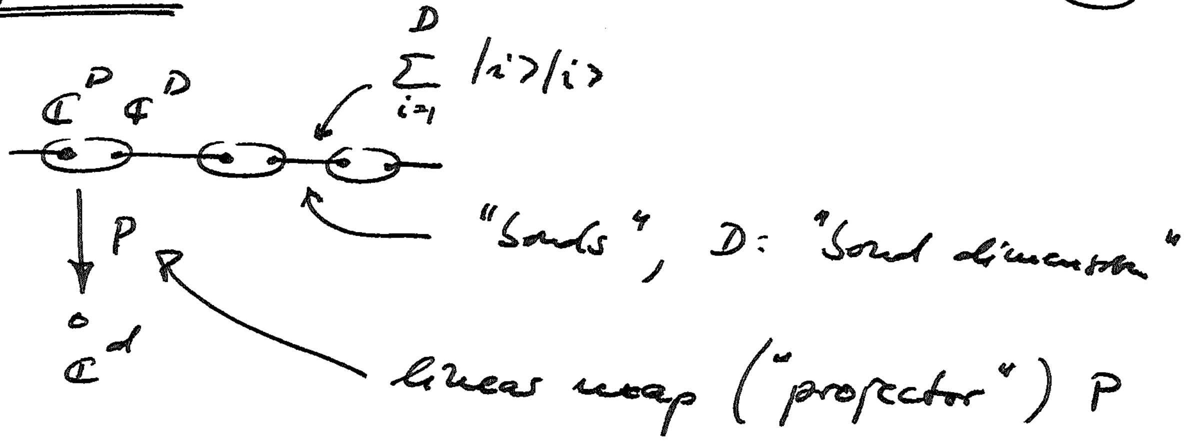
Properties of MPS

MPS:



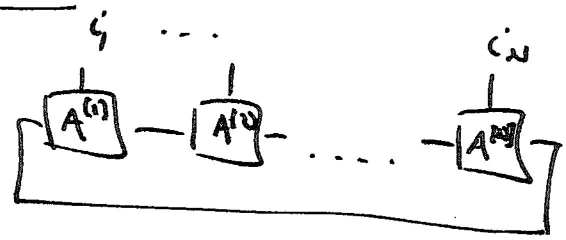
$$|\psi\rangle = \sum c_{i_1 \dots i_N} |i_1, \dots, i_N\rangle$$

with $c_{i_1 \dots i_N} = \mathrm{tr}\left[A^{[1]i_1} \cdots \cdots A^{[N]i_N} \right]$ (PBC)

or $c_{i_1 - i_N} = \langle l | A^{[1]i_1} \cdots \cdots A^{[N]i_N} | r \rangle$ (OBC)

Tensor network notation:

$c_{i_1 \dots i_N}$ =



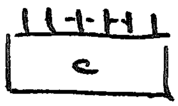
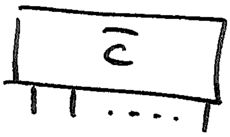
Normalization of MPS

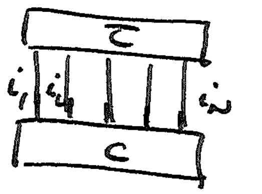
$$|\psi\rangle = \sum_{i_1 - i_N} c_{i_1 \dots i_N} \, |i_1, \dots, i_N\rangle$$

$$\langle\psi|\psi\rangle = \sum_{\substack{i_1, \dots, i_N \\ j_1, \dots, j_N}} \langle j_1, \dots, j_N| \, \bar{c}_{j_1 \dots j_N} \, c_{i_1, \dots, i_N} \, |i_1, \dots, i_N\rangle$$

