II. Matrix Product States

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

with states

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

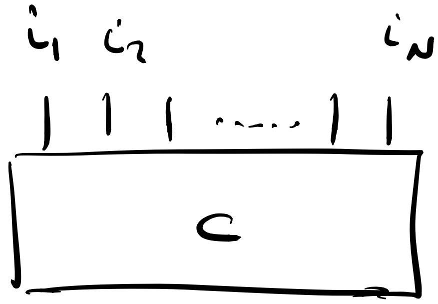
1. Construction

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

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

Graphical notation:

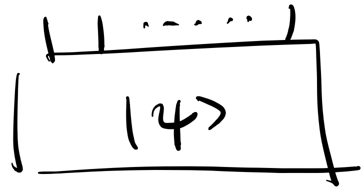
$c_{i_1 \ldots i_N}$ =



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

$$c_{i_1 i_2 \dots i_N} = c_{i_1 (i_2 \dots i_N)}$$ 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 $C = U \Lambda V$),

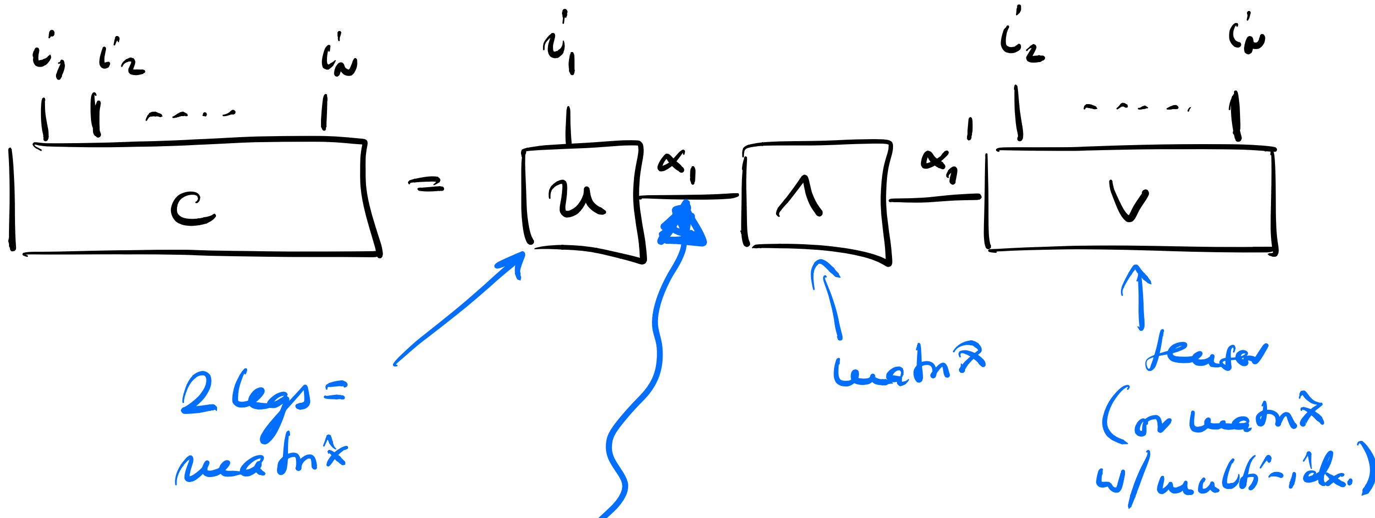
with Λ a diagonal matrix, $\Lambda_{\alpha_1, \alpha_1'} = \delta_{\alpha_1 \alpha_1'} \cdot \overset{\geq 0}{\lambda_{\alpha_1}}$

and U, V isometries:

$$\sum_{i_1} \overline{U}_{i_1,\beta_1} \, U_{i_1,\alpha_1} = \delta_{\alpha_1,\beta_1} ,$$

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

<u>Graphically</u>:



