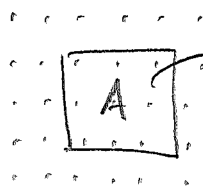
Projected Entangled Pair States

MPS: good description for 1D ground states, useful for numerical simulations and to build analytical models.

Can we generalize this to 2D?

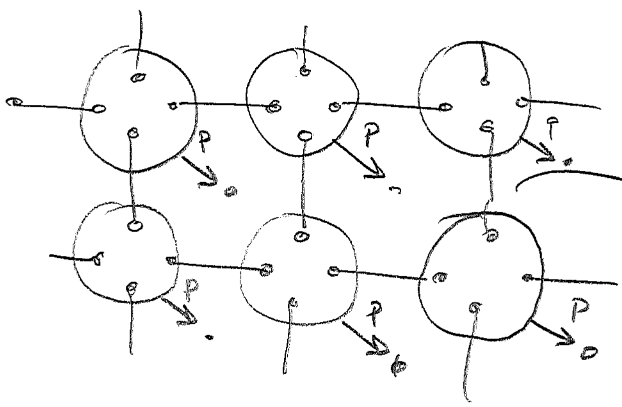
Recall area law (→ Lecture 2):

ground state $|\psi\rangle$:



$S(\rho_A) \sim \partial A \quad \longleftrightarrow$ entanglement concentrated around boundary. (Motivated MPS constr.)

Construct state again from entanglement properties:



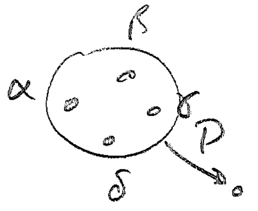
$$|\omega_D\rangle \equiv \sum_{i=1}^{D} |i\rangle|i\rangle$$

$$P: \mathbb{C}^D \times \mathbb{C}^D \times \mathbb{C}^D \times \mathbb{C}^D \to \mathbb{C}^d$$

(Note: P can depend on lattice site: $P \rightsquigarrow P^{[x,y]}$)

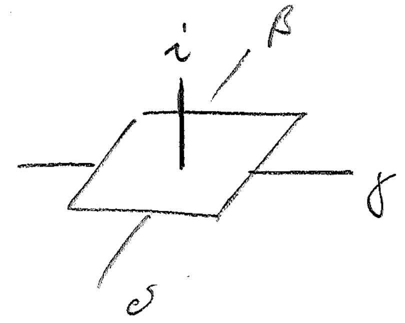
$$\boxed{\text{"Projected Entangled Pair State (PEPS)"}}$$

We can again use tensors to express this:

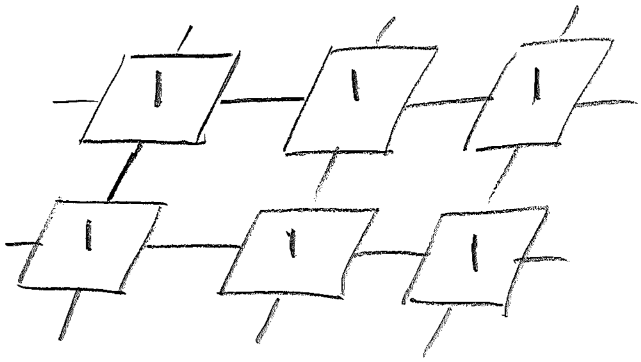


$$\longleftrightarrow P^{[x,y]} = \sum_{i\alpha\beta\gamma\delta} A^{[x,y]}_{i;\alpha\beta\gamma\delta}\, |i\rangle\langle \alpha,\beta,\gamma,\delta|$$

$$\longleftrightarrow \quad A^{[x,y]}_{i;\alpha\beta\gamma\delta} \equiv$$



$\longleftrightarrow$ The whole PEPS can be written as a 2D tensor network



Hastings (cond-mat/0508554, cond-mat/0701055):

Ground (and thermal) states are well approximated by PEPS.

