Matrix Product States: Basic properties

Matrix Product State (open boundary conditions (OBC)):
1D chain of N d-level systems:

$$|\psi\rangle = \sum_{i_1,\dots,i_N} A^{[1]i_1} A^{[2]i_2} \cdot \ldots \cdot A^{[N]i_N} \, |i_1, i_2, \dots, i_N\rangle$$

with $A^{[1]i_1}$ $1\times D$ matrix (vector)

$A^{[s]i_s}$ $D\times D$ matrix, $s=2,\dots,N-1$

$A^{[N]i_N}$ $D\times 1$ matrix

D: virtual dimension, bond dimension

Last lecture: Every state $|\psi\rangle$ has an MPS representation with
$D =$ max. Schmidt rank of $|\psi\rangle$ across any cut $1\dots k|k+1\dots N$.

General state: Schmidt rank $D \sim d^{N/2}$ $\Rightarrow$
$\Rightarrow$ # of parameters $\sim NdD^2 = Nd^{2N+1/2}$: exp. in N!
$\Rightarrow$ no improvement over $|\psi\rangle = \sum c_{i_1\dots i_N}|i_1\dots i_N\rangle$ (d^N parameters)

State with bounded Schmidt rank:
# of parameters $\sim NdD^2$, D const. : linear in N!
$\Rightarrow$ exponential improvement over $c_{i_1\dots i_N}$.

Will see later: low entanglement (area law) $\rightarrow$ good MPS approximation to $|\psi\rangle$ with low D exists.

MPS: Efficient approximation of states with low entanglement, in particular ground states of gapped local Hamiltonians!

Generalization: MPS with periodic boundary conditions (PBC):

$$|\psi\rangle = \sum_{i_1 \dots i_N} \mathrm{tr}\left[A^{[1]i_1} A^{[2]i_2} \cdot \dots \cdot A^{[N]i_N}\right] |i_1, \dots, i_N\rangle$$

Graphical notation for MPS:

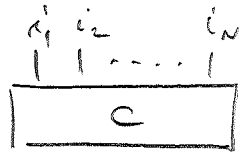
$$|\psi\rangle = \sum_{i_1 \dots i_N} c_{i_1 \dots i_N} |i_1 \dots i_N\rangle$$

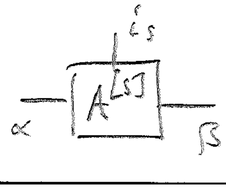
$c_{i_1 \dots i_N}$: Tensor w/ N indices (very large!)

MPS: Express $c_{i_1 \dots i_N}$ as summation ("contraction") over a set of simple tensors.

Graphical notation:

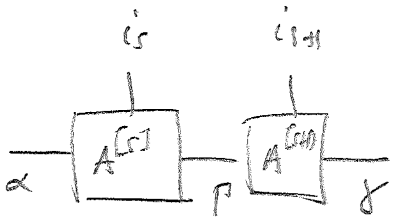
Tensor = "box w/ legs":

$c_{i_1 \dots i_N} =$ 

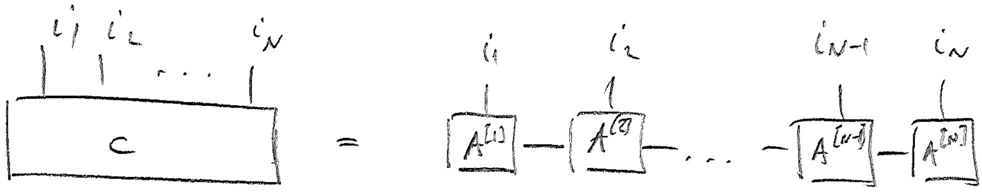
$A^{[s]i_s}_{\alpha\beta} =$ 

Summation (contraction) = connect legs:

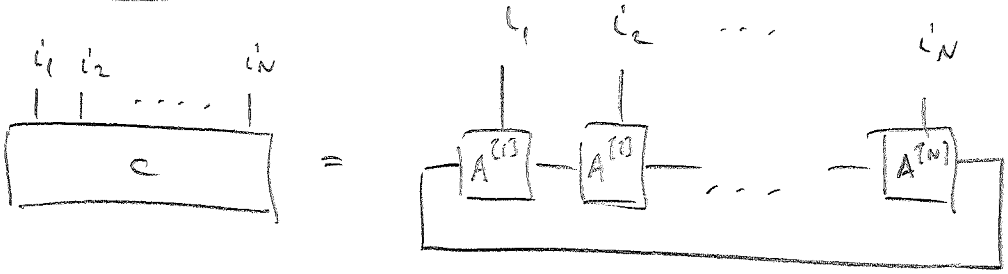
$$\sum A^{[s]\,i_s}_{\alpha\beta} \, A^{[s+1]\,i_{s+1}}_{\beta\gamma} \; = $$



MPS (OBC):



MPS (PBC):



Re-express $c_{i_1 \dots i_N}$ as <u>Tensor Network</u> $\rightarrow$ <u>"Tensor Network States"</u>.

$\rightarrow$ Structure of TN reproduces locality structure of system!

Examples:

Ex. 1: GHZ: $\frac{1}{\sqrt{2}}\left(|0\ldots 0\rangle + |1\ldots 1\rangle\right)$

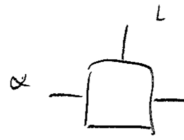
PBC: $A^{[s],0} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |0\rangle\langle 0|$; $A^{[s],1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = |1\rangle\langle 1|$

$$\longrightarrow \quad A^{[s],i_s} \cdot A^{[s+1],i_{s+1}} = \delta_{i_s, i_{s+1}} \, A^{[s+1] i_{s+1}} \quad \text{etc.}$$

$$\longrightarrow \quad \mathrm{tr}\left[A^{[1] i_1} \cdot \ldots \cdot A^{[N] i_N} \right] = \delta_{i_1 \ldots i_N}$$

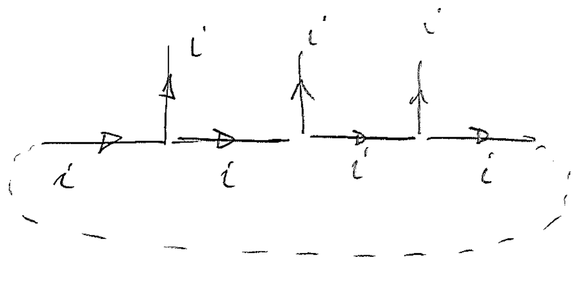
Note:
- MPS is not normalized.
- We can normalize by e.g. choosing $A^{[1],i} = \frac{1}{\sqrt{2}}(\ldots)$.
- Normalization breaks transl. invariance (or dep. on N).

Graphical:



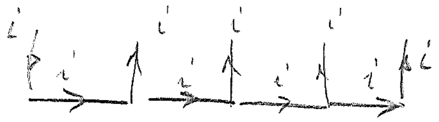
$\equiv \delta_{\alpha\beta i}$

"Algorithmic" interpretation: Tensor "transports" information on virtual index from left to right & copies it to physical index.



In particular: Map from α to (i,β) is isometry: can be implemented deterministically $\rightarrow$ preparation scheme (if we had OBC)

Can we write GHZ w/ OBC?

