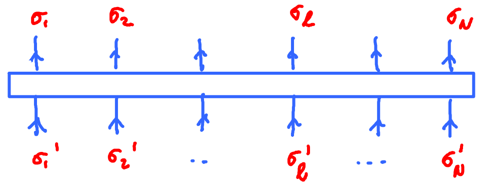
MPS-V: Matrix product operators

[Schollwöck2011, Sec. 5]

MPS-V.1

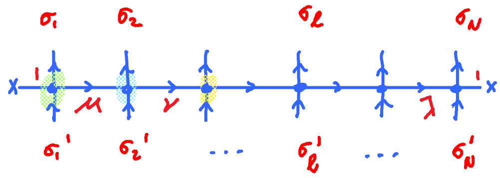
Consider an operator acting on N-site chain:

$$\hat O = |\vec\sigma'\rangle\, O^{\vec\sigma'}{}_{\vec\sigma}\, \langle\vec\sigma| \tag{1}$$

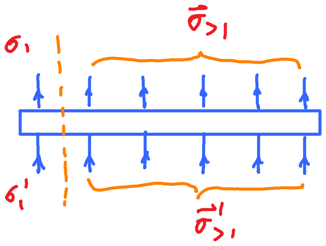


It can always be written as 'matrix product operator' (MPO),

$$\hat O = |\vec\sigma'\rangle\, \underbrace{W^{1\sigma_1'}{}_{\mu\sigma_1} W^{\mu\sigma_2'}{}_{\nu\sigma_2}}\cdots W^{\lambda\sigma_N'}{}_{\sigma_N 1}\,\langle\vec\sigma| \equiv |\vec\sigma'\rangle \prod_\ell W^{\sigma_\ell'}{}_{\sigma_\ell}\,\langle\vec\sigma| \tag{2}$$



using a sequence of QR decompositions:



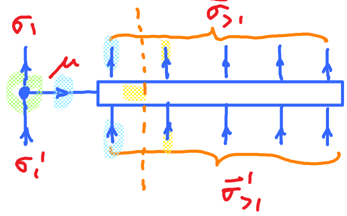
reshape as matrix with composite indices

QR decomposition

$$\equiv (\sigma_1',\sigma_1) \to\bullet\to (\vec\sigma_{>1}',\vec\sigma_{>1}) = (\sigma_1',\sigma_1) \xrightarrow[d^2]{Q} \bullet \xrightarrow[d^2]{\mu} \bullet \xrightarrow[(d^{N-1})^2]{R} (\vec\sigma_{>1}',\vec\sigma_{>1}) \tag{3}$$

reshape again

$$= \tag{4}$$

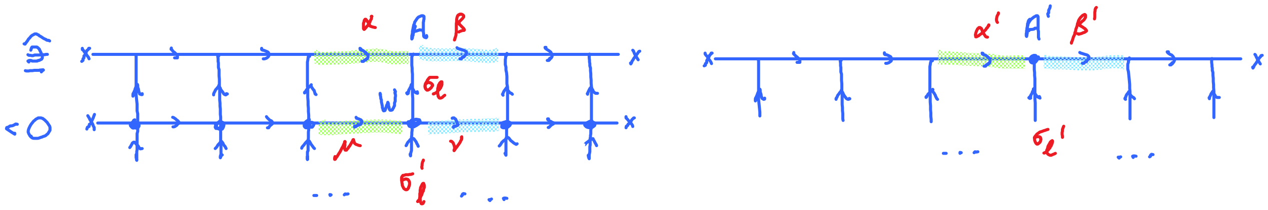


In general, this produces MPO with growing bond dimensions: $d^2,\ (d^2)^2,\ (d^2)^3,\ \ldots$

But for short-ranged Hamiltonians, bond dimension is typically very small, $\mathcal{O}(1)$.

1. Applying MPO to MPS yields MPS

$$|\psi'\rangle = \hat O|\psi\rangle \tag{5}$$

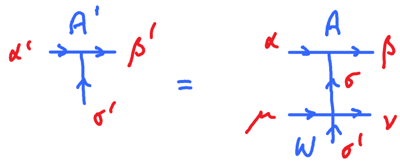


$$\tag{6}$$

$$|\psi\rangle = |\vec\sigma\rangle \prod_\ell A_{[\ell]}^{\alpha_\ell\sigma_\ell}{}_{\beta_\ell} \tag{7}$$

$$|\psi'\rangle = \hat O|\psi\rangle = |\vec\sigma\rangle \prod_\ell A'^{\,\alpha_\ell'\sigma_\ell'}_{[\ell]\;\beta_\ell'} \tag{8}$$

$$A'^{\,\alpha'\sigma'}{}_{\beta'} = W^{\mu\sigma'}{}_{\nu\sigma} A^{\alpha\sigma}{}_{\beta} \tag{9}$$



with composite indices, $\alpha_\ell' = (\alpha,\mu)$, $\beta_\ell' = (\beta,\nu)$, of increased dimension: $\tilde D_{A'} = D_W \cdot D_A$ (10)

