MPS I: Basic properties of matrix product states

MPS-I.1

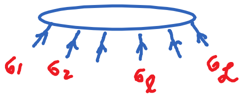
1. Overlaps, matrix elements $\langle\tilde\psi|\psi\rangle$

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

General ket: $|\psi\rangle = |\sigma_\mathscr{L}\rangle \dots |\sigma_2\rangle|\sigma_1\rangle C^{\sigma_1,\dots,\sigma_\mathscr{L}} =: |\vec\sigma\rangle C^{\vec\sigma}$

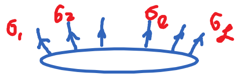
$(\in \mathcal{H}^\mathscr{L})$

summation over repeated indices implied



(1)

General bra: $\langle\psi| = \underbrace{\overline{C^{\sigma_1,\dots,\sigma_\mathscr{L}}}}_{=:\,C^\dagger_{\vec\sigma_R}} \langle\sigma_1|\langle\sigma_2|\dots\langle\sigma_\mathscr{L}| =: \underbrace{C^\dagger_{\vec\sigma_R}}_{:=\,\overline{C^{\vec\sigma}}}\langle\vec\sigma|$

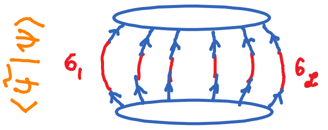


(2)

Overlap: $\langle\tilde\psi|\psi\rangle = \overline{\tilde C^{\sigma'_1,\dots,\sigma'_\mathscr{L}}}\langle\sigma'_1|\langle\sigma'_2|\dots\underbrace{\langle\sigma'_\mathscr{L}|\sigma_\mathscr{L}\rangle}\dots|\sigma_2\rangle|\sigma_1\rangle C^{\sigma_1,\dots,\sigma_\mathscr{L}}$ (3a)

These unit matrices lead to contractions, depicted graphically by connected legs! $\rightsquigarrow \mathbb{1}^{\sigma'_1}{}_{\sigma_1}\mathbb{1}^{\sigma'_2}{}_{\sigma_2}\ \mathbb{1}^{\sigma'_\mathscr{L}}{}_{\sigma_\mathscr{L}} = \mathbb{1}^{\vec\sigma'}{}_{\vec\sigma}$

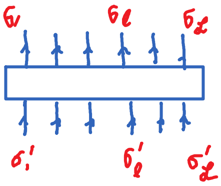
$$= \tilde C^\dagger_{\vec\sigma_R}\, C^{\vec\sigma}$$



(3b)

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

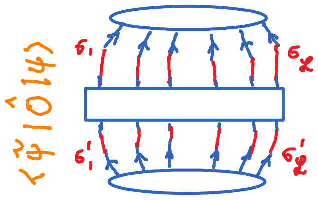
General operator: $\hat O = |\vec\sigma'\rangle O^{\vec\sigma'}{}_{\vec\sigma}\langle\vec\sigma|$



(4)

Matrix elements: $\langle\tilde\psi|\hat O|\psi\rangle = C^\dagger_{\tilde{\vec\sigma}'_R}\underbrace{\langle\tilde{\vec\sigma}'|\vec\sigma'\rangle}_{\mathbb{1}^{\tilde{\vec\sigma}'}{}_{\vec\sigma'}} O^{\vec\sigma'}{}_{\vec\sigma}\underbrace{\langle\vec\sigma|\tilde{\vec\sigma}\rangle}_{\mathbb{1}^{\vec\sigma}{}_{\tilde{\vec\sigma}}} C^{\tilde{\vec\sigma}}$ (5a)

$$= C^\dagger_{\vec\sigma'_R}\, O^{\vec\sigma'}{}_{\vec\sigma}\, C^{\vec\sigma}$$



(5b)

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

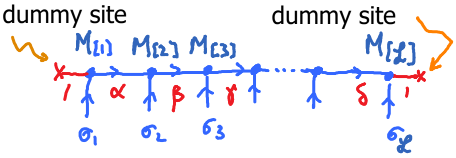
Now consider matrix product states:

Ket:

dummy index

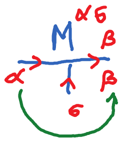
$$|\psi\rangle = |\vec\sigma\rangle M^{1\sigma_1}_{[1]\alpha}\underbrace{\ M^{\alpha\sigma_2}_{[2]}}\ \beta\underbrace{M^{\beta\sigma_3}_{[3]}}\gamma\dots M^{\gamma\sigma_\mathscr{L}}_{[\mathscr{L}]1}$$

dummy index



(6)

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



index-reading order

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

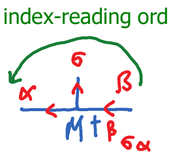
Add dummy sites at left and right, so that first and last M's have two virtual indices, just like other M's .

Bra:

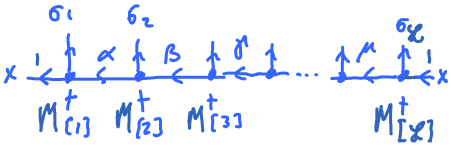
$$\langle\psi| = \overline{M_{[1]}^{1\sigma_1}{}_{\alpha}}\;\overline{M_{[2]}^{\alpha\sigma_2}{}_{\beta}}\;\overline{M_{[3]}^{\beta\sigma_3}{}_{\gamma}}\cdots\overline{M_{[\mathscr{L}]}^{\mu\sigma_{\mathscr{L}}}{}_{1}}\,\langle\vec\sigma|$$

$$= M^{\dagger 1}_{[\mathscr{L}]\sigma_{\mathscr{L}}\mu}\cdots M^{\dagger\gamma}_{[3]\sigma_3\beta}\, M^{\dagger\beta}_{[2]\sigma_2\alpha}\, M^{\dagger\alpha}_{[1]\sigma_1 1}$$

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



(7a)

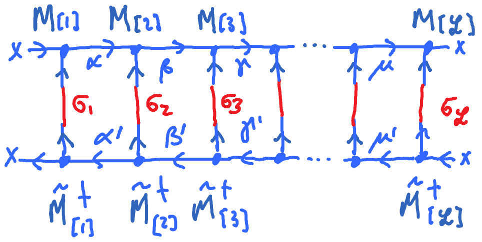


(7b)

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 opposite order as the vertices in the diagram.

