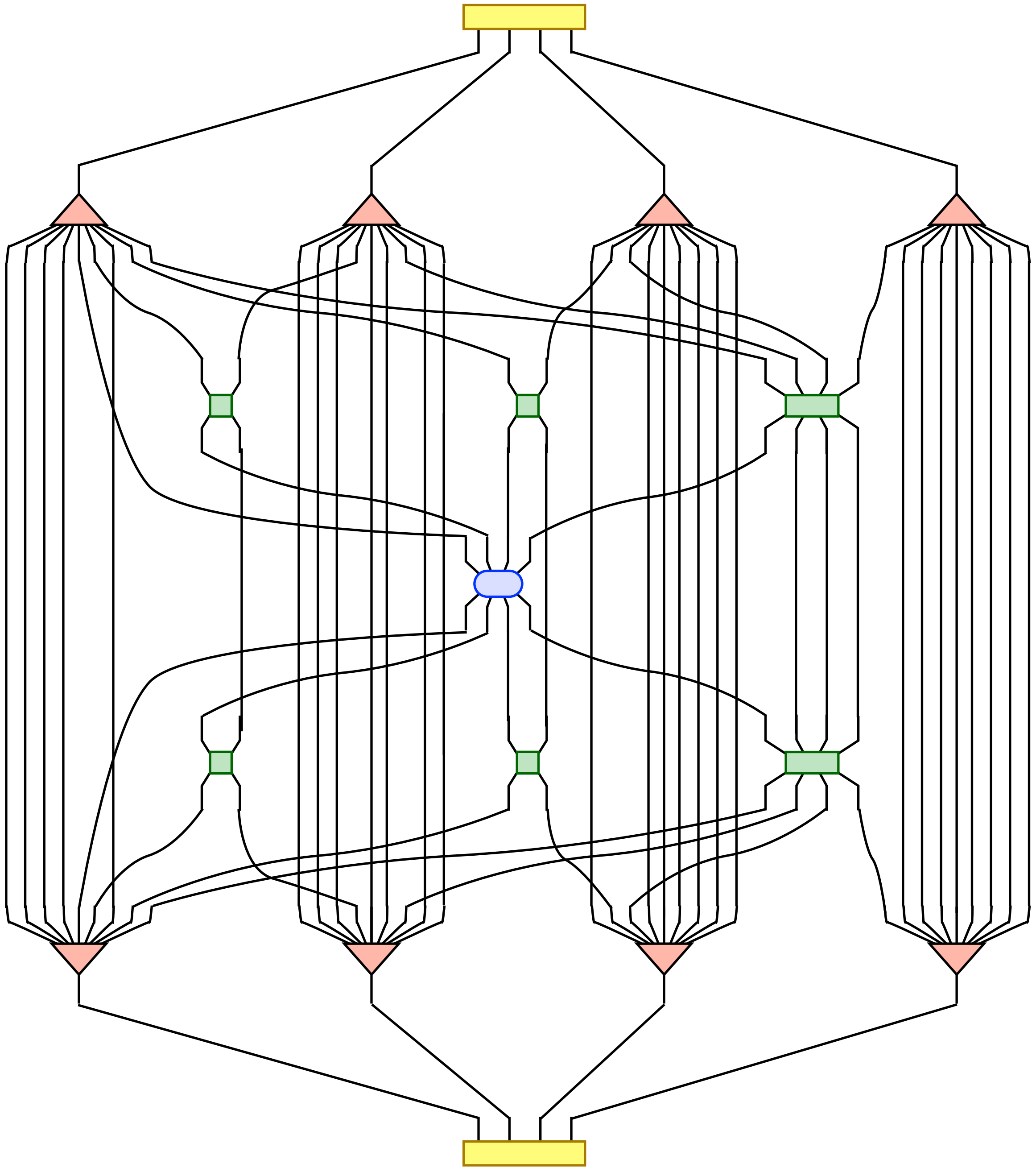
Example 3:



$$\sum_{ijk} A_{uik} B_{ij} C_{vjk} \quad = \quad T_{uv}$$

★ The rank of the resulting tensor corresponds to the number of open legs in the network

Diagrammatic notation



- ★ Hard to write down with all indices...
- ★ We know the result is going to be a number

Introduction to tensor networks

➡ **Aim**: Efficient representation of quantum many-body states

$\mathbb{V}$: local Hilbert space e.g. $\{|\uparrow\rangle, |\downarrow\rangle\}$

Lattice with N sites: 1 2 3 4 5 .... N-1 N

Full Hilbert space: $\mathbb{V}\otimes\mathbb{V}\otimes\mathbb{V}\otimes\mathbb{V}\otimes\mathbb{V}\otimes \dots \otimes\mathbb{V}\otimes\mathbb{V}$

dimension 2^N grows exponentially with N

Hamiltonian: $\hat{H} = \sum_{\langle ij\rangle} \hat{h}_{ij}$ sum of local terms

Represent the ground state: $|\Psi\rangle = \sum_{\substack{i_1 i_2 \dots i_N \\ i_k \in \{\uparrow,\downarrow\}}} \Psi_{i_1 i_2 \dots i_N} |i_1 \otimes i_2 \otimes \cdots \otimes i_N\rangle$

2^N coefficients

Complexity: **~exp(N) many numbers ⟶ inefficient!**

Tensor network ansatz for a wave function

Lattice: ● 1 ● 2 ● 3 ● 4 ● 5 ● 6

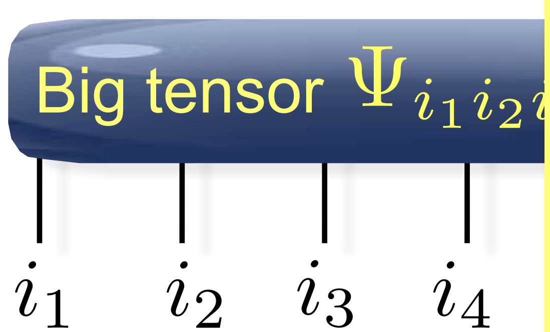
2 basis states per site: $\{|\uparrow\rangle, |\downarrow\rangle\}$

2^6 basis states

2^6 coefficients

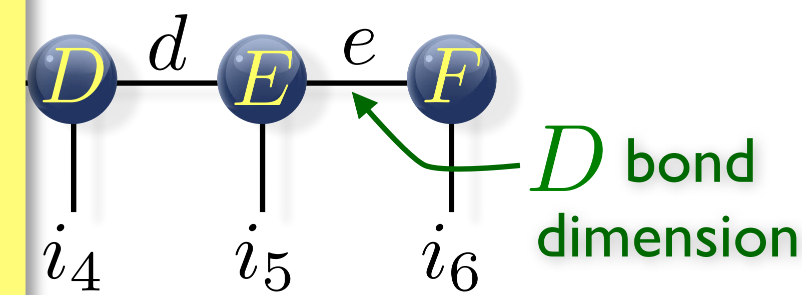
State: $|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4 i_5 i_6} \Psi_{i_1 i_2 i_3 i_4 i_5 i_6} |i_1 \otimes i_2 \otimes i_3 \otimes i_4 \otimes i_5 \otimes i_6\rangle$

Tensor/multidimensi



Why is this possible??

atrix product state (**MPS**)

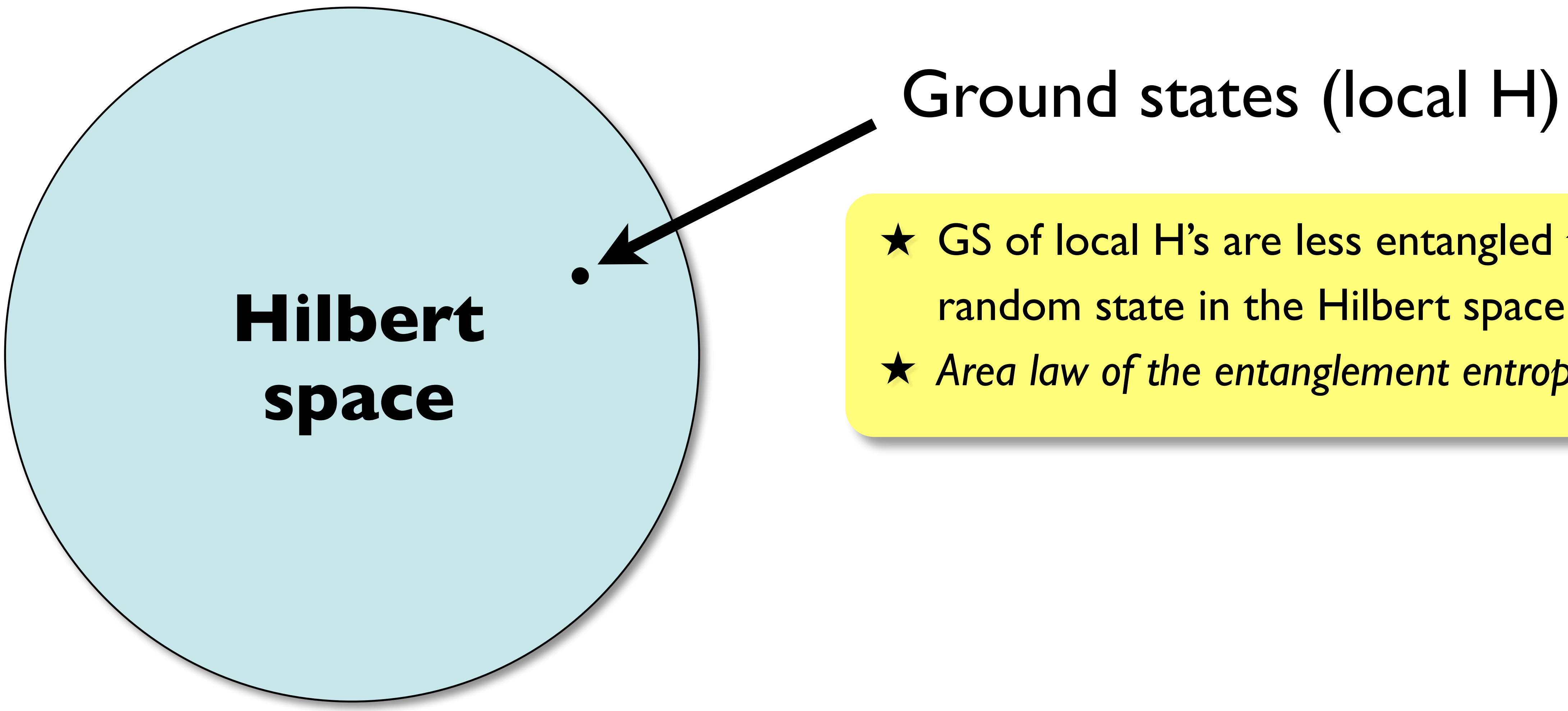


$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6} \approx \sum_{abcde} A^{a}_{i_1} B^{ab}_{i_2} C^{bc}_{i_3} D^{cd}_{i_4} E^{de}_{i_5} F^{e}_{i_6} = \tilde{\Psi}_{i_1 i_2 i_3 i_4 i_5 i_6}$$

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

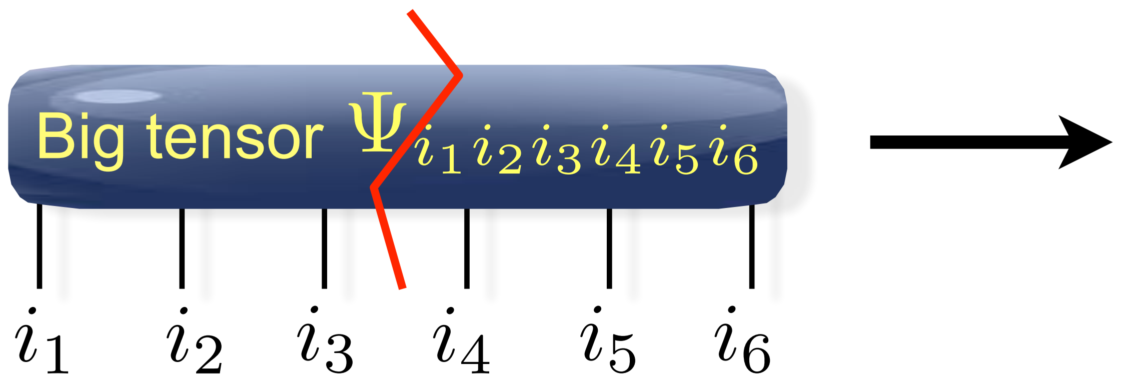
Efficient representation!

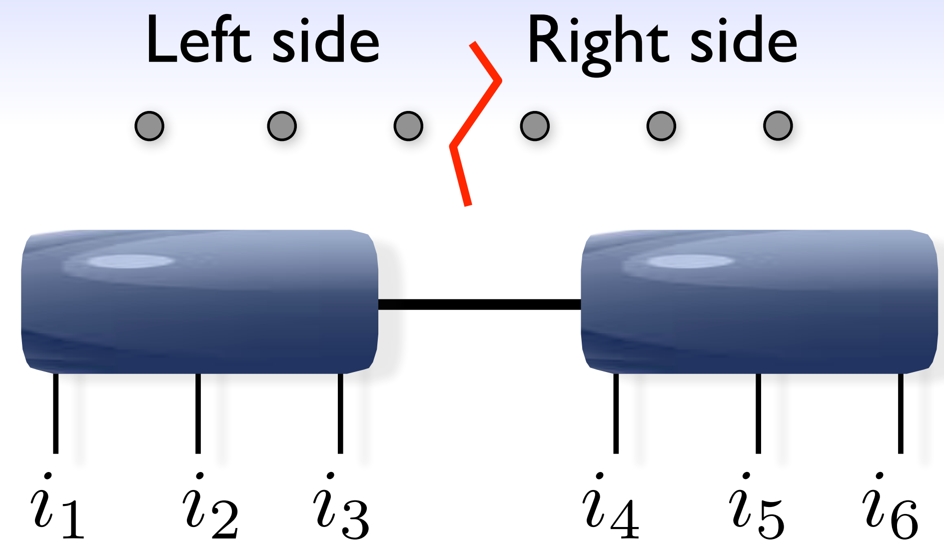
"Corner" of the Hilbert space

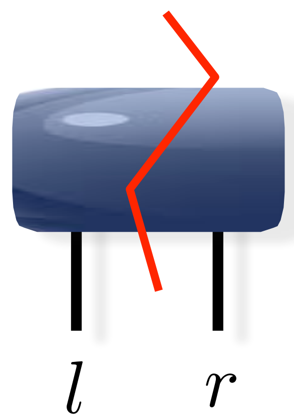


- ★ GS of local H's are less entangled than a random state in the Hilbert space
- ★ *Area law of the entanglement entropy*

Splitting in the middle

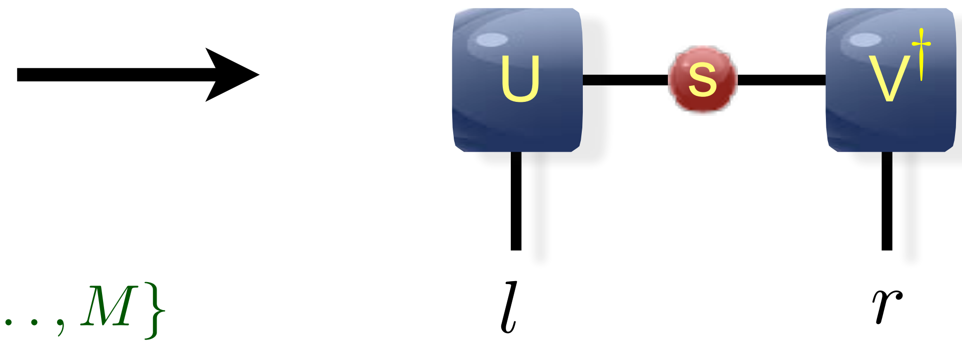






$l, r \in \{1, \ldots, M\}$

$M = 2^{N/2}$



Singular value decomposition

$$\Psi = U s V^\dagger$$

$$s_{kk} \geq 0$$

diagonal matrix!

$$\Psi_{lr} = \sum_k U_{lk} s_{kk} V^*_{rk}$$

$$|\Psi\rangle = \sum_{lr} \Psi_{lr} |l\rangle |r\rangle = \sum_{lr} \sum_k U_{lk} s_{kk} V^*_{rk} |l\rangle |r\rangle$$

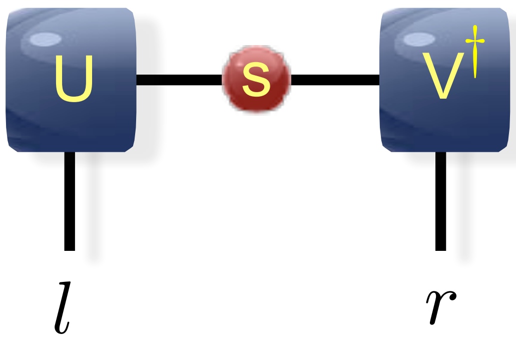
$$= \sum_k s_{kk} |u_k\rangle |v_k\rangle$$

Schmidt decomposition

How many relevant singular values?

$$|\Psi\rangle = \sum_{k}^{M} s_{kk} |u_k\rangle |v_k\rangle$$

how many non-zero singular values?



★ Special cases:

$$s_{11} = 1, \quad s_{kk} = 0 \quad \text{for} \quad k > 1$$

$$|\Psi\rangle = 1|u_1\rangle|v_1\rangle$$

Product state

$$s_{11} = \frac{1}{\sqrt{2}}, \quad s_{22} = \frac{1}{\sqrt{2}}, \quad s_{kk} = 0 \quad \text{for} \quad k > 2$$

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|u_1\rangle|v_1\rangle + \frac{1}{\sqrt{2}}|u_2\rangle|v_2\rangle$$

Entangled state

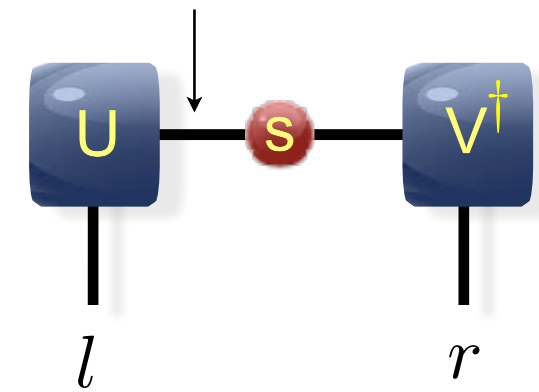
$$s_{kk} = \frac{1}{\sqrt{M}}, \quad \text{for all } k$$

Maximally entangled state

How many relevant singular values?

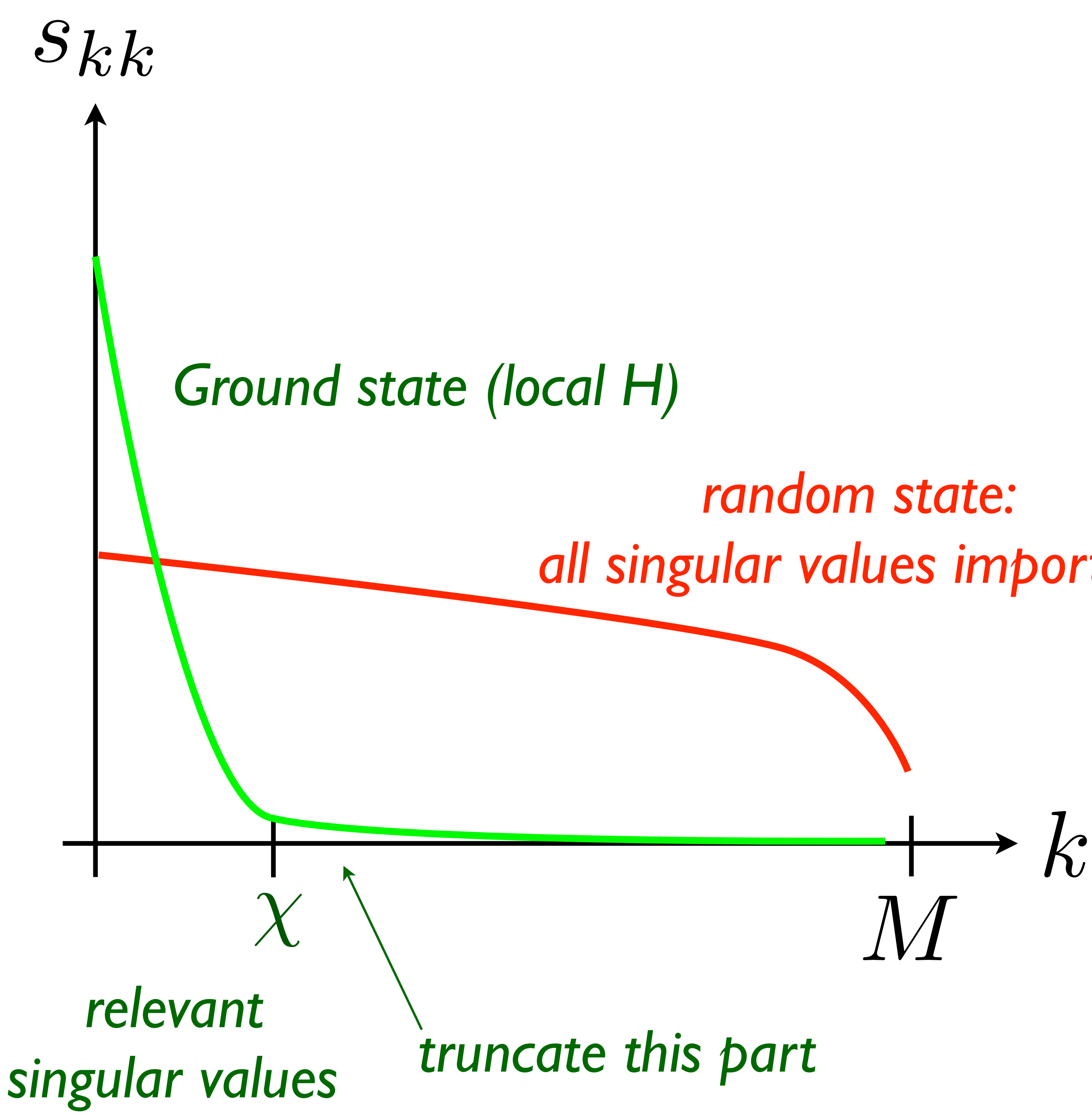
bond dimension

$D = \chi$



$$|\Psi\rangle = \sum_{k}^{M} s_{kk} |u_k\rangle |v_k\rangle$$

*how many **relevant** singular values?*



$$|\Psi\rangle \approx |\tilde{\Psi}\rangle = \sum_{k}^{\chi} s_{kk} |u_k\rangle |v_k\rangle$$

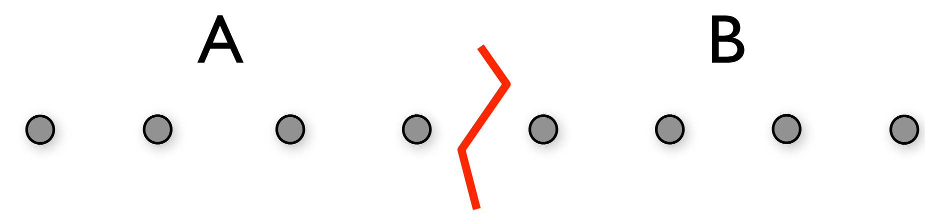
keeping the χ largest singular values minimizes the error

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

KEY IDEA OF DMRG!