Yes: 

$$\rightarrow \quad A^{[1],0} = (1,0) = \langle 0| = \langle +| A^{[s],0} \qquad (\langle +| = (\langle 0| + \langle 1|))$$

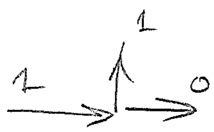
$$A^{[1],1} = (0,1) = \langle 1| = \langle +| A^{[s],1}$$

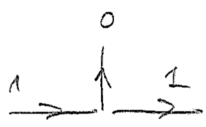
$$A^{[N],0} = \begin{pmatrix}1\\0\end{pmatrix} = |0\rangle = A^{[s],0}|+\rangle$$

$$A^{[N],1} = \begin{pmatrix}0\\1\end{pmatrix} = |1\rangle = A^{[s],1}|+\rangle$$

Example 2: W State

$$|W\rangle \propto |100\ldots\rangle + |010\ldots\rangle + |0010\ldots\rangle + \ldots + |00\ldots01\rangle$$



or


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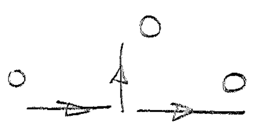
and 

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Start with 1, end with 0:

1 will be exactly at one position

$$A^{[s],0} = |0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}$$

$$A^{[s],1} = |1\rangle\langle 0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \sigma^+$$

$$A^{[1],i} = \langle 1| A^{[s],i} \quad ; \quad A^{[N],i} = A^{[s],i} |0\rangle$$

$$\Rightarrow c_{i_1 \ldots i_N} = \langle 1| \underbrace{A^{[1]i_1} A^{[2]i_2} \cdots A^{[N]i_N}}_{} |0\rangle$$

each: $\mathbb{1}$ or σ^+, and $\sigma^+\sigma^+ = 0$

$\Rightarrow$ exactly one σ^+ $\Rightarrow$ W state!

Note: No PBC representation of W state exists (unless D grows w/ N).

AKLT state: $d=3$ (spin-1), $D=2$. (states: $|+1\rangle$, $|0\rangle$, $|-1\rangle$)

$$A^{[s],+1} = \sqrt{2}\sigma^+ \; ; \; A^{[s],-1} = -\sqrt{2}\sigma^- \; ; \; A^{[s],0} = \sigma_z .$$

Ground state: Σ of $|(+1)\,0\ldots0\,(-1)\,0\ldots0\,(+1)\,0\ldots0\,(-1)\ldots\rangle$

$\rightarrow$ alternating $(+1)$ and (-1) w/ arb. # of 0 inbetween!

$\rightarrow$ sign dep. on # of zeros!

$\rightarrow$ some type of long-range order/information?

AKLT: ∘ First example of MPS.

∘ Gives interesting solvable model.

∘ Will meet it again later.

Properties of Matrix Product States:

① Normalization:

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

$$\langle\psi|\psi\rangle = \sum_{\substack{i_1 \ldots i_N \\ j_1 \ldots j_N}} \langle \underbrace{j_1 \ldots j_N | \bar{c}_{j_1 \ldots j_N} c_{i_1 \ldots i_N} | i_1 \ldots i_N}_{\delta_{i_k j_k}} \rangle$$

$$= \sum_{i_1 \ldots i_N} c_{i_1 \ldots i_N} \bar{c}_{i_1 \ldots i_N}$$

$$= \sum_{i_1 \ldots i_N} \mathrm{tr}\left[A^{[1]i_1} \cdot A^{[2],i_2} \cdot \ldots\right] \cdot \mathrm{tr}\left[\bar{A}^{[1]i_1} \cdot \bar{A}^{[2]i_2} \cdot \ldots\right]$$

$$\boxed{\begin{aligned} \underline{NB}: \quad & \mathrm{tr}[A]\,\mathrm{tr}[B] = \mathrm{tr}[A \otimes B], \\ & (AC) \otimes (BD) = (AB) \otimes (CD) \end{aligned}}$$

$$= \sum_{i_1 \ldots i_N} \mathrm{tr}\left[\left(A^{[1]i_1} \otimes \bar{A}^{[1],i_1}\right) \cdot \left(A^{[2]i_2} \otimes \bar{A}^{[2]i_2}\right) \cdot \ldots\right]$$

$$= \mathrm{tr}\left[\left(\sum_{i_1} A^{[1]i_1} \otimes \bar{A}^{[1]i_1}\right) \cdot \ldots\right]$$

