ETH

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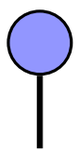
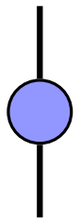
Matrix product states, why DMRG works in 1d, and how to make it work in 2d.

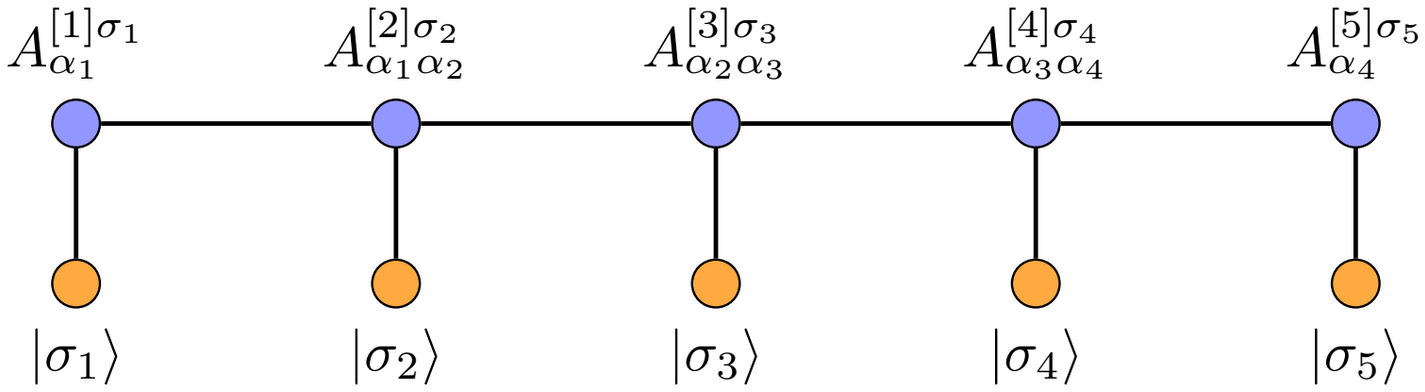
Representing linear algebra pictorially


Scalar


Vector


Matrix

Matrix product states



$$|\Psi\rangle = \sum_{\{\sigma_i\}} \left(A^{[1]\sigma_1} A^{[2]\sigma_2} A^{[3]\sigma_3} A^{[4]\sigma_4} A^{[5]\sigma_5} \right) |\sigma_1 \dots \sigma_5\rangle$$

- These states occur automatically as the fixed points of DMRG calculations
- They can also be used as variational ansatz in their own merit!

Variational ansatz

- Remember Ritz' variational principle

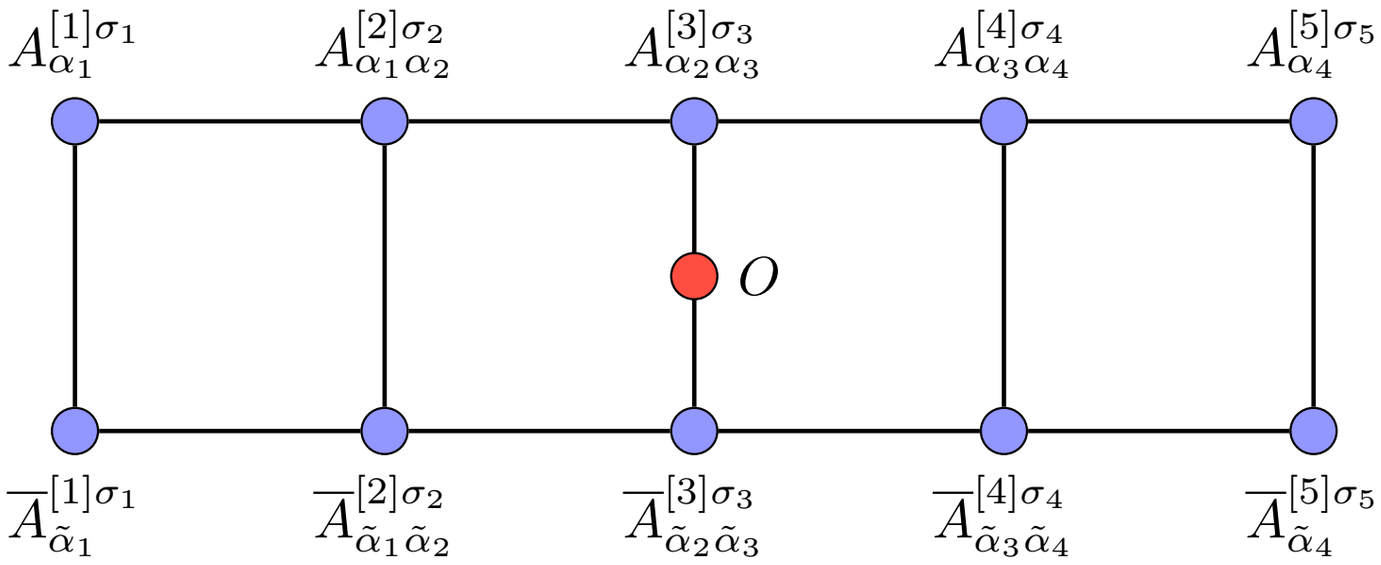
$$E_0 \leq E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

  for any state $|\Psi\rangle$

- We can always
  - optimize with Monte Carlo (stochastic methods), DMRG, conjugate gradient, ...
  - give upper bound on the energy
- **We can never give an estimate of systematic errors!**
- We need good reason to believe our ansatz is good!

