VI. Tensor Networks in two and higher dimensions

1) Projected Entangled Pair States (PEPS)

MPS: - good approx. for ground states in 1D
- basis for powerful numerical methods
- framework for analytical modelling

Can we generalize this to 2D (and higher)?

What is the same?

What is different?

Basic intuition behind MPS:

Area law ⇒ entanglement distributed locally

Idea: Build 2D ansatz based on locality of entanglement.

a) Definition

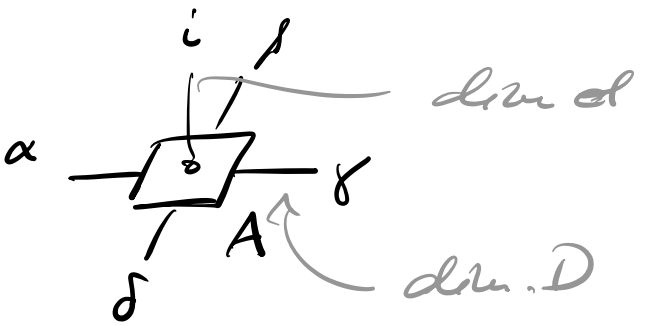
Consider 2D lattice

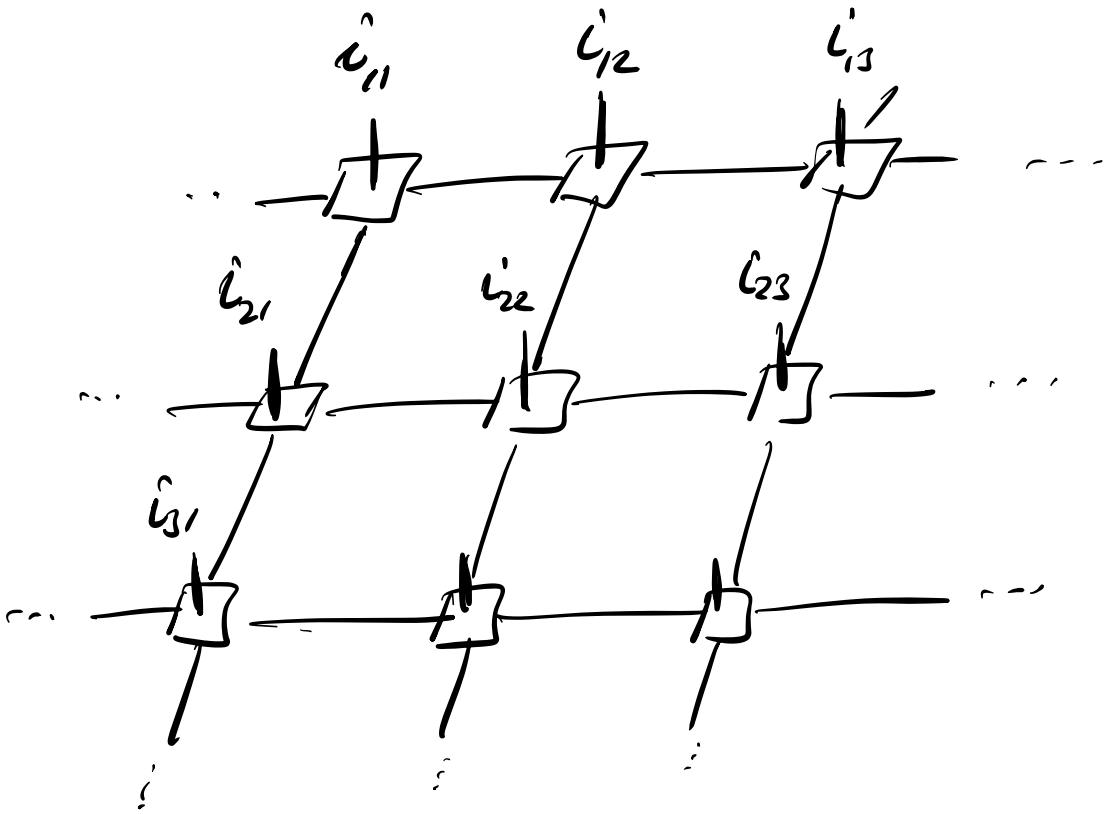
(here: square lattice: easiest to draw)

$$|\psi\rangle = \sum_{i_1 \dots i_N} c_{i_1 \dots i_N} |i_1, \dots, i_N\rangle$$

