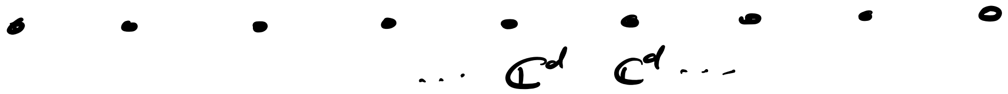
III. Matrix Product States

In this chapter, we will consider one-dimensional spin chains, i.e. $\mathcal{H} = (\mathbb{C}^d)^{\otimes N}$,



with states

$$|\psi\rangle = \sum_{i_1,\dots,i_N=0}^{d-1} c_{i_1\dots i_N} |i_1,\dots,i_N\rangle$$

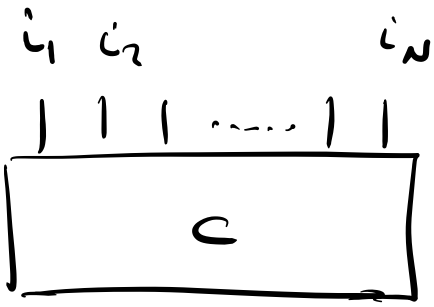
1. Construction

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

We can think of $c_{i_1\dots i_N}$ as a <u>tensor</u> with N indices; each index can take d values.

Graphical notation:

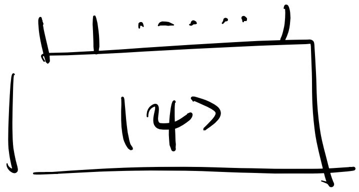
$c_{i_1\dots i_N}$ =



Box = tensor

legs = indices

Since $|\psi\rangle$ and $c_{i_1 \dots i_N}$ are the same object (once we fix a basis), can can also write



.

We can also consider

$$C_{i_1 i_2 \dots i_N} = C_{i_1 (i_2 \dots i_N)} \quad \text{as a matrix}$$

with row-index i_1 and column-index $(i_2 \dots i_N)$ (i.e., a multi-index).

Now perform an SVD of $C_{i_1(i_2 \dots i_N)}$:

$$C_{i_1(i_2 \dots i_N)} = \sum_{\alpha_1, \alpha_1'} U_{i_1, \alpha_1} \Lambda_{\alpha_1, \alpha_1'} V_{\alpha_1', (i_2, \dots, i_N)}$$

can replace by λ_{α_1} & $V_{\alpha_1,(\dots)}$

(or $C = U \Lambda V$),

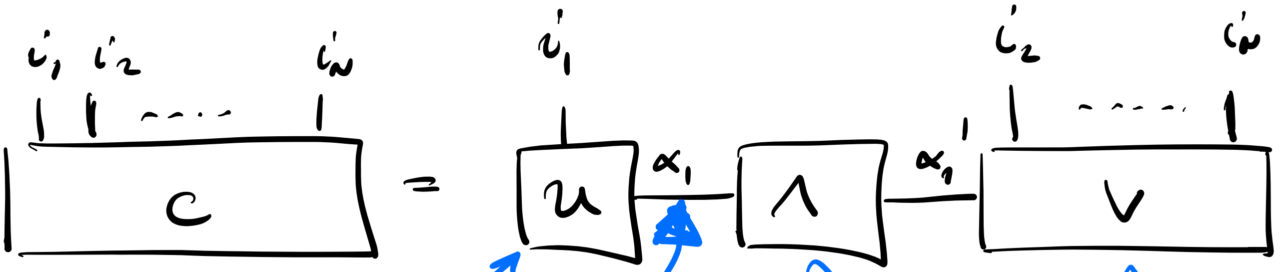
with Λ a diagonal matrix, $\Lambda_{\alpha_1, \alpha_1'} = \delta_{\alpha_1 \alpha_1'} \cdot \overset{\geq 0}{\lambda_{\alpha_1}}$

and U, $V^\dagger$ isometries

$$\sum_{i_1} \overline{U}_{i_1,\beta_1} U_{i_1,\alpha_1} = \delta_{\alpha_1,\beta_1} \quad (\text{i.e. } U^\dagger U = \mathbb{1})$$

$$\sum_{i_2 \dots i_N} \overline{V}_{\beta_1,(i_2,\dots,i_N)} V_{\alpha_1,(i_2,\dots,i_N)} = \delta_{\alpha_1,\beta_1} \quad (\text{i.e. } V V^\dagger = \mathbb{1})$$

Graphically:



2 legs = matrix

matrix

tensor (or matrix w/ multi-idx.)

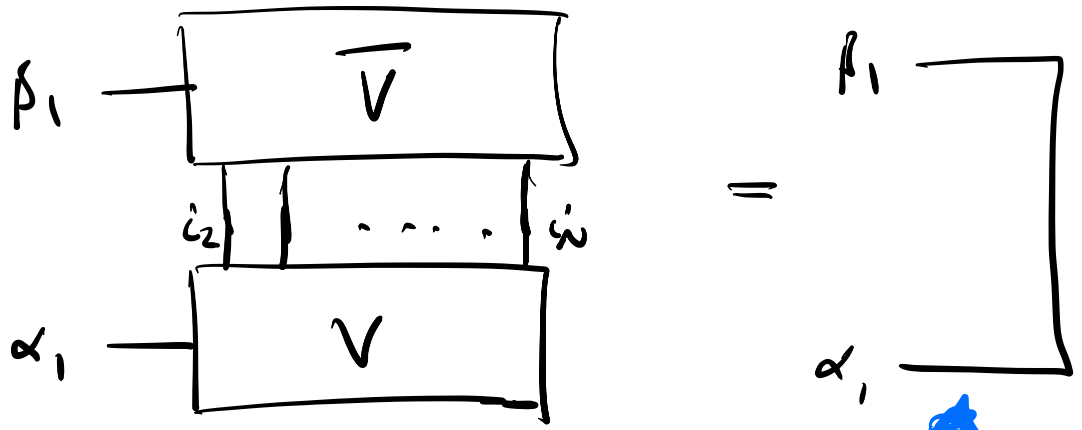
connecting legs denotes <u>contraction</u>: The legs are <u>identified</u> and summed over

E.g.: $i - \boxed{A} - \boxed{B} - j = \sum_k A_{ik} B_{kj} = (A \cdot B)_{ij}$

(matrix product!

The isometry conditions read graphically:

$$\sum_{i_2 \dots i_N} \overline{V}_{\beta_1,(i_2,\dots,i_N)} V_{\alpha_1,(i_2,\dots,i_N)} = \delta_{\alpha_1,\beta_1} .$$



simple line = identity matrix

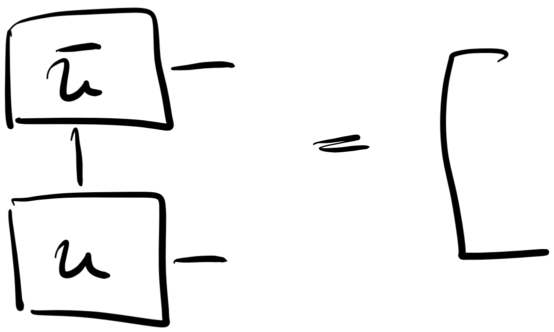
(consistent:

$-\boxed{A}-\boxed{B}- = A \cdot B$

$= A \cdot \mathbb{1} \cdot B$

$= \mathbb{1} \cdot A \cdot B = \dots)$

and



Express state $|\psi\rangle$ with U, Λ, V:

$$|\psi\rangle = \sum_{\substack{i_1, i_2, \dots, i_N \\ \alpha_1}} U_{i_1 \alpha_1} \Lambda_{\alpha_1, \alpha_1} V_{\alpha_1, (i_2, \dots, i_N)} |i_1, i_2, \dots, i_N\rangle$$

$$\circledast \quad = \sum_{\alpha_1} \Lambda_{\alpha_1 \alpha_1} \underbrace{\left(\sum_{i_1} U_{i_1 \alpha_1} |i_1\rangle\right)}_{=: |\ell_{\alpha_1}\rangle} \underbrace{\left(\sum_{i_2, \dots, i_N} V_{\alpha_1, (i_2, \dots, i_N)} |i_2, \dots, i_N\rangle\right)}_{=: |r_{\alpha_1}\rangle}$$

$$\Rightarrow \langle \ell_\beta | \ell_\alpha \rangle = \sum_{i, j, \alpha, \beta} U_{i\alpha} \overline{U_{j\beta}} \underbrace{\langle j | i \rangle}_{= \delta_{ij}}$$

$$= \sum U_{i\alpha} \overline{U_{i\beta}} = \delta_{\alpha\beta}$$

$\Rightarrow$ $|\ell_\alpha\rangle$ (and $|r_\alpha\rangle$) ONS!

$\Rightarrow$ $\circledast$ is the Schmidt decomposition of $|\psi\rangle$

in the partition $\underbrace{1}_{A} | \underbrace{2 3 \dots N}_{B}$, with

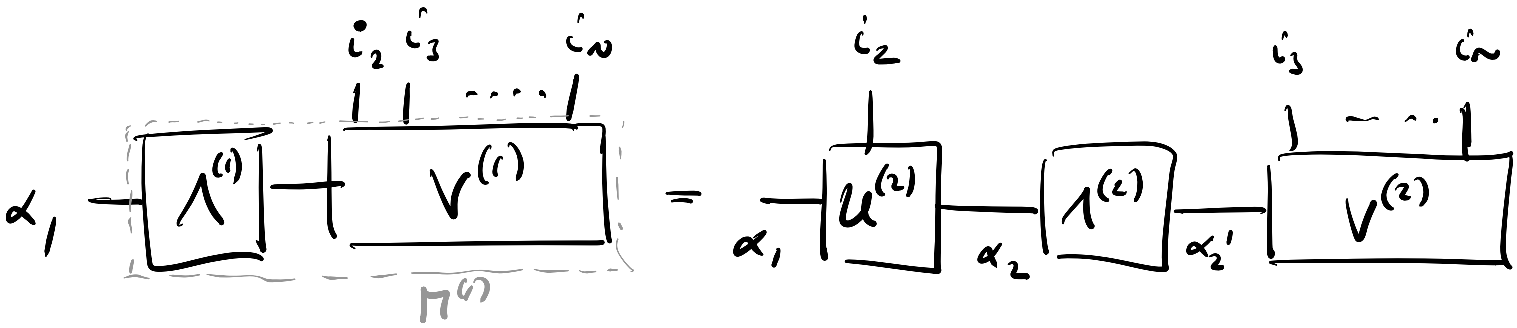
$\Lambda_{\alpha_1 \alpha_1}$ the Schmidt coefficients!

Now call $\mathcal{U} = \mathcal{U}^{(1)}$, $\Lambda = \Lambda^{(1)}$, $V = V^{(1)}$

Consider $M^{(1)}_{\underbrace{\alpha_1 i_2}, \underbrace{(i_3 \dots i_N)}} := \sum_{\alpha_1'} \Lambda_{\alpha_1, \alpha_1'} V_{\alpha_1', (i_2 \dots i_N)}$

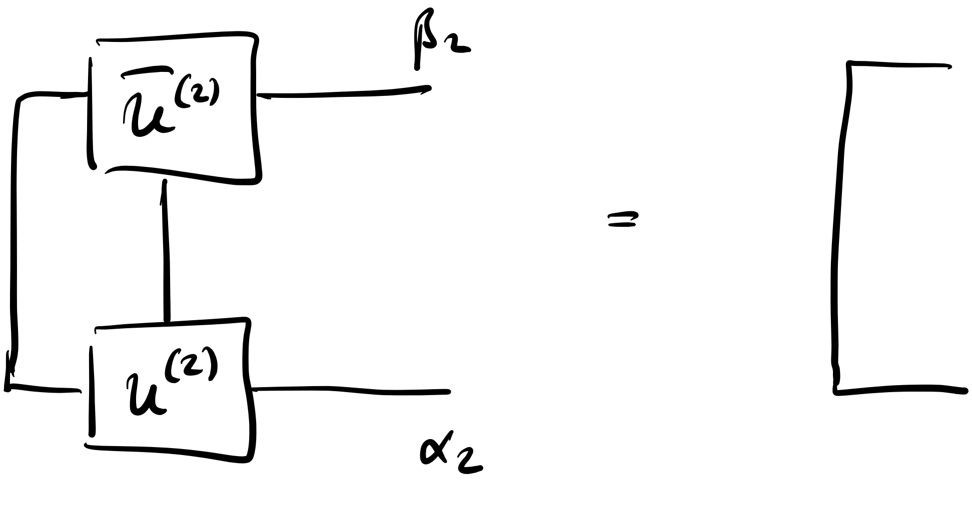
new row/col. indices

Perform SVD of $M^{(1)} \equiv$ "$\Lambda^{(1)} \cdot V^{(1)}$":