Reduced density matrix

$$|\Psi\rangle = \sum_k^M s_{kk} |u_k\rangle |v_k\rangle$$



★ Reduced density matrix of left side: *describes system on the left side*

$$\rho_A = \mathrm{tr}_B[\rho] = \mathrm{tr}_B[|\Psi\rangle\langle\Psi|] = \sum_k \lambda_k |u_k\rangle\langle u_k| \qquad \lambda_k = s_{kk}^2 \qquad \textit{probability}$$

★ **Entanglement entropy:** $S(A) = -\mathrm{tr}[\rho_A \log \rho_A] = -\sum_k \lambda_k \log \lambda_k$

- Product state: $S(A) = -1 \log 1 = 0$

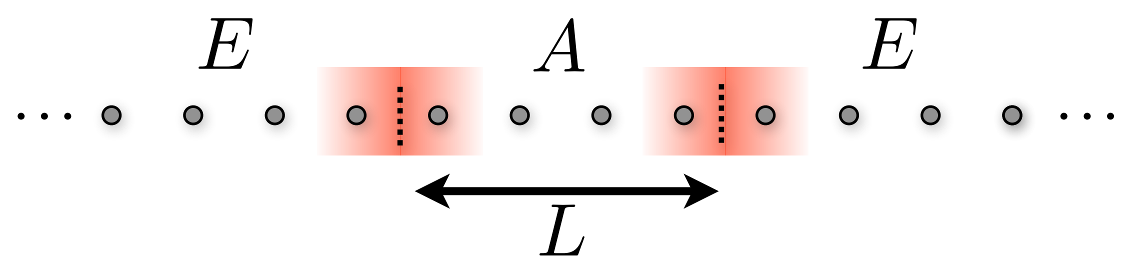
⋮

- Maximally entangled state: $S(A) = -\sum_k \frac{1}{M} \log \frac{1}{M} = logM$

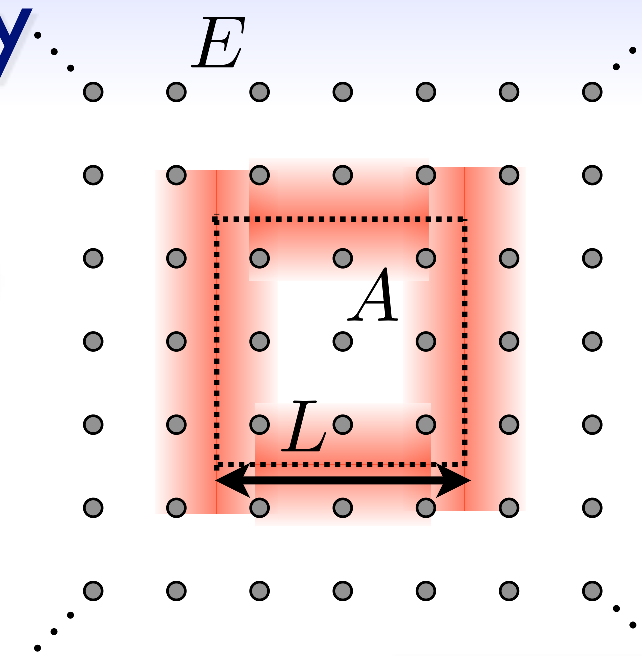
How large is S in a ground state? How does it ***scale*** *with system size?*

Area law of the entanglement entropy

1D



2D



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

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

General (random) state

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

Ground state (local Hamiltonian)

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

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

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

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

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

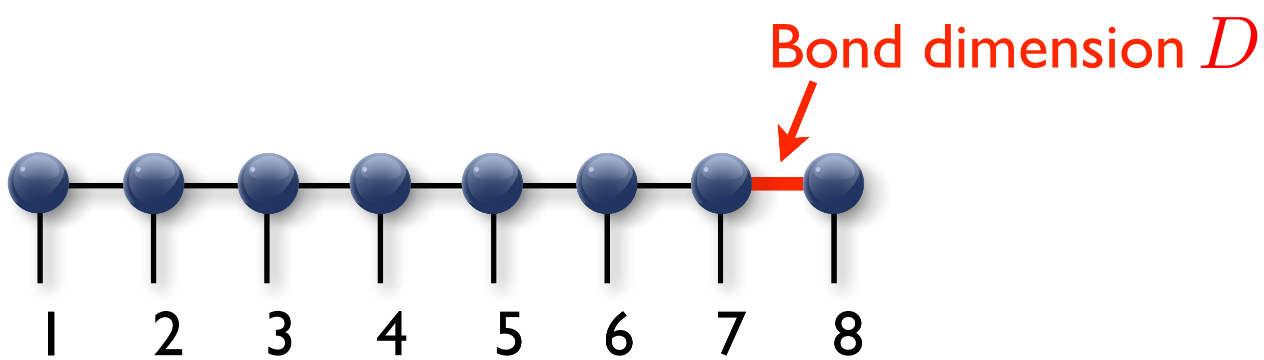
2D $S(L) \sim \alpha L$ $\chi \sim \exp(\alpha L)$

MPS & PEPS

1D

MPS

Matrix-product state



Physical indices (lattices sites)

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

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

Östlund, Rommer, PRL 75, 3537 (1995)

✓ Reproduces area-law in 1D

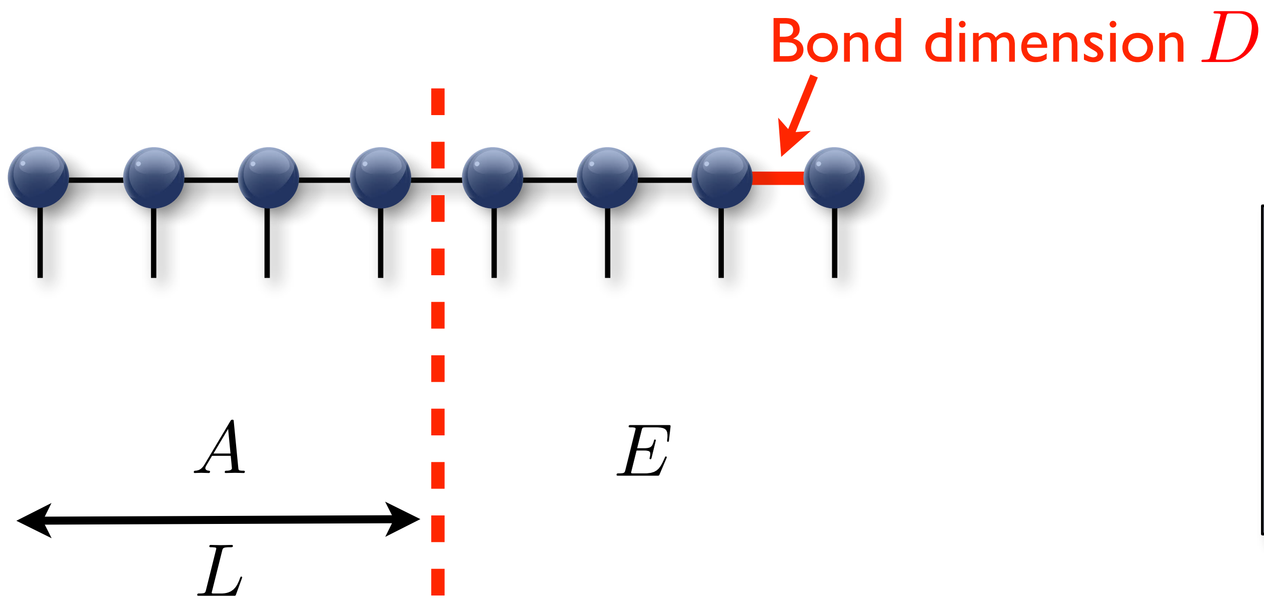
$$S(L) = const$$

MPS & PEPS

1D

MPS

Matrix-product state



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

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

✓ Reproduces area-law in 1D

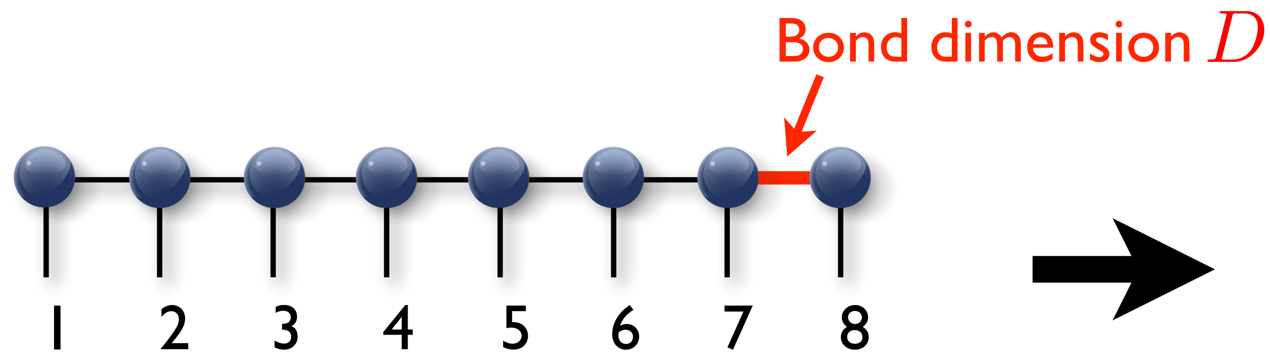
$$S(L) = const$$

MPS & PEPS

1D

MPS

Matrix-product state



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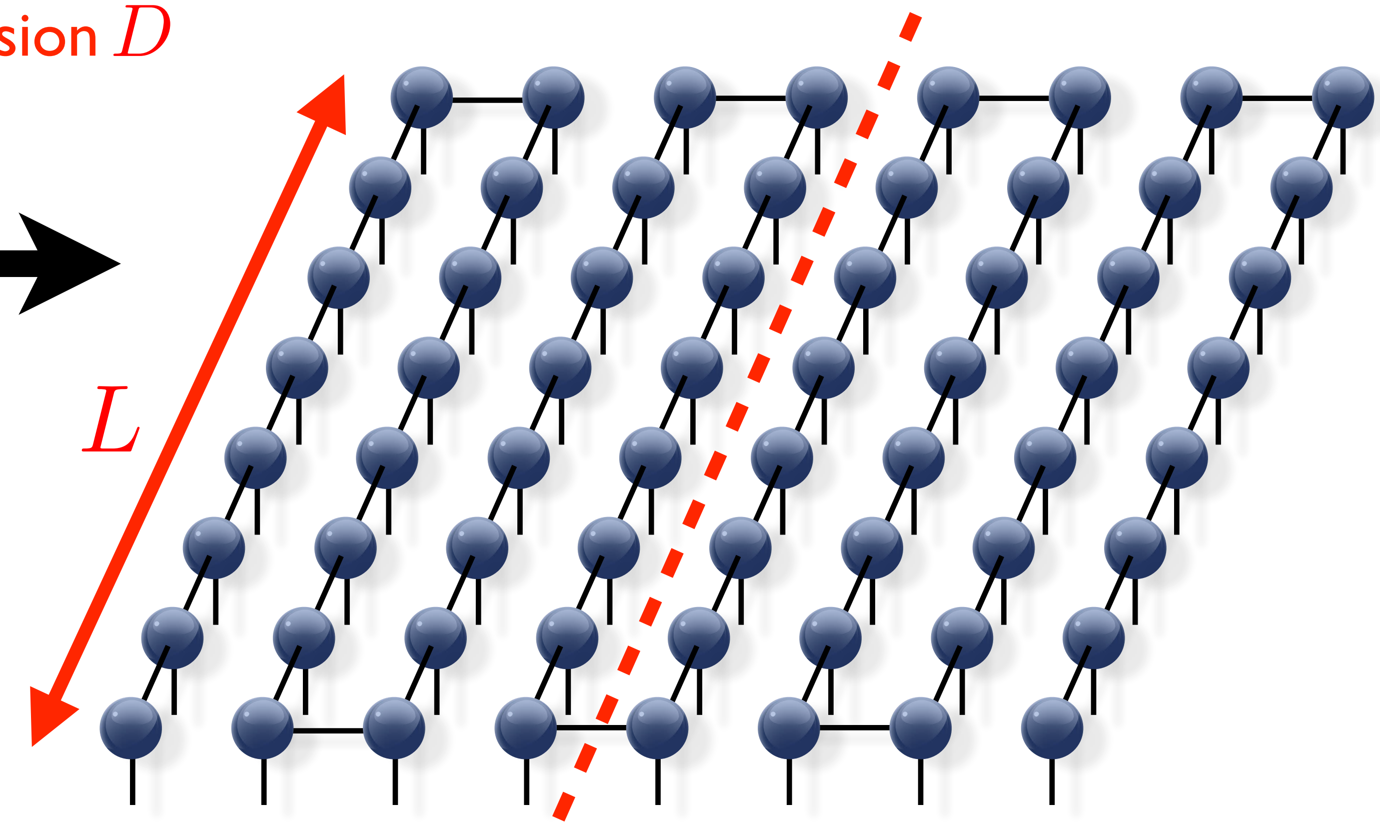
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

can we use an MPS?



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

$$S(L) \sim L$$

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

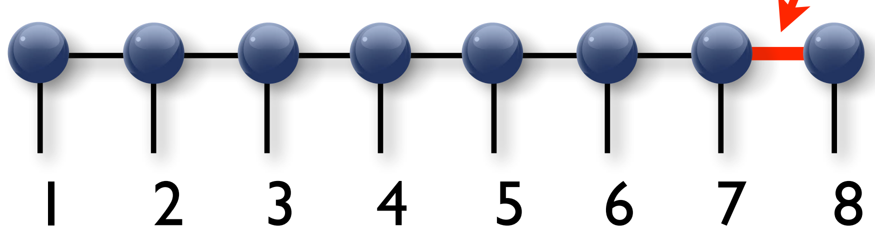
MPS & PEPS

1D

MPS

Matrix-product state

Bond dimension D



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✓ Reproduces area-law in 1D

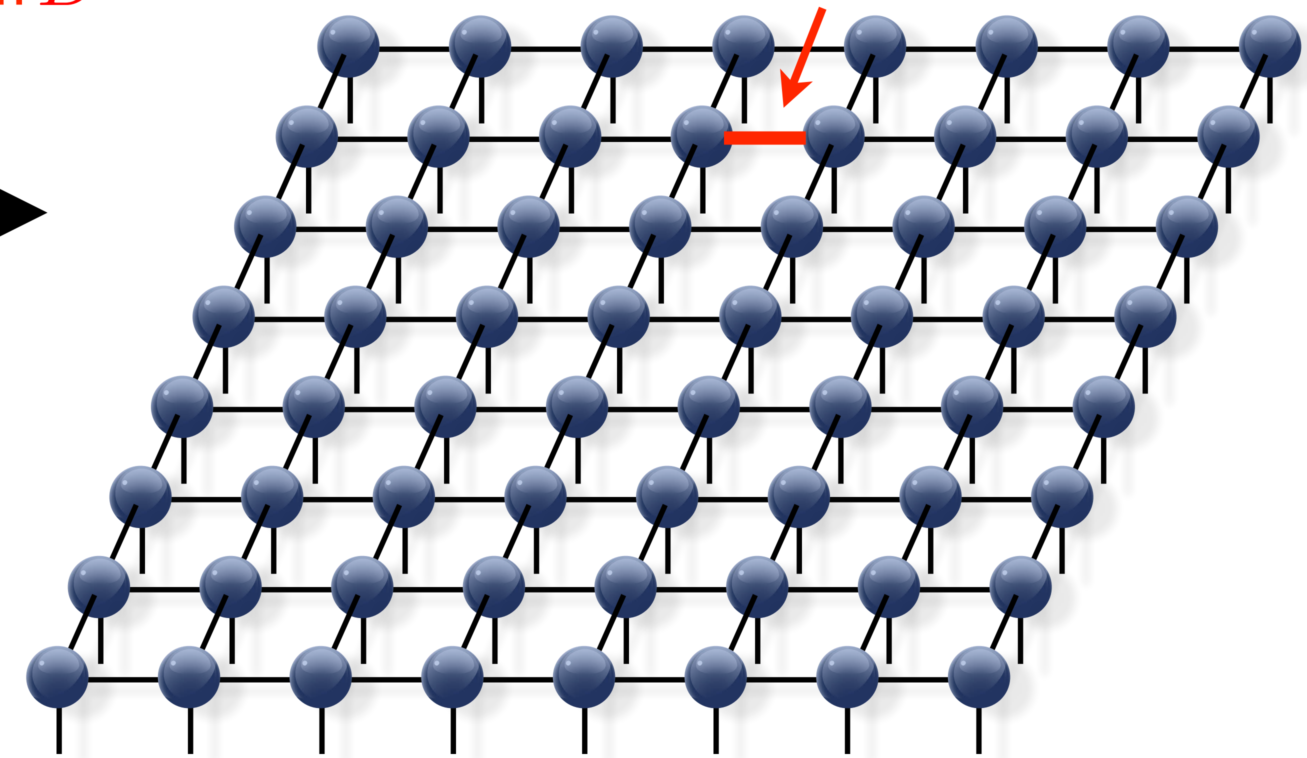
$$S(L) = const$$

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)