Express $c_{i_1 \dots i_N}$ as 2D tensor network

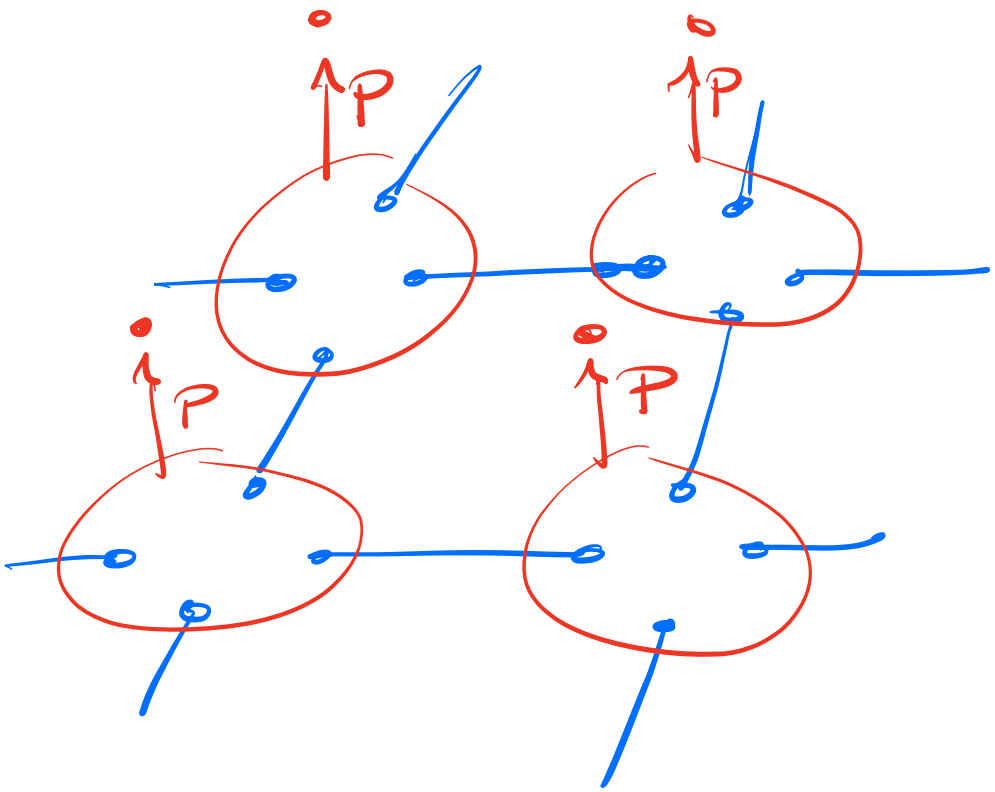
with tensor





As in 1D, we can either do this with PBC, terminate the boundaries, or choose site-dep. tensors $A^{[ij]}$.

We can also express such states in the "AKLT way", i.e. with ent. states $|\omega\rangle$ and maps $P: \mathbb{C}^D \otimes \mathbb{C}^D \otimes \mathbb{C}^D \otimes \mathbb{C}^D \to \mathbb{C}^d$,



(e.g., $|\omega\rangle = \sum_{i=1}^{D} |i\rangle|i\rangle$; $P = \sum A^{i}_{\alpha\beta\gamma\delta} |i\rangle\langle\alpha\beta\gamma\delta|$)

Because of this, these states are also called "Projected Entangled Pair States" (PEPS) — even though I need not be a projector — or simply "Tensor Network States" (TNS).

Note: The same constructs can be used on other lattices, higher dimensions, or any graph.

b) Approximability by PEPS

In 1D, area law ⇒ ent. distr. locally ⇒ good MPS approx.

In 2D, "area law ⇒ ent. local" does not automatically hold.

Do PEPS still provide a good approx. of ground states of 2D local Hamiltonians?

Yes! – Using more direct techniques (Trotter or Taylor expansion, which is truncated) we can get similar result:

Ground states are well approximated to error ε with a bond dimension

$$D \sim \left(\frac{N}{\varepsilon}\right)^{\log N}$$

i.e., <u>almost</u> polynomial.

(Terms & conditions apply, see arXiv: 1406.2973)

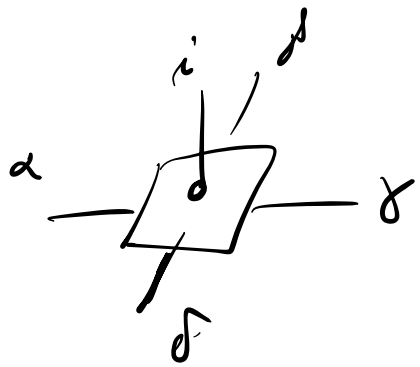
$\Rightarrow$ PEPS form a good class of states to approximate ground states.

2. Examples

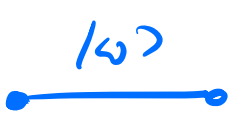
a) The GHZ state

$$|\psi\rangle = |0\ldots0\rangle + |1\ldots1\rangle$$

$$A^{i}_{\alpha\beta\gamma\delta} = \begin{cases} 1: & i=\alpha=\beta=\gamma=\delta \\ 0: & \text{otherwise} \end{cases}$$

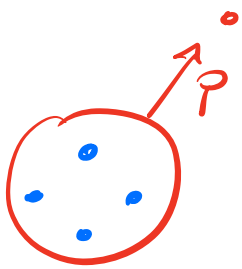


b) AKLT state:



$$|\omega\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

$\mathfrak{su}(2)$ singlet (spin ½)



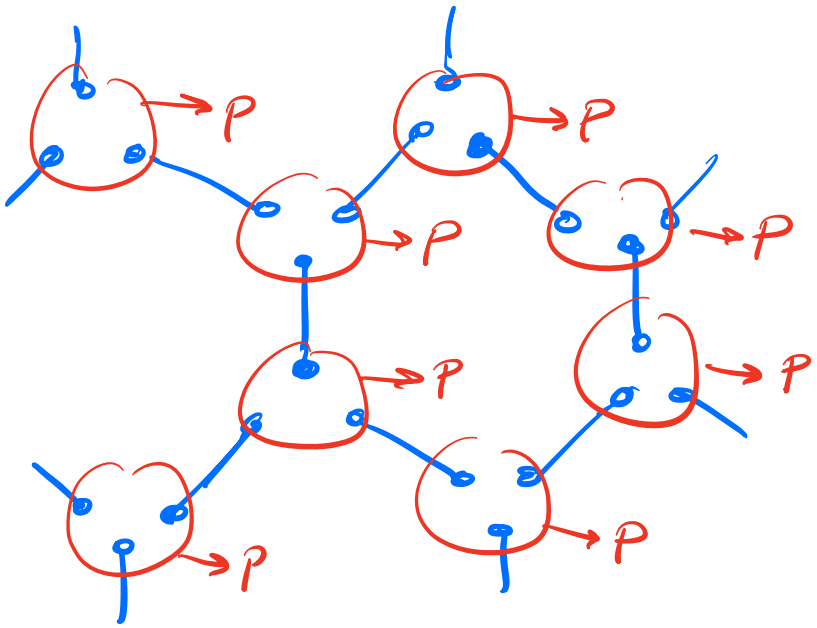
$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2}$: spin 0, 1, 2

$$P = \Pi_{S=2}$$

proj. onto perm.-sym. space!

⟶ $\mathfrak{su}(2)$-invariant spin-2 state.

Alternatively: honeycomb lattice.