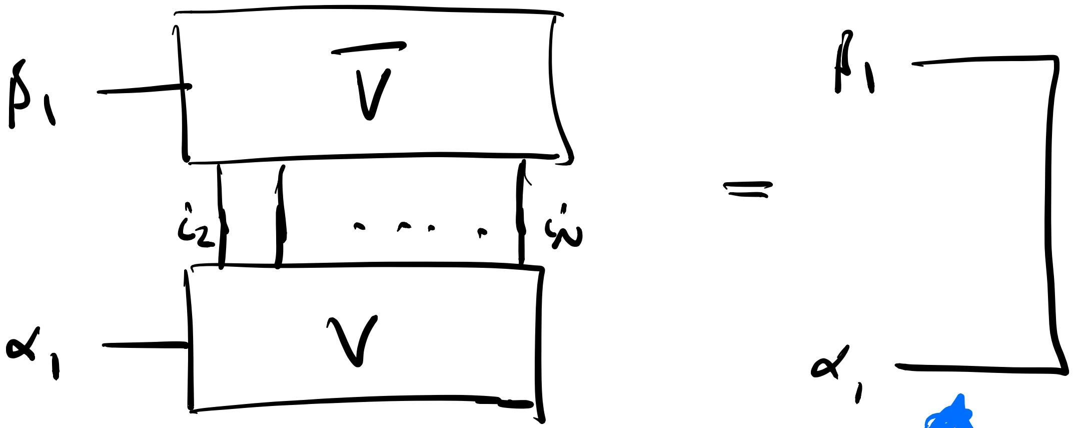
connecting legs denotes <u>contraction</u>: The legs are <u>identified</u> and summed over

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

matrix product!

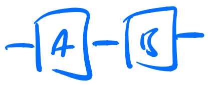
The isometry conditions read graphically:

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



simple line = identity matrix

(consistent:

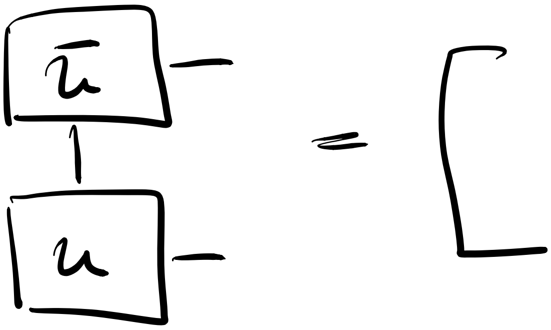


$= A \cdot B$

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

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

and



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

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

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

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

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

$\Rightarrow$ $|l_\alpha\rangle$ (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

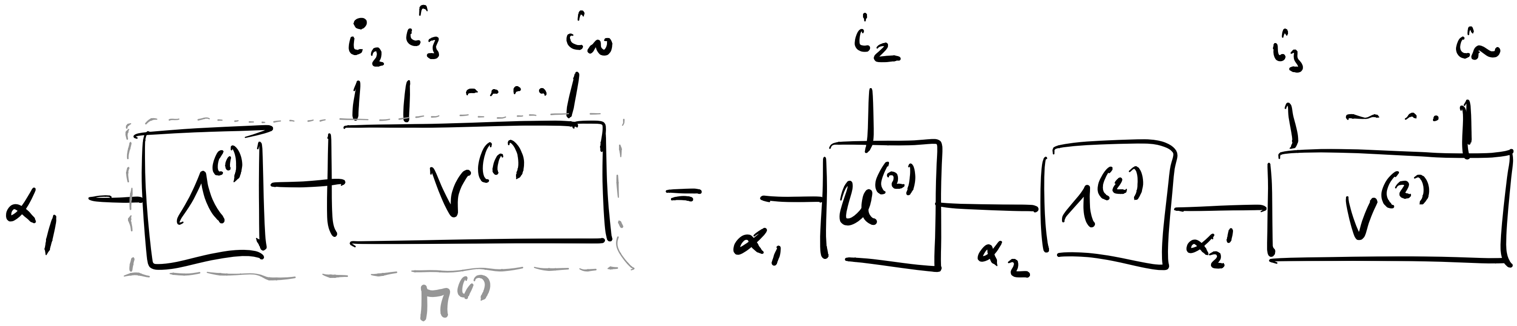
$\Lambda_{\alpha_1 \alpha_1} = \operatorname{eig}(\Lambda)$ the Schmidt coefficients!

