Matrix product states (MPS)

MPS.1 Reshaping generic tensor into MPS form

A generic tensor of arbitrary rank can be expressed as an MPS through repeated matrix factorizations,

using QR decomposition, $M \overset{\text{TNB-III.2}}{=} QR$, or singular value decomposition (SVD): $M \overset{\text{TNB-III.2}}{=} USV^\dagger$

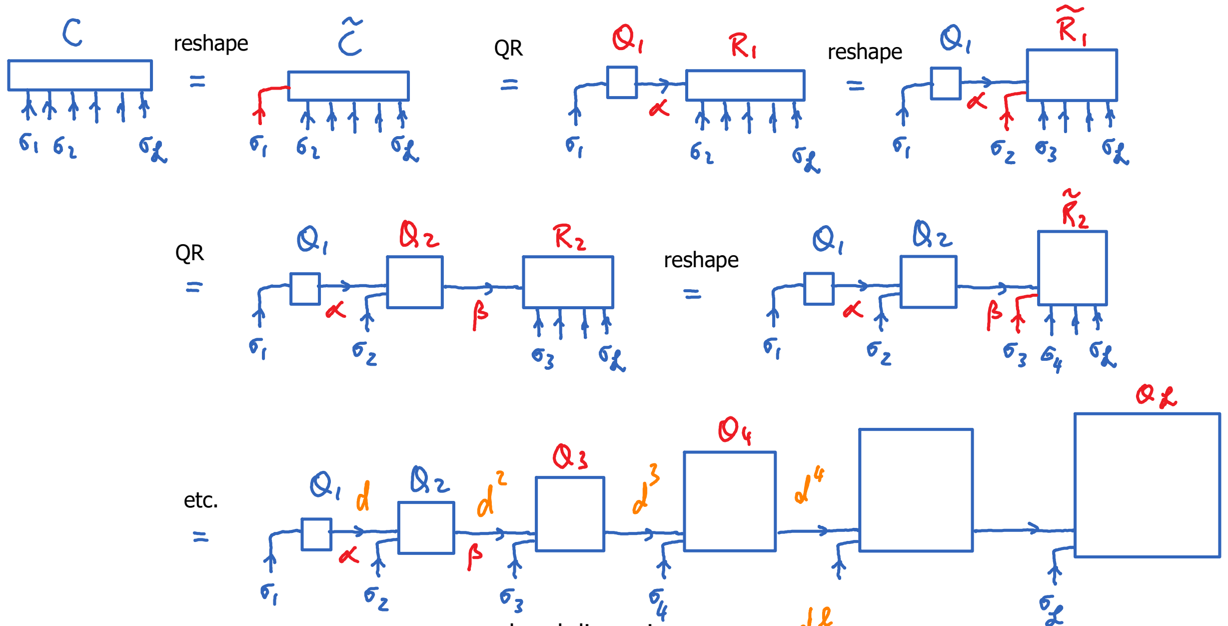
$$M^a{}_b = Q^a{}_c R^c{}_b \qquad\qquad M^a{}_b = U^a{}_c S^c{}_d V^{\dagger d}{}_e$$

$$C^{\sigma_1\ldots\sigma_\mathcal{L}} \overset{\substack{\text{reshape}\\ \text{(= regroup indices)}}}{=} \tilde{C}^{\sigma_1,\sigma_2\ldots\sigma_\mathcal{L}} \overset{\text{QR}}{=} Q_1^{\sigma_1}{}_\alpha R_1^{\alpha,\sigma_2\ldots\sigma_\mathcal{L}} \overset{\text{reshape}}{=} Q_1^{\sigma_1}{}_\alpha \tilde{R}_1^{\alpha\sigma_2,\sigma_3\ldots\sigma_\mathcal{L}} \qquad (1)$$

$$\overset{\text{QR}}{=} Q_1^{\sigma_1}{}_\alpha Q_2^{\alpha\sigma_2}{}_\beta R_2^{\beta,\sigma_3\ldots\mathcal{L}} \overset{\text{reshape}}{=} Q_1^{\sigma_1}{}_\alpha Q_2^{\alpha\sigma_2}{}_\beta \tilde{R}_2^{\beta\sigma_3,\sigma_4\ldots\mathcal{L}} \overset{\text{etc.}}{=} \ldots \qquad (2)$$

$$= Q_1^{\sigma_1}{}_\alpha Q_2^{\alpha\sigma_2}{}_\beta Q_3^{\beta\sigma_3}{}_\gamma \ldots R_{\mathcal{L}-1}^{\mu\sigma_\mathcal{L}} \qquad (3)$$