Define $\mathbb{E}^{[s]} := \sum_i A^{[s]i} \otimes \bar{A}$: "transfer operator"

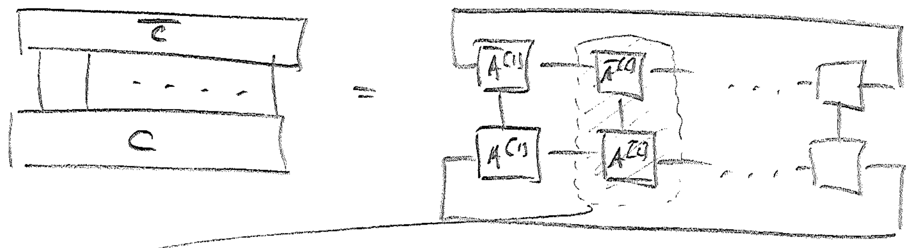
$$\Longrightarrow \langle\psi|\psi\rangle = \mathrm{tr}\left[\mathbb{E}^{[1]} \cdot \mathbb{E}^{[2]} \cdot \ldots \cdot \mathbb{E}^{[N]}\right]$$

$\Rightarrow \langle\psi|\psi\rangle \equiv$ matrix multiplication of $D^2\times D^2$-matrices

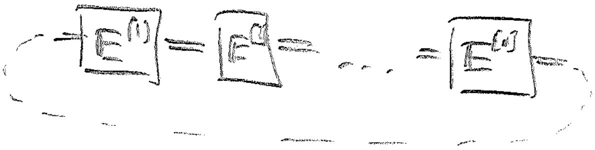
$\Rightarrow$ efficient (as compared to $\sum_{i_1\ldots i_N} |c_{i_1\ldots i_N}|^2$).

Alternative graphical derivation:

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



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



(2) Expectation values of local observables

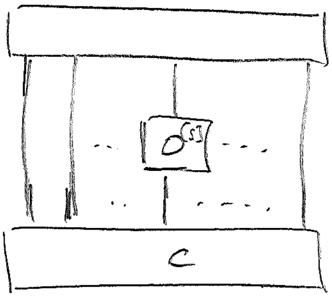
(for simplicity: single-site observables.
Otherwise: block sites, or write $O = \sum A^i \otimes B^i$)

$$\langle\psi|O^{[s]}|\psi\rangle = \sum \langle j_1\ldots j_N|\bar{c}_{j_1\ldots j_N}\, O^{[s]}\, c_{i_1\ldots i_N}|i_1\ldots i_N\rangle$$

$$= \sum \underbrace{\langle j_1\ldots j_N|O^{[s]}|i_1\ldots i_N\rangle}_{=\langle j_s|O^{[s]}|i_s\rangle \prod_{k\neq s}\delta_{i_k j_k}} c_{i_1\ldots i_N}\,\bar{c}_{j_1\ldots j_N}.$$

$$= \sum_{\substack{i_1 \dots i_N \\ j_s}} c_{i_1 \dots i_N} \, \overline{c_{i_1 \dots j_s \dots i_N}} \, \langle j_s | O^{[s]} | i_s \rangle .$$

$=$



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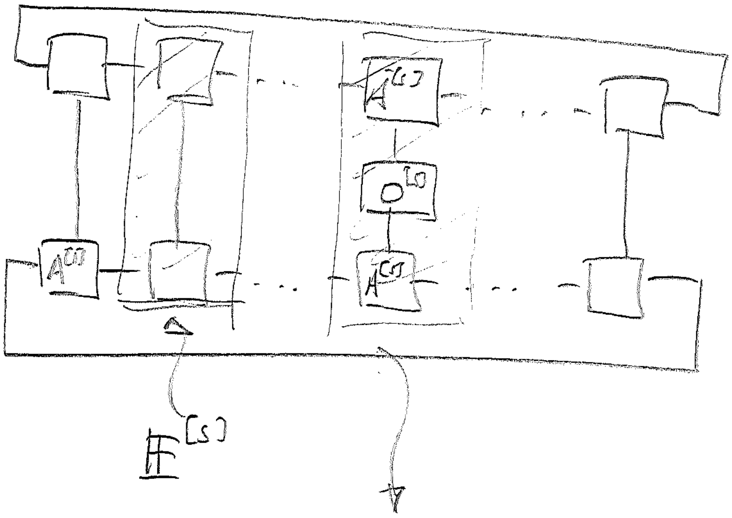
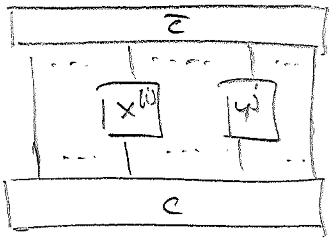


