7. Translational invariant infinite MPS: Construction and correlations

Knowing the transfer operator, we can now revisit tinv. MPS in the thermodyn. limit.

a) Construction

Consider a tinv. PBC MPS with tensor A,

$\mathbb{E} = \sum A^i \otimes \bar{A}^i$, on a chain of length N.

The expectation value of an operator O

at position 1 (Note: tinv. $\Rightarrow$ all positions equiv.!) is

tinv: all $\mathbb{E}$ the same!

$$\langle\psi|O|\psi\rangle = \mathrm{tr}\Big[\mathbb{E}_O \cdot \underbrace{\mathbb{E} \cdot \ \ldots\ldots \ \cdot \mathbb{E}}_{N-1 \text{ times}}\Big]$$

$$= \mathrm{tr}\left[\mathbb{E}_O \, \mathbb{E}^{N-1}\right].$$

and the normalization

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

Assume $\mathbb{E}$ diagonalizable (generic!):

$$\mathbb{E} = \sum \lambda_i \, |r_i\rangle\langle l_i|$$

eigenvalue decomposition.

(<u>Note:</u> $\langle l_i | r_j\rangle = \delta_{ij}$, but

$\langle l_i | l_j\rangle$, $\langle r_i | r_j\rangle$ arbitrary!)

Wlog: $|\lambda_1| \geq |\lambda_2| \geq \dots$

Then, $\mathbb{E}^{\ell} = \sum \lambda_i^{\ell} \, |r_i\rangle\langle l_i|$.

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

largest eigenval. non-degen.
(in absolute value)

Then, as $\ell \gg 1$,

$$\mathbb{E}^{\ell} \longrightarrow \lambda_1^{\ell} |r_1\rangle\langle \ell_1| .$$

Thus, as $N \to \infty$:

$$\frac{\langle \psi | O | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\mathrm{tr}\left[\mathbb{E}_0 \, \mathbb{E}^{N-1} \right]}{\mathrm{tr}\left[\mathbb{E}^{N} \right]}$$

$$= \frac{\sum_i \mathrm{tr}\left[\mathbb{E}_0 \, \lambda_i^{N-1} |r_i\rangle\langle \ell_i| \right]}{\sum_i \mathrm{tr}\left[\lambda_i^{N} |r_i\rangle\langle \ell_i| \right]}$$

$$= \frac{\sum_i \lambda_i^{N-1} \langle \ell_i | \mathbb{E}_0 | r_i \rangle}{\sum \lambda_i^{N} \underbrace{\langle \ell_i | r_i \rangle}_{=1}}$$

$$\longrightarrow \frac{\lambda_1^{N-1} \langle \ell_1 | \mathbb{E}_0 | r_1 \rangle}{\lambda_1^{N}}$$

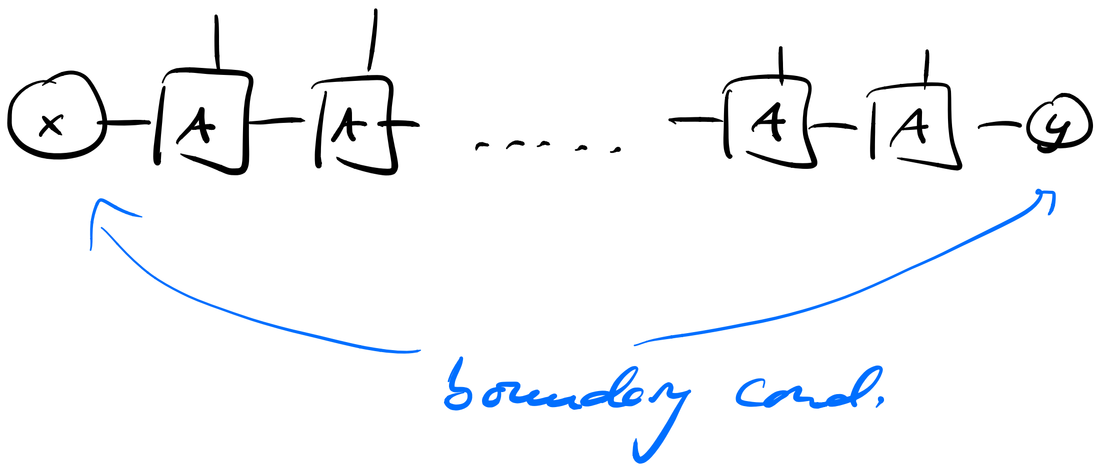
$$= \frac{1}{\lambda_1} \langle \ell_1 | \mathbb{E}_0 | r_1 \rangle .$$