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

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

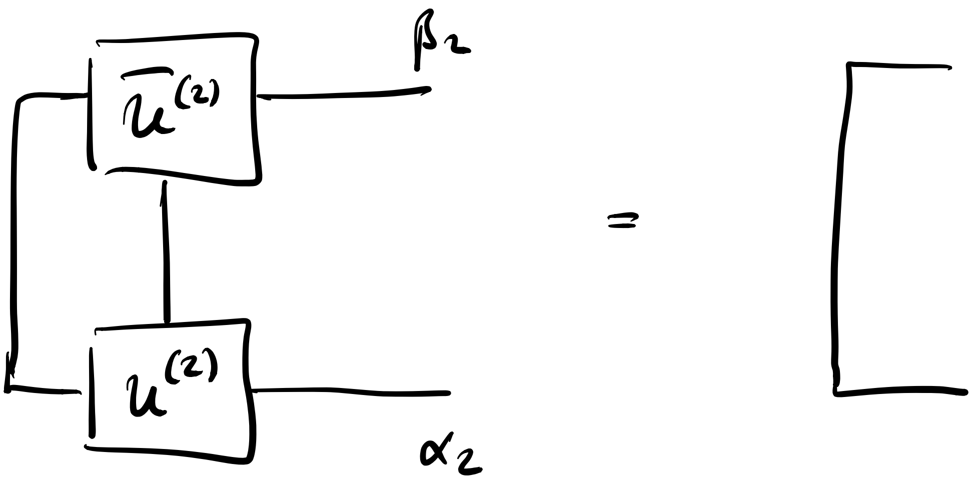
new row/col. indices

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

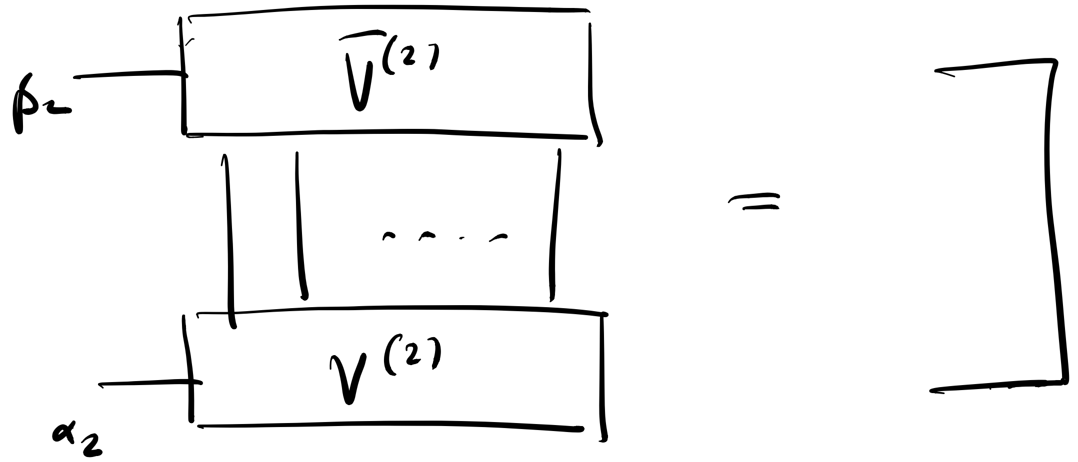


$\Lambda^{(2)}$ is diagonal ≥ 0

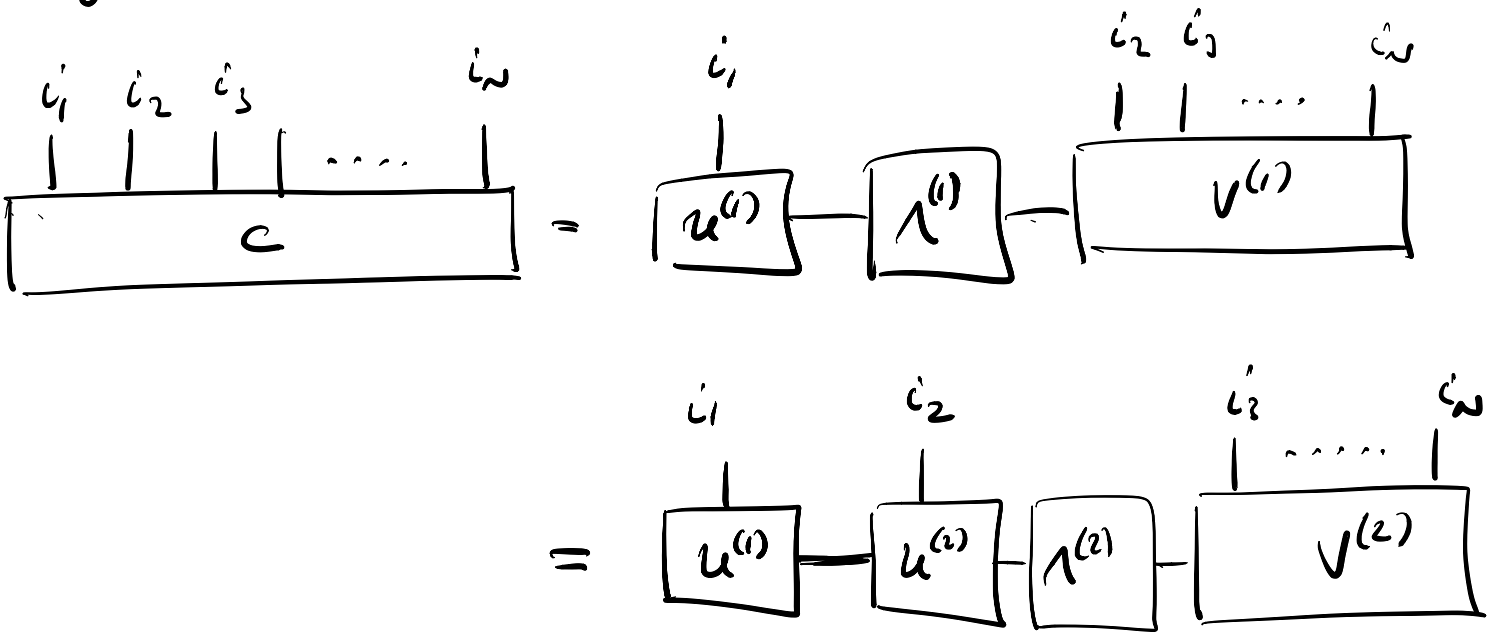
$\mathcal{U}^{(2)}, V^{(2)}$ isometries:



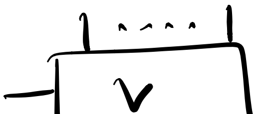
(or: $\sum_{\alpha_1 i_2} \mathcal{U}^{(2)}_{(\alpha_1 i_2)\alpha_2} \, \overline{\mathcal{U}}^{(2)}_{(\alpha_1 i_2)\beta_2} = \delta_{\alpha_2 \beta_2}$)