Bond dimension D

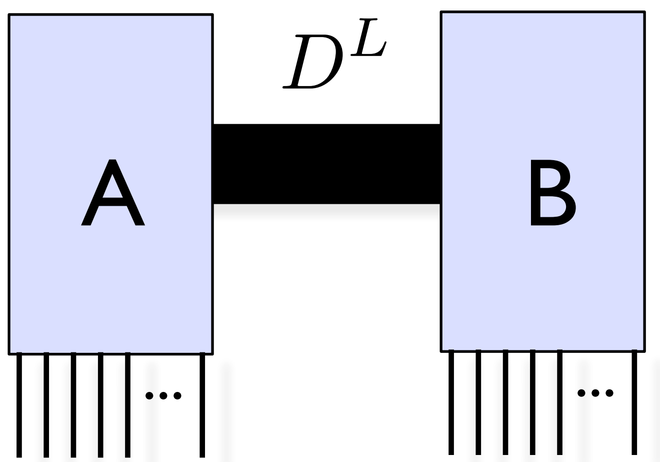


F. Verstraete, J. I. Cirac, cond-mat/0407066
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

✓ Reproduces area-law in 2D

$$S(L) \sim L$$

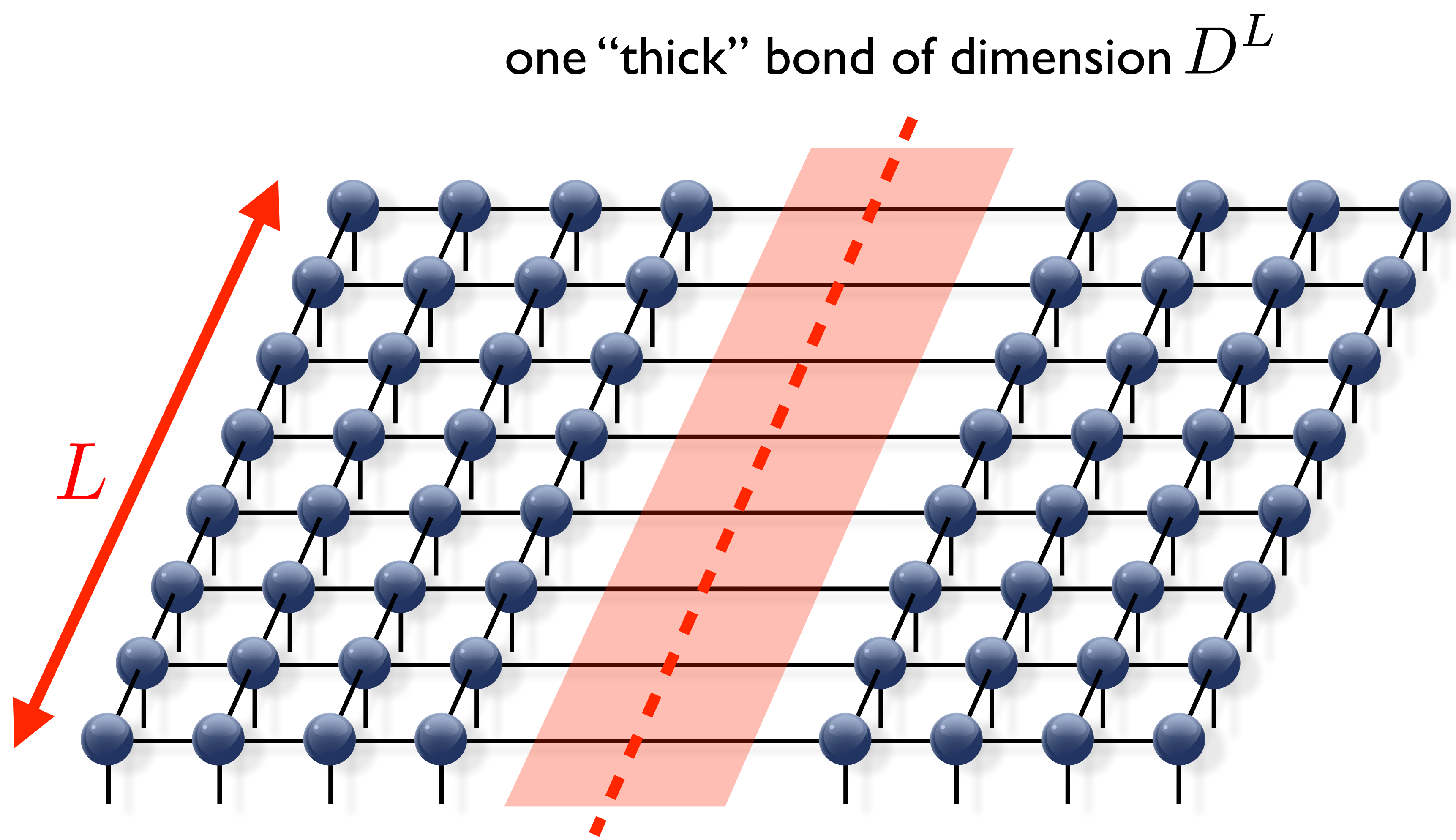
PEPS: Area law



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

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

The number of cuts scales with the cut length



✓ Reproduces area-law in 2D

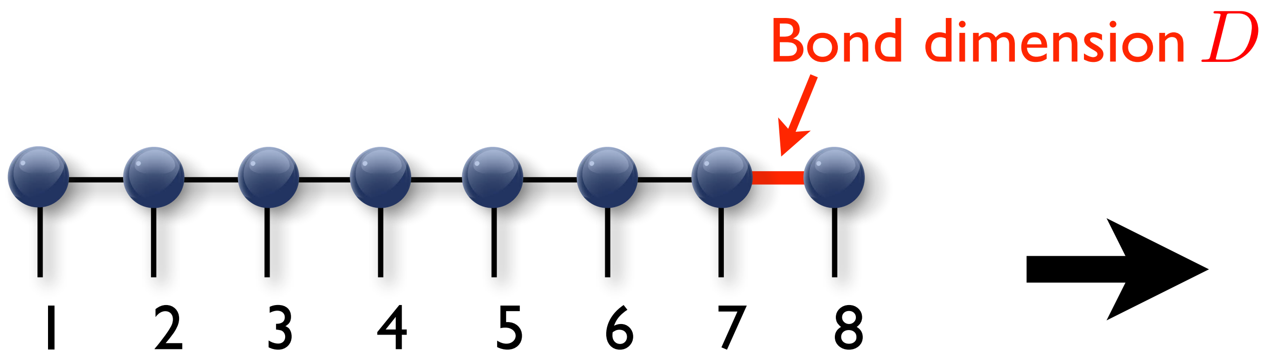
$$S(L) \sim L$$

MPS & PEPS

1D

MPS

Matrix-product state



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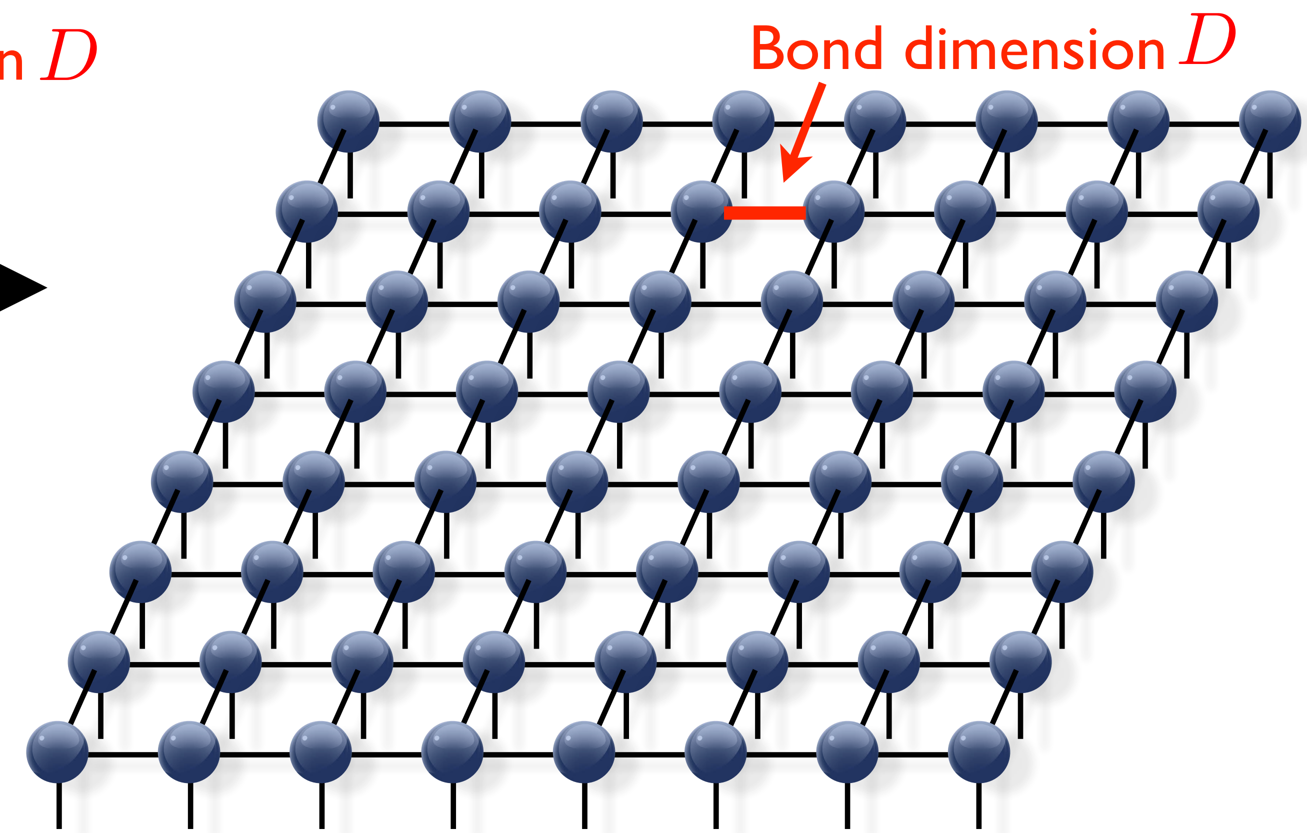
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



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

✓ Reproduces area-law in 2D

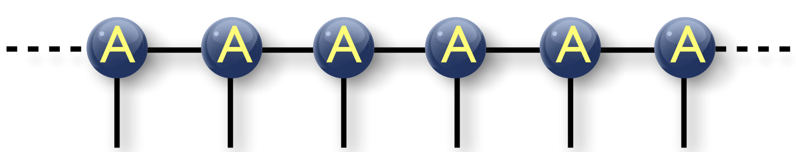
$$S(L) \sim L$$

Infinite PEPS (iPEPS)

1D

iMPS

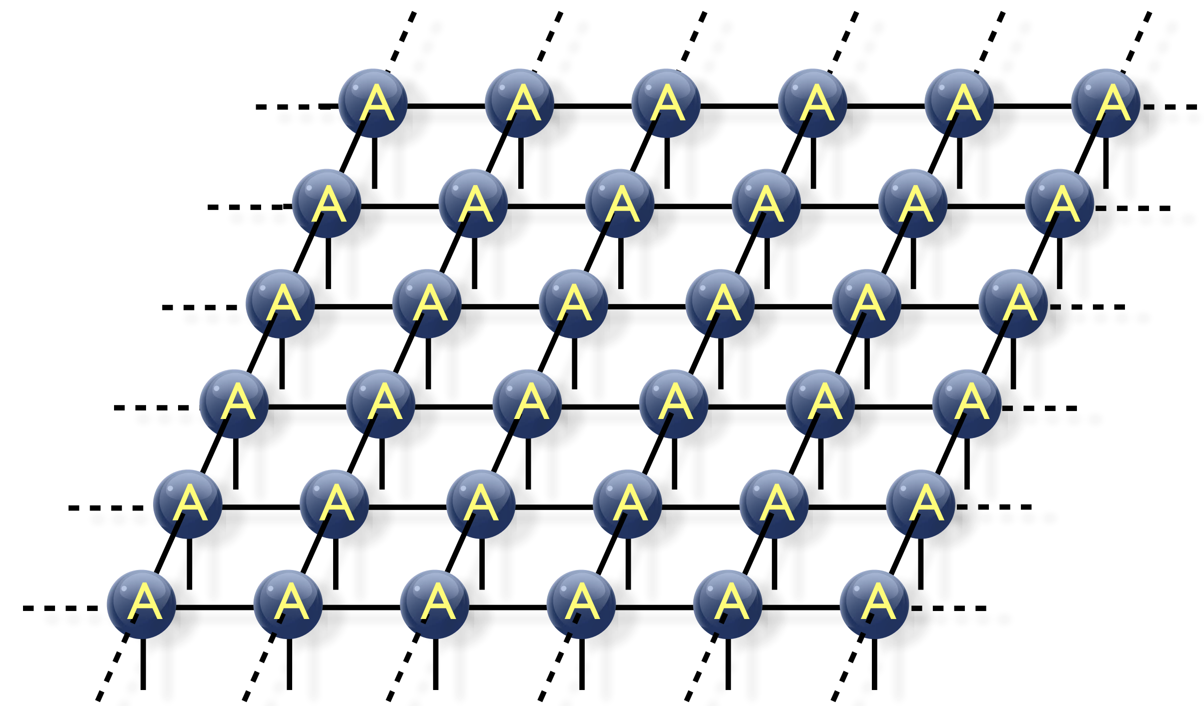
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

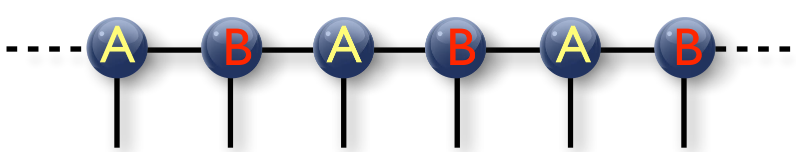
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

Infinite PEPS (iPEPS)

1D

iMPS

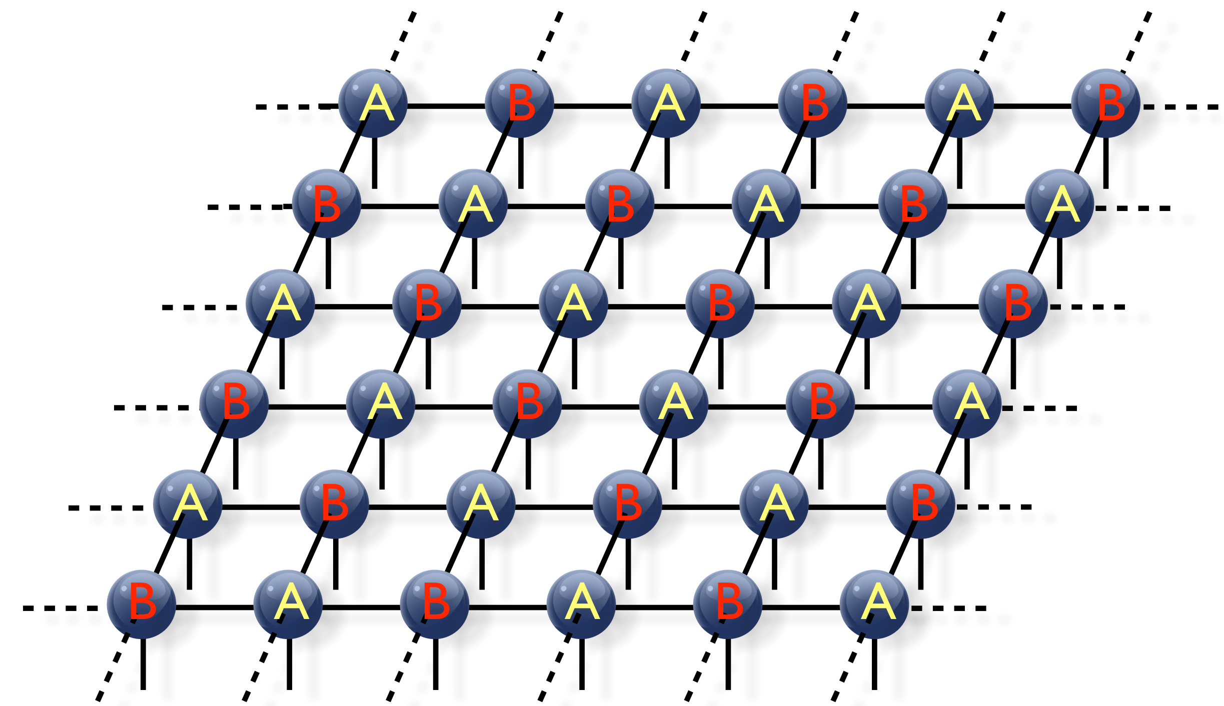
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

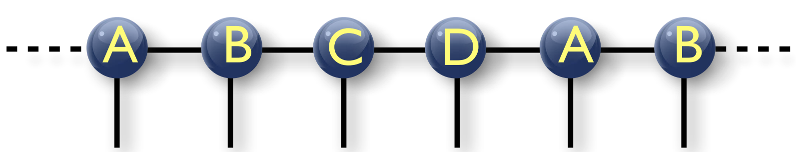
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

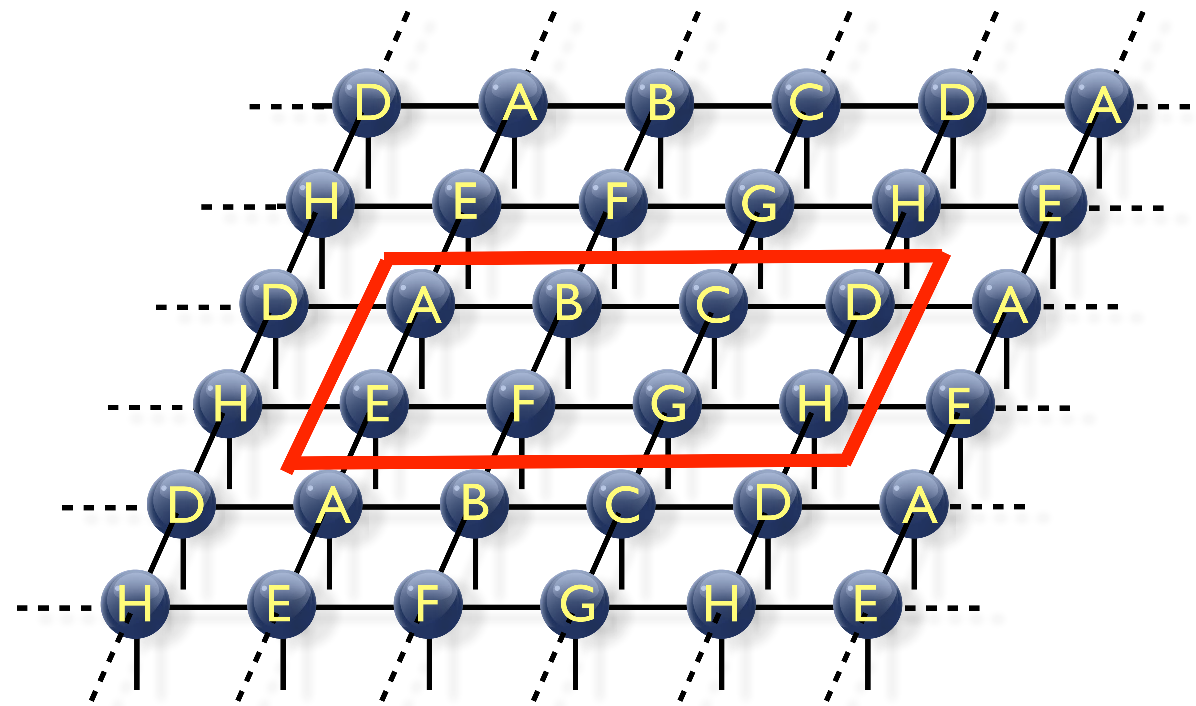
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



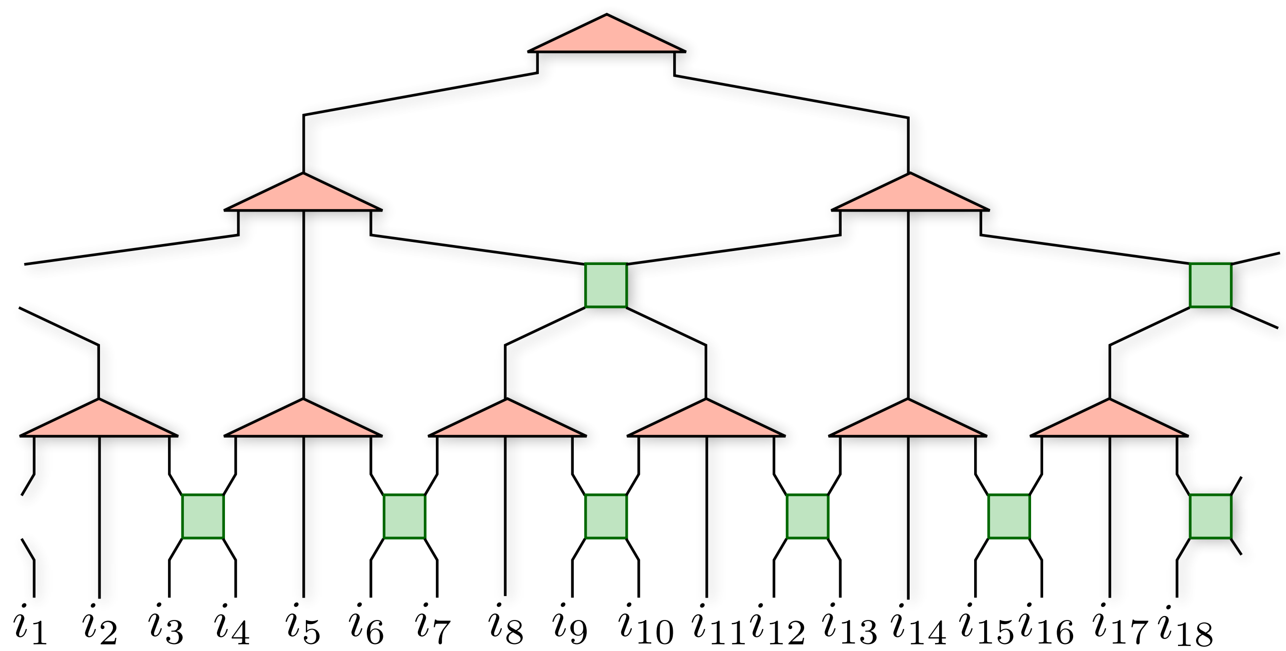
here: 4x2 unit cell

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

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

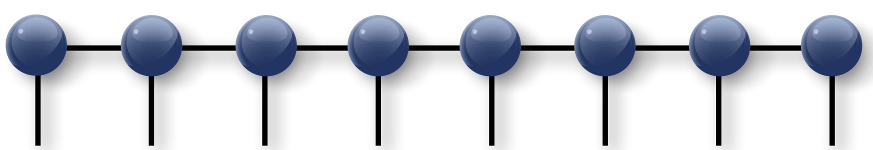
Hierarchical tensor networks (TTN/MERA)

