MPS I: Matrix product states

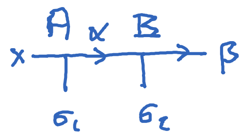
MPS-I.1

$|\alpha\rangle = |\sigma_1\rangle A^{|\sigma_1}{}_{\alpha}$ $\qquad \left(\begin{matrix}\cdot\\ \vdots \end{matrix}\right) = A_\alpha = A'_\alpha$

1. Overlaps and normalization

$\langle \tilde{\psi} | \psi \rangle$

Consider overlap of 2-site MPS:



dummy index

$$|\beta\rangle = |\sigma_2\rangle|\sigma_1\rangle A^{1\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta} \tag{1}$$

$$\langle\beta'|\beta\rangle = \overline{A^{1\sigma_1'}{}_{\alpha'}}\, \overline{B^{\alpha'\sigma_2'}{}_{\beta'}} \langle\sigma_1'|\langle\sigma_2'|\sigma_2\rangle|\sigma_1\rangle A^{1\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta} \tag{2}$$

$\delta^{\sigma_2'}{}_{\sigma_2}$ $\quad \delta^{\sigma_1'}{}_{\sigma_1}$

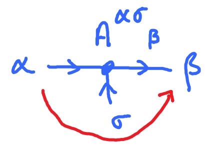
introduce $A^\dagger$'s: $\qquad A^{\dagger\alpha'}{}_{\sigma_1' 1} \quad B^{\dagger\beta'}{}_{\sigma_2'\alpha'}$ (3)

reorder $A^\dagger$'s: $\qquad B^{\dagger\beta'}{}_{\sigma_2'\alpha'} A^{\dagger\alpha'}{}_{\sigma_1' 1} A^{1\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta} = \left(B^\dagger_{\sigma_2} A^\dagger_{\sigma_1}\right)^{\beta'}{}_{1} \left(A^{\sigma_1} B^{\sigma_2}\right)_{1\beta}$ (4)

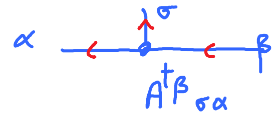
$A^\dagger B^\dagger \neq B^\dagger A^\dagger$

Ket: $\qquad |\beta\rangle = |\sigma\rangle|\alpha\rangle A^{\alpha\sigma}{}_{\beta}$

Use diagrammatic rules to keep track of contraction patterns: (5)



Bra: $\qquad \langle\beta| = \langle\alpha|\langle\sigma|\, \overline{A^{\alpha\sigma}{}_{\beta}} \equiv A^{\dagger\beta}{}_{\sigma\alpha} \langle\alpha|\langle\sigma|$ (6)



We accommodated complex conjugation via Hermitian conjugation and index transposition:

$$A^{\dagger\beta}{}_{\sigma\alpha} = \overline{A^{\alpha\sigma}{}_{\beta}}$$

This moves upstairs indices downstairs and vice versa, i.e. invents all arrows in diagram.
Note that in diagram vertex, α sits left, β right, whereas on $A^\dagger$, β sits left, α right.
This convention may seem initially awkward, but it greatly simplifies the structure of diagrams representing overlaps.

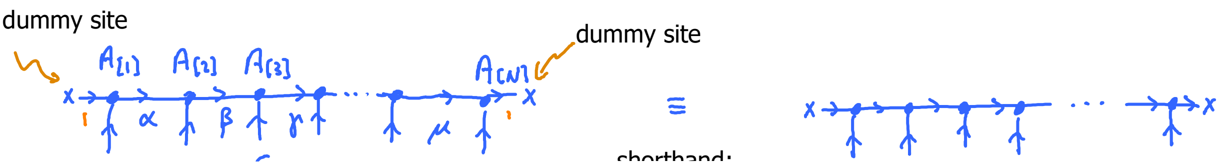
Generalization to many-site MPS:

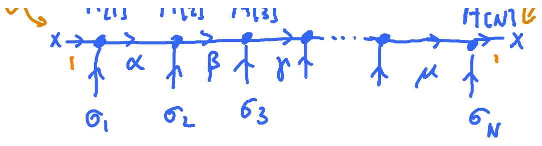
$|\sigma_N\rangle \ldots |\sigma_2\rangle|\sigma_1\rangle$ $\qquad$ dummy index

$$|\psi\rangle = |\vec{\sigma}\rangle_N A^{1\sigma_1}_{[1]\,\alpha} A^{\alpha\sigma_2}_{[2]\,\beta} A^{\beta\sigma_3}_{[3]\,\gamma} \ldots A^{\mu\sigma_N}_{[N]\,1} \tag{7}$$

dummy index

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





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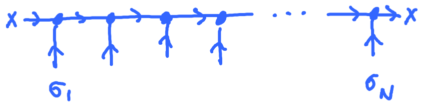
shorthand:
omit indices



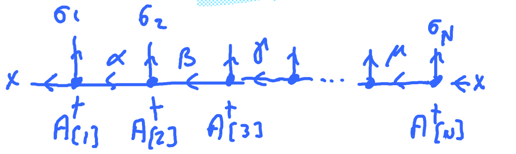
(8)

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

$\langle\sigma_1|\langle\sigma_2|\ldots\langle\sigma_N|$

Bra:

$$\langle\psi| = \underset{N}{\langle\vec\sigma|}\, \overline{A_{[1]\alpha}^{1\sigma_1}}\, \overline{A_{[2]\beta}^{\alpha\sigma_2}}\, \overline{A_{[3]\gamma}^{\beta\sigma_3}} \cdots \overline{A_{[N]1}^{\mu\sigma_N}} = A^{\dagger 1}_{[N]\sigma_N\mu} \cdots A^{\dagger\gamma}_{[3]\sigma_3\beta}\, A^{\dagger\beta}_{[2]\sigma_2\alpha}\, A^{\dagger\alpha}_{[1]\sigma_1 1}\, \underset{N}{\langle\vec\sigma|} \qquad (9)$$



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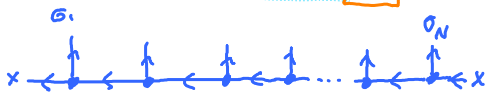
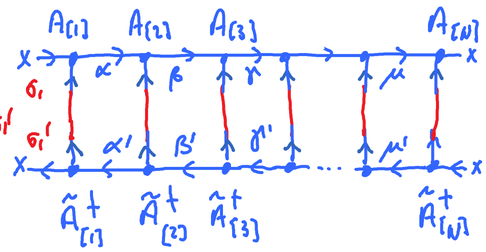


We expressed all ~~makes~~ matrices via their Hermitian conjugates by transposing indices and inverting arrows. To recover a matrix product structure, we ordered the Hermitian conjugate matrices to appear in the <u>opposite</u> order as the vertices in the diagram.

Recipe for bra formula: as chain grows, attach new matrices $A^\dagger$ on the left, opposite to vertex order in diagram.

Now consider overlap between two MPS:

$$\langle\tilde\psi|\psi\rangle = \delta^{\sigma_1}_{\sigma_1'}$$



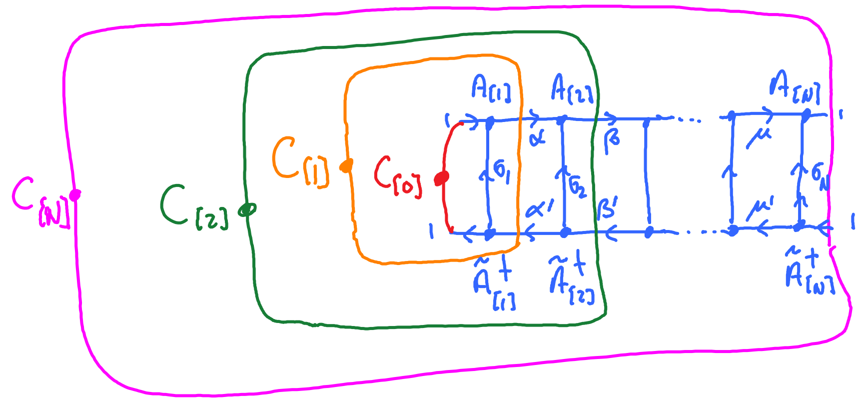
Recipe: contract all physical indices!