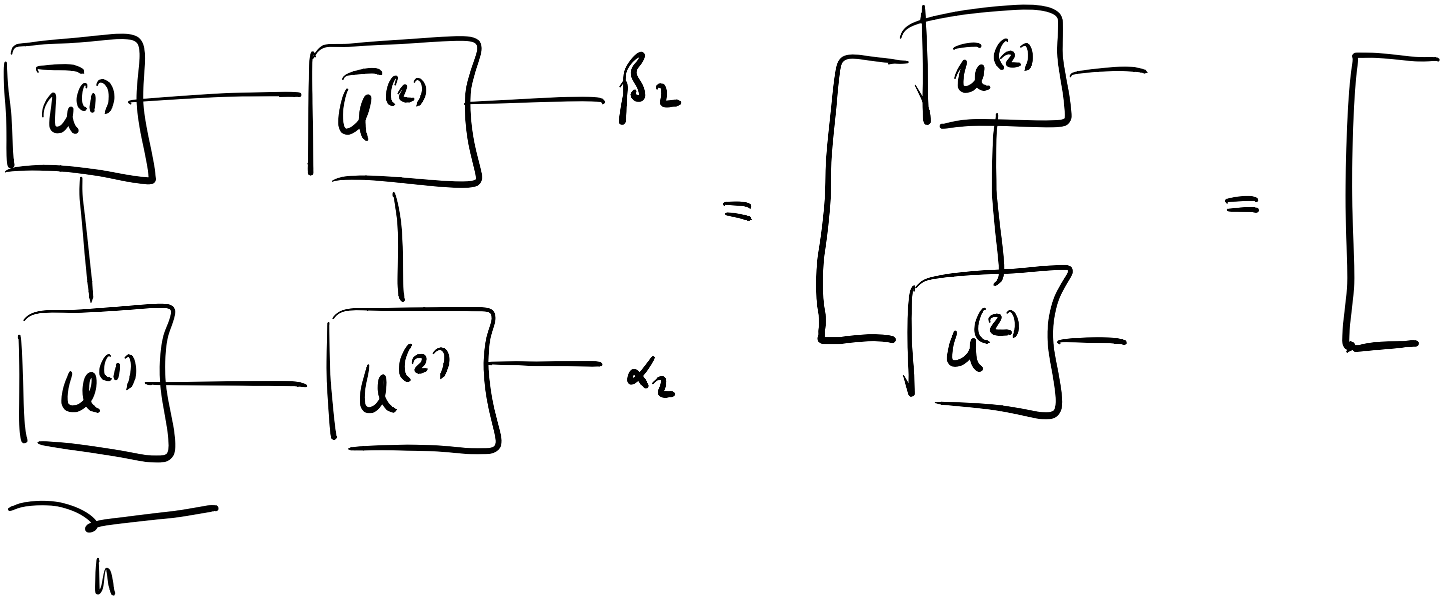


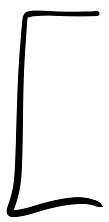
<u>Together:</u>



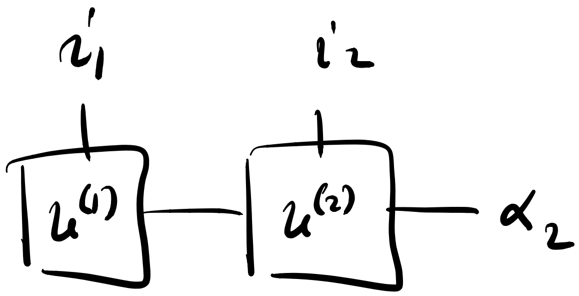
What is the form of the decomposition in the cut $12|3\ldots N$?

$V^{(2)}$ isometry $\Rightarrow$ right basis α_2  is ONB.





$\Longrightarrow$

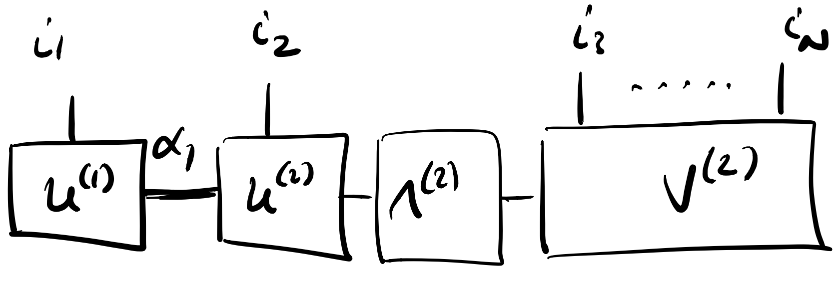


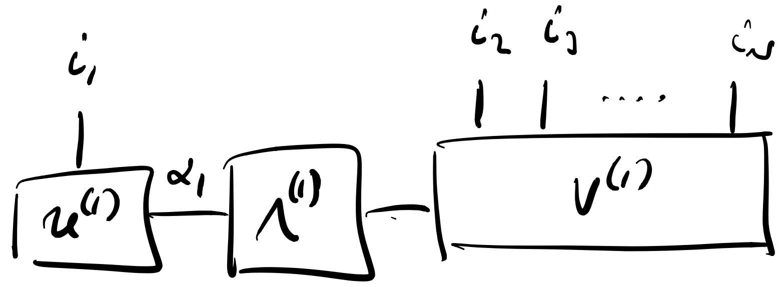
