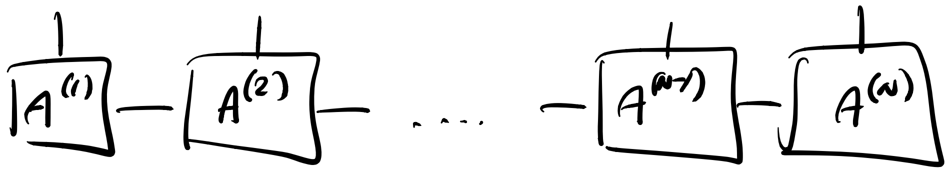
3. Canonical forms

Definition (from now on):

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

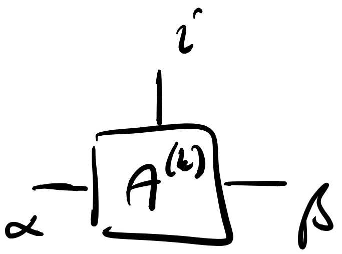
$$|\psi\rangle = \sum_{i_1,\dots,i_N} A^{i_1,(1)} A^{i_2,(2)} \cdots A^{i_N,(N)} |i_1,\dots,i_N\rangle,$$

$=$ 

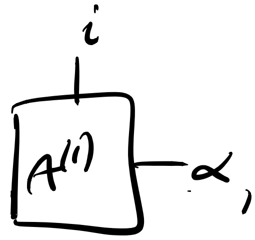
with $A^{i_k,(k)}$, $k=2,\dots,N-1$ $D\times D$-matrices, and $A^{i_1,(1)}$ $1\times D$, $A^{i_N,(N)}$ $D\times 1$ (i.e. vectors)

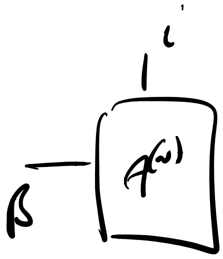
More generally, $A^{i_k,(k)}$ can be a $D_{k-1}\times D_k$-matrix $D_0 = D_N = 1$.

Terminology:



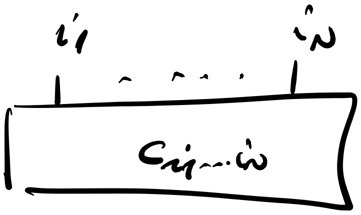
are 3-index (3-leg) tensors.



, 

are 2-index tensors.

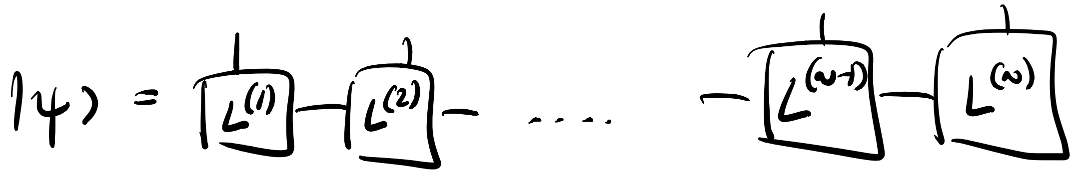
We call i the **physical index** (or degree of freedom, DoF), and α, β the **virtual** or **auxiliary** **indices/DoFs.**

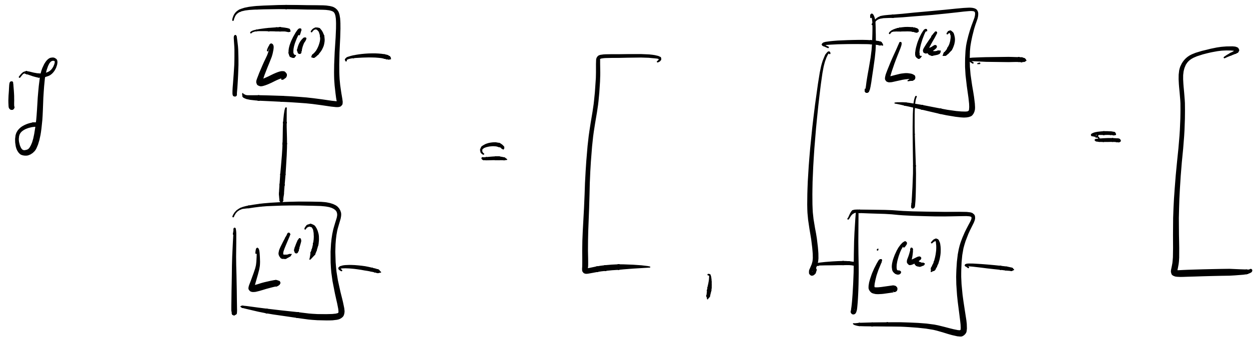
Since  is expressed as a network of elementary tensors, such states are also called **Tensor Network States.**