$$= \tilde A^{\dagger 1}_{[N]\sigma_N\mu'} \cdots \tilde A^{\dagger\mu'}_{[3]\sigma_3\beta'}\, \tilde A^{\dagger\beta'}_{[2]\sigma_2\alpha'}\, \tilde A^{\dagger\alpha'}_{[1]\sigma_1 1}\, A^{1\sigma_1}_{[1]\alpha}\, A^{\alpha\sigma_2}_{[2]\beta}\, A^{\beta\sigma_3}_{[3]\gamma} \cdots A^{\mu\sigma_N}_{[N]1} \qquad (10)$$

Exercise: derive this result algebraically from (7), (9),

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:

$$\langle \tilde\psi | \psi \rangle = $$  (11)

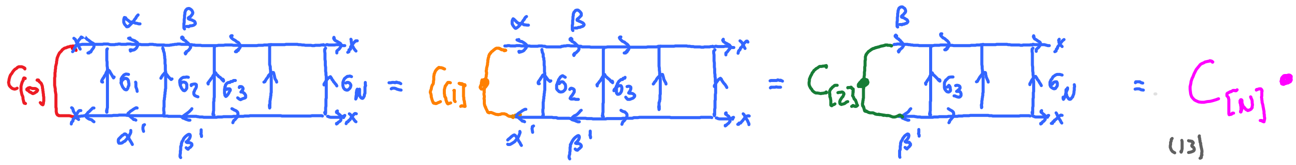
$$= \tilde A^{\dagger 1}{}_{\sigma_N \mu'} \cdots \tilde A^{\dagger \beta'}{}_{\sigma_2 \alpha'} \underbrace{A^{\dagger \alpha'}{}_{\sigma_1 1} \cdot \overbrace{1}^{\equiv C_{[0]}{}^{1}{}_{1} = 1} \cdot A_{[1]}{}^{1\sigma_1}{}_{\alpha}}_{\equiv C_{[1]}{}^{\alpha'}{}_{\alpha}} A_{[2]}{}^{\alpha\sigma_2}{}_{\beta} \cdots A_{[N]}{}^{\mu\sigma_N}{}_{1} \qquad (12)$$

$$\equiv C_{[2]}{}^{\beta'}{}_{\beta}$$

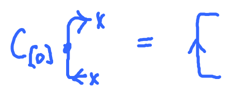
$$\vdots$$

$$\equiv C_{[N]}{}^{1}{}_{1}$$

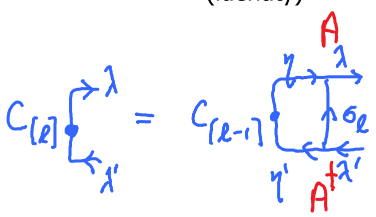
Diagrammatic depiction: 'closing zipper' from left to right.

 (13)

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

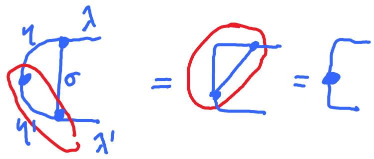
Initialization:  $C_{[0]}{}^{1}{}_{1} = 1$ (14)

(identity)

Iteration step:  $C_{[\ell]}{}^{\lambda'}{}_{\lambda} = \tilde A^{\dagger \lambda'}{}_{\sigma_\ell \eta'} \, C_{[\ell-1]}{}^{\eta'}{}_{\eta} \, A^{\eta \sigma_\ell}{}_{\lambda}$ (15)

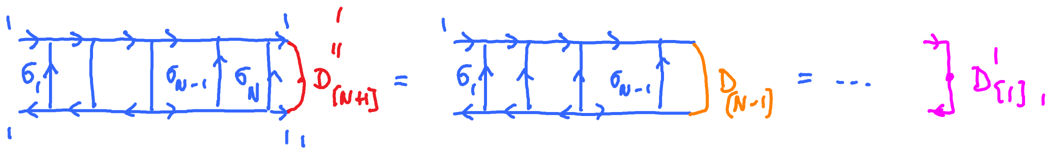
Final answer: $\langle \tilde\psi | \psi \rangle = C_{[N]}{}^{1}{}_{1}$ (16)

