

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

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


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-facing diagonals' at vertices



$$(2b)$$

identity matrix

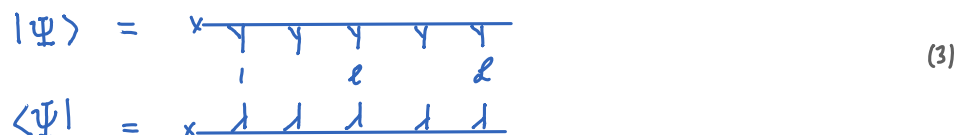
The right-angled triangle contains complete information about all arrows attached to it:

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:

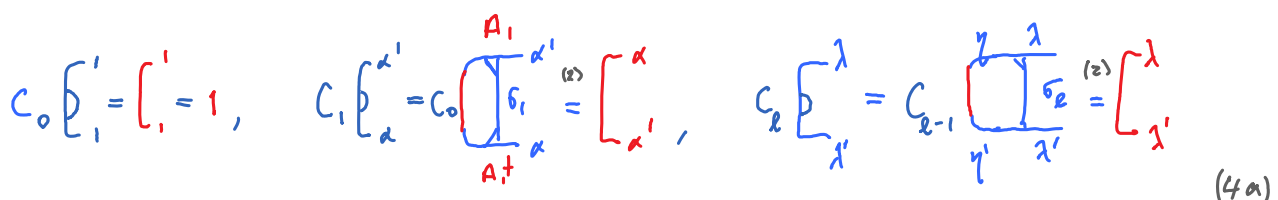
Hence, there is no need to draw arrows explicitly when using  $\nabla$ ,  $\perp$  !

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 constituent  $A$ s.

$$A_i^\dagger \quad \lambda \quad \gamma \quad \lambda \quad (4a)$$

We suppress arrows for  $C$ , too, since they can be reconstructed from arrows of constituent  $A$ s.

Hence:

$$\langle \Psi | \Psi \rangle = \text{diagram} = \text{diagram} = \text{diagram} = \begin{bmatrix} x \\ x \end{bmatrix} = 1 \quad \text{smiley face} \quad (4b)$$

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

$$\text{diagram} \quad |\Psi_\lambda\rangle_\ell = |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \dots \otimes |\sigma_\ell\rangle [A_1^{\sigma_1} A_2^{\sigma_2} \dots A_\ell^{\sigma_\ell}]'_\lambda \quad (5)$$

$$\text{diagram} = \begin{bmatrix} \lambda \\ \lambda' \end{bmatrix} \quad \langle \Psi^{\lambda'} | \Psi_\lambda \rangle_\ell = \mathbb{1}^{\lambda'}_\lambda \quad \text{smiley face} \quad (6)$$

close the zipper

Call this state space  $V_\ell = \text{span} \{ |\Psi_\lambda\rangle_\ell \} \subseteq V_1 \otimes V_2 \otimes \dots \otimes V_\ell \quad (7)$

where  $V_\ell = \text{span} \{ |\sigma_\ell\rangle \}$  is local state space of site  $\ell$

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

Each  $A_\ell$  defines an isometric map to a new (possibly smaller) basis:

$$A_\ell: V_{\ell-1} \otimes V_\ell \rightarrow V_\ell, \quad |\Psi_{\lambda'}\rangle_{\ell-1} |\sigma_\ell\rangle \mapsto |\Psi_\lambda\rangle_\ell = |\Psi_{\lambda'}\rangle_{\ell-1} |\sigma_\ell\rangle [A_\ell]^{\lambda\sigma_\ell}_{\lambda'} \quad (8)$$

old basis                      new basis

If  $A_\ell$  is a unitary, then  $\dim(V_\ell) = \dim(V_{\ell-1}) \cdot \dim(V_\ell) \Rightarrow$  no truncation  $(9)$

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

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

Hence  $V_\ell = V_1 \otimes V_2 \otimes \dots \otimes V_\ell$  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.

