MPS I: Basic properties of matrix product states

MPS-I.1

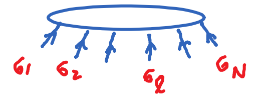
1. Overlaps, matrix elements $\langle\tilde\psi|\psi\rangle$

We first consider general quantum states, then matrix product states (MPSs):

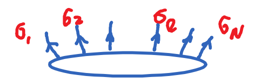
General ket: $|\psi\rangle = |\sigma_N\rangle \ldots |\sigma_2\rangle|\sigma_1\rangle C^{\sigma_1,\ldots,\sigma_N} := |\vec\sigma\rangle C^{\vec\sigma}$ (1)

$(\in \mathcal{H}^N)$

summation over repeated indices implied



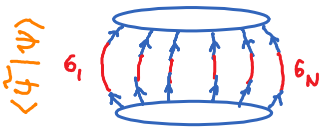
General bra: $\langle\psi| = \underbrace{\overline{C^{\sigma_1,\ldots,\sigma_N}}}_{:= C^\dagger_{\sigma_N}} \langle\sigma_1|\langle\sigma_2|\ldots\langle\sigma_N| := \underbrace{C^\dagger_{\vec\sigma_R}}_{:= \overline{C^{\vec\sigma}}}\langle\vec\sigma|$ (2)



Overlap: $\langle\tilde\psi|\psi\rangle = \overline{\tilde C^{\sigma_1',\ldots,\sigma_N'}}\langle\sigma_1'|\langle\sigma_2'|\ldots\underbrace{\langle\sigma_N'|\sigma_N\rangle}\ldots|\sigma_2\rangle|\sigma_1\rangle C^{\sigma_1,\ldots,\sigma_N}$ (3a)

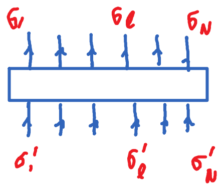
$$\delta^{\sigma_1'}_{\sigma_1}\delta^{\sigma_2'}_{\sigma_2}\ldots\delta^{\sigma_N'}_{\sigma_N} = \delta^{\vec\sigma'}_{\vec\sigma}$$

$$= \tilde C^\dagger_{\vec\sigma_R}\, C^{\vec\sigma}$$ (3b)



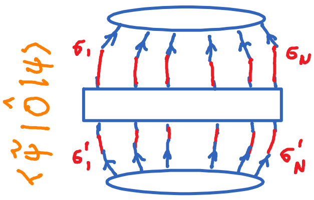
Recipe for overlaps: contract all physical legs of bra and ket.

General operator: $\hat O = |\vec\sigma'\rangle O^{\vec\sigma'}{}_{\vec\sigma}\langle\vec\sigma|$ (4)



Matrix elements: $\langle\tilde\psi|\hat O|\psi\rangle = \tilde C^\dagger_{\tilde{\vec\sigma}_R}\underbrace{\langle\tilde{\vec\sigma}|\vec\sigma'\rangle}_{\delta^{\tilde{\vec\sigma}}_{\vec\sigma'}} O^{\vec\sigma'}{}_{\vec\sigma}\underbrace{\langle\vec\sigma|\tilde{\tilde{\vec\sigma}}\rangle}_{\delta^{\vec\sigma}_{\tilde{\tilde{\vec\sigma}}}} C^{\tilde{\tilde{\vec\sigma}}}$ (5a)

$$= \tilde C^\dagger_{\vec\sigma'_R}\, O^{\vec\sigma'}{}_{\vec\sigma}\, C^{\vec\sigma}$$ (5b)



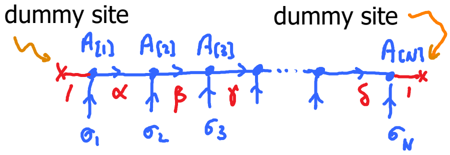
Recipe for matrix elements: contract all physical legs of bra and ket with operator.

Now consider matrix product states:

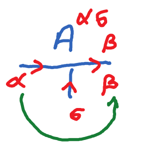
Ket: (dummy index)

$$|\psi\rangle = |\vec\sigma\rangle A_{[1]}^{1\sigma_1}{}_{\alpha}\, A_{[2]}^{\alpha\sigma_2}{}_{\beta}\, A_{[3]}^{\beta\sigma_3}{}_{\gamma}\ldots A_{[N]}^{\gamma\sigma_N}{}_{1}$$ (6)

dummy index



Recipe for ket formula: as chain grows, attach new matrices A^σ on the right (in <u>same</u> order as vertices in diagram), resulting in a matrix product of A^σ matrices .



Square brackets indicate that each site has a different A^σ matrix. We will often omit them and use the shorthand, $A^{\alpha\sigma_\ell}{}_\beta \equiv A_{[\ell]}^{\alpha\sigma_\ell}{}_\beta$, since the ℓ on σ_ℓ uniquely identifies the site.

Add dummy sites at left and right, so that first and last A's have two virtual indices, just like other A's .

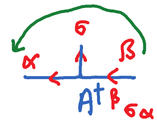
Bra:

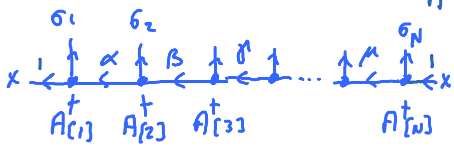
$$\langle\psi| = \overline{A^{1\sigma_1}_{[1]\alpha}}\;\overline{A^{\alpha\sigma_2}_{[2]\beta}}\;\overline{A^{\beta\sigma_3}_{[3]\gamma}}\cdots\overline{A^{\mu\sigma_N}_{[N]1}}\;\langle\vec\sigma|$$

$$= A^{\dagger 1}_{[N]\sigma_N\mu}\cdots A^{\dagger\gamma}_{[3]\sigma_3\beta}\,A^{\dagger\beta}_{[2]\sigma_2\alpha}\,A^{\dagger\alpha}_{[1]\sigma_1 1}$$

index-reading order

$$\overline{A^{\alpha\sigma}{}_{\beta}} =: A^{\dagger\beta}{}_{\sigma\alpha} \qquad (7a)$$



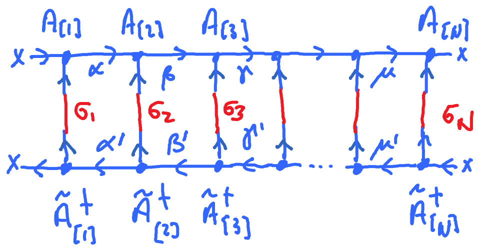


(7b)

We expressed all matrices via their Hermitian conjugates by transposing indices and inverting arrows. To recover a matrix product structure, we ordered the Hermitian conjugate matrices to appear in the <u>opposite</u> order as the vertices in the diagram.