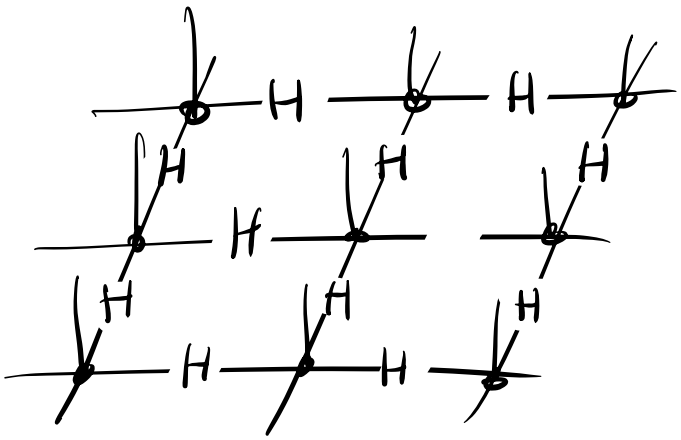


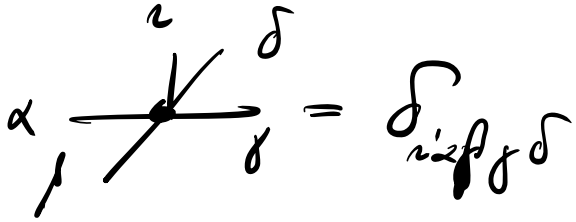
$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{1}{2} \text{ or } \frac{3}{2} \Longrightarrow P = \Pi_{3/2}$$

perm.-sym. space!

c) 2D cluster state

The 2D cluster state – obtained by acting with $CZ = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$ on $|+\rangle^{\otimes N}$ on all edges of the lattice is a PEPS with

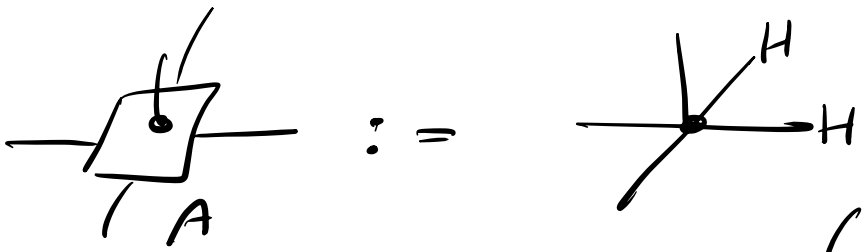




$$-H- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

(Can be brought into conv. form

e.g. by blocking



(→ Homework)

f) PEPS from classical models

Let $H(s_1, \dots, s_N)$ be a <u>classical statistical model</u>, e.g. the 2D Ising model

$$H = -\sum_{\langle ij \rangle} s_i s_j \quad , s_i = \pm 1$$

N.N.

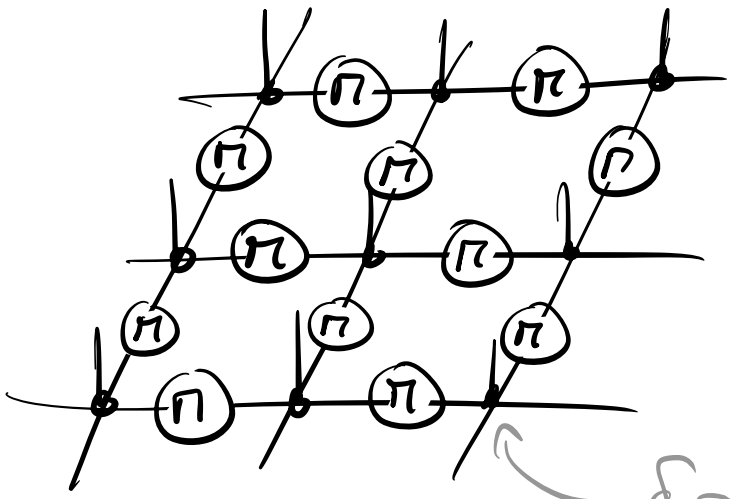
Define

$$|\psi(\beta)\rangle = \sum_{s_1,\dots,s_N} e^{-\beta/2 H(s_1,\dots,s_N)} |s_1,\dots,s_N\rangle$$

This state is a PEPS:

E.g. for the Ising model:

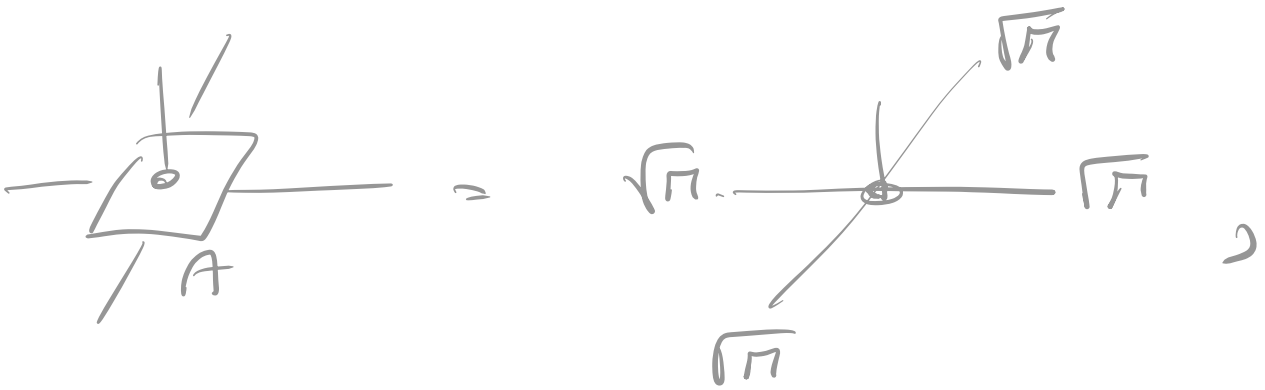
$|\psi(\beta)\rangle$ =



$$\pi = \begin{pmatrix} e^{\beta/2} & e^{-\beta/2} \\ e^{-\beta/2} & e^{\beta/2} \end{pmatrix}$$

(Can be written as "conventional" PEPS

with 

or 

i.e. $P = |0\rangle\langle\alpha,\alpha,\alpha,\alpha| + |1\rangle\langle\beta,\beta,\beta,\beta|$,

$|\alpha\rangle = \sqrt{\pi}\,|0\rangle$; $|\beta\rangle = \sqrt{\pi}\,|1\rangle$.)