Observables

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



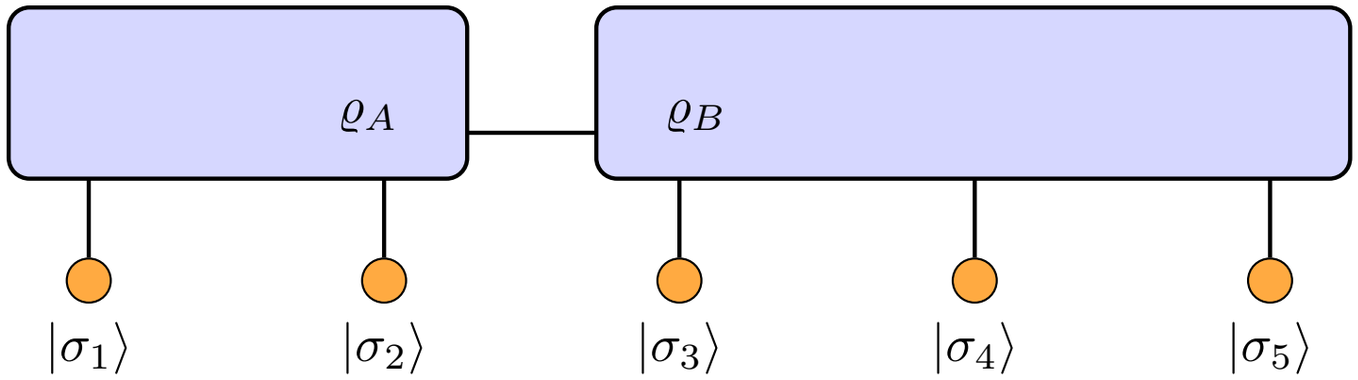
- No transformation of operators necessary - once the state is found, one can calculate just about anything!

Extensions

- **Variational Monte Carlo** methods are sign free and can be applied to systems with periodic boundary conditions without additional cost
- **Time evolution** algorithms can be easily devised using MPS
  - Many relevant applications e.g. in optical lattice systems
- MPS can also be written down for **finite temperature** systems, removing the limitation of DMRG to low-lying eigenstates

...why DMRG works in 1d...

Renormalization group



$$|\Psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$$

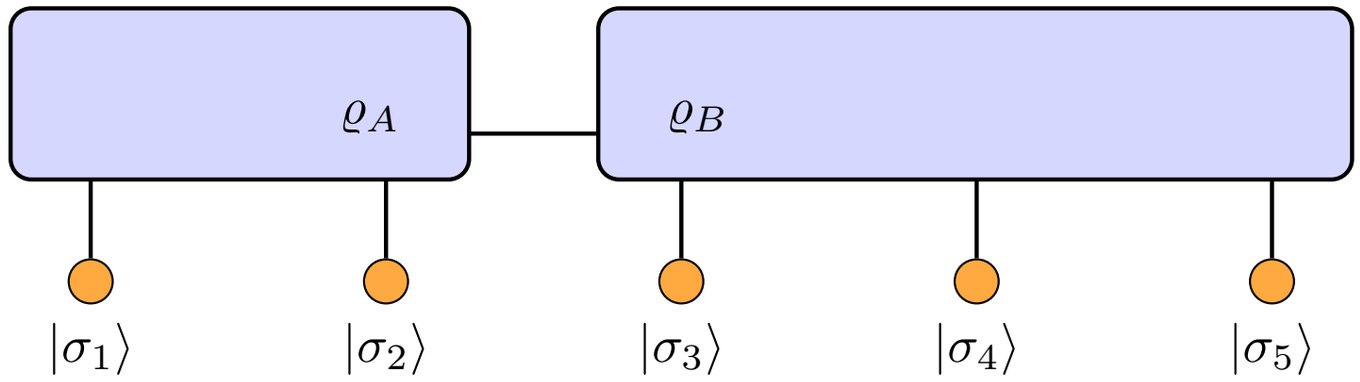
$$|\Psi_{AB}\rangle = \sum_{ij} c_{ij} |u_i\rangle \otimes |v_j\rangle$$

- Renormalization group idea: *choose a smaller set of basis states* for both subsystems that still captures important properties

Renormalization group

$$|\Psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$$

$$|\Psi_{AB}\rangle = \sum_{ij} c_{ij} |u_i\rangle \otimes |v_j\rangle$$



- What renormalized basis to choose for A and B?
  - Low-energy eigenstates: only works in very special cases. Why not? Remember particle-in-a-box that was discussed in lecture.
  - Eigenvectors of reduced density matrices: seems to work very well!

