Full update optimization in symmetry-broken and symmetry-preserving phases

Juraj Hasik, Federico Becca

Tensor Networks | Motivation

Complete information about a ground state (or any other state) ...

$$|\psi\rangle = \sum_I c_I |n_i\rangle$$

.... we need a **basis** and **coefficients**

Problem ? **Dimensionality** grows exponentially with the system size !

$$dim(\mathcal{H}) = dim(\mathcal{H}_{site})^N$$

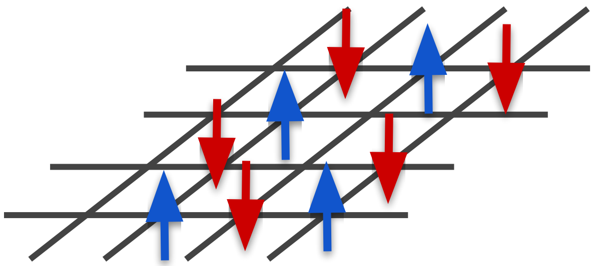
Moreover we are interested in the thermodynamic limit - **N ⟶ ∞**

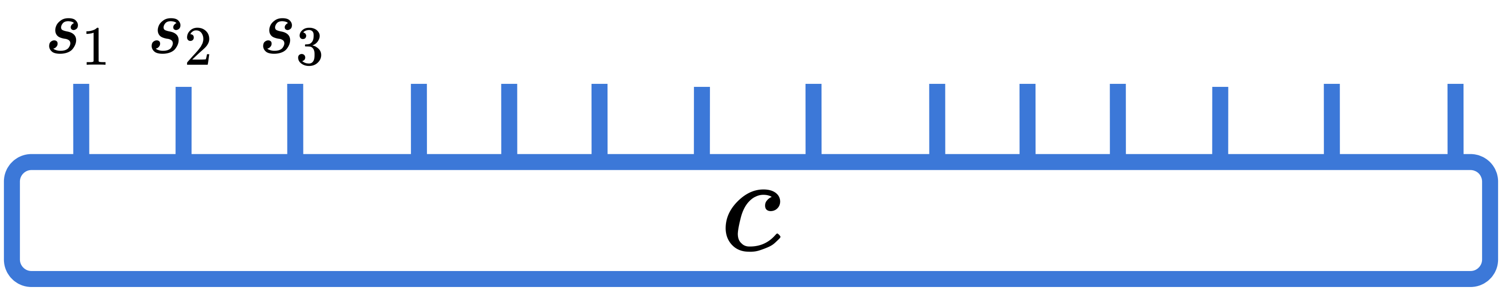
Just for comparison: Size of **ALL the data** on the internet ≂ **10^18** “numbers”
Hilbert space of 10x10 lattice of spins **10^30**

Tensor Networks | A proposal - iPEPS

Generic wavefunction on a square lattice in the spin basis

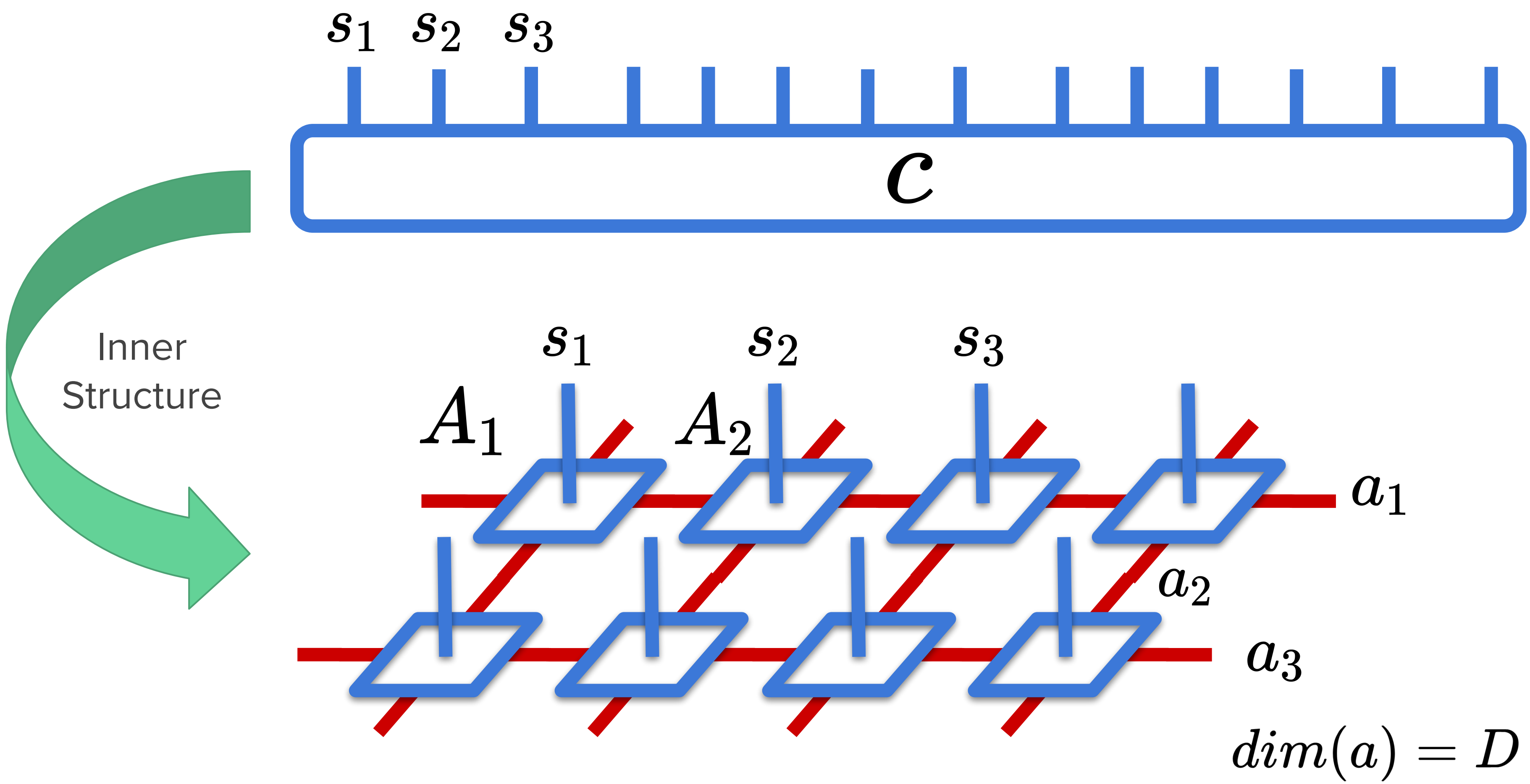
$$|\psi\rangle = \sum_{s_1 s_2 \ldots} c_{s_1 s_2 \ldots} |s_1 s_2 \ldots\rangle$$





Number of parameters: $2^{\#spins}$

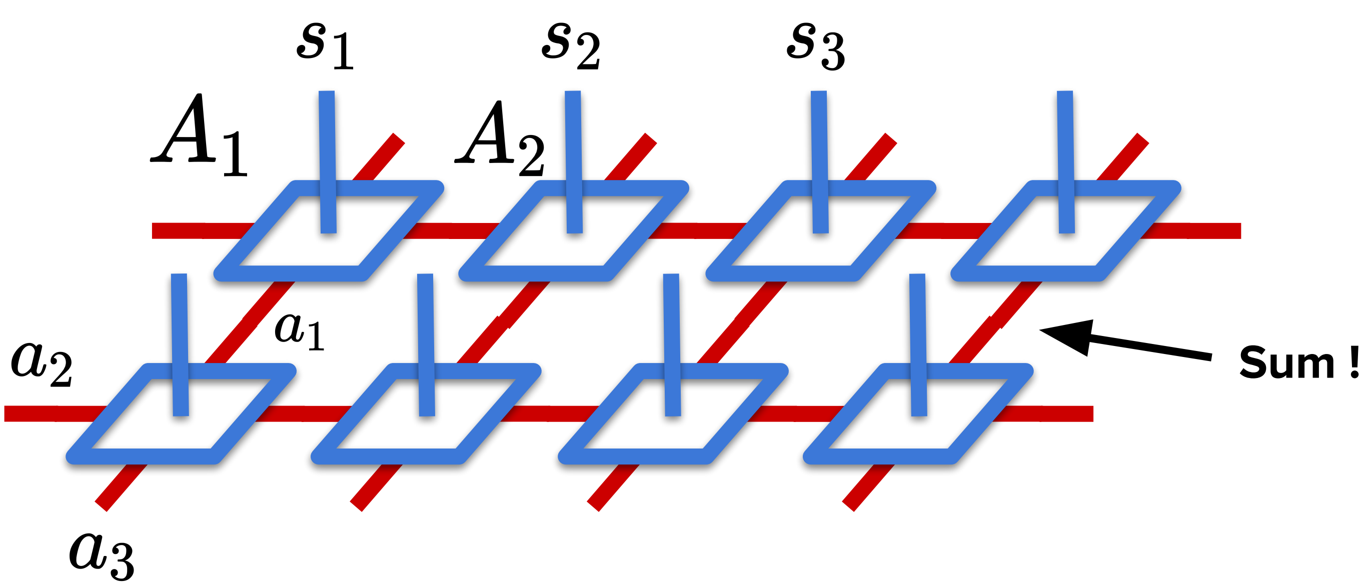
Tensor Networks | A proposal - iPEPS



where each **A** is D x D x D x D x d tensor holding variational parameters

Tensor Networks | A proposal - iPEPS

We express **all** coefficients through tensors $c_{s_1 s_2 \ldots} = Tr_{aux}(A^{s_1} A^{s_2} \ldots)$



$$|\psi\rangle = \sum_{|s_1 s_2 \ldots\rangle} Tr_{aux}(A^{s_1} A^{s_2} \ldots)|s_1 s_2 \ldots\rangle$$

Tensor Networks | Properties of iPEPS

Variational wavefunction targeting **ground states** of fermionic or spin lattice models with local Hamiltonian

- **systematically improvable** with bond dimension D
- satisfy **area law** by construction
- **no** sign problem
- can break or impose **translational symmetry**
- or **internal symmetries**
- good compression properties