For these states $|\psi(s)\rangle$,

$$\langle\psi(s)|\,\sigma_i^z\,\sigma_j^z\,|\psi(s)\rangle =$$

$$= \sum_{s_1,\dots,s_N} e^{-\beta H(s_1,\dots,s_N)}\, \langle s_1,\dots,s_N|\,\sigma_i^z s_j^z\,|s_1,\dots,s_N\rangle$$

$\Rightarrow$ $\langle \psi(\beta) | \sigma_i^z \sigma_j^z | \psi(\beta) \rangle$ equals the correlation in the classical Gibbs state $e^{-\beta H}$!

(Same for more complex σ^z correlators.)

Such a construction for $|\psi(\beta)\rangle$ can be done for any classical Hamiltonian — this can be seen e.g. since

$$|\psi(\beta)\rangle = \prod e^{-\beta/2 h_i} |+\rangle^{\otimes N}$$

↑ commute, & any of these operators can be written as a small local TN.

g) PEPS with critical correlations

2D classical models, e.g. Ising model, undergo phase transitions at some crit. temperature β_{crit}.

$\Rightarrow e^{-\beta_{crit} H}$ has algebraically decaying correlations!

$$\langle \psi(\beta_{crit}) | \sigma_i^z \sigma_j^z | \psi(\beta_{crit}) \rangle \sim \frac{1}{|i-j|^{2\Delta_\sigma}}$$

with some exponent ("scaling dimension") Δ_σ.

$\Rightarrow$ PEPS can exhibit critical correlations.

Exponential clustering theorem: H gapped $\Rightarrow$ ground state of H has exp. decaying correlations.

⟹ PEPS can describe states which are not ground states of gapped local Hamiltonians.

b) Partition functions of class. statistical models

H class. Ham., e.g. Ising ($H = -\sum_{\langle i,j\rangle} s_i s_j$).

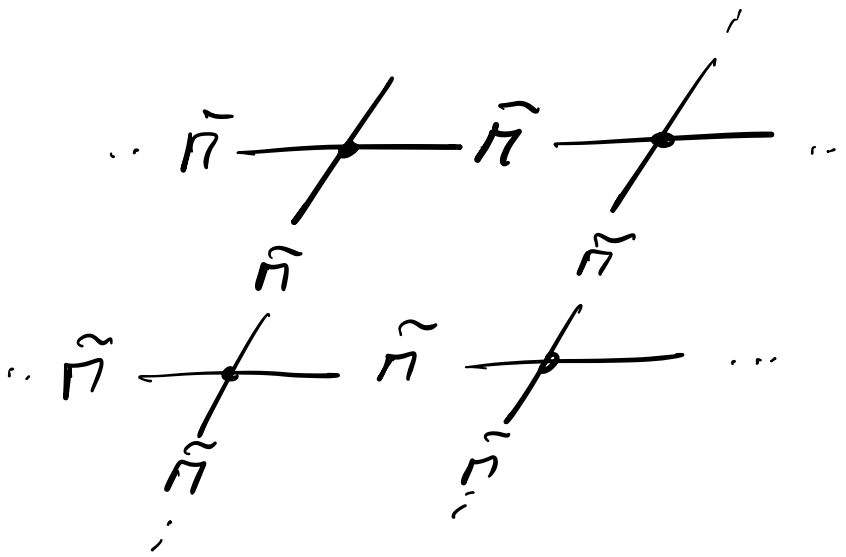
Partition function $Z = \mathrm{tr}(e^{-\beta H})$

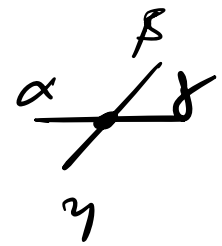
$$= \sum_{s_1,\dots,s_N} e^{-\beta H(s_1,\dots,s_N)}$$

Z is a tensor network:

e.g. since $Z = \langle \psi(\beta) | \psi(\beta) \rangle$,

or (more efficiently), e.g. for Ising:



and  $= \delta_{\alpha=\beta=\gamma=\eta}$,

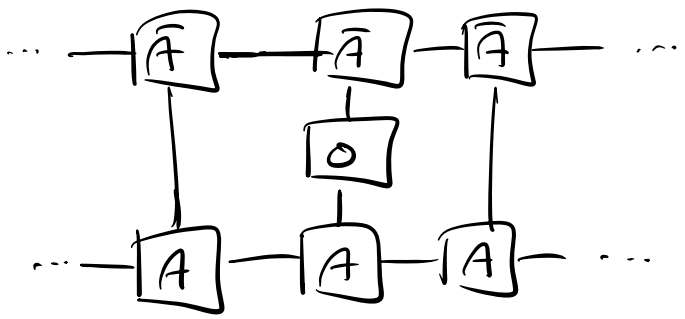
and $\Pi = \begin{pmatrix} e^{+\beta} & e^{-\lambda} \\ e^{-\lambda} & e^{+\beta} \end{pmatrix}$.