$D^2 d \cdot \ell$

## 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:

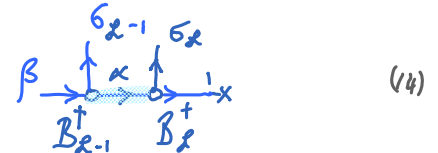
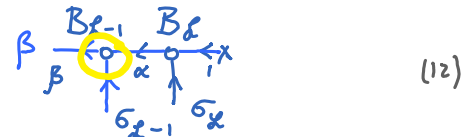
$$|\alpha\rangle = |\sigma_x\rangle [B_x]_{\alpha}^{\sigma_x'} \quad \text{left-to-right index order as in diagram}$$

$$|\beta\rangle = |\sigma_{x-1}\rangle |\sigma_x\rangle [B_{x-1}]_{\beta}^{\sigma_{x-1}'} [B_x]_{\alpha}^{\sigma_x'}$$

$$\langle\alpha| = [B_x^\dagger]_{\sigma_x}^{\alpha} \langle\sigma_x|$$

$$:= [B_x]_{\alpha}^{\sigma_x'}$$

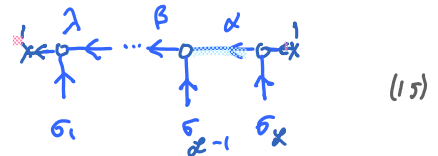
$$\langle\beta| = [B_x^\dagger]_{\sigma_x}^{\alpha} [B_{x-1}^\dagger]_{\sigma_{x-1}}^{\beta} \langle\sigma_x| \langle\sigma_{x-1}|$$



Iterating this, we obtain kets and bras of the form

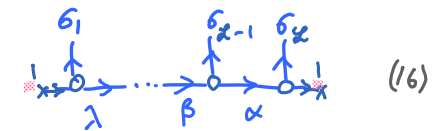
$$|\psi\rangle = |\sigma_1\rangle |\sigma_2\rangle \dots |\sigma_x\rangle [B_1]_{\sigma_1}^{\sigma_1'} \dots [B_{x-1}]_{\sigma_{x-1}}^{\sigma_{x-1}'} [B_x]_{\alpha}^{\sigma_x'}$$

$$= |\bar{\sigma}\rangle [B_1^{\sigma_1'} \dots B_{x-1}^{\sigma_{x-1}'} B_x^{\sigma_x'}]_{\alpha}$$



$$\langle\psi| = [B_1^\dagger]_{\sigma_1}^{\alpha} [B_2^\dagger]_{\sigma_2}^{\beta} \dots [B_x^\dagger]_{\sigma_x}^{\alpha} \langle\sigma_1| \dots \langle\sigma_2| \langle\sigma_1|$$

$$= [B_x^{\sigma_x} B_{x-1}^{\sigma_{x-1}} \dots B_1^{\sigma_1}]_{\alpha} \langle\bar{\sigma}|$$

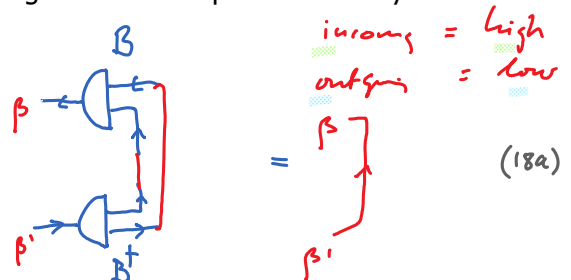
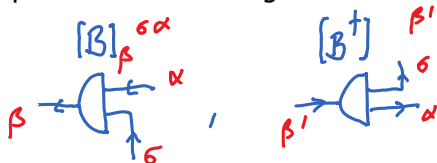


A three-leg tensor  $B_\beta^{\sigma\alpha}$  is called right-normalized if it is a right isometry, i.e. if it satisfies

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

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

Graphical notation for right-normalization:



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



$$(18b)$$

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:

$$(19)$$

Moreover, the matrices for site  $l$  to any site  $l' = 1, \dots, L$  define an orthonormal state space:

$$(20)$$

$$(21)$$

Call this state space  $W_l = \text{span} \{ |\Phi_\lambda\rangle_l \} \subseteq V_l \otimes V_{l+1} \otimes \dots \otimes V_{L'}$  (22)

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

Each  $\frac{B_l}{\sqrt{\lambda}}$  defines an isometric map to a new (possibly smaller) basis:

$$(23)$$

$W_l = V_l \otimes V_{l+1} \otimes \dots \otimes V_{L'}$  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. 😊