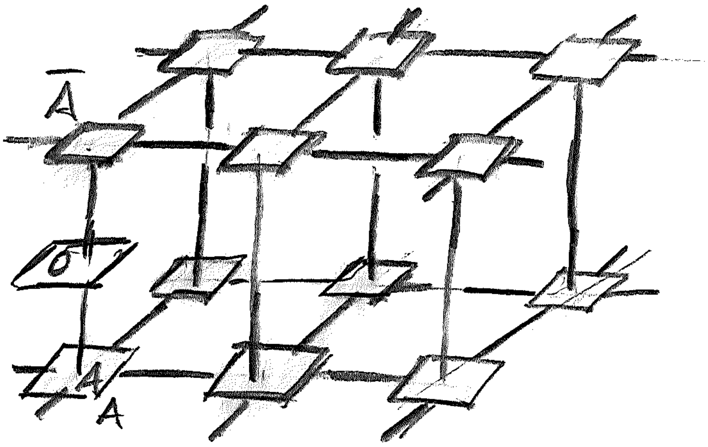
<u>Concretely:</u>

$$D_{max} \sim \left(\left(\frac{N}{\epsilon}\right)\log\left(\frac{N}{\epsilon}\right)\right)^{c\log\left(\frac{N}{\epsilon}\right)}$$

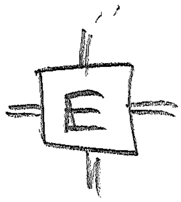
(as long as density of states grows at most like $N^E/E!$).

Computation of expectation values:

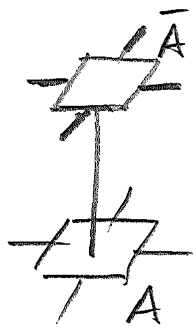
$\langle\psi|O|\psi\rangle =$



With "transfer operators"



$:=$



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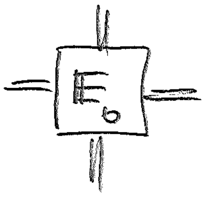

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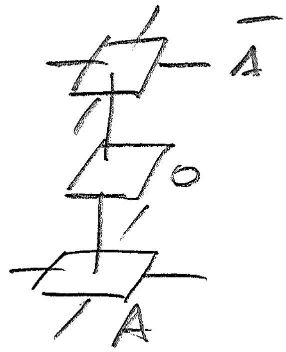
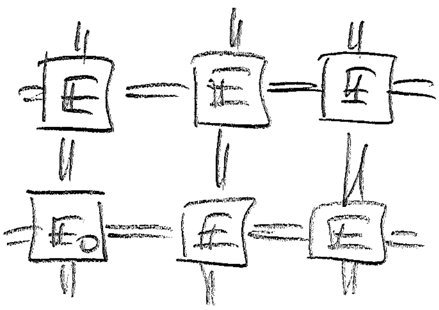


,

we have

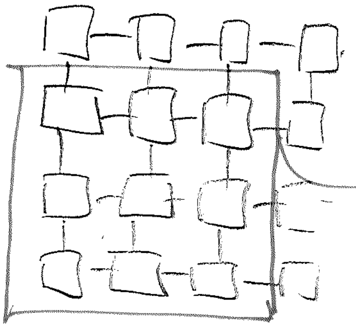
$\langle\psi|O|\psi\rangle =$



⇒ Exp. value in 2D is obtained by contracting 2D tensor network.

In 1D, we had to multiply matrices (1D TN) ⇒ efficient.

Here: For exact contraction, we need to store intermediate tensor with $O(\sqrt{N})$ indices, i.e., size $(D^2)^{\sqrt{N}}$ → exponential!