3. Numerical PEPS algorithms

a) Computation of expectation values

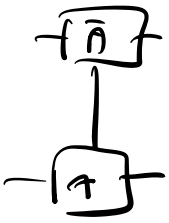
Exp. values for MPS:

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



Transfer operator

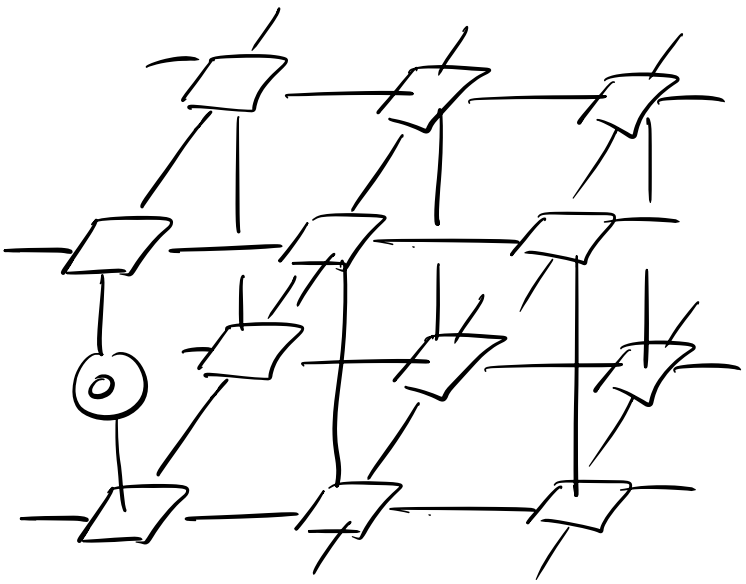
$E =$



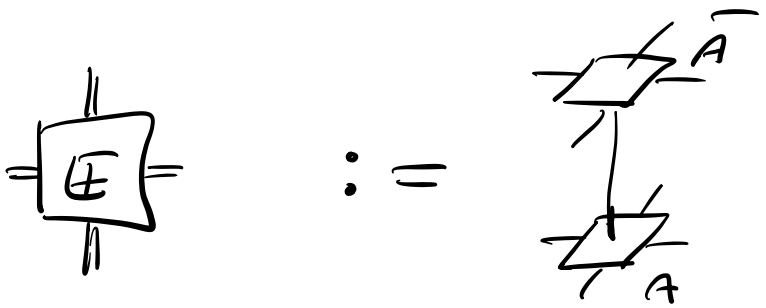
$\Rightarrow \langle \psi | O | \psi \rangle = \ldots E \cdot E \cdot E_O \cdot E \ldots$

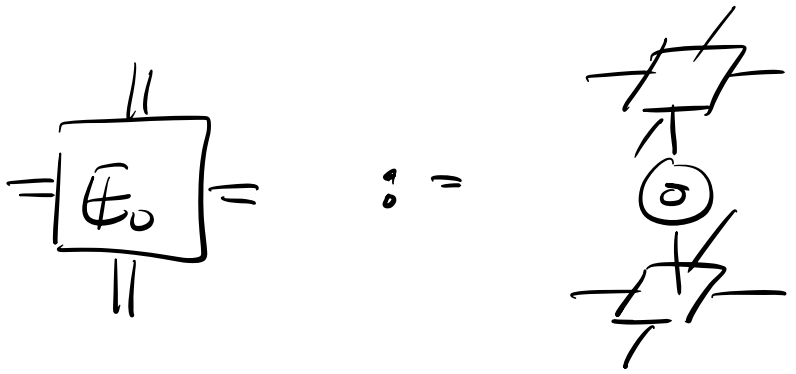
Exp. values for PEPS:

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



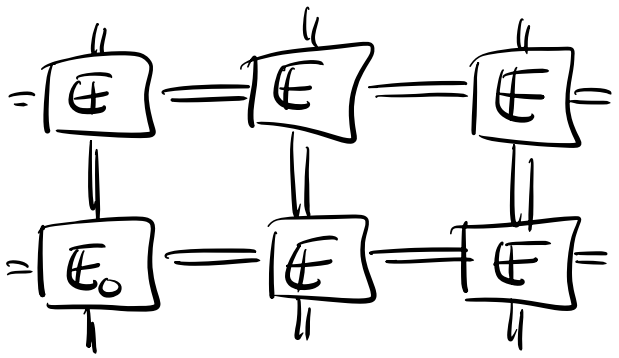
Define transfer operators:





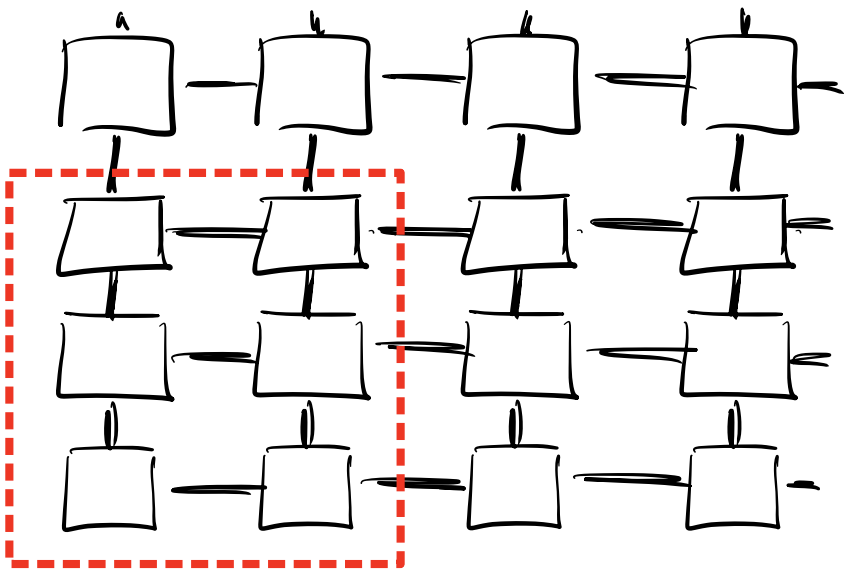
Then,

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



$\Rightarrow$ 2D expectation values map to contraction of 2D tensor network (vs. 1D TN in MPS = matrix multiplication)

Can this still be done efficiently?



contracting cuts # of indices prop. to length of boundary

⇒ no efficient choice possible — for any contraction order length of boundary will go up to to $O(L)$ for $L \times L$ system.

Contraction of 2D PEPS is "exponentially hard!"

More precisely: It is NP-hard, in fact,

it is a #P-complete (or rather: GapP-

the difference of two #P functions) problem.

($\hat{=}$ evaluating path integrals)

$\Rightarrow$ We need to resort to approximate contraction methods!

