6. Properties of MPS: Norms, expectation values, correlations.

How can we evaluate properties of MPS:

* normalization
* expectation values, energies
* correlation functions

...

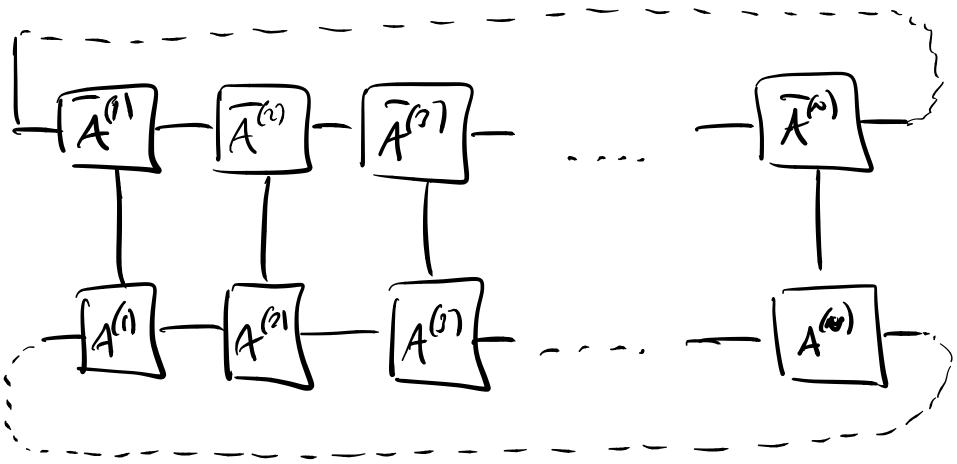
What do they depend on?

Can this be done efficiently – that is, without having to compute $c_{i_1,\dots,i_N}$, but rather in time poly(D)?

a) Normalization

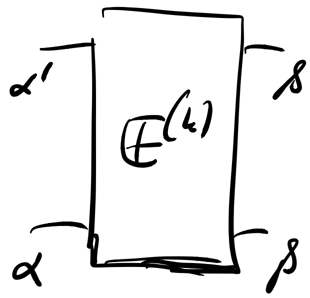
Consider wlog PBC MPS (OBC is special case with $D_0 = D_N = 1$).

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



Define

$\mathbb{E}^{(k)} =$



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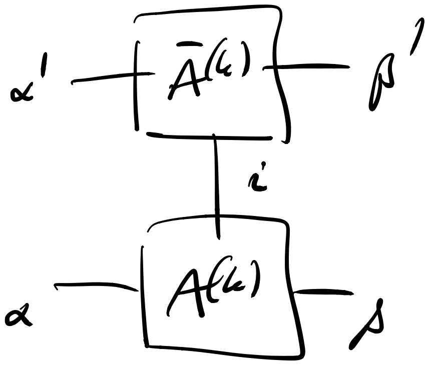


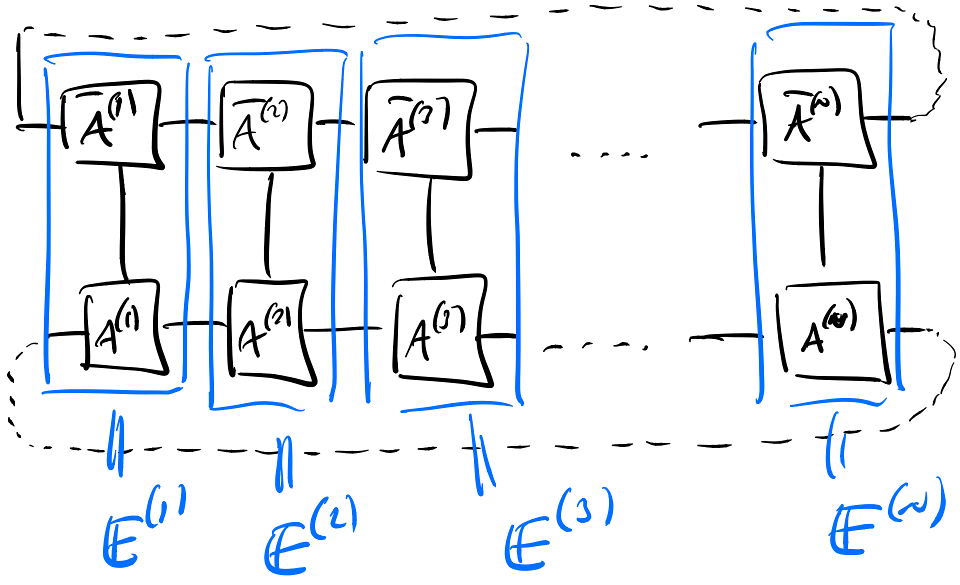
$$= \sum A^{i,(k)} \otimes \bar{A}^{i,(k)}$$