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

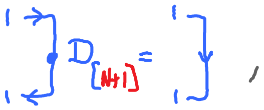
One iteration: $\underbrace{D \cdot D \cdot d}_{\text{fixed}} \cdot \underbrace{D}_{\text{sum}} + \underbrace{D \cdot D}_{\text{fixed}} \; \underbrace{d \cdot D}_{\text{sum}}$  (17)

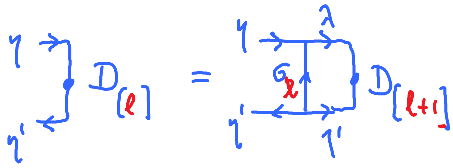
Total cost: $\sim D^3 \cdot d \cdot N$ (18)

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



(19)

Initialization:  (identity)

Iteration step: 

(20)

<u>Normalization</u> $\langle\psi|\psi\rangle = ?$

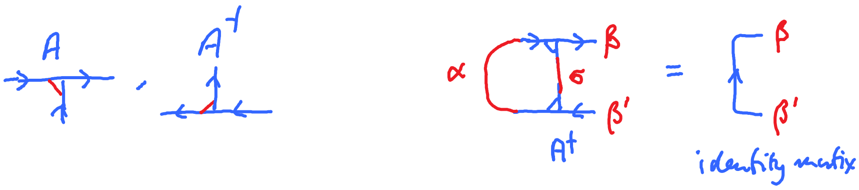
Use above scheme, with $\tilde{A} = A$

<u>Left-normalization</u>

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

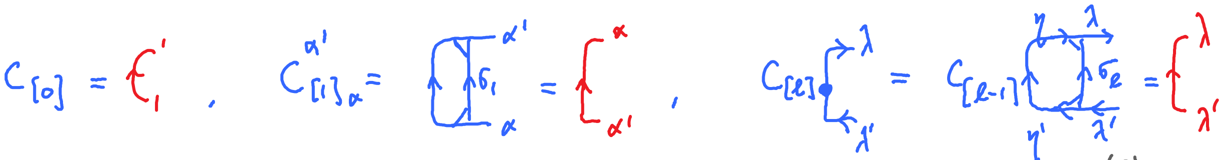
$\boxed{A^\dagger A = \mathbb{1}}$. Explicitly: $(A^\dagger A)^{\beta'}{}_{\beta} = \underbrace{A^{\dagger\beta'}{}_{\sigma\alpha} A^{\alpha\sigma}}{}_{\beta} = \mathbb{1}^{\beta'}{}_{\beta}$ (21)

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



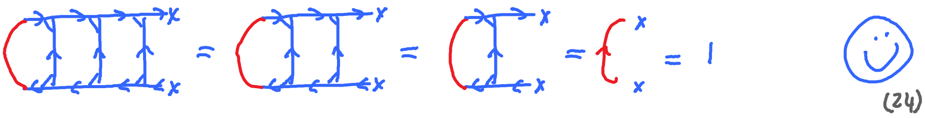
(22)

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



(23)

Hence:

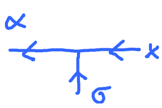
$\langle\psi|\psi\rangle =$  $= 1$

(24)

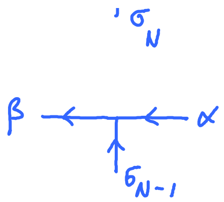
<u>Right-normalization</u>

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:

$|\alpha\rangle = |\sigma_N\rangle B^{\sigma_N 1}_{\alpha}$ 

(25)

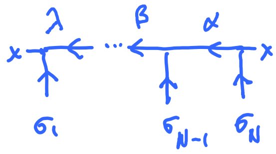
$$|\beta\rangle = |\sigma_N\rangle|\sigma_{N-1}\rangle\, B_\beta{}^{\sigma_{N-1}\alpha}\, B_\alpha{}^{\sigma_N 1}$$  (26)