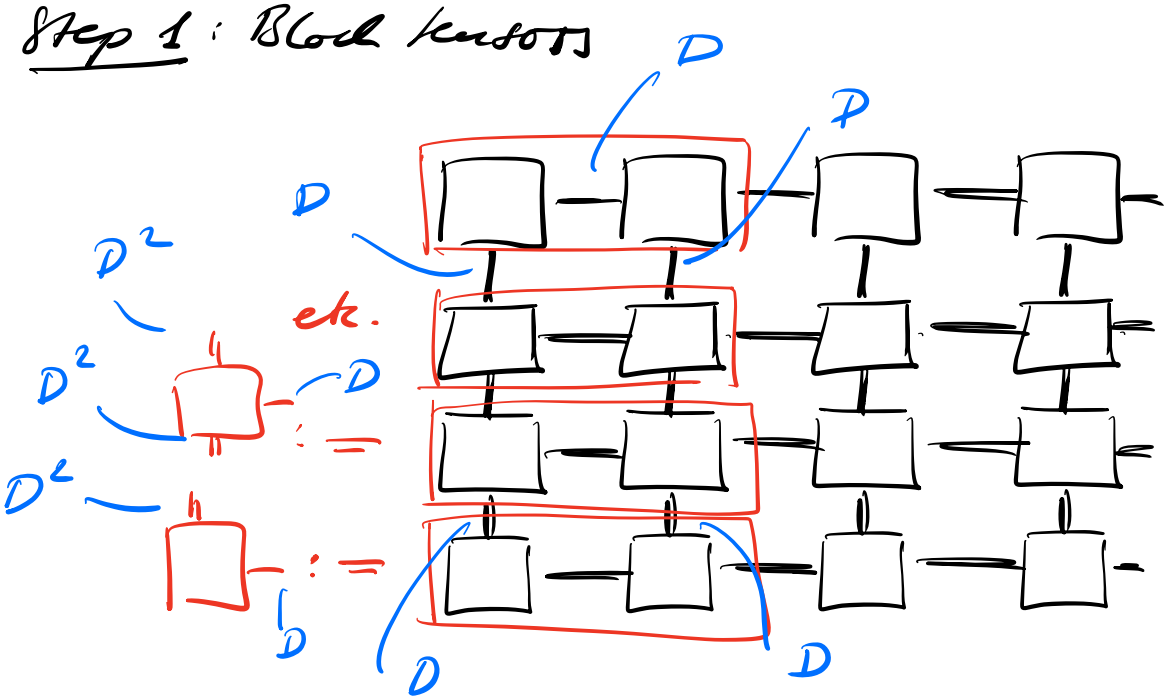
b) Approximate contraction schemes

Two different types of schemes.

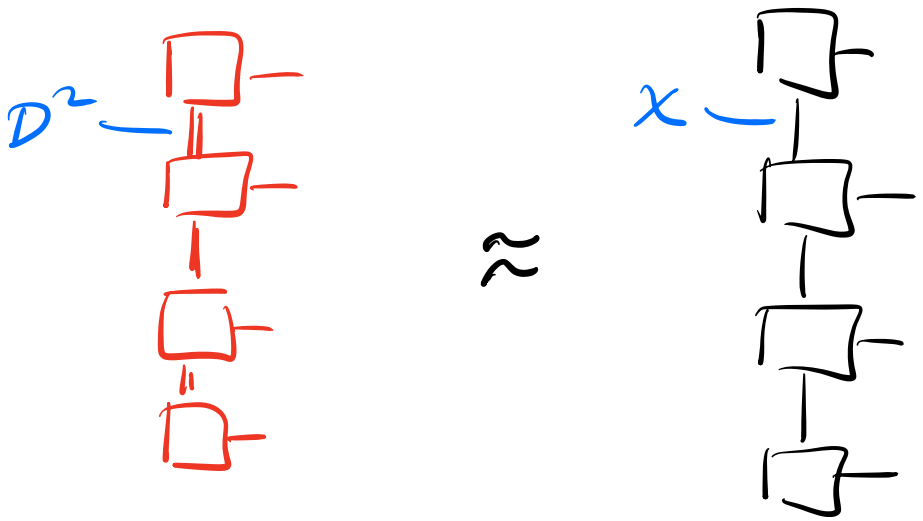
i) Column-wise contraction

Case I: Finite (non-hom.) Systems

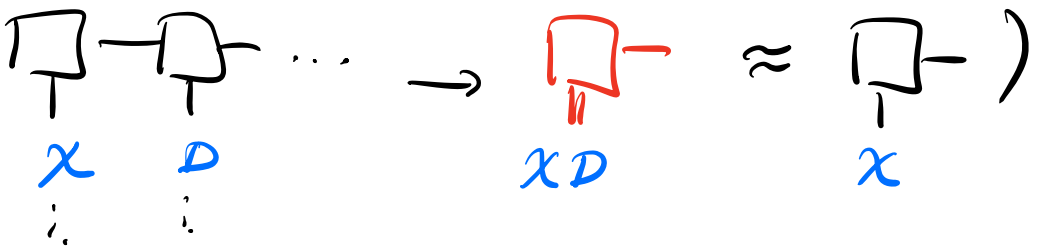
Step 1: Block tensors



Step 2 : Truncate new knots



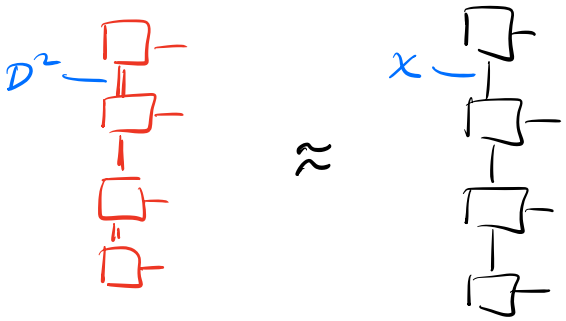
and iterate ... (in the next steps, this

becomes 

)

X controls accuracy of approximation.