Recipe for bra formula: as chain grows, attach new matrices $A^\dagger_\sigma$ on the left, (in opposite order as vertices in diagram), resulting in a matrix product of $A^\dagger_\sigma$ matrices.

Overlap: $\langle\tilde\psi|\psi\rangle \overset{(3b)}{=}$



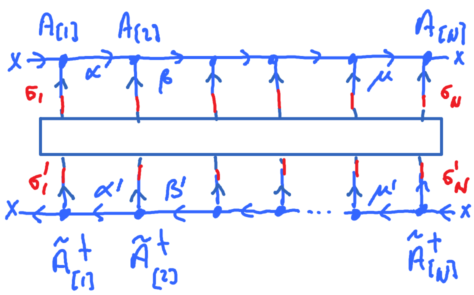
Recipe: contract all physical indices! (8a)

$$= \tilde A^{\dagger 1}_{[N]\sigma'_N\mu'}\cdots\tilde A^{\dagger\beta'}_{[2]\sigma'_2\alpha'}\,\tilde A^{\dagger\alpha'}_{[1]\sigma'_1 1}\,A^{1\sigma_1}_{[1]\alpha}\,A^{\alpha\sigma_2}_{[2]\beta}\cdots A^{\mu\sigma_N}_{[N]1} \qquad (8b)$$

Recipe: contract all physical indices with each other, and all virtual indices of neighboring tensors.

Matrix elements:

$$\langle\tilde\psi|\hat O|\psi\rangle \overset{(5b)}{=}$$



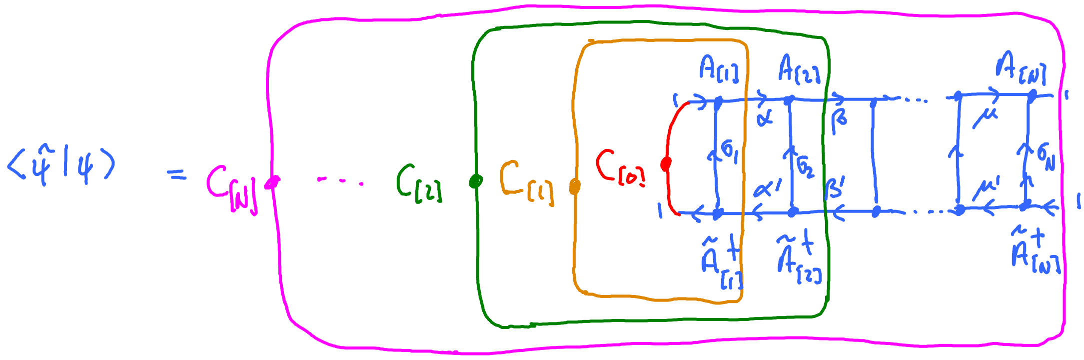
(9)

$$= \tilde A^{\dagger 1}_{[N]\sigma'_N\mu'}\cdots\tilde A^{\dagger\beta'}_{[2]\sigma'_2\alpha'}\,\tilde A^{\dagger\alpha'}_{[1]\sigma'_1 1}\,O^{\sigma'_1\sigma'_2\dots\sigma'_N}{}_{\sigma_1\sigma_2\dots\sigma_N}\,A^{1\sigma_1}_{[1]\alpha}\,A^{\alpha\sigma_2}_{[2]\beta}\cdots A^{\mu\sigma_N}_{[N]1} \qquad (10)$$

Exercise: derive this result algebraically from (7a), (8a)!

If we would perform the matrix multiplication first, for fixed $\vec\sigma$, and then sum over $\vec\sigma$, we would get d^N terms, each of which is a product of $2N$ matrices. Exponentially costly! ☹

But calculation becomes tractable if we rearrange summations:



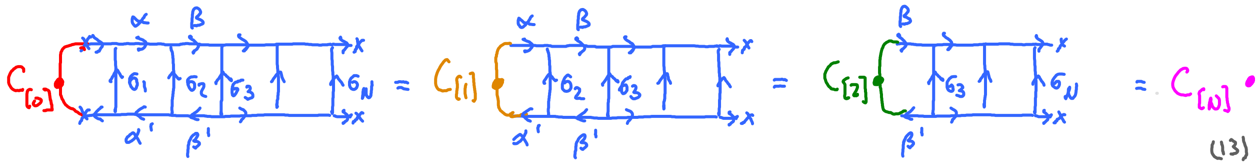
(11)

$$= \tilde{A}^{\dagger 1}{}_{\sigma_N \mu'} \cdots \tilde{A}^{\dagger \beta'}{}_{\sigma_2 \alpha'} \underbrace{\underbrace{A^{\dagger \alpha'}{}_{\sigma_1 1} \cdot \overbrace{1}^{\equiv C'_{[0]1}} \cdot A^{1\sigma_1}_{[1]\ \alpha}}_{:= C^{\alpha'}_{[1]\alpha}} A^{\alpha\sigma_2}_{[2]\ \beta}}_{:= C^{\beta'}_{[2]\beta}} \cdots A^{\mu\sigma_N}_{[N]\ 1} \tag{12}$$

$$\vdots$$

$$:= C'_{[N]1}$$

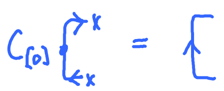
Diagrammatic depiction: 'closing zipper' from left to right.