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

Left-canonical form:

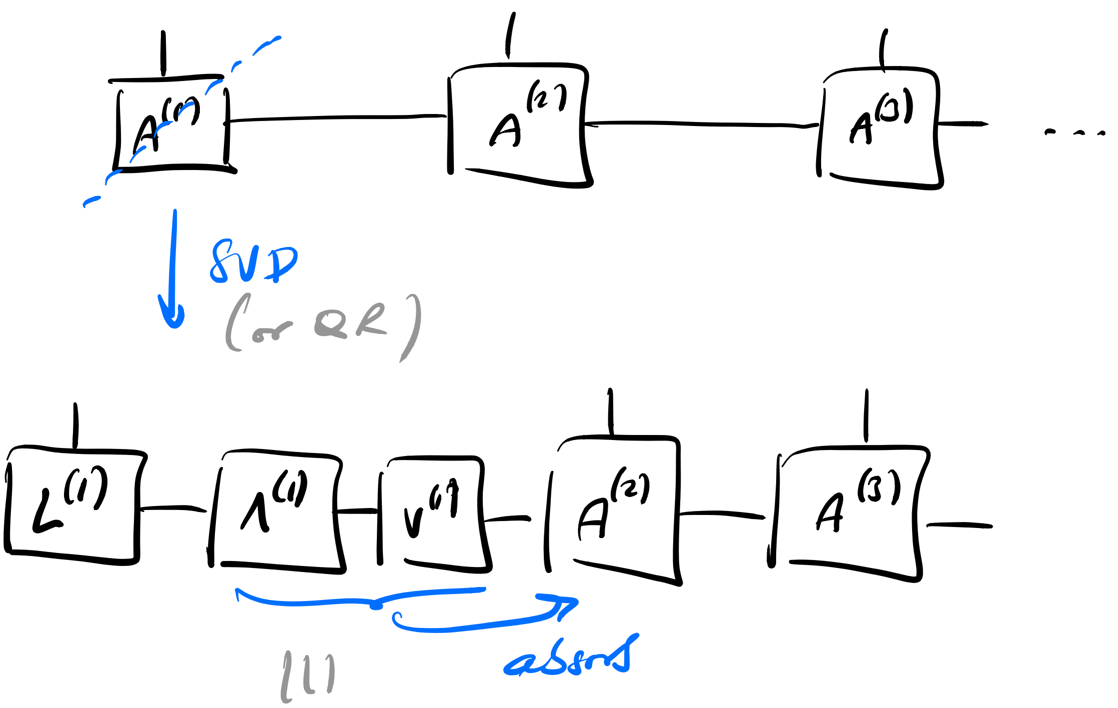
An MPS is said to be in left-canonical form,