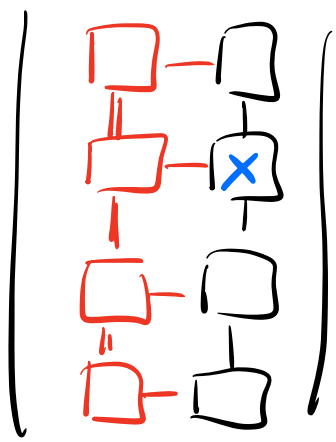
Approximating



can be done in different ways, which

can be derived from 1D algorithms:

- truncate by SVD
- maximization of overlap

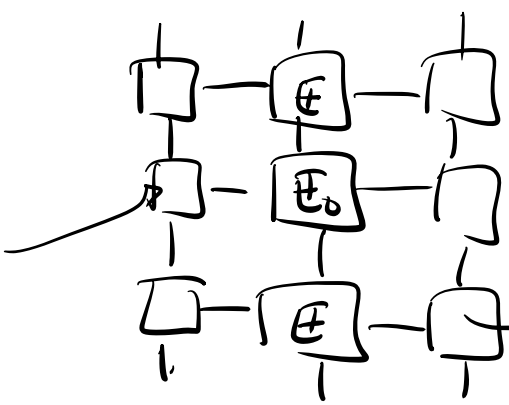


(quadratic in any tensor X $\Rightarrow$ can be solved using DMRG!!)

Case II: infinite systems

Works the same way, but use infinite 1D algorithms for contraction (including more sophisticated methods, such as tangent space/VUMPS).

After contracting  from left & right infinity, one has



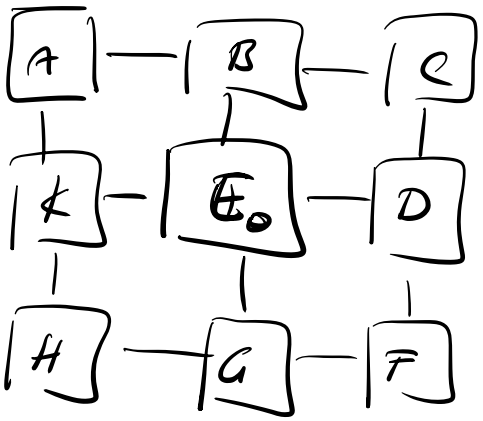
(X)

which is a 1D problem ⇒ eff. contractate.

— If the transfer matrix is hermitian, one can also find its leading eigenvalue variationally, i.e. by maximizing ⟨x|x⟩ w/ same left + right vector.

ii) Corner transfer matrix (CTM)

- method for infinite systems
- approximate the "environment" of the bit of interest by



- environment tensors are determined by matching rows/columns of  , absorbing them in boundary tensors, and truncating.

c) Variational method

Can use this as basis for variational algorithm.

Idea as in 1D:

Finite system: $|\psi\rangle$ linear in each tensor $\Rightarrow$ energy

$$E(x) = \frac{\langle \psi[x] | H | \psi[x] \rangle}{\langle \psi[x] | \psi[x] \rangle}$$

$$= \frac{\vec{x} \cdot \Pi \vec{x}}{\vec{x} \cdot N \vec{x}}$$

can be minimized by generalized eigenvalue problem

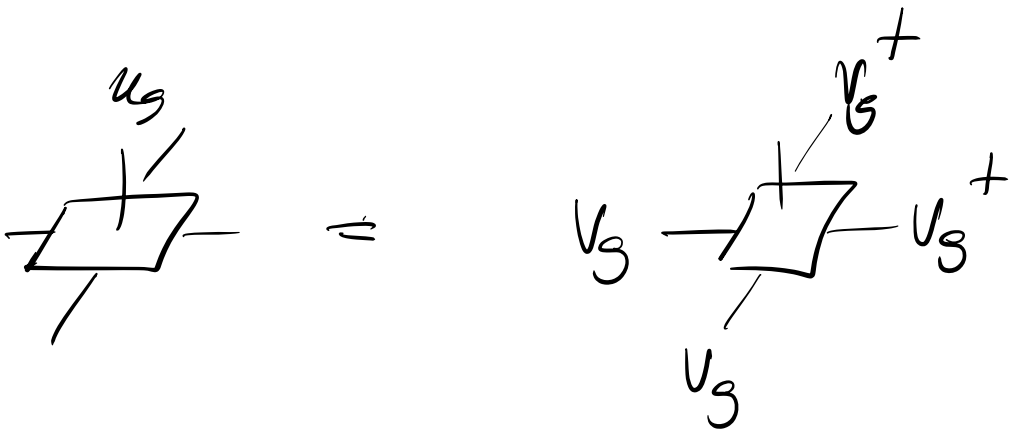
$\Rightarrow$ DMRG-type algorithm

Infinite system: Similar to 1D:

Use either imag. time evolution (then absorb into tensor & cut D), or gradient search.

4. Analytical properties of PEPS

a) Symmetries



$\Downarrow$

PEPS has symmetry: $|\psi\rangle = U_g^{\otimes N} |\psi\rangle$.

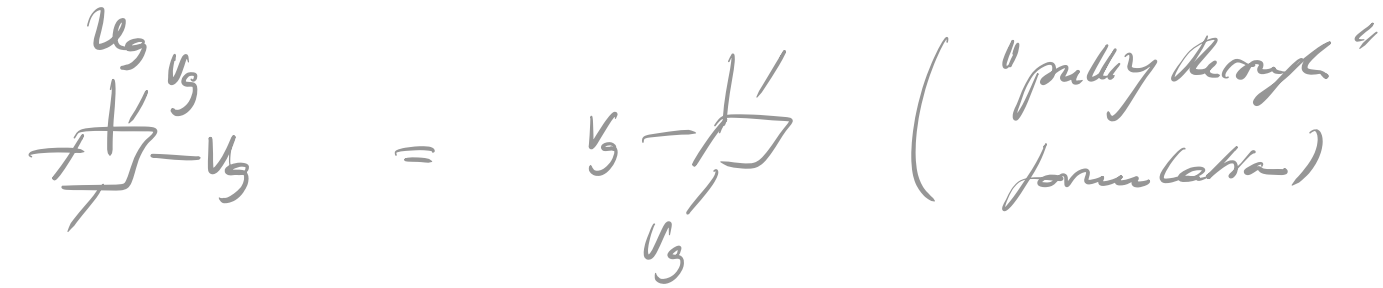
$\Longrightarrow$ Symmetries can be encoded locally?