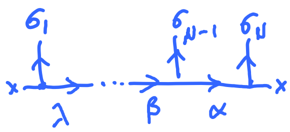
left-to-right index order as in diagram

$$\langle\alpha| = \underbrace{B^\dagger{}_{1\sigma_N}{}^{\alpha}}_{\equiv\, \overline{B_\alpha{}^{\sigma_N 1}}}\, \langle\sigma_N|$$  (27)

$$\langle\beta| = B^\dagger{}_{1\sigma_N}{}^{\alpha}\, B^\dagger{}_{\alpha\sigma_{N-1}}{}^{\beta}\, \langle\sigma_{N-1}|\langle\sigma_N|$$  (28)

Iterating this, we obtain kets and bras of the form

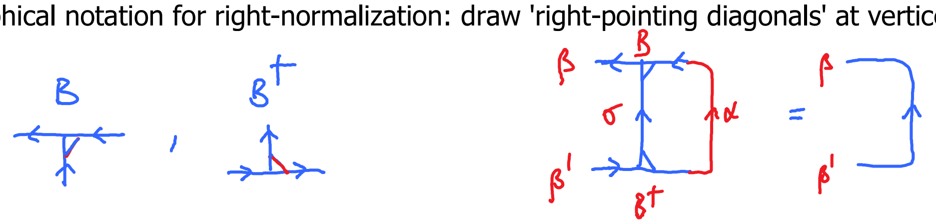
$$|\psi\rangle = |\sigma_N\rangle|\sigma_{N-1}\rangle\dots|\sigma_1\rangle\, B_1{}^{\sigma_1\lambda}\dots B_\beta{}^{\sigma_{N-1}\alpha}\, B_\alpha{}^{\sigma_N 1}$$  (29)

$$\langle\psi| = B^\dagger{}_{1\sigma_N}{}^{\alpha}\, B^\dagger{}_{\alpha\sigma_{N-1}}{}^{\beta}\dots B^\dagger{}_{\lambda\sigma_1}{}^{1}\, \langle\sigma_1|\dots\langle\sigma_{N-1}|\langle\sigma_N|$$  (30)

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

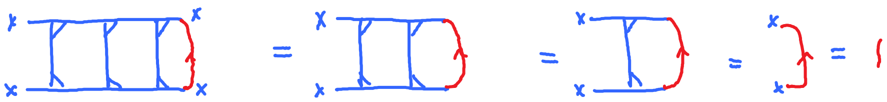
$$BB^\dagger = \mathbb{1}. \quad \text{Explicitly:} \quad (BB^\dagger) = B_\beta{}^{\sigma\alpha}\, B^\dagger{}_{\alpha\sigma}{}^{\beta'} = \mathbb{1}_\beta{}^{\beta'} \qquad (31)$$

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



(32)

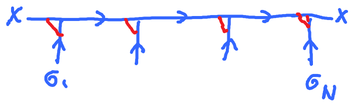
When all B's are right-normalized, closing the zipper right-to-left is easy:

$\langle\psi|\psi\rangle =$ 
(33)

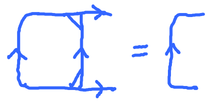
Conclusion: MPS built purely from left-normalized A 's or purely from right-normalized B 's are automatically normalized to 1. 

2. Various canonical MPS forms

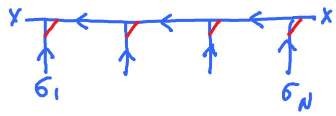
Left-canonical (lc-) MPS:



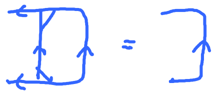
$$|\psi\rangle = |\vec{\sigma}\rangle_N (A^{\sigma_1} \dots A^{\sigma_N}) \qquad A^\dagger A = \mathbb{1}$$

 (1)

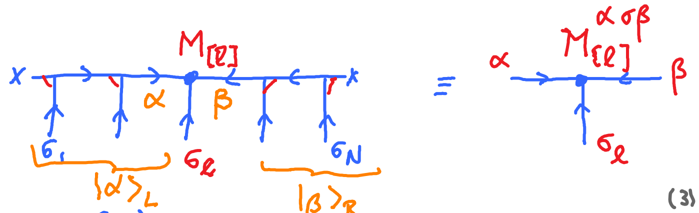
Right-canonical (rc-) MPS:



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

 (2)