MERA



tensors at different length scales

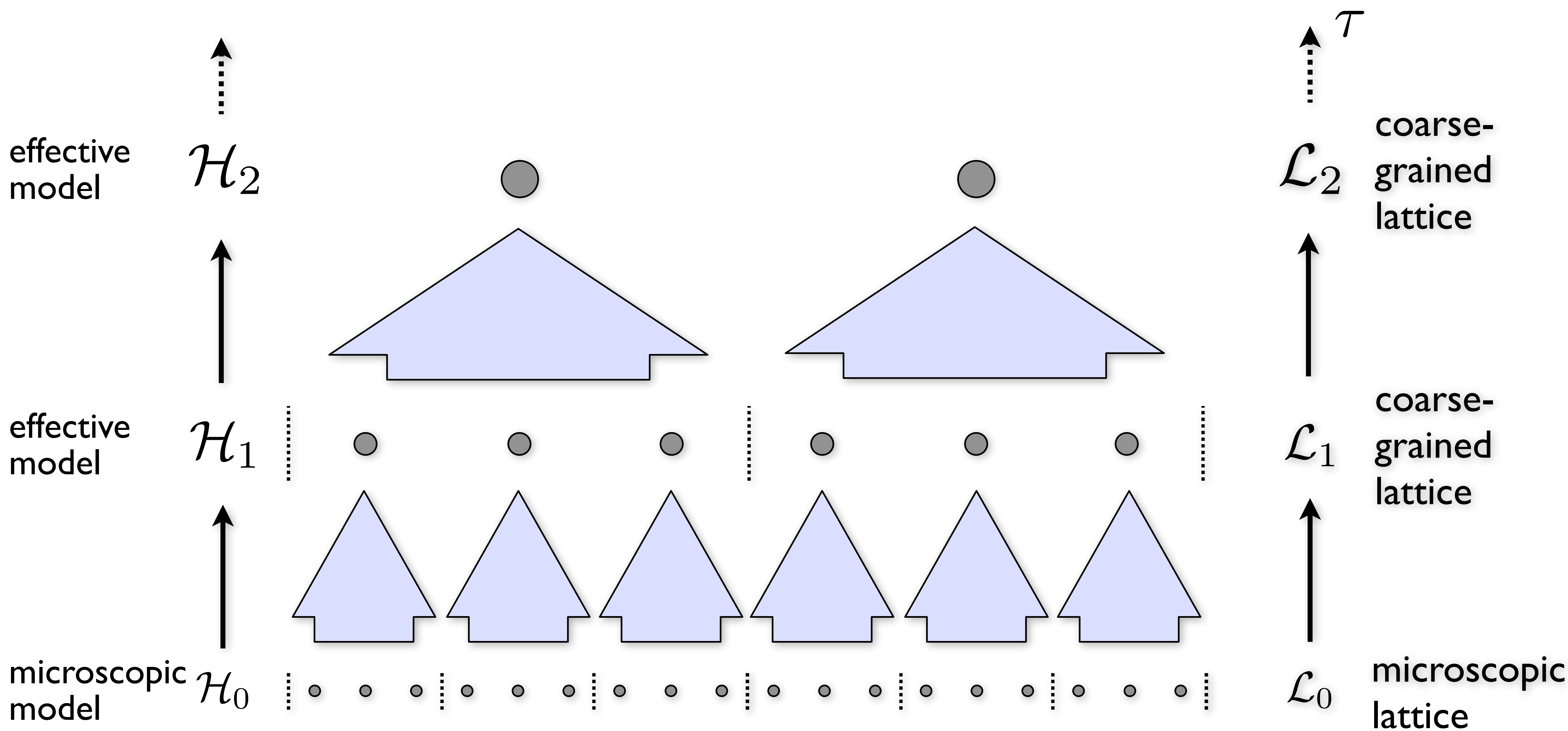
MPS



"flat"

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

Real-space renormalization group transformation

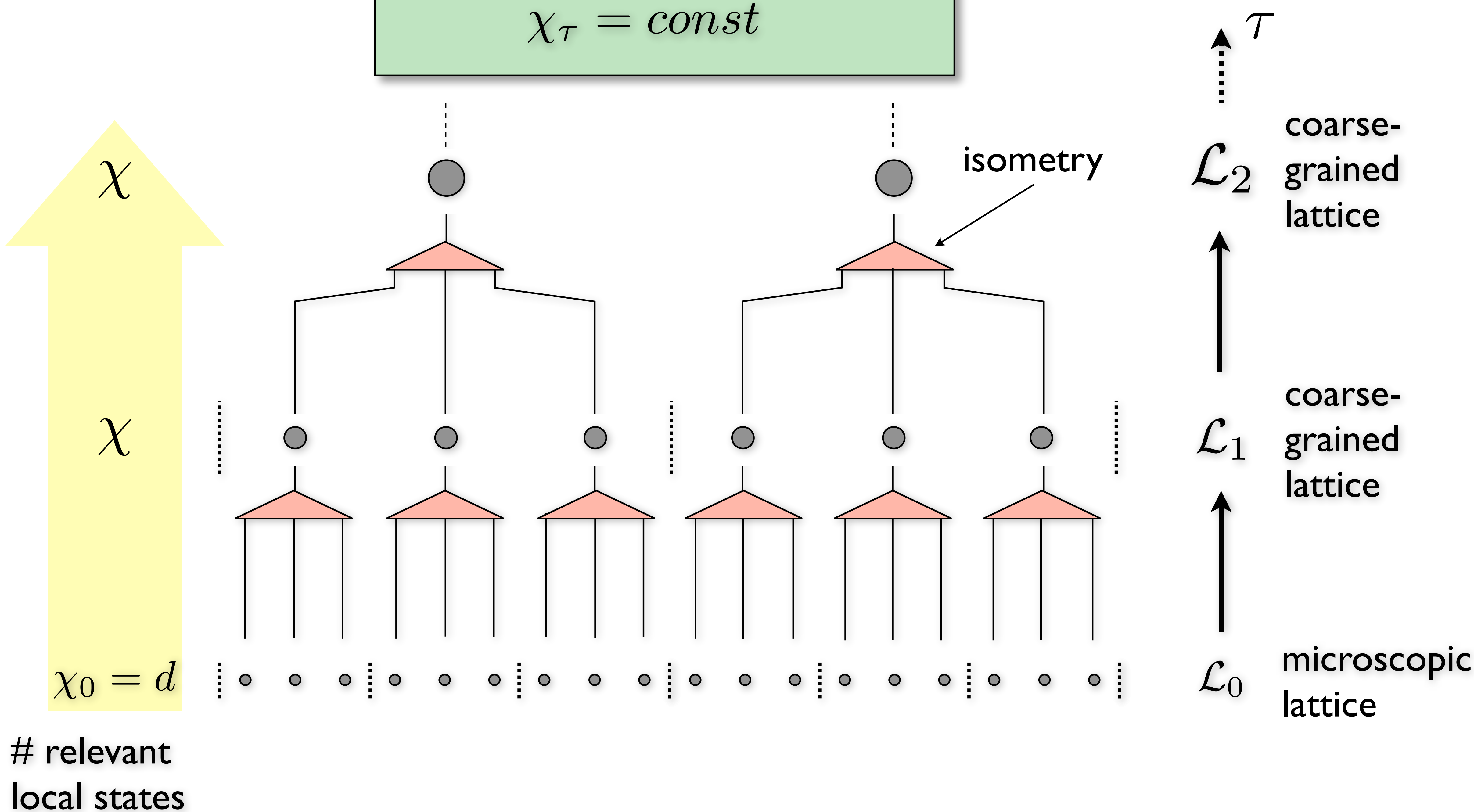


Tree Tensor Network (1D)

1D systems (non-critical)

$$S(L) = const$$

$$\chi_\tau = const$$

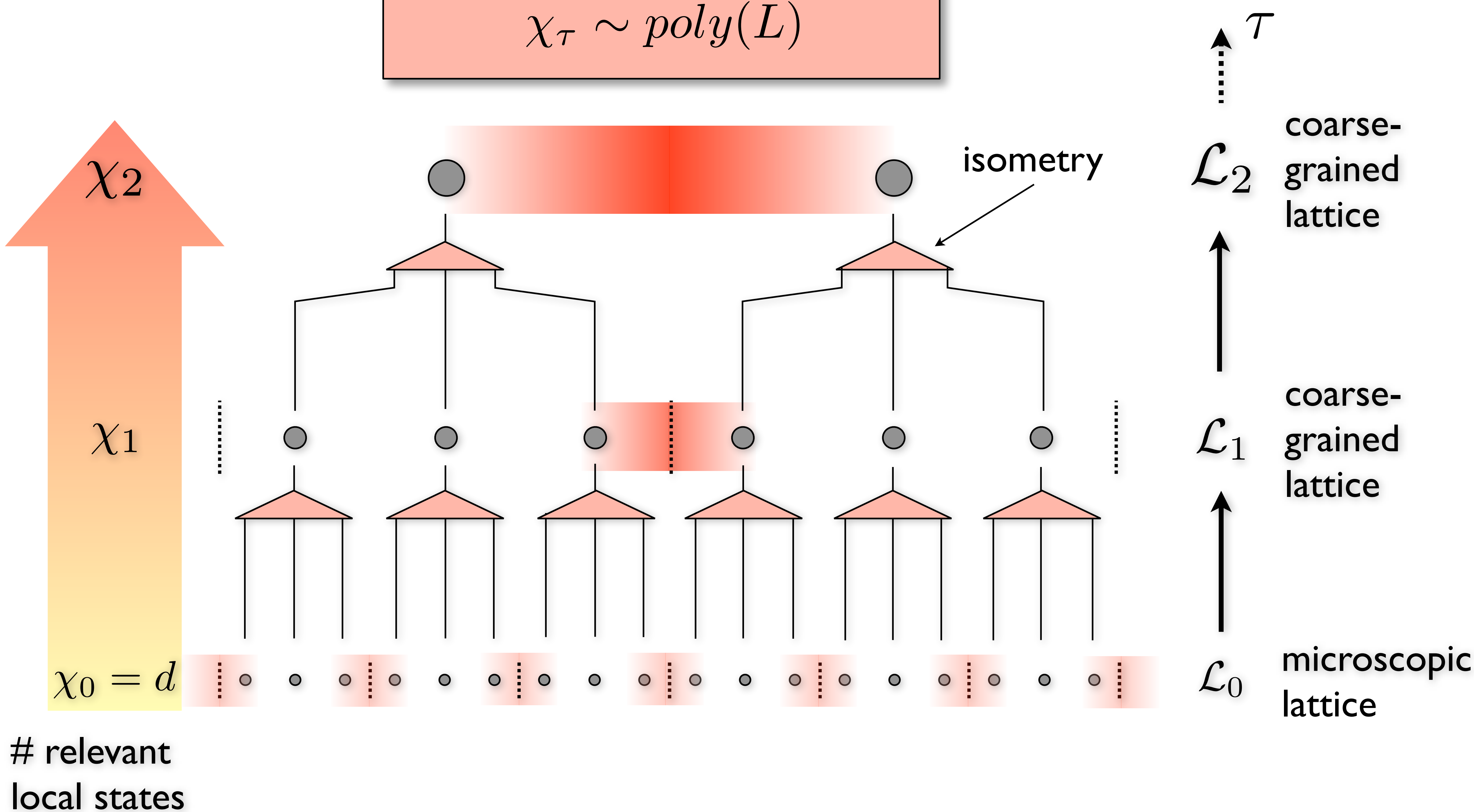


Tree Tensor Network (1D)

1D critical systems

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

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



The MERA (The multi-scale entanglement renormalization ansatz)

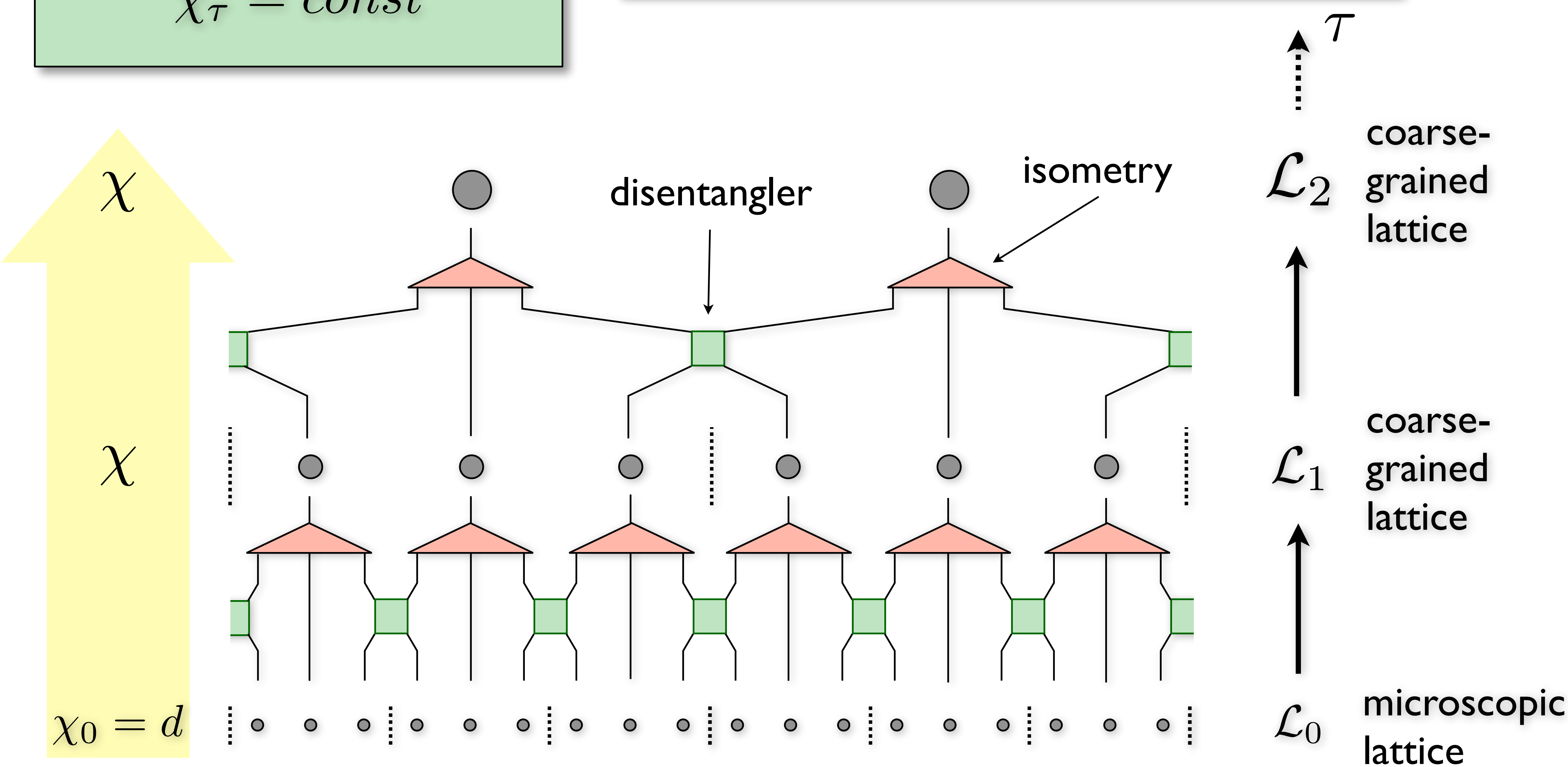
G. Vidal, PRL 99, 220405 (2007)
G. Vidal, PRL 101, 110501 (2008)

1D systems (critical)

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

$$\chi_\tau = const$$

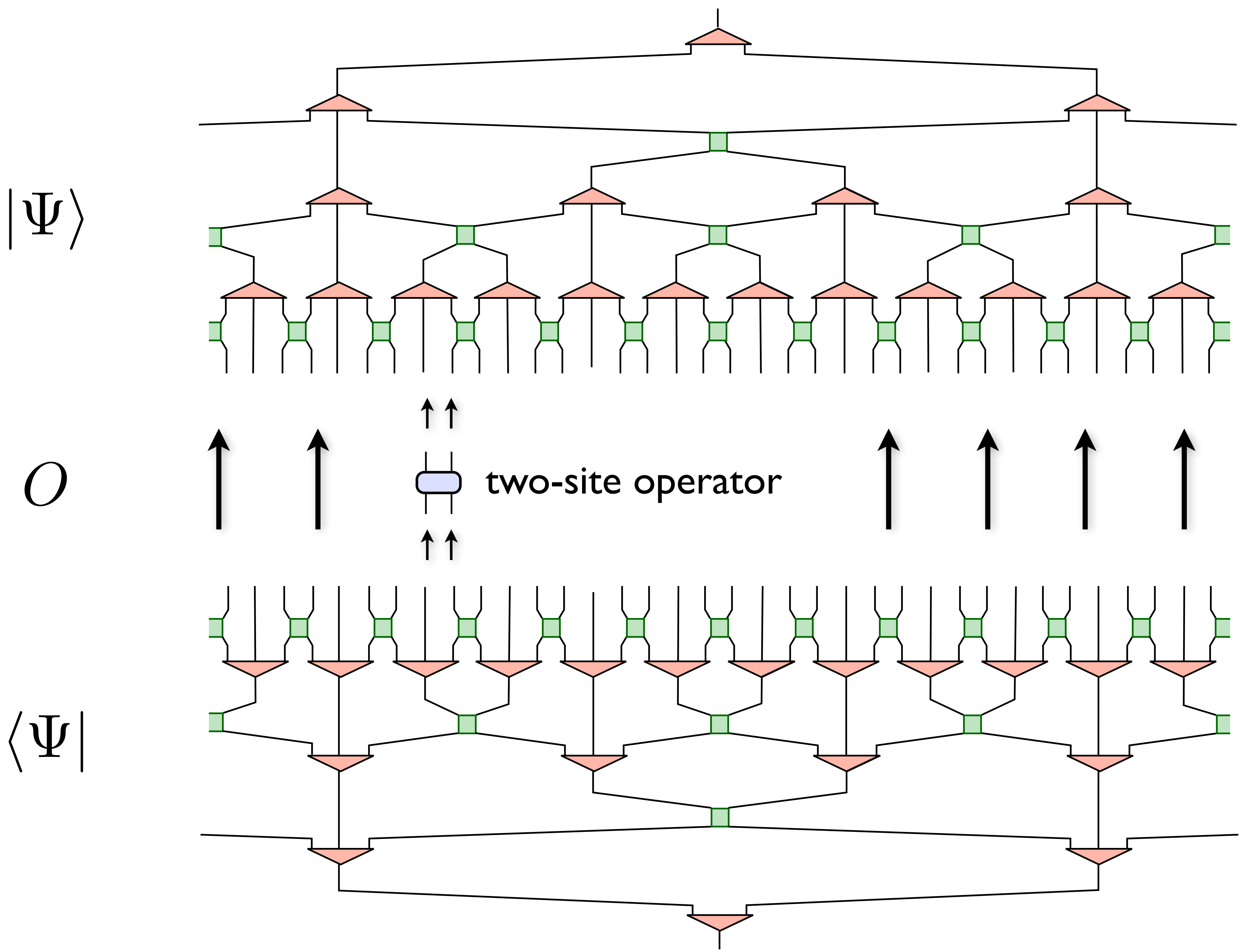
KEY: disentanglers reduce the amount of short-range entanglement