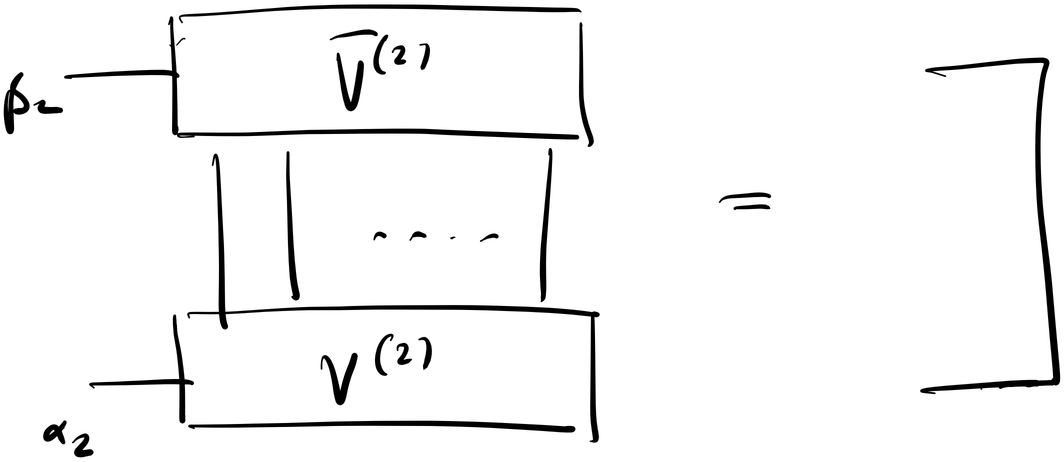


$\Lambda^{(2)}$ is diagonal ≥ 0

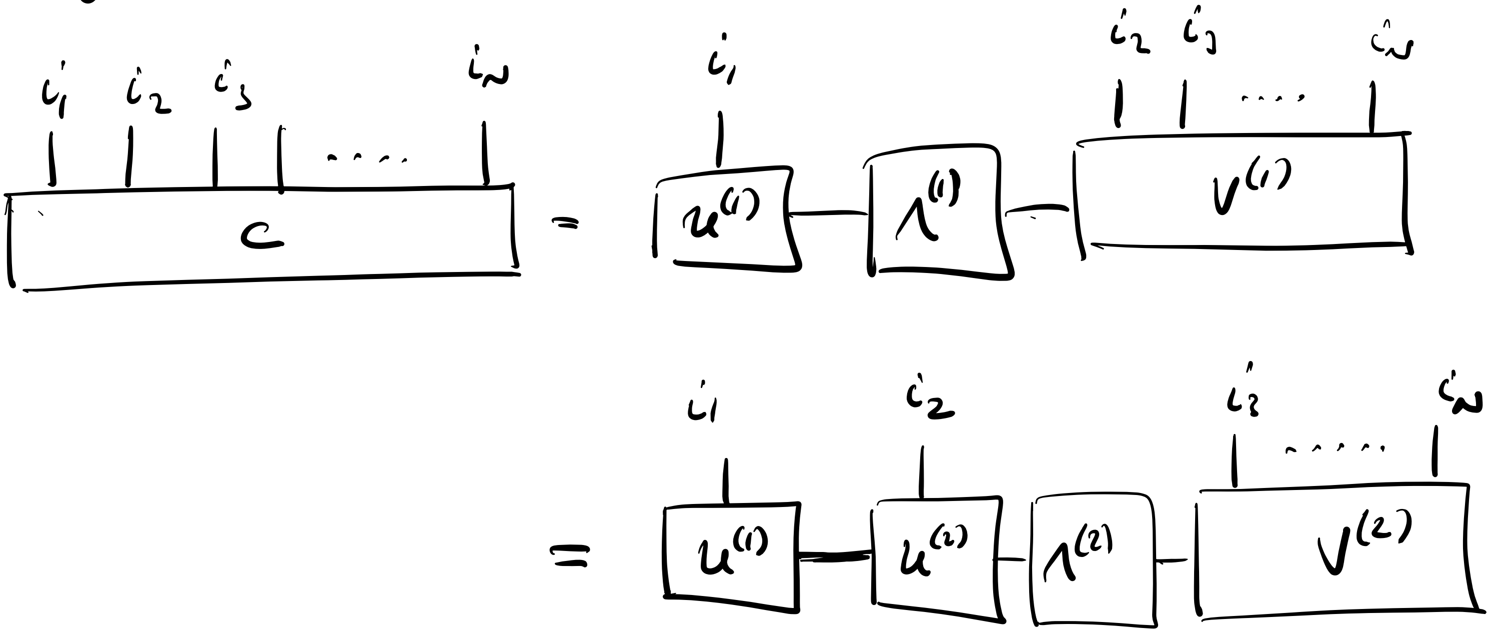
$\mathcal{U}^{(2)}$, $V^{(2)}$ isometries:



(or: $\sum_{\alpha_1 i_2} \mathcal{U}^{(2)}_{(\alpha_1 i_2)\alpha_2} \bar{\mathcal{U}}^{(2)}_{(\alpha_1 i_2)\beta_2} = \delta_{\alpha_2 \beta_2}$)

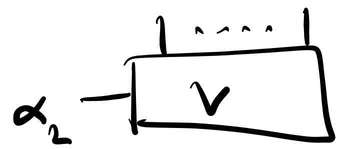


Together:

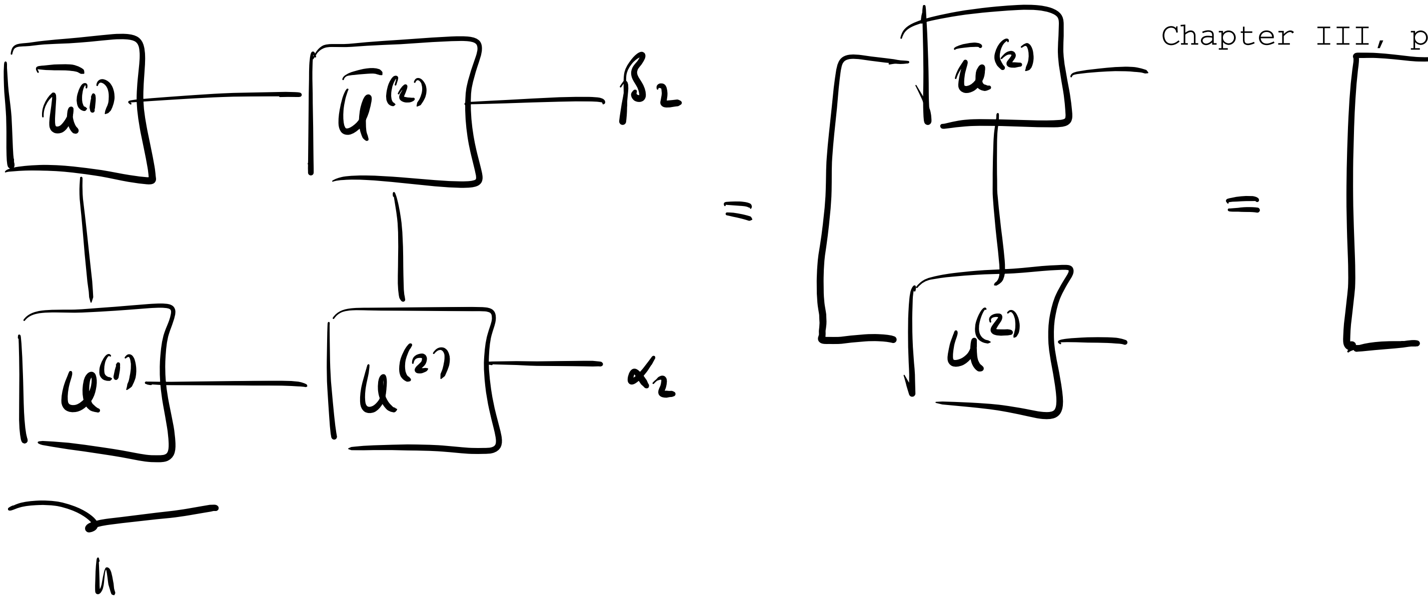


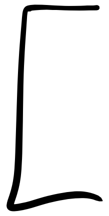
What is the form of the decomposition in the cut $12|3\ldots N$?

$V^{(2)}$ isometry $\Rightarrow$ right basis

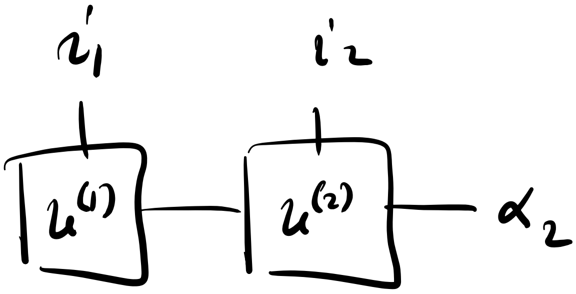


is ONB.





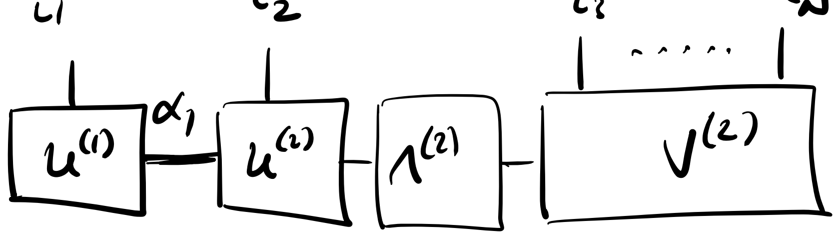
$\Longrightarrow$



is <u>also</u> an isometry (as a map from $\alpha_2 \to (i_1 i_2)$)

$\Longrightarrow$ this is <u>again</u> a Schmidt decomposition, now in the cut $12|3 \ldots\ldots N$.

<u>Moreover</u>, if we consider



across the cut $1|2\ldots N$, then this <u>still</u> gives a Schmidt-like decomposition

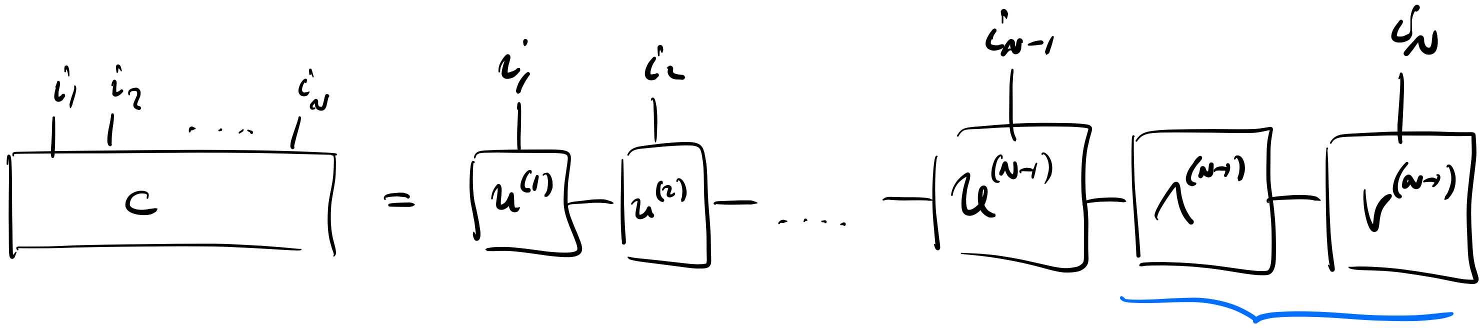
$$|\psi\rangle = \sum |e^{(1)}_{\alpha_1}\rangle \, |\tilde{r}^{(1)}_{\alpha}\rangle$$

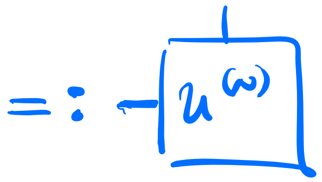
with $\langle e^{(1)}_{\alpha} | e^{(1)}_{\beta}\rangle = \delta_{\alpha\beta}$

and $\langle \tilde{r}^{(1)}_{\alpha} | \tilde{r}^{(1)}_{\beta}\rangle = \Lambda_{\alpha\alpha}\,\delta_{\alpha\beta}$

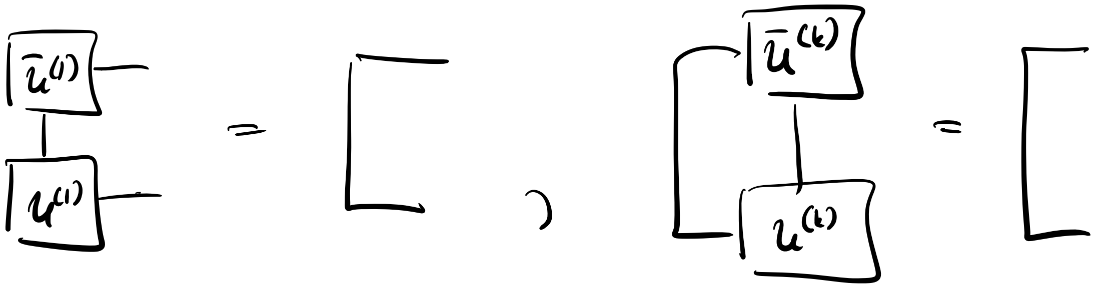
Orthonormal, and the Schmidt coefficient <u>absorbed</u> in $|\tilde{r}_\alpha\rangle$ s

We can now *iterate* this scheme and get:



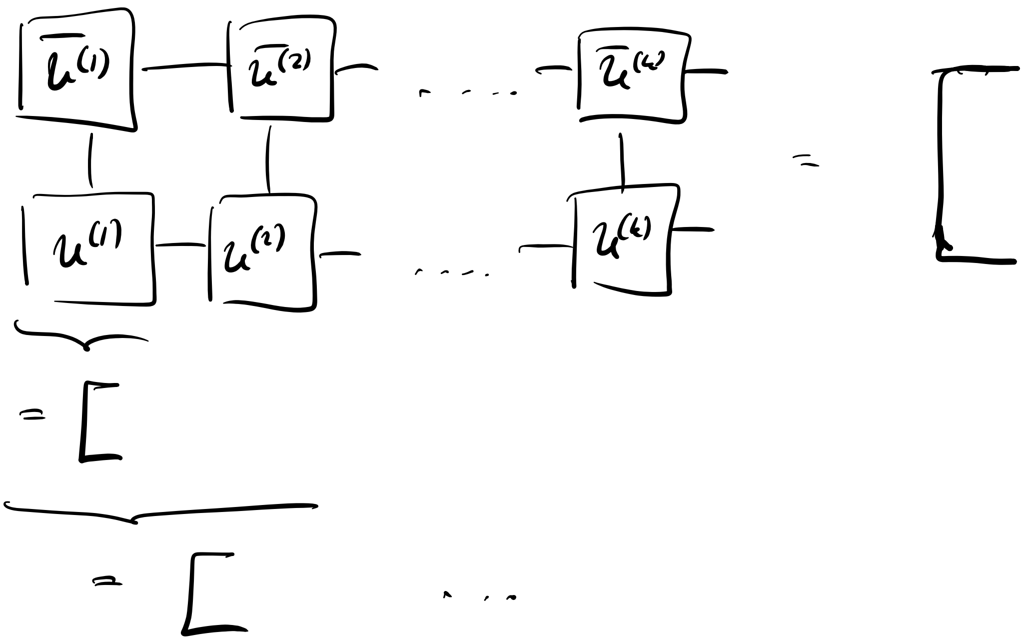


with



$(k=2,\dots,N-1)$

and thus also



— i.e., this representation gives a quasi-Schmidt decomposition on every cut $1\ldots k|(k+1)\ldots N$, $k=1,\ldots,N-1$:

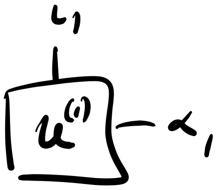
$$\sum |l_\alpha^{(k)}\rangle\, |\tilde{r}_\alpha^{(k)}\rangle ,$$

$$\langle l_\beta^{(k)} | l_\alpha^{(k)}\rangle = \delta_{\alpha\beta}$$

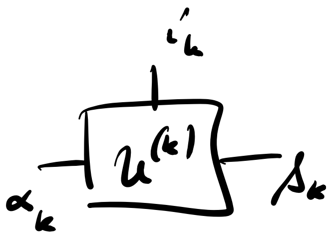
$$\langle \tilde{r}_\beta^{(k)} | \tilde{r}_\alpha^{(k)}\rangle = \lambda_\alpha^{(k)}\, \delta_{\alpha\beta}$$

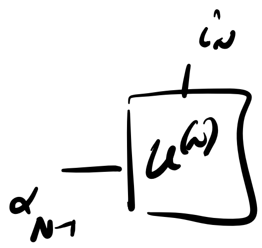
Schmidt coeffs for cut k.