- interpreted as a $D^2 \times D^2$ matrix with row index (α, α'), col. index (β, β').

$\mathbb{E}$ is also called the transfer matrix or transfer operator.

Then,

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



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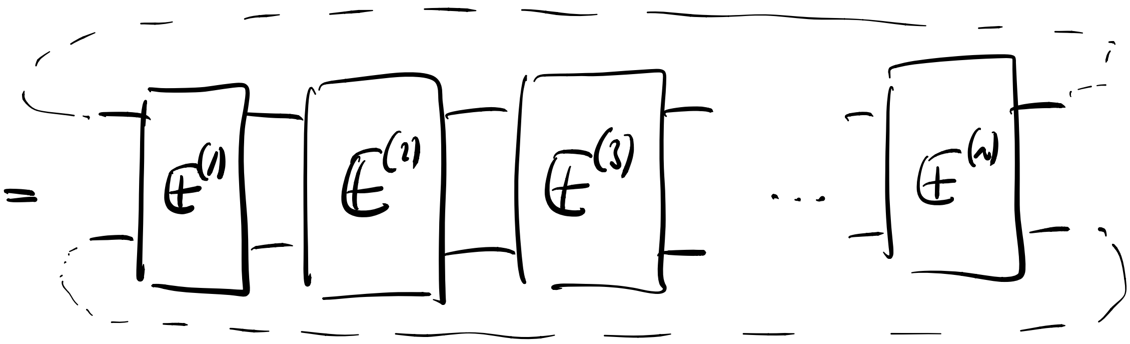


$$= \mathrm{tr}\left(\mathbb{E}^{(1)}\cdot\mathbb{E}^{(2)}\cdot\mathbb{E}^{(3)}\cdot\ldots\cdot\mathbb{E}^{(N)}\right)$$

For OBC, $\mathbb{E}^{(1)}$ & $\mathbb{E}^{(N)}$ are <u>vectors</u>.

What is the comp. cost (for simplicity, $D_k \equiv D$ $\forall k$)?

<u>PBC</u>: Need to multiply two $D^2 \times D^2$

matrices in each step.

Comp. cost of a matrix product of a $(a \times b) \times (b \times c)$ matrix:

$a \cdot b \cdot c$ operations.

$\Rightarrow$ Computational cost is D^6 per step, i.e. ND^6 in total (vs. d^N for building $c_{i_1 \dots i_N}$).

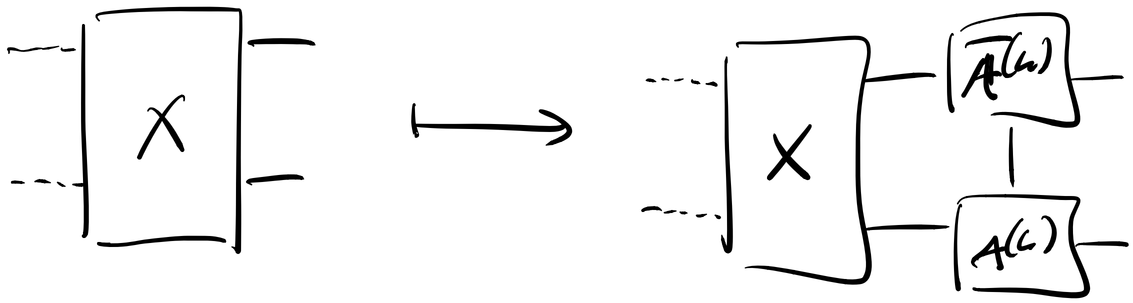
<u>OBC</u>: If we start from the right:

$$\underbrace{\underbrace{E^{(N-1)}}_{D^2 \times D^2} \underbrace{E^{(N)}}_{D^2 \times 1}}_{D^2 \times 1\text{-vector}} \Rightarrow D^4 \text{ operations.}$$