F. Verstraete and J. I. Cirac, arXiv:cond-mat/0407066, (2004)
R. Orús, Annals of Physics, 349 (2014)

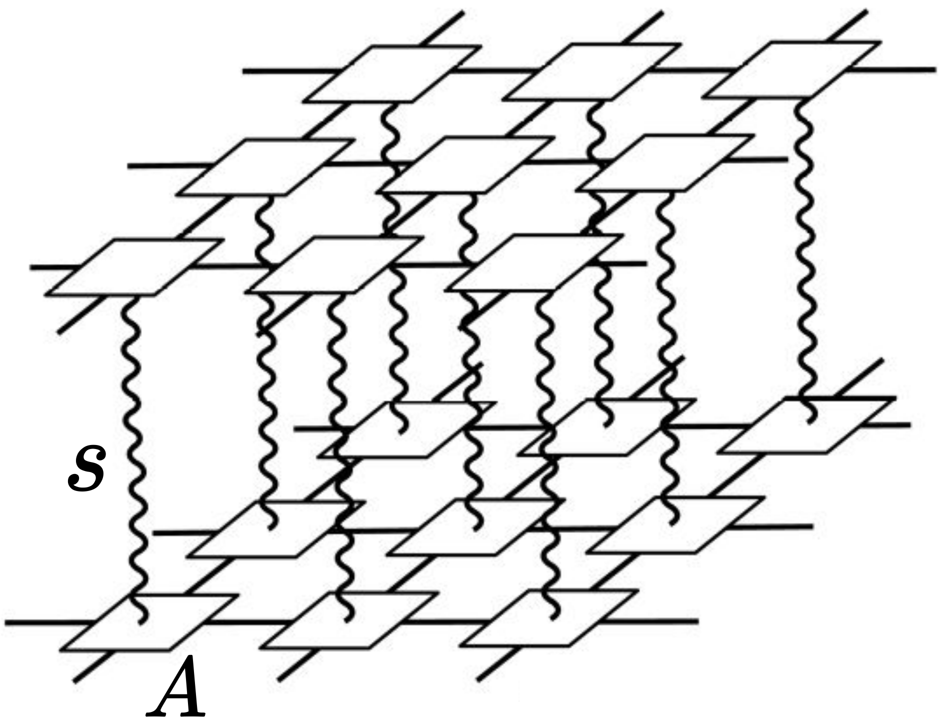
Properties of iPEPS | Area Law

Area law: property of ground states of **local** and **gapped** Hamiltonians

$$Tr(\rho_R log \rho_R) \propto |\partial R|$$

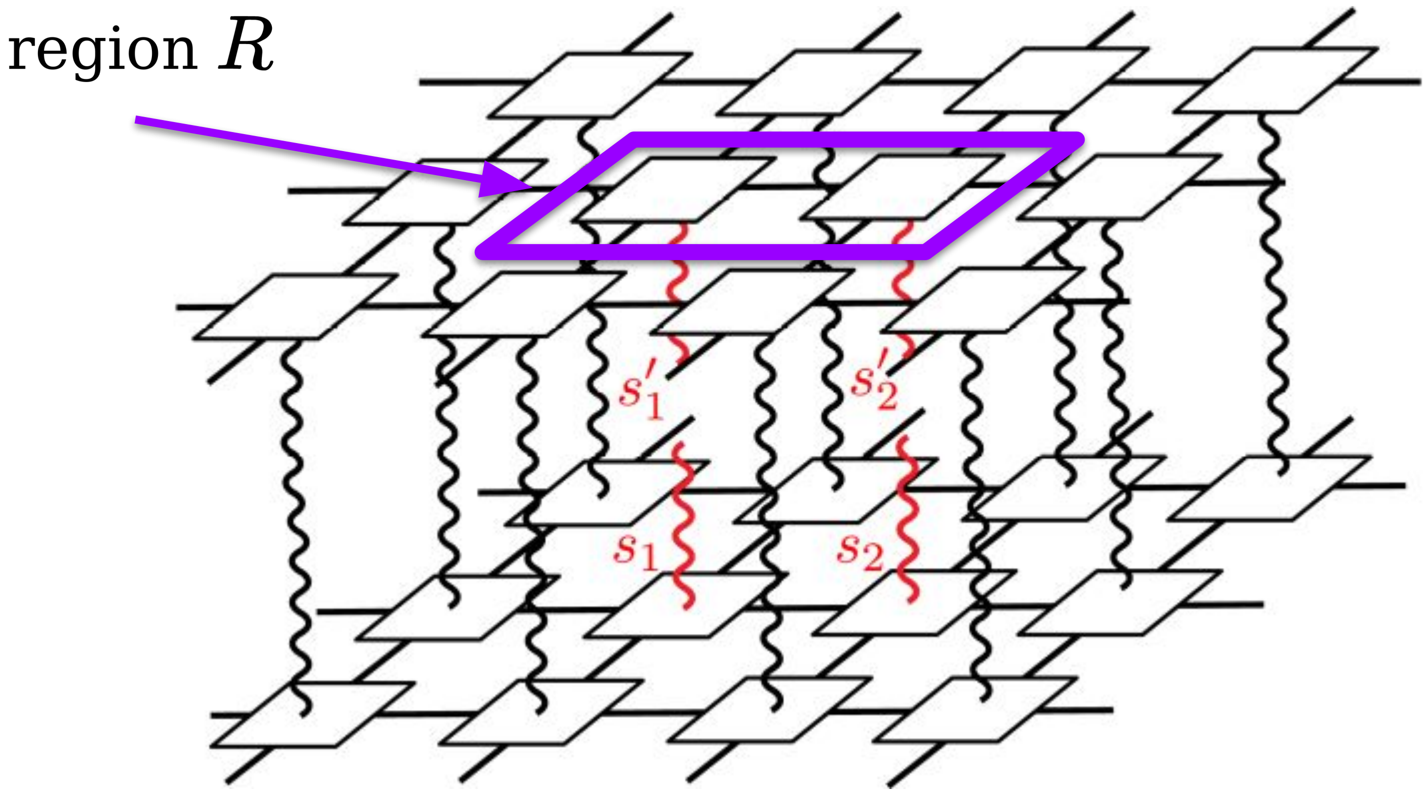
How to see this ? Let's start with a norm ...

$$\langle\psi|\psi\rangle =$$



Properties of iPEPS | Area Law

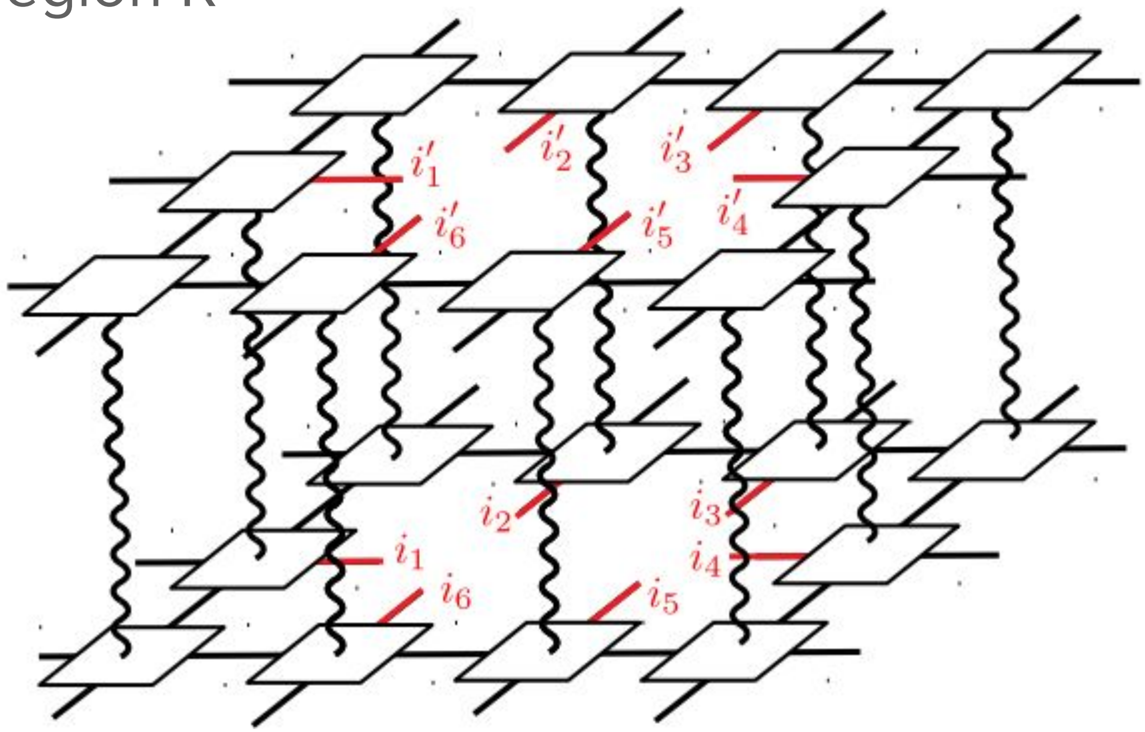
$$\rho_{s_1 s_2; s_1' s_2'} = \sum\nolimits_{\notin s_1 s_2; s_1' s_2'} c^*_{s_1' s_2' s_3' \ldots} c_{s_1 s_2 s_3 \ldots}$$