(13)

The set of two-leg tensors $C_{[\ell]}$ can be computed iteratively:

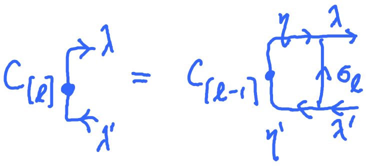
Initialization:



(identity)

$$C'_{[0]1} = 1 \tag{14}$$

Iteration step:
sum over σ_ℓ
yields $C_{[\ell]}$

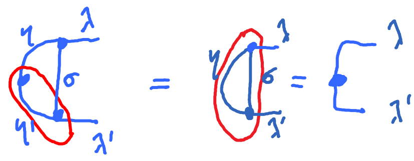


$$C_{[\ell]}{}^{\lambda'}{}_{\lambda} = \tilde{A}^{\dagger \lambda'}{}_{\sigma_\ell \eta'} C^{\eta'}_{[\ell-1]\eta} A^{\eta \sigma_\ell}{}_{\lambda} \tag{15}$$

Final answer: $$\langle \tilde{\psi} | \psi \rangle = C'_{[N]1} \tag{16}$$

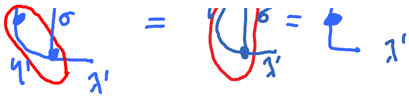
Cost estimate (if all A's are $D \times D$):

One iteration: $$\underbrace{D^2 d}_{\text{fixed } \lambda' \eta \sigma} \cdot \underbrace{D}_{\text{sum } \eta'} + \underbrace{D^2}_{\text{fixed } \lambda' \lambda} \underbrace{dD}_{\text{sum } \eta \sigma}$$



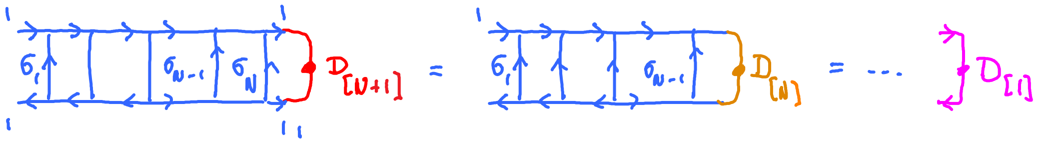
(17)

fixed $\lambda'\eta\sigma$ sum η' fixed $\lambda'\lambda$ sum $\eta\sigma$

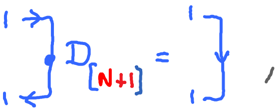

(17)

Total cost: $\sim D^3 d \cdot N$ (18)

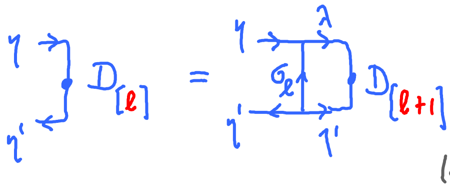
Remark: a similar iteration scheme can be used to 'close zipper from right to left':


(19)

Initialization:


(identity)

Iteration step:
sum over σ_ℓ
yields $D_{[\ell]}$


(20)

Normalization $\langle\psi|\psi\rangle = ?$ Use above scheme, with $\tilde{A} = A$

2. Left- and right-normalized states

MPS-I.2

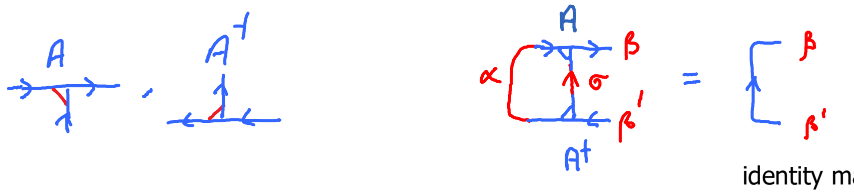
Computation of expectation and matrix elements is simpler if the MPS is built from tensors relating orthonormal spaces. Such tensors are called 'left-normalized' or 'right-normalized.

Left-normalization

A 3-leg tensor $A^{\alpha\sigma}{}_{\beta}$ is called 'left-normalized' if it satisfies

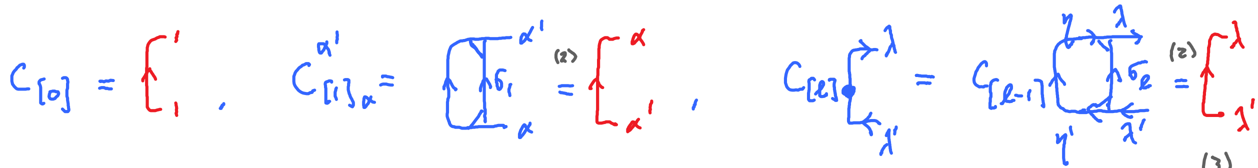
$\boxed{A^\dagger A = \mathbb{1}}$. Explicitly: $(A^\dagger A)^{\beta'}{}_{\beta} = A^{\dagger\beta'}{}_{\sigma\alpha} A^{\alpha\sigma}{}_{\beta} = \mathbb{1}^{\beta'}{}_{\beta}$ (1)

Graphical notation for left-normalization: draw 'left-pointing diagonals' at vertices



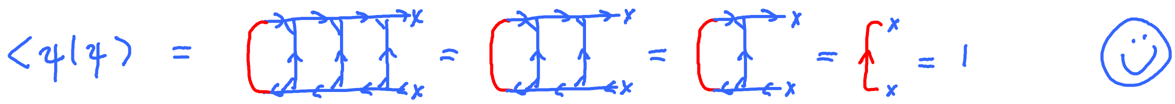
identity matrix (2)

When all A's are left-normalized, closing the zipper left-to-right is easy, since all $C_{[\ell]}$ reduce to identity matrices:



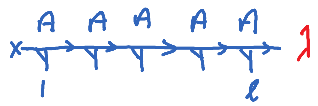
(3)

Hence:

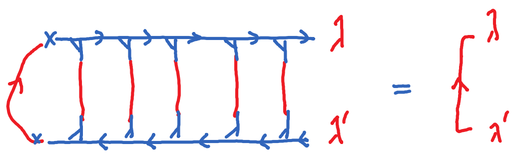


(4)

When all matrices of a MPS are left-normalized, the matrices for site 1 to any site $\ell = 1, \dots, N$ define an orthonormal state space:



$$|\lambda\rangle = |\vec{\sigma}_\ell\rangle \left[A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_\ell}\right]^{1}{}_{\lambda} \quad (5)$$



close the zipper

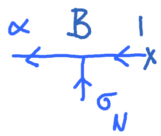
$$\langle\lambda'|\lambda\rangle = \mathbb{1}^{\lambda'}{}_{\lambda} \quad (6)$$

Right-normalization

So far we have viewed an MPS as being built up from left to right, hence used right-pointing arrows on ket diagram. Sometimes it is useful to build it up from right to left, running left-pointing arrows.