Why does DMRG work?

$$\begin{aligned}
\text{Let} \quad \rho_S = \mathrm{Tr}_E \rho &= \sum_\alpha w_\alpha |w_\alpha\rangle\langle w_\alpha| \\
\text{where} \quad \rho_S |w_\alpha\rangle &= w_\alpha |w_\alpha\rangle \\
\text{then} \quad \langle A\rangle = \mathrm{Tr}(\rho_S A) &= \sum_\alpha w_\alpha \langle w_\alpha|A|w_\alpha\rangle
\end{aligned}$$

- Error in expectation value is controlled by truncation in α and the decay of the density matrix eigenvalues w_α
- Understanding the decay of the density matrix eigenvalues will lead to understanding of accuracy of DMRG

Density matrix spectra

$$\rho_S |w_\alpha\rangle = w_\alpha |w_\alpha\rangle$$

- Is there some physical understanding of the decay of those eigenvalues?
  - Consider von Neumann entropy/entanglement entropy

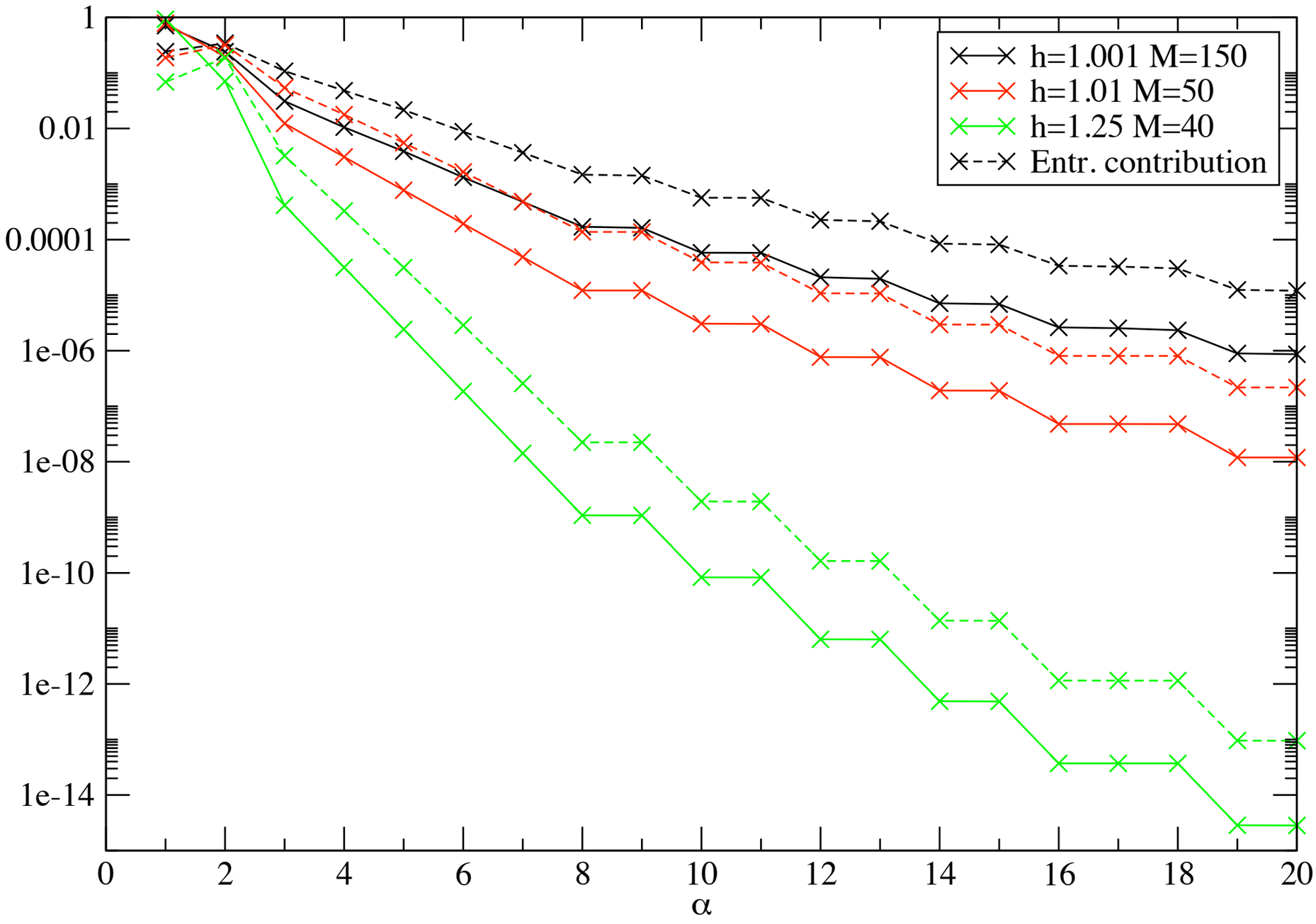
$$S = -\sum w_\alpha \ln w_\alpha$$

  - Decay of the eigenvalues is related to entropy: a slow decay corresponds to large entropy!