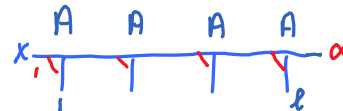
Any matrix product can be expressed in infinitely many different ways without changing the product:

$$M M' = (M U U^{-1} M') = \tilde{M} \tilde{M}' \quad \text{'gauge freedom'} \quad (1)$$

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

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

[all tensors are left-normalized, denoted  $A$ ]



$$(2)$$

$$|\Psi_\alpha\rangle = |\sigma_1\rangle \dots |\sigma_L\rangle [A_1^{\sigma_1} \dots A_L^{\sigma_L}]'_\alpha$$

$$A^\dagger A = \mathbb{1}$$

$$\boxed{\text{A}} = \text{[ ]} \quad (3)$$

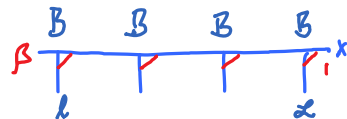
These states form an orthonormal set:

$$\langle \Psi^{\alpha'} | \Psi_\alpha \rangle = \mathbb{1}^{\alpha' \alpha} \quad (\text{MPS-I.2.6}) \quad (4)$$

In general,  $\mathbb{V}_L \subset \mathbb{H}^L$ .  
true subset

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

[all tensors are right-normalized, denoted  $B$ ]



$$(5)$$

$$|\Phi_\beta\rangle = |\sigma_1\rangle \dots |\sigma_L\rangle [B_1^{\sigma_1} \dots B_L^{\sigma_L}]'_\beta$$

$$B B^\dagger = \mathbb{1}$$

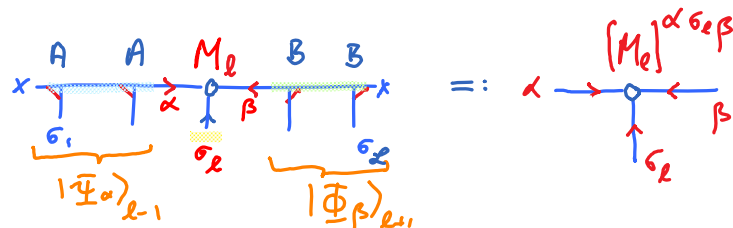
$$\boxed{\text{B}} = \text{[ ]} \quad (6)$$

These states form an orthonormal set:

$$\langle \Phi^{\beta'} | \Phi_\beta \rangle = \mathbb{1}^{\beta' \beta} \quad (\text{MPS-I.2.18}) \quad (7)$$

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

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



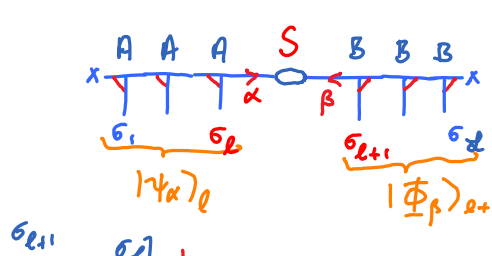
$$(8)$$

$$|\Psi\rangle = |\bar{\sigma}\rangle_l [A_1^{\sigma_1} \dots A_{l-1}^{\sigma_{l-1}}]'_\alpha [M_l]^{\alpha \sigma_l \beta} [B_{l+1}^{\sigma_{l+1}} \dots B_L^{\sigma_L}]'_\beta = |\Psi_\alpha\rangle_{l-1} |\sigma_l\rangle |\Phi_\beta\rangle_{l+1} [M_l]^{\alpha \sigma_l \beta} \quad (9)$$

The states  $|\alpha, \sigma_l, \beta\rangle := |\Psi_\alpha\rangle_{l-1} |\sigma_l\rangle |\Phi_\beta\rangle_{l+1}$  form an orthonormal set:  $\langle \alpha', \sigma'_l, \beta' | \alpha, \sigma_l, \beta \rangle = \mathbb{1}_\alpha \mathbb{1}_{\sigma'_l \sigma_l} \mathbb{1}_{\beta' \beta}$   
 $M_l^{\alpha \sigma_l \beta}$  can be viewed as the wavefunction of  $|\Psi\rangle$  in this basis. (10)