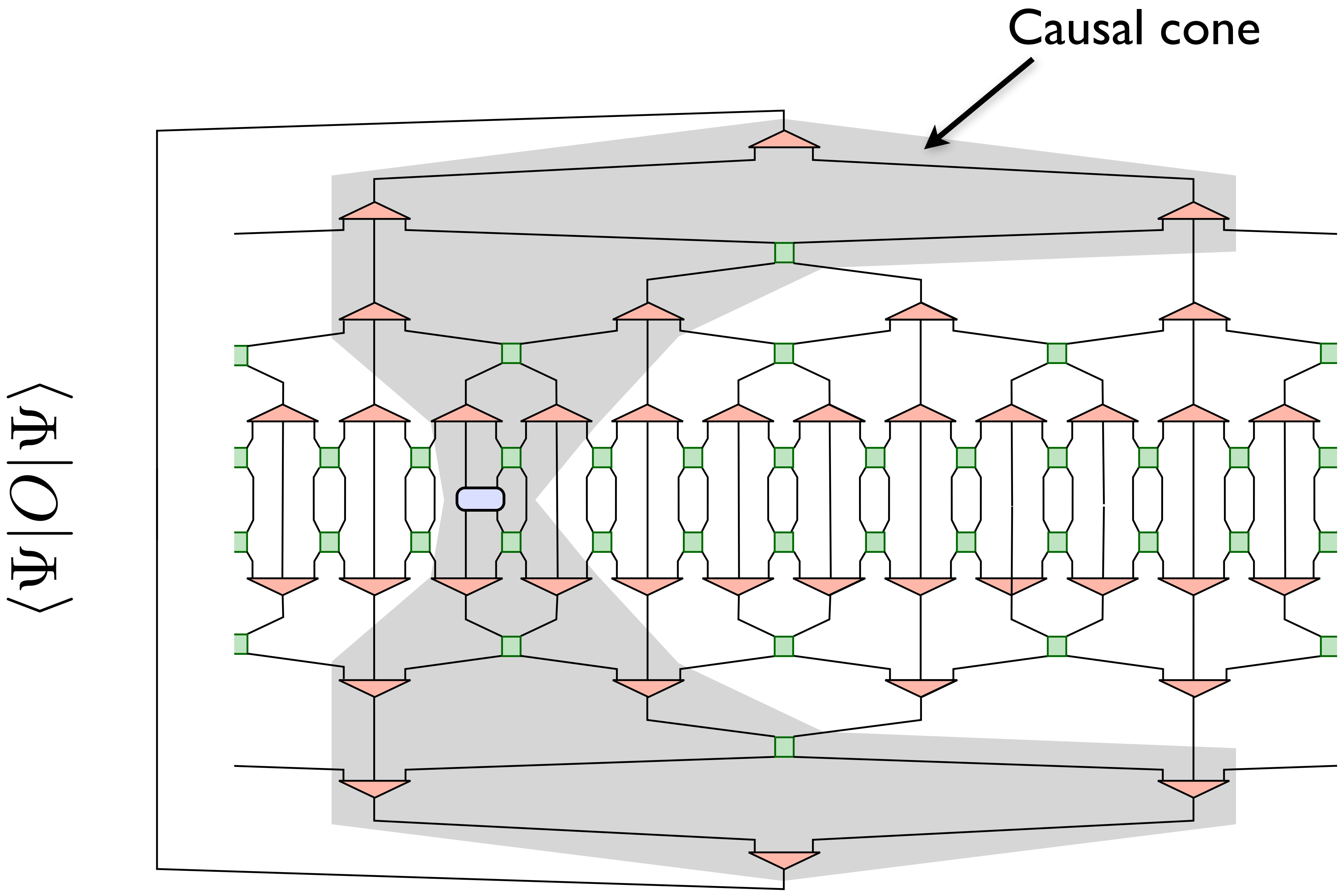
relevant local states

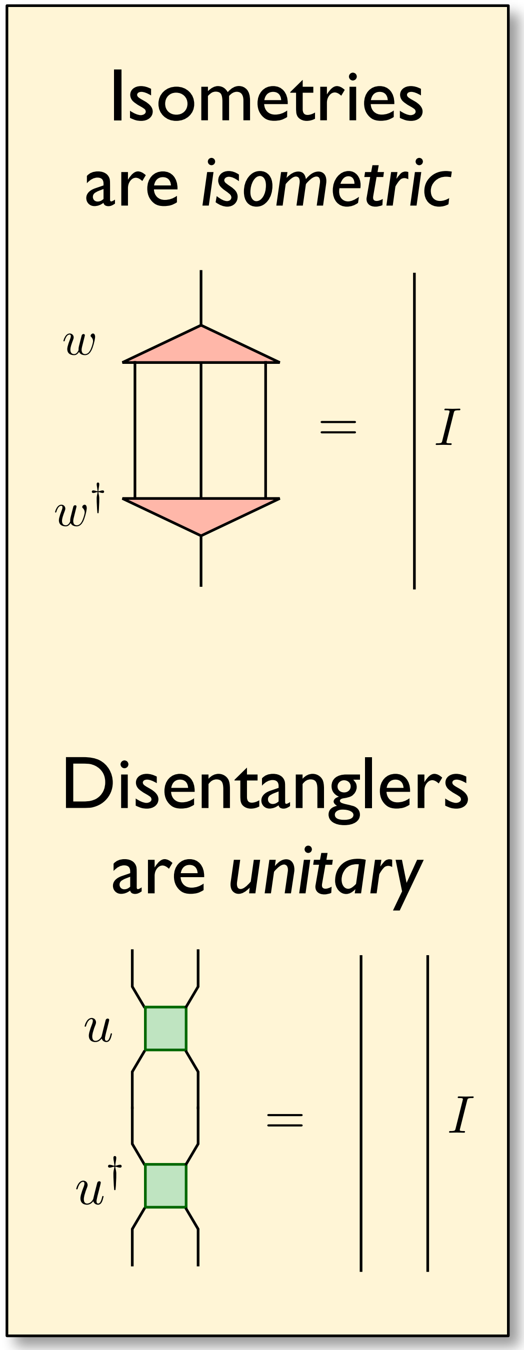
MERA: Properties

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



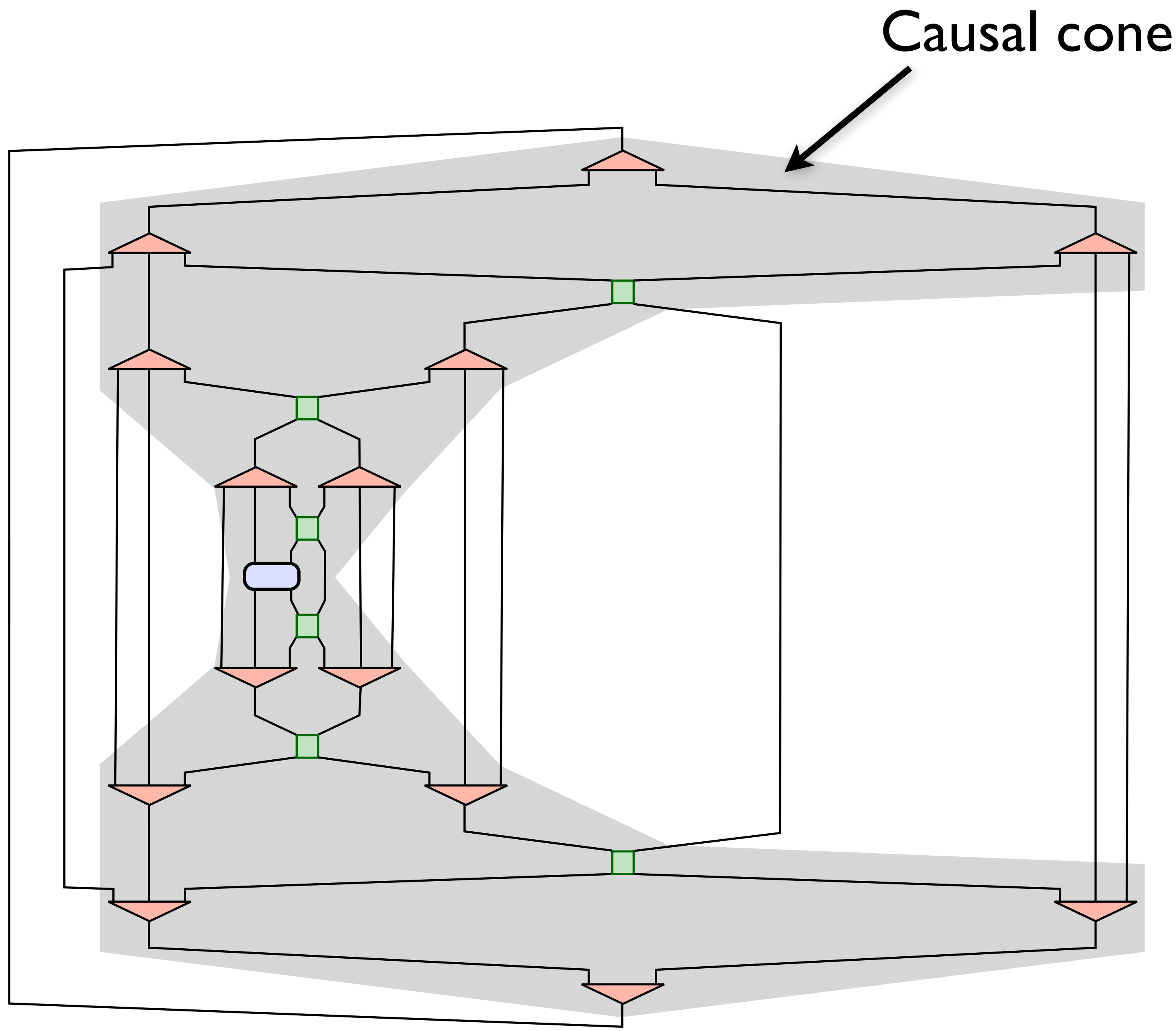
MERA: Properties



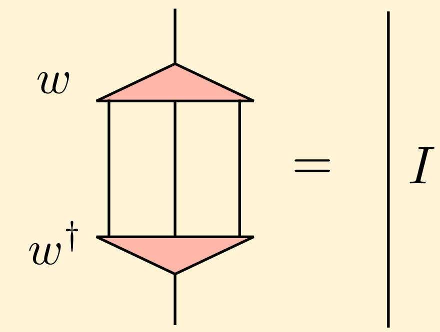


MERA: Properties

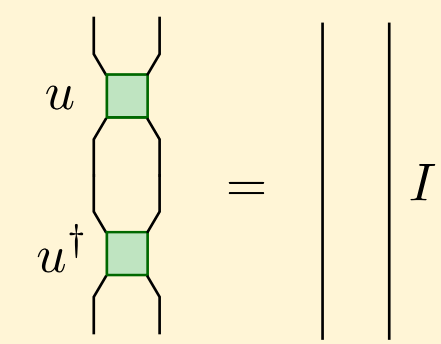
$\langle \Psi | O | \Psi \rangle$



Isometries are *isometric*



Disentanglers are *unitary*

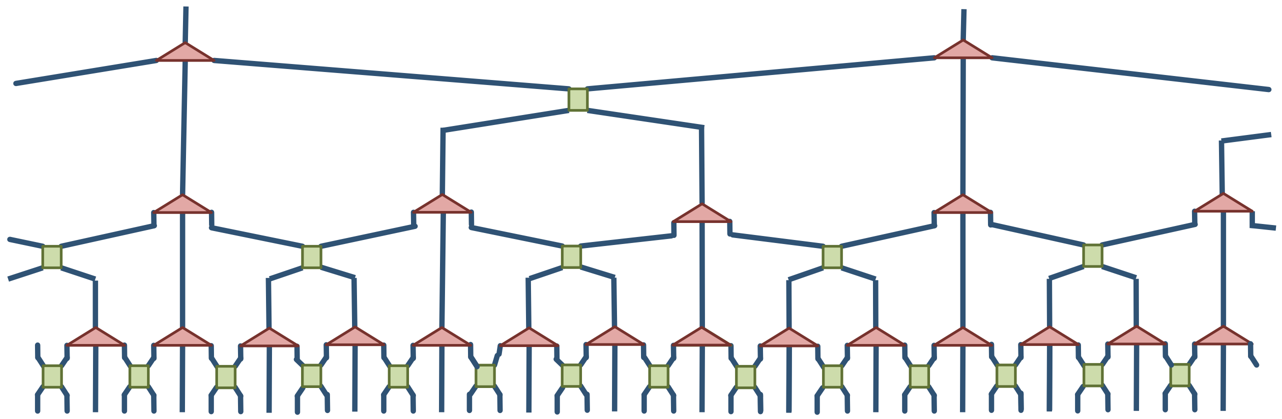


Efficient computation of expectation values of observables!

Different types of MERA's

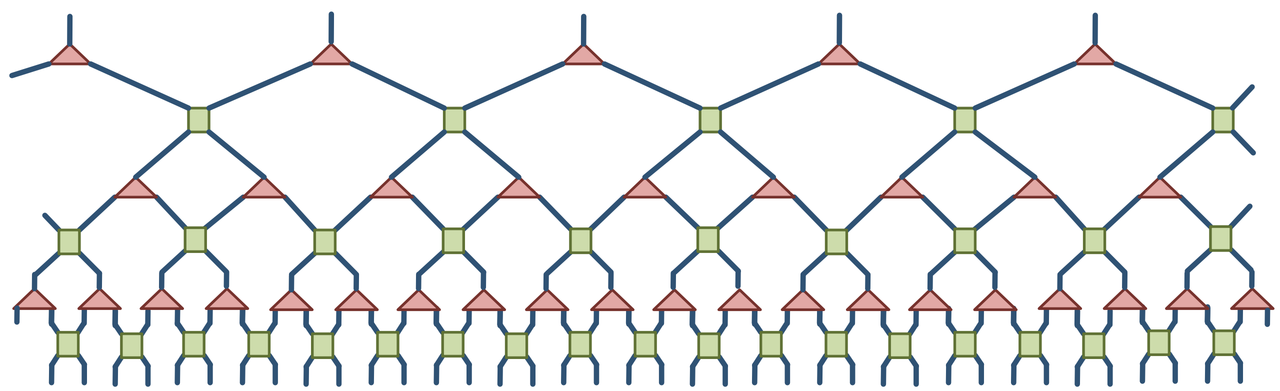
Figures by G. Evenbly

Ternary MERA:
3-to-1 blocking



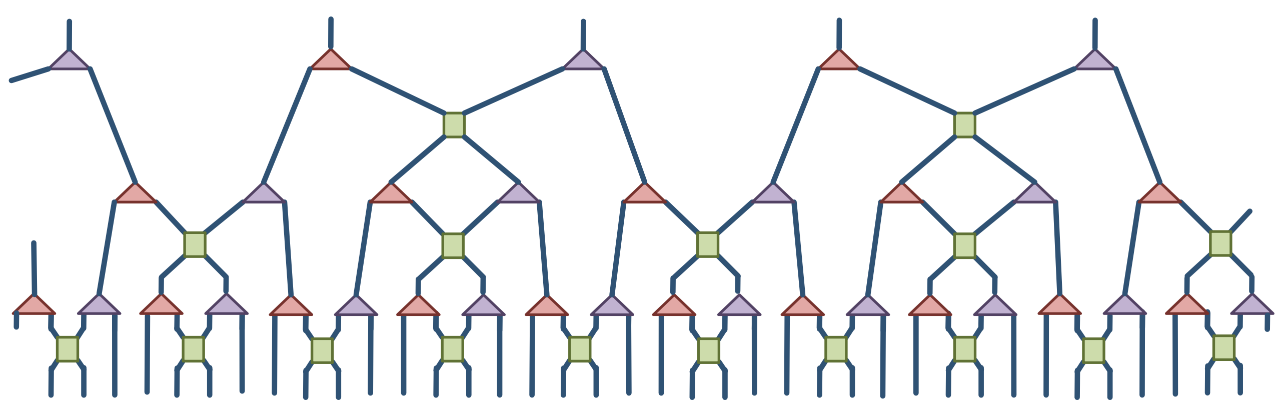
$O\left(\chi^8\right)$

Binary MERA:
2-to-1 blocking



$O\left(\chi^9\right)$

Modified binary MERA:
2-to-1 blocking



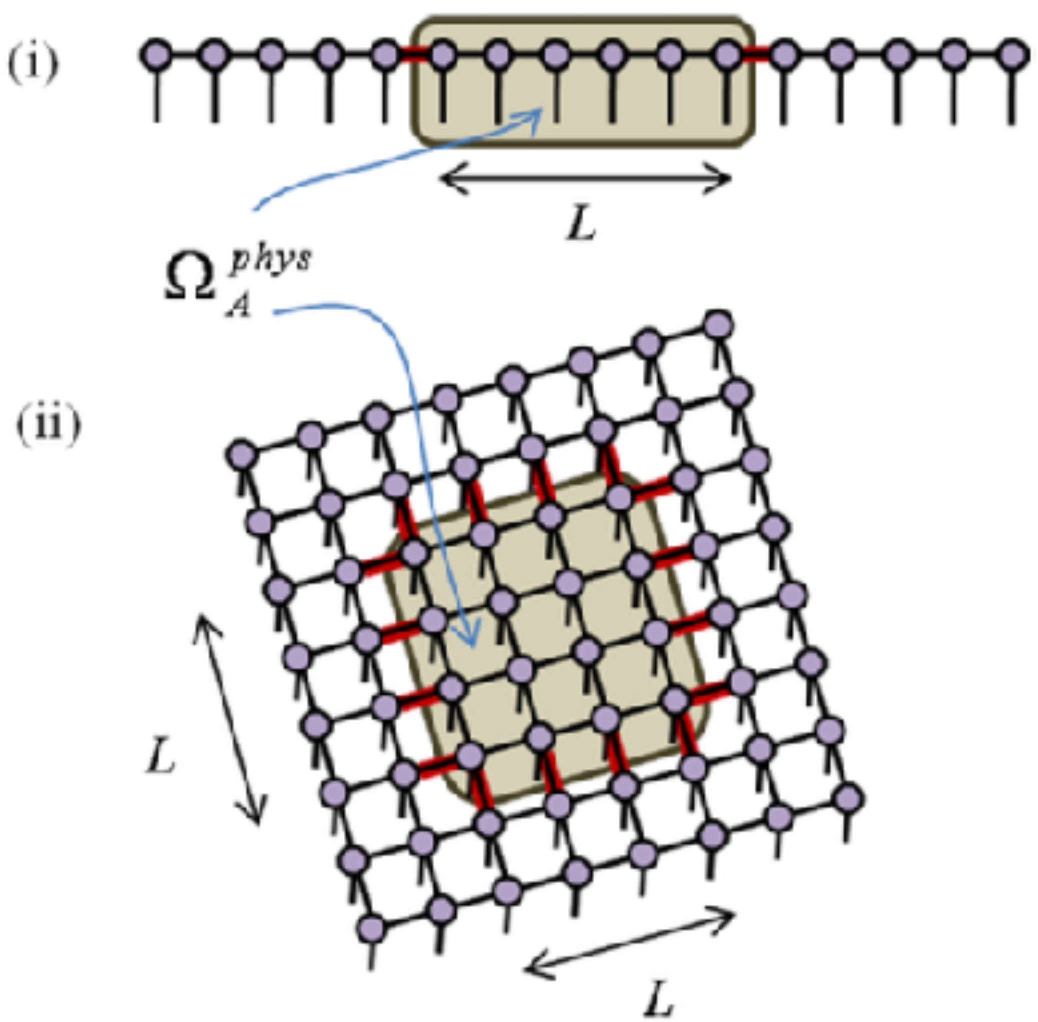
$O\left(\chi^7\right)$

TRADEOFF: computational cost vs efficiency of coarse-graining

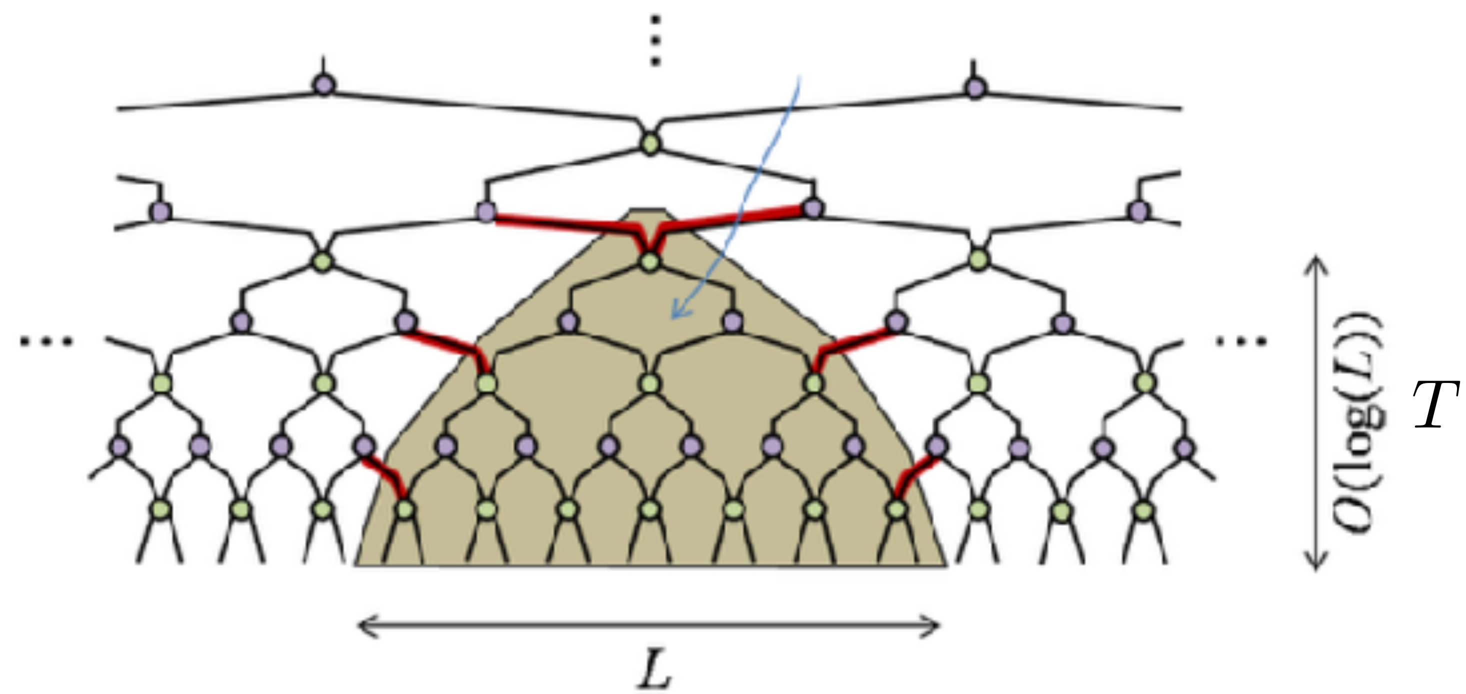
MERA: Entanglement entropy

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

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



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



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

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

Reproduces log(L) scaling of 1D critical systems

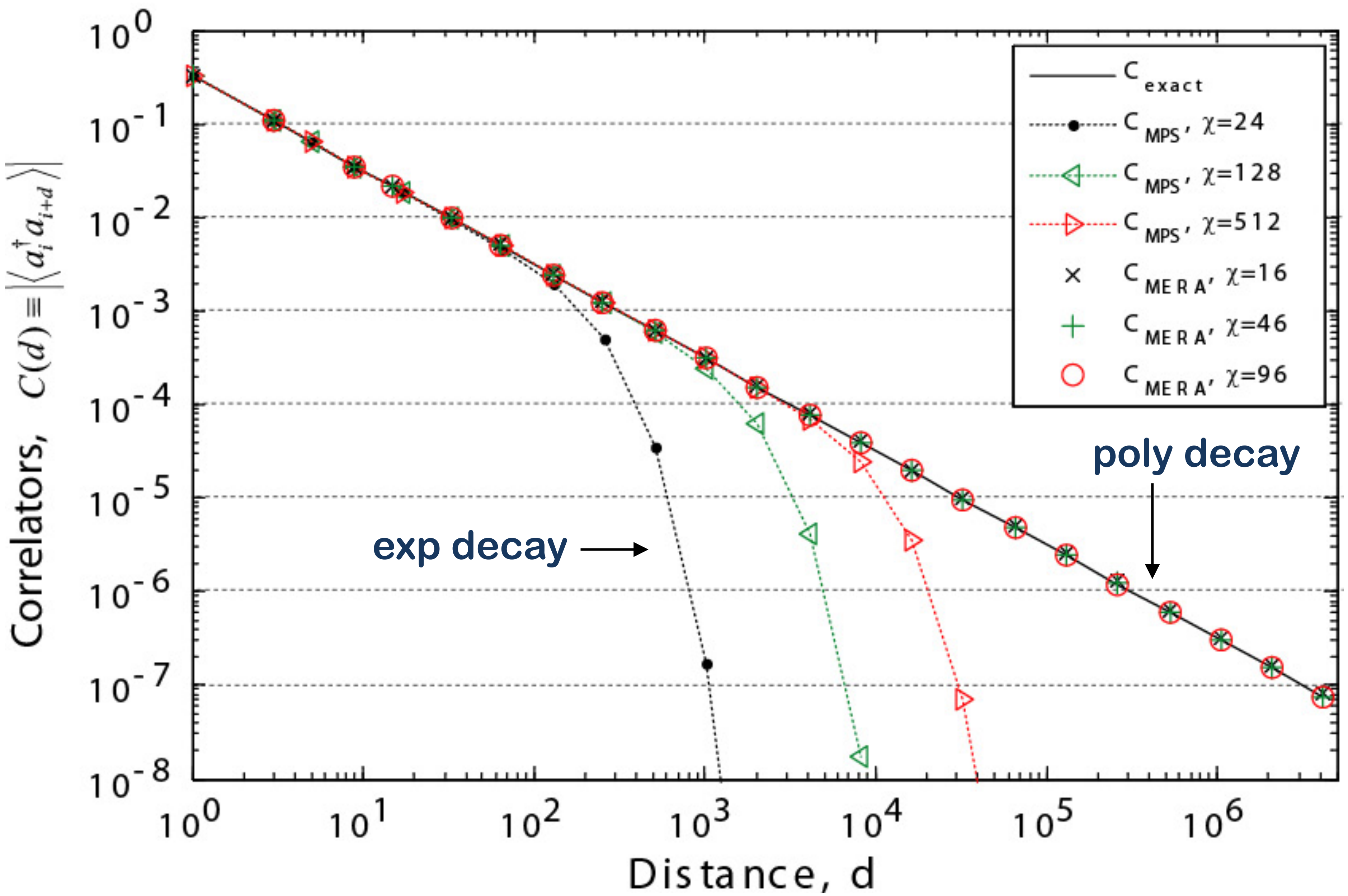
figures from Evenbly & Vidal, J Stat Phys **145** (2011)