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

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



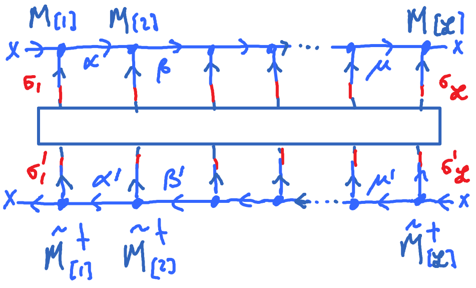
Recipe: contract all physical indices! (8a)

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

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

Matrix elements:

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



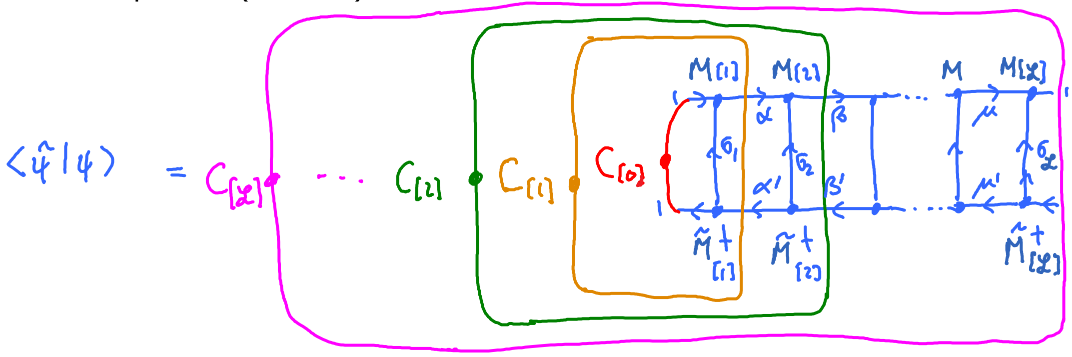
(9)

$$= \tilde M^{\dagger 1}_{[\mathscr{L}]\sigma'_{\mathscr{L}}\mu'}\cdots\tilde M^{\dagger\beta'}_{[2]\sigma'_2\alpha'}\,\tilde M^{\alpha'\dagger}_{[1]\sigma'_1 1}\,O^{\sigma'_1\sigma'_2\ldots\sigma'_{\mathscr{L}}}{}_{\sigma_1\sigma_2\ldots\sigma_{\mathscr{L}}}\,M_{[1]}^{1\sigma_1}{}_{\alpha}\,M_{[2]}^{\alpha\sigma_2}{}_{\beta}\cdots M_{[\mathscr{L}]}^{\mu\sigma_{\mathscr{L}}}{}_{1} \qquad (10)$$

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 $d^{\mathscr{L}}$ terms, each of which is a product of $2\mathscr{L}$ matrices. Exponentially costly! ☹

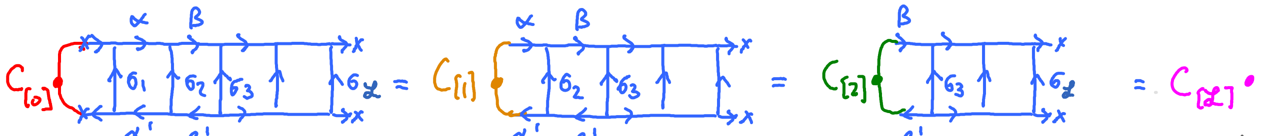
But calculation becomes tractable if we rearrange summations, to keep number of 'open legs' as small as possible (here = 2):



(11)

$$= \underbrace{\tilde M^{\dagger 1}_{[\mathcal L]\sigma_{\mathcal L}\mu'} \cdots \underbrace{\tilde M^{\dagger\beta'}_{[2]\sigma_2\alpha'} \underbrace{\tilde M^{\dagger\alpha'}_{[1]\sigma_1 1} \cdot \overset{=:C'_{[0]1}}{1} \cdot \tilde M^{1\sigma_1}_{[1]\alpha}}_{=:C^{\alpha'}_{[1]\alpha}} M^{\alpha\sigma_2}_{[2]\beta}}_{=:C^{\beta'}_{[2]\beta}} \cdots M^{\mu\sigma_{\mathcal L}}_{[\mathcal L]1}}_{=:C'_{[\mathcal L]1}} \qquad (12)$$

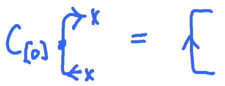
Diagrammatic depiction: 'closing zipper' from left to right.



(13)

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

Initialization:



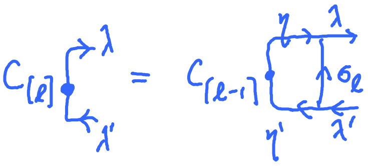
(identity)

$$C'_{[0]1} = 1 \qquad (14)$$

Iteration step:

sum over σ_ℓ

yields $C_{[\ell]}$



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

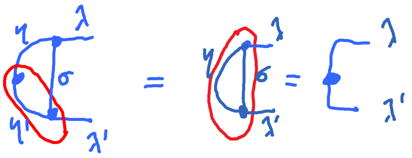
Final answer:

$$\langle\tilde\psi|\psi\rangle = C'_{[\mathcal L]1} \qquad (16)$$

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

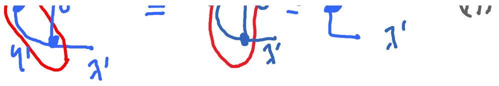
One iteration:

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



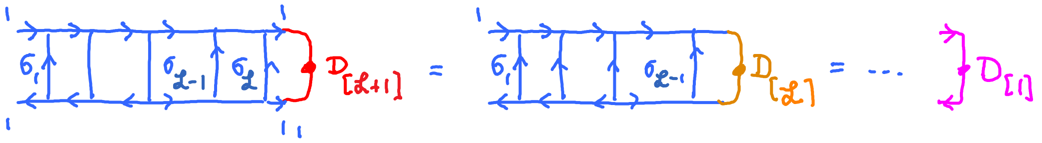
(17)