Density matrix spectra

Typical spectrum

(1d Ising model in transverse field)



Classical entropy

- Entropy measures *ignorance about state*

$$S = k_B \ln \Omega$$

where Ω is the number of microstates compatible with thermodynamic observables

- Consider ground state:
  - Classically, Ω is ground state degeneracy. In general, only thermal states have large entropy
  - In a quantum system, ground states are in general superpositions of many states; therefore, ground states can have large entropy!

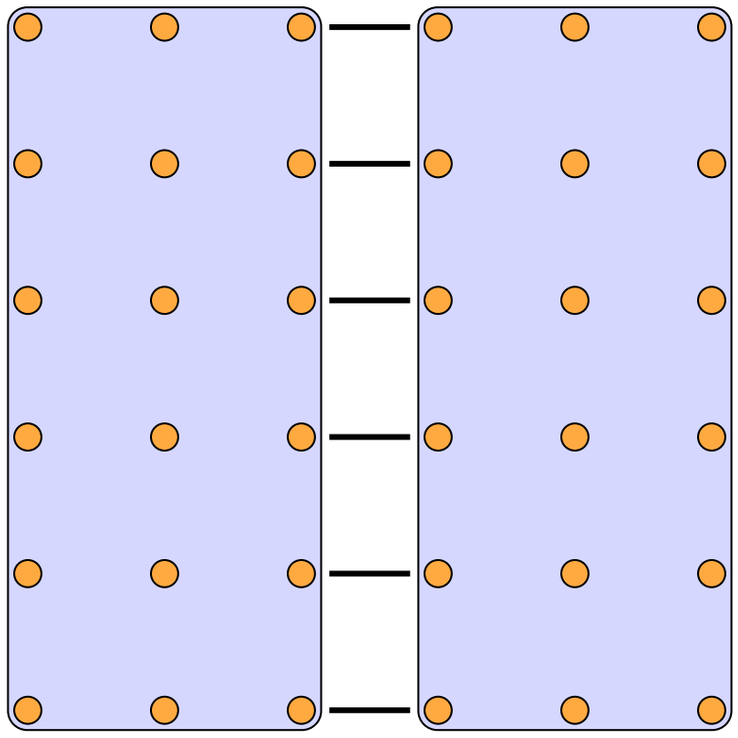
Entanglement in 1d

- If the entanglement of our system is not too large and the eigenvalues of the density matrix decay quickly, we can find a good MPS approximation to the ground state!
- In one dimension, we are lucky: for most systems, the entanglement saturates as a function of system size!
- Bond dimension necessary to capture entanglement

$$S \leq \ln M$$

...and how to extend it to higher dimensions.

Scaling of entanglement



- Scaling of bipartite entanglement of left with right block?