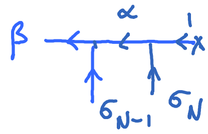
Building blocks:

$$|\alpha\rangle = |\sigma_N\rangle B_\alpha{}^{\sigma_N 1} \qquad (7)$$

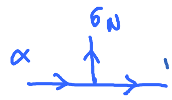


left-to-right index order as in diagram

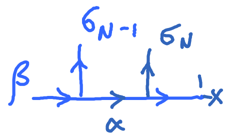
$$|\beta\rangle = |\sigma_N\rangle|\sigma_{N-1}\rangle B_\beta{}^{\sigma_{N-1}\alpha} B_\alpha{}^{\sigma_N 1} \qquad (8)$$



$$\langle\alpha| = \underbrace{B^\dagger{}_{1\sigma_N}{}^{\alpha}}_{\equiv \overline{B_\alpha{}^{\sigma_N 1}}} \langle\sigma_N| \qquad (9)$$

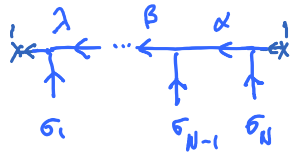


$$\langle\beta| = B^\dagger{}_{1\sigma_N}{}^{\alpha} B^\dagger{}_{\alpha\sigma_{N-1}}{}^{\beta} \langle\sigma_{N-1}|\langle\sigma_N| \qquad (10)$$

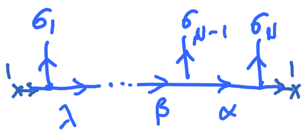


Iterating this, we obtain kets and bras of the form

$$|\psi\rangle = |\sigma_N\rangle|\sigma_{N-1}\rangle\dots|\sigma_1\rangle B_1{}^{\sigma_1\lambda}\dots B_\beta{}^{\sigma_{N-1}\alpha} B_\alpha{}^{\sigma_N 1} \qquad (11)$$



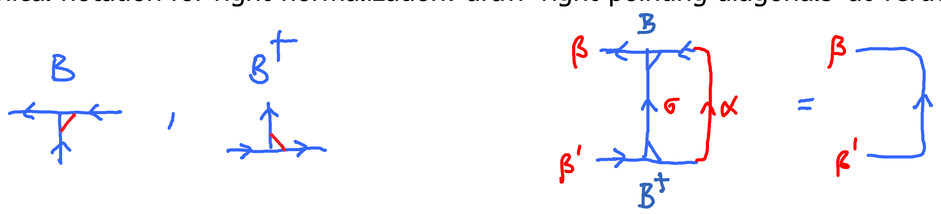
$$\langle\psi| = B^\dagger{}_{1\sigma_N}{}^{\alpha} B^\dagger{}_{\alpha\sigma_{N-1}}{}^{\beta} \dots B^\dagger{}_{\lambda\sigma_1}{}^{1} \langle\sigma_1|\dots\langle\sigma_{N-1}|\langle\sigma_N| \qquad (12)$$



A three-leg terror $B_\beta{}^{\sigma\alpha}$ is called right-normalized if it satisfies

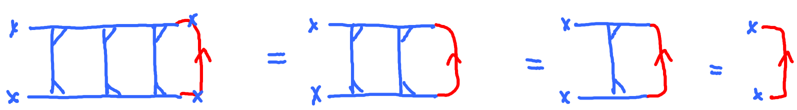
$$BB^\dagger = \mathbb{1}. \qquad \text{Explicitly:} \quad (BB^\dagger)_\beta{}^{\beta'} = B_\beta{}^{\sigma\alpha} B^\dagger{}_{\alpha\sigma}{}^{\beta'} = \mathbb{1}_\beta{}^{\beta'} \qquad (13)$$

Graphical notation for right-normalization: draw 'right-pointing diagonals' at vertices



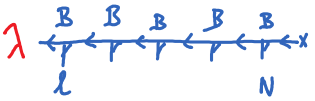
(14)

When all B's are right-normalized, closing the zipper right-to-left is easy:

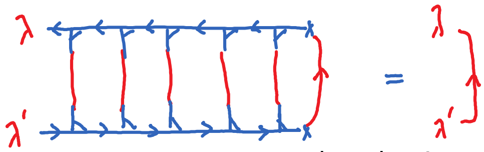
$\langle\psi|\psi\rangle =$  $= 1$ (15)

When all matrices of a MPS are right-normalized, the matrices for site N to any site $\ell = 1, \dots N$

When all matrices of a MPS are right-normalized, the matrices for site N to any site $\ell = 1, \dots, N$ define an orthonormal state space:



$$|\lambda\rangle = |\vec{\sigma}_\ell\rangle \left[B^{\sigma_\ell} B^{\sigma_{\ell+1}} \cdots B^{\sigma_N} \right]_{\lambda}^{\;1} \qquad (16)$$



close the zipper

$$\langle \lambda' | \lambda \rangle = \mathbb{1}^{\lambda'}{}_{\lambda} \qquad (17)$$

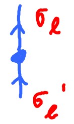
Conclusion: MPS built purely from left-normalized A's or purely from right-normalized B's are automatically normalized to 1. Shorter MPSs built on subchains automatically define orthonormal state spaces.

3. Matrix elements of local operators

Local operators act non-trivially only on a few sites (e.g. only one, or two nearest neighbors).

One-site operator

$$\hat{O}_{[\ell]} = |\sigma_\ell'\rangle \, O^{\sigma_\ell'}{}_{\sigma_\ell} \langle \sigma_\ell|$$

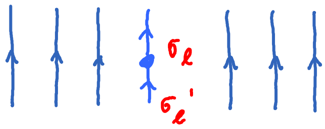


(1)

E.g. for spin $1/2$: $(S_z)^{\sigma'}{}_{\sigma} = \frac{1}{2}\begin{pmatrix}1 & \\ & -1\end{pmatrix}$, $(S_+)^{\sigma'}{}_{\sigma} = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}$, $(S_-)^{\sigma'}{}_{\sigma} = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}$ (2)

In the Hilbert space of full system, one-site operator acts as unit operator on all sites except ℓ :

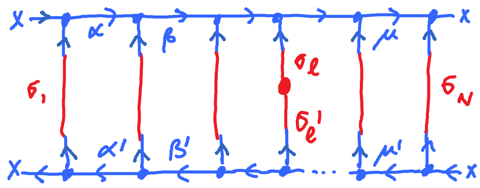
$$\hat{O}_{[\ell]} = |\vec{\sigma}'\rangle \underbrace{\delta^{\sigma_1'}{}_{\sigma_1} \cdots O^{\sigma_\ell'}{}_{\sigma_\ell} \cdots \delta^{\sigma_N'}{}_{\sigma_N}}_{O^{\vec{\sigma}'}{}_{\vec{\sigma}}} \langle \vec{\sigma}|$$



(3)

Matrix element between two MPS:

$$\langle \tilde{\psi} | \hat{O}_{[\ell]} | \psi \rangle =$$

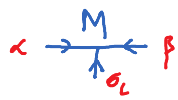


(4)