$\Rightarrow$ normalization can be computed <u>efficiently</u>.

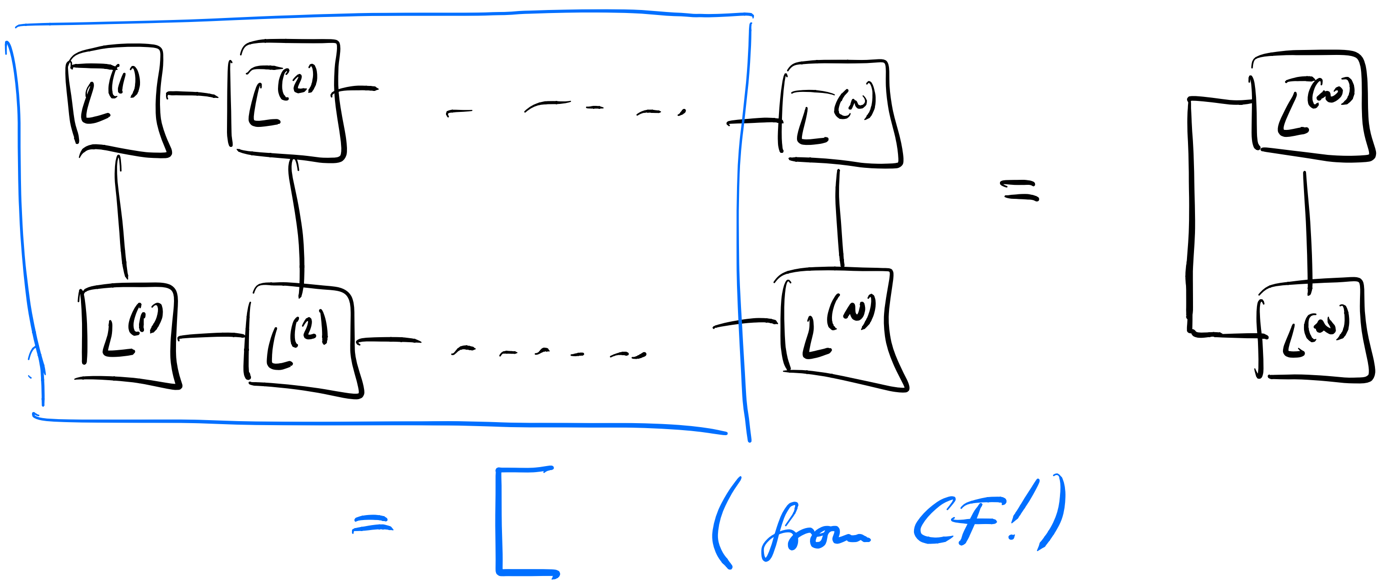
Important points for numerical simulations:

* The PBC/OBC scaling can be improved to D^5/D^3 by applying

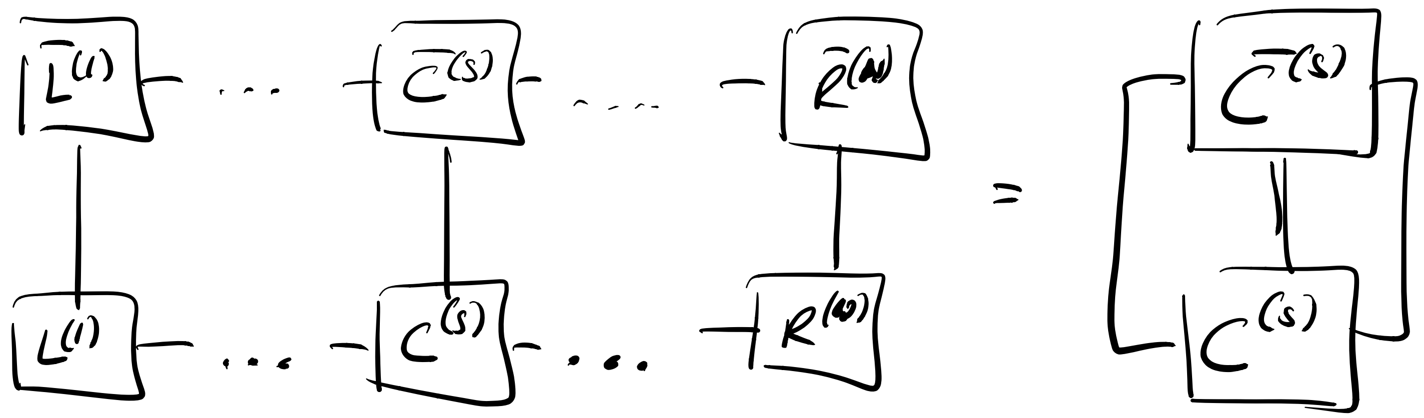


without building $E^{(l)}$. (→ Exercise #7)

* By using the left- (or right-) canonical form, the computation can be done in $O(1)$ steps:



* Similarly, for a mixed CF:



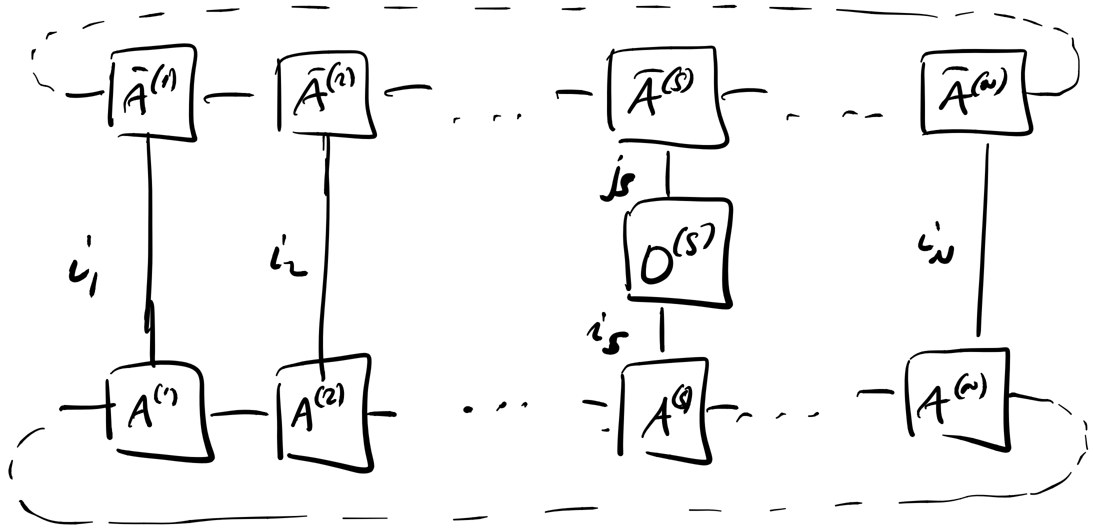
$$= \| C^{(s)} \|_2^2 = \sum_{i_s, \alpha, \beta} \left| C^{i_s (s)}_{\alpha\beta} \right|^2$$

b) Expectation values

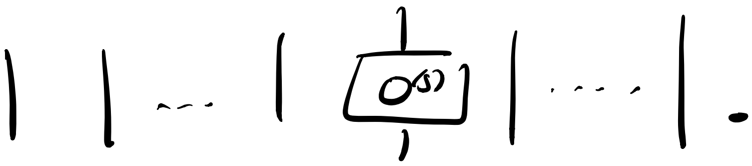
Expectation values $\langle \psi | O | \psi \rangle$ of local observables, e.g. single-site observables $O^{(s)}$ such as $O^{(s)} = \sigma_z^{(s)}$:

$$\langle \psi | O^{(s)} | \psi \rangle = \sum \bar{c}_{j_1 \dots j_N} c_{i_1 \dots i_N} \langle j_1, \dots, j_N | O^{(s)} | i_1, \dots, i_N \rangle$$

$$= \sum_{\substack{i_1 \dots i_N \\ j_s}} \bar{c}_{i_1 \dots i_{s-1} j_s i_{s+1} \dots i_N} \, c_{i_1 \dots i_N} \underbrace{O^{(s)}_{j_s i_s}}_{= \langle j_s | O^{(s)} | i_s \rangle}$$

$=$ 

... can also be understood by noting that

$O^{(s)} = \mathbb{1} \otimes O^{(s)} \otimes \mathbb{1} =$ 

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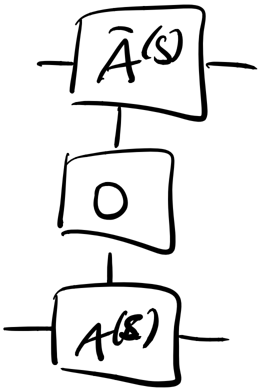
Can it be computed efficiently?

Define again $E^{(k)}$ as before, and additionally

$E_O^{(s)} =$ 

$= \sum_{i,j} A^{i,(s)} \otimes \bar{A}^{j,(s)} \langle j|O|i\rangle$

(Note that $E_{\mathbb{1}}^{(s)} \equiv E^{(s)}$.)

Then, we have that

$$\langle\psi|O|\psi\rangle = \mathrm{tr}\left[\mathbb{E}^{(1)} \cdots \mathbb{E}^{(s-1)}\, \mathbb{E}_O^{(s)}\, \mathbb{E}^{(s+1)} \cdots \mathbb{E}^{(N)}\right]$$

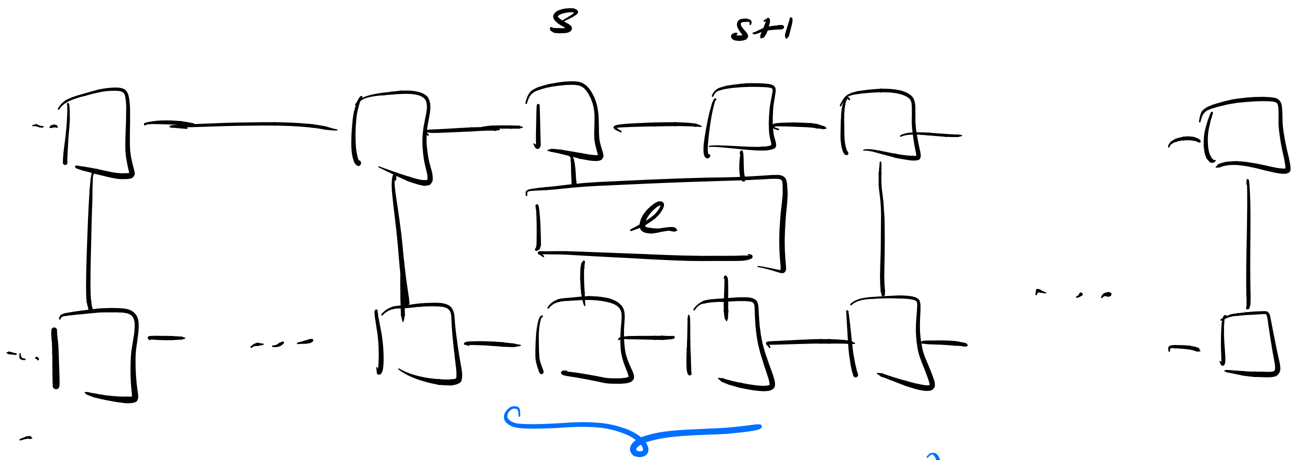
(PBC)

or for OBC,

$$\langle\psi|O|\psi\rangle = \mathbb{E}^{(1)} \cdots \mathbb{E}^{(s-1)}\, \mathbb{E}_O^{(s)}\, \mathbb{E}^{(s+1)} \cdots \mathbb{E}^{(N)}$$

$\Longrightarrow$ expectation values can be <u>computed efficiently</u>.