Power-law decaying correlations

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

quantum XX model: (critical, c=1)

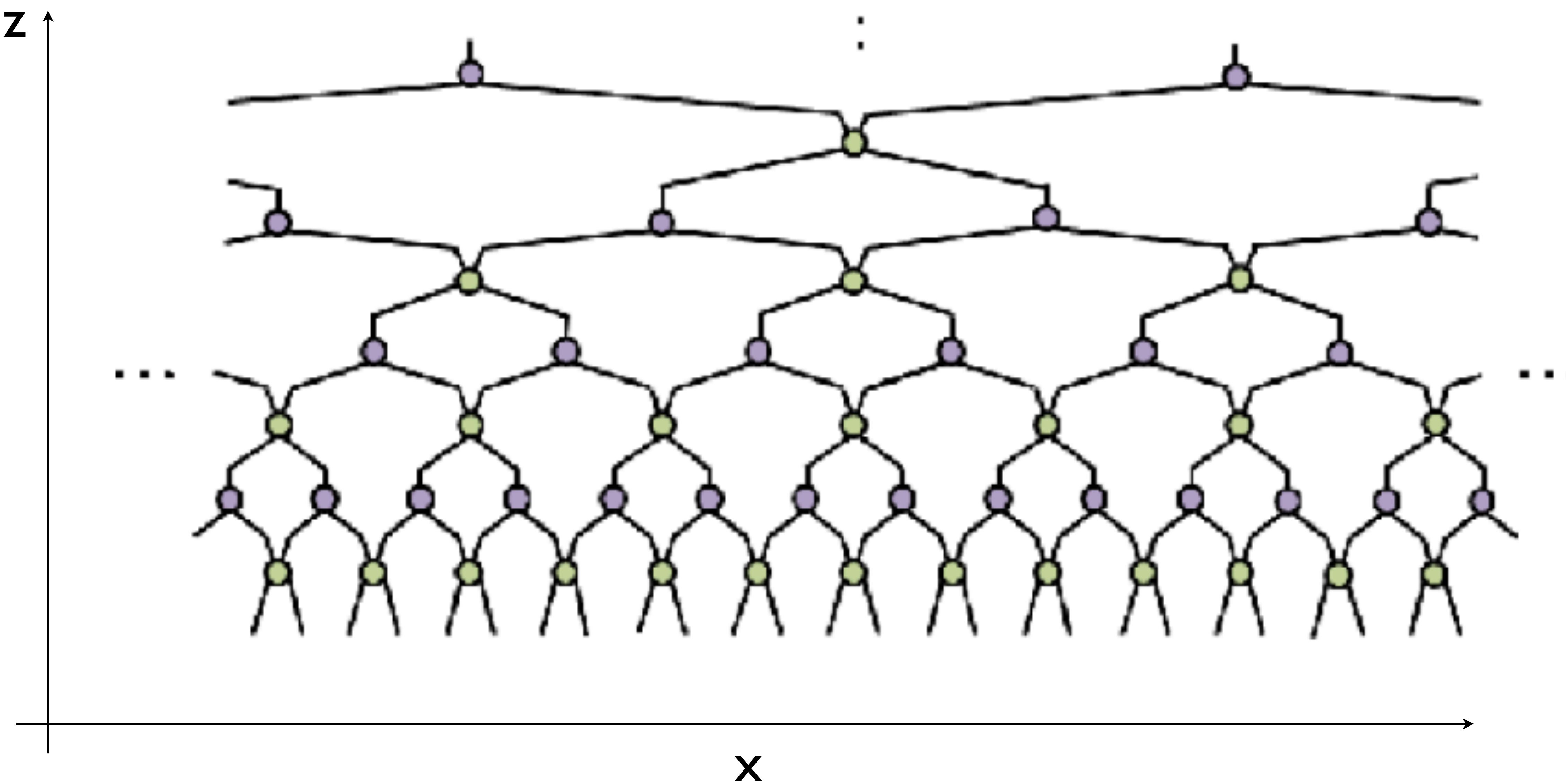
$$H_{XX} = \sum_r \left(\sigma_r^X \sigma_{r+1}^X + \sigma_r^Y \sigma_{r+1}^Y \right)$$



However, critical systems can still be studied with MPS!

slide from Glen Evenbly

Scale invariant MERA

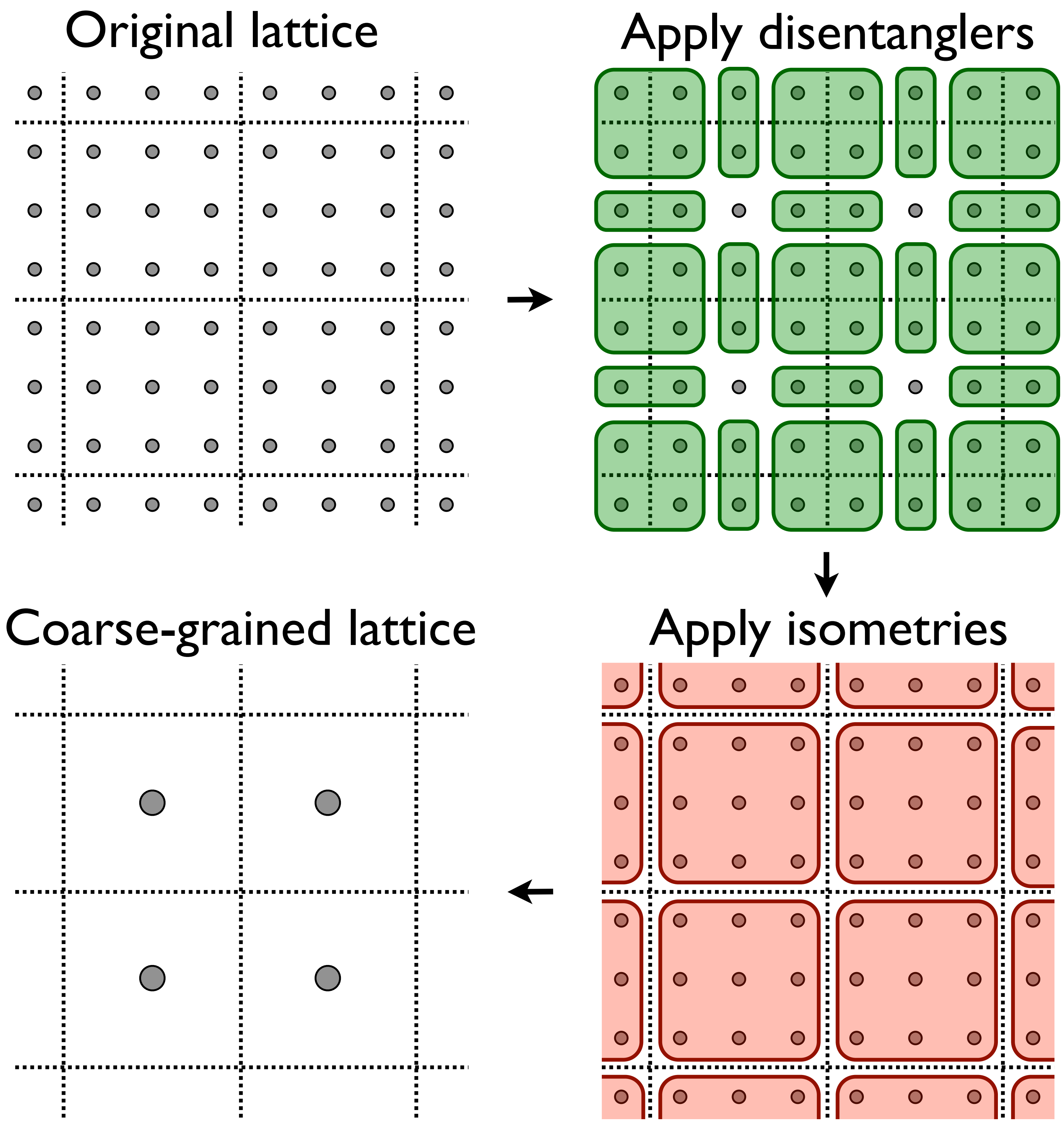


Translational invariance: *same tensors along x*

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

2D MERA (top view)

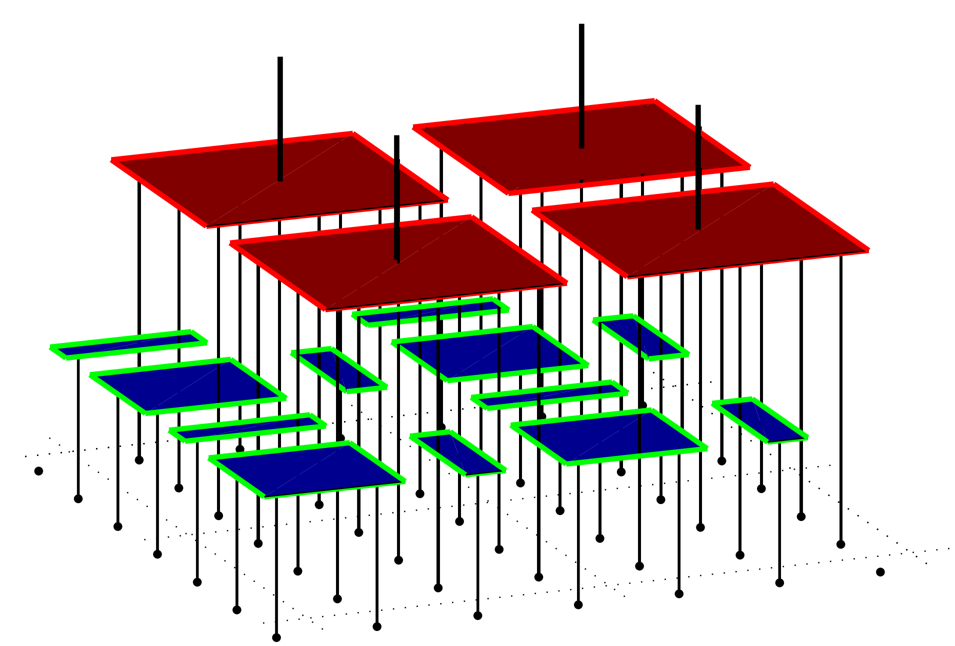
Evenbly, Vidal. PRL 102, 180406 (2009)



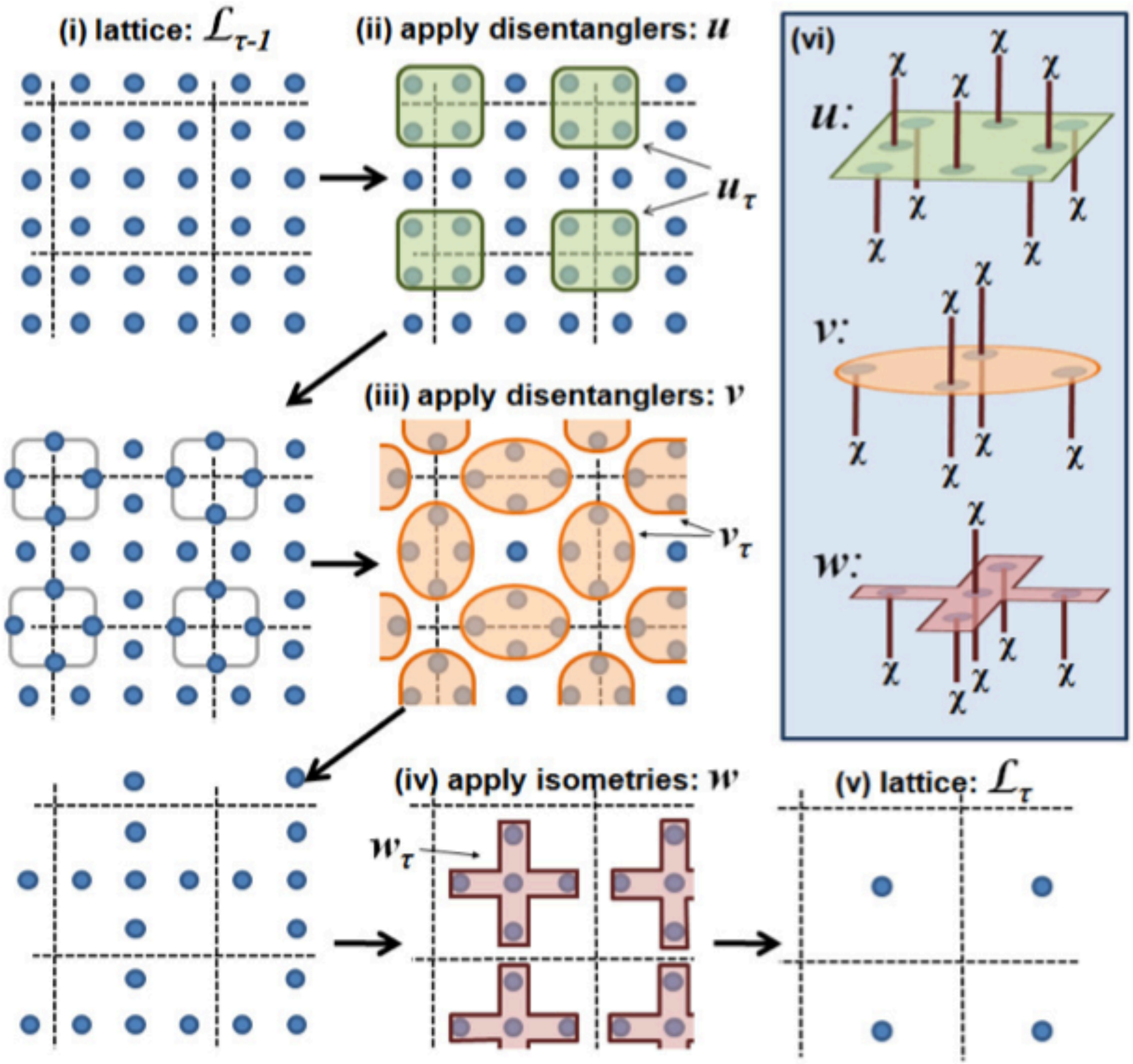
✓ Accounts for area-law in 2D systems

$$S(L) \sim L$$

$$\chi_\tau = const$$

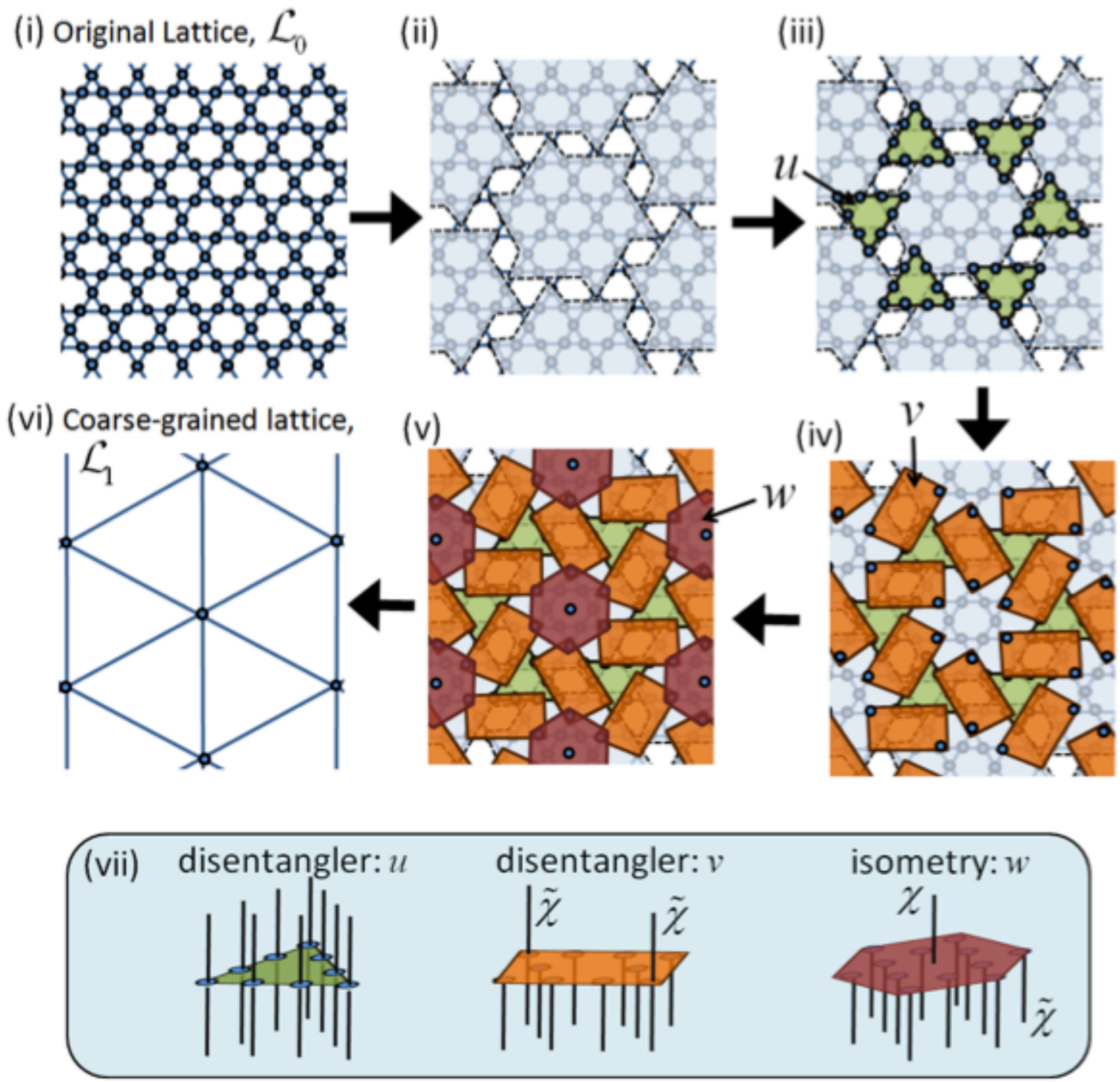


Different structures of the 2D MERA...