Alternatively, we can consider

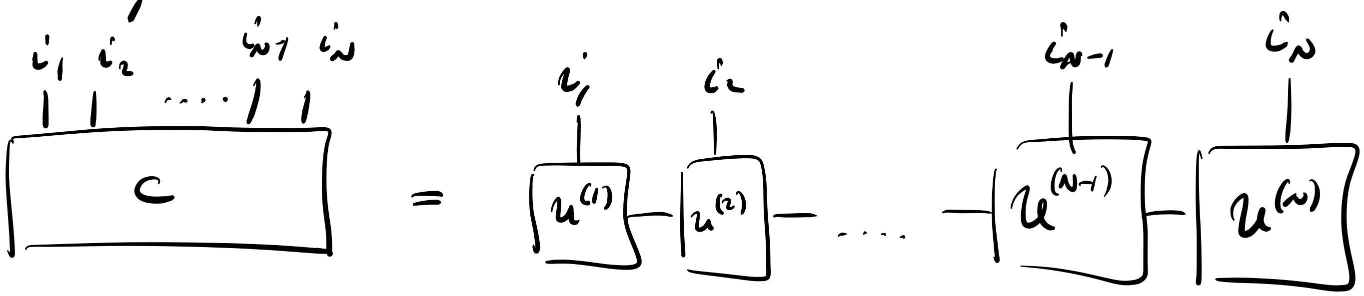


as a set of row vectors $(U_{i_1}^{(1)})_{\alpha_1}$,

and  as matrices $(U_{i_k}^{(k)})_{\alpha_k\beta_k}$,

and  as a set of col. vectors $(U_{i_N}^{(N)})_{\alpha_{N-1}}$.

Then,



$$= \underbrace{U^{(1)}_{i_1} \cdot U^{(2)}_{i_2} \cdot \ldots \cdot U^{(N-1)}_{i_{N-1}} \, U^{(N)}_{i_N}}_{\text{vector} \,\cdot\, \text{matrix} \,\cdot\, \text{matrix} \,\cdot \ldots \cdot\, \text{vector}\,!}$$

$$\Longrightarrow \boxed{|\psi\rangle = \sum U^{(1)}_{i_1} \cdot U^{(2)}_{i_2} \cdot \ldots \cdot U^{(N-1)}_{i_{N-1}} \cdot U^{(N)}_{i_N} \, |i_1, \ldots, i_N\rangle}$$

$$\boxed{\text{"Matrix Product State" (MPS)}}$$

In general, we have:

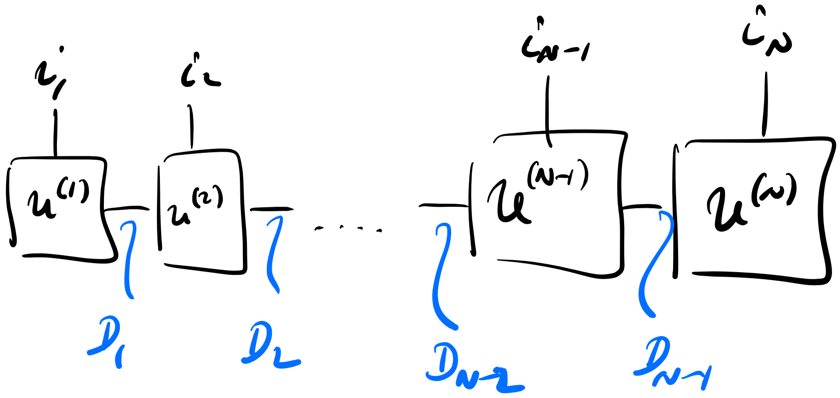
$U^{(1)}_{i_1}$: $1 \times D_1$ – vector

$U^{(2)}_{i_2}$: $D_1 \times D_2$ – matrix

$U^{(k)}_{i_k}$: $D_{k-1} \times D_k$ – matrix

$\vdots$

$U^{(N)}_{i_N}$: $D_{N-1} \times 1$ - vector



We call D_i the "bond dimension".

Observation: We have re-phrased $c_{i_1 \ldots i_N}$ as a vector-matrix product!

Did this reduce the # of parameters?

No, this cannot be – this decomposition is exact & cannot reduce # of params.

In fact: At each cut, the bond dimension will generically be min(dim(left), dim(right)), e.g. $\min(d^k, d^{N-k})$, since D_k is the summation range of the Schmidt decomposition!

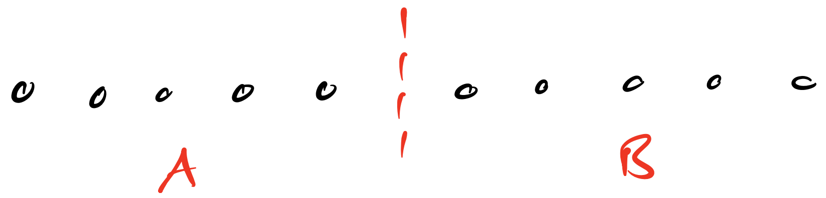
$\Rightarrow$ the bond dimension will be <u>exponentially big</u> when we decompose an arbitrary state

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

2. Truncation of the bond dimension & approximability by MPS

Can we reduce the # of parameters for states with small entanglement?

Have seen: for any partition



$|\psi_{AB}\rangle$

we can cut the Schmidt decomposition

$$|\psi_{AB}\rangle = \sum_{i=1}^{r} s_i \, |l_i\rangle \otimes |r_i\rangle$$

to a smaller # of terms,

$$|\psi(\chi)\rangle = \sum_{i=1}^{\chi} s_i \, |l_i\rangle \otimes |r_i\rangle \, ,$$

at an error $\varepsilon(\chi)$ which scales moderately.

<u>Step I</u> Assume $\varepsilon(\chi) = 0$ (i.e.: S_0-Renyi-entropy is bounded by $S_0 \le \log \chi$):

Then, Schmidt decomposition at each cut k,

$$|\psi\rangle = \sum_{i=1}^{D_k} s_i |l_i\rangle |r_i\rangle$$

has only χ non-zero terms, $D_k \leq \chi \ \forall k$!

$\Rightarrow$ In each step of the previous construction, the dimensions D_k of the matrices are $D_k \leq \chi$

(or, alternatively: The rank of the SVD is $\leq \chi$.)

$\Rightarrow$ For 1D states $|\psi\rangle$ with an area law for the 0-Rényi entropy, $S_0(\rho_A) \leq \log \chi$,

the exact MPS decomposition of $|\psi\rangle$ has bond dimension $\leq \chi$, i.e.,

$$|\psi\rangle = \sum_{i_1 \ldots i_N} U^{(1)}_{i_1} U^{(2)}_{i_2} \cdot \ldots \cdot U^{(N)}_{i_N} |i_1, \ldots, i_N\rangle,$$

with $U^{(k)}_{i_k}$, $2 \le k \le N-1$ $\chi \times \chi$-matrices.

(Note: If a D_k is smaller than χ, we can always pad it with zeros to obtain $\chi \times \chi$ matrices everywhere – if we want.

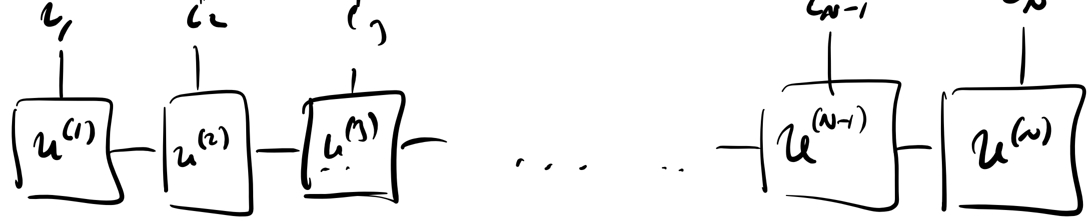
More generally, "bond dimension χ" should generally be read as "bond dimension at most χ".)

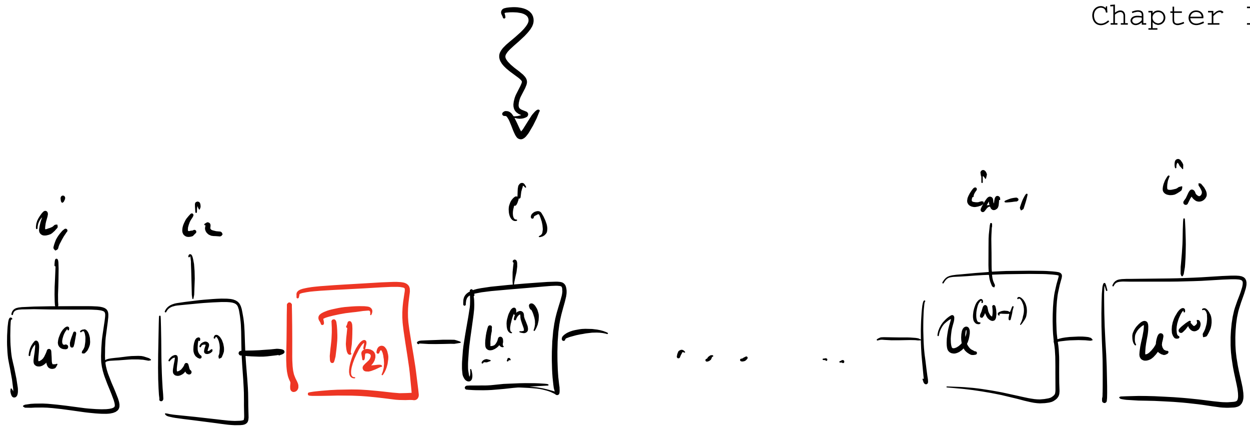
Step II: What happens if the truncation is approximate, with error

differs from prev. ε by factor 2.

$$\varepsilon(\chi) = \| \, |\psi\rangle - |\psi(\chi)\rangle \, \|^2$$

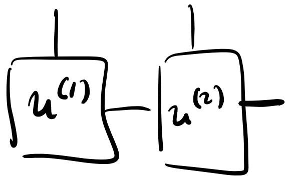
We can think of cutting the Schmidt rank at any given cut as changing



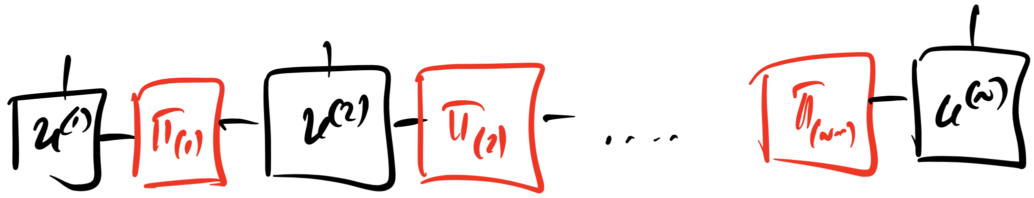


where $\Pi_{(2)}$ is the projector onto the χ largest Schmidt vectors!

... which again equals

with same projector $P_{(2)}$ (since  is an isometry).

Then, define the truncated MPS as

$|\hat{\phi}(\chi)\rangle =$ 

$= P_{(1)} \cdot P_{(2)} \cdot \ldots \cdot P_{(N-1)} \; |\psi\rangle$

We know that $\| P_{(s)} |\psi\rangle - |\psi\rangle \| \leq \sqrt{\varepsilon(x)}$,

or $P_{(s)}|\psi\rangle = |\psi\rangle + |\delta_s\rangle$, $\| |\delta_s\rangle \| \leq \sqrt{\varepsilon}$,

and thus

$$\| P_{(N-2)} \underbrace{P_{(N-1)} |\psi\rangle}_{= |\psi\rangle + |\delta_{N-1}\rangle} - |\psi\rangle \| \leq \underbrace{\| P_{(N-2)} |\psi\rangle - |\psi\rangle \|}_{\leq \sqrt{\varepsilon}} + \underbrace{\| |\delta_{N-1}\rangle \|}_{\leq \sqrt{\varepsilon}},$$

and doing this telescopically:

$$\| P_{(1)} \cdot \ldots \cdot P_{(N-1)} |\psi\rangle - |\psi\rangle \| \leq \sqrt{\varepsilon} \cdot N.$$

In fact, with a bit more care, we can find that the errors are independent, and thus

$$\varepsilon_{tot} := \| |\psi\rangle - |\phi(x)\rangle \|^2 \leq N \cdot \varepsilon$$

State where we have used the truncated Schmidt dec. at all cuts.

We can now combine this with the fact that

$$\varepsilon(\chi) \sim \left(\frac{e^{S_\alpha}}{\chi}\right)^{\eta} :$$

strict area law, $S_\alpha \leq$ const:

$$\varepsilon(\chi) \sim \frac{1}{\chi^{\eta}},$$ and thus

$$\varepsilon_{tot}(\chi) \sim \frac{N}{\chi^{\eta}},$$

or $\chi \sim \mathrm{poly}\left(N, \frac{1}{\varepsilon_{tot}}\right)$,

i.e. the χ ($\leftrightarrow$ # of parameters) required to describe a ground state to global error ε_{tot} scales polynomially with system size & accuracy.

For gapless systems with

$S \leq c \log L \leq c \log N$:

$$\varepsilon(\chi) \sim \left(\frac{e^{c \log N}}{\chi}\right)^{n}$$

$$\sim \mathrm{poly}(\chi, N),$$

and thus

$$\varepsilon_{tot}(\chi) \sim \mathrm{poly}(\chi, N),$$

and $\chi \sim \mathrm{poly}\left(\frac{1}{\varepsilon}, N\right)$

$\Longrightarrow$ same type of (efficient) scaling even for critical systems!

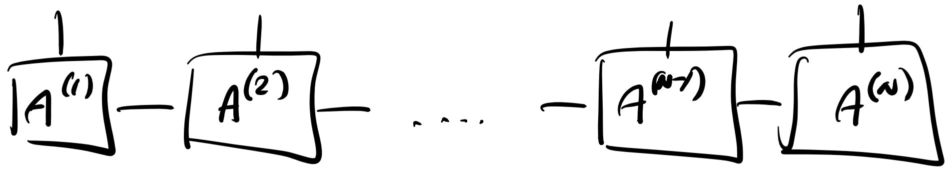
(Compare this to <u>exponential</u> scaling of parameters in N for <u>exact</u> state!)