Visualization:

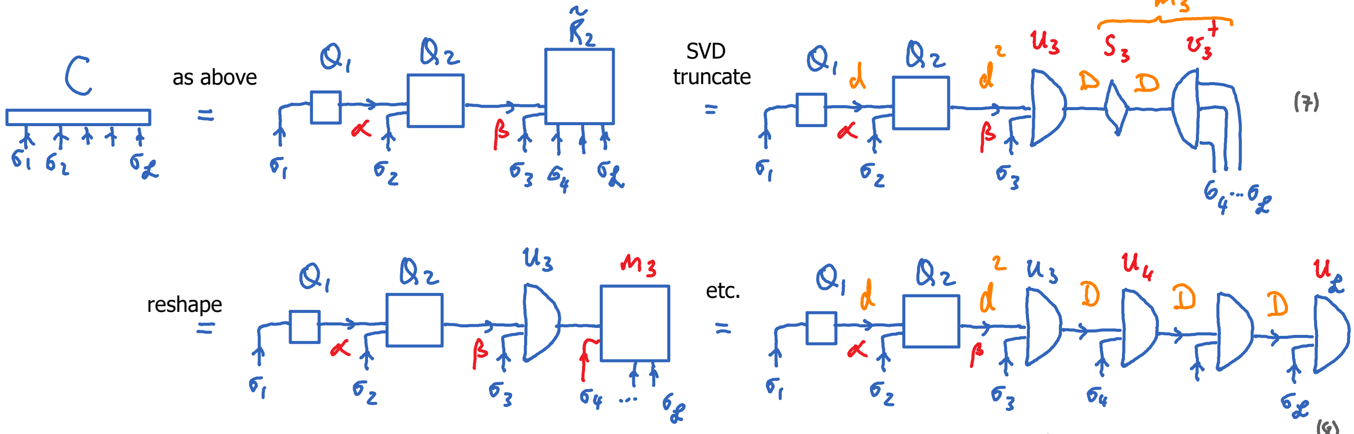


bond dimensions grow as $d^\mathcal{L}$

If a maximal bond dimension of $D_\alpha < D$ is desired, this can be achieved using SVD instead of QR decompositions, and truncating by retaining only largest D singular values at each step:

$R \overset{\text{SVD}}{=} US'V^\dagger$ (U and V are isometries, S' is diagonal, with non-negative elements)

$\overset{\text{truncate}}{\simeq} usv^\dagger$ where s contains only largest D singular values of S'



truncated representation

MPS.2 Overlaps, matrix elements

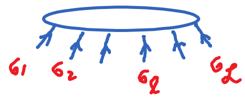
Overlaps $\langle\tilde\psi|\psi\rangle$

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

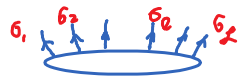
General ket: $|\psi\rangle = |\sigma_1\rangle|\sigma_2\rangle\ldots|\sigma\rangle\, C^{\sigma_1,\ldots,\sigma_\mathscr{L}} =: |\vec\sigma\rangle\, C^{\vec\sigma}$ (1)

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

summation over repeated indices implied



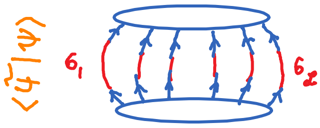
General bra: $\langle\psi| = \underbrace{\overline{C^{\sigma_1,\ldots,\sigma_\mathscr{L}}}}_{=:\, C^\dagger_{\vec\sigma_R}}\langle\sigma_\mathscr{L}|\ldots\langle\sigma_2|\langle\sigma_1| =: \underbrace{C^\dagger_{\vec\sigma_R}}_{:=\, \overline{C^{\vec\sigma}}}\langle\vec\sigma|$ (2)