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



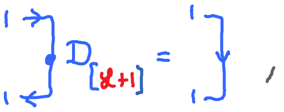
Total cost: $\sim D^3 d \cdot \mathcal{L}$ (18)

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



(19)

Initialization:

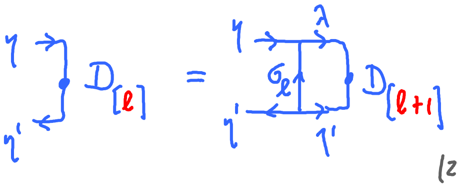


(identity)

iteration step:

sum over σ_ℓ

yields $D_{[\ell]}$



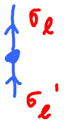
(20)

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

'Closing the zipper' is also useful for computing expectation values of local operators, i.e. operators acting non-trivially only on a few sites (e.g. only one, or two nearest neighbors).

One-site operator (acts non-trivially only on one site, ℓ)

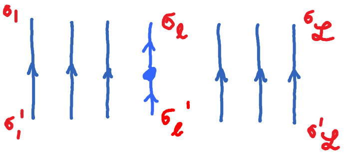
Action on site ℓ : $\hat{O}_{[\ell]} = |\sigma'_\ell\rangle \, O^{\sigma'_\ell}{}_{\sigma_\ell} \langle\sigma_\ell|$



(21)

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

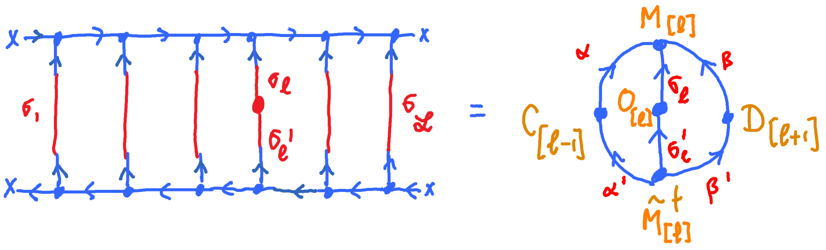
Action on full chain: $\hat{O}_{[\ell]} = |\vec{\sigma}'\rangle \underbrace{\mathbb{1}^{\sigma'_1}{}_{\sigma_1} \dots O^{\sigma'_\ell}{}_{\sigma_\ell} \cdots \mathbb{1}^{\sigma'_\mathcal{L}}{}_{\sigma_\mathcal{L}}}_{O^{\vec{\sigma}'}{}_{\vec{\sigma}}} \langle\vec{\sigma}|$



(22)

Matrix element between two MPS:

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



(23)

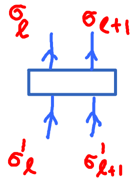
Close zipper from left using $C_{[\ell-1]}$ [see (15)] and from right using $D_{[\ell+1]}$ [see (20)].

$$= \tilde{M}^{\dagger}_{\beta'\sigma_\ell'\alpha'} \, C_{[\ell-1]}{}^{\alpha'}{}_{\alpha} \, M^{\alpha\sigma_\ell\beta} \, D_{[\ell+1]}{}_{\beta}{}^{\beta'} \, O^{\sigma_\ell'}{}_{\sigma_\ell} \tag{24}$$

<u>Two-site operator</u> (acts nontrivally only on two sites, ℓ and $\ell+1$) [e.g. for spin chain: $\vec{S}_\ell \cdot \vec{S}_{\ell+1}$]

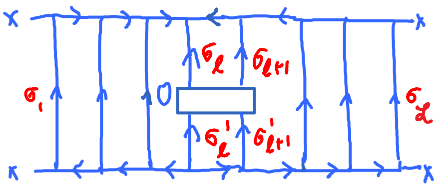
Action on sites ℓ , $\ell+1$:

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



Matrix elements:

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



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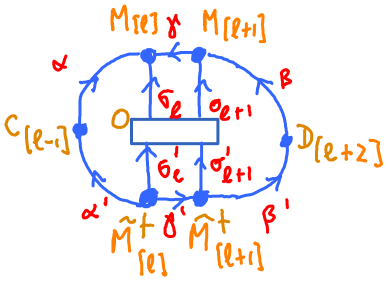


(11)

$$= \tilde{M}^{\dagger}_{\beta'\sigma_{\ell+1}'}{}^{\gamma'} \, \tilde{M}^{\dagger}_{\gamma'\sigma_\ell'\alpha'} \, C_{[\ell-1]}{}^{\alpha'}{}_{\alpha} \, M^{\alpha\sigma_\ell\gamma} \, M_{\gamma}{}^{\sigma_{\ell+1}\beta} D_{[\ell+2]}{}_{\beta}{}^{\beta'} \, O^{\sigma_\ell'\sigma_{\ell+1}'}{}_{\sigma_\ell\sigma_{\ell+1}} \tag{12}$$

2. Left- and right-normalized MPS

MPS-I.2

Computation of normalization and matrix elements of local operators is simpler if the MPS is built from tensors with special normalization properties, called 'left-normalized' or 'right-normalized' tensors.

Left-normalization

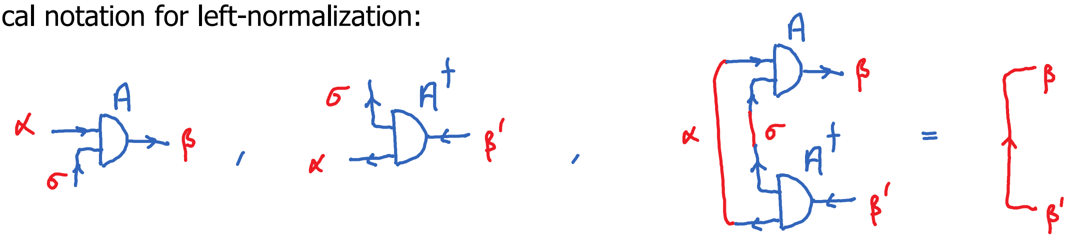
A 3-leg tensor $A^{\alpha\sigma}{}_{\beta}$ is called 'left-normalized' if it is a left isometry, i.e. if it satisfies