3. Canonical forms

Definition (from now on):

A Matrix Product State (MPS) of bond dimension D is a state of the form

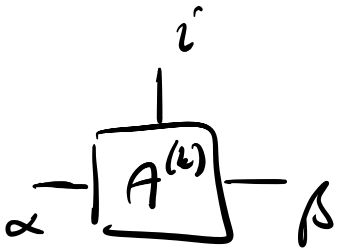
$$|\psi\rangle = \sum_{i_1,\dots,i_N} A^{i_1,(1)} A^{i_2,(2)} \cdots A^{i_N,(N)} |i_1,\dots,i_N\rangle,$$

$=$ 

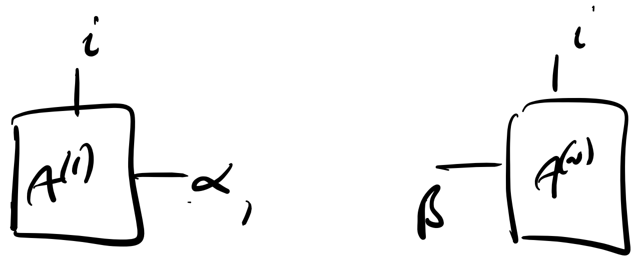
with $A^{i_k,(k)}$, $k=2,\dots,N-1$ $D\times D$ - matrices, and $A^{i_1,(1)}$ $1\times D$, $A^{i_N,(N)}$ $D\times 1$ (i.e. vectors)

More generally, $A^{i_k,(k)}$ can be a $D_{k-1}\times D_k$ - matrix $D_0 = D_N = 1$.

Terminology:



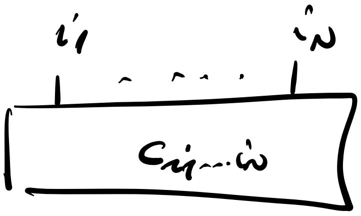
are 3-index (3-leg) tensors.



are 2-index tensors.

We call i the physical index (or degree of freedom, DoF), and α, β the virtual or auxiliary indices/DoFs.

Since

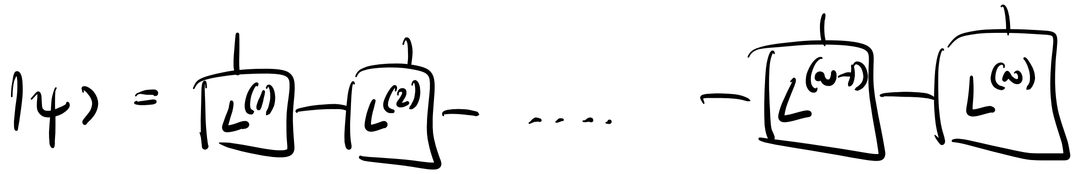


is expressed as a network of elementary tensors, such states are also called Tensor Network States.

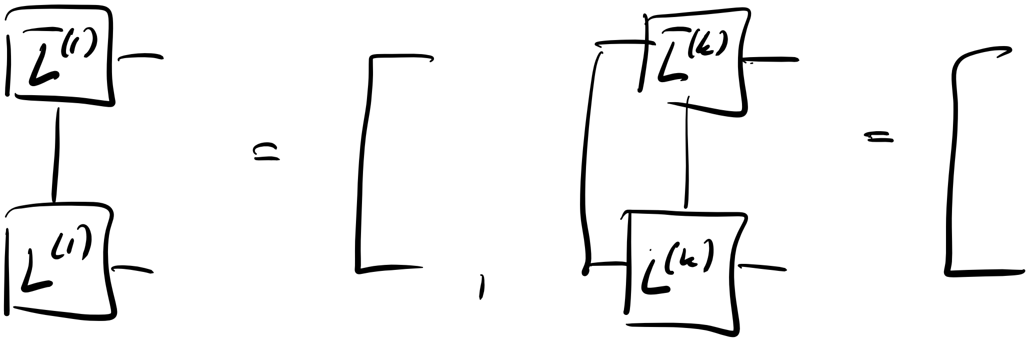
A priori, the matrices $A^{i_k,(k)}$ are unrestricted. However, they can be brought into canonical forms.

Left-canonical form:

An MPS is said to be in left-canonical form,

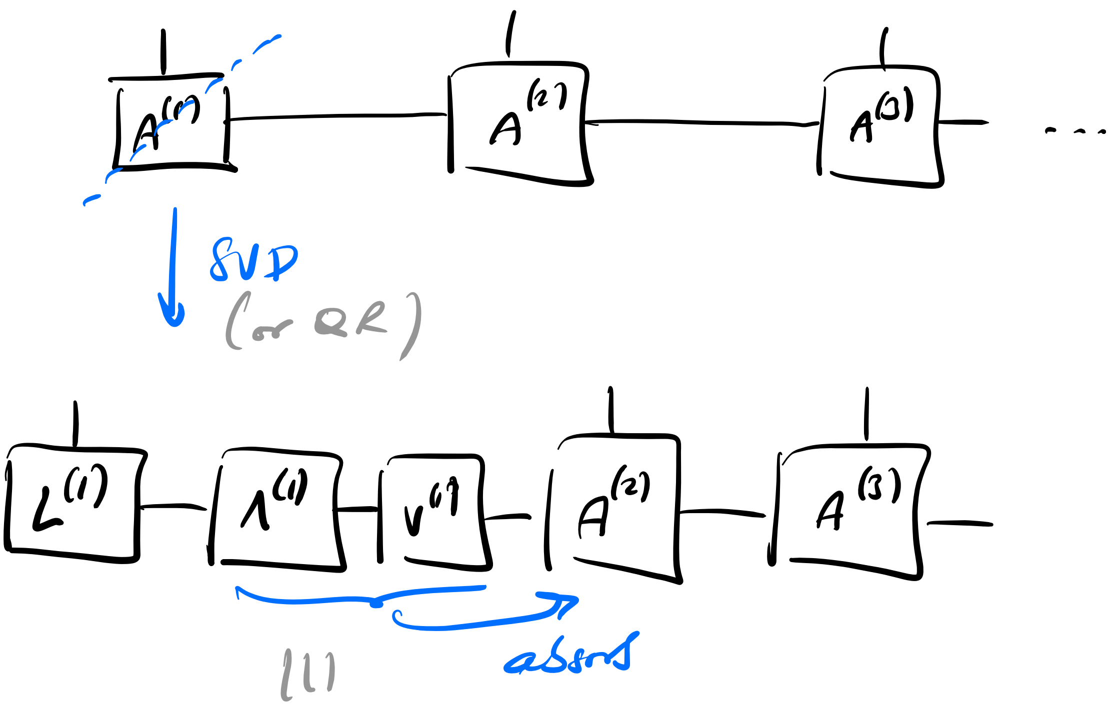


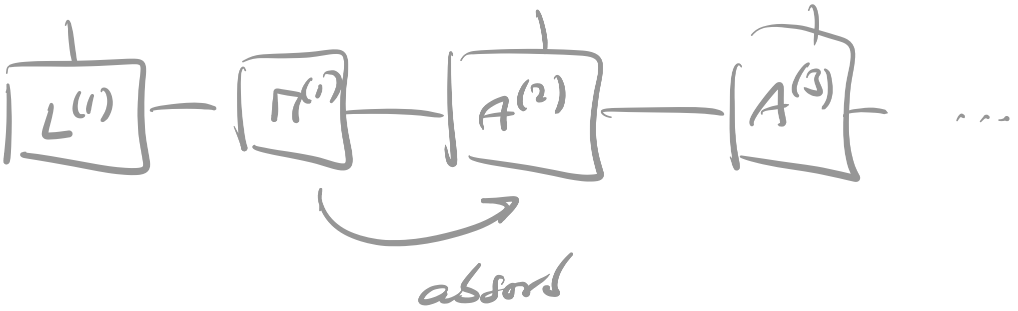
if

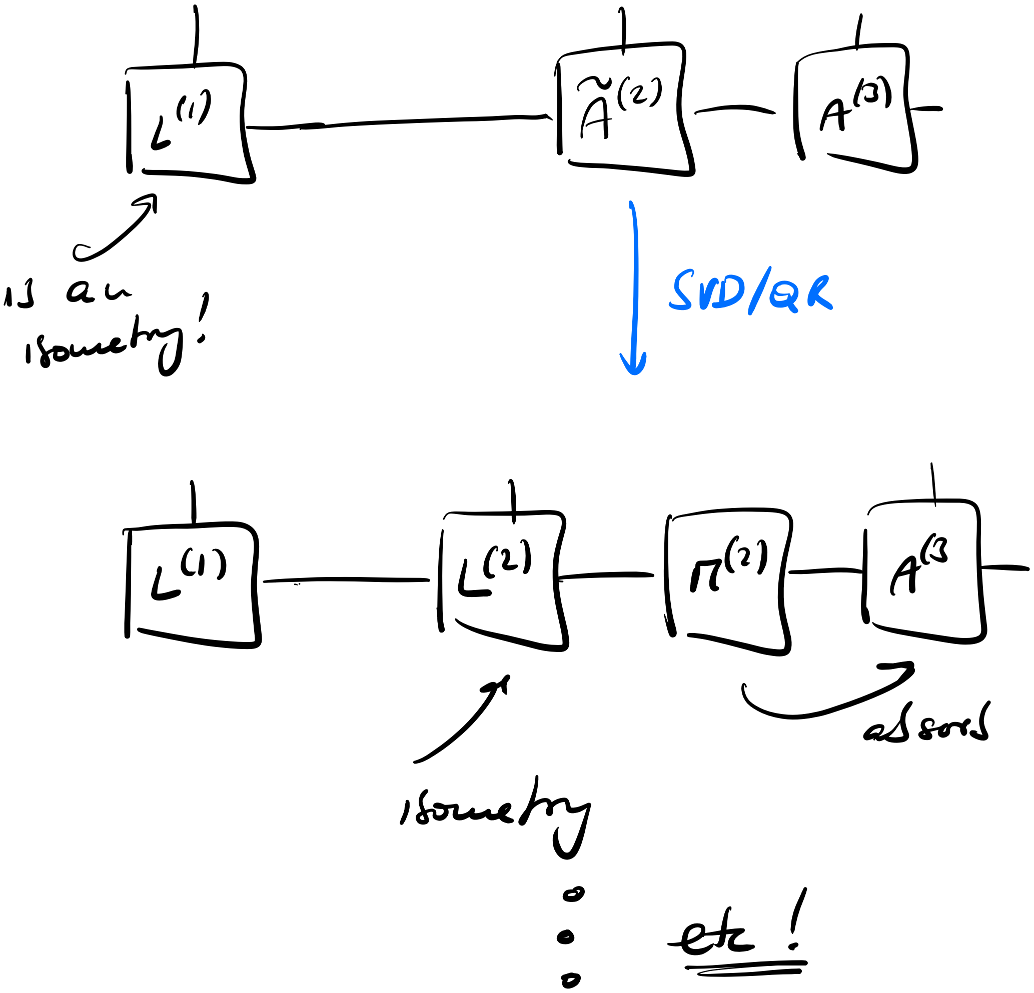


$(k<N)$.

Every MPS can be brought into left-can. form by a sequence of local transformations (Exercise problem 3a):







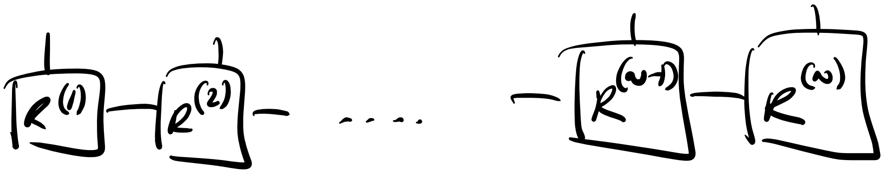
Important: Size of matrices for SVD is $D \times dD$, i.e. indep. of system size, & comp. cost $\sim D^3$

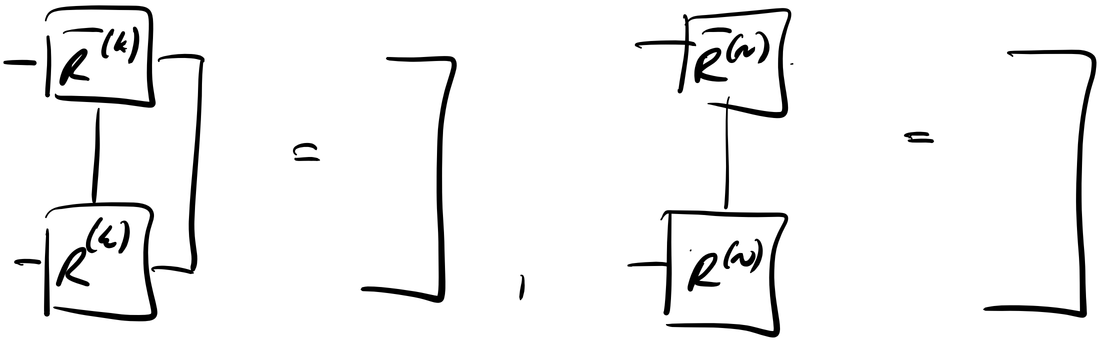
$\Rightarrow$ MPS can be brought into can. form **efficiently**.

Analogously, we can define the

Right-canonical form (CF):

An MPS is said to be in right-canonical form,

$|\psi\rangle =$ 

if 

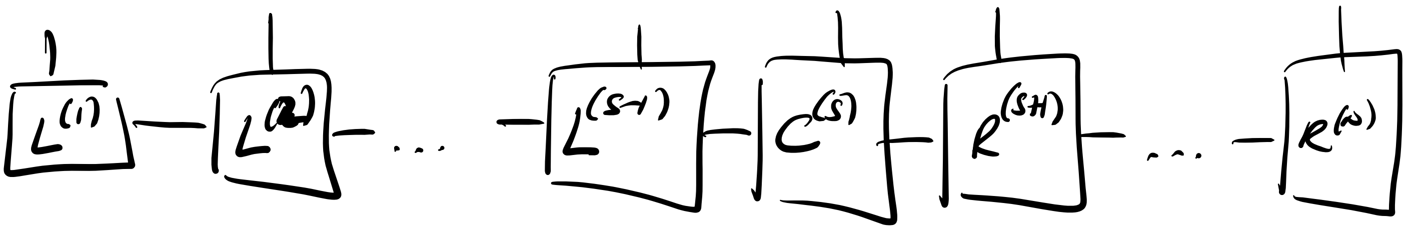
$(1 < k < N)$

... and it can be brought into right-CF in an analogous way.