We find:

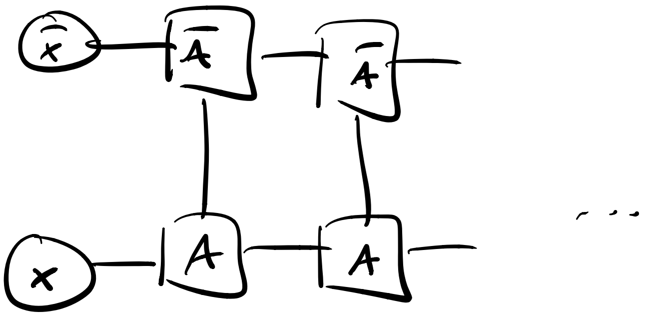
- $\dfrac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle}$ is well-defined in the thermodynamic limit.

- This can be used to compute exp. values for any quantity, by choosing left/right boundaries $\langle l_1|$ and $|r_1\rangle$ (example – correlations – in a moment!)

- The same result can be obtained from OBC:



Let $X = x\otimes\bar{x}$, $Y = y\otimes\bar{y}$ the two-layer boundary condition:



$$\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\langle x|\mathbb{E}^{n}\,\mathbb{E}_0\,\mathbb{E}^{n}|y\rangle}{\langle x|\,\mathbb{E}^{2n+1}|y\rangle}.$$

Using $\mathbb{E}^{\ell} = \sum \lambda_i^{\ell}|r_i\rangle\langle l_i| \to \lambda_1^{\ell}|r_1\rangle\langle l_1|$,

for $n \to \infty$ we have

$$\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} \longrightarrow \frac{\lambda_1^{2n}\langle x|r_1\rangle\langle l_1|y\rangle\,\langle l_1|\mathbb{E}_0|r_1\rangle}{\lambda_1^{2n+1}\langle x|r_1\rangle\langle l_1|y\rangle}$$

$$= \frac{1}{\lambda_1}\langle l_1|\mathbb{E}_0|r_1\rangle.$$

b) Correlation functions

How do correlations in a transl. inv. (infinite) MPS look like?

$$\frac{\langle\psi|X_1 Y_\ell|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\mathrm{tr}\left[\mathbb{E}_X \, \mathbb{E}^{\ell-2} \, \mathbb{E}_Y \, \mathbb{E}^{N-\ell}\right]}{\mathrm{tr}\left[\mathbb{E}^N\right]}$$

$$\xrightarrow{N\to\infty} \frac{\lambda_1^{N-\ell}\langle \ell_1|\mathbb{E}_X \, \mathbb{E}^{\ell-2}\mathbb{E}_Y|r_1\rangle}{\lambda_1^N}$$

assume diagonalizable

$$= \frac{1}{\lambda_1^\ell}\langle \ell_1|\mathbb{E}_X \left(\sum \lambda_i |r_i\rangle\langle \ell_i|\right)^{\ell-2}\mathbb{E}_Y|r_1\rangle$$

$$= \sum_i \left(\frac{\lambda_i}{\lambda_1}\right)^{\ell-2} \frac{\langle \ell_1|\mathbb{E}_X|r_i\rangle}{\lambda_1}\frac{\langle \ell_i|\mathbb{E}_Y|r_1\rangle}{\lambda_1}$$

If both $|\lambda_1|$ and $|\lambda_2|$ are non-degenerate, then for $\ell \gg 1$:

$$\approx \underbrace{\frac{\langle e_1 | \mathbb{E}_x | r_1 \rangle}{\lambda_1}}_{= \langle \psi | X | \psi \rangle} \underbrace{\frac{\langle e_1 | \mathbb{E}_y | r_1 \rangle}{\lambda_1}}_{= \langle \psi | y | \psi \rangle} +$$

$$\underbrace{\frac{\langle e_1 | \mathbb{E}_x | r_2 \rangle}{\lambda_1} \frac{\langle e_2 | \mathbb{E}_y | r_1 \rangle}{\lambda_1}}_{=: C} \left(\frac{\lambda_2}{\lambda_1} \right)^{\ell - 2}$$

$$= \langle \psi | X | \psi \rangle \langle \psi | y | \psi \rangle + C \cdot \left(\frac{\lambda_2}{\lambda_1} \right)^{-2} \cdot e^{-\ell/\xi},$$

where $\xi = -\dfrac{1}{\log(\lambda_2/\lambda_1)}$.