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

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



$$(11)$$

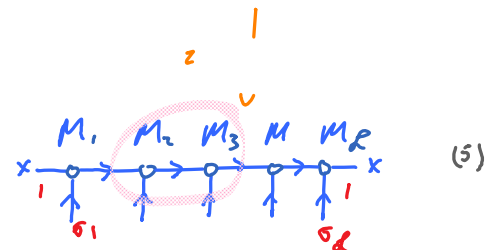
$$|\psi\rangle = |\vec{\sigma}\rangle_{\mathcal{L}} [A_1 \dots A_{\ell}]^{\sigma_1 \dots \sigma_{\ell}} = \underbrace{|\psi_{\alpha}\rangle_{\mathcal{L}}}_{\text{can be chosen diagonal}} \underbrace{|\Phi_{\beta}\rangle_{\mathcal{R}}}_{\text{can be chosen diagonal}} S^{\alpha\beta} \quad (12)$$

The states  $|\alpha, \beta\rangle := |\psi_{\alpha}\rangle_{\mathcal{L}} |\Phi_{\beta}\rangle_{\mathcal{R}}$  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 site-normalized form

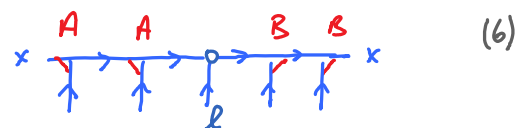
Given:  $|\psi\rangle = |\vec{\sigma}\rangle_{\mathcal{L}} [M_1 \dots M_{\ell}]^{\sigma_1 \dots \sigma_{\ell}}$



[or with index:  $|\psi_{\alpha}\rangle = \text{[diagram with index } \alpha]$ ]

Goal (i): left-normalize  $M_1$  to  $M_{\ell-1}$

Goal (ii): right-normalize  $M_{\ell}$  to  $M_{\ell+1}$



(i) take a pair of adjacent tensors,  $MM'$ , and use SVD to yield left isometry on the left:

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

$U^{\dagger}U = \mathbb{1}$  (QR decomposition of  $M'$ )

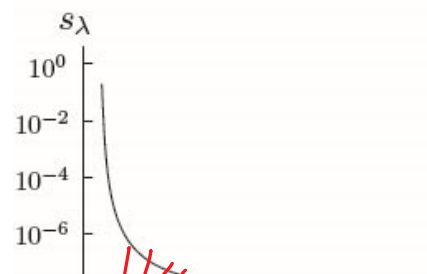
$$\alpha \rightarrow M \rightarrow M' \rightarrow \alpha' \xrightarrow{\text{SVD}} \alpha \rightarrow A \rightarrow \tilde{M}' \rightarrow \alpha' \quad (8)$$

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

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, using  $USV^{\dagger} \approx U'SV'^{\dagger}$

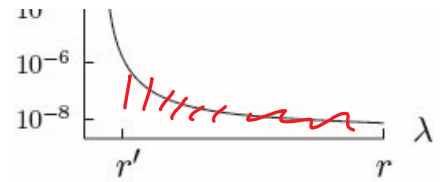
$$\sum_{\lambda=1}^{\tau} \rightarrow \sum_{\lambda=1}^{\tau'} \quad (\text{but (10) remains valid!})$$



$$\sum_{\lambda=1} \rightarrow \sum_{\lambda=1}$$

(but (10) remains valid!)

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



Starting from  $M_1 M_2 = A_1 \tilde{M}_2$ , move rightward up to  $\tilde{M}_{l-1} M_l = A_{l-1} \tilde{M}_l$

$$x \begin{array}{c} M_1 \\ \downarrow \\ \sigma_1 \end{array} \begin{array}{c} M_2 \\ \downarrow \\ \sigma_2 \end{array} \begin{array}{c} M_3 \\ \downarrow \\ \sigma_3 \end{array} \begin{array}{c} M \\ \downarrow \\ \sigma \end{array} \begin{array}{c} M_2 \\ \downarrow \\ \sigma_2 \end{array} x = x \begin{array}{c} A_1 \\ \downarrow \\ \sigma_1 \end{array} \begin{array}{c} A_2 \\ \downarrow \\ \sigma_2 \end{array} \begin{array}{c} \tilde{M} \\ \downarrow \\ \sigma_l \end{array} \begin{array}{c} M \\ \downarrow \\ \sigma \end{array} \begin{array}{c} M \\ \downarrow \\ \sigma \end{array} x = \begin{array}{c} A_l \\ \downarrow \\ \sigma_l \end{array} \begin{array}{c} \tilde{M} \\ \downarrow \\ \sigma_l \end{array} x = QR \quad \begin{array}{c} A A A R B B \\ \hline \end{array}$$