Finally, we can define a

Mixed canonical form:

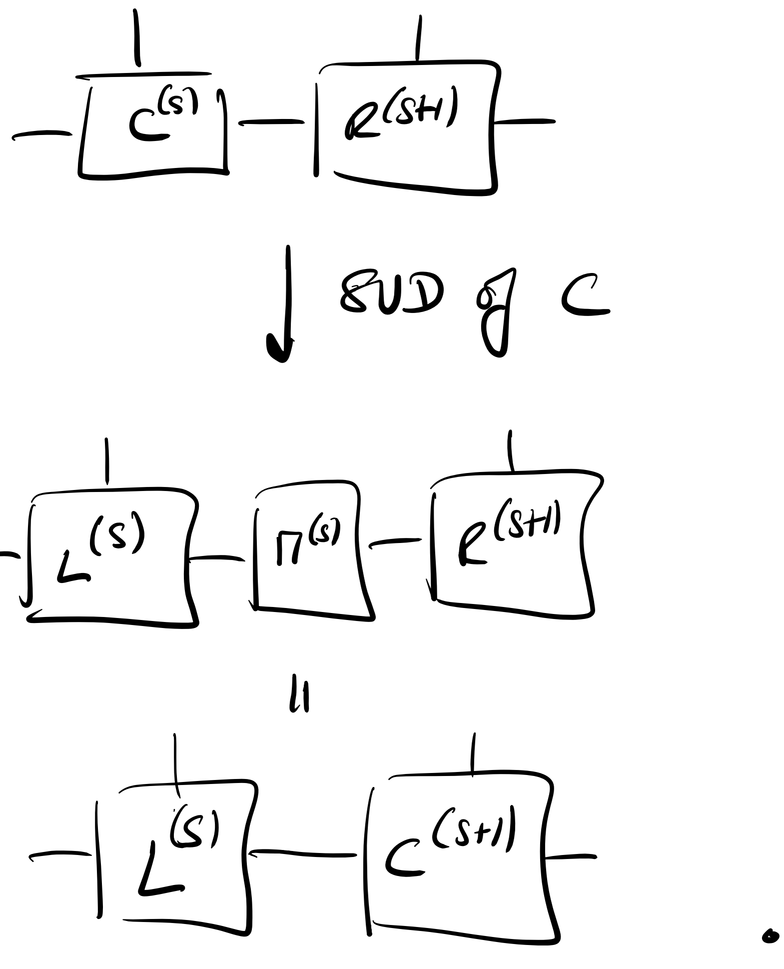
An MPS is in mixed CF,



where the $L^{(n)}$ are in left-CF, and the $R^{(n)}$ are in right-CF.

s is called the "working site".

<u>Important:</u> The working site can be moved to the left/right, $s \to s \pm 1$, by updating only two tensors, e.g.



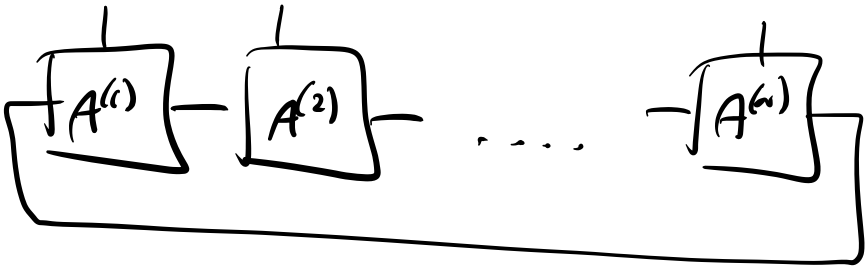
More can. forms $\longrightarrow$ Exercise #36.

4. Periodic, translational invariant, & infinite MPS

MPS can also be defined with periodic boundary conditions (PBC):

Periodic MPS: A PBC MPS is of the form

$|\psi\rangle =$

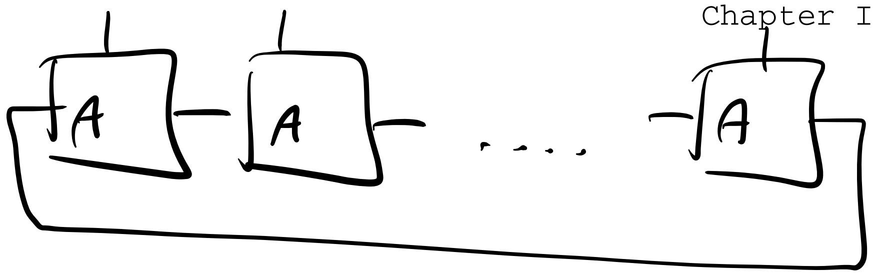


$$= \sum_{i_1,\dots,i_N} \mathrm{tr}\left[A^{i_1,(1)} \cdot A^{i_2,(2)} \cdot \ldots \cdot A^{i_N,(N)}\right] |i_1,\dots,i_N\rangle$$

In particular, PBC MPS can be chosen to be translational invariant:

Translational invariant (t.inv) PBC MPS:

A t.inv. PBC MPS is obtained by choosing all tensors $A^{(n)}$ to be identical, $A^{(n)} \equiv A$:

$|\psi\rangle =$ 

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

We can also use this to define tr.inv. states directly in the "thermodynamic limit" $N \to \infty$, i.e., on infinite chains.

More on this later.

<u>Important advantage</u> of tr.inv. MPS:

State is described by $O(1)$ parameters, indep. of system size N, and we can describe state on <u>any</u> system size N with <u>one</u> set of parameters

5. Examples

a) Product States

Product State

$$|\psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \dots \otimes |\phi_N\rangle .$$

$$\text{Let } |\phi_s\rangle = \sum_{i_s=0}^{d-1} a^{i_s,(s)} |i_s\rangle$$

Then,

$$|\psi\rangle = \left(\sum_{i_1=0}^{d-1} a^{i_1,(1)} |i_1\rangle \right) \otimes \left(\sum_{i_2=0}^{d-1} a^{i_2,(2)} |i_2\rangle \right) \otimes \dots$$

$$= \sum_{i_1,\dots i_N=0}^{d-1} a^{i_1,(1)} a^{i_2,(2)} , \dots , a^{i_N,(N)} |i_1, \dots, i_N\rangle ,$$

$\Rightarrow$ MPS with $D = 1$, where the matrices $A^{i_s,(s)}$ are numbers,

$$A^{i_s,(s)} = a^{i_s,(s)} .$$

$\Rightarrow$ Product states are a special case (in fact, the simplest instance) of MPS.

b) The GHZ state

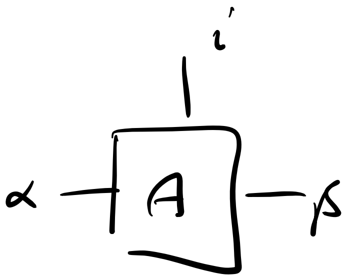
$$|GHZ\rangle = \frac{1}{\sqrt{2}}\left(|00\ldots 0\rangle + |11\ldots 1\rangle\right) \qquad (d=2)$$

PBC transl. inv. MPS:

$$A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |0\rangle\langle 0|$$

$$A^1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = |1\rangle\langle 1|$$

or



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

we have
$$A^0 A^0 = A^0$$
$$A^1 A^1 = A^1$$
$$A^0 A^1 = 0$$

$$\Rightarrow \quad \mathrm{tr}\left[A^{i_1} A^{i_2} \ldots A^{i_N}\right] = \begin{cases} 1 & i_1 = i_2 = \ldots = i_N \\ 0 & \text{else} \end{cases}$$

$$\Rightarrow |\psi\rangle = \sum \operatorname{tr}\left[A^{i_1} A^{i_2} \cdots\cdots A^{i_N}\right] |i_1, \ldots, i_N\rangle$$

$$= |0 \ldots\ldots 0\rangle + |1 \ldots\ldots 1\rangle$$

GHZ state up to normalization.

Can normalize e.g. by setting $A^{i_1,(1)} = \frac{1}{\sqrt{2}} A^{i_1}$, $A^{i_k,(k)} = A^{i_k}$. But: this breaks transl. inv. of representation.

Note: MPS are generally not normalized (cf. later).

Can also be written with OBC:

$$\langle + | A^{i_1} \cdots\cdots A^{i_N} | + \rangle =$$

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$= \delta_{i_1 \ldots i_N} \langle + | A^{i_1} | + \rangle = \frac{1}{2}.$$

$\Rightarrow$ MPS with

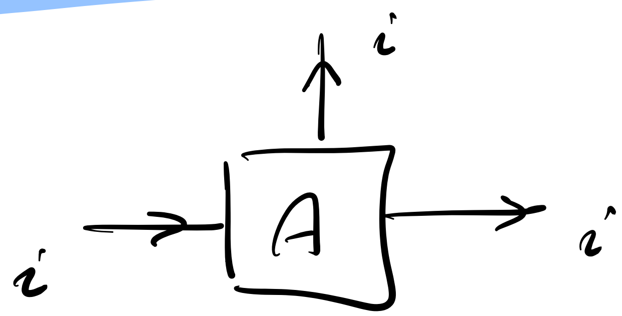
$$B^{i_1,(1)} := \sqrt{2}\langle +| A^{i_1}$$

$$B^{i_k,(k)} := A^{k}$$

$$B^{i_N,(N)} := A^{i_N}|+\rangle$$

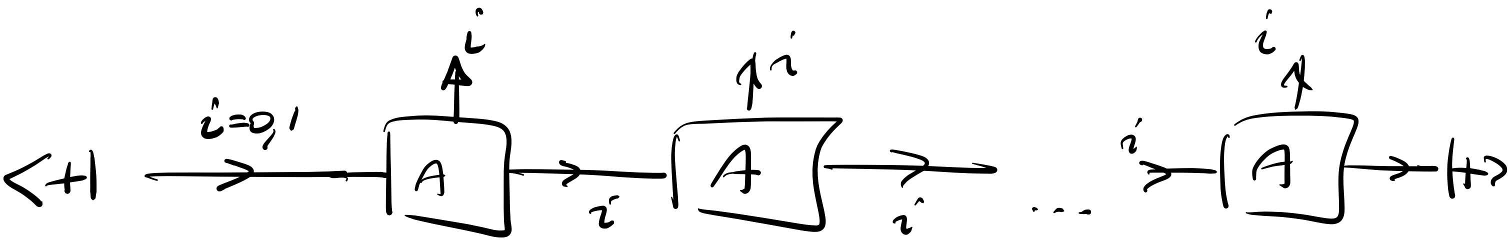
gives OBC rep. of GHZ state.

"Agent" interpretation:



A takes input i, and outputs i as a physical system, and i as a virtual system.

Total GHZ state in OBC rep.:



Each process has an amplitude associated to it; the total amplitude is the product of the amplitudes (cf. path integral).

Sometimes this gives a very natural perspective on MPS.

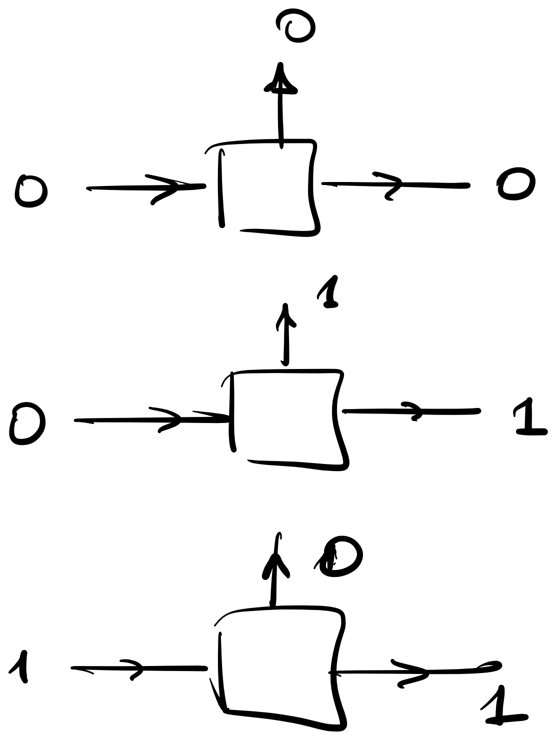
c) The W state

$$|W\rangle = \frac{1}{\sqrt{N}}\left(|100\ldots0\rangle + |010\ldots0\rangle + \ldots + |00\ldots01\rangle\right)$$

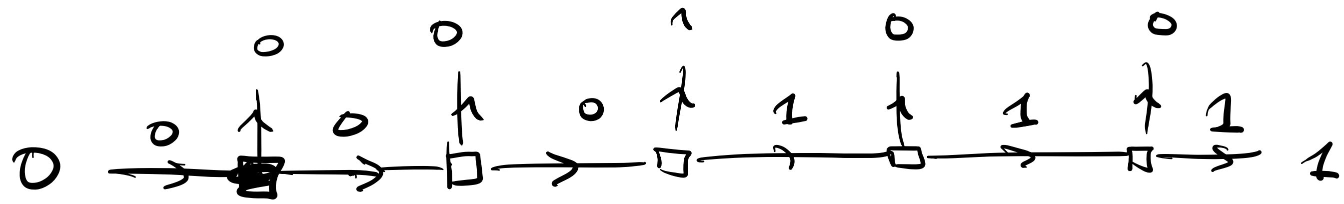
Agent picture:

① Start with 0.

② valid transitions:



③ final configuration: 1



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

$$A^1 = |0\rangle\langle 1| = \sigma^-$$

$$|\psi\rangle = \sum_{i_1,\dots,i_N} \underbrace{\langle 0| A^{i_1}}_{\equiv B^{i_1,(1)}} \underbrace{A^{i_2} \cdots\cdots}_{\equiv B^{i_k,(k)}} \underbrace{A^{i_N} |1\rangle}_{\equiv B^{i_N,(N)}} |i_1,\dots,i_N\rangle$$

$$(\sigma^-)^2 = 0, \quad \langle 0|\sigma^-|1\rangle = 1.$$

$$\Rightarrow |\psi\rangle \propto |W\rangle$$

Note: No tr.inv. PBC rep. of $|W\rangle$ exists, unless D grows with N.

(Any tr.inv. OBC MPS can be transformed in a tr.inv. PBC MPS with $D_{PBC} = N D_{OBC}$.)

d) The cluster state

The <u>cluster state</u> is obtained by acting with

$$CZ_{i,i+1} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \quad \text{on} \quad |+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}},$$

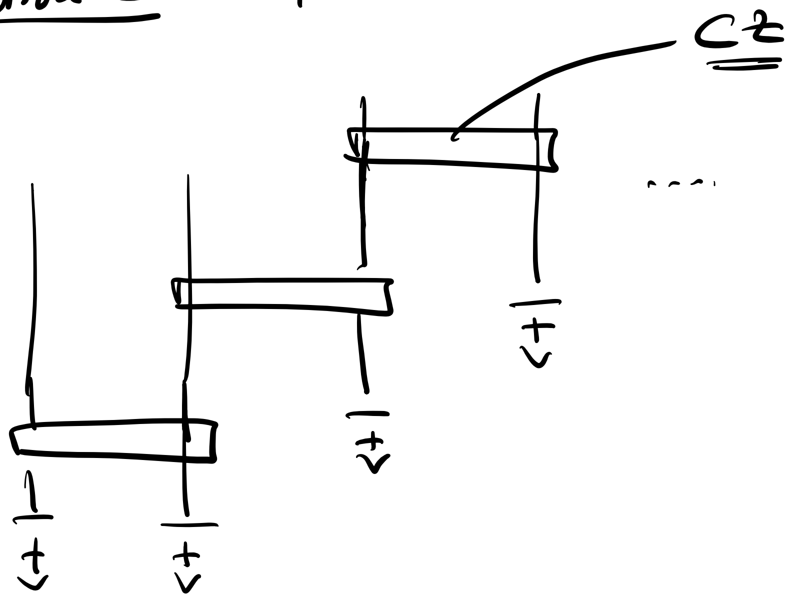
$$|\mathcal{C}\rangle = \prod_{i=1}^{N-1} CZ_{i,i+1} \, |+\rangle^{\otimes N} \quad (\text{w/ OBC}).$$

(<u>Note</u>: All $CZ_{i,i+1}$ commute – any order ok.)