$$S(L) = ?$$

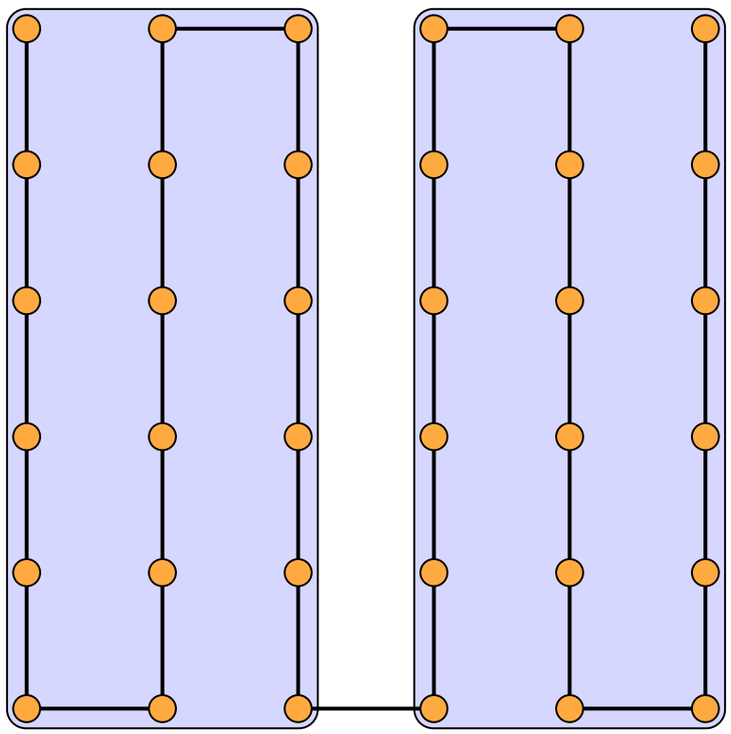
- Trivially expect volume scaling

$$S(L) \propto V = L^2/2$$

- Conjecture: area law

$$S(L) \propto L$$

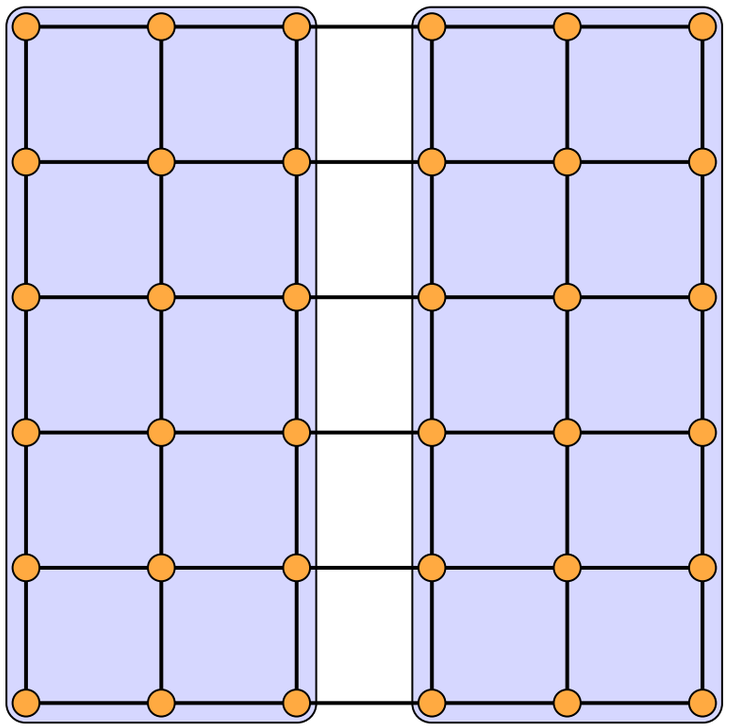
MPS in 2D



- Entanglement encoded in MPS between the two blocks does not grow with system size
  - Density matrix eigenvalues of the blocks decay very slowly
- Exponential number of states necessary in DMRG calculation

$$S_N \leq \ln N \longrightarrow N \geq e^{S_N} \sim e^L$$

MPS in 2D



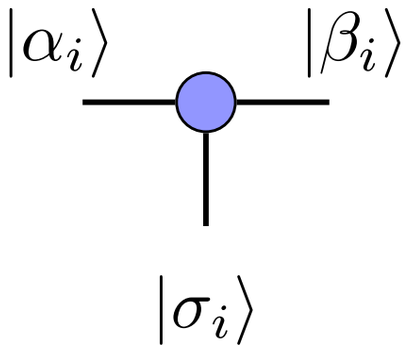
- Replacing matrices by tensors, we can put maximally entangled bond on each physical bond

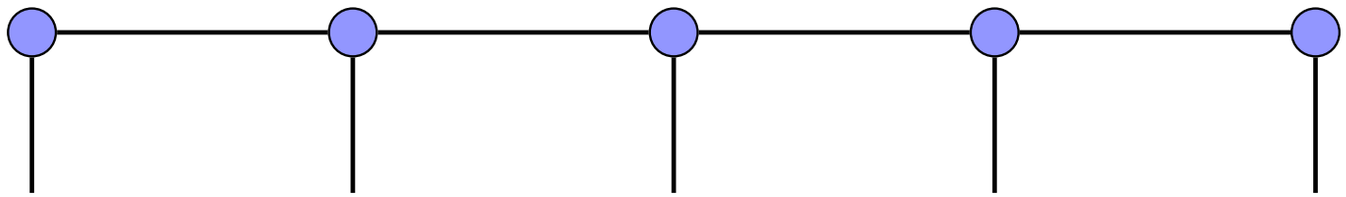
- Entanglement between blocks scales linearly in system size

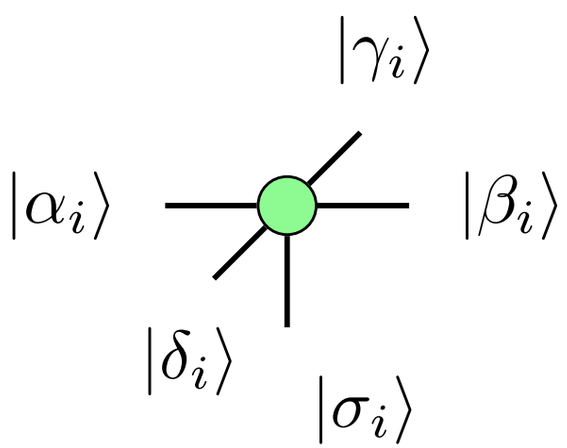
- Achieved with **PEP states** (projected entangled pair states)