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

Such an A defines an 'isometry' from space labeled by its left indices to space labeled by its right indices.

distance-preserving map (in index-free notation: if $y = Ax$, then $y^\dagger y = x^\dagger A^\dagger A x = x^\dagger x$)

Graphical notation for left-normalization:



(2a)

More compact notation: draw 'left-pointing diagonals' at vertices

(2b)

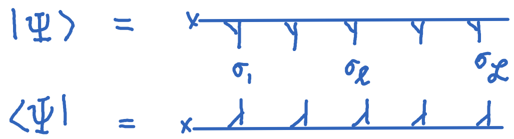
The right-angled triangle contains <u>complete</u> information about all arrows attached to it:

for A , incoming arrows to sharp angles, outgoing arrow from right angle,

for $A^\dagger$, outgoing arrows from sharp angles, incoming to from right angle:

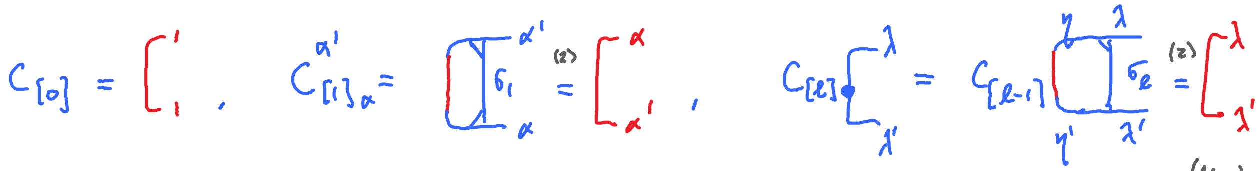
Hence, there is no need to draw arrows explicitly when using $\top$, $\perp$!

Consider a 'left-normalized MPS', i.e. one constructed purely from left isometries:



(3)

Then, closing the zipper left-to-right is easy, since all $C_{[\ell]}$ reduce to identity matrices:



(4a)

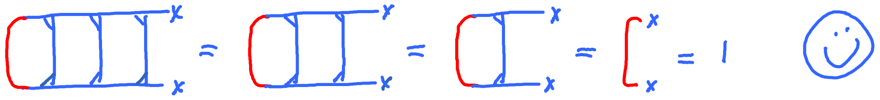
We suppress arrows for C, too, since they can be reconstructed from arrows of constitutent As.

Hence:

We suppress arrows for C, too, since they can be reconstructed from arrows of constitutent As.

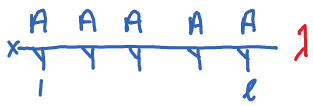
Hence:

$\langle\Psi|\Psi\rangle =$

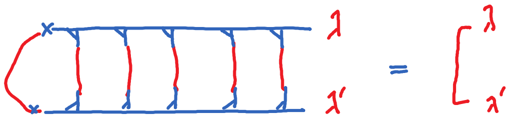


(4b)

Moreover, the matrices for site 1 to any site $\ell = 1,\ldots,N$ define an <u>orthonormal state space</u>:



$$|\Psi_\lambda\rangle_\ell = \overset{|\sigma_1\rangle\otimes\ldots\otimes|\sigma_\ell\rangle}{|\vec{\sigma}_{1\ldots\ell}\rangle}\,[A^{\sigma_1}A^{\sigma_2}\ldots A^{\sigma_\ell}]^1{}_\lambda \qquad (5)$$



close the zipper

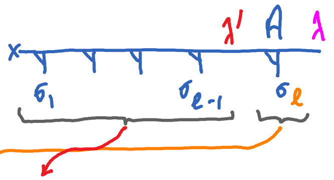
$$ {}_\ell\langle\Psi^{\lambda'}|\Psi_\lambda\rangle_\ell = \mathbb{1}^{\lambda'}{}_\lambda \qquad ☺ \qquad (6)$$

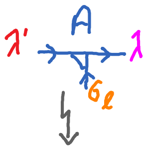
Call this state space $\mathbb{V}_\ell = \mathrm{span}\{|\Psi_\lambda\rangle_\ell\} \subseteq \mathbb{V}_1\otimes\mathbb{V}_2\otimes\ldots\otimes\mathbb{V}_\ell$ (7)

where $\mathbb{V}_\ell = \mathrm{span}\{|\sigma_\ell\rangle\}$ is local state space of site ℓ

These state spaces are built up iteratively from left to right through left-isometric maps:

Each  defines an isometric map to a new (possibly smaller) basis:





$$A_\ell : \mathbb{V}_\ell\otimes\mathbb{V}_{\ell-1} \to \mathbb{V}_\ell, \qquad \underbrace{|\sigma_\ell\rangle|\Psi_{\lambda'}\rangle_{\ell-1}}_{\text{old basis}} \mapsto \underbrace{|\Psi_\lambda\rangle_\ell}_{\text{new basis}} = |\sigma_\ell\rangle|\Psi_{\lambda'}\rangle_{\ell-1}A^{\lambda'\sigma_\ell}{}_\lambda \qquad (8)$$

If A_ℓ is a unitary, then $\dim(\mathbb{V}_\ell) = \dim(\mathbb{V}_\ell)\cdot\dim(\mathbb{V}_{\ell-1})$ $\Rightarrow$ no truncation (9)

$$D_\ell = d\cdot D_{\ell-1}$$

If A_ℓ is an isometry, then $D_\ell < d\cdot D_{\ell-1}$ $\Rightarrow$ truncation was involved! (10)

Hence $\mathbb{V}_\ell = \mathbb{V}_1\otimes\mathbb{V}_2\otimes\ldots\otimes\mathbb{V}_\ell$ only if all A's are not only isometries but unitaries.

$D_\ell = d^\ell$

truncation possible

no truncation!

Even if truncation is involved, the resulting MPS are useful, precisely because they are parametrized by a limited number of parameters (namely elements of A tensors). E.g., they can be optimized variationally by minimizing energy $\Rightarrow$DMRG).