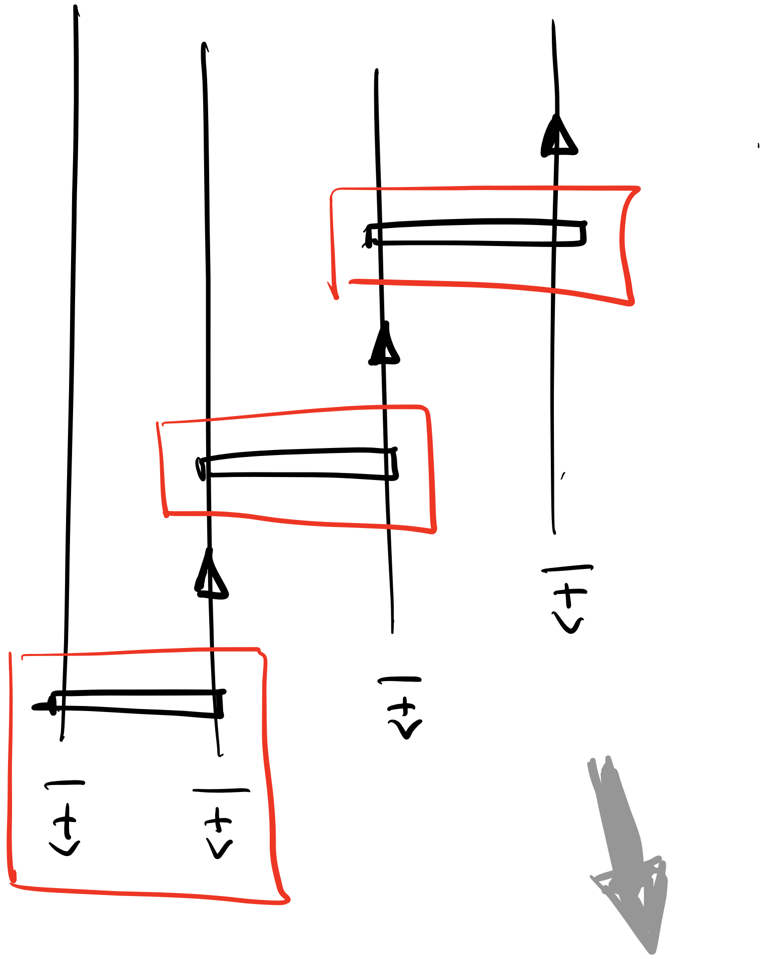
How can we find MPS representation?

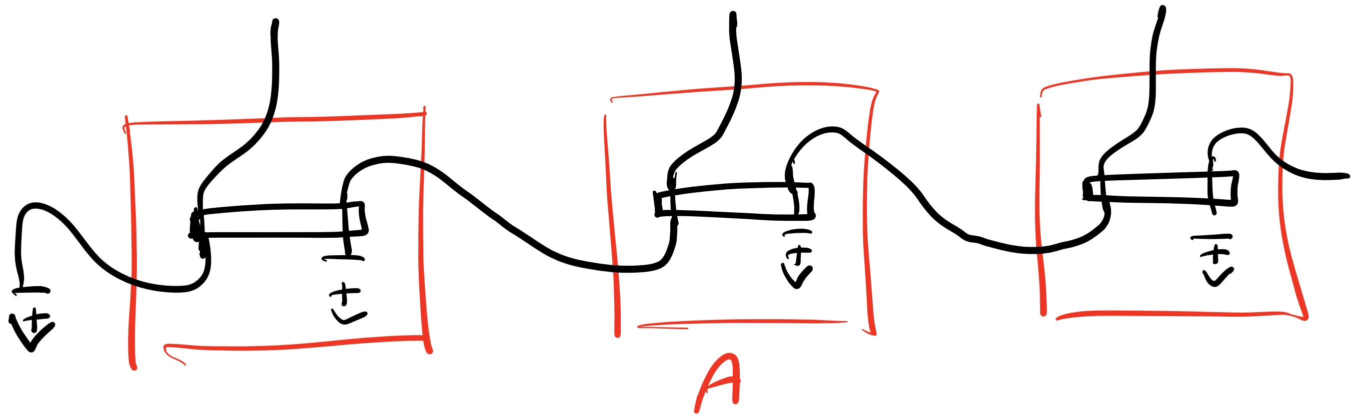
Different approaches possible ...

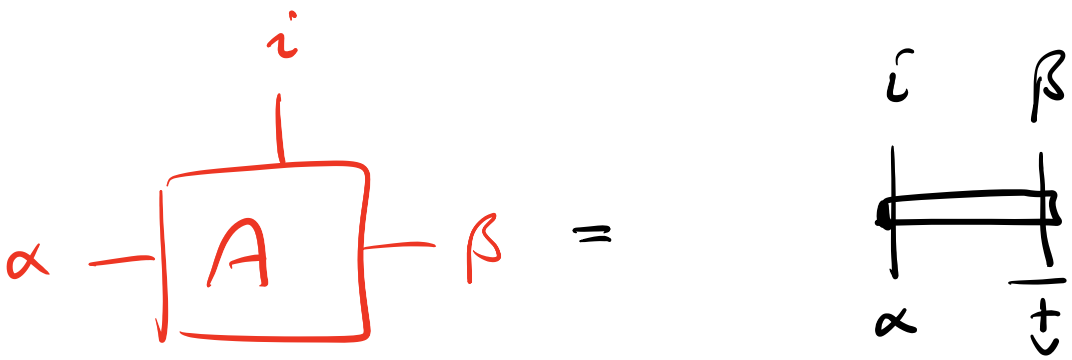
<u>Option 1</u>: $|\mathcal{C}\rangle =$



Adjoint picture:







$$= \langle i| \otimes \langle\beta|\, CZ\, \underbrace{|\alpha\rangle \otimes |+\rangle}_{\frac{|\alpha 0\rangle + |\alpha 1\rangle}{\sqrt{2}}}$$

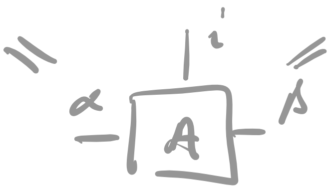
$$\alpha = 0 \swarrow \qquad \searrow \alpha = 1$$

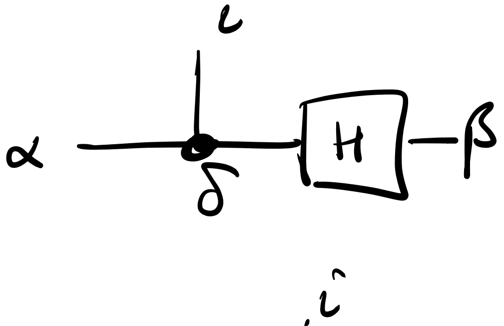
$$\frac{|\alpha 0\rangle + |\alpha 1\rangle}{\sqrt{2}} \qquad\qquad \frac{|\alpha 0\rangle - |\alpha 1\rangle}{\sqrt{2}}$$

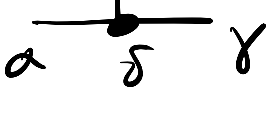
$\langle i,\beta|\dots\rangle \Rightarrow$

$$\frac{\delta_{\alpha i}}{\sqrt{2}} \cdot (+1)^{\beta} \qquad\qquad \frac{\delta_{\alpha i}}{\sqrt{2}} (-1)^{\beta}$$

for $\alpha = 0$ $\qquad$ for $\alpha = 1$





with 

the δ-tensor:

$$\delta_{\alpha i \gamma} = \begin{cases} 1 & \alpha = i = \gamma \\ 0 & \text{otherwise} \end{cases}$$

and $H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} = |0\rangle\langle +| + |1\rangle\langle -|$

the Hadamard matrix/transformation.

i.e.:

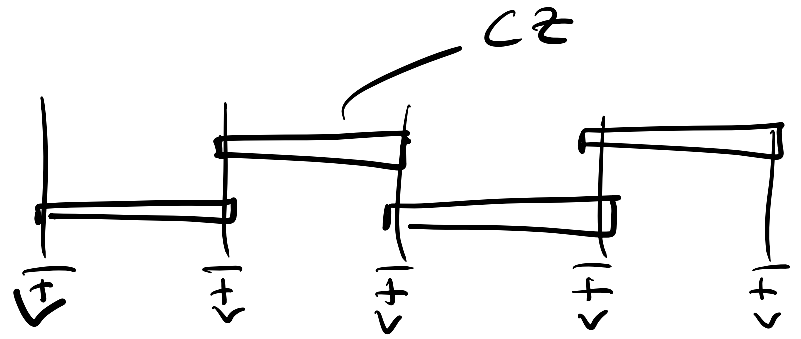
or

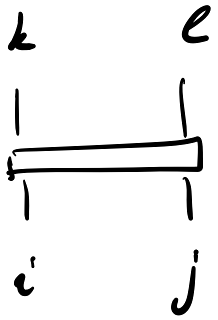
$$A^0 = |0\rangle\langle 0| \cdot H = |0\rangle\langle +|$$

$$A^1 = |1\rangle\langle 1|\, H = |1\rangle\langle -| .$$

$$|\mathrm{cl}\rangle = \sum_{i_1,\dots,i_N} \langle +| A^{i_1} \dots A^{i_N} |0\rangle\, |i_1,\dots,i_N\rangle$$

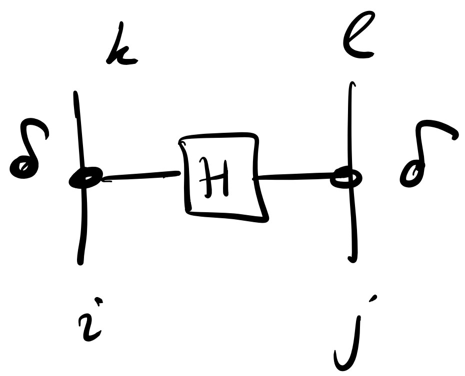
Option 2:

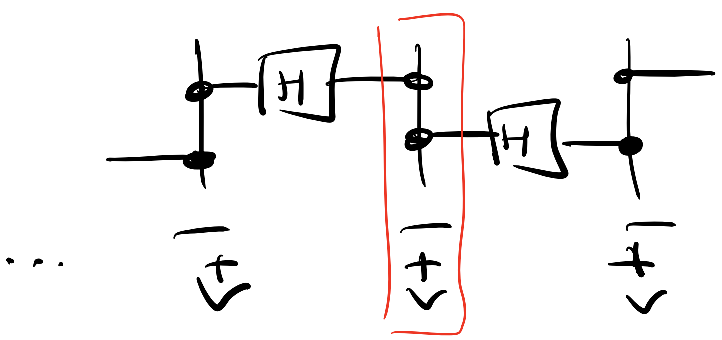
$|\psi\rangle =$ 

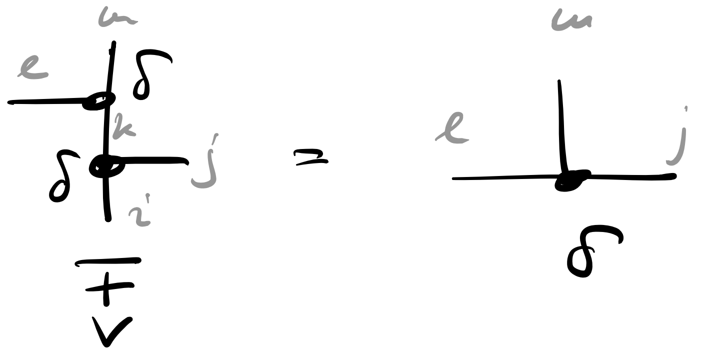


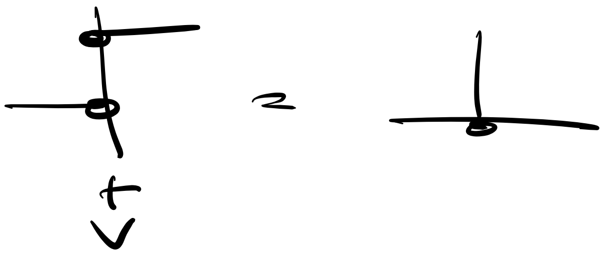
$$= \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

$$= \delta_{ik}\, \delta_{jl}\, \underbrace{(H)_{ij}}_{= (-1)^{i \cdot j}}$$

$=$ 

$\Rightarrow |\psi\rangle =$ 

and  !

(and same for )

$\Longrightarrow$ same MPS representation

(but this also works for PBC).

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

How can we evaluate properties of MPS:

* normalization
* expectation values, energies
* correlation functions

...

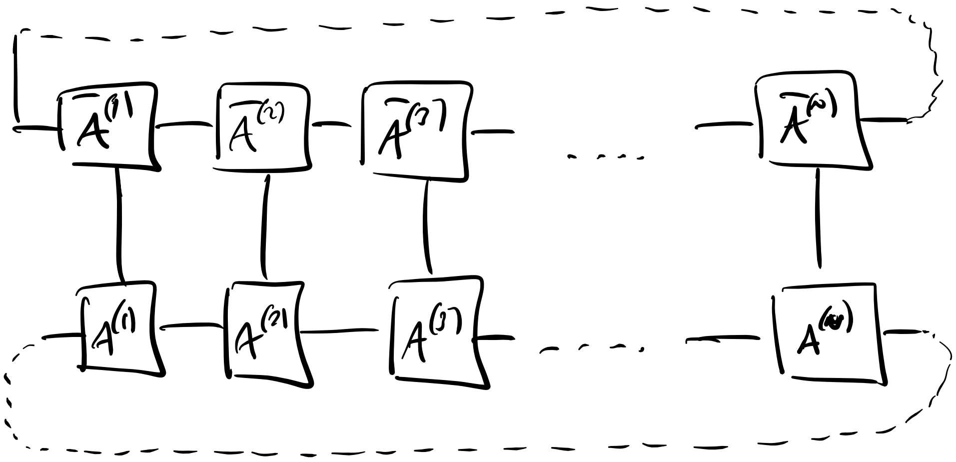
What do they depend on?