is <u>also</u> an isometry (as a map from $\alpha_2 \to (i_1 i_2)$)

$\Longrightarrow$ this is <u>again</u> a Schmidt decomposition,

now in the cut $12|3 \ldots. N$.

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



$=$ 

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

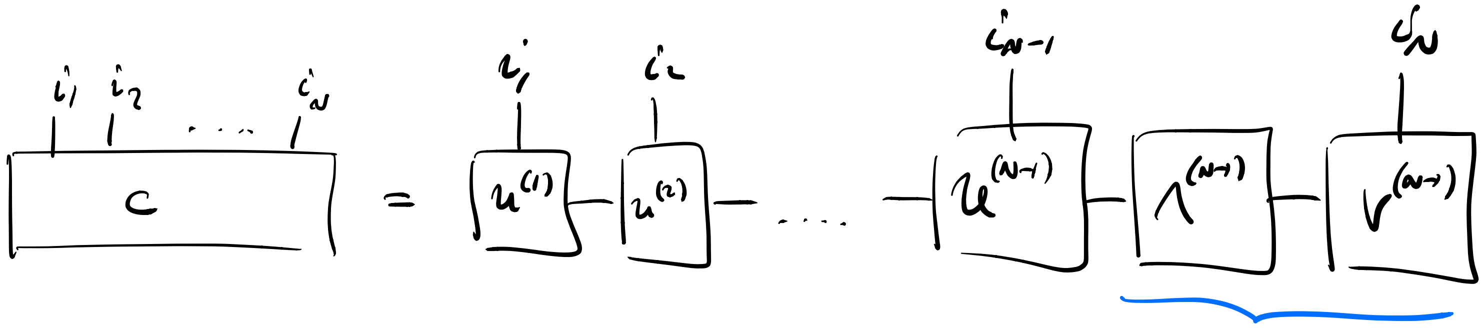
$$|\psi\rangle = \sum |\ell^{(1)}_{\alpha_1}\rangle\, |\tilde{r}^{(1)}_{\alpha}\rangle$$