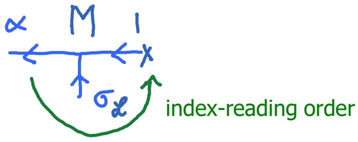
Right-normalization

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, using left-pointing arrows.

Building blocks:

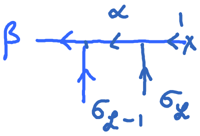
$$|\alpha\rangle = |\sigma_\mathcal{L}\rangle M_\alpha{}^{\sigma_\mathcal{L} 1}$$

left-to-right index order as in diagram



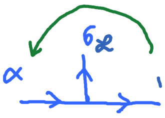
(11)

$$|\beta\rangle = |\sigma_\mathcal{L}\rangle|\sigma_{\mathcal{L}-1}\rangle M_\beta{}^{\sigma_{\mathcal{L}-1}\alpha} M_\alpha{}^{\sigma_\mathcal{L} 1}$$



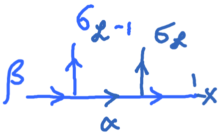
(12)

$$\langle\alpha| = \underbrace{M^\dagger{}_{1\sigma_\mathcal{L}}{}^{\alpha}}_{:= \overline{M_\alpha{}^{\sigma_\mathcal{L} 1}}} \langle\sigma_\mathcal{L}|$$



(13)

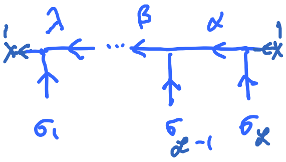
$$\langle\beta| = M^\dagger{}_{1\sigma_\mathcal{L}}{}^{\alpha} M^\dagger{}_{\alpha\sigma_{\mathcal{L}-1}}{}^{\beta} \langle\sigma_{\mathcal{L}-1}|\langle\sigma_\mathcal{L}|$$



(14)

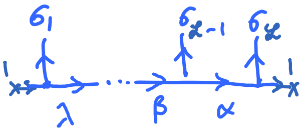
Iterating this, we obtain kets and bras of the form

$$|\psi\rangle = |\sigma_\mathcal{L}\rangle|\sigma_{\mathcal{L}-1}\rangle\dots|\sigma_1\rangle M_1{}^{\sigma_1\lambda}\dots \underbrace{M_\beta}_{}{}^{\sigma_{\mathcal{L}-1}\alpha} \underbrace{M_\alpha}_{}{}^{\sigma_\mathcal{L} 1}$$



(15)

$$\langle\psi| = M^\dagger{}_{\underbrace{1\sigma_\mathcal{L}}_{}}{}^{\alpha} M^\dagger{}_{\alpha\sigma_{\mathcal{L}-1}}{}^{\beta}\underbrace{\;\;}_{} \dots M^\dagger{}_{\lambda\sigma_1}{}^{1} \langle\sigma_1|\dots\langle\sigma_{\mathcal{L}-1}|\langle\sigma_\mathcal{L}|$$



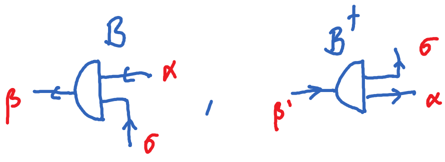
(16)

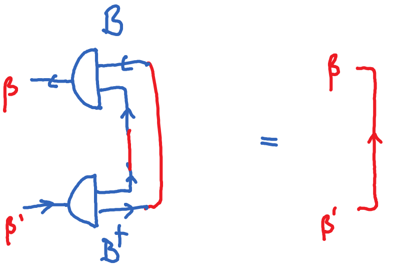
A three-leg tensor $B_\beta{}^{\sigma\alpha}$ is called right-normalized if it is a right isometry, i.e. if it satisfies

$$B B^\dagger = \mathbb{1} . \quad \text{Explicitly:} \quad (BB^\dagger)_\beta{}^{\beta'} = B_\beta{}^{\sigma\alpha} B^\dagger{}_{\alpha\sigma}{}^{\beta'} = \mathbb{1}_\beta{}^{\beta'} \tag{17}$$

Such a $B^\dagger$ defines an 'isometry' from space labeled by its left indices to space labeled by its right indices.

Graphical notation for right-normalization:





(18a)

More compact notation: draw 'right-pointing diagonals' at vertices

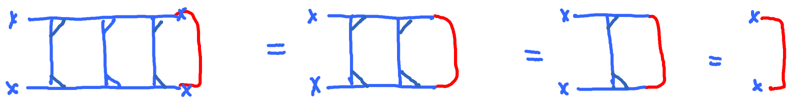
(18b)

(18b)

Again, right-angled triangles complete information on arrows, so arrows can be suppressed.

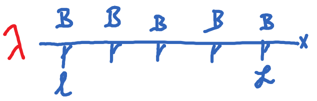
For 'right-normalized MPS', constructed purely from right isometries, closing zipper right-to-left is easy:

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

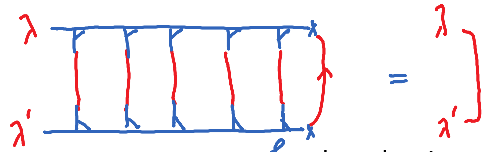


$$= 1 \qquad (19)$$

Moreover, the matrices for site N to any site $\ell = 1, \dots, N$ define an orthonormal state space:



$$|\Phi_\lambda\rangle_\ell = \overset{|\sigma_\ell\rangle\otimes\dots\otimes|\sigma_\mathcal{N}\rangle}{|\vec{\sigma}_{\ell\dots\mathcal{N}}\rangle} \left[B^{\sigma_\ell} B^{\sigma_{\ell+1}}\dots B^{\sigma_\mathcal{N}}\right]_\lambda{}' \qquad (20)$$

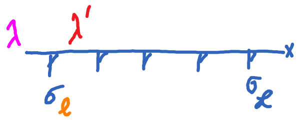


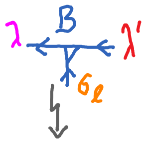
$${}_\ell\langle\Phi^{\lambda'}|\Phi_\lambda\rangle_\ell = \mathbb{1}^{\lambda'}{}_\lambda \qquad ☺ \qquad (21)$$