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

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

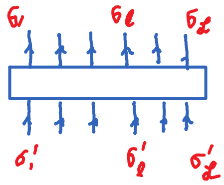
$$= \tilde C^\dagger_{\vec\sigma_R}\, C^{\vec\sigma}$$



(3b)

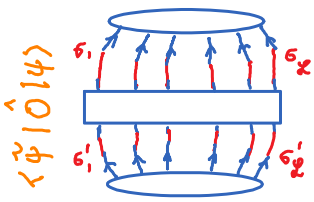
Recipe for overlaps: contract all physical legs of bra and ket.

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



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

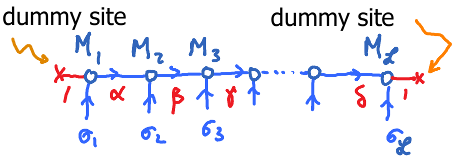
Now consider matrix product states:

Ket:

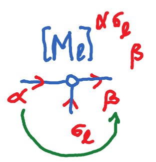
dummy index

$|\psi\rangle = |\vec\sigma\rangle\underbrace{[M_1]^{1\sigma_1}{}_\alpha[M_2]^{\alpha\sigma_2}{}_\beta}\underbrace{[M_3]^{\beta\sigma_3}{}_\gamma}\ \ [M_\mathscr{L}]^{\gamma\sigma_\mathscr{L}}{}_1$

dummy index



(6)



index-reading order

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

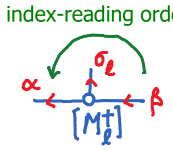
The subscript ℓ on M_ℓ indicates that the tensors differ from site to site. The tensor M_ℓ has elements $[M_\ell]^{\alpha\sigma_\ell}{}_\beta$, indicated using square brackets.

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

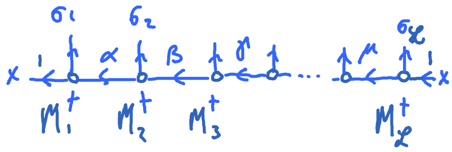
Bra:

$$\langle\psi| = \overline{[M_1]}^{1\sigma_1}{}_{\alpha}\,\overline{[M_2]}^{\alpha\sigma_2}{}_{\beta}\,\overline{[M_3]}^{\beta\sigma_3}{}_{\gamma}\;\overline{[M_\mathcal{L}]}^{\gamma\sigma_\mathcal{L}}{}_{1}\,\langle\vec\sigma|$$

$$\overline{M^{\alpha\sigma}{}_{\beta}} =: M^{\dagger\beta}{}_{\sigma\alpha} \tag{7a}$$



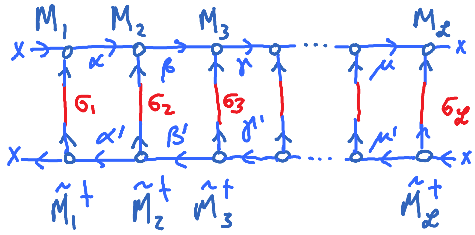
$$= [M^\dagger_\mathcal{L}]^{1}{}_{\sigma_\mathcal{L}\mu}\cdots[M^\dagger_3]^{\gamma}{}_{\sigma_3\beta}\,[M^\dagger_2]^{\beta}{}_{\sigma_2\alpha}\,[M^\dagger_1]^{\alpha}{}_{\sigma_1 1} \tag{7b}$$



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 $M^\dagger_\sigma$ on the left, (in opposite order as vertices in diagram), resulting in a matrix product of $M^\dagger_\sigma$ matrices.