In practice, application of MPO is usually followed by SVD+truncation, to 'bring bond dimension back down':

$$A'\,A' \overset{\text{SVD}}{=} U\,S\,V^\dagger A' \overset{\text{truncate}}{\simeq} U\,(\tilde S\,V^\dagger A) \equiv \tilde A'\,\tilde A' \tag{11}$$

Addition of MPOs $\hat O + \hat{\tilde O}$

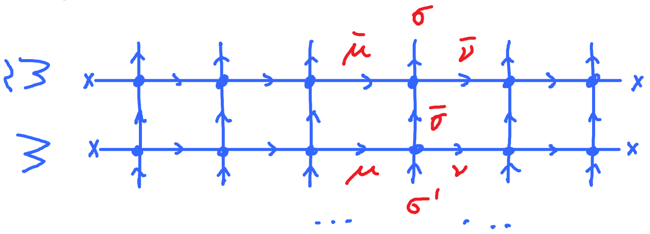
Let $\hat O = |\vec\sigma'\rangle \prod_\ell W^{\sigma'_\ell}{}_{\sigma_\ell} \langle\vec\sigma|$ $\qquad \hat{\tilde O} = |\vec\sigma'\rangle \prod_\ell \tilde W^{\sigma'_\ell}{}_{\sigma_\ell} \langle\vec\sigma|$

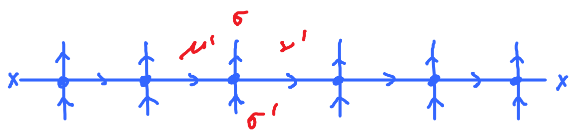
$$\hat O + \hat{\tilde O} = |\vec\sigma'\rangle \left[W W \dots W + \tilde W \tilde W \dots \tilde W \right] \langle\vec\sigma|$$

$$= |\vec\sigma'\rangle \, \mathrm{Tr} \begin{pmatrix} W & \\ & \tilde W \end{pmatrix} \begin{pmatrix} W & \\ & \tilde W \end{pmatrix} \dots \begin{pmatrix} W & \\ & \tilde W \end{pmatrix} \langle\vec\sigma|$$

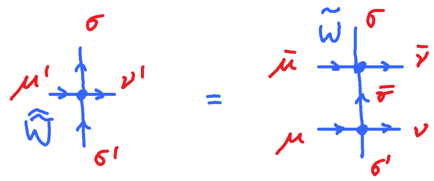
= MPO in enlarged space

Multiplication of MPOs $\qquad W \tilde W = \tilde{\tilde W}$





$$\tilde{\tilde W}^{\mu'\sigma'}{}_{\nu'\sigma} = W^{\mu\sigma'}{}_{\nu\bar\sigma} \, \tilde W^{\bar\mu\bar\sigma}{}_{\bar\nu\sigma}$$



with composite indices, $\mu' = (\mu, \bar\mu)$, $\nu' = (\nu, \bar\nu)$, of increased dimension: $D_{\tilde{\tilde W}} = D_W \cdot D_{\tilde W}$

2. MPO representation of Heisenberg Hamiltonian

$$\hat{H} = \sum_{\ell=1}^{N-1}\left[J^z \hat{S}^z_\ell \hat{S}^z_{\ell+1} + \tfrac{1}{2}J\,\hat{S}^+_\ell \hat{S}^-_{\ell+1} + \tfrac{1}{2}J\,\hat{S}^-_\ell \hat{S}^+_{\ell+1}\right] - h\sum_{\ell=1}^{L} S^z_\ell$$

is shorthand for
$$= J^z\, \hat{S}^z_1 \otimes \hat{S}^z_2 \otimes \hat{\mathbb{1}} \otimes \dots \otimes \hat{\mathbb{1}}$$
$$+\; J^z\, \mathbb{1} \otimes \hat{S}^z_2 \otimes \hat{S}^z_3 \otimes \dots \otimes \mathbb{1} \qquad + \dots$$

Contains sum of one- and two-site operators. How can we bring this into the form of an MPO?

Solution: introduced operator-valued matrices, whose product reproduces the above form!

$$\hat{H} = |\vec{\sigma}'\rangle \prod_\ell W_{[\ell]}{}^{\sigma'_\ell}{}_{\sigma_\ell} \langle\vec{\sigma}|$$
$$= \left(|\sigma'_1\rangle W_{[1]}{}^{\sigma'_1}{}_{\sigma_1}\langle\sigma_1|\right)\otimes\left(|\sigma'_2\rangle W_{[2]}{}^{\sigma'_2}{}_{\sigma_2}\langle\sigma_2|\right)\otimes\dots\otimes\left(|\sigma'_N\rangle W_{[N]}{}^{\sigma'_N}{}_{\sigma_N}\langle\sigma_N|\right)$$
$$= \hat{W}_{[1]}\,\hat{W}_{[2]} \otimes \dots \otimes \hat{W}_{[N]}$$
= product of one-site operators.