Call this state space $W_\ell = \mathrm{span}\{|\Phi_\lambda\rangle_\ell\} \subseteq V_\ell \otimes V_{\ell+1} \otimes \dots \otimes V_\mathcal{N}$ (22)

These state spaces are built up iteratively from right to left through right-isometric maps:

Each  defines an isometric map to a new (possibly smaller) basis:





$$B_\ell : W_{\ell+1} \otimes V_\ell \to W_\ell , \qquad \underset{\text{old basis}}{|\Phi_{\lambda'}\rangle_{\ell+1}|\sigma_\ell\rangle} \mapsto \underset{\text{new basis}}{|\Phi_\lambda\rangle_\ell} = |\Phi_{\lambda'}\rangle_{\ell+1}|\sigma_\ell\rangle B_\lambda{}^{\sigma_\ell\lambda'} \qquad (23)$$

$\mathbb{V}_\ell = \mathbb{V}_\ell \otimes \mathbb{V}_{\ell+1} \otimes \dots \otimes \mathbb{V}_\mathcal{N}$ only if all B's are not only isometries but unitaries. (24)

Summary: 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. Various canonical MPS forms

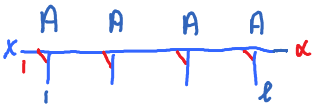
Any matrix product can be expressed in infinitely many different ways without changing the product:

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

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

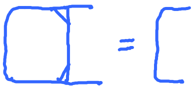
(i) Left-canonical (lc-) MPS:

[all tensors are left-normalized, denoted A]



(2)

$$|\Psi_\alpha\rangle_\ell = |\vec\sigma\rangle_\ell \,(A^{\sigma_1}\cdots A^{\sigma_\ell})^1{}_\alpha \qquad A^\dagger A = \mathbb{1}$$



(3)

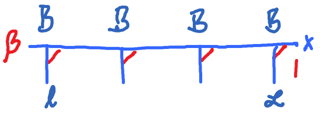
These states form an orthonormal set: $\;{}_\ell\langle\Psi^{\alpha'}|\Psi_\alpha\rangle_\ell \overset{\text{(MPS-I.2.6)}}{=} \mathbb{1}^{\alpha'}{}_\alpha$ (4)

In general, $\mathbb{V}_\ell \subset \mathcal{H}^\ell$.

true subset

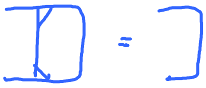
(ii) Right-canonical (rc-) MPS:

[all tensors are right-normalized, denoted B]



(5)

$$|\Phi_\beta\rangle_\ell = |\vec\sigma\rangle_\ell \,(B^{\sigma_1}\cdots B^{\sigma_{\mathcal{L}}})_\beta{}^1 \qquad BB^\dagger = \mathbb{1}$$

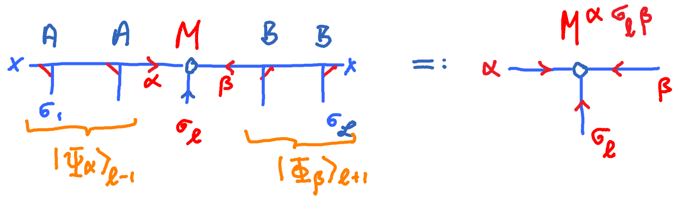


(6)

These states form an orthonormal set: $\;{}_\ell\langle\Phi^{\beta'}|\Phi_\beta\rangle_\ell \overset{\text{(MPS-I.2.18)}}{=} \mathbb{1}^{\beta'}{}_\beta$ (7)

(iii) Site-canonical (sc-) MPS:

[left-normalized to left of site ℓ ,
right-normalized to right of site ℓ]



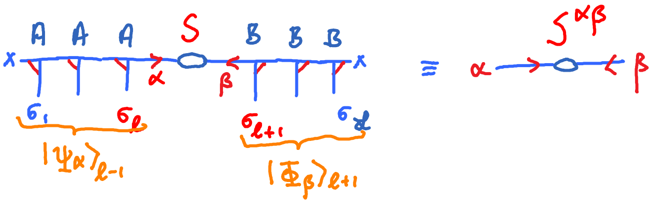
(8)

$$|\Psi\rangle = |\vec\sigma\rangle_{\mathcal{L}}(A^{\sigma_1}\cdots A^{\sigma_{\ell-1}})^1{}_\alpha M^{\alpha\sigma_\ell\beta}(B^{\sigma_{\ell+1}}\cdots B^{\sigma_{\mathcal{L}}})_\beta{}^1 = |\Phi_\beta\rangle_{\ell+1}|\sigma_\ell\rangle|\Psi_\alpha\rangle_{\ell-1}M^{\alpha\sigma_\ell\beta} \qquad (9)$$

The states $|\alpha,\sigma,\beta\rangle := |\Phi_\beta\rangle_{\ell+1}|\sigma_\ell\rangle|\Psi_\alpha\rangle_{\ell-1}$ form an orthonormal set: $\langle\alpha',\sigma',\beta'|\alpha,\sigma,\beta\rangle = \mathbb{1}^{\alpha'}{}_\alpha\mathbb{1}^{\sigma'}{}_\sigma\mathbb{1}^{\beta'}{}_\beta$ (10)

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

[left-normalized from sites 1 to ℓ ,
right-normalized from sites $\ell+1$ to N]



(11)

$$|\psi\rangle = |\vec\sigma\rangle_{\mathcal{L}}(A^{\sigma_1}\cdots A^{\sigma_\ell})^1{}_\alpha S^{\alpha\beta}(B^{\sigma_{\ell+1}}\cdots B^{\sigma_{\mathcal{L}}})_\beta{}^1 = \sum_{\alpha\beta}|\Phi_\beta\rangle_{\ell+1}|\Psi_\alpha\rangle_{\ell-1}S^{\alpha\beta} \qquad (12)$$

can be chosen diagonal

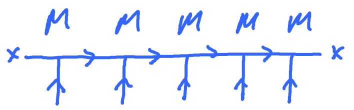
↳ can be chosen diagonal

The states $|\alpha,\beta\rangle := |\Phi_\beta\rangle_{\ell+1}|\Psi_\alpha\rangle_\ell$ form an orthonormal set: $\langle\alpha',\beta'|\alpha,\beta\rangle = \mathbb{1}^{\alpha'}{}_{\alpha}\,\mathbb{1}^{\beta'}{}_{\beta}$ (13)