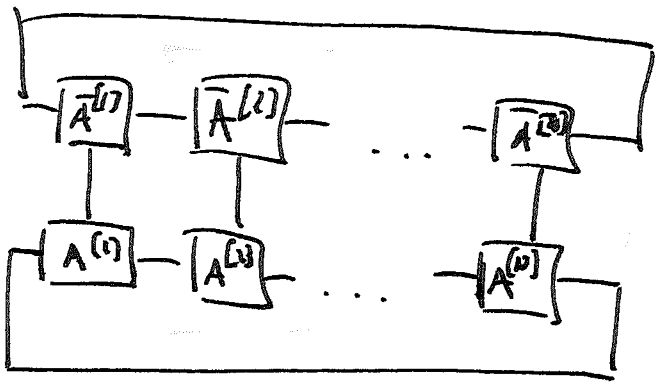
$$\langle j_1, \dots, j_N | i_1, \dots, i_N\rangle \equiv \delta_{i_1 j_1} \dots \delta_{i_N j_N}$$

$$= \sum \bar{c}_{i_1, \dots, i_N} \cdot c_{i_1, \dots, i_N} .$$

$c_{i_1 \dots i_N} =$  ; $\bar{c}_{i_1 \dots i_N} =$ 

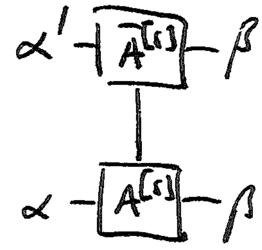
$\Rightarrow \langle\psi|\psi\rangle = \sum \bar{c}_{i_1 - i_N} \, c_{i_1, - i_N} =$ 

for MPS :

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

$(*)$

Consider



$$=: \mathbb{E}^{[s]}$$

This can be understood as a linear map (i.e., matrix) from the "double index" (α,α') to (β,β').

In formulas:

$$\mathbb{E}^{[s]}_{(\alpha\alpha')(\beta\beta')} = \sum_i A^{[s]i}_{\alpha\beta} \cdot \bar{A}^{[s]i}_{\alpha'\beta'}$$

or

$$\boxed{\mathbb{E}^{[s]} = \sum_i \bar{A}^{[s]i} \otimes \bar{A}^{[s]i}}$$

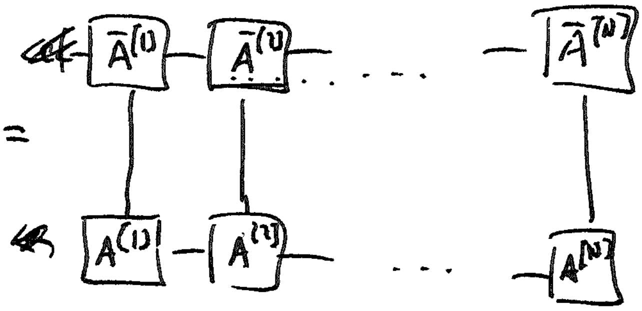
From $(*)$, we see that

$$\langle\psi|\psi\rangle = \mathrm{tr}\left[\mathbb{E}^{[1]}\,\mathbb{E}^{[2]} \cdots\cdots \mathbb{E}^{[N]}\right].$$

(In particular: $\langle\psi|\psi\rangle$ can be evaluated by multiplying N matrices of size $D^2 \times D^2 \Longrightarrow$ computation time is ND^6, i.e. efficient in N!)

OBC:

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



$$= \mathbb{E}^{[1]} \cdot \mathbb{E}^{[2]} \cdot \ldots \cdot \mathbb{E}^{[N]}$$

$1 \times D^2$ $\quad$ $D^2 \times D^2$ $\quad$ $D^2 \times 1$

$\Rightarrow$ OBC: ~~scales as~~ multiplication of D^2-vectors w/ $D^2 \times D^2$ matrix

$\Rightarrow$ scaling ND^4!

Note: We could have done the same only with formulas:

Using $\mathrm{tr}(X \otimes Y) = \mathrm{tr}X \cdot \mathrm{tr}Y$ and $(AC) \otimes (BD) = (A \otimes C)(B \otimes D)$, we find

$$\langle\psi|\psi\rangle = \sum_{i_1 - i_N} \mathrm{tr}\left[A^{[1]i_1} \cdots A^{[N]i_N}\right] \cdot \mathrm{tr}\left[\bar{A}^{[1]i_1} \cdots \bar{A}^{[N]i_N}\right]$$

$$= \sum \mathrm{tr}\left[\underbrace{\left(A^{[1]i_1} \otimes \bar{A}^{[1]i_1}\right)}_{\equiv \mathbb{E}^{[1]}} \cdots \left(A^{[N]i_N} \otimes \bar{A}^{[N]i_N}\right)\right]$$