Observation: In a translational invariant MPS with transfer matrix spectrum $\{\lambda_1, \lambda_2, \ldots\}$, if $|\lambda_1|$ is non-degenerate, correlation functions decay exponentially, with correlation length $\xi = -1/\log|\lambda_2/\lambda_1|$.

In particular, the connected correlation function

$$\langle (X_1 - \langle X_1\rangle)(Y_\ell - \langle Y_\ell\rangle)\rangle$$

$$= \langle X_1 Y_\ell\rangle - \langle X_1\rangle\langle Y_\ell\rangle$$

(where $\langle \cdot \rangle = \langle \psi | \cdot | \psi \rangle$) decays exponentially to zero.

Note: We can avoid the normalization & rescaling by λ_1 by replacing

$$A \longrightarrow \frac{1}{\sqrt{\lambda_1}} A \text{ ; the new } \mathbb{E} \text{ has } \lambda_1 = 1.$$

c) Long-range order in tru. MPS

Conversely, if $|\lambda_1|$ is degenerate, i.e.

$|\lambda_1| = |\lambda_2| > |\lambda_3| \geq \dots$, then

$$\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum \lambda_i^{N-1}\langle l_i|\mathbb{E}_O|r_i\rangle}{\sum \lambda_i^N}$$

$$\xrightarrow{N\to\infty} \frac{\lambda_1^{N-1}\langle l_1|\mathbb{E}_O|r_1\rangle + \lambda_2^{N-1}\langle l_2|\mathbb{E}_O|r_2\rangle}{\lambda_1^N + \lambda_2^N}$$

If we assume $\lambda_1 = \lambda_2$, then this means

$$\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{1}{2}\left(\frac{\langle l_1|\mathbb{E}_O|r_1\rangle}{\lambda_1} + \frac{\langle l_2|\mathbb{E}_O|r_2\rangle}{\lambda_2}\right),$$

– this looks like an <u>average</u> of two states.

In fact, with OBC, we have

$$\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{i=1,2}\langle x|r_i\rangle\langle l_i|y\rangle \;\; \langle l_i|\mathbb{E}_O|r_i\rangle}{\sum_{i=1,2}\langle x|r_i\rangle\langle l_i|y\rangle \;\; \lambda_i}$$

$$= \frac{\langle l(x)|\mathbb{E}_O|r(y)\rangle}{\langle l(x)|r(y)\rangle\,\lambda_1}$$

with $|r(y)\rangle = \sum_{i=1,2} |r_i\rangle\langle l_i|y\rangle$,

$$\langle l(x)| = \langle x| \sum_{i=1,2} |r_i\rangle\langle l_i|$$

i.e. by choosing the boundary conditions x and y we can <u>change</u> the expectation value in the middle: The system is sensitive to boundary conditions!

Now consider the correlation function for some given boundary condition:

$$\frac{\langle\psi|X_1 Y_\ell|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\langle l(x)|\,\mathbb{E}_X\,\mathbb{E}^{\ell-2}\,\mathbb{E}_Y\,|r(y)\rangle}{\lambda_1^{\ell}\langle l(x)|r(y)\rangle}$$

$$= \frac{\langle l(x)|\,\mathbb{E}_X\left(\sum_i \lambda_i^{\ell-2}\,|r_i\rangle\langle l_i|\right)\mathbb{E}_Y\,|r(y)\rangle}{\lambda_1^{\ell}\,\langle l(x)|r(y)\rangle}$$

$$\xrightarrow{\ell \gg 1} \frac{\langle \ell(x)| \mathbb{E}_x \left(\lambda_1^{\ell-2} |r_1\rangle\langle \ell_1| + \lambda_2^{\ell-2} |r_2\rangle\langle \ell_2| \right) \mathbb{E}_y | r(y)\rangle}{\lambda_1^{\ell} \langle \ell(x)|r(y)\rangle}$$