Goal (ii): now right-normalize  $M_l$  to  $M_{l+1}$

$$x \begin{array}{c} A \\ \downarrow \\ \sigma \end{array} \begin{array}{c} A \\ \downarrow \\ \sigma \end{array} \begin{array}{c} \tilde{M} \\ \downarrow \\ \sigma_l \end{array} \begin{array}{c} B \\ \downarrow \\ \sigma \end{array} \begin{array}{c} B \\ \downarrow \\ \sigma \end{array} x$$

Take a pair of adjacent tensors,  $M M'$ , and use SVD to yield right isometry on the right:

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

$$\alpha \begin{array}{c} M \\ \downarrow \\ \sigma \end{array} \begin{array}{c} M' \\ \downarrow \\ \sigma' \end{array} \alpha' \xrightarrow{\text{SVD}} \alpha \begin{array}{c} M \\ \downarrow \\ \sigma \end{array} \begin{array}{c} U \\ \downarrow \\ \lambda \end{array} \begin{array}{c} S \\ \downarrow \\ \lambda' \end{array} \begin{array}{c} V^\dagger \\ \downarrow \\ \sigma' \end{array} \alpha' = \alpha \begin{array}{c} \tilde{M} \\ \downarrow \\ \sigma \end{array} \begin{array}{c} B \\ \downarrow \\ \sigma' \end{array} \alpha' \quad (14)$$

$$M_{\alpha}^{\sigma\beta} M'_{\beta}^{\sigma'\alpha'} = (M_{\alpha}^{\sigma\beta} U_{\beta}^{\lambda} S_{\lambda}^{\lambda'}) (V_{\lambda'}^{\dagger} \sigma' \alpha') = \tilde{M}_{\alpha}^{\sigma\lambda'} B_{\lambda'}^{\sigma'\alpha'} \quad (15)$$


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

Starting from  $M_{l-1} M_l = \tilde{M}_{l-1} B_l$ , move leftward up to  $\tilde{M}_l \tilde{M}_{l+1} = \tilde{M}_l B_{l+1}$

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

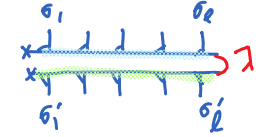
$$M M' = A \tilde{M}' = \tilde{M} B \quad (18)$$

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

Recall: a set of MPS  $|\Psi_\lambda\rangle_e = |e_1\rangle \otimes \dots \otimes |e_\ell\rangle [A_1^{\sigma_1} \dots A_\ell^{\sigma_\ell}]^\lambda_\lambda =$   (1)  
specified by given left-normalized tensors

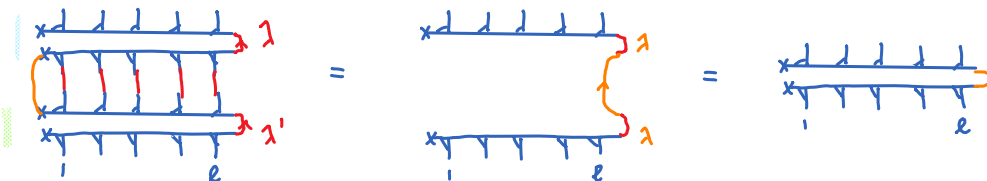
defines an orthonormal basis for a state space  $V_e = \text{span}\{|\Psi_\lambda\rangle_e\} \subseteq V_1 \otimes V_2 \otimes \dots \otimes V_\ell =: V^{\otimes \ell}$  (2)

since  $\langle \Psi^{\lambda'} | \Psi^\lambda \rangle_e =$    $\stackrel{\text{close zipper}}{=} \left\{ \begin{matrix} \lambda \\ \lambda' \end{matrix} \right\} = \mathbb{I}^{\lambda'}_\lambda$  (3)