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



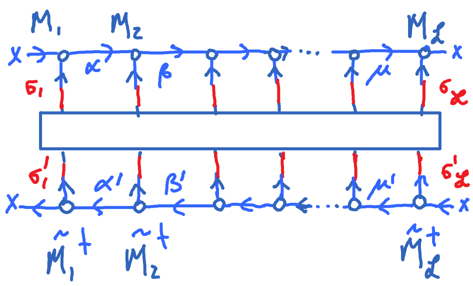
Recipe: contract all physical indices! (8a)

$$= [\tilde M^\dagger_\mathcal{L}]^{1}{}_{\sigma_\mathcal{L}\mu'}\cdots[\tilde M^\dagger_2]^{\beta'}{}_{\sigma_2\alpha'}\,[\tilde M^\dagger_1]^{\alpha'}{}_{\sigma_1 1}\,[M_1]^{1\sigma_1}{}_{\alpha}\,[M_2]^{\alpha\sigma_2}{}_{\beta}\cdots[M_\mathcal{L}]^{\mu\sigma_\mathcal{L}}{}_{1} \tag{8b}$$

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

<u>Matrix elements</u>

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



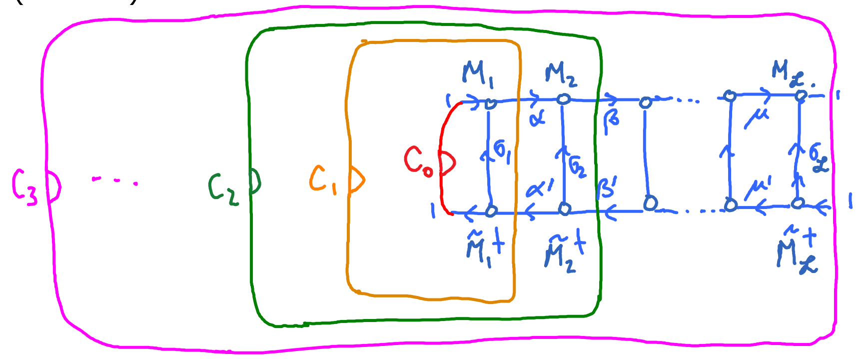
(9)

$$= [\tilde M^\dagger_\mathcal{L}]^{1}{}_{\sigma'_\mathcal{L}\mu'}\cdots[\tilde M^\dagger_2]^{\beta'}{}_{\sigma'_2\alpha'}\,[\tilde M^\dagger_1]^{\alpha'}{}_{\sigma'_1 1}\;O^{\sigma'_1\sigma'_2\ldots\sigma'_\mathcal{L}}{}_{\sigma_1\sigma_2\ldots\sigma_\mathcal{L}}\;[M_1]^{1\sigma_1}{}_{\alpha}\,[M_2]^{\alpha\sigma_2}{}_{\beta}\cdots[M_\mathcal{L}]^{\mu\sigma_\mathcal{L}}{}_{1} \tag{10}$$

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

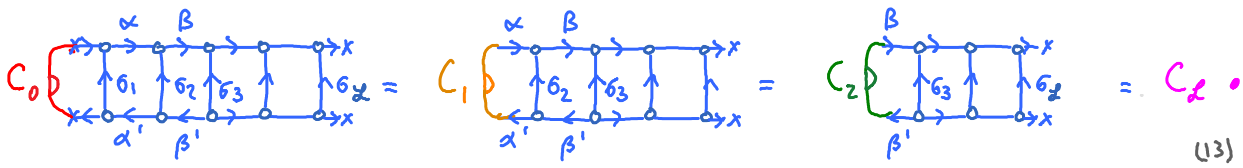
But calculation becomes tractable if we rearrange summations, to keep number of 'open legs' as small as possible (here = 2):

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

(11)