The computation of such matrix element is simplest if $|\psi\rangle$ and $|\tilde{\psi}\rangle$ are in 'site-canonical form',
i.e. constructed from left- or right-normalized tensors for sites earlier or later than ℓ , respectively

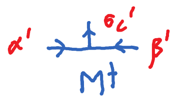
site ℓ is special:

$$|\psi\rangle = |\sigma_N\rangle \left(A^{\sigma_1} \cdots A^{\sigma_{\ell-1}} M^{\sigma_\ell} B^{\sigma_{\ell+1}} \cdots B^{\sigma_N}\right)$$



(5)

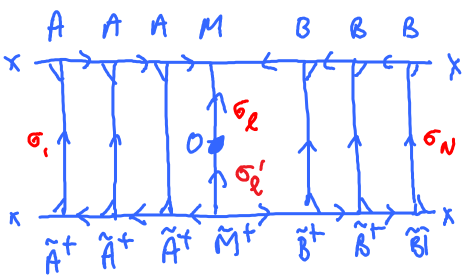
$$|\tilde{\psi}\rangle = |\sigma_N'\rangle \left(\tilde{A}^{\sigma_1'} \cdots \tilde{A}^{\sigma_{\ell-1}'} \tilde{M}^{\sigma_\ell'} \tilde{B}^{\sigma_{\ell+1}'} \cdots \tilde{B}^{\sigma_N'}\right)$$



(6)

Matrix element:

$$\langle \tilde{\psi} | \hat{O} | \psi \rangle =$$



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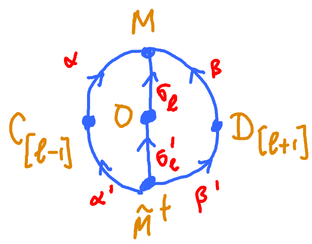


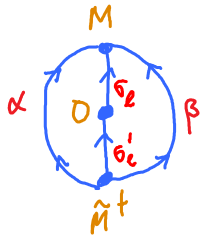
(7)

Close zipper from left using $C_{[\ell-1]}$ from left-normalized A's [see MPS-I.1-(15)],
and from right using $D_{[\ell+1]}$ from right-normalized B's [analogous to MPS-I.1-(20)].

$$= \tilde{M}^{\dagger}_{\beta'\sigma_\ell'\alpha'}\, C^{\alpha'}_{[\ell-1]\,\alpha}\, M^{\alpha\sigma_\ell\beta}\, D_{[\ell+1]\,\beta}{}^{\beta'}\, O^{\sigma_\ell'}{}_{\sigma_\ell} \qquad (8)$$

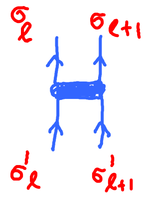
Now consider the expectation value, $\langle\psi|\hat{O}|\psi\rangle$ (i.e. drop all tilde's). The left-normalization of A's guarantees that $C_{[\ell-1]} = \mathbb{1}$, and right-normalization of B's that $D_{[\ell+1]} = \mathbb{1}$.

Hence $$\langle\psi|\hat{O}|\psi\rangle = M^{\dagger}_{\beta\sigma_\ell'\alpha}\, M^{\alpha\sigma_\ell\beta}\, O^{\sigma_\ell'}{}_{\sigma_\ell} \qquad (9)$$

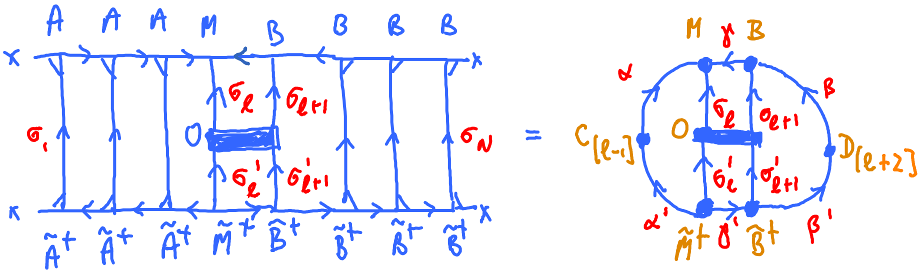


<u>Two-site operator</u> (e.g. for spin chain: $\vec{S}_\ell \cdot \vec{S}_{\ell+1}$)

$$\hat{O}_{[\ell,\ell+1]} = |\sigma_{\ell+1}'\rangle|\sigma_\ell'\rangle\, O^{\sigma_\ell'\sigma_{\ell+1}'}{}_{\sigma_\ell\sigma_{\ell+1}}\, \langle\sigma_\ell|\langle\sigma_{\ell+1}| \qquad (10)$$



Matrix elements:

$\langle\tilde{\psi}|\hat{O}_{[\ell,\ell+1]}|\psi\rangle =$  (11)

$$= \tilde{B}^{\dagger}_{\beta'\sigma_{\ell+1}'}{}^{\gamma'}\, \tilde{M}^{\dagger}_{\gamma'\sigma_\ell'\alpha'}\, C^{\alpha'}_{[\ell-1]\,\alpha}\, M^{\alpha\sigma_\ell\gamma}\, B_{\gamma}{}^{\sigma_{\ell+1}\beta}\, D_{[\ell+2]\,\beta}{}^{\beta'}\, O^{\sigma_\ell'\sigma_{\ell+1}'}{}_{\sigma_\ell\sigma_{\ell+1}} \qquad (12)$$

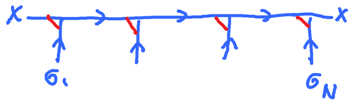
4. Various canonical MPS forms

Any matrix product can be expressed through different matrices without changing the product:

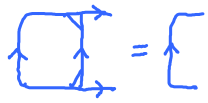
$$M M' = (\underbrace{M\, U}_{\tilde M})(\underbrace{U^{-1} M'}_{\tilde M'}) = \tilde M \tilde M' \qquad \text{'gauge freedom'}$$

Gauge freedom can be exploited to 'reshape' MPSs into particularly convenient, 'canonical' forms:

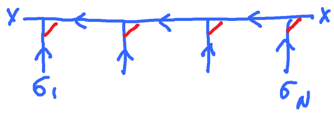
Left-canonical (lc-) MPS:



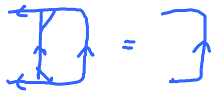
$$|\psi\rangle = |\vec\sigma\rangle_N (A^{\sigma_1} \dots A^{\sigma_N}) \qquad A^\dagger A = \mathbb{1} \tag{1}$$