Projector onto  $V_e$ :  $\hat{P}_e = |\Psi_\lambda\rangle_e \langle \Psi^\lambda| =$   (4)  
(sum over  $\lambda$  implied)

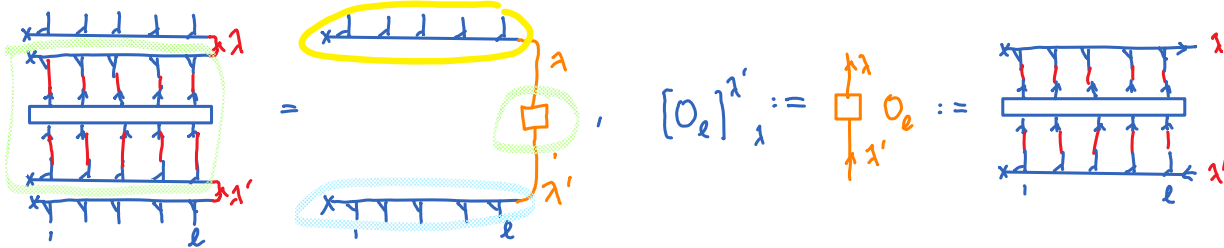
Indeed:

$$\hat{P}_e \hat{P}_e = |\Psi_{\lambda'}\rangle_e \langle \Psi^{\lambda'}| \cdot |\Psi_\lambda\rangle_e \langle \Psi^\lambda| = \hat{P}_e \quad \checkmark \quad (5)$$


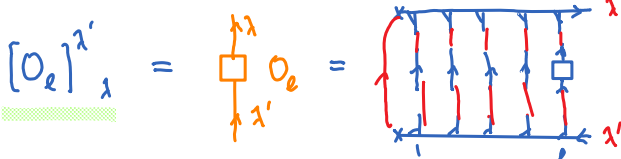
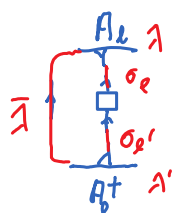
$$=$$
  (6)

Operators defined on  $V_e^{\otimes \ell}$  can be mapped to  $V_e$  using these projectors:

$$\hat{O} =$$
   $\xrightarrow{\hat{P}_e} \hat{O}_e =: \hat{P}_e \hat{O} \hat{P}_e =: |\Psi_{\lambda'}\rangle_e [O_e]^{\lambda'}_{\lambda} \langle \Psi^\lambda|$  (7)

$$\hat{O}_e =$$
  (8)

Simplest case: 1-site operator acting only on site  $\ell$ :

$$\hat{o}_\ell =$$
   $, \quad [O_e]^{\lambda'}_\lambda =$    $\stackrel{\text{close zipper}}{=} \bar{\lambda}$   (9)

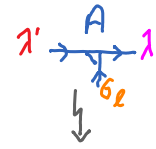
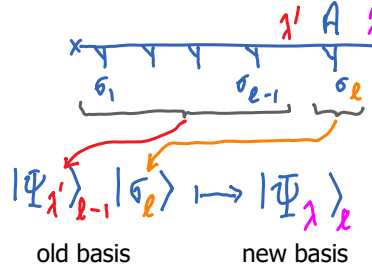
During iterative diagonalization, the space  $V_e$  is constructed through a sequence of isometric maps: (possibly involving truncation)



During iterative diagonalization, the space  $\mathbb{V}_\ell$  is constructed through a sequence of isometric maps: (possibly involving truncation)

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

$$A_\ell: \mathbb{V}_{\ell-1} \otimes \mathbb{V}_\ell \rightarrow \mathbb{V}_\ell,$$