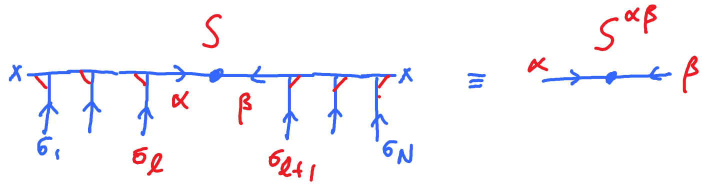
Site-canonical (sc-) MPS:



(3)

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

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



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

can be chosen diagonal

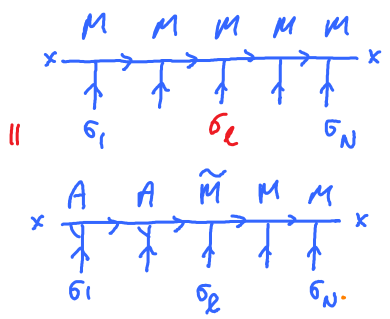
How can we bring an arbitrary MPS into one of these forms?

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

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

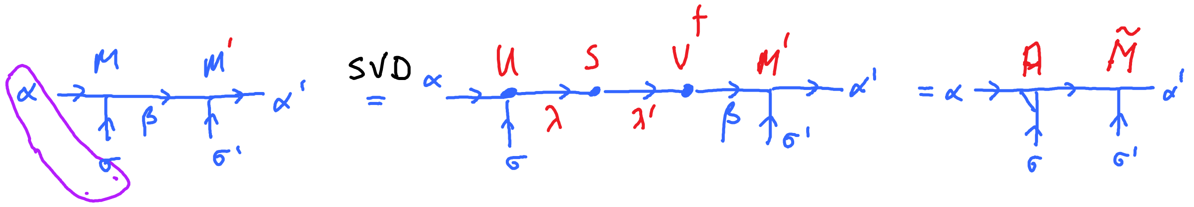
[or with index: $|s_N\rangle =$  s_N]

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



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

$$M M' = U S V^\dagger M' \equiv A \tilde{M}, \quad \text{with} \quad A = U, \quad \tilde{M} = S V^\dagger M' \qquad (7)$$



(8)

$$M^{\alpha\sigma}{}_{\beta}\, M'^{\beta\sigma'}{}_{\alpha'} = U^{\alpha\sigma}{}_{\lambda}\, S^{\lambda}{}_{\lambda'}\, V^{\dagger\lambda'}{}_{\beta}\, M'^{\beta\sigma'}{}_{\alpha'} = A^{\alpha\sigma}{}_{\lambda}\, \hat{M}^{\lambda\sigma'}{}_{\alpha'} \qquad (9)$$

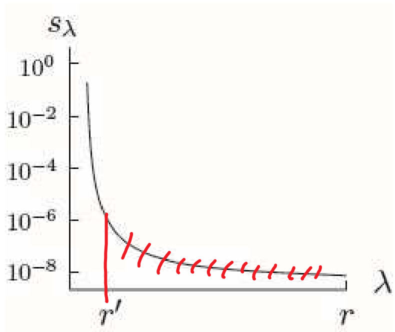
The properly $U^\dagger U = \mathbb{1}$ ensures left-normalization: $A^\dagger A = \mathbb{1}$ (10)

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

The smallest singular values,

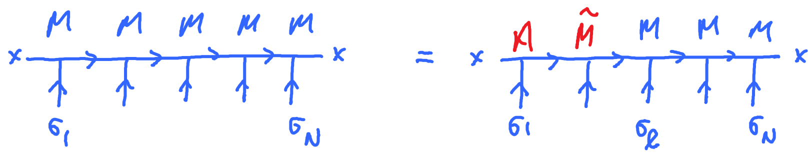
$$\sum_{\lambda=1}^{r} \longrightarrow \sum_{\lambda=1}^{r'}$$

(but (10) remains valid!)