Same for 2-site observables, e.g. 2-body Hamiltonians:



$$=: \mathbb{E}_h^{(s,s+1)}$$

* define transfer operator for block on which h acts, then

$$\langle\psi|h|\psi\rangle = \mathbb{E}^{(1)}\cdot\ldots\,\mathbb{E}^{(s-1)}\,\mathbb{E}_h^{(s,s+1)}\,\mathbb{E}^{(s+2)}\cdot\ldots$$

* or decompose $h = \sum_i a_i \otimes b_i$, and use

$$\langle\psi|h|\psi\rangle = \sum_{i,j} \mathbb{E}^{(1)}\cdot\ldots\cdot\mathbb{E}^{(s-1)}\mathbb{E}_{a_i}^{(s)}\mathbb{E}_{b_i}^{(s+1)}\cdot\ldots$$

<u>Possible optimizations</u> (e.g. for numerics):

* We can again use a gauge condition – ideally mixed gauge around h – to reduce the computational cost to $O(1)$.

* For $\langle\psi|H|\psi\rangle = \sum_s \langle\psi|h_s|\psi\rangle$, there is no single "good" gauge, but we can still re-use results, e.g.:

$$\langle\psi|h_{s-1,s}|\psi\rangle = \boxed{\mathbb{E}_1\cdot\mathbb{E}_2\cdot\ldots\cdot\mathbb{E}^{(s-2)}}\,\mathbb{E}_h^{(s-1,s)}\,\mathbb{E}_h^{(s+1)}\,\boxed{\mathbb{E}_h^{(s+2)}\cdot\ldots}$$

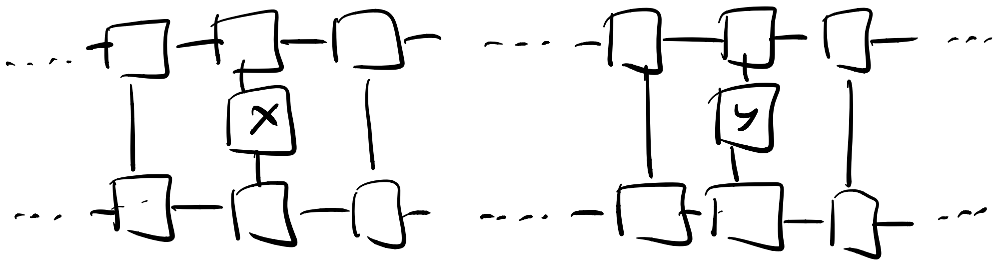
$$\langle\psi|h_{s-1,s}|\psi\rangle = \boxed{\mathbb{E}_1\cdot\mathbb{E}_2\cdot\ldots\cdot\mathbb{E}^{(s-2)}}\,\mathbb{E}^{(s-1)}\,\mathbb{E}_h^{(s,s+1)}\,\boxed{\mathbb{E}_h^{(s+2)}\cdot\ldots}$$

same for both h also same

$\Rightarrow$ total effort to compute $\langle\psi|H|\psi\rangle = \sum_s \langle\psi|h_s|\psi\rangle$ scales proportional with N!

c) Correlation functions

What about correlation functions between operators X_i, Y_j at sites i & j?

$\langle\psi|X_i Y_j|\psi\rangle =$ 

$$= E^{(1)} \cdots E^{(i-1)} \cdot E_X^{(i)} E^{(i+1)} \cdots E^{(j-1)} E_Y^{(j)} E^{(j+1)} \cdots$$

$\Rightarrow$ again efficient.

d) State vs. transfer operator

Properties of state apparently determined mostly by $\{\mathbb{E}^{(k)}\}$, together with $\mathbb{E}_0^{(k)}$.

How much information about the state does $\{\mathbb{E}^{(k)}\}$ encode?