Expectation values (energies, corr. functions, ...) for MPS

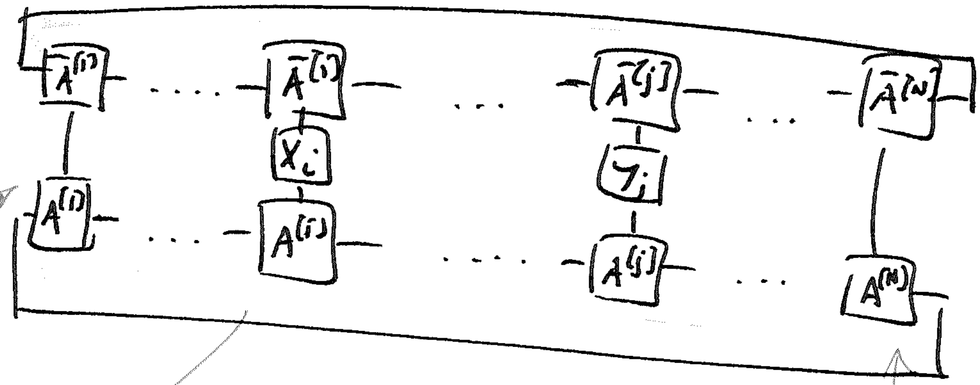
How can we compute exp. values $\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle}$,

for O e.g. Hamiltonian $H = \sum h_i$ (e.g.: $h_i = \vec{S}_i \cdot \vec{S}_{i+1}$),

or $O = X_i \otimes X_j$ (corr. function)

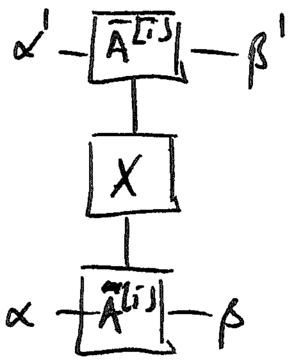
We focus wlog. on $O = \sum X_i \otimes Y_j$ (includes Ham. etc.)

$\langle\psi|X_i \otimes X_j|\psi\rangle =$



$\equiv \mathbb{E}^{[1]}$

$\equiv \mathbb{E}^{[N]}$



$$\boxed{\;\equiv: \mathbb{E}_X^{[i]} \equiv \sum_{j,k} A^{[i]j} \otimes \bar{A}^{[i]k} \langle j|X|k\rangle\;}$$

(Note: $\mathbb{E}_{\mathbb{1}}^{[i]} \equiv \mathbb{E}^{[i]}$.)

$$\Rightarrow \quad \langle\psi|X_i\otimes X_j|\psi\rangle = \mathrm{tr}\Big[\mathbb{E}^{[1]}\cdots\mathbb{E}^{[i-1]}\,\mathbb{E}_X^{[i]}\cdot\mathbb{E}^{[i+1]}\cdots$$
$$\cdots\mathbb{E}^{[j-1]}\,\mathbb{E}_Y^{[j]}\,\mathbb{E}^{[j+1]}\cdots\mathbb{E}^{[N]}\Big]$$

$\Rightarrow$ energies, corr. functions, etc. can be computed just as the normalization. In part., the scaling in N is efficient (quadratic for Ham., but there are tricks!)

Scaling of correlations for MPS

Consider a tr. inv. PBC MPS w/ tensors $A \equiv A^i_{\alpha\beta}$.

What can we say about the scaling of correlations

$$\frac{\langle\psi|X_i\otimes Y_j|\psi\rangle}{\langle\psi|\psi\rangle} = c(i,j) \quad \text{as a function of } i-j\,?$$

$$c(i,j) = \frac{\mathrm{tr}\Big[\overbrace{\mathbb{E}\cdots\mathbb{E}}^{i-1}\cdot\overset{i}{\mathbb{E}_X}\cdot\overbrace{\mathbb{E}\cdots\mathbb{E}}^{j-i-1}\,\overset{j}{\mathbb{E}_Y}\,\overbrace{\mathbb{E}\cdots\mathbb{E}}^{N-(j)}\Big]}{\mathrm{tr}\Big[\underbrace{\mathbb{E}\cdots\mathbb{E}}_{N}\Big]}$$

$$= \frac{\mathrm{tr}\Big[\mathbb{E}_X\cdot\mathbb{E}^{j-i-1}\,\mathbb{E}_Y\cdot\mathbb{E}^{N+i-j-1}\Big]}{\mathrm{tr}\Big[\mathbb{E}^N\Big]}.$$