Properties of iPEPS | Area Law

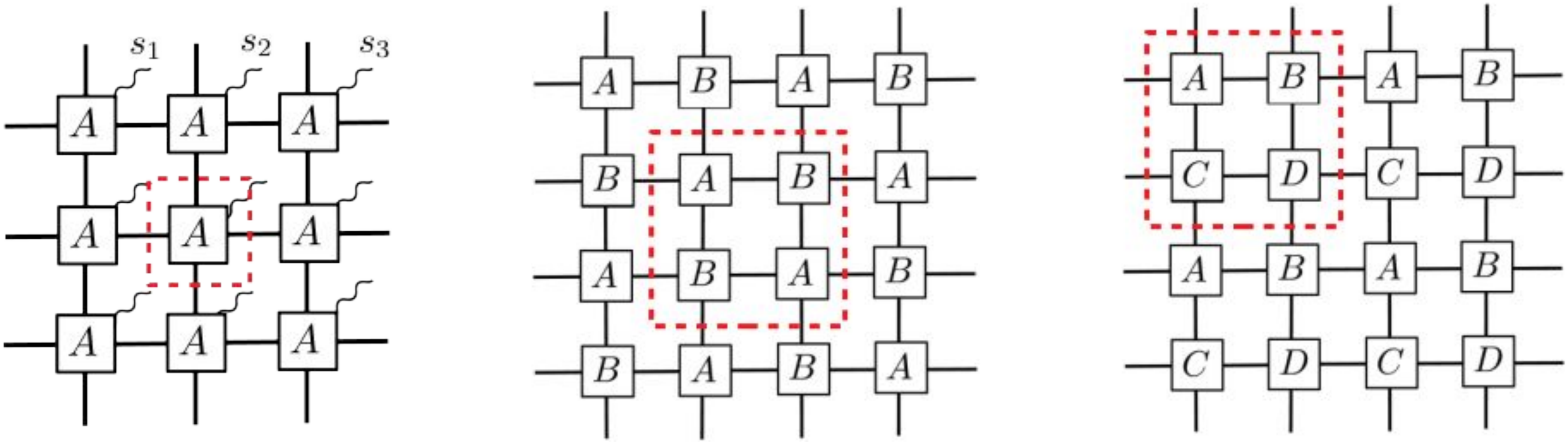
Environment of region R

$$E :=$$



Entanglement entropy proportional to $D^{\#aux} \approx D^{|\partial R|}$

Properties of iPEPS | Translational symmetry



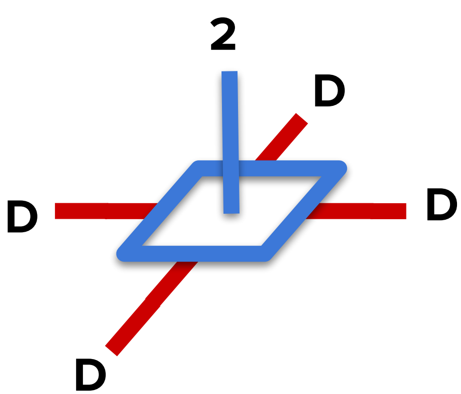
iPEPS: Class of (non)linear functions of many variables

$$c_{s_1 s_2 \ldots} = Tr_{aux}(A^{s_1} B^{s_2} C^{s_3} D^{s_4} A^{s_5} \ldots)$$

Properties of iPEPS | Compression properties

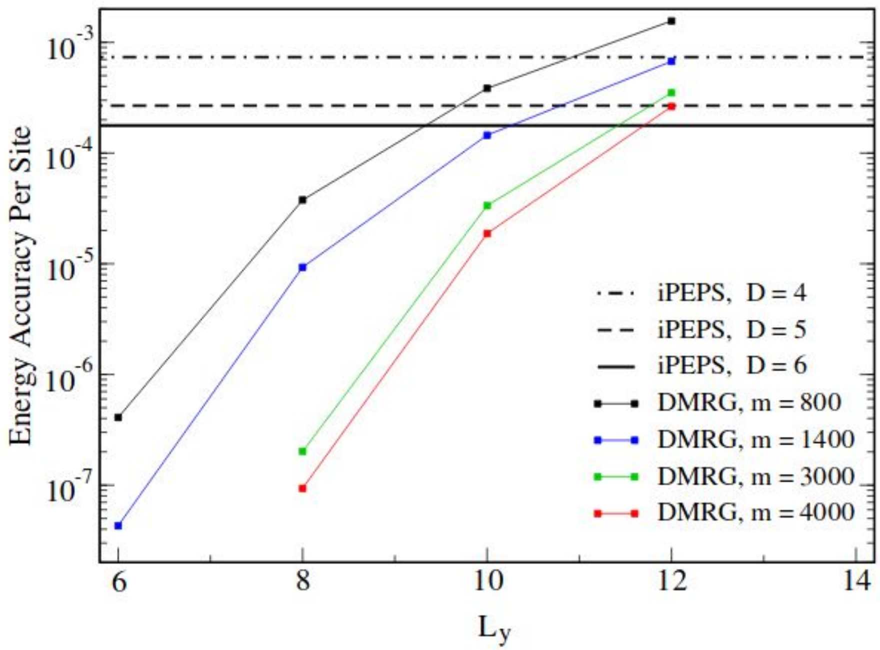
Take iPEPS with **bond dimension D**.

How many elements do we have ?



Parameters: $2D^4$

2D Heisenberg



E.M. Stoudenmire, Steven R. White, Annu. Rev. Condens. Matter Phys., 3 (2011)

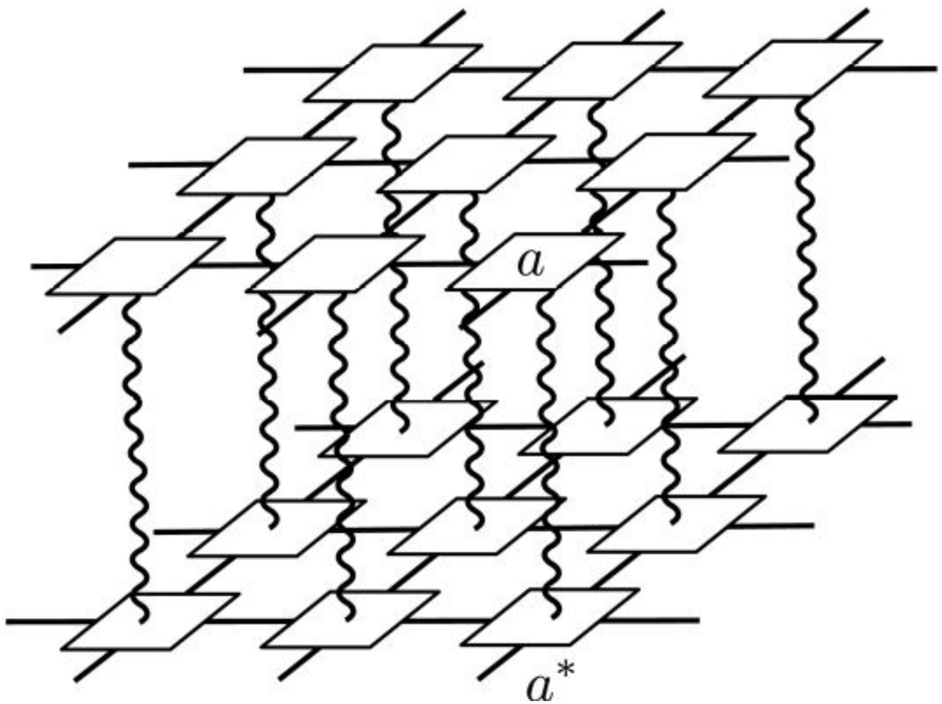
J. O. Iregui, M. Troyer, P. Corboz, *PRB 96 (2017)*

For large system - DMRG **O(10^6)** vs iPEPS **O(10^3)**

iPEPS | Expectation values

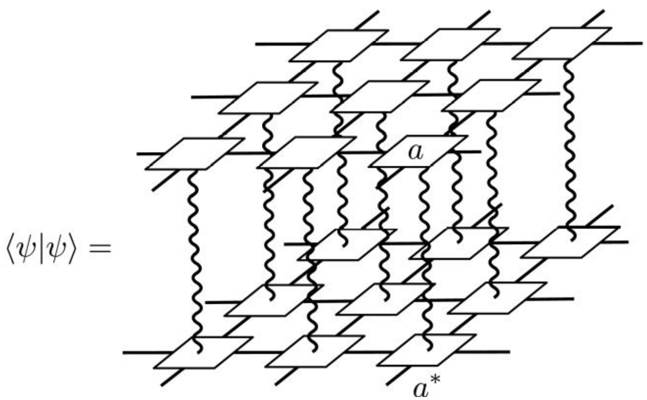
Let's again look at the network representing a norm **from above**