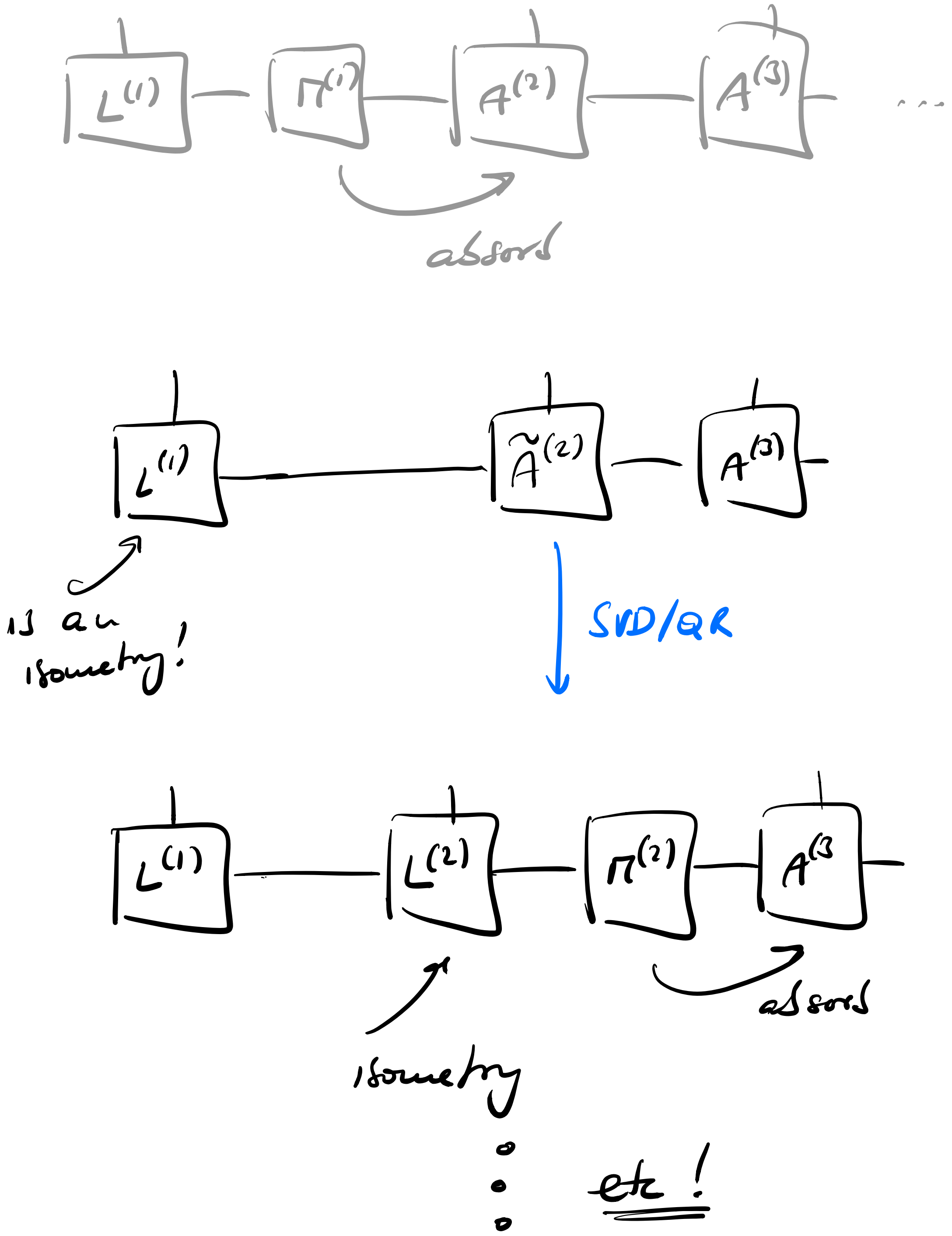




(k<N).

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





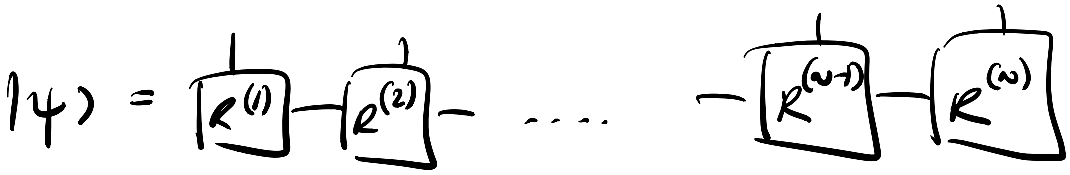
<u>Important</u>: Size of matrices for SVD is $D \times dD$, i.e. indep. of system size, & comp. cost $\sim D^3$

$\Rightarrow$ MPS can be brought into can. form <u>efficiently</u>.