Theorem: A given transfer matrix $\mathbb{E} \equiv \mathbb{E}^{(k)}$ fixes the tensor $A \equiv A^{(k)}$ up to a local basis transformation on the physical system, i.e., for any pair A^i, B^i s.th.

$$\mathbb{E} = \sum A^i \otimes \bar{A}^i = \sum B^i \otimes \bar{B}^i ,$$

$$\exists U_{ij} \text{ unitary}: \quad A^i = \sum_j U_{ij} B^j$$

In fact, this even holds when the physical dimensions are different, with U a (partial) isometry.

<u>Proof:</u> $\longrightarrow$ Exercise #6

(If you know Q. Information:

$\sum A^i_{\alpha\beta} |\alpha,\beta\rangle \otimes |i\rangle$ is a purification of

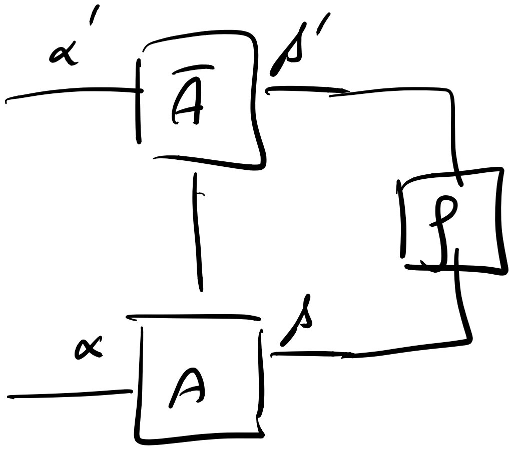
$\rho = \sum \mathbb{E}_{(\alpha\alpha'),(\beta\beta')} |\alpha\beta\rangle\langle\alpha'\beta'|$) $\boxtimes$

$\Rightarrow$ all <u>non-local properties</u> of an MPS are encoded in the $\{\mathbb{E}^{(n)}\}$.

e) Transfer operator as a CP map

And one more bit of Q. Info:

The transfer operator $\mathbb{E}$ defines a map $\rho \longmapsto \mathcal{E}(\rho)$ by virtue of



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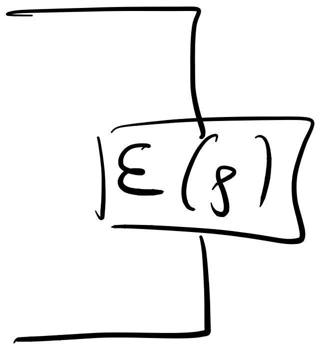


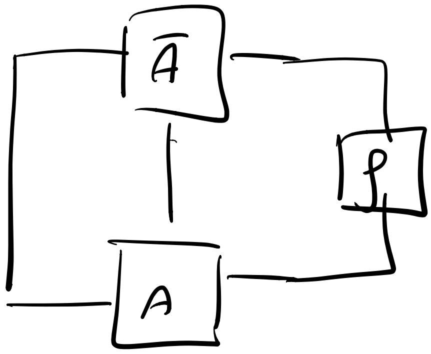
We have $\mathcal{E}(\rho) = \sum A^{i}_{\alpha\beta} \, \bar{A}^{i}_{\alpha'\beta'} \, \rho_{\beta\beta'} \, |\alpha\rangle\langle\alpha'|$

$$= \sum A^{i} \cdot \rho \cdot (A^{i})^{\dagger}$$

$\Rightarrow$ $\mathcal{E}(\cdot)$ is a <u>completely positive map.</u>

(If the MPS is in left-canonical form, then $\mathcal{E}(\cdot)$ is also trace-preserving:

$\mathrm{tr}(\mathcal{E}(\rho)) =$



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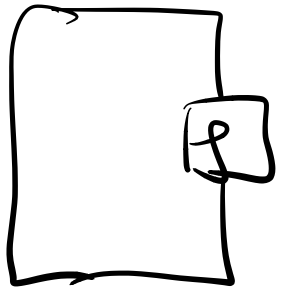

$= \mathrm{tr}(\rho)$