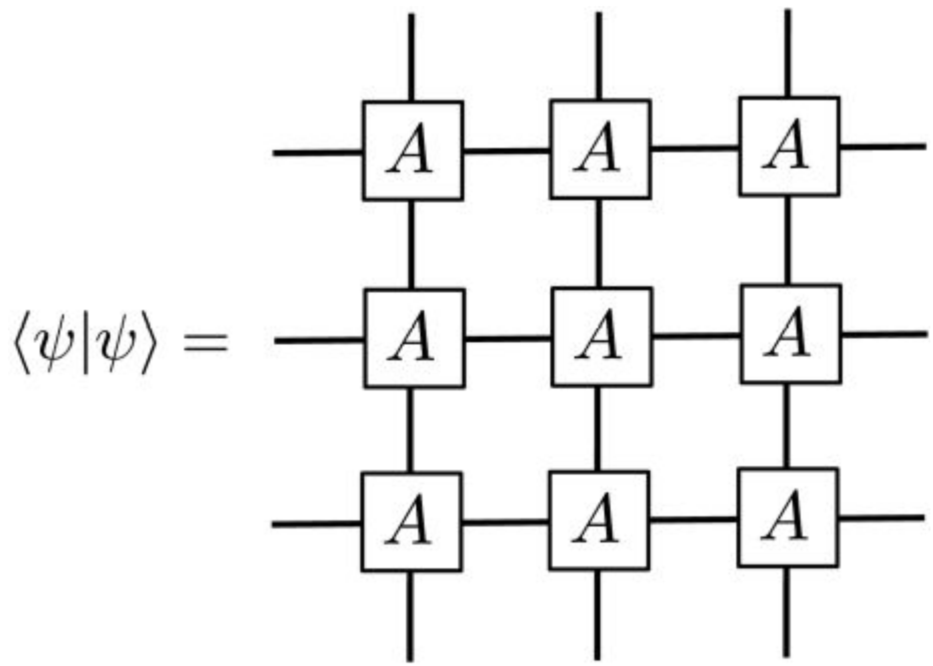
$$\langle\psi|\psi\rangle =$$



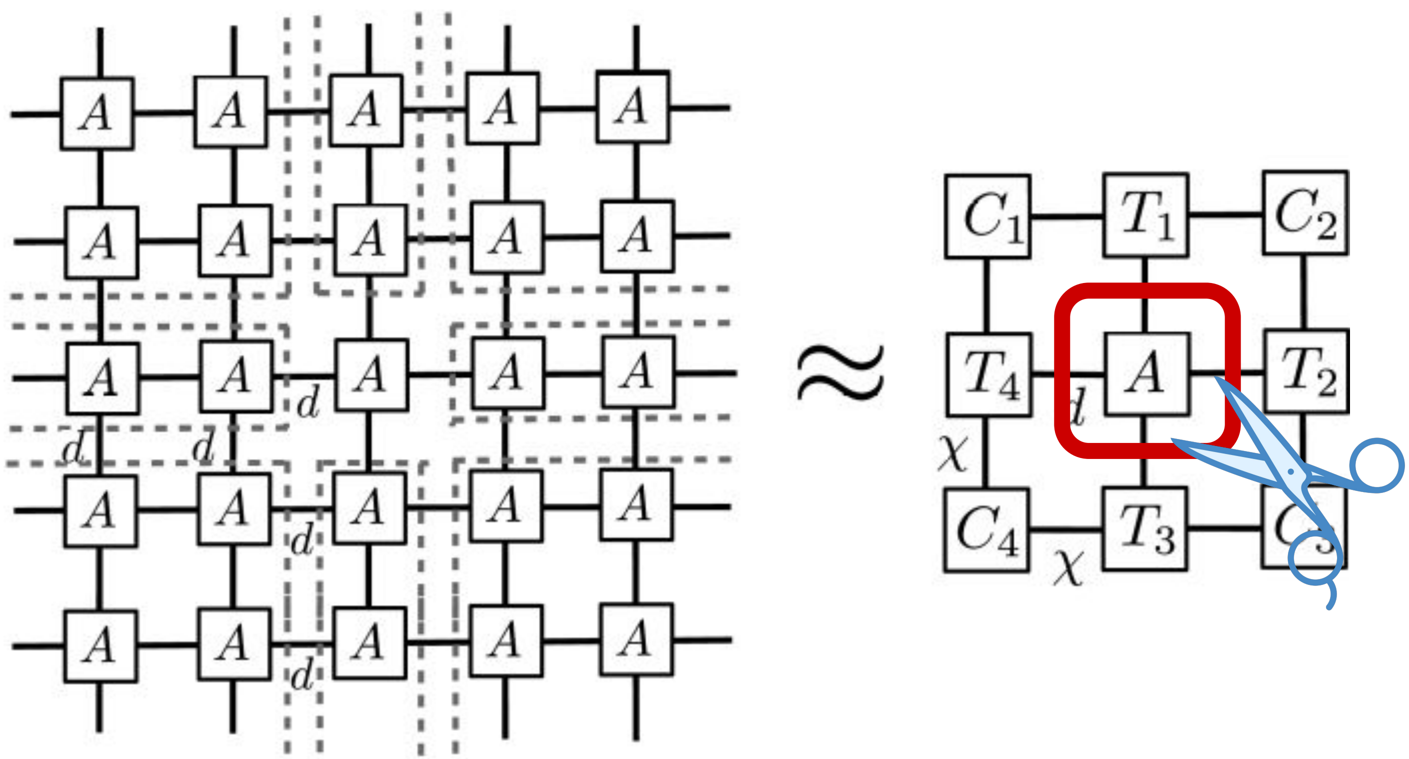
iPEPS | Expectation values

Let's again look at the network representing a norm **from above**



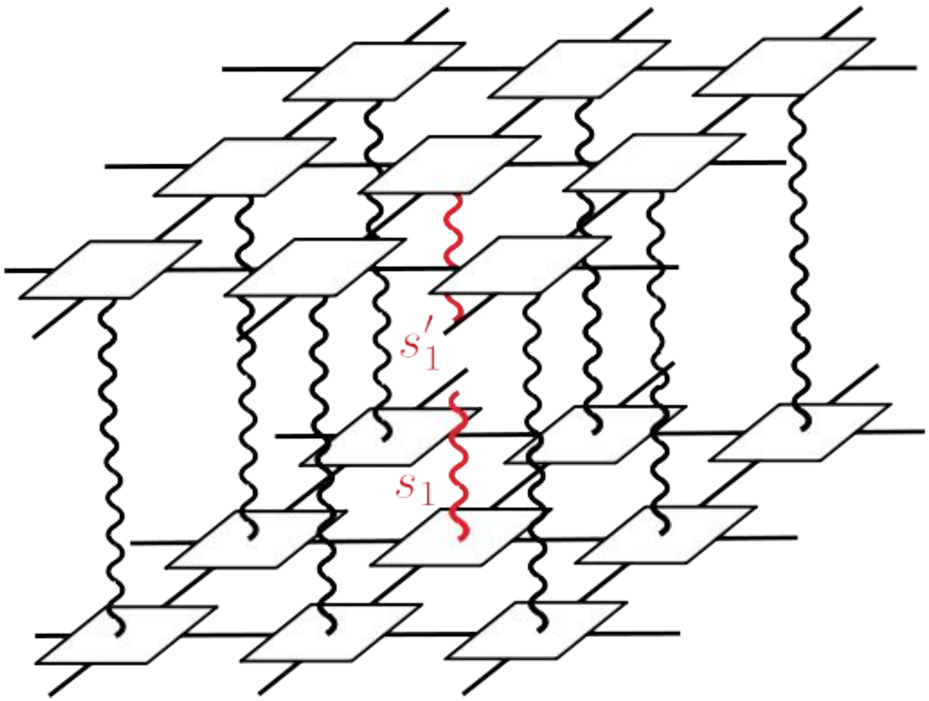


iPEPS | Expectation values

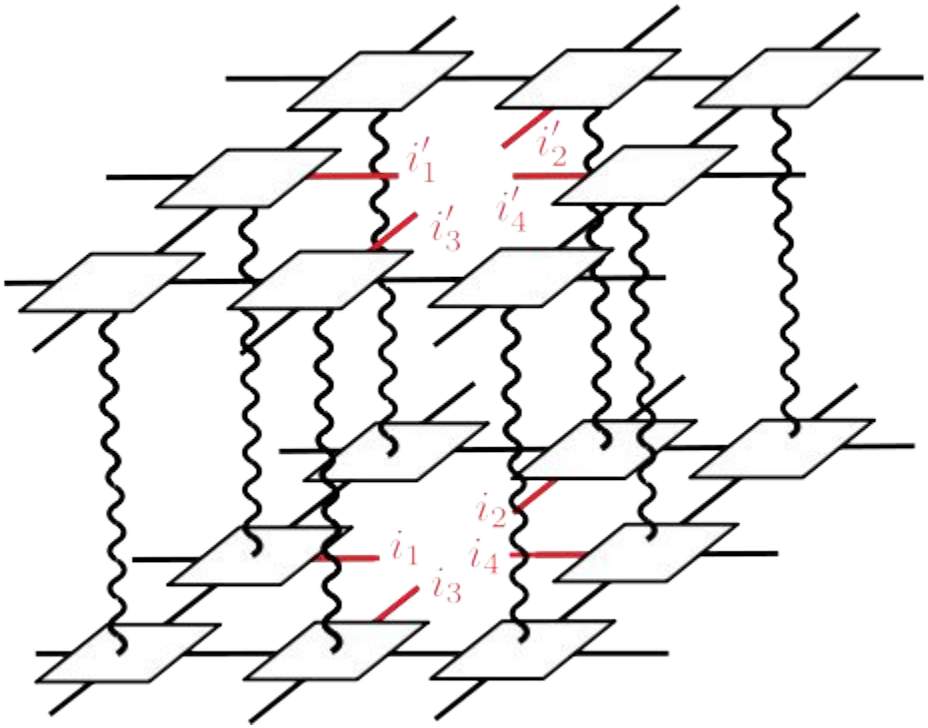


$$\langle\psi|\psi\rangle = \sum(A\ldots A\ldots) \rightarrow \sum(C_1 T_1 C_2 \ldots A)$$