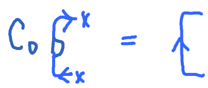
$$\underbrace{[\tilde M_\mathcal{L}^\dagger]^{1'}{}_{\sigma_\mathcal{L}\mu'}\cdots\underbrace{[\tilde M_2^\dagger]^{\beta'}{}_{\sigma_2\alpha'}\underbrace{[\tilde M_1^\dagger]^{\alpha'}{}_{\sigma_1 1'}\,\overbrace{1'\cdot 1}^{=:[C_0]^{1'}{}_1}\,[M_1]^{1\sigma_1}{}_{\alpha}}_{=:[C_1]^{\alpha'}{}_\alpha}[M_2]^{\alpha\sigma_2}{}_{\beta}}_{=:[C_2]^{\beta'}{}_\beta}\cdots[M_\mathcal{L}]^{\mu\sigma_\mathcal{L}}{}_1}_{=:[C_\mathcal{L}]^{1'}{}_1} \qquad (12)$$

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



(13)

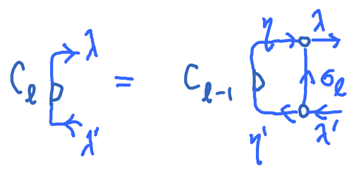
The set of two-leg tensors C_ℓ can be computed iteratively:

Initialization: 

(identity)

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

Iteration step:
sum over σ_ℓ
yields C_ℓ

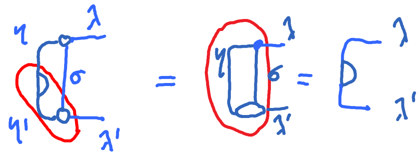


$$[C_\ell]^{\lambda'}{}_{\lambda} = [\tilde M_\ell^\dagger]^{\lambda'}{}_{\sigma_\ell\eta'}\,[C_{\ell-1}]^{\eta'}{}_{\eta}\,[M_\ell]^{\eta\sigma_\ell}{}_{\lambda} \qquad (15)$$

Final answer: $\langle\tilde\psi|\psi\rangle = [C_\mathcal{L}]^{1'}{}_1$ (16)

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

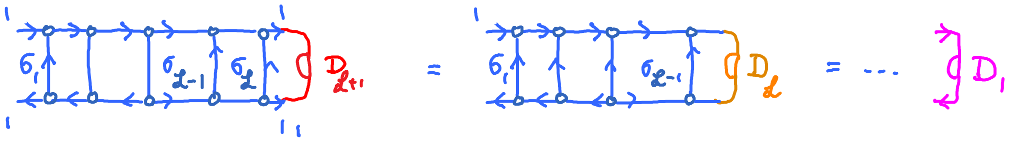
One iteration: $\underbrace{D^2 d}_{\substack{\text{fixed}\\ \lambda'\eta\sigma}}\cdot\underbrace{D}_{\substack{\text{sum}\\ \eta'}} + \underbrace{D^2}_{\substack{\text{fixed}\\ \lambda'\lambda}}\underbrace{dD}_{\substack{\text{sum}\\ \eta\sigma}}$

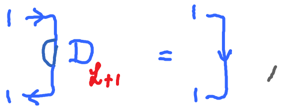

(17)

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

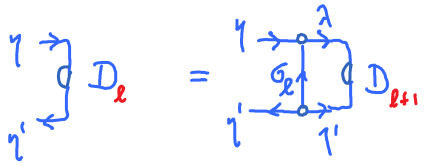
Total cost: $\sim D^3 d \cdot \mathcal{L}$ (18)

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

 (19)

Initialization: 

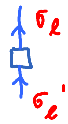
(identity)

iteration step: sum over σ_ℓ yields D_ℓ  (20)

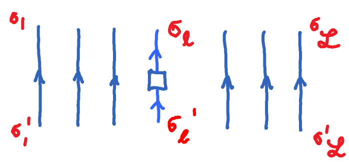
<u>Normalization</u> $\langle \psi | \psi \rangle = ?$ Use above scheme, with $\tilde{M} = M$

'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).