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

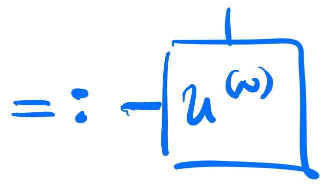
and $\langle \tilde{r}^{(1)}_{\alpha} | \tilde{r}^{(1)}_{\beta}\rangle = \Lambda_{\alpha\alpha}\, \delta_{\alpha\beta}$

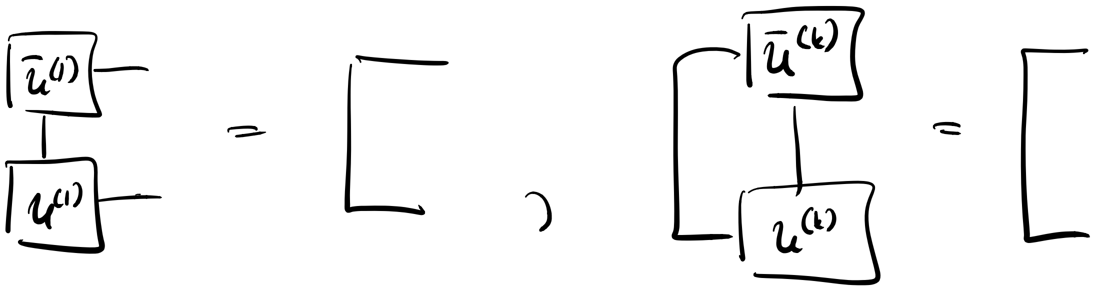
Orthonormal, and the Schmidt coefficient <u>absorbed</u> in $|\tilde{r}_{\alpha}\rangle$ 6

We can now *iterate* this scheme and get:



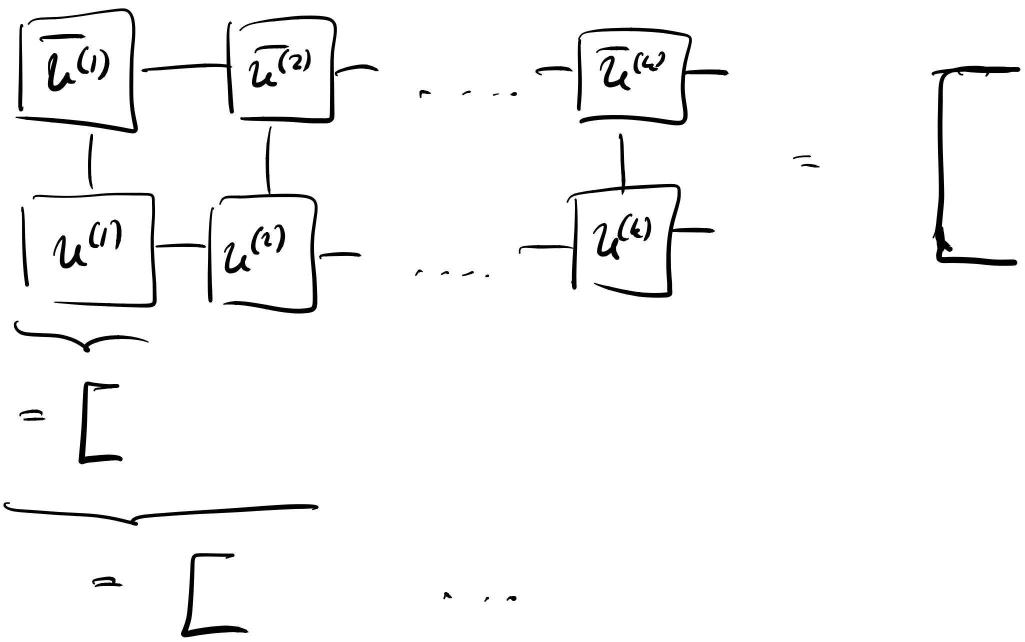
with





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

and thus also



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

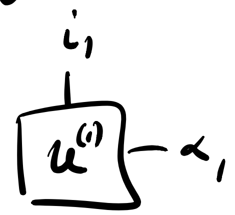
$$\sum |l_\alpha^{(k)}\rangle\, |\tilde{r}_\alpha^{(k)}\rangle \,,$$