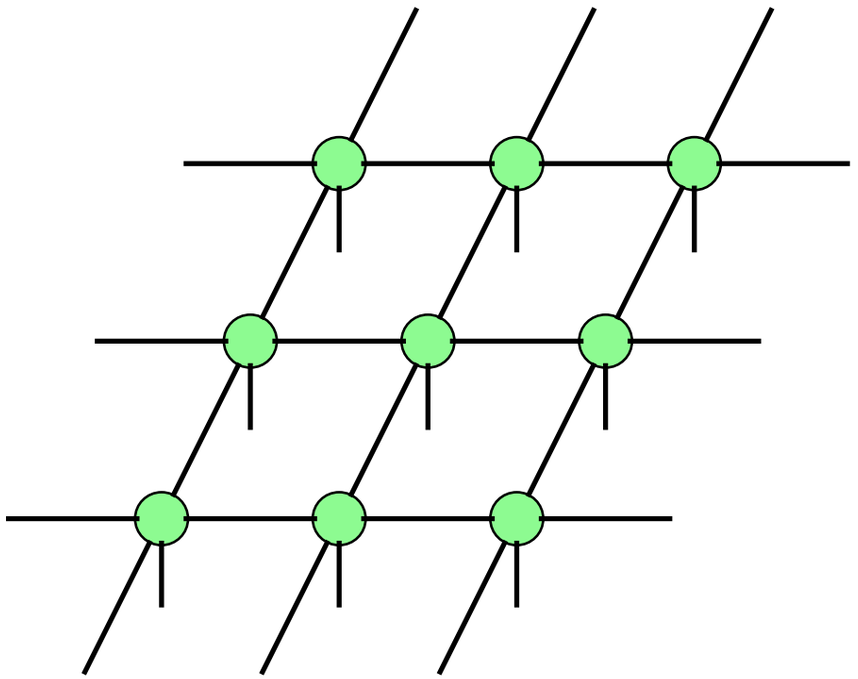
From MPS to PEPS

F. Verstraete and J.I. Cirac, arXiv:cond-mat/0407066v1



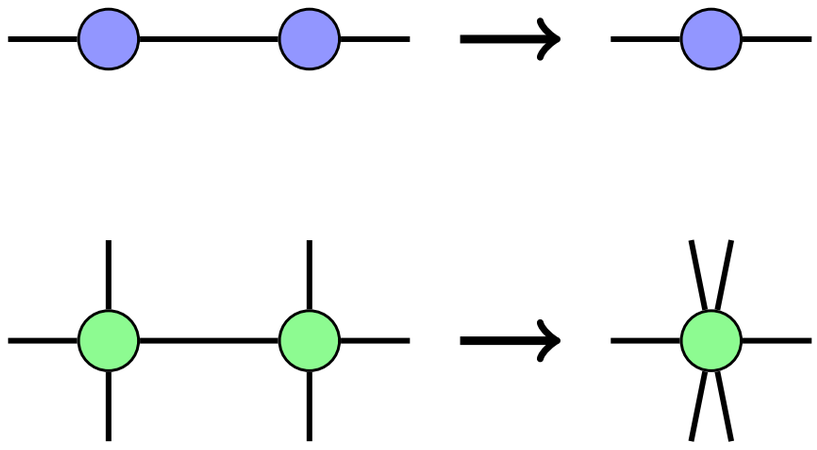






Another problem

- Contracting a tensor network is an exponentially hard problem
  - Matrix x Matrix = Matrix
  - Tensor x Tensor = Bigger Tensor