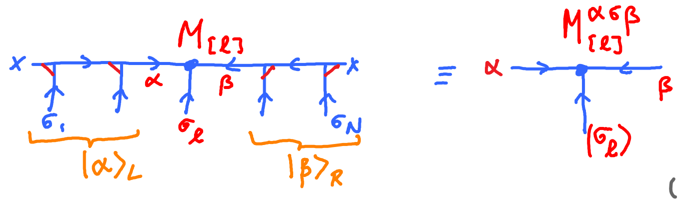
Right-canonical (rc-) MPS:



$$|\psi\rangle = |\vec\sigma\rangle_N (B^{\sigma_1} \dots B^{\sigma_N}) \qquad B B^\dagger = \mathbb{1} \tag{2}$$



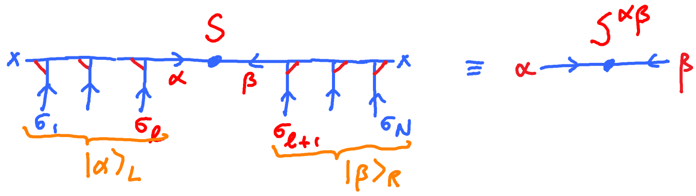
Site-canonical (sc-) MPS:



(3)

$$|\psi\rangle = |\vec\sigma\rangle_N (A^{\sigma_1} \dots A^{\sigma_{\ell-1}} M^{\sigma_\ell}_{[\ell]} B^{\sigma_{\ell+1}} \dots B^{\sigma_N}) = |\beta\rangle_R |\sigma_\ell\rangle |\alpha\rangle_L M^{\alpha\sigma_\ell\beta}$$

Bond-canonical (bc-) (or mixed) MPS:



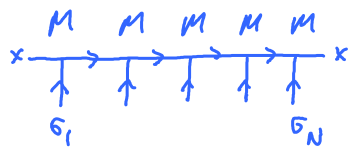
$$|\psi\rangle = |\vec\sigma\rangle_N (A^{\sigma_1} \dots A^{\sigma_\ell})_\alpha S^{\alpha\beta}_{[\ell]\beta} (B^{\sigma_{\ell+1}} \dots B^{\sigma_N}) = \sum_{\alpha\beta} |\beta\rangle_R |\alpha\rangle_L S^{\alpha\beta}_{[\ell]} \tag{4}$$

can be chosen diagonal

How can we bring an arbitrary MPS into one of these forms?

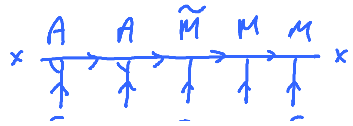
Transforming to left-normalized form

Given: $|\psi\rangle = |\vec\sigma\rangle_N (M^{\sigma_1} \dots M^{\sigma_N})$



(5)

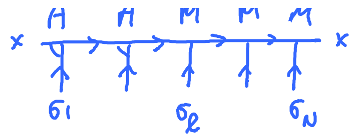
[or with index: $|s_N\rangle =$ ]



(6)

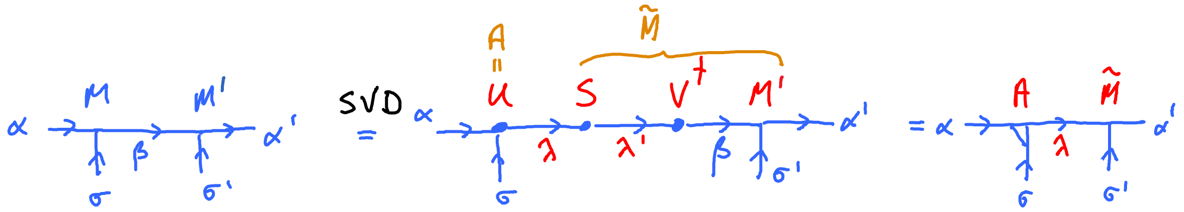
Goal : left-normalize M^{σ_1} to $M^{\sigma_{\ell-1}}$

Goal : left-normalize M^{σ_1} to $M^{\sigma_{\ell-1}}$



Strategy: take a pair of adjacent tensors, MM', and use SVD,

$$MM' = USV^\dagger M' \equiv A\tilde{M}, \qquad \text{with } A = U, \quad \tilde{M} = SV^\dagger M' \tag{7}$$



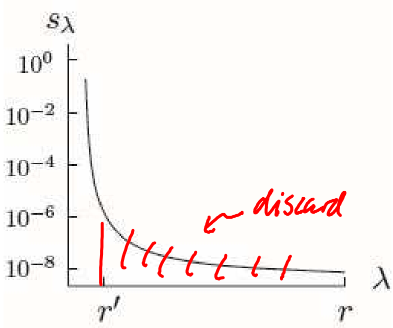
$$M^{\alpha\sigma}{}_{\beta}\, M'^{\beta\sigma'}{}_{\alpha'} = \left(U^{\alpha\sigma}{}_{\lambda}\right)\left(S^{\lambda}{}_{\lambda'}\, V^{\dagger\lambda'}{}_{\beta}\, M'^{\beta\sigma'}{}_{\alpha'}\right) = A^{\alpha\sigma}{}_{\lambda}\, \tilde{M}^{\lambda\sigma'}{}_{\alpha'} \tag{9}$$

The properly $U^\dagger U = \mathbb{1}$ ensures left-normalization: $A^\dagger A = \mathbb{1}$ (10)

Truncation, if desired, can be performed by discarding some of

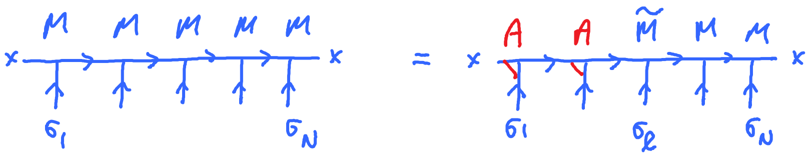
The smallest singular values,

$$\sum_{\lambda=1}^{r} \longrightarrow \sum_{\lambda=1}^{r'}$$ (but (10) remains valid!)



Note: instead of SVD, we could also me QR (cheaper!)

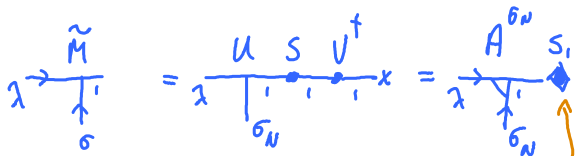
By iterating, starting from $M^{\sigma_1} M^{\sigma_2}$, we left-normalize M^{σ_1} to $M^{\sigma_{\ell-1}}$,



To left-normalize the <u>entire</u> MPS, choose $\ell = N$.