indices ∝ boundary ∝ $\sqrt{N}$

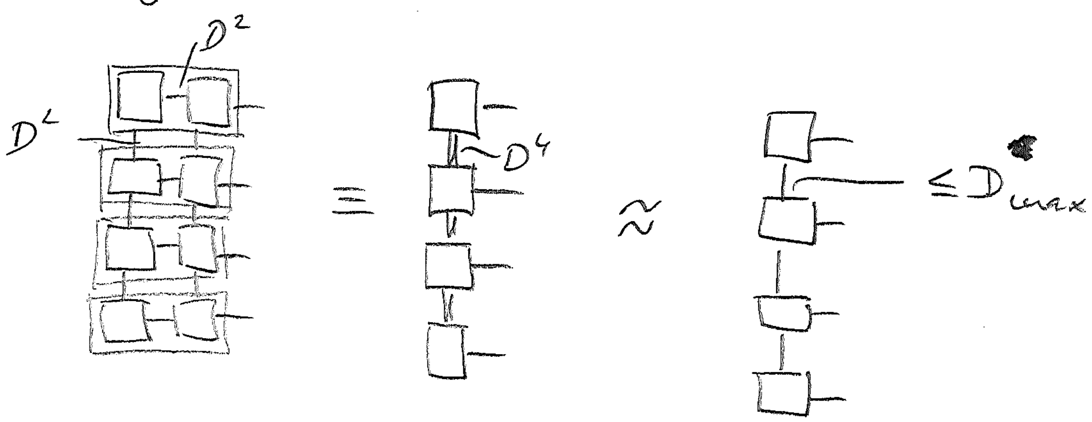
sites.

⇒ We need to use approximate contraction schemes!

Approximate contraction:

Similar to simulation of time evol w/ MPS (→ lecture 6):

Contract column-wise and approximate by an MPS w/ D_{max} after every step:



, etc.

* Truncation can be done using DMRG or local truncation w/ SVD (cf. time evol.).

* Resources for contraction scale like $\propto D^8$ (for $D_{max} = \propto D^2$)
(→ homework!)

* Truncation error is known and (in practice) very small.
* Allows to compute local observables, correlation functions, ...

Variational method:

We have again that

$|\psi[A^{[1,1]}, A^{[1,2]}, \ldots, A^{[N_x,N_y]}]\rangle$ is linear in each $A^{[x,y]}$.

$\Rightarrow$

$$E(A^{[x,y]}) = \frac{\langle\psi[\ldots, A^{[x,y]}, \ldots]|H|\psi[\ldots, A^{[x,y]}, \ldots]\rangle}{\langle\psi[\ldots A^{[x,y]}, \ldots]|\psi[\ldots, A^{[x,y]}, \ldots]\rangle}$$

$$= \frac{\vec{A}^{[x,y]} \cdot M \vec{A}^{[x,y]}}{\vec{A}^{[x,y]} \cdot N \vec{A}^{[x,y]}}$$

can be minimized by solving generalized eigenvalue problem $M\vec{A}^{[x,y]} = E N \vec{A}^{[x,y]}$

$\Rightarrow$ Numerical method for simulating 2D systems!

Using approximate contraction, we can use PEPS for

* variational ground state calculations
* simulation of time evolution
* imaginary time evolution for ground states
* etc. ... (cf. 1D)

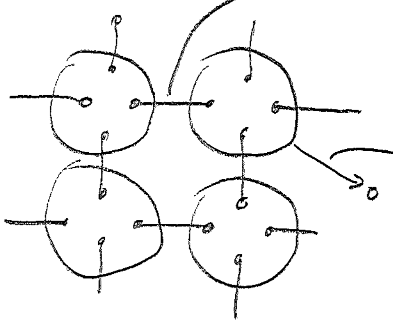
Examples of PEPS:

* 2D GHZ state:

$$P = |0\rangle\langle 0000| + |1\rangle\langle 1111|$$

* AKLT state:

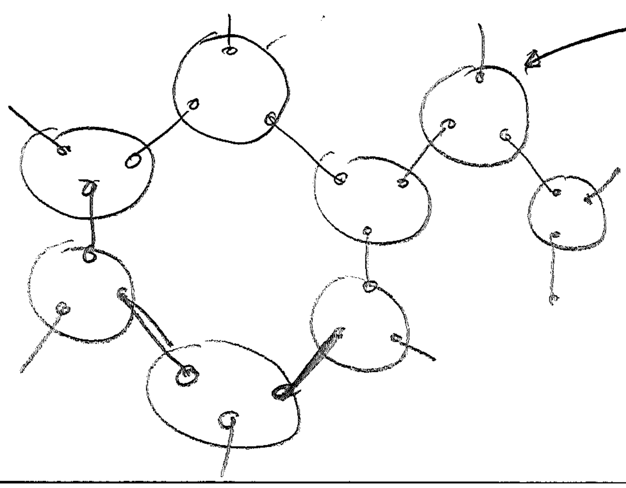
$|01\rangle - |10\rangle$ $(S=0)$



P: Proj. onto $S=2$ (max. spin)

alternatively: AKLT on hex. lattice (PEPS work on any lattice!)