- Need **approximate scheme**

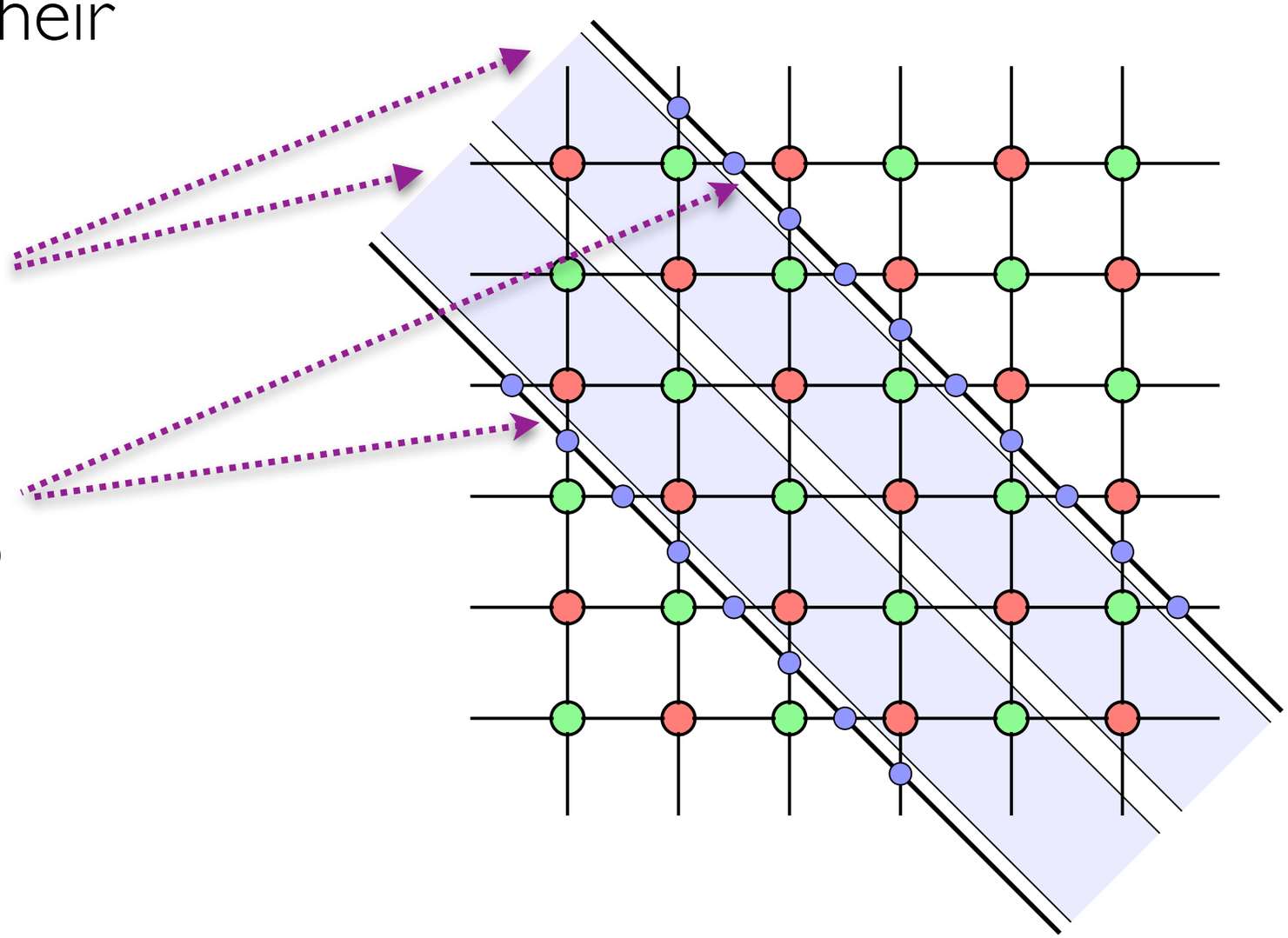
iPEPS: 2d to 1d

- Lattice is made up of transfer operators and can be approximated by their eigenvectors

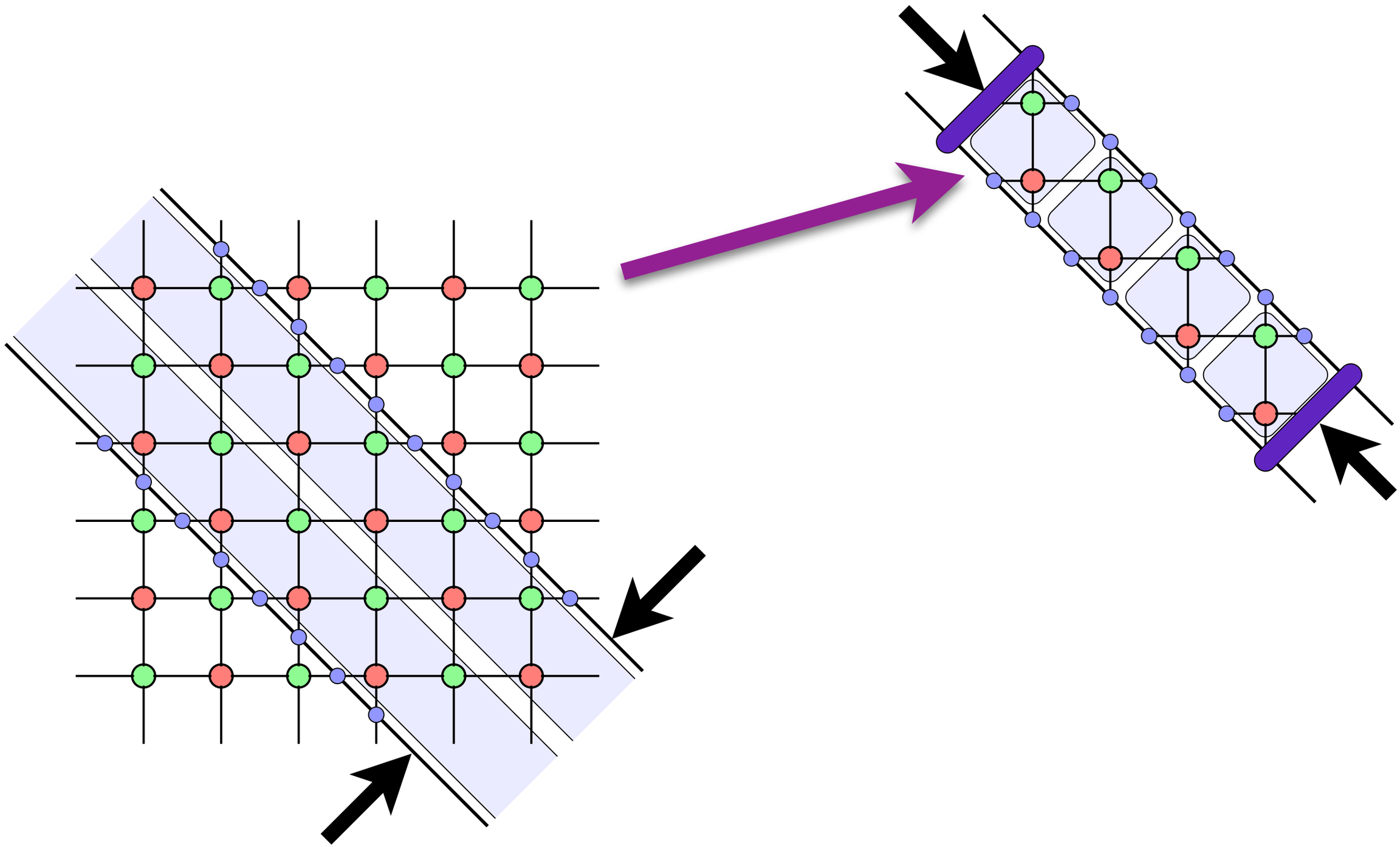
J. Jordan, R. Orus, G. Vidal, F. Verstraete and J.I. Cirac, arXiv:cond-mat/0703788v4