As last step, left-normalize last site using SVD on final $\tilde{M}$:

$$\tilde{M}^{\lambda\sigma_N}{}_{1} = \underbrace{U^{\lambda\sigma_N}{}_{1}}_{A^{\lambda\sigma_N}{}_{1}}\ \underbrace{S^{1}{}_{1}}_{s_1}\ \underbrace{V^{\dagger 1}{}_{1}}_{1}$$



diamond indicates single number

lc-form: $|\psi\rangle = |\vec{\sigma}\rangle_N \left(A^{\sigma_1} \dots A^{\sigma_N}\right) s_1$

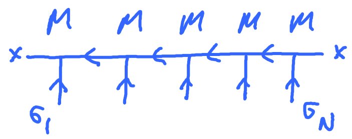
diamond indicates
single number

lc-form: $|\psi\rangle = |\vec{\sigma}\rangle_N \left(A^{\sigma_1} \dots A^{\sigma_N}\right) s_1$

The final singular value, s_1 determines normalization: $\langle\psi|\psi\rangle = |s_1|^2$. (12)

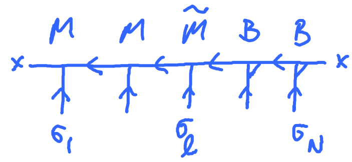
<u>Transforming to right-normalized form</u>

Given: $|\psi\rangle = |\vec{\sigma}\rangle_N \left(M^{\sigma_1} \dots M^{\sigma_N}\right)$



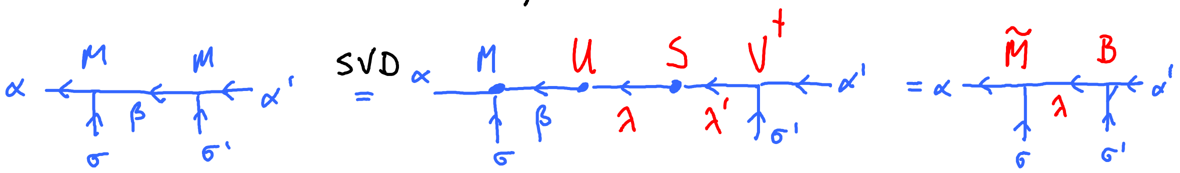
[or with index: $|S_1\rangle = S_1$ ]

Goal : right-normalize M^{σ_N} to $M^{\sigma_{\ell+1}}$



Strategy: take a pair of adjacent tensors, $M M'$, and use SVD:

$$M M' = M U S V^\dagger \equiv \tilde{M} B \,, \quad \text{with} \quad \tilde{M} = M' U S \,, \quad B = V^\dagger \,. \qquad (13)$$



(14)

$$M_\alpha{}^{\sigma\beta} \, M'_\beta{}^{\sigma'\alpha'} = \left(M_\alpha{}^{\sigma\beta} \, U_\beta{}^\lambda \, S_\lambda{}^{\lambda'}\right)\left(V^\dagger{}_{\lambda'}{}^{\sigma'\alpha'}\right) = \tilde{M}_\alpha{}^{\sigma\lambda'} \, B_{\lambda'}{}^{\sigma'\alpha'} \qquad (15)$$

Here, $V^\dagger V = \mathbb{1}$ ensures right-normalization: $B B^\dagger = \mathbb{1}$. (16)

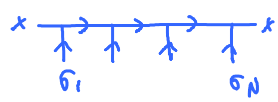
Starting form $M^{\sigma_{N-1}} M^{\sigma_N}$, move leftward up to $M^{\sigma_\ell} M^{\sigma_{\ell+1}}$.

To right-normalize entire chain, choose / and at last site, $\ell = 1$

$$\tilde{M}_1{}^{\sigma_1\lambda} = \underbrace{U_1'}_{=1} \, \underbrace{S_1'}_{S_1} \, \underbrace{V^\dagger{}_1{}^{\sigma_1\lambda}}_{B_1{}^{\sigma_1\lambda}} \,. \qquad S_1 \text{ determines normalization.} \qquad (17)$$

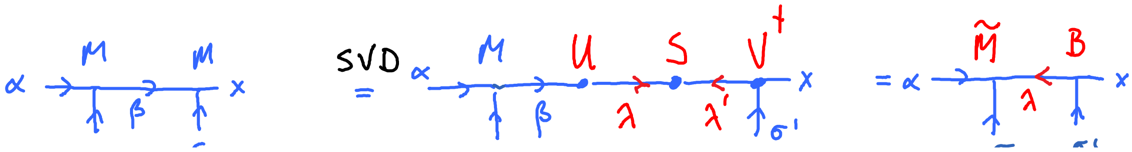
<u>Exercise</u>

(a) Right-normalize a state with right-pointing arrows!

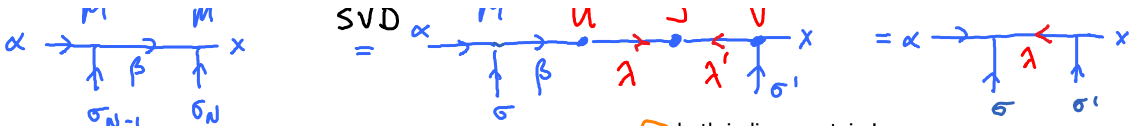


Hint: start at $M^{\sigma_{N-1}} M^{\sigma_N}$

and note the up $\leftrightarrow$ down changes in index placement.



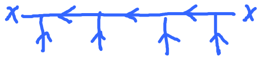
(18)

 (18)

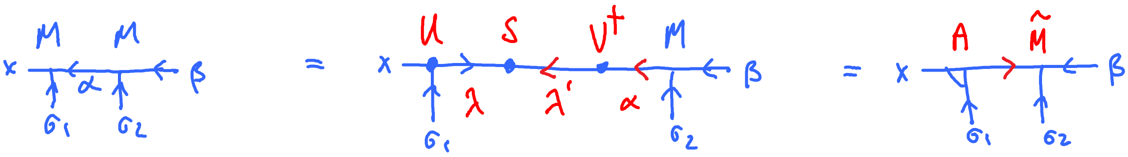
both indices upstairs!

$$M^{\alpha\sigma}{}_{\beta}\, M^{\beta\sigma'}{}_{1} = \left(M^{\alpha\sigma}{}_{\beta}\, U^{\beta}{}_{\lambda}\, S^{\lambda\lambda'}\right)\left(V^{\dagger}{}_{\lambda'}{}^{\sigma'}\right) = \tilde{M}^{\alpha\sigma\lambda}\, B_{\lambda}{}^{\sigma'} \qquad (19)$$

(b) Left-normalize a state with left-pointing arrows!