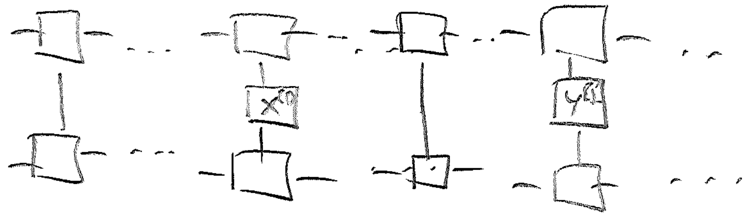
Define $\mathbb{E}_O^{[s]} = \sum_{ij} A^{[s]i} \otimes \overline{A}^{[s]j} \langle j | O^{[s]} | i \rangle$

$$\Longrightarrow \langle \psi | O | \psi \rangle = \mathrm{tr}\left[\mathbb{E}^{[1]} \mathbb{E}^{[2]} \cdots \mathbb{E}_O^{[s]} \cdot \mathbb{E}^{[s+1]} \cdots \mathbb{E}^{[N]} \right]$$

(3) Correlation functions:

$\langle \psi | X^{[i]} Y^{[j]} | \psi \rangle =$

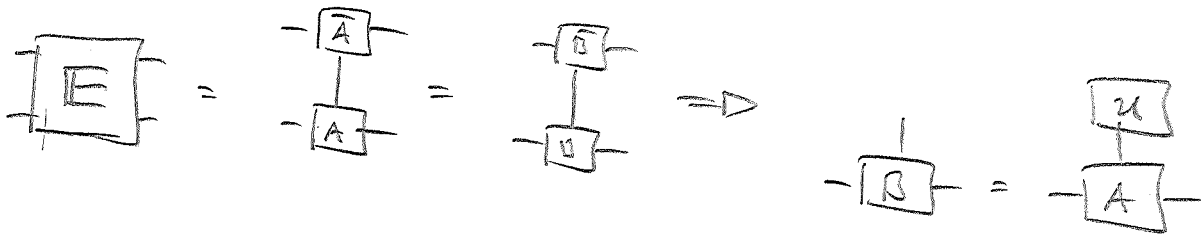


$=$ 

$$= \mathrm{tr}\left[\mathbb{E}^{[1]}\,\mathbb{E}^{[2]}\cdots\mathbb{E}_X^{[i]}\cdots\mathbb{E}_Y^{[j]}\,\mathbb{E}^{[j+1]}\cdots\right]$$

$\Rightarrow$ all information about correlation function etc. contained in transfer operator.

<u>In fact:</u> Transfer op. $\mathbb{E}^{[s]}$ determines state <u>uniquely</u> up to local basis transformation (i.e., basis choice)



$\Rightarrow$ all non-local properties contained in $\mathbb{E}$!

(Proof: Homework!)

Scaling of correlations in MPS

Consider transl. invariant MPS (PBC), i.e. $A^{[i]} \equiv A$.