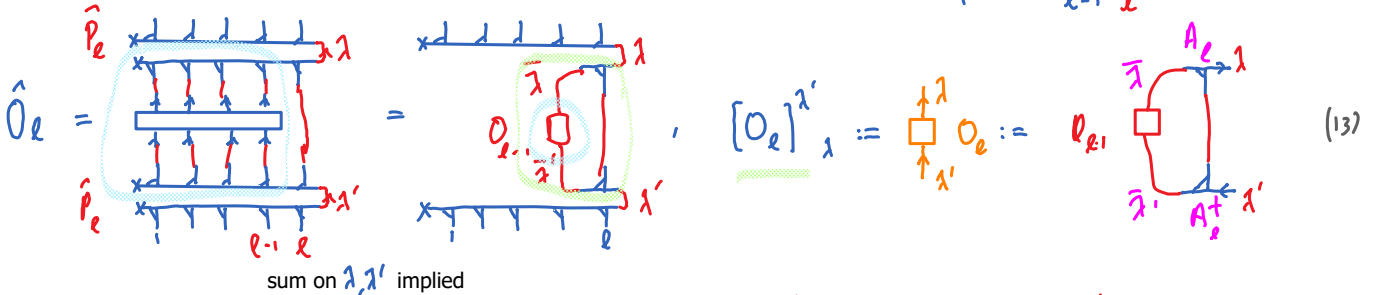


(10)

Each such map also induces a transformation of operators defined on its domain of definition. It is useful to have a graphical depiction for how operators transform under such maps.

Consider an operator defined on  $\mathbb{V}^{\otimes(\ell-1)}$ , represented on  $\mathbb{V}_{\ell-1}$  by  $\hat{O}_{\ell-1} = \hat{P}_{\ell-1} \hat{O} \hat{P}_{\ell-1}$  (11)

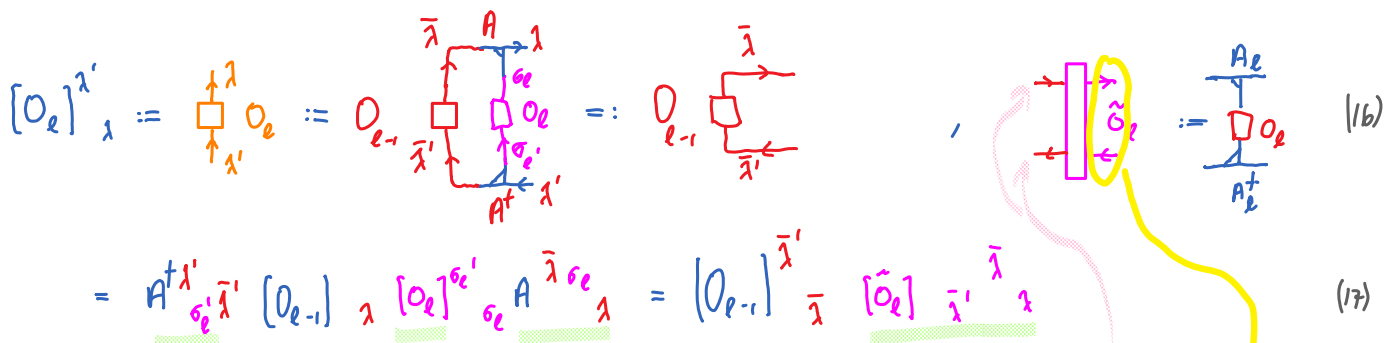
What is its representation on  $\mathbb{V}_\ell$ ?  $\hat{O}_\ell = \hat{O}_{\ell-1} \otimes \mathbb{1}_\ell =$  (12)



Explicitly:  $\hat{O}_\ell = |\Psi_{\lambda'}\rangle_\ell [O_\ell]^{\lambda'}_\lambda \langle \Psi^\lambda|$ ,  $[O_\ell]^{\lambda'}_\lambda = A^{\dagger \lambda' \sigma_\ell \bar{\lambda}'} [O_{\ell-1}]^{\bar{\lambda}'}_{\bar{\lambda}} A^{\bar{\lambda} \sigma_\ell}_\lambda$  (14)

Similarly, for operator with non-trivial action also on site :  $\hat{O}_\ell = \hat{O}_{\ell-1} \otimes \hat{\sigma}_\ell =$  (15)

Just replace  $\uparrow$  by in (9):



Thus, the isometry  $A_\ell$  maps the local operator into an effective basis associated with  $\mathbb{V}_{\ell-1}$  and  $\mathbb{V}_\ell$