iPEPS | Expectation values

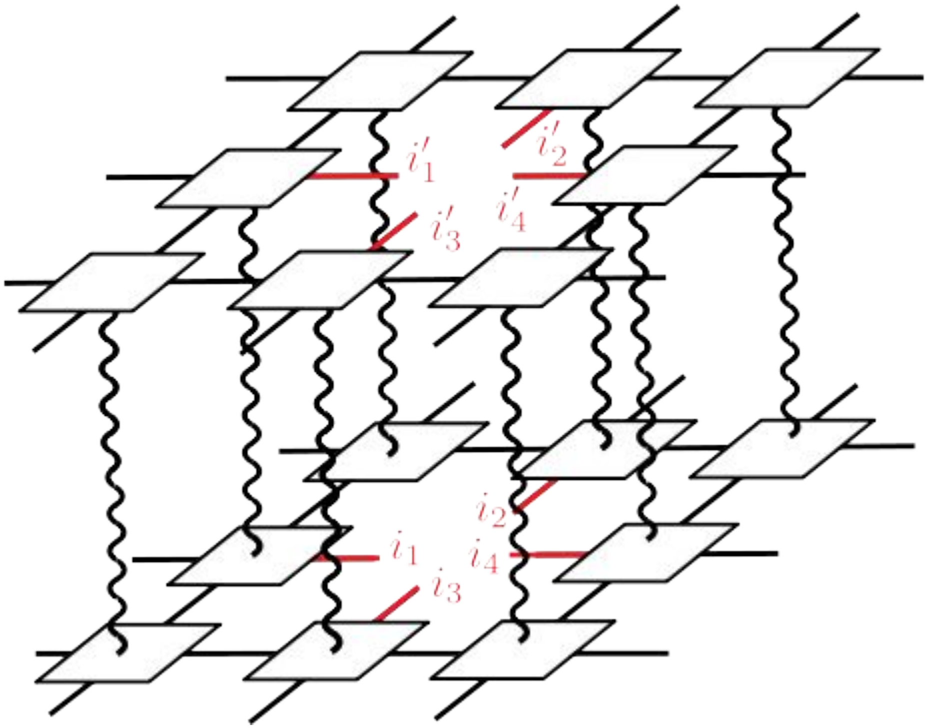


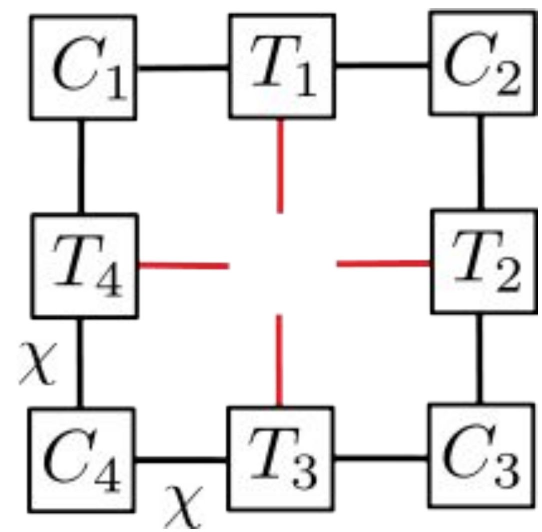
$\rho_{phys}(1site)$



$\rho_{aux}(1site)$

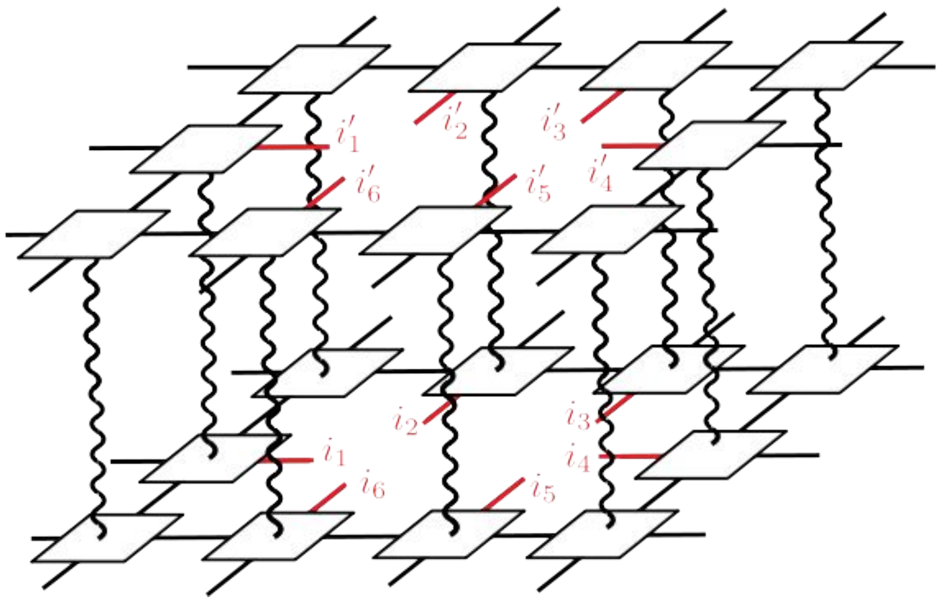
iPEPS | Expectation values

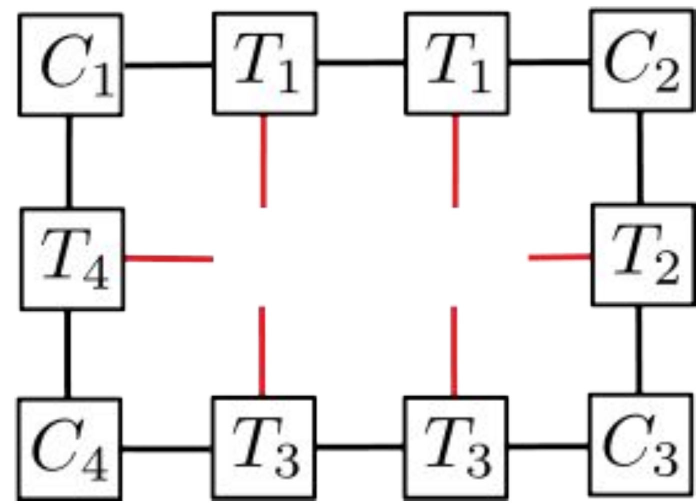




$$\rho_{aux}(1site) \rightarrow \sum(C_1 T_1 C_2 \ldots)$$

iPEPS | Expectation values

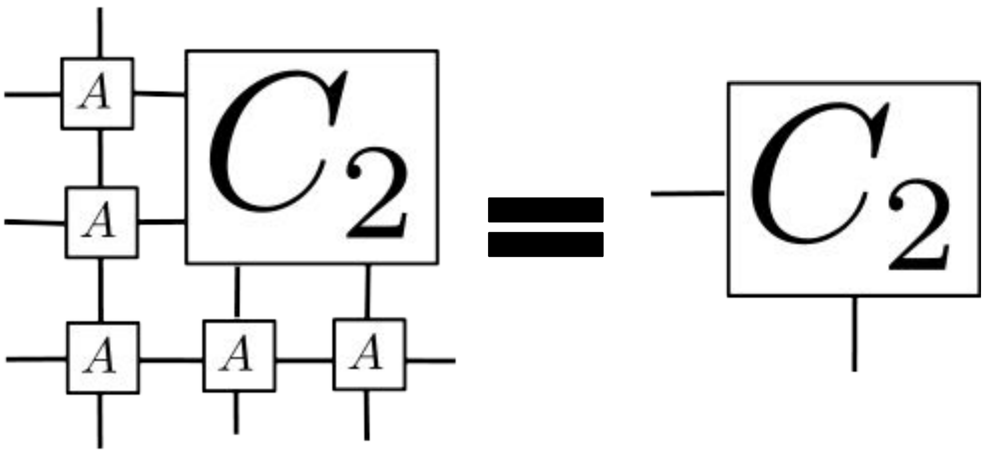


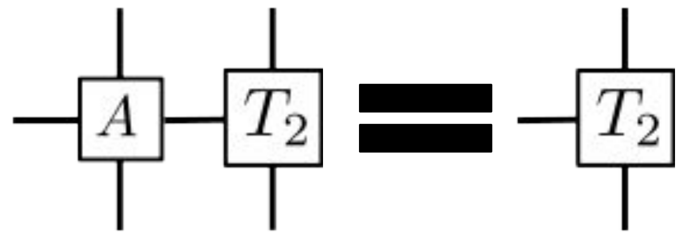


$$\rho_{aux}(2site) \rightarrow \sum(C_1 T_1 T_1 C_2 T_2 \dots)$$

iPEPS | Getting the environment

Solve **fixed point** equations





foundations:

T. Nishino, K. Okunishi, J. Phys. Soc. Jpn. 65 (1996)

iPEPS:

R. Orús, G. Vidal, PRB 80 (2009)

P. Corboz, T.M. Rice, M. Troyer, PRL 113 (2014)

Alternative approach - channel environments

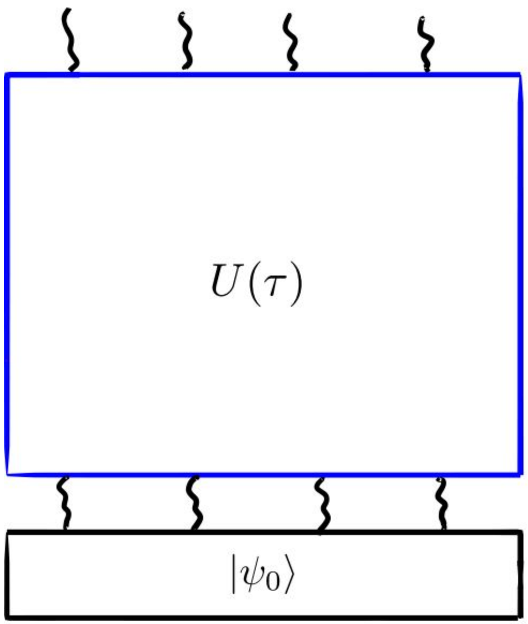
L. Vanderstraeten et. al, Phys. Rev. B 94 (2016)

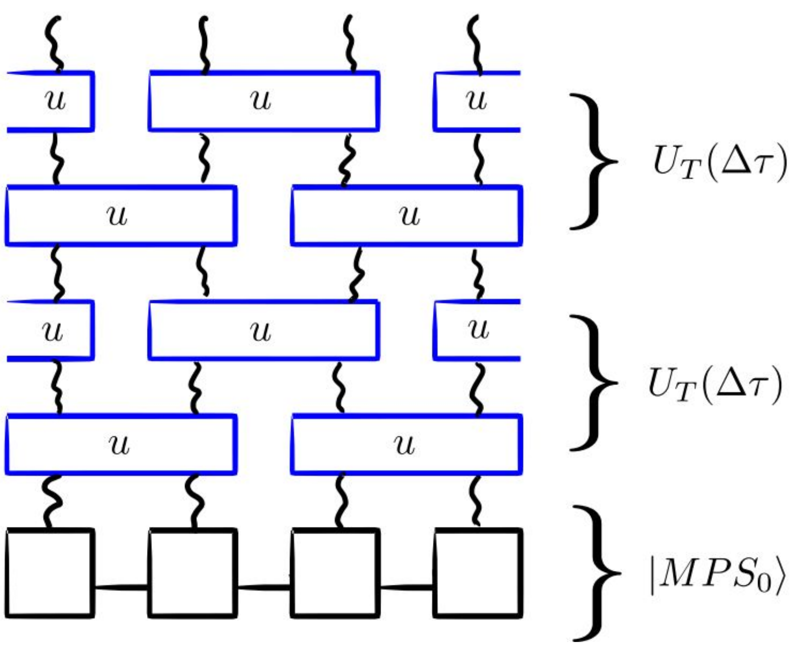
iPEPS | Optimization (sketch)

Ground state is equivalent to **fixed point** of imaginary time evolution operator

$$U(\tau) := exp(-\tau H)$$

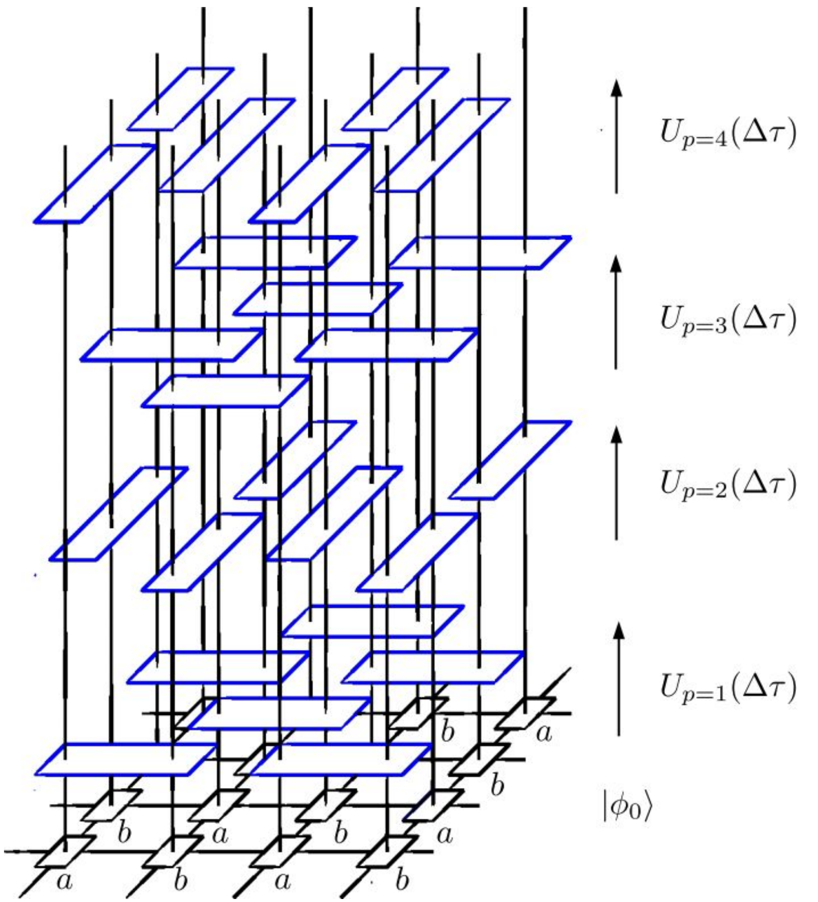
... but that's a too complicated object: perform **Trotter decomposition**