(for $\lambda_1 = \lambda_2$)

$$= \frac{\langle \ell(x)|\mathbb{E}_x|r_1\rangle\langle \ell_1|\mathbb{E}_y|r_1\rangle + \langle \ell_1|\mathbb{E}_x|r_2\rangle\langle \ell_2|\mathbb{E}_y|r(y)\rangle}{\lambda_1^2 \langle \ell(x)|r(y)\rangle}$$

This is generally non-zero even for the connected correlation functions:

$$\langle (x - \langle x\rangle)(y - \langle y\rangle)\rangle$$

$$= \langle xy\rangle - \langle x\rangle\langle y\rangle$$

$$\frac{\langle \ell(x)|\mathbb{E}_x \left(\sum_{i=1,2} |r_i\rangle\langle \ell_i| \right) \mathbb{E}_y |r(x)\rangle}{\lambda_1^2 \langle \ell(x)|r(y)\rangle} \neq \frac{\langle \ell(x)|\mathbb{E}_x|r(y)\rangle\langle \ell(x)|\mathbb{E}_y|r(y)\rangle}{\lambda_1^2 \langle \ell(x)|r(y)\rangle^2}$$

Observation:

MPS with a degenerate leading eigenvalue always have long-range correlations

$$\langle X_1 Y_\ell \rangle \longrightarrow \text{const} \underbrace{\neq 0}_{\text{for suitable } X, Y.}$$

Observation:

MPS always have either

* exponentially decaying correlations or
* long range correlations.

Translational invariant MPS with finite D cannot exactly reproduce states with algebraically decaying correlations

$$\langle X_1 Y_\ell \rangle \sim \frac{1}{\ell^\alpha},$$

and thus cannot exactly reproduce

ground states of critical Hamiltonians.

But: Correlation functions in MPS are the sum of D^2 exponentials, which can be used to approximate algebraic correlations within a certain range.

d) Limitations to approximability

Exponential Clustering Theorem:

(Hastings & Koma 2005: https://arxiv.org/abs/math-ph/0507008
Nachtergaele & Sims 2005: https://arxiv.org/abs/math-ph/0506030)

(Colloquially:)

If $H = \sum h_i$ is local with gap Δ, then all connected correlation functions in the ground state decay exponentially,

$$\left|\langle (x_i - \langle x_i\rangle)(y_j - \langle y_j\rangle)\rangle\right| \leq c(x,y)\cdot e^{-|i-j|/\xi},$$

with $\xi \sim \frac{1}{\Delta}$.

Conversely: Gapless Hamiltonians typically have algebraically decaying correlations ("critical correlations"/"critical Ham.")

$\Rightarrow$ tr.inv. MPS cannot describe critical states exactly.

$\Rightarrow$ "folk knowledge": MPS cannot capture critical correlations.

(Though not obvious what this exactly means for non-tr.inv. MPS.)

Does this imply a limitation for using MPS to study critical systems?

- algebraic correlations must (and can) be approximated by sum of exponentials (# of terms $= D^2$!!)

- also generic gapped states cannot be exactly written as MPS, since the Schmidt rank for generic systems in the ground state is maximal.

- Moreover, also gapped systems typ. don't have corrs. w/ exact exponential decay, but rather of Ornstein-Zernike form

$$\langle X_i Y_j \rangle \sim \frac{1}{\sqrt{\ell}} e^{-\ell/\xi} \;, \quad \ell = |i-j| .$$

$\Longrightarrow$ must also be approx. by exponentials.

- <u>Approximability vs. area law:</u>

$$D \sim \mathrm{poly}\left(\frac{N}{\varepsilon}\right) \cdot e^{S_{max}}$$

$$S_{max} \begin{cases} \xrightarrow{\text{gapped}} \sim \text{const.} \\ \xrightarrow{\text{gapless}} \sim \alpha \log N \end{cases}$$

$\Rightarrow$ in both cases, $D \sim \mathrm{poly}\left(\frac{N}{\varepsilon}\right)$

(just with different polynomial, dep. on α)