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

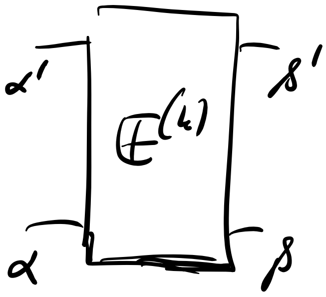
Consider wlog PBC MPS (OBC is special case with $D_0 = D_N = 1$).

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

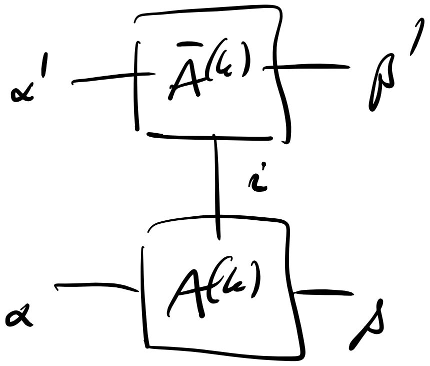


Define

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



$=$



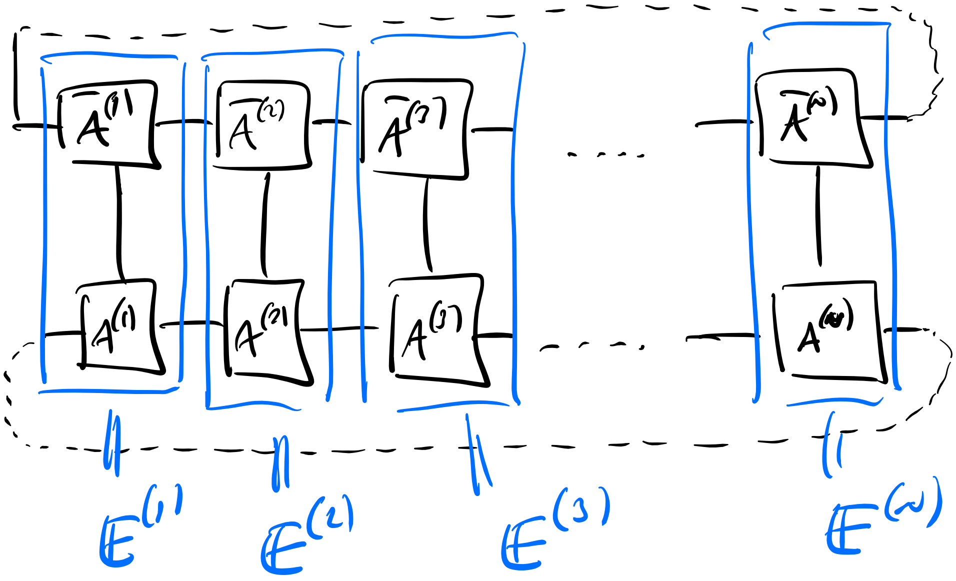
$$= \sum A^{i,(k)} \otimes \bar{A}^{i,(k)}$$

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

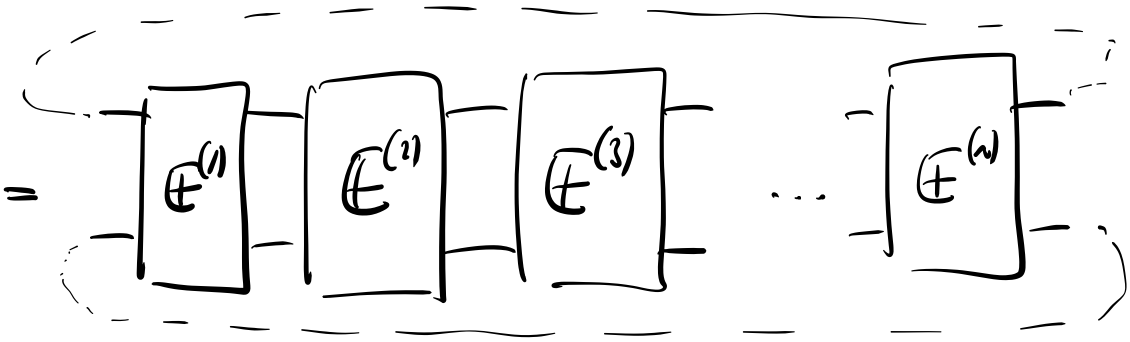
$\mathbb{E}$ is also called the transfer matrix or transfer operator.

Then,

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



$=$



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

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. $N D^6$ in total (vs. d^N for building
$c_{i_1 \ldots i_N}$).

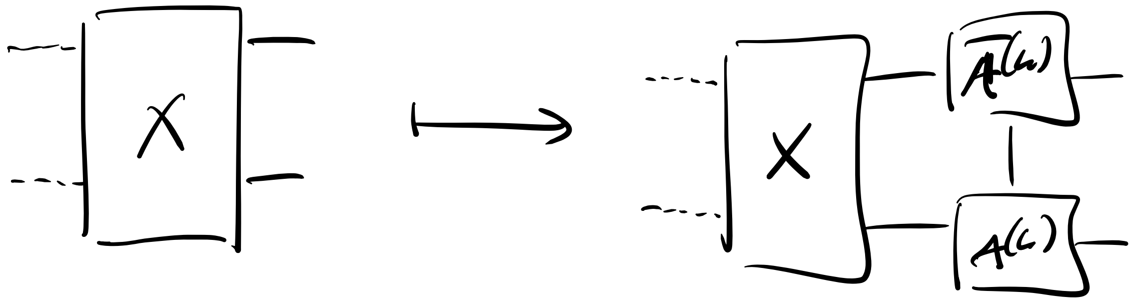
<u>OBC</u>: If we start from the right:

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

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

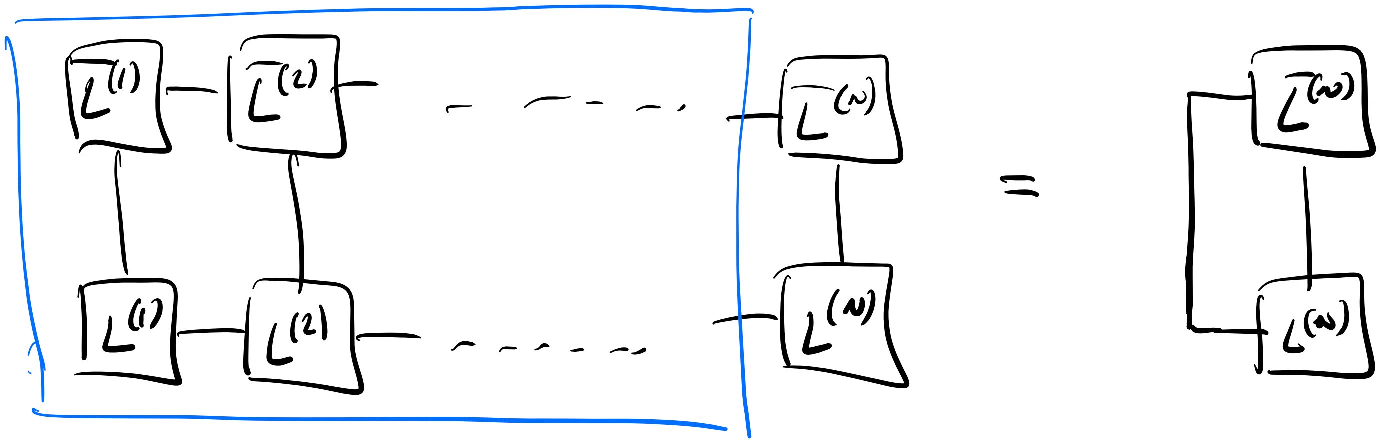
Important points for numerical simulations:

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



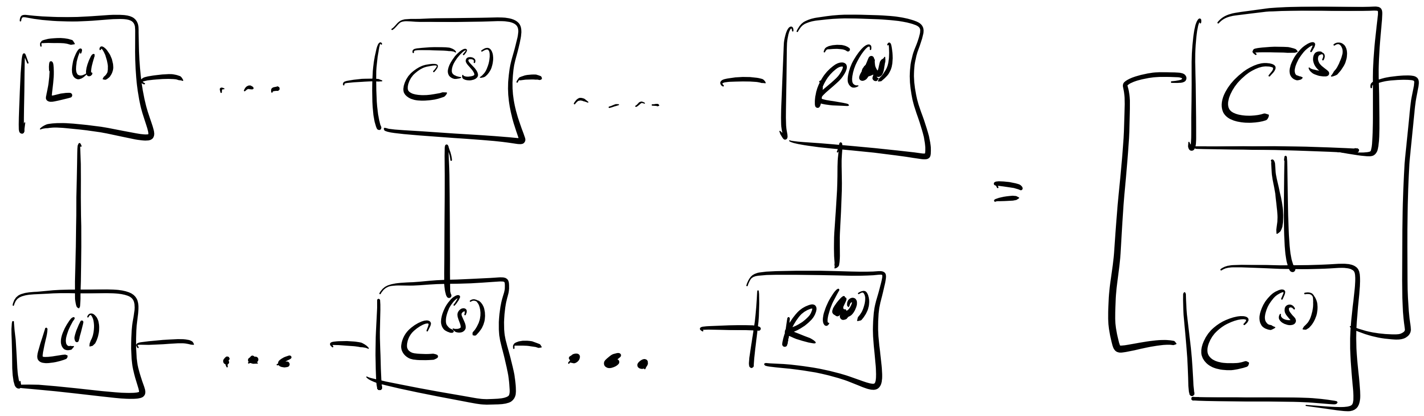
without building $E^{(l)}$.

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



= [(from CF!)

* Similarly, for a mixed CF:



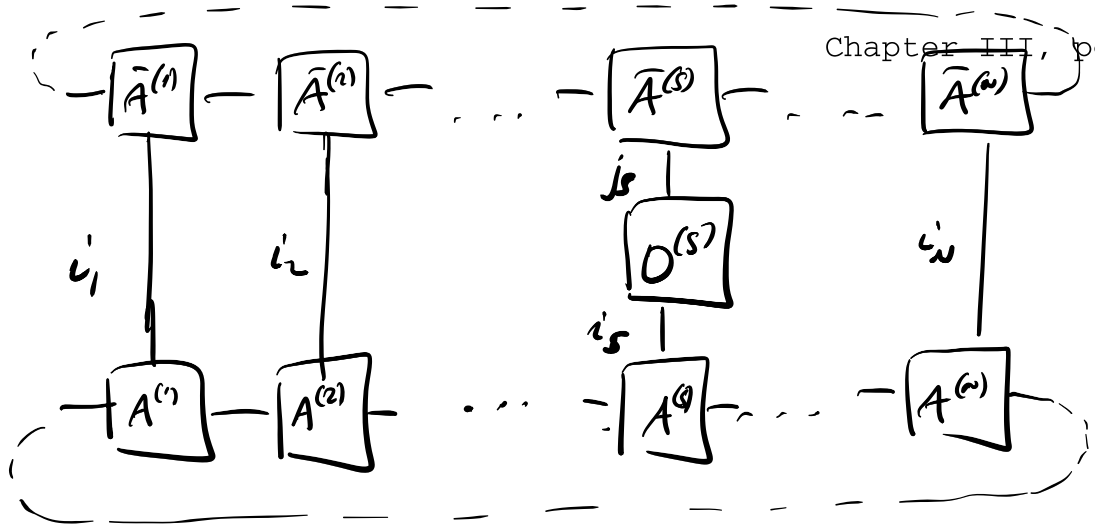
$$= \| C^{(s)} \|_2^2 = \sum_{i_s,\alpha,\beta} \left| C^{i_s (s)}_{\alpha\beta} \right|^2$$

b) Expectation values

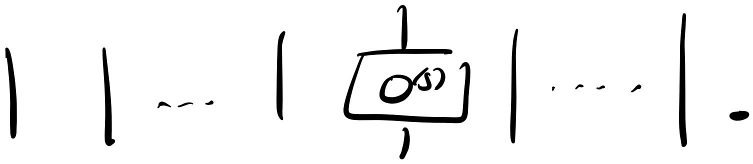
Expectation values $\langle\psi|O|\psi\rangle$ of local observables, e.g. single-site observables $O^{(s)}$ such as $O^{(s)} = \sigma_z^{(s)}$:

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

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

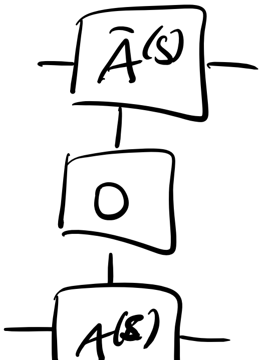
$=$ 

... can also be understood by noting that

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

Can it be computed efficiently?

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

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

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

Then, we have that

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

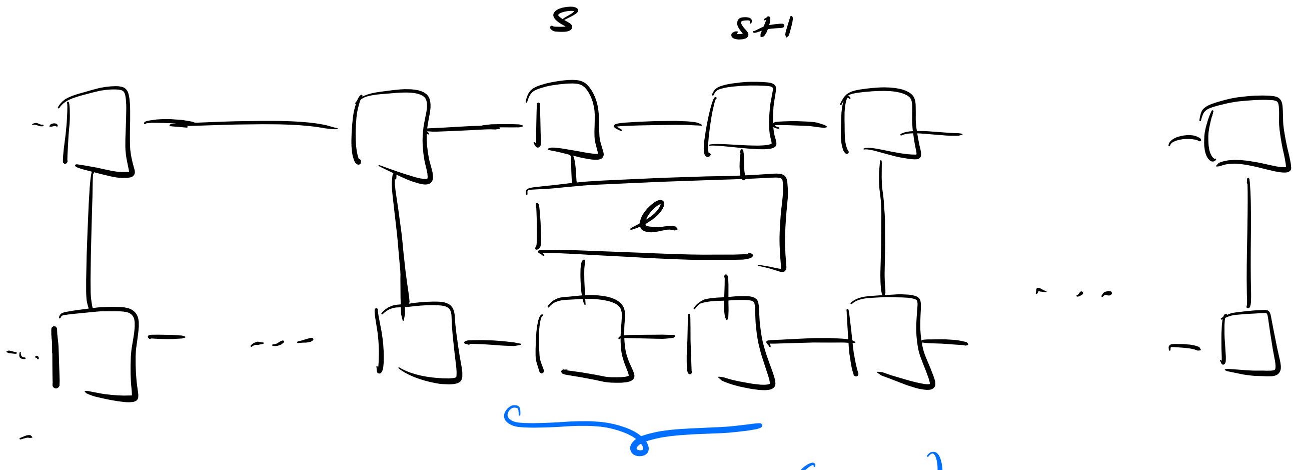
(PBC)

or for OBC,

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

$\Rightarrow$ expectation values can be computed efficiently.