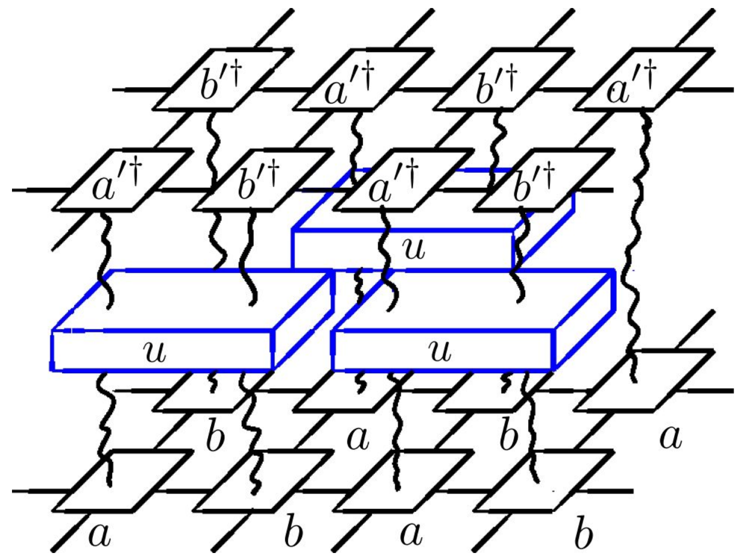
iPEPS | Optimization (sketch)

Infinite stack - impossible to handle efficiently ...



... proceed **layer by layer:**

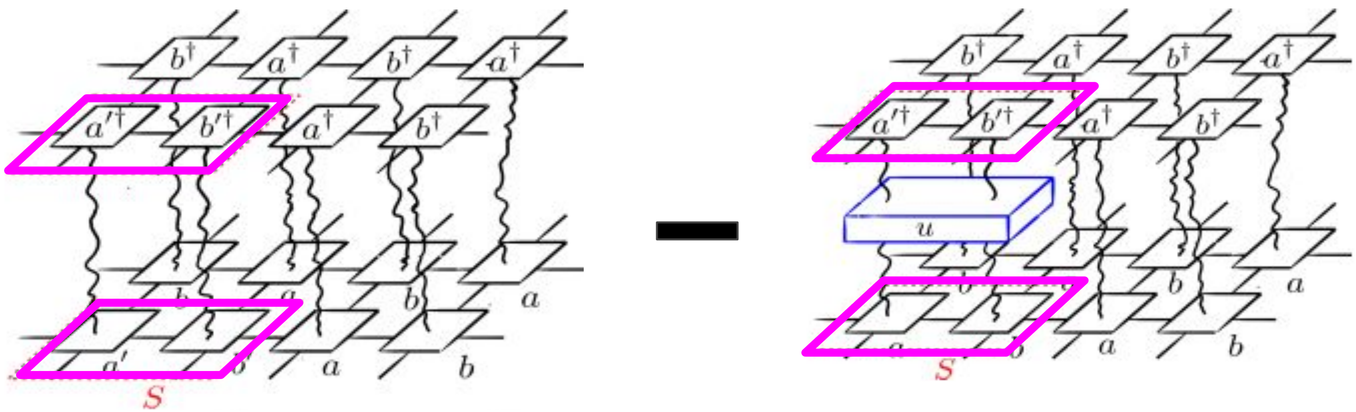
$$\langle a'b'|U(\Delta\tau)|ab\rangle$$



iPEPS | Optimization (sketch)

Reduce the problem problem even more - treat only
single gate

$$|a_{n+1}, b_{n+1}, \ldots; \bar{\phi}_n\rangle = \underset{a', b', \ldots \in \mathcal{H}_t}{\operatorname{argmin}} \left| |a', b', \ldots; \bar{\phi}_n\rangle - u_{ij} |a_n, b_n, \ldots; \bar{\phi}_n\rangle \right| .$$

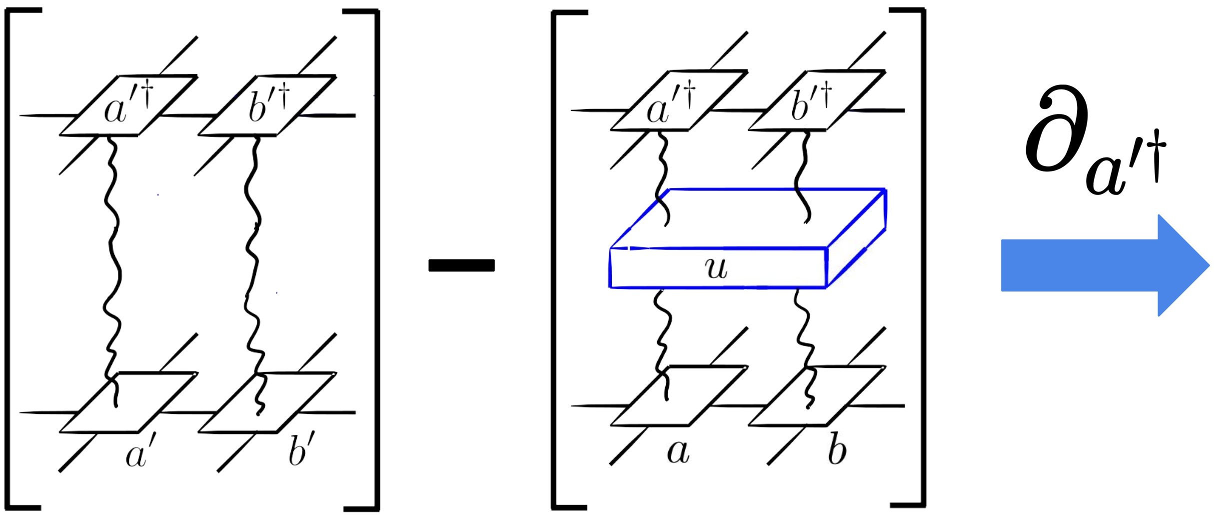


$\langle a', b', \ldots; \bar{\phi}_n | a', b', \ldots; \bar{\phi}_n \rangle$ − $\langle a', b', \ldots; \bar{\phi}_n | u_{ij} | a, b, \ldots; \bar{\phi}_n \rangle$

J. Jordan et. al, PRL 101 (2008), M. Lubasch; H. N. Phien et. al, PRB 92 (2015)
J. I. Cirac, M. C. Bañuls, PRB 90, (2014)

iPEPS | Optimization (sketch)

ALS: Break up the optimization problem into **series of linear problems**



$$\rho_{2site}(a,b) \qquad \rho_{2site}(a,b)$$

$$Ma' = K$$

Controls governing the optimization:

- precision of the environment:
  how many CTM iterations per step,
  initialize from scratch everytime ?
  cutoff on singular values
- ALS:
  tolerance on the cost function,
  regularization and precondioning
  of the linear system
  initialization of tensor a', b'
- Trotter Decomposition:
  time step,
  order of the Trotter gates

iPEPS | Algorithms

All of this and a bit more is implemented here

(CTM on arbitrary unit cells, 2-site and 3-site simple and full update, ...)

github.com/jurajHasik/pi-peps

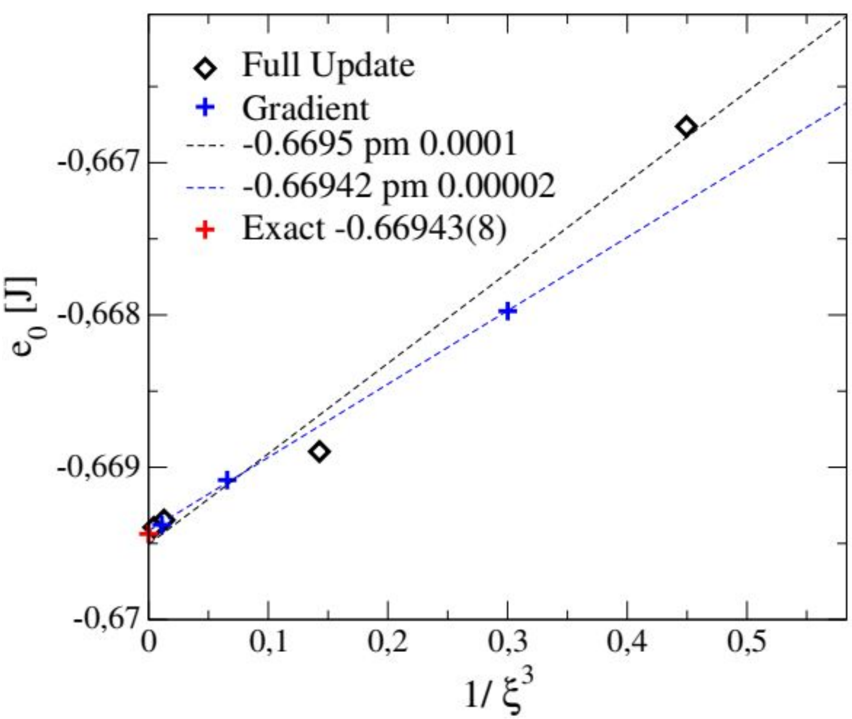
Caveat: Documentation is still work in progress