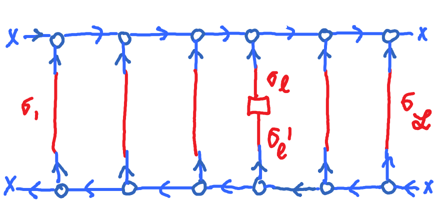
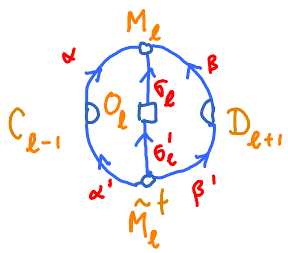
<u>One-site operator</u> (acts non-trivially only on one site, ℓ)

Action on site ℓ : $\hat{O}_\ell = |\sigma'_\ell\rangle [O]^{\sigma'_\ell}{}_{\sigma_\ell} \langle \sigma_\ell|$  (21)

E.g. for spin $\frac{1}{2}$: $[S^z]^{\sigma'}{}_{\sigma} = \frac{1}{2}\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$, $[S^+]^{\sigma'}{}_{\sigma} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $[S^-]^{\sigma'}{}_{\sigma} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

Action on full chain: $\hat{O}_\ell = |\vec{\sigma}'\rangle \underbrace{\mathbb{1}^{\sigma'_1}{}_{\sigma_1} \cdots [O]^{\sigma'_\ell}{}_{\sigma_\ell} \cdots \mathbb{1}^{\sigma'_\mathcal{L}}{}_{\sigma_\mathcal{L}}}_{O^{\vec{\sigma}'}{}_{\vec{\sigma}}} \langle \vec{\sigma}|$  (22)

<u>Matrix element</u> between two MPS:

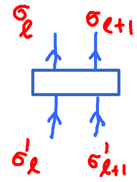
$\langle \tilde{\psi} | \hat{O}_\ell | \psi \rangle =$  $=$  (23)

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

$$= \left[\tilde{M}_\ell^\dagger\right]_{\beta'\sigma_\ell'\alpha'} \left[C_{\ell-1}\right]^{\alpha'}{}_{\alpha} \left[M_\ell\right]^{\alpha\sigma_\ell\beta} \left[D_{\ell+1}\right]_{\beta}{}^{\beta'} \left[O\right]^{\sigma_\ell'}{}_{\sigma_\ell} \qquad (26)$$

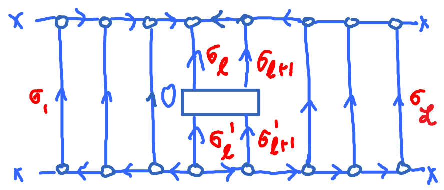
<u>Two-site operator</u> (acts nontrivally only on two sites, ℓ and $\ell+1$) [e.g. for spin chain: $\vec{S}_\ell \cdot \vec{S}_{\ell+1}$]

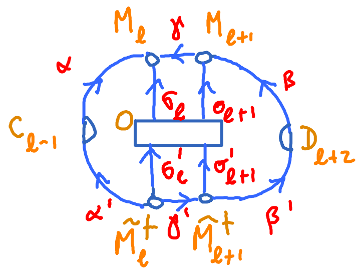
Action on sites ℓ , $\ell+1$: $\hat{O}_{\ell,\ell+1} = |\sigma_\ell'\rangle|\sigma_{\ell+1}'\rangle \left[O\right]^{\sigma_\ell'\sigma_{\ell+1}'}{}_{\sigma_\ell\sigma_{\ell+1}} \langle\sigma_{\ell+1}|\langle\sigma_\ell|$



(10)

Matrix elements:

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

$=$ 

(11)

$$= \left[\tilde{M}_{\ell+1}^\dagger\right]_{\beta'\sigma_{\ell+1}'}{}^{\gamma'} \left[\tilde{M}_\ell^\dagger\right]_{\gamma'\sigma_\ell'\alpha'} \left[C_{\ell-1}\right]^{\alpha'}{}_{\alpha} \left[M_\ell\right]^{\alpha\sigma_\ell\gamma} \left[M_{\ell+1}\right]_{\gamma}{}^{\sigma_{\ell+1}\beta} \left[D_{\ell+2}\right]_{\beta}{}^{\beta'} \left[O\right]^{\sigma_\ell'\sigma_{\ell+1}'}{}_{\sigma_\ell\sigma_{\ell+1}} \qquad (12)$$