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

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

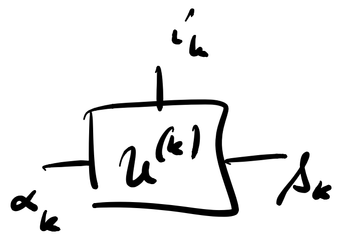
Schmidt coeffs for cut k.

Alternatively, we can consider



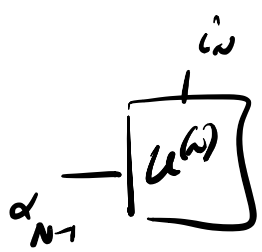
as a set of row vectors $(U^{(1)}_{i_1})_{\alpha_1}$,

and



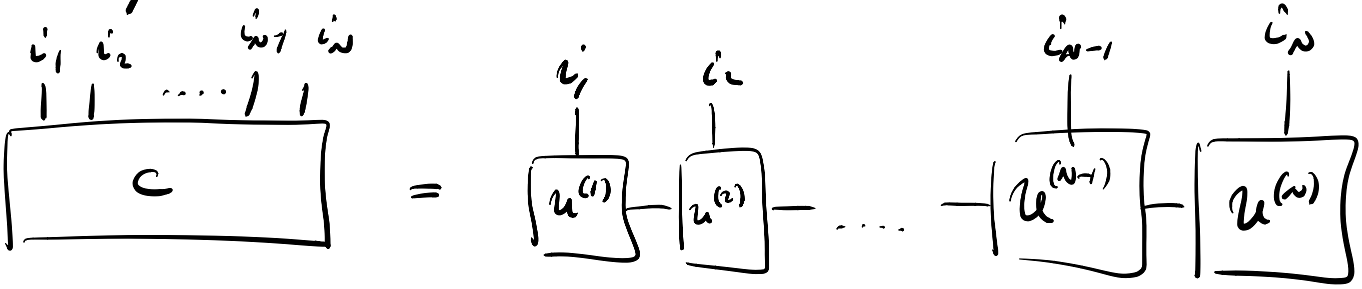
as matrices $(U^{(k)}_{i_k})_{\alpha_k\beta_k}$,

and



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

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:

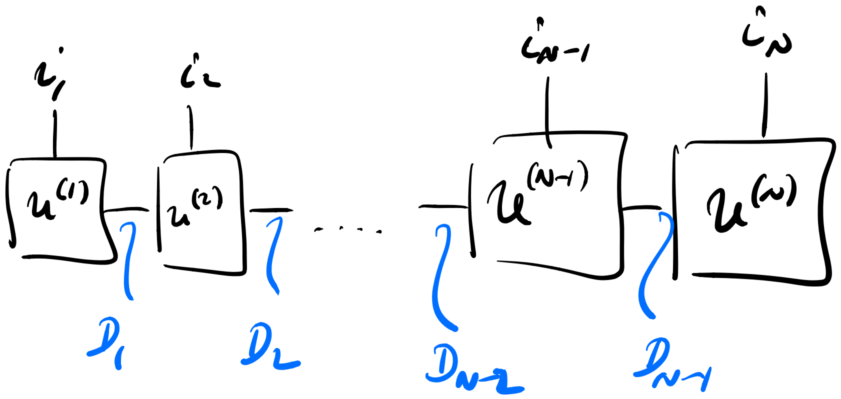
$u^{(1)}_{i_1}$: $1 \times D_1$ – vector

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

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

⋮

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



We call D_i the "<u>bond dimension</u>".

<u>Observation:</u> We have re-phrased $c_{i_1 \dots i_N}$ as a <u>vector-matrix product!</u>

Did this <u>reduce</u> the <u># of parameters</u>?

<u>No</u>, this <u>cannot be</u> — this decomposition is exact & cannot reduce # of params.

<u>In fact:</u> 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

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