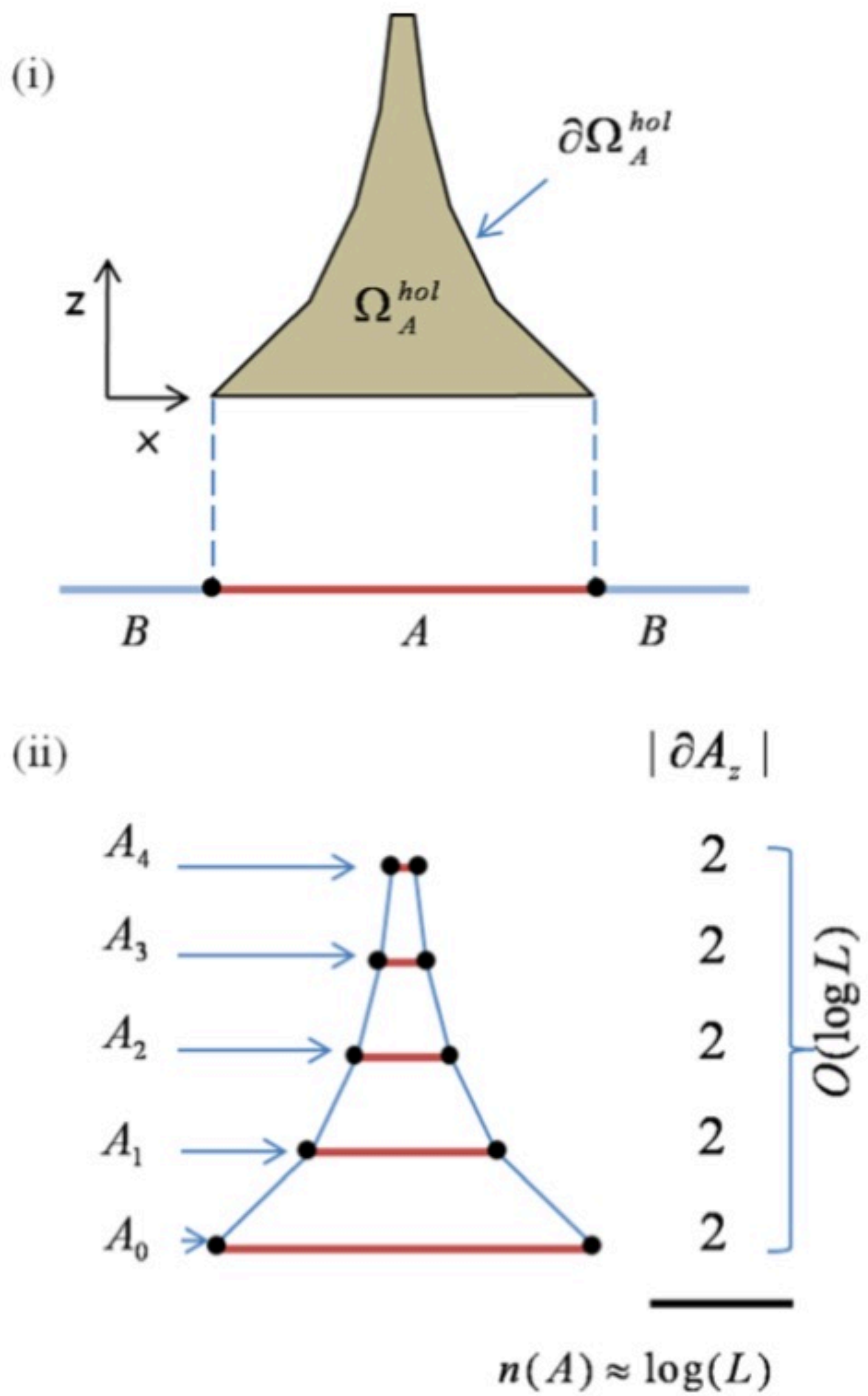
Evenbly & Vidal, PRL **102**, 180406 (2009)

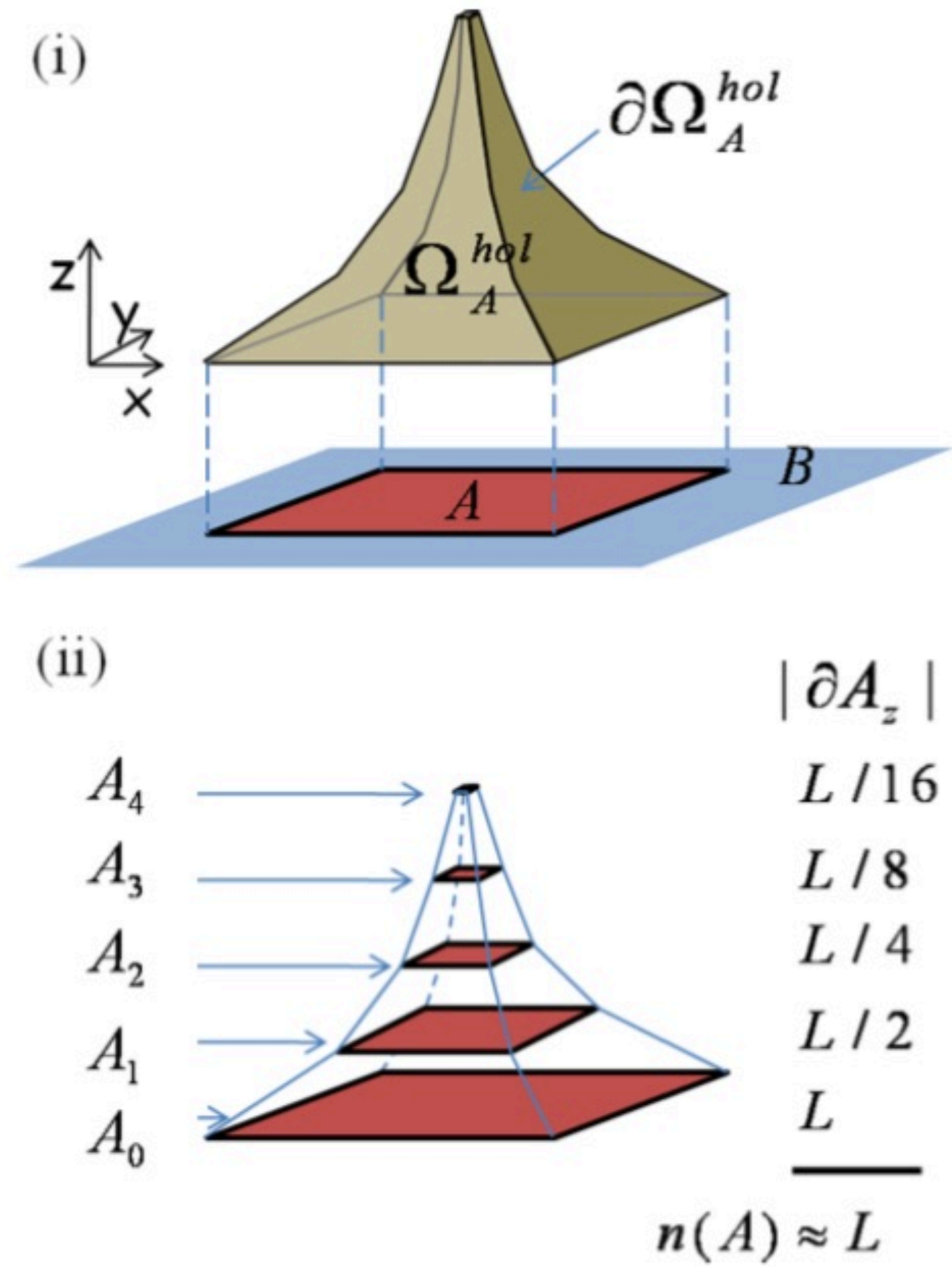
2D MERA on the Kagome lattice



Evenbly & Vidal, PRL 104, 187203 (2010)

1D vs 2D MERA



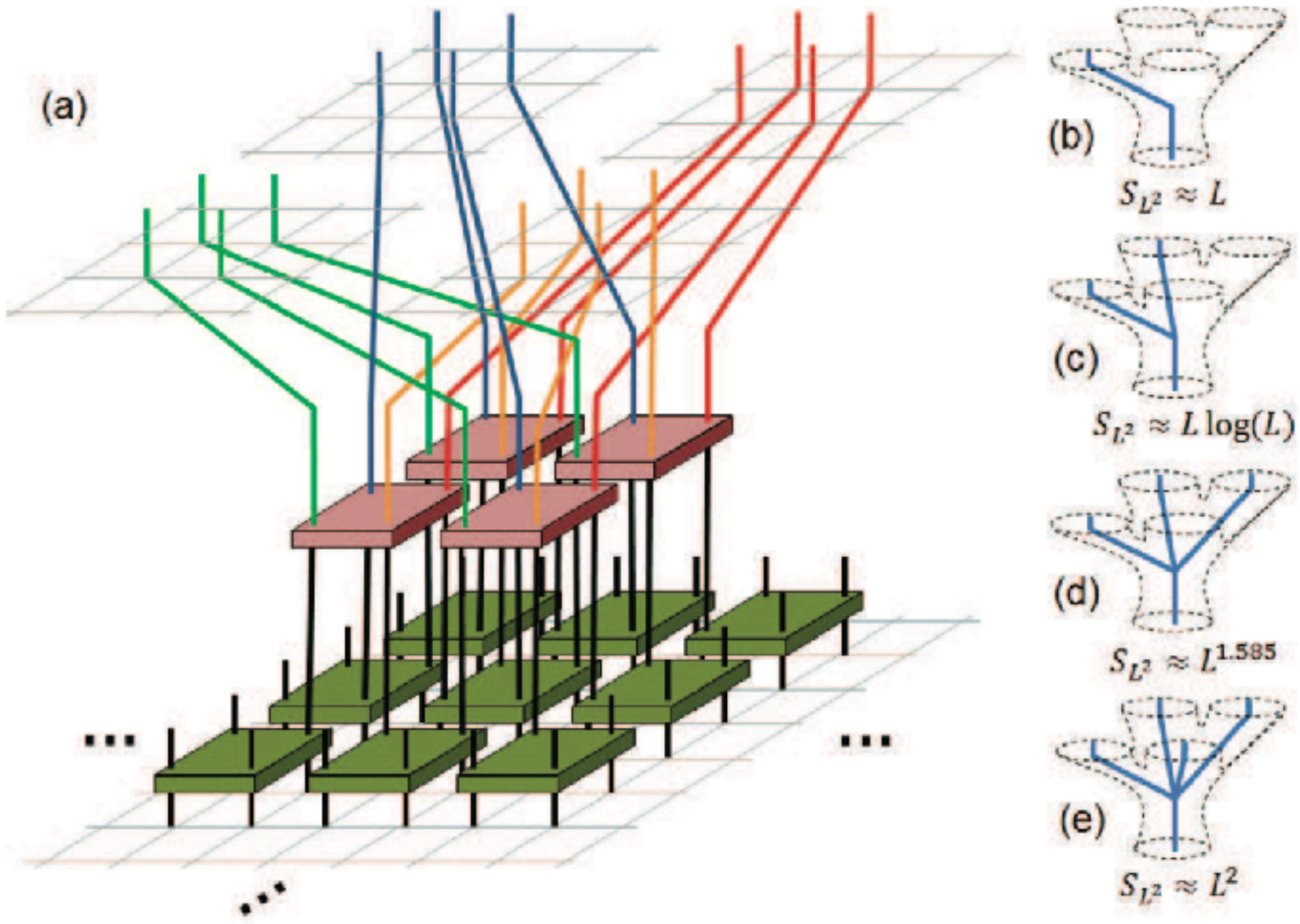


same number of connections in each layer

decreasing number of connections

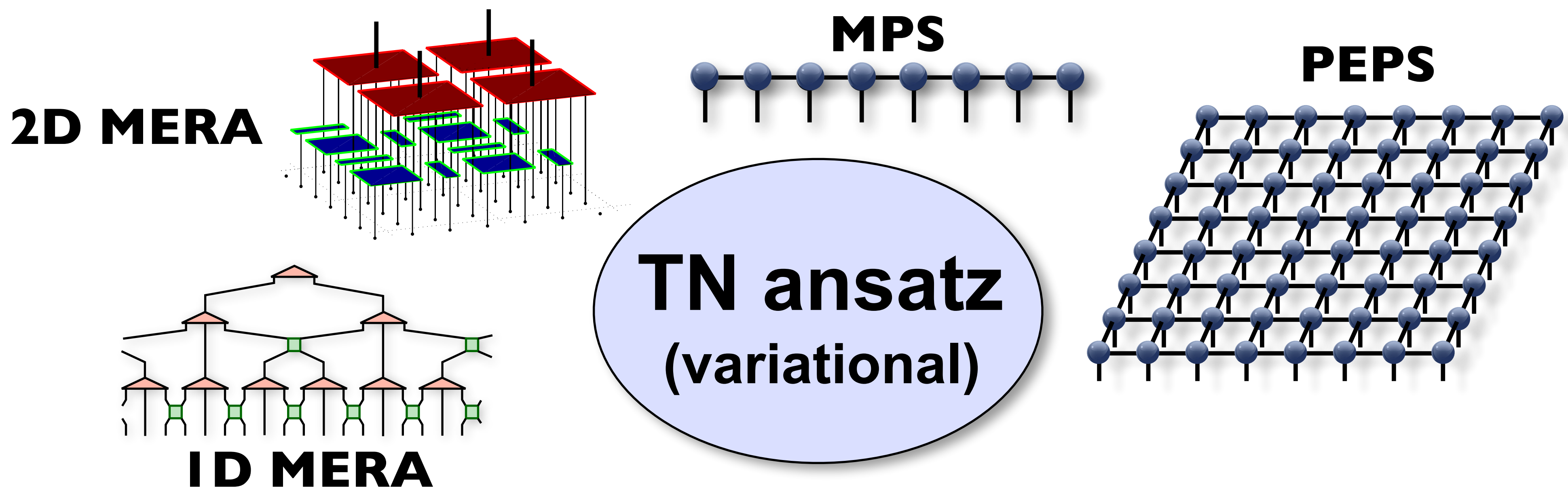
Evenbly and G. Vidal, J Stat Phys **145**, 891(2011).

Branching MERA: beyond area law scaling in 2D



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

Summary: Tensor network ansätze



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

➡ Different tensor networks can reproduce different entanglement entropy scaling:

★ MPS: area law in 1D

★ MERA: log L scaling in 1D (critical systems)

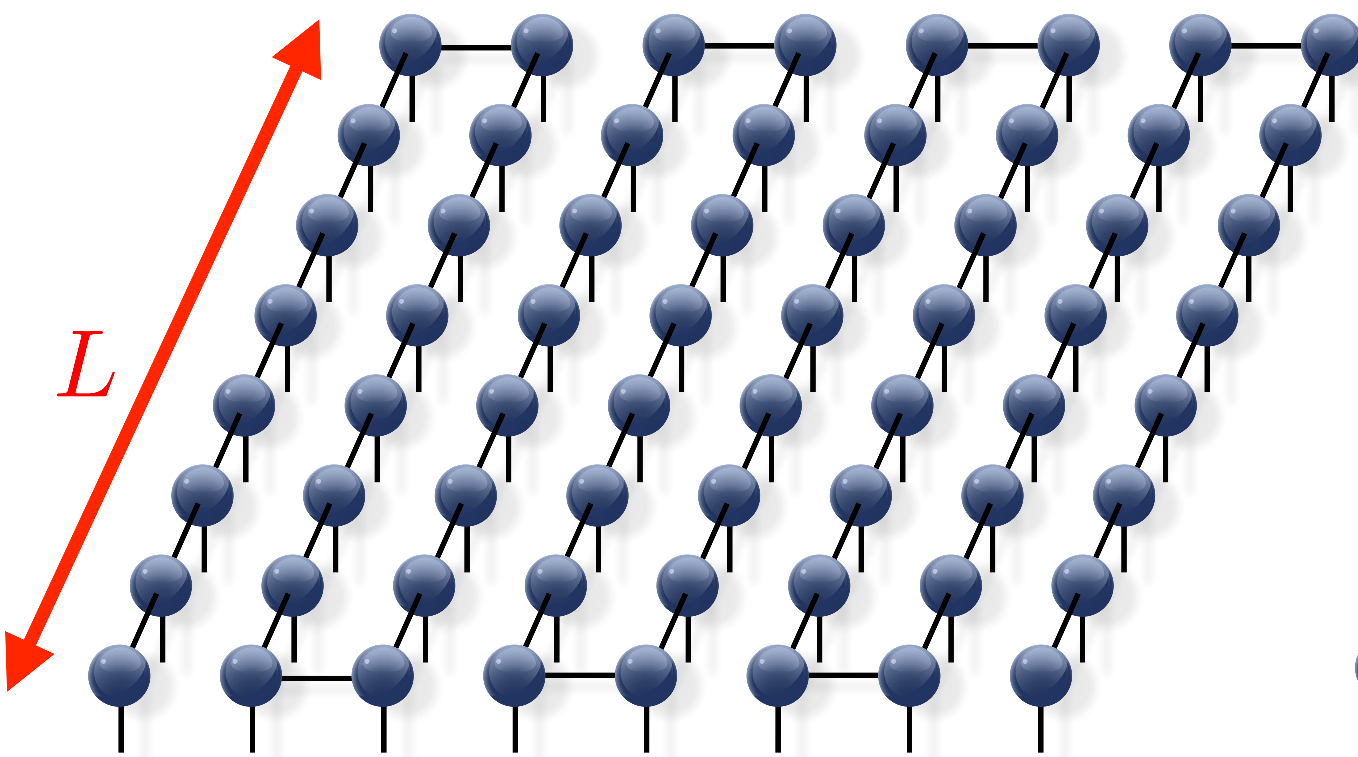
★ PEPS/iPEPS: area law in 2D

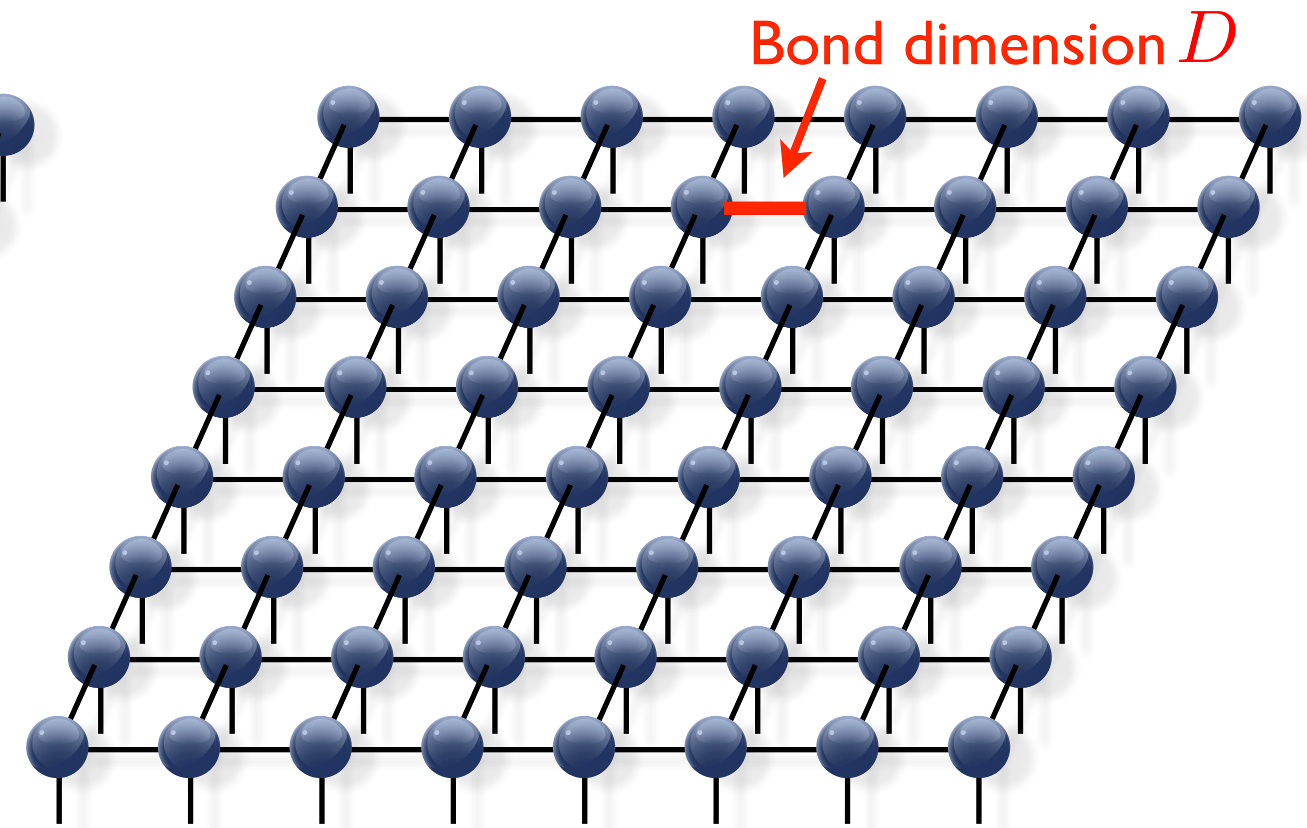
★ 2D MERA: area law in 2D

★ branching MERA: beyond area law in 2D (e.g. L log L scaling) (Evenbly & Vidal, 2014)

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~exp(L)*

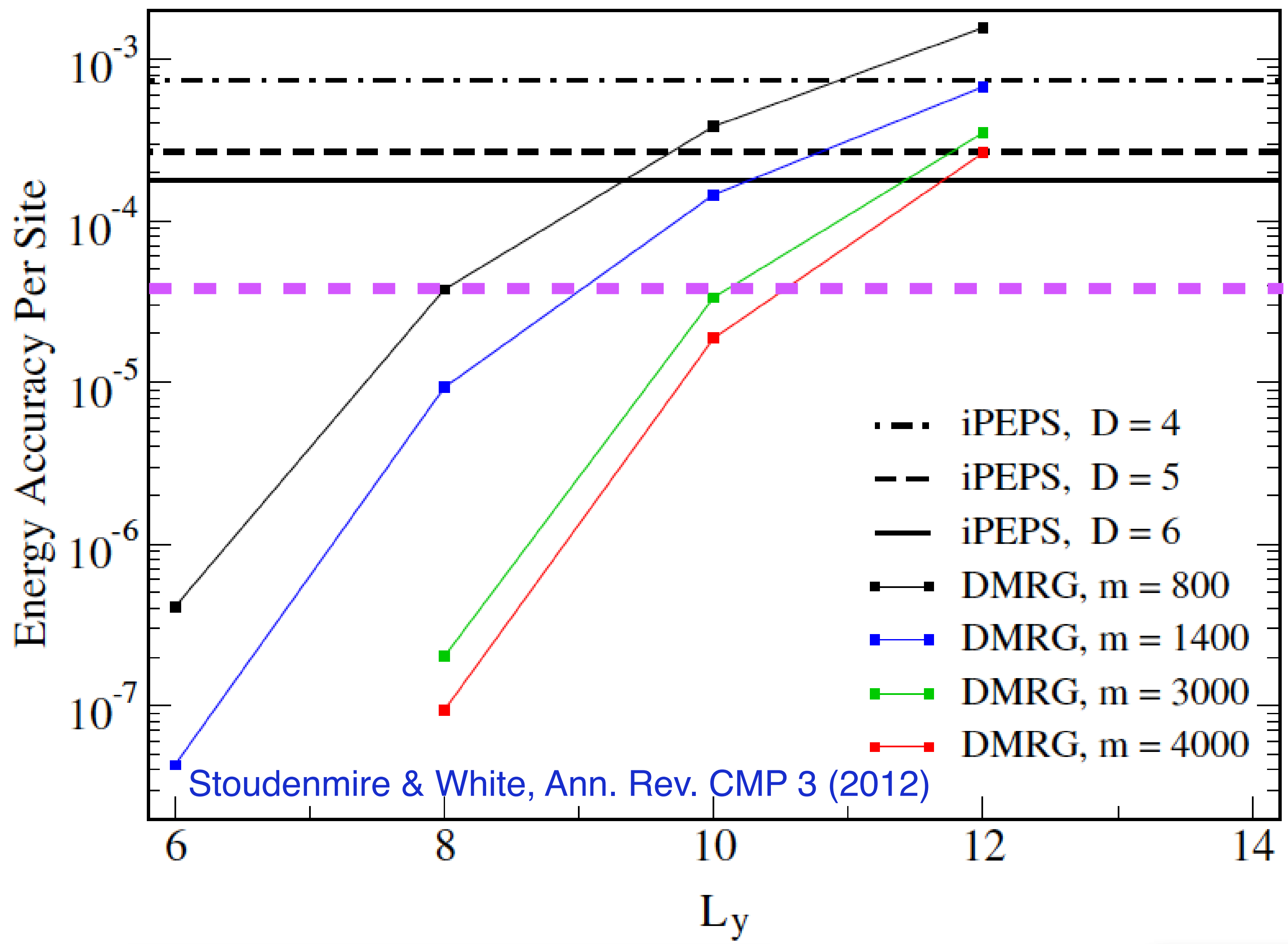
★ Large / infinite systems (scalable)!