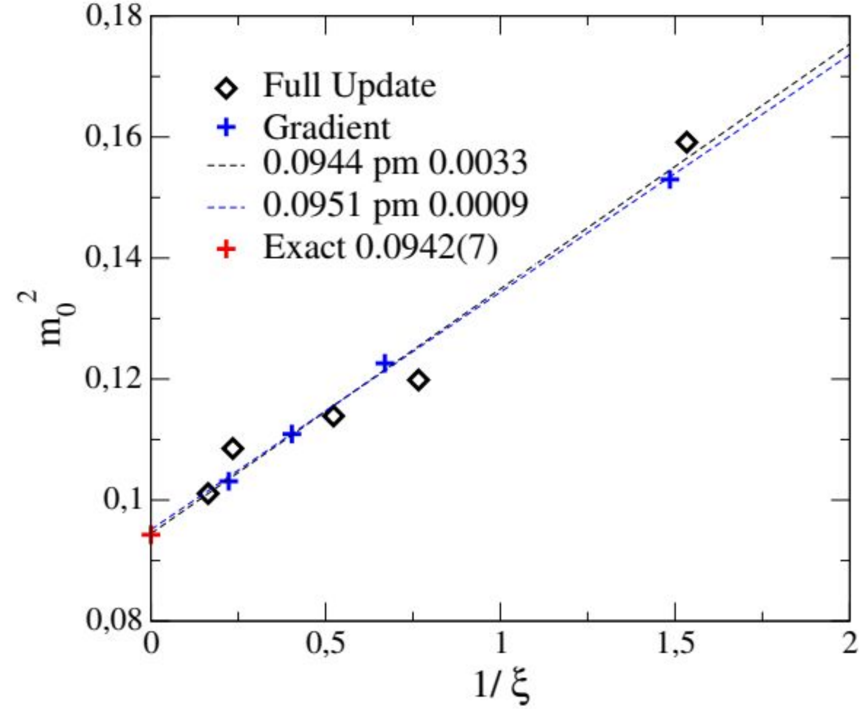
iPEPS | Symmetry-broken phase

Case: Heisenberg model $$H = \sum_{\langle i,j \rangle} S_i \,.\, S_j$$

Can we use **finite-size** scaling ? Q: Let's try, but what is the **length scale** ?

A: **Correlation length** !





A. W. Sandvik, PRB 56 (1997); M. Rader and A. M. Läuchli, PRX 8 (2018), P. Corboz et. al, PRX 8 (2018)

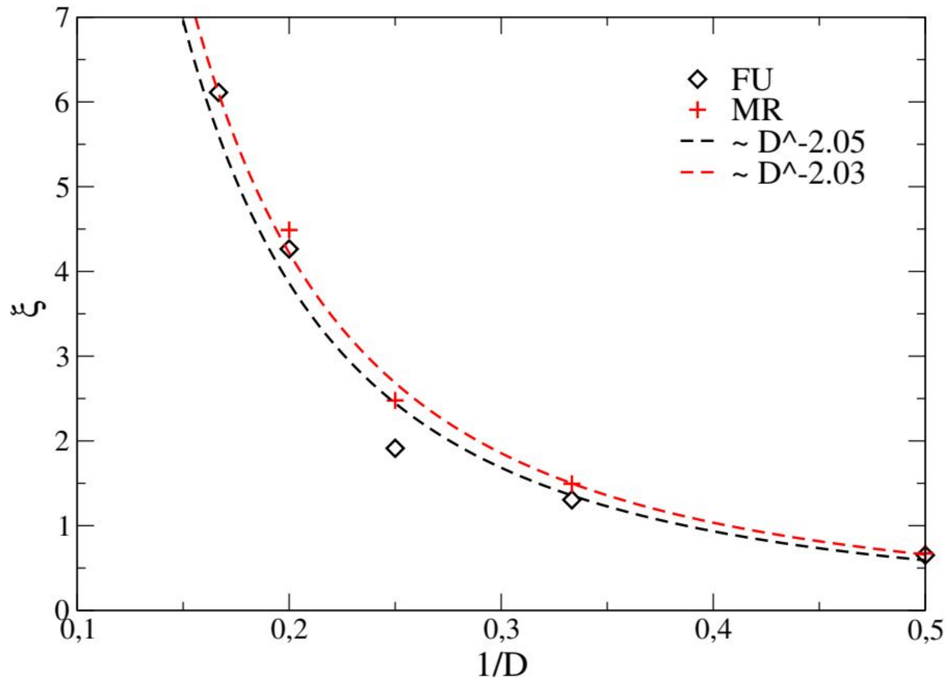
iPEPS | Symmetry-broken phase

Case: Heisenberg model $$H = \sum_{\langle i,j \rangle} S_i \, . \, S_j$$

True ground state is **gapless** ⇔ **diverging correlation length**

- not FU nor gradient optimization gives **finite D iPEPS** with diverging correlation length

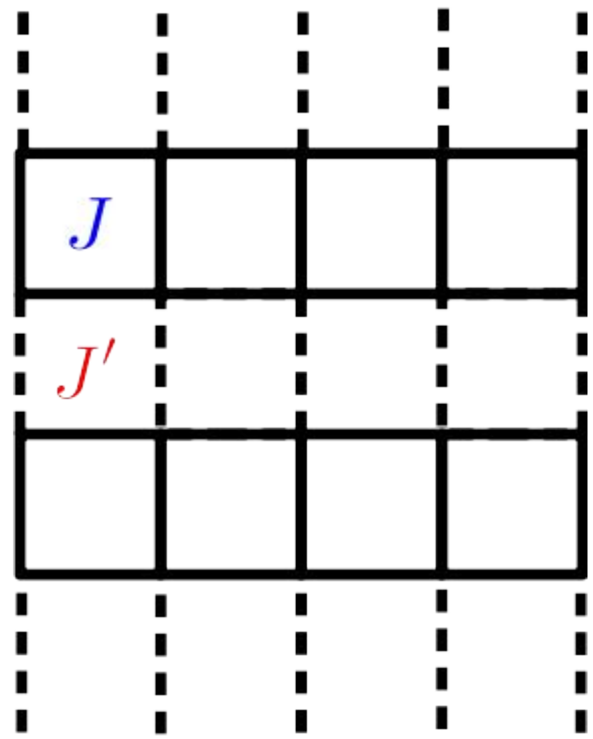
- iPEPS correlation length **diverges** with D



iPEPS | SU(2) symmetric phase

Spin ½ coupled ladders

$$H = J \sum_{r} \vec{S}_r . \vec{S}_{r+\hat{x}} + J \sum_{r|r_y \in even} \vec{S}_r . \vec{S}_{r+\hat{y}} + J' \sum_{r|r_y \in odd} \vec{S}_r . \vec{S}_{r+\hat{y}}$$



- Quantum order-disorder phase transition for **critical J’ ≈ 0.314**
- For small inter-ladder coupling GS is a gapped VBS

QMC: M. Matsumoto et. al, PRB 65 (2001); L. Capriotti, F. Becca, PRB 65 (2002)

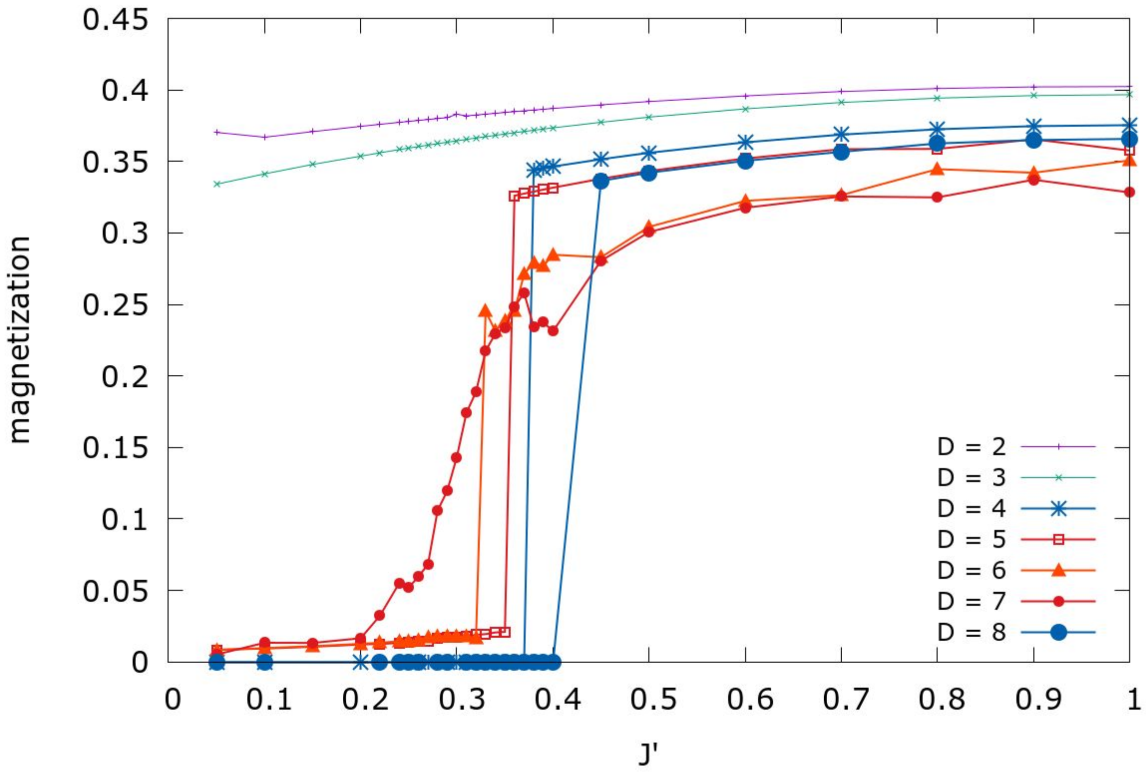
iPEPS | SU(2) symmetric phase

Initial analysis - **simple update**

- seed by AFM state or VBS formed by singlets on the rungs of ladders

Behaviour is **not** monotonic with **D**:

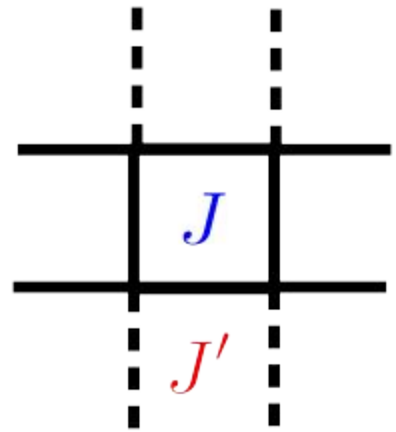
- D = 4,8 captures non-magnetic phase
- D = 5,6,7 develops **finite magnetization** even for J’ < J’crit



iPEPS | SU(2) symmetric phase

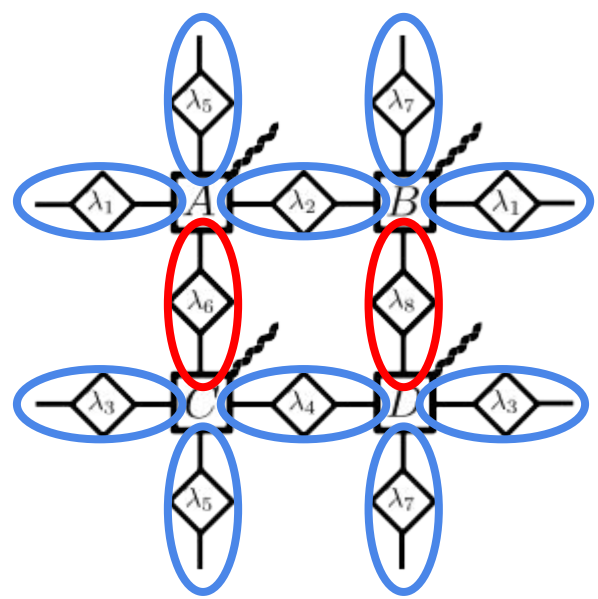
What is going on ?