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

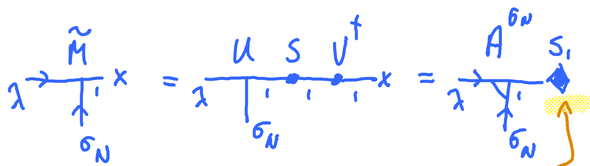
By iterating, starting from $M^{\sigma_1} M^{\sigma_2}$, we left-normalize M^{σ_1} to $M^{\sigma_{\ell-1}}$,



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

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

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



(11)

diamond indicates single number

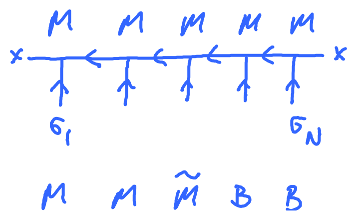
lc-form: $|\psi\rangle = |\vec{\sigma}\rangle_N \left(A^{\sigma_1} \dots A^{\sigma_N}\right) s_1$

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

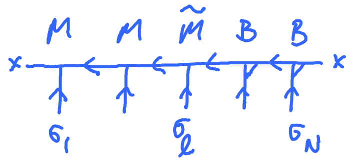
<u>Transforming to right-normalized form</u>

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

[or with index: $|s_1\rangle = s_1$ ]



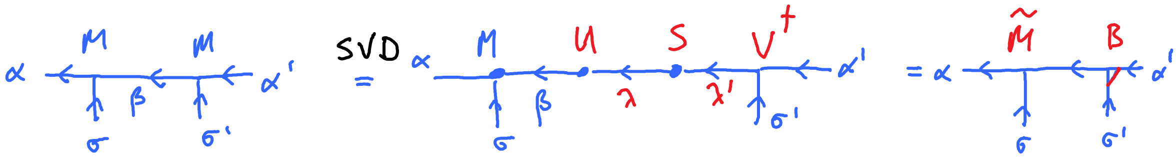
[or with index: $|s_1)$ = ]



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

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

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



(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 $M^{\sigma_\ell} M^{\sigma_{\ell+1}}$.

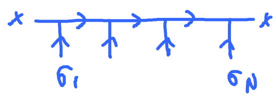
To right-normalize entire chain, choose / and at last site, $\ell = 1$

$$\tilde{M}_1{}^{\sigma_1\lambda} = \underbrace{U_1{}^1}_{=1} \underbrace{S_1{}^1}_{s_1} \underbrace{V^\dagger{}_1{}^{\sigma_1\lambda}}_{B_1{}^{\sigma_1\lambda}} \,.$$

s_1 determines normalization. (17)

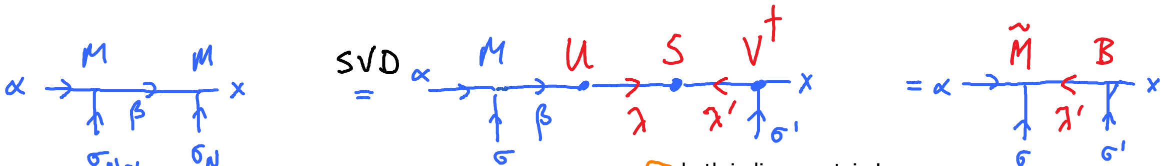
<u>Exercise</u>

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



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

and note the up ⟷ down changes in index placement.

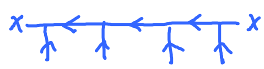


(18)

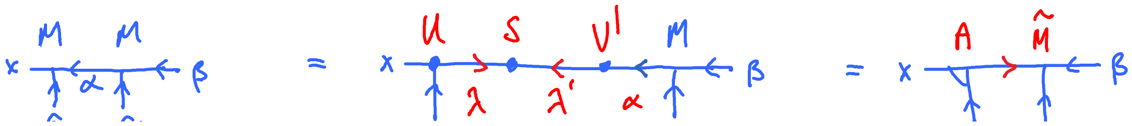
both indices upstairs!

$$M^{\alpha\sigma}{}_\beta M^{\beta\sigma'}{}_1 = \left(M^{\alpha\sigma}{}_\beta U^\beta{}_\lambda S^{\lambda\lambda'}\right)\left(V^\dagger{}_{\lambda'}{}^{\sigma'}{}_1\right) = \tilde{M}^{\alpha\sigma\lambda'} B_{\lambda'}{}^{\sigma'}{}_1 \qquad (19)$$