★ 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

~

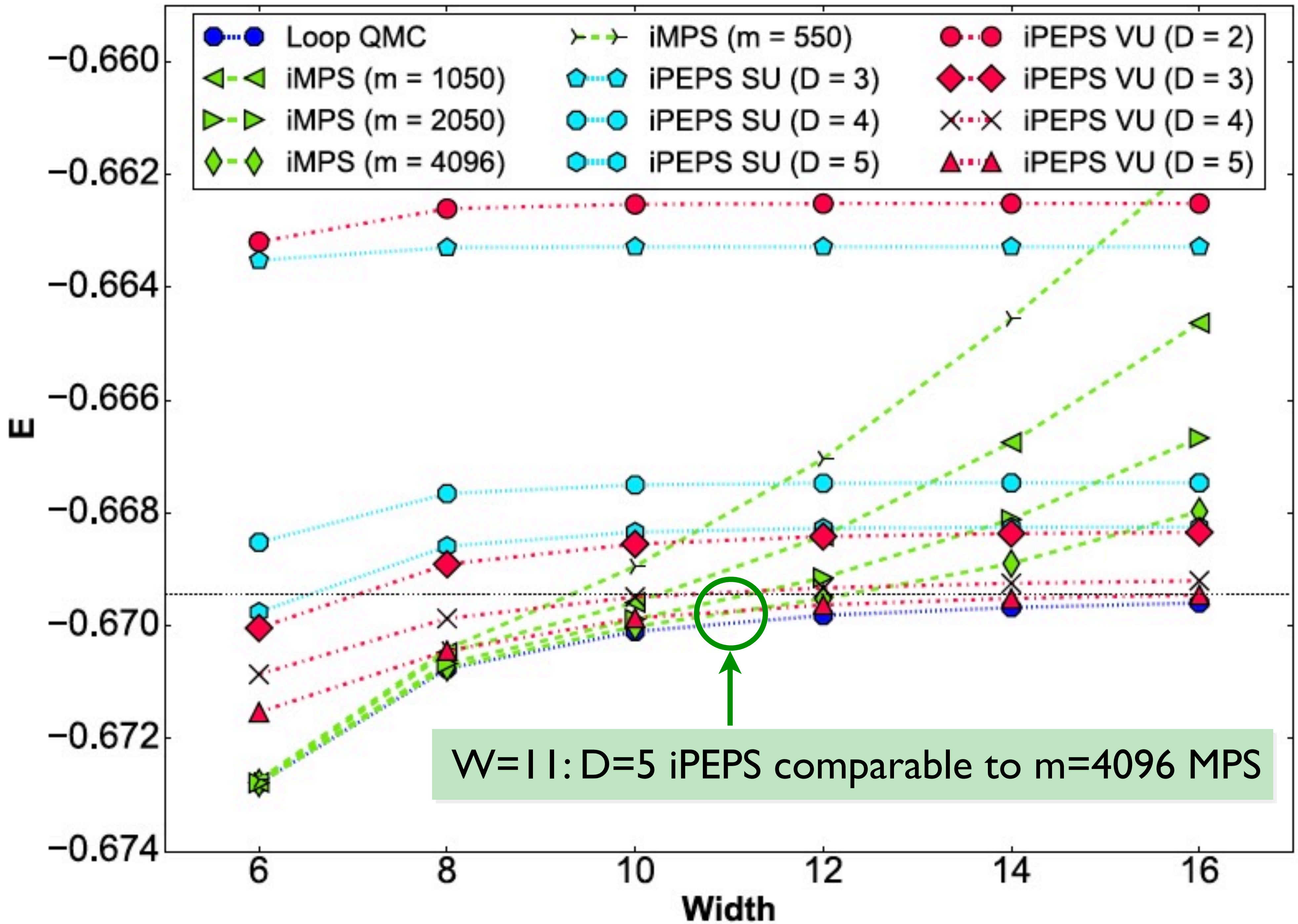
MPS D=3000 on finite Ly=10 cylinder

~ 18'000'000

4 orders of magnitude fewer parameters (per tensor)

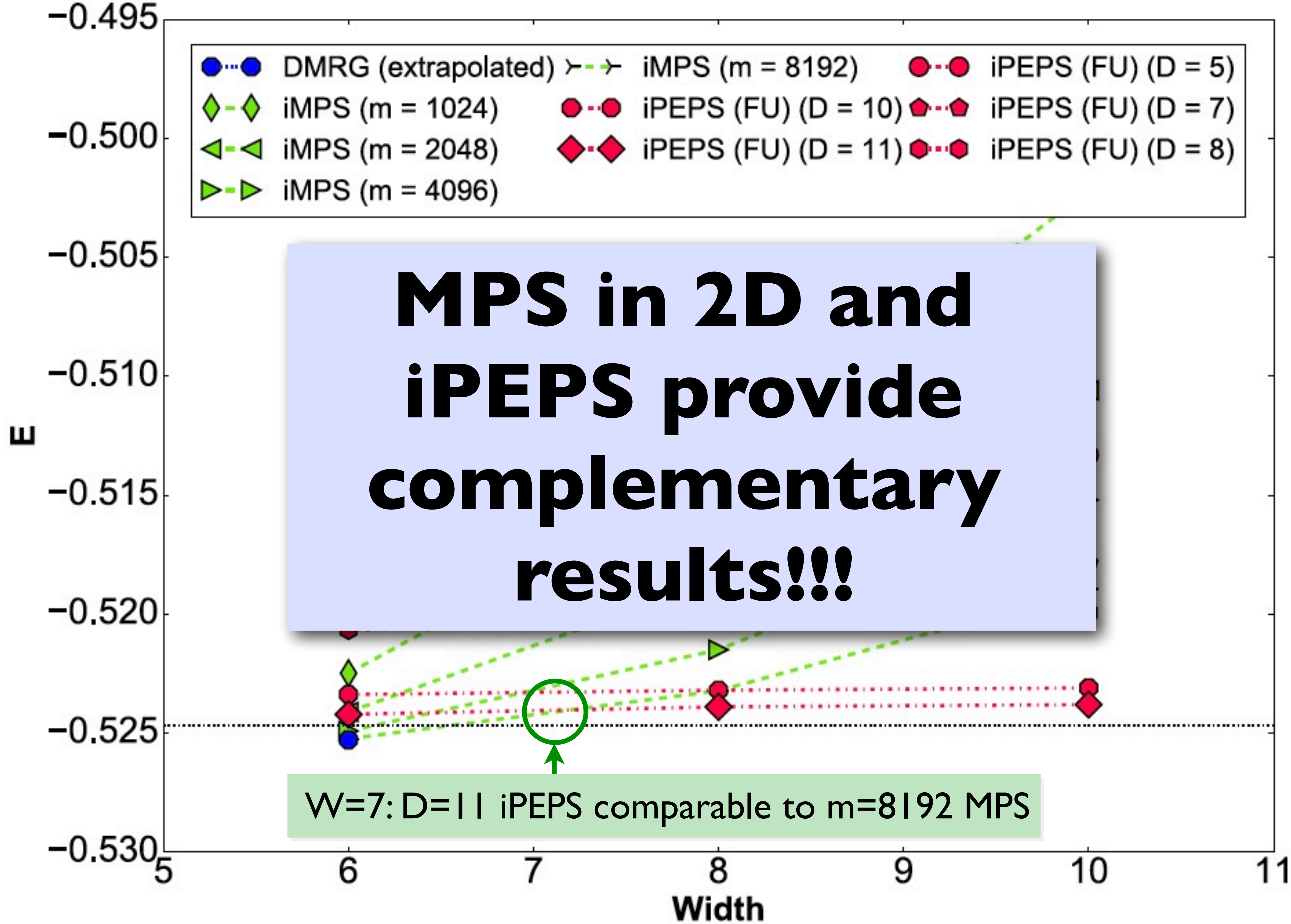
iMPS vs iPEPS on infinite cylinders: Heisenberg model

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)



Classification by entanglement (2D)

- How large does D have to be?

▶ It depends on the amount of entanglement in the system!

Entanglement

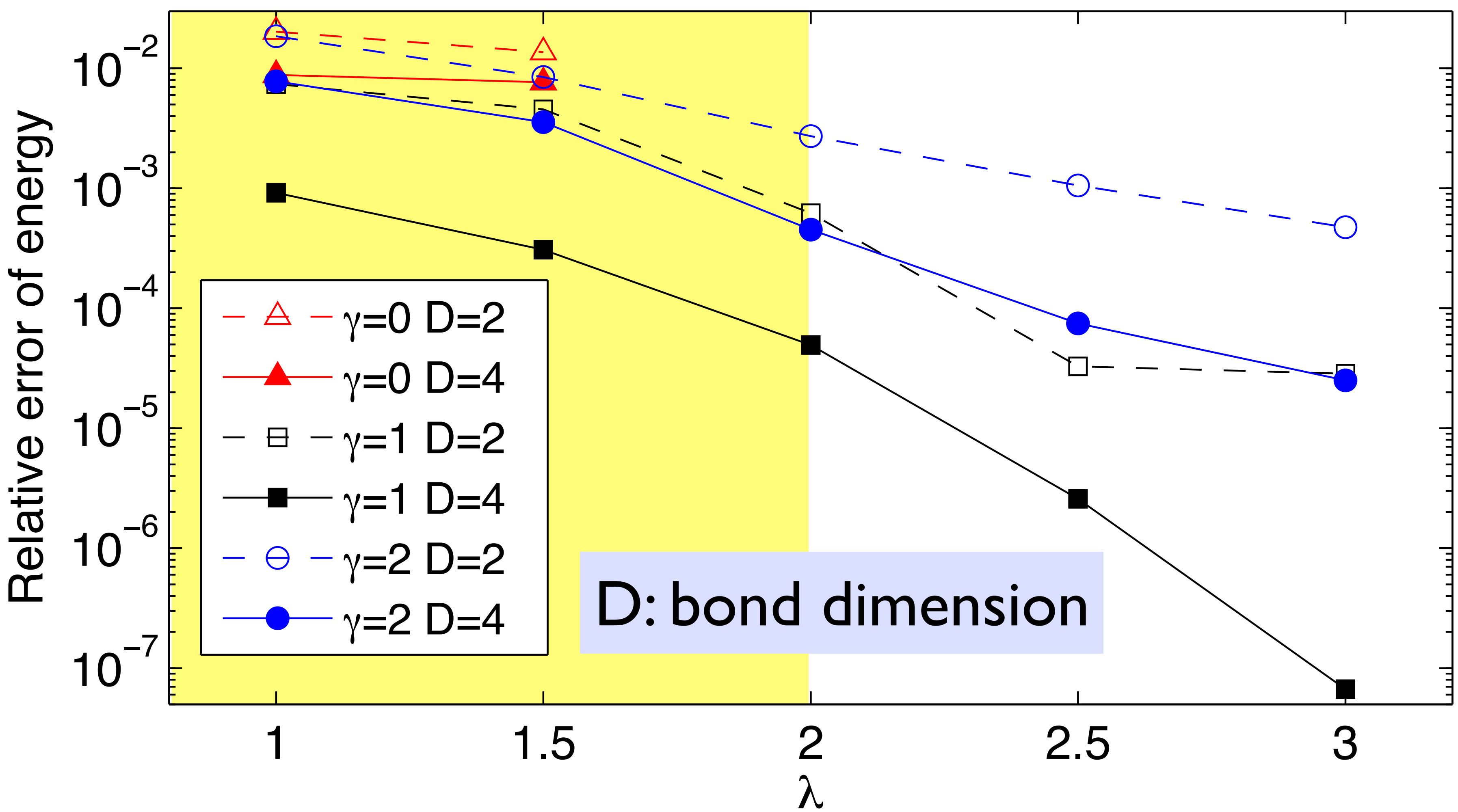
low	**gapped systems**	band insulators, valence-bond crystals, s-wave superconductors, ...
	gapless systems with area law	Heisenberg model, d-wave / p-wave SC, Dirac Fermions, ...
high	**systems with "1D fermi surface"**	free Fermions, Fermi-liquid type phases, bose-metals?

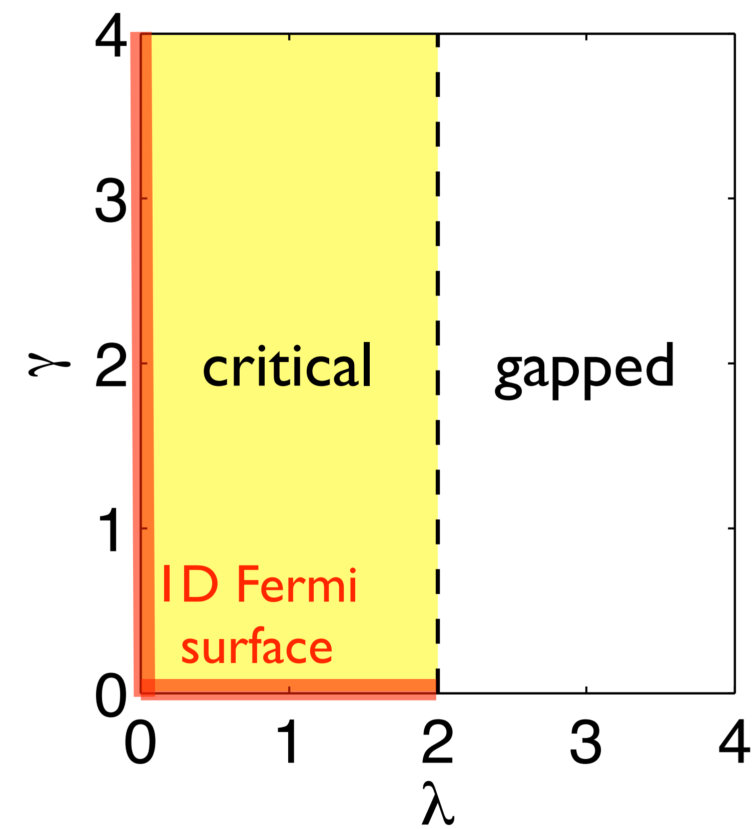
$$S(L) \sim L \log L$$

Non-interacting spinless fermions (old iPEPS results)

Corboz, Orús, Bauer, and Vidal, PRB 81 (2010)

$$H_{\text{free}} = \sum_{\langle rs \rangle} [c_r^\dagger c_s + c_s^\dagger c_r - \gamma(c_r^\dagger c_s^\dagger + c_s c_r)] - 2\lambda \sum_r c_r^\dagger c_r$$





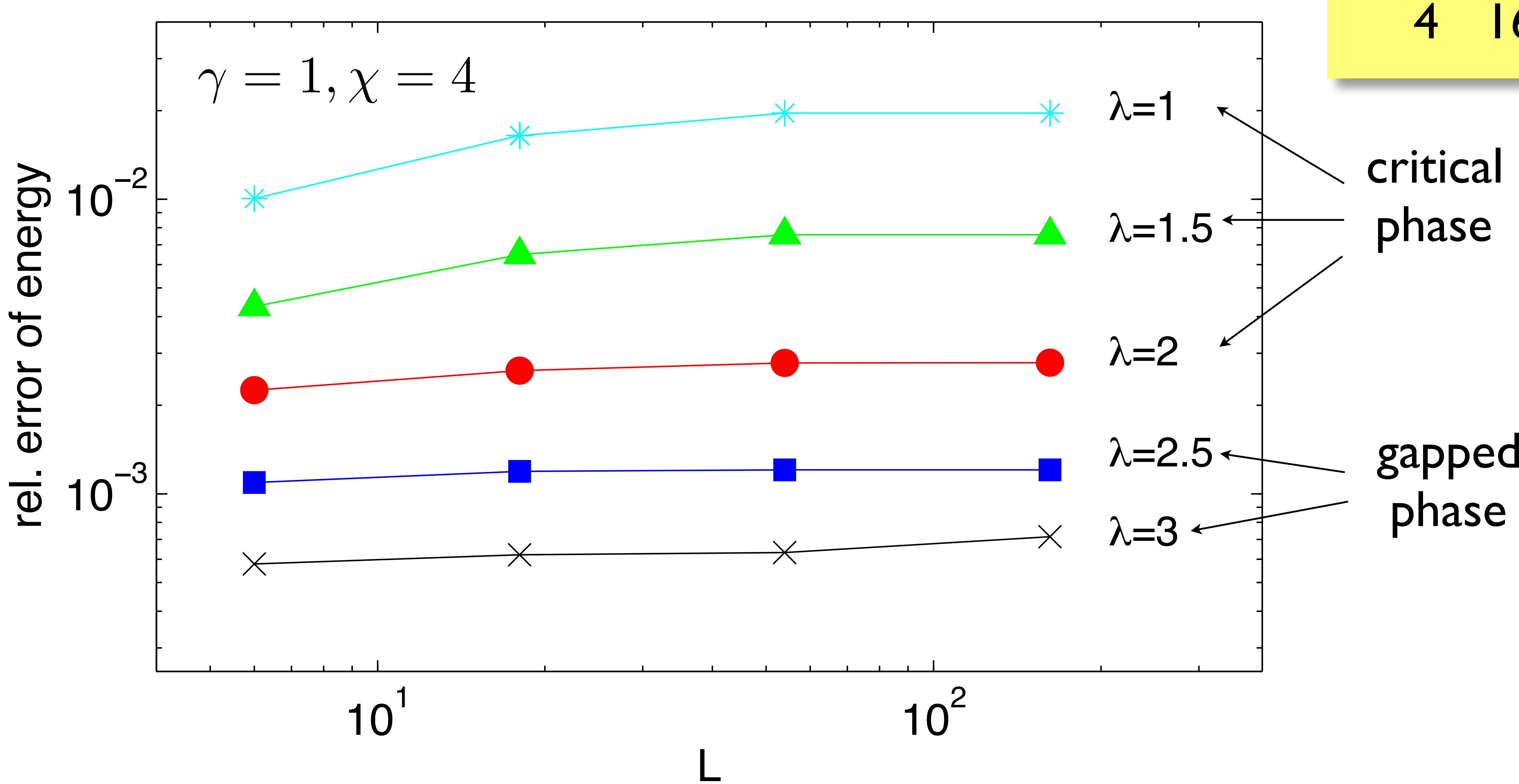
Li et al., PRB 74, 073103 (2006)

fast convergence with D in gapped phases

slow convergence in phase with 1D Fermi surface

Non-interacting fermions (2D MERA)

Layers	Size
1	6x6
2	18x18
3	54x54
4	162x162



Error ≈ constant with L → 2D MERA is scalable!