Looking at the weights - rigid **block structure** appears



Strong rungs $\quad \mathbf{2} \oplus \mathbf{2} \oplus \mathbf{4} + \ldots$

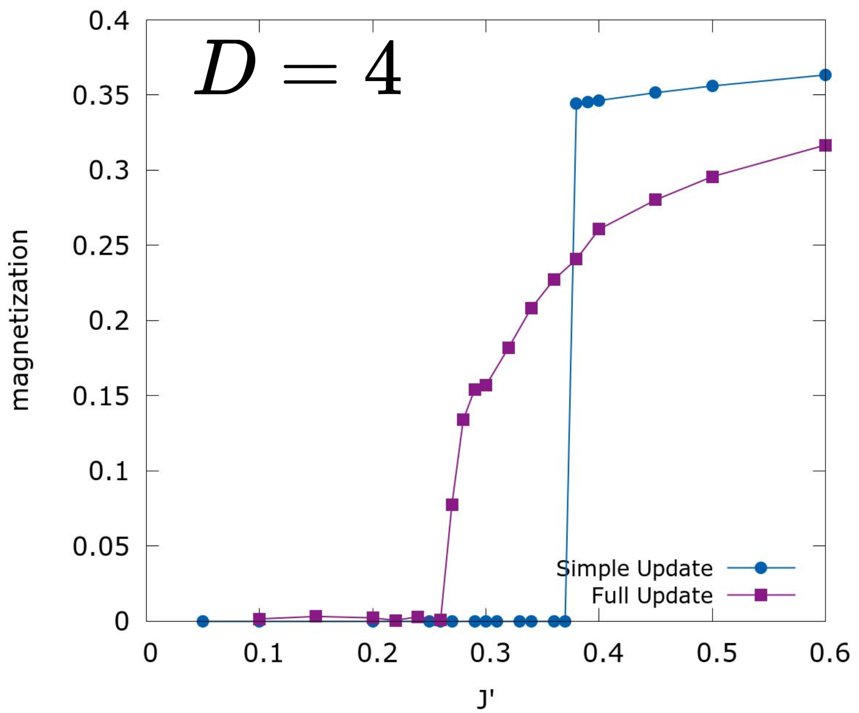
Other $\quad \mathbf{1} \oplus \mathbf{3} \oplus \mathbf{3} \oplus \mathbf{1} + \ldots$

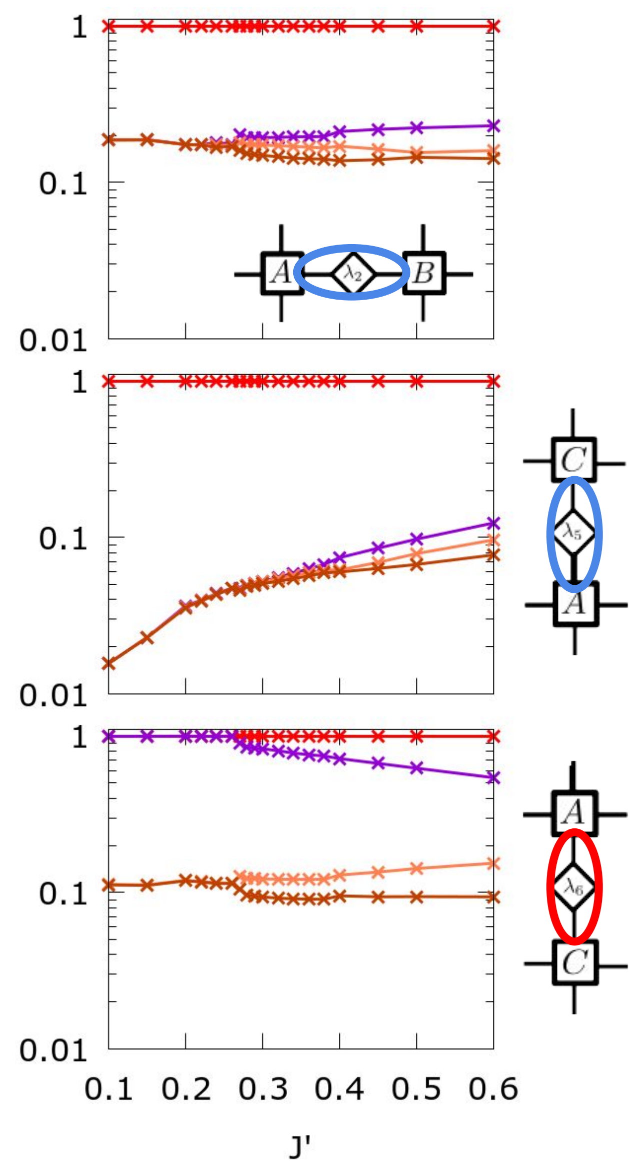


Smallest commensurate D's are exactly **D=4** and **D=8**

iPEPS | SU(2) symmetric phase

- Full update improves the picture - we have second order phase transition
- Symmetry breaking shows up in the blocks on the bonds

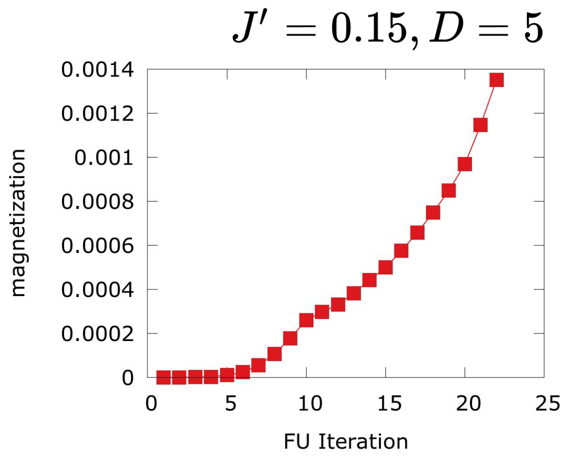


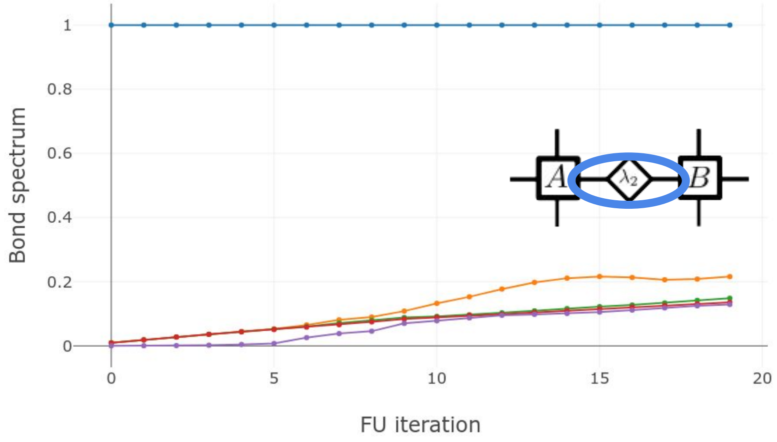


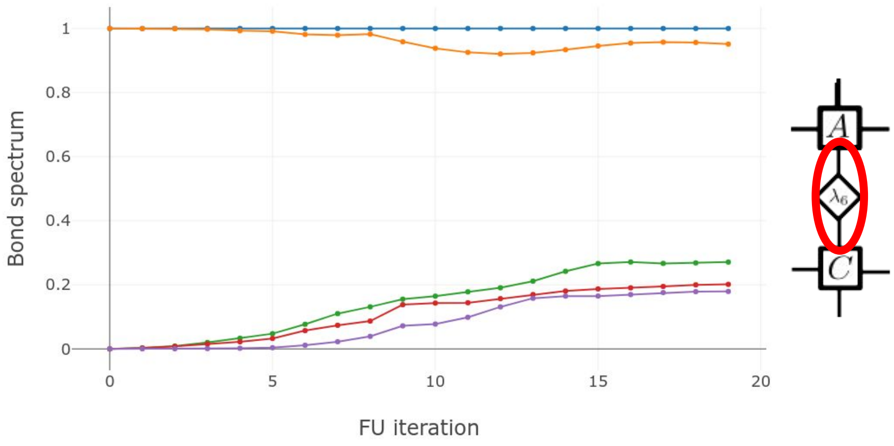
iPEPS | SU(2) symmetric phase

Unrestricted optimization (no blocks) makes sense only for **commensurate D**

To describe SU(2) symmetric phases **block structure** is necessary







iPEPS | Nasty parts & what’s ahead

- Computation of observables scales polynomially ... as **D^12 !!!**
- Still large redundancy ⇔ **gauge freedom**. Why ? Because of the **loops**
- variational parameters have no interpretation

  Partially addressable by imposing symmetric ansatz and/or block structure on auxiliary indices

- **Optimization, optimization, optimization:**

Compute gradients !

- Algorithmically challenging
- Scale to clusters - MPI & GPUs

Thank you!