How do correlation functions scale?

$$c(i,j) = \frac{\langle\psi| X^{[i]} Y^{[j]} |\psi\rangle}{\langle\psi|\psi\rangle} \quad \text{as function of } i-j\text{?}$$

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

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

Assume $\mathbb{E}$ has no Jordan blocks ($\rightarrow$ cf. HW):

$$\mathbb{E} = \sum_{k=1}^{D^2} \lambda_k\, |r_k\rangle\langle l_k| \quad : \text{eigenvalue decomposition,} \quad \langle l_i|r_j\rangle = \delta_{ij}$$

wlog $|\lambda_1| \geq |\lambda_2| \geq \ldots$

Assume first $|\lambda_1| > |\lambda_2|$:

Then, $\mathbb{E}^M \longrightarrow \lambda_1^M |r_1\rangle\langle l_1|$ for $M \rightarrow \infty$.

$$\Rightarrow \quad c(i,j) \overset{N\ \text{large}}{\approx} \frac{\operatorname{tr}\left[\mathbb{E}_X\, \mathbb{E}^{j-i-1}\, \mathbb{E}_Y\, \lambda_1^{N+i-j-1} |r_1\rangle\langle l_1|\right]}{\operatorname{tr}\left[\lambda_1^N |r_1\rangle\langle l_1|\right]}$$

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

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

$$\Rightarrow \quad c(i,j) = \sum_{k=1}^{D^2} \left(\frac{\lambda_k}{\lambda_1}\right)^{j-i-1} \frac{\langle l_1|\mathbb{E}_X|r_k\rangle\langle l_k|\mathbb{E}_Y|r_1\rangle}{\lambda_1^2}$$

$\Rightarrow$ all <u>correlation functions</u> <u>decay exponentially</u>.

Largest eigenvalue of $\mathbb{E}$ degenerate (up to phase, $|\lambda_1| = |\lambda_2| = \dots$):

$$\mathbb{E}^M \longrightarrow \underbrace{\sum_{k=1}^{K}{}'}_{\text{Sum over degen. eigenvalues}} \lambda_k^M |r_k\rangle\langle l_k|$$

$$c(i,j) \overset{\substack{\text{large } N\\ \text{large } |j-i|}}{\approx} \frac{\operatorname{tr}\left[\mathbb{E}_X \left(\sum_{k=1}^{K} \lambda_k^{j-i-1} |r_k\rangle\langle l_k|\right) \mathbb{E}_Y \left(\sum_{k=1}^{K} \lambda_k^{N+i-j-1} |r_k\rangle\langle l_k|\right)\right]}{\operatorname{tr}\left[\sum_{k=1}^{K} \lambda_k^N |r_k\rangle\langle l_k|\right]}$$

$$= \frac{\sum_{k,l=1}^{K} \lambda_k^{j-i-1} \lambda_l^{N-i-j-1} \langle l_l | E_x | r_k \rangle \langle l_k | E_y | r_l \rangle}{\sum_{k=1}^{K} \lambda_k^N}$$

$\Longrightarrow$ this term is <u>constant</u> for $|j-i| \to \infty$,

up to <u>oscillations</u> if $\arg(\lambda_k) \neq \arg(\lambda_l)$.

<u>Examples:</u>

<u>AKLT state:</u>

$$A^{+1} = \sqrt{2}\,\sigma^+ ; \quad A^{-1} = \sqrt{2}\,\sigma^- ; \quad A^0 = \sigma_z .$$

$$\mathbb{E} = 2\sigma^+ \otimes \sigma^+ + 2\sigma^- \otimes \sigma^- + \sigma_z \otimes \sigma_z$$

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

$\Longrightarrow \lambda_1 = 3 ; \quad |r_1\rangle = |l_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} ; \quad |\lambda_2| = |\lambda_3| = |\lambda_4| = 1$

$\Longrightarrow$ Correlations decay as $\left(\frac{1}{3}\right)^l = e^{-l/\xi}$

$\Longrightarrow$ correlation length $\xi = -\frac{1}{\log(1/3)} \simeq 0.910$

GHZ state: $A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$; $A^1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

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

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

$\Rightarrow$ long-range correlations!