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

Transforming to left-normalized form

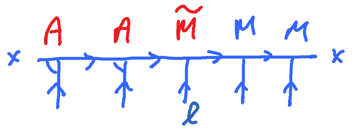
Given: $|\psi\rangle = |\vec{\sigma}\rangle_{\mathscr{L}}(M^{\sigma_1}\dots M^{\sigma_{\mathscr{L}}})$



(5)

[or with index: $|\Psi_\alpha\rangle =$ ]

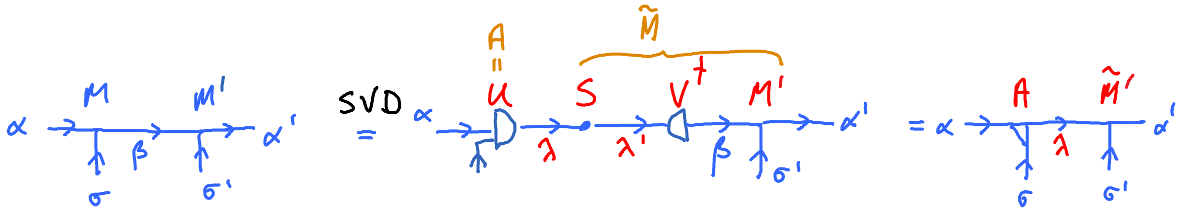
Goal : left-normalize M^{σ_1} to $M^{\sigma_{\mathscr{L}-1}}$



(6)

Strategy: take a pair of adjacent tensors, MM', and use SVD to yield left isometry on the left:

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



(8)

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

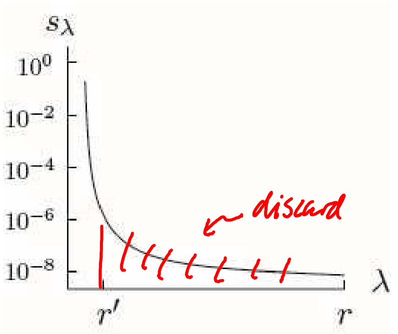
The property $U^\dagger U = \mathbb{1}$ ensures left-normalization: $A^\dagger A = \mathbb{1}$ (10)

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!)



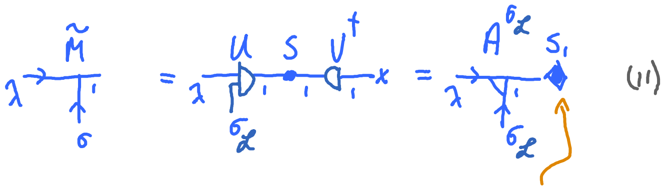
Note: instead of SVD, we could also me QR (cheaper!)

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

To left-normalize the entire MPS, choose $\ell = \mathscr{L}$.

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

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



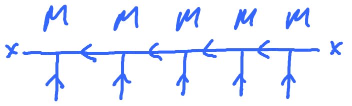
diamond indicates single number

lc-form: $|\psi\rangle = |\vec{\sigma}\rangle_{\mathscr{L}} \left(A^{\sigma_1} \dots A^{\sigma_{\mathscr{L}}}\right) s_1$

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

Transforming to right-normalized form

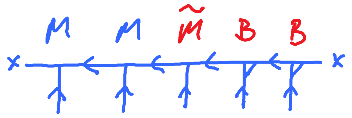
Given: $|\psi\rangle = |\vec{\sigma}\rangle_{\mathscr{L}} \left(M^{\sigma_1} \dots M^{\sigma_{\mathscr{L}}}\right)$



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

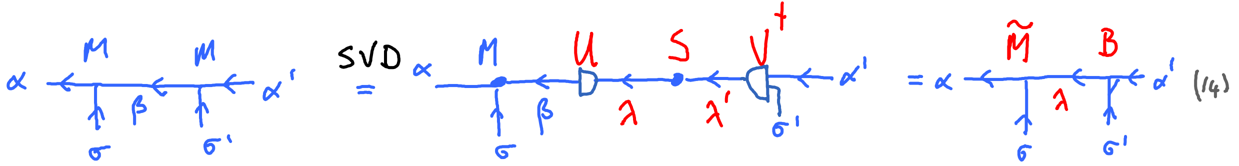
]

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



Strategy: take a pair of adjacent tensors, MM', and use SVD to yield right isometry on the right:

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



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

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

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

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

$$\tilde{M}_{1}{}^{\sigma_1\lambda} = \underbrace{U_{1}{}^{1}} \underbrace{S_{1}{}^{1}} \underbrace{V^{\dagger}{}_{1}{}^{\sigma_1\lambda}} \ .$$

s_1 determines normalization. (17)

$$\underbrace{\quad}_{=1}\underbrace{\quad}_{S_1}\underbrace{\qquad}_{B_1{}^{\sigma_1\lambda}}$$

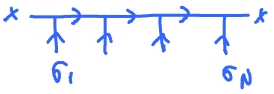
Summary: using SVD, products of two matrices can be converted into forms containing a left isometriy on the left or right isometry on the right:

$$M\,M' = A\,\tilde{M}' = \tilde{M}\,B \qquad (18)$$

This can be used iteratively to convert any of the four canonical forms into any other one.

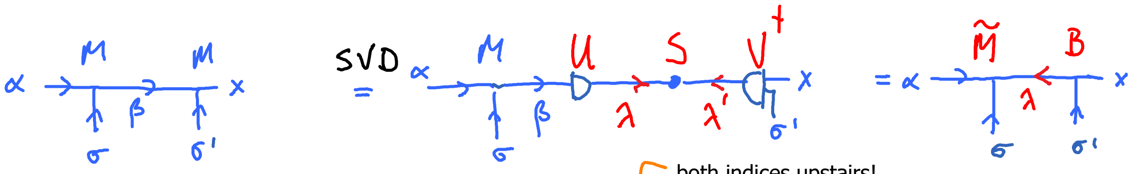
Examples [self-study!]