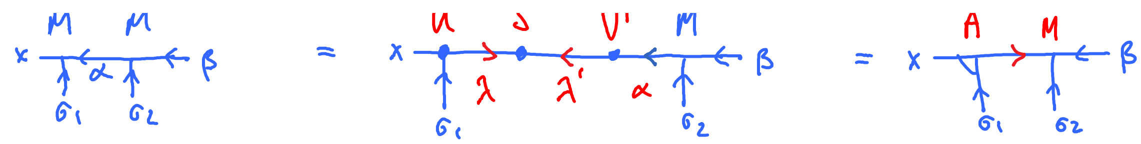
(b) Left-normalize a state with left-pointing arrows!



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



(20)

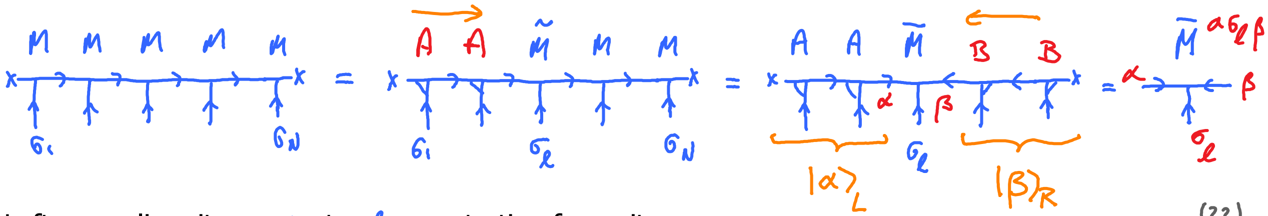


(20)

both indices upstairs!

$$M_1{}^{\sigma_1\alpha}\, M_\alpha{}^{\sigma_2\beta} = \left(U^{1\sigma_1}{}_{\lambda}\right)\left(S^{\lambda\lambda'}\, V^{\dagger}_{\lambda'}{}^{\alpha} M_\alpha{}^{\sigma_2\beta}\right) = A_1{}^{\sigma_1\lambda}\, \tilde{M}_\lambda{}^{\sigma_2\beta} \qquad (21)$$

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



(22)

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

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

$$M M' = M \underbrace{U^\dagger U}_{\mathbb{1}} M' = \tilde{M}\tilde{M}'$$

Result:

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

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

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

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

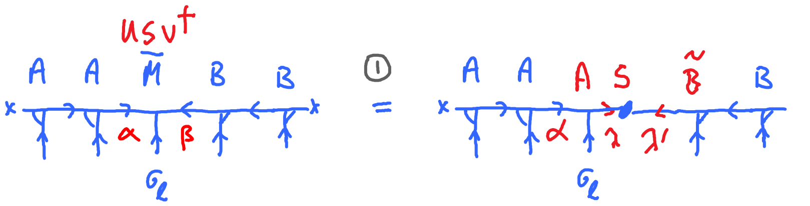
(Exercise: verify this, using $A^\dagger A = \mathbb{1}$ and $B B^\dagger = \mathbb{1}$.)

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.

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

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

or ② U with neighboring A .



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

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

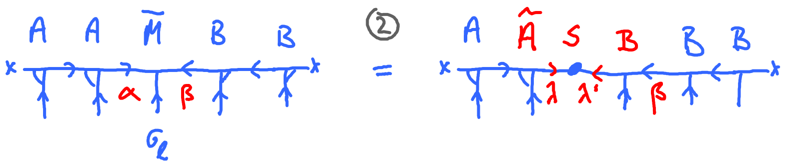
(Exercise: add indices!) (27)

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

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

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).



$$= \underbrace{|\lambda'\rangle_R}_{\text{involves sites } \ell \text{ to } N}\ \overbrace{\underbrace{|\lambda\rangle_L}_{\text{involves sites } 1 \text{ to } \ell-1}\, S^{\lambda\lambda'}}^{G_\ell} \tag{29}$$

$\tilde M = U S V^\dagger$ $\qquad$ $\tilde A = AU$, $\; B = V^\dagger$ $\qquad$ (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).