Does the converse also hold? Is there a fund. theorem for PEPS?

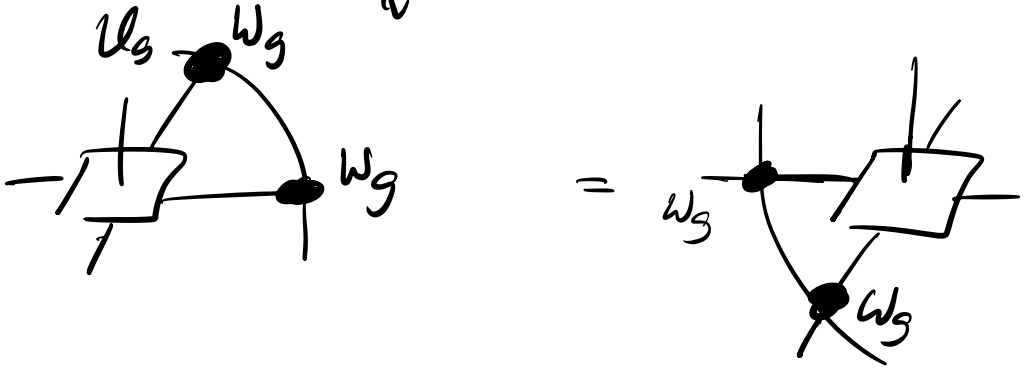
For generic ("injective") PEPS: Yes! – All such PEPS encode the sym. as above!

However, in 2D there can be fundamentally different ways to encode symmetries:

E.g., sym. can be encoded by 1D Matrix Product Operators (MPOs):

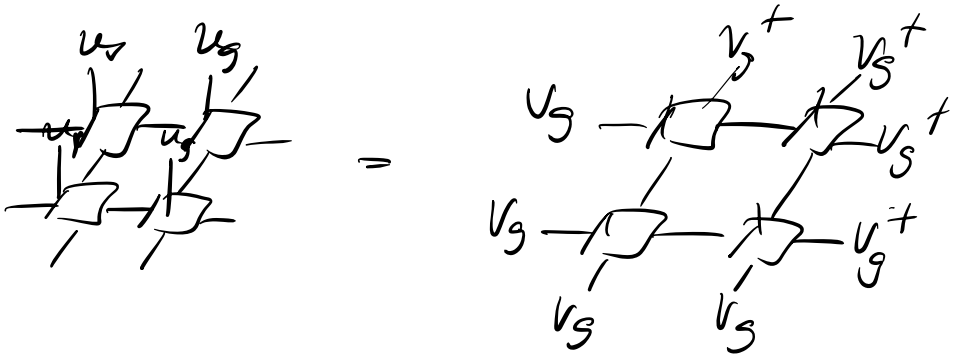


} generalize to



Gives rise to a (partial) class. of 2D phases phases by studying MPO representations of sym. group G.

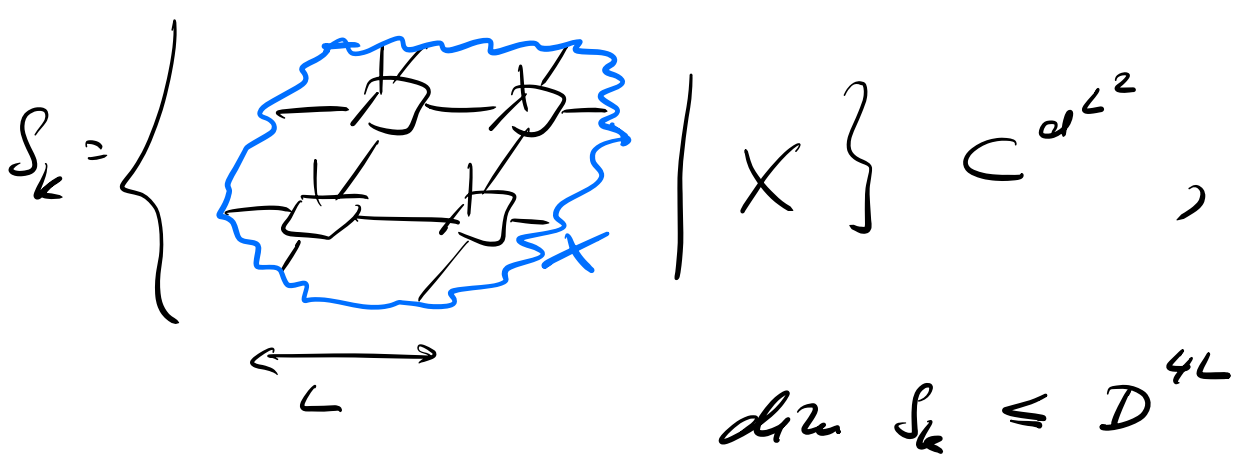
Note: In the product encoding V_g, the 2-cocycle is not a good class. of phases, since blocking:



gives inequivalent proj. representation $V_g \otimes V_g$ (e.g. $\frac{1}{2} \otimes \frac{1}{2}$ is integer spin).

5) Parent Hamiltonians

Parent Hamiltonians can be defined as in 4D:



$$\dim S_k \leq D^{4L}$$

$\Rightarrow$ S_L not full space as soon as

$$D^{4L} < d^{L^2} \quad \text{or}$$

$$L > 4 \log D / \log d$$

$\Rightarrow$ $H = \sum (\mathbb{1} - \Pi_{S_L})$ is parent Ham.

Again, for generic PEPS, H (defined on a big enough patch) has a unique ground state.

But: Not always gapped

(e.g. "cluster PEPS" at crit. point

$\Rightarrow$ algebraic corrs. $\Rightarrow$ cannot be ground state of gapped Ham.

(once the "exponential clustering theorem" states: gap $\Rightarrow$ exp. decay of corrs. in g. state).