Infinite propagator

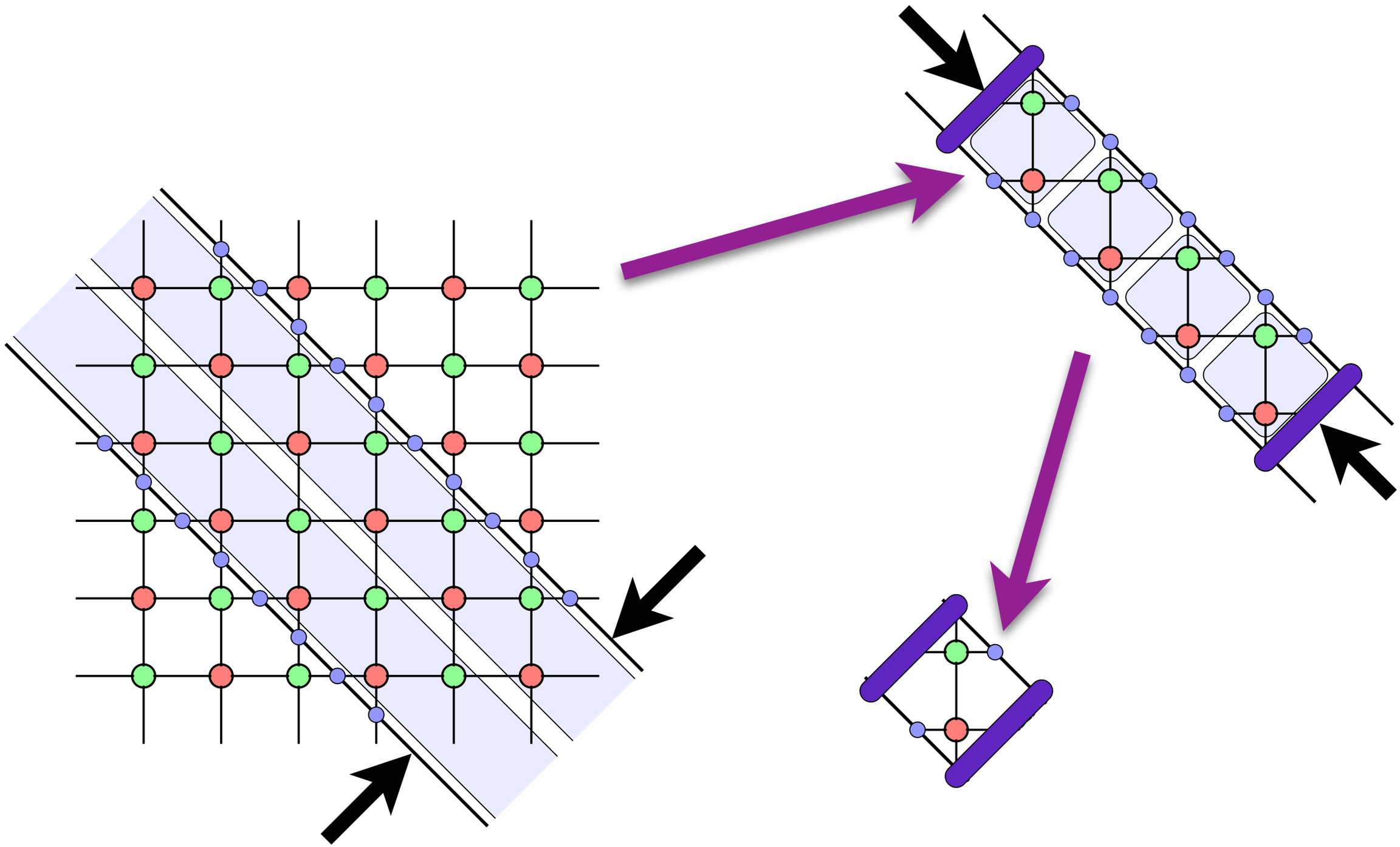
Boundary iMPS



iPEPS: 1d to 0d



iPEPS: 1d to 0d



Thank you
for your attention