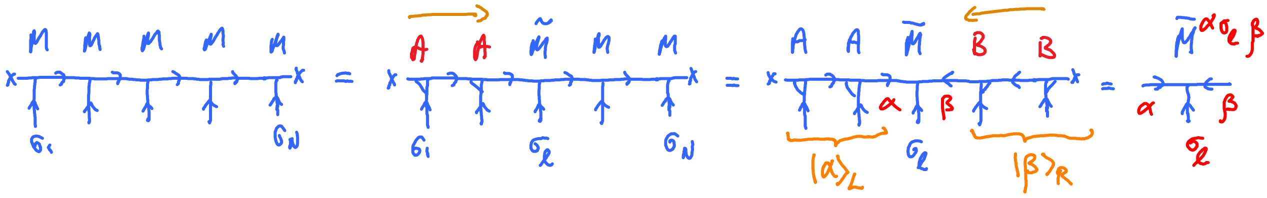
Hint: start at $M^{\sigma_1} M^{\sigma_2}$:

 (20)

both indices upstairs!

$$M_{1}{}^{\sigma_1\alpha}\, M_{\alpha}{}^{\sigma_2\beta} = \left(U^{1\sigma_1}{}_{\lambda}\right)\left(S^{\lambda\lambda'}\, V^{\dagger}{}_{\lambda'}{}^{\alpha}\, M_{\alpha}{}^{\sigma_2\beta}\right) = A_{1}{}^{\sigma_1\lambda}\, \tilde{M}_{\lambda}{}^{\sigma_2\beta} \qquad (21)$$

Transforming to site-canonical form

 (22)

Left-normalize sites 1 to $\ell-1$, starting from site .

Then right-normalize sites N to $\ell+1$, starting from site N .

Result:

$$|\psi\rangle = \underbrace{|\sigma_N\rangle \ldots |\sigma_{\ell+1}\rangle \left(B^{\sigma_{\ell+1}} \ldots B^{\sigma_N}\right)'_{\beta}}_{|\beta\rangle_R}\, |\sigma_\ell\rangle \underbrace{|\sigma_{\ell-1}\rangle \ldots |\sigma_1\rangle \left(A^{\sigma_1} \ldots A^{\sigma_{\ell-1}}\right)'_{\alpha}}_{|\alpha\rangle_L}\, \tilde{M}^{\alpha\sigma_\ell\beta} \qquad (23)$$

$$= |\beta\rangle_R\, |\sigma_\ell\rangle\, |\alpha\rangle_L\, \tilde{M}^{\alpha\sigma_\ell\beta} \qquad (24)$$

The states $|\alpha, \sigma_\ell, \beta\rangle \equiv |\beta\rangle_R |\sigma_\ell\rangle |\alpha\rangle_L$ form an orthonormal set:

$$\langle \alpha', \sigma_\ell', \beta' | \alpha, \sigma_\ell, \beta\rangle = \delta^{\alpha'}{}_{\alpha}\, \delta^{\sigma_\ell'}{}_{\sigma_\ell}\, \delta^{\beta'}{}_{\beta} \qquad (25)$$

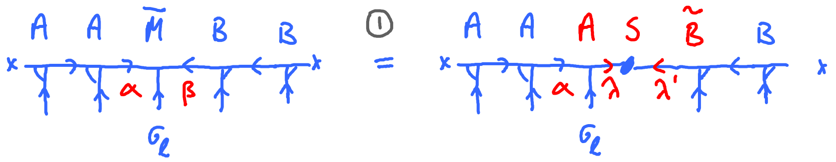
(Exercise: verify this, using $A^\dagger A = \mathbb{1}$ and $B B^\dagger = \mathbb{1}$.)

This is 'local site basis' for site ℓ . Its dimension $D_\alpha \cdot d \cdot D_\beta$ is usually $\lll d^N$ of full Hilbert space.

Transforming to bond-canonical form

<u>Transforming to bond-canonical form</u>

Start from (e.g.) sc-form, use SVD for $\bar{M} = USV^\dagger$, combine ① $V^\dagger$ with neighboring B, or ② U with neighboring A.



$$= \underbrace{|\lambda'\rangle_R}_{\text{involves sites } \ell+1 \text{ to } N} \cdot \underbrace{|\lambda\rangle_L}_{\text{involves sites } 1 \text{ to } \ell} S^{\lambda\lambda'} \qquad (26)$$

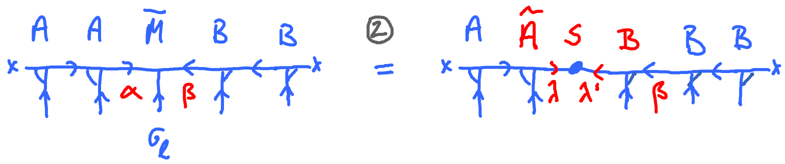
$$\bar{M} = USV^\dagger \qquad A = U, \quad \hat{B} = V^\dagger B$$

(Exercise: add indices!) (27)

The states $|\lambda, \lambda'\rangle \equiv |\lambda\rangle_R |\lambda'\rangle_L$ form an orthonormal set.

$$\langle \bar{\lambda}, \bar{\lambda}' | \lambda, \lambda' \rangle = \delta^{\bar{\lambda}}{}_{\lambda} \, \delta^{\bar{\lambda}'}{}_{\lambda} \qquad (28)$$

This is called the 'local bond basis for bond ℓ' (from site ℓ to $\ell+1$). It has dimension $r \cdot r$ (r = dimension of singular matrix S).



$$= \underbrace{|\lambda'\rangle_R}_{\text{involves sites } \ell \text{ to } N} \cdot \underbrace{|\lambda\rangle_L}_{\text{involves sites } 1 \text{ to } \ell-1} S^{\lambda\lambda'} \qquad (29)$$

$$\bar{M} = USV^\dagger \qquad \tilde{A} = AU, \quad B = V^\dagger$$

(Exercise: add indices!) (30)

$|\lambda, \lambda'\rangle \equiv |\lambda'\rangle_R |\lambda\rangle_L$ form 'local bond basis' for bond $\ell-1$ (from site $\ell-1$ to ℓ).