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



Hint: start at $M^{\sigma_{\mathcal{L}-1}}\,M^{\sigma_{\mathcal{L}}}$

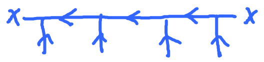
and note the up ↔ down changes in index placement.



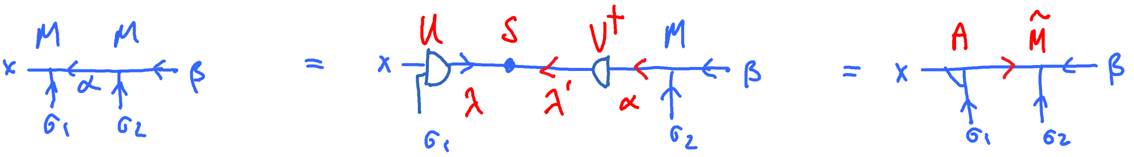
both indices upstairs!

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

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



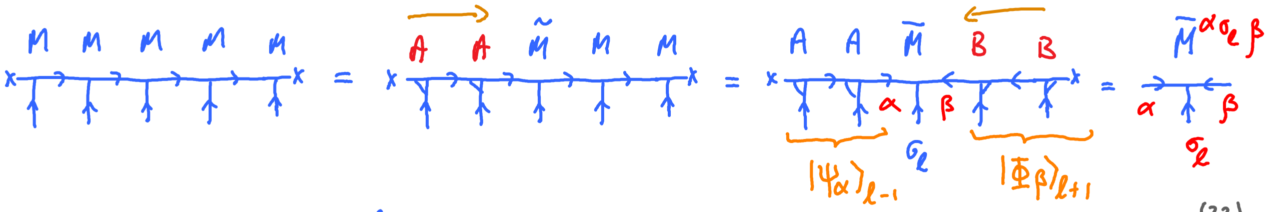
Hint: start at $M^{\sigma_1}M^{\sigma_2}$:



both indices upstairs!

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

(c) Transforming to site-canonical form



(22)

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

Then right-normalize sites $\mathcal{L}$ to $\ell+1$, starting from site $\mathcal{L}$.

Result:

$$|\psi\rangle = \underbrace{|\sigma_N\rangle\ldots|\sigma_{\ell+1}\rangle\left(B^{\sigma_{\ell+1}}\ldots B^{\sigma_N}\right)_{\beta}{}^{1}}_{|\Phi_\beta\rangle_{\ell+1}}\;|\sigma_\ell\rangle\;\underbrace{|\sigma_{\ell-1}\rangle\ldots|\sigma_1\rangle\left(A^{\sigma_1}\ldots A^{\sigma_{\ell-1}}\right)^{1}{}_{\alpha}}_{|\Psi_\alpha\rangle_{\ell-1}}\;\bar{M}^{\alpha\sigma_\ell\beta} \qquad (23)$$

$$= |\Phi_\beta\rangle_{\ell+1}\,|\sigma_\ell\rangle\,|\Psi_\alpha\rangle_{\ell-1}\,\bar{M}^{\alpha\sigma_\ell\beta} \qquad (24)$$

The states $|\alpha,\sigma_\ell,\beta\rangle := |\Phi_\beta\rangle_{\ell+1}\,|\sigma_\ell\rangle\,|\Psi_\alpha\rangle_{\ell-1}$ form an orthonormal set:

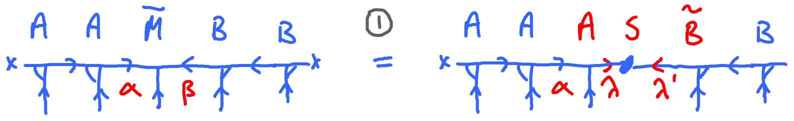
$$\langle\alpha',\sigma_\ell',\beta'|\alpha,\sigma_\ell,\beta\rangle = \delta^{\alpha'}{}_{\alpha}\,\delta^{\sigma_\ell'}{}_{\sigma_\ell}\,\delta^{\beta'}{}_{\beta} \qquad (25)$$

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

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

(d) Transforming to bond-canonical form

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 .



$$= \underbrace{|\Phi_{\lambda'}\rangle_{\ell+1}}_{\text{involves sites } \ell+1 \text{ to } \mathcal{L}}\cdot\underbrace{|\Psi_\lambda\rangle_\ell}_{\text{involves sites } 1 \text{ to } \ell}\,S^{\lambda\lambda'} \qquad (26)$$

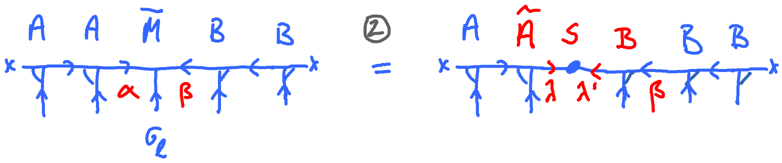
$$\bar{M} = USV^\dagger \qquad A = U\,,\quad \hat{B} = V^\dagger B$$ (Exercise: add indices!) (27)

The states $|\lambda,\lambda'\rangle := |\Phi_{\lambda'}\rangle_{\ell+1}\cdot|\Psi_\lambda\rangle_\ell$ 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).



$$= \underbrace{|\Phi_{\lambda'}\rangle_{\ell}}_{\text{involves sites } \ell \text{ to } \mathcal{L}}\;\underbrace{|\Psi_\lambda\rangle_{\ell-1}}_{\text{involves sites } 1 \text{ to } \ell-1}\,S^{\lambda\lambda'} \qquad (29)$$

$$\bar{M} = USV^\dagger \qquad \tilde{A} = AU\,,\quad B = V^\dagger$$ (Exercise: add indices!) (30)

$|\lambda,\lambda'\rangle := |\Phi_{\lambda'}\rangle_\ell\cdot|\Psi_\lambda\rangle_{\ell-1}$ form 'local bond basis' for bond $\ell-1$ (from site $\ell-1$ to ℓ).