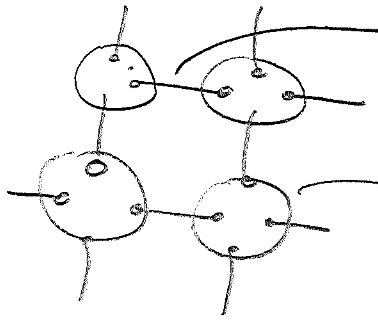
P = Proj. onto $S=3/2$.



* The <u>cluster state</u> used in measurement based quantum computing (→ cf later lecture).

* <u>Topological models</u> such as Kitaev's toric code (→ homework)

* <u>Resonating valence bond states</u>, i.e., the superposition of all ways of putting singlets between adjacent sites:



$|01\rangle - |10\rangle + |22\rangle$

$P = |0\rangle(\langle 0222| + \langle 2022| + \dots) + |1\rangle(\langle 1222| + \langle 2122| + \dots)$

(→ homework)

<u>PEPS from classical models:</u>

Let $H(s_1, \dots, s_N)$ be a <u>classical statistical model</u>

(e.g.: $\underbrace{s_i = \pm 1}_{\substack{+1 \,\hat{=}\, |0\rangle \\ -1 \,\hat{=}\, |1\rangle}}$; $H \equiv -\frac{1}{2}\sum_{\langle ij\rangle} s_i s_j$: Ising model).

Define

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

This state:

i) has the same correlation functions (in the z basis) as the Gibbs state $e^{-\beta H(s_1,\dots,s_N)}$:

$$\langle\psi|\sigma_z^i\sigma_z^j|\psi\rangle = \sum_{s_1,\dots,s_N} e^{-\beta H(s_1,\dots,s_N)} \langle s_i|\sigma_z^i|s_i\rangle\langle s_j|\sigma_z^j|s_j\rangle.$$

ii) Is a PEPS ("Ising PEPS") (with e.g. for the Ising model: $D=2$).

$$|\omega\rangle = |00\rangle + |11\rangle$$

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

with
$$|\alpha\rangle = \cosh(\phi)|0\rangle + \sinh(\phi)|1\rangle$$
$$|\beta\rangle = \sinh(\phi)|0\rangle + \cosh(\phi)|1\rangle,$$

where $\tanh(2\phi) = e^{-\beta/2}$. ($\rightarrow$ homework)

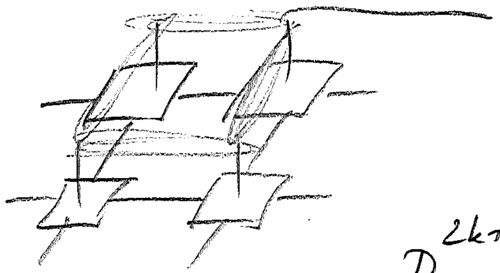
<u>Consequences:</u>

PEPS can exhibit <u>critical correlations</u> (for $\beta=\beta_{crit}$), which decay with a power law, and thus must come from <u>gapless Hamiltonians.</u>

($\longleftrightarrow$ Contrast to 1D where all correlations decay exponentially!)

PEPS & parent Hamiltonians:

PEPS can also be used to construct solvable models:



$\rho_{k\times l}$: dimension of space d^{kl},

but rank $\propto$ boundary: D^{2k+2l}

$D^{2k+2l} < d^{kl}$: rank deficit

$\Rightarrow$ parent Ham. as $\mathbb{1} - \mathrm{Proj}(\mathrm{supp}(\rho_{k\times l}))$.

Again: * Injectivity of P (after blocking) ensures unique G.S. (argument similar to MPS, lecture 9).

* Criteria for topological g.s. structure are also known.

Gap of H: We can argue as for MPS (Lecture 9) that

$H^2 \geq \gamma H$ is satisfied is $h_i h_j + h_j h_i \geq -c\,(h_i + h_j)$

for small enough c.

But: i) this is harder to check numerically (larger blocks needed!)

ii) not always true (e.g. the parent for the critical Ising PEPS must be gapless!)