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

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

Possible optimizations (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.:

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

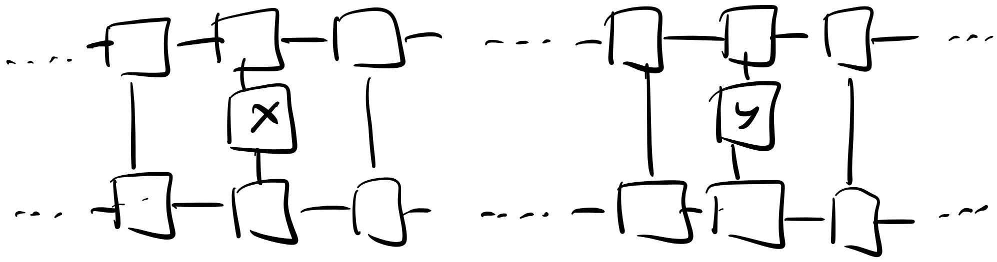
$$\langle\psi|h_{s,s+1}|\psi\rangle = \boxed{\mathbb{E}^{(1)}\cdot\mathbb{E}^{(2)}\cdot\ldots\cdot\mathbb{E}^{(s-2)}}\,\mathbb{E}^{(s-1)}\mathbb{E}_h^{(s,s+1)}\boxed{\mathbb{E}^{(s+2)}\cdot\ldots}$$

same for both ... 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.

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

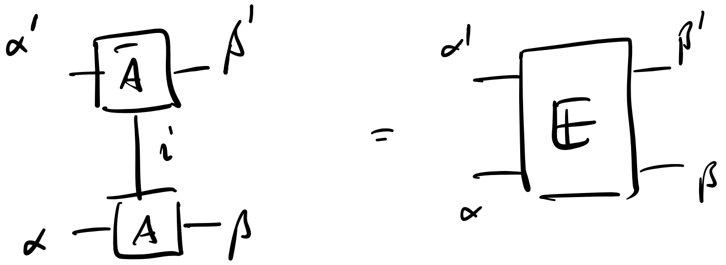
$$\exists U_{ij} \text{ unitary}: \quad A^i = \sum_j U_{ij} B^j$$

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

Isometry.

$\Rightarrow$ all non-local properties of an MPS are encoded in the $\{\mathbb{E}^{(k)}\}$.

Proof sketch:



interpret $A^{i}_{\alpha\beta}$ as matrix $\hat{A}_{(\alpha\beta),i}$

interpret $\mathbb{E}$ as matrix $\hat{\mathbb{E}}_{(\alpha\beta),(\alpha'\beta')}$

$$\hat{\mathbb{E}} = \hat{A} \cdot \hat{A}^{\dagger}.$$

What is relation betw. $\hat{A}, \hat{B}$ with $\hat{A}\hat{A}^{\dagger} = \hat{B}\hat{B}^{\dagger}$?

$\hat{\mathbb{E}} \geq 0$, and thus $\hat{\mathbb{E}} = U D^{2} U^{\dagger}$, with

U isometry, $D = \begin{pmatrix} s_1 & & \\ & \ddots & \\ & & s_r \end{pmatrix}$, $s_1 \geq \dots s_r > 0$

(as in construction of SVD). Then,

$\hat{A}\hat{A}^\dagger = \hat{B}\hat{B}^\dagger = \hat{\mathbb{E}}$ $\Longrightarrow$ SVDs of $\hat{A}$ and $\hat{B}$ are

$$\hat{A} = U D V_A^\dagger$$
$$\hat{B} = U D V_B^\dagger \quad , \; V_A, V_B \text{ isometries}$$

$\boxtimes$

(From a quantum information perspective, this is equivalent to the ambiguity of purifications, as

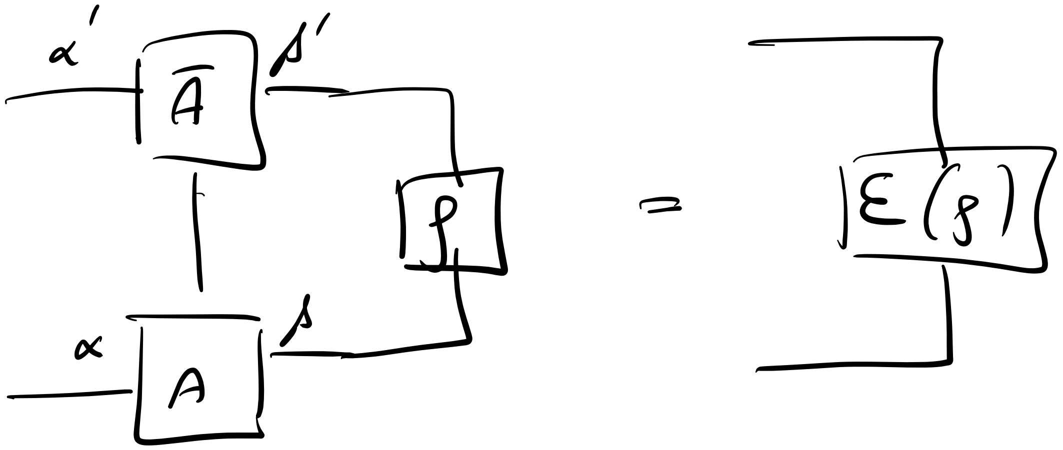
$$\sum A^i_{\alpha\beta} |\alpha,\beta\rangle \otimes |i\rangle \text{ is a purification of}$$

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

e) Transfer operator as a CP map

One more connection to quantum information:

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

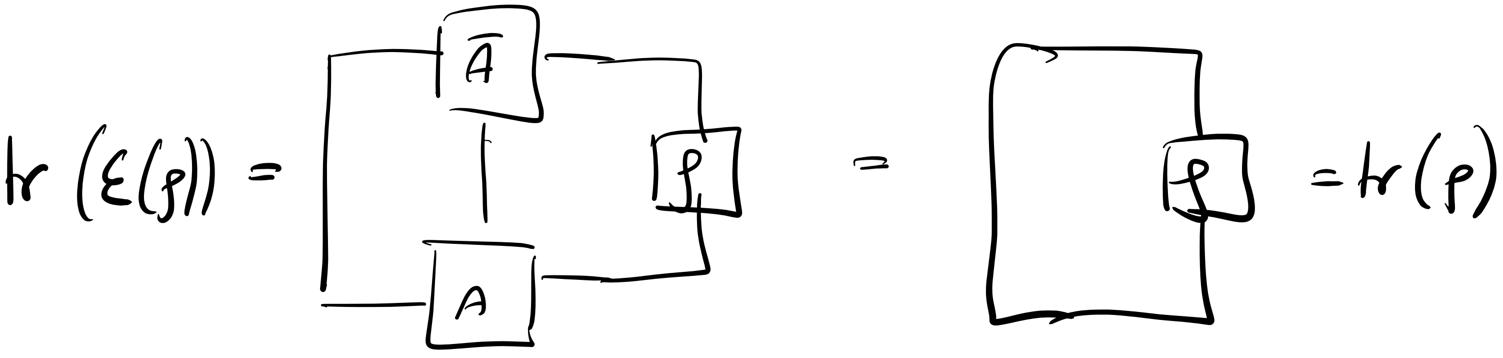


We have $\mathcal{E}(\rho) = \sum A^i_{\alpha\beta} \bar{A}^i_{\alpha'\beta'} \rho_{\beta\beta'} |\alpha\rangle\langle\alpha'|$

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

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

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



7. Translational invariant infinite MPS: Construction and correlations

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

a) Construction

Consider a t.i. 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: t.i. $\Rightarrow$ all positions equiv.!) is

t.i.: all $\mathbb{E}$ the same!

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

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

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.

(Note: $\langle l_i|r_j\rangle = \delta_{ij}$, 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 $l \gg 1$,

$$\mathbb{E}^l \longrightarrow \lambda_1^{\,l}\, |r_1\rangle\langle l_1|.$$

Note: This even holds for non-diagonalizable $\mathbb{E}$, since for CP maps, the largest eigenvalue cannot have a Jordan block. I.e.: The following argument always applies, given that $|\lambda_1|$ is non-degenerate.

Thus, as $N \to \infty$:

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

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

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

$$\longrightarrow \frac{\lambda_1^{N-1}\langle l_1|\mathbb{E}_O|r_1\rangle}{\lambda_1^N}$$

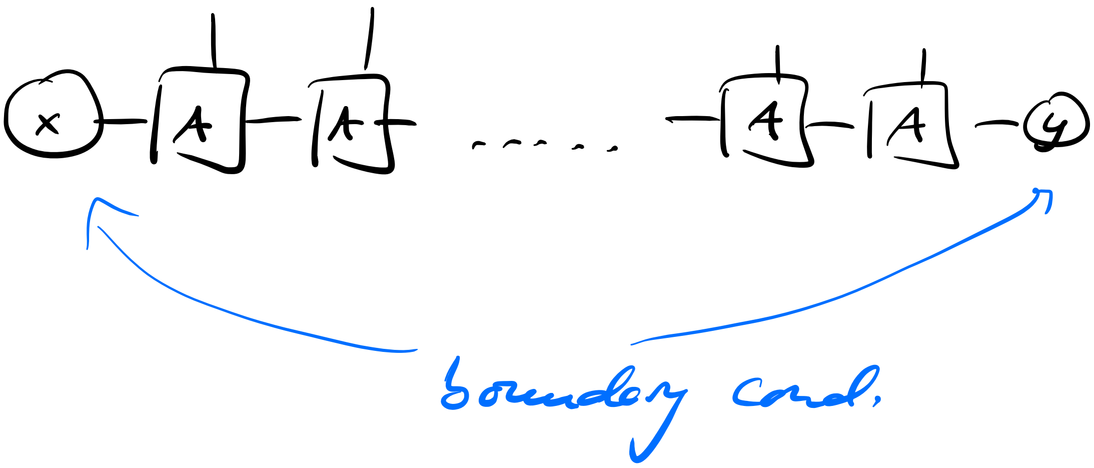
$$= \frac{1}{\lambda_1}\langle l_1|\mathbb{E}_O|r_1\rangle.$$

We find:

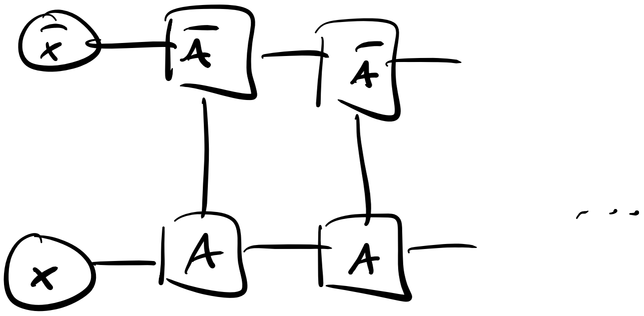
- $\dfrac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle}$ is well-defined in the thermodynamic limit.

- 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 $\mathbb{E}^{e} = \sum \lambda_i^{e} |r_i\rangle\langle e_i| \to \lambda_1^{e} |r_1\rangle\langle e_1|$,

for $n \to \infty$ we have

$$\frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} \longrightarrow \frac{\lambda_1^{2n}\langle x|r_1\rangle\langle e_1|y\rangle\,\langle e_1|\mathbb{E}_0|r_1\rangle}{\lambda_1^{2n+1}\langle x|r_1\rangle\langle e_1|y\rangle}$$

$$= \frac{1}{\lambda_1}\langle e_1|\mathbb{E}_0|r_1\rangle.$$

b) Correlation functions

How do correlations in a translationally invariant (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 $\ell \gg 1$:

$$\approx \underbrace{\frac{\langle \ell_1 | \mathbb{E}_x | r_1 \rangle}{\lambda_1}}_{= \langle \psi | X | \psi \rangle} \underbrace{\frac{\langle \ell_1 | \mathbb{E}_y | r_1 \rangle}{\lambda_1}}_{= \langle \psi | Y | \psi \rangle} +$$

$$\underbrace{\frac{\langle \ell_1 | \mathbb{E}_x | r_2 \rangle}{\lambda_1} \frac{\langle \ell_2 | \mathbb{E}_y | r_1 \rangle}{\lambda_1}}_{=: C} \left(\frac{\lambda_2}{\lambda_1} \right)^{\ell - 2}$$

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

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

Observation: In a translational invariant MPS with transfer matrix spectrum $\{\lambda_1, \lambda_2, \dots\}$, 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

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

c) Long-range order in trv. 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 change the expectation value in the middle: The system is sensitive to boundary conditions!

Now consider the correlation function for some given boundary condition:

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

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

$$\ell \gg 1 \quad \longrightarrow \quad \frac{\langle \ell(x)|E_x\left(\lambda_1^{\ell-2}|r_1\rangle\langle \ell_1| + \lambda_2^{\ell-2}|r_2\rangle\langle \ell_2|\right)E_y|r(y)\rangle}{\lambda_1^{\ell}\langle \ell(x)|r(y)\rangle}$$

(for $\lambda_1 = \lambda_2$)

$$= \frac{\langle \ell(x)|E_x|r_1\rangle\langle \ell_1|E_y|r(y)\rangle + \langle \ell(x)|E_x|r_2\rangle\langle \ell_2|E_y|r(y)\rangle}{\lambda_1^2\langle \ell(x)|r(y)\rangle}$$

This is generally <u>non-zero</u> even for the <u>connected</u> correlation functions:

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

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

$$\frac{\langle \ell(x)|E_x\left(\sum_{i=1,2}|r_i\rangle\langle \ell_i|\right)E_y|r(y)\rangle}{\lambda_1^2\langle \ell(x)|r(y)\rangle} \neq \frac{\langle \ell(x)|E_x|r(y)\rangle}{\lambda_1\langle \ell(x)|r(y)\rangle} \times \frac{\langle \ell(x)|E_y|r(y)\rangle}{\lambda_1\langle \ell(x)|r(y)\rangle}$$

$\parallel$ A $\qquad$ $\parallel$ B $\qquad$ $\parallel$ C

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

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

$\lambda_1 = \lambda_2 = 1, \quad \lambda_3 = \lambda_4 = 0.$

leading eigenvectors: $|r_1\rangle = |l_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$,

$|r_2\rangle = |l_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

Let $X = Y = \sigma_z$:

$$\mathbb{E}_X = \mathbb{E}_Y = \mathbb{E}_{\sigma_z} = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{pmatrix}$$

Choose $|l(x)\rangle = |r(x)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

Then, $A = 1$,

$B = C = 0$.

<u>Observation:</u>

MPS with a degenerate leading eigenvalue have <u>long-range correlations</u>

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

<u>Observation:</u>

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.

Note: There are also constraints to the ability of MPS to exactly capture ground states of generic gapped systems:

- 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.