Analogously, we can define the

Right-canonical form (CF):

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



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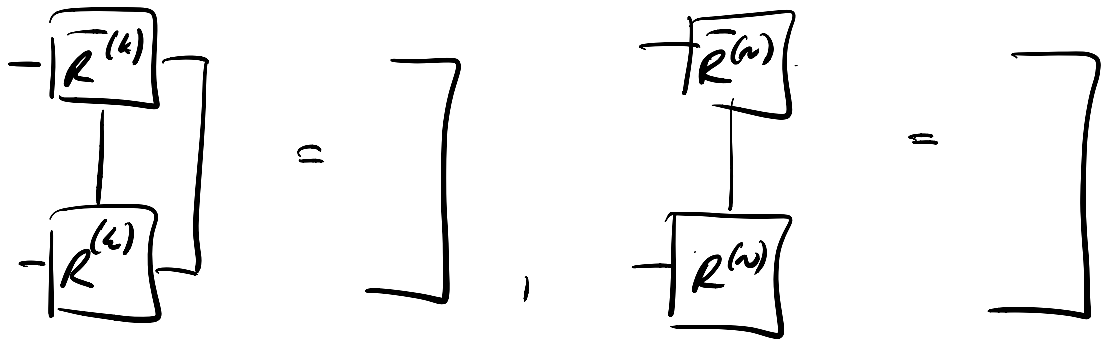


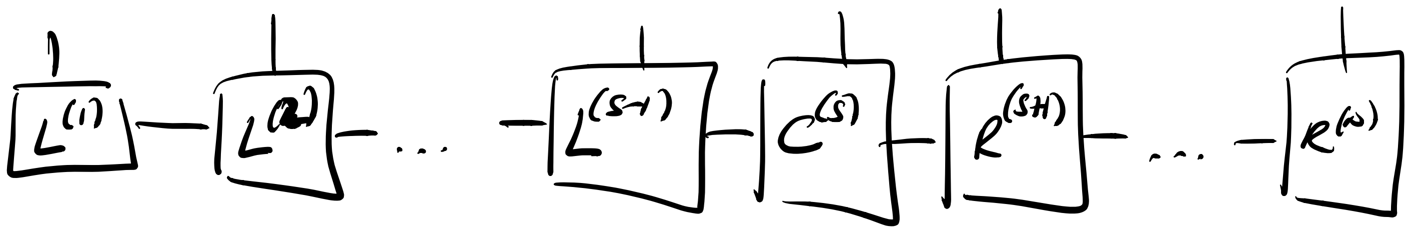
$(1 < k < N)$

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

Finally, we can define a

Mixed canonical form:

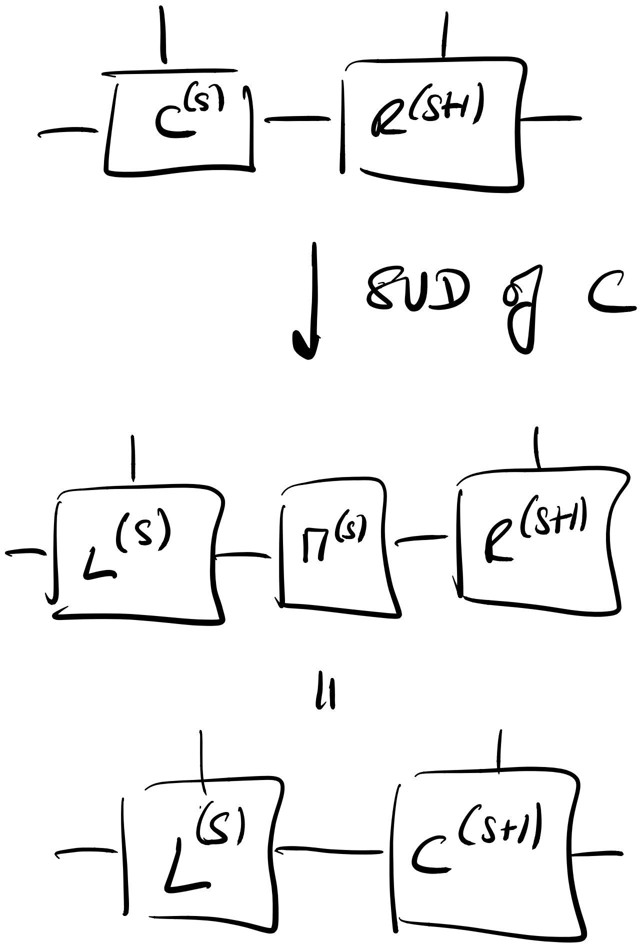
An MPS is in mixed CF,



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.



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