Eigendecomposition of $\mathbb{E}$ (assume no Jordan blocks!)

$$\mathbb{E} = \sum_k \lambda_k |r_k\rangle\langle l_k| \, ;$$

Focus first on unique max. eigenvalue:

$$|\lambda_1| > |\lambda_2| \geq \dots .$$

Then, $\mathbb{E}^M \longrightarrow \lambda_1^M |r_1\rangle\langle l_1|$ for large M!

$$\Rightarrow \quad c(i,j) \overset{N\,\text{large}}{\approx} \frac{\mathrm{tr}\left[\mathbb{E}_x \, \mathbb{E}^{j-i-1} \cdot \mathbb{E}_y \cdot \lambda_1^{N+i-j-1} |r_1\rangle\langle l_1|\right]}{\cancel{\mathrm{tr}\,\mathbb{E}^N} \; \mathrm{tr}\left[\lambda_1^N |r_1\rangle\langle l_1|\right]}$$

$$= \frac{\langle l_1 | \mathbb{E}_x \, \mathbb{E}^{j-i-1} \, \mathbb{E}_y | r_1\rangle}{\lambda_1^{j-i+1}}$$

Now use that $\mathbb{E}^{j-i-1} = \sum_k \lambda_k^{j-i-1} |r_k\rangle\langle l_k|$

$$\Rightarrow \quad c(i,j) = \sum_k \left(\frac{\lambda_k}{\lambda_1}\right)^{j-i-1} \frac{\langle l_1|\mathbb{E}_x|r_k\rangle\langle l_k|\mathbb{E}_y|r_1\rangle}{\lambda_1^2}$$

$\Rightarrow$ <u>all</u> correlations decay <u>exponentially</u>

If the largest eigenval. of $\mathbb{E}$ is <u>degenerate</u>

$\Rightarrow$ state has long-range correlations.

(let $\sum'$ denote sum over largest eigenvalues)

For $N \to \infty$, $j-i \to \infty$:

$$c(i,j) \approx \frac{\mathrm{tr}\left[\mathbb{E}_X \left(\sum' \lambda_k^{j-i-1} |r_k\rangle\langle l_k|\right) \mathbb{E}_Y \left(\sum' \lambda_l^{N+i-j-1} |r_l\rangle\langle l_l|\right)\right]}{\mathrm{tr}\left[\mathbb{E}_X \sum' \lambda_k^{N} |r_k\rangle\langle l_k|\right]}$$

$$= \frac{\sum_{kl} \lambda_k^{j-i-1} \lambda_l^{N-i-j-1} \langle l_l|\mathbb{E}_X|r_k\rangle\langle l_k|\mathbb{E}_Y|r_l\rangle}{\sum' \lambda_k^N}$$

$$= \text{const. (up to oscillations).}$$

<u>Examples:</u>

<u>AKLT state:</u> $A^{+1} = \sigma_{xy}$; $A^0 = \sigma_z$; $A^{-1} = \sigma_x$

$$\mathbb{E} = \sigma_x \otimes \bar{\sigma}_x + \sigma_y \otimes \bar{\sigma}_y + \sigma_z \otimes \sigma_z$$

$$= \begin{pmatrix} 1 & & & 2 \\ & 1 & 0 & \\ & 0 & 1 & \\ 2 & & & 1 \end{pmatrix}$$

$$\lambda_1 = 3; \quad |r_1\rangle = |\ell_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$|\lambda_2| = |\lambda_3| = |\lambda_4| = 1$$

$\Rightarrow$ Correlations decay like $\left(\frac{1}{3}\right)^{\ell} \equiv e^{-\ell/\xi}$

$\Rightarrow$ corr. length $\xi = -1/\log(1/3) = 0.91\ldots$

<u>GHZ state:</u> $A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; \quad A^1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

$$\mathbb{E} = A^0 \otimes \bar{A}^0 + A^1 \otimes \bar{A}^1 = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & 1 \end{pmatrix}$$

$\Rightarrow \quad |\lambda_1| = |\lambda_2| = 1; \quad \lambda_3 = \lambda_4 = 0$

$\Rightarrow$ Long-range correlations!