Each $\hat{W}_{[\ell]}$ acts only on site ℓ ; their tensor product gives the full MPO.

Viewed from any given bond, the string of operators in each term of $\hat{H}$ can be in one of 'states':

$$\hat{\mathbb{1}} \overset{5}{\otimes} \hat{\mathbb{1}} \overset{5}{\otimes} \hat{\mathbb{1}} \overset{5}{\otimes} -hS^z \overset{1}{\otimes} \hat{\mathbb{1}} \overset{1}{\otimes} \hat{\mathbb{1}}$$
$$\hat{\mathbb{1}} \overset{5}{\otimes} \hat{\mathbb{1}} \overset{5}{\otimes} \tfrac{J}{2}\hat{S}^- \overset{2}{\otimes} \hat{S}^+ \overset{1}{\otimes} \hat{\mathbb{1}} \overset{1}{\otimes} \hat{\mathbb{1}}$$
$$\hat{\mathbb{1}} \overset{5}{\otimes} \hat{\mathbb{1}} \overset{5}{\otimes} \tfrac{J}{2}\hat{S}^+ \overset{3}{\otimes} \hat{S}^- \overset{1}{\otimes} \hat{\mathbb{1}} \overset{1}{\otimes} \hat{\mathbb{1}}$$
$$\hat{\mathbb{1}} \overset{5}{\otimes} \hat{\mathbb{1}} \overset{5}{\otimes} J^z\hat{S}^z \overset{4}{\otimes} \hat{S}^z \overset{1}{\otimes} \hat{\mathbb{1}} \overset{1}{\otimes} \hat{\mathbb{1}}$$

"state 1": only $\mathbb{1}$ to the right

state 2: one $\hat{S}^+$ just to the right

state 3: one $\hat{S}^-$ just to the right

state 4: one $\hat{S}^z$ just to the right

state 5: one $-h\hat{S}^z$ or completed interaction somewhere to the right

Build matrix whose element ij implements 'transition' from 'state' j to i ~~left~~ on its left:

$$\hat{W}_{[\ell]} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}\!\!\begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} \mathbb{1} & 0 & 0 & 0 & 0 \\ \hat{S}^+ & 0 & 0 & 0 & 0 \\ \hat{S}^- & 0 & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 & 0 \\ -h\hat{S}^z & \tfrac{J}{2}\hat{S}^- & \tfrac{J}{2}\hat{S}^+ & J^z\hat{S}^z & \mathbb{1} \end{bmatrix} \end{array}$$

On site N: and also column 1 of $\hat{W}_{[\ell]}$

$$\hat{W}_{[N]} = \begin{bmatrix} \mathbb{1} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -h S^z \end{bmatrix}\begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}$$

One site 1 (= row 5 of $\hat{W}_{[\ell]}$):

$$\hat{W}^{[1]} = \left[-hS^z,\ \tfrac{J}{2}\hat{S}^-,\ \tfrac{J}{2}\hat{S}^+,\ J^z S^z,\ \mathbb{1}\right]$$

Check: multiplying out a product of such $\hat{W}$'s yields desired result:

$$\hat W_{[1]}\hat W_{[2]}\hat W_{[3]}\hat W_{[4]} = \hat W_{[1]}\hat W_{[2]}\begin{bmatrix} \hat{\mathbb{1}} & 0 & & & \\ \hat S^+ & 0 & & & \\ \hat S^- & 0 & & & \\ \hat S^z & 0 & & & \\ -h\hat S^z & \frac{J}{2}\hat S^- & \frac{J}{2}\hat S^+ & J^z\hat S^z & \hat{\mathbb{1}} \end{bmatrix}\begin{bmatrix} \hat{\mathbb{1}} \\ \hat S^+ \\ \hat S^- \\ \hat S^z \\ -h S_z \end{bmatrix}$$

$$= \hat W_{[1]}\begin{bmatrix} \hat{\mathbb{1}} & 0 & & & \\ \hat S^+ & 0 & & & \\ \hat S^- & 0 & & & \\ \hat S^z & 0 & & & \\ -h\hat S^z & \frac{J}{2}\hat S^- & \frac{J}{2}\hat S^+ & J^z\hat S^z & \hat{\mathbb{1}} \end{bmatrix}\begin{bmatrix} \mathbb{1}\otimes\mathbb{1} \\ \hat S^+\otimes\mathbb{1} \\ \hat S^-\otimes\mathbb{1} \\ \hat S^z\otimes\mathbb{1} \\ -h\hat S^z\otimes\mathbb{1} + \frac{J}{2}\hat S^-\otimes\hat S^+ + \frac{J}{2}\hat S^+\otimes\hat S^- + J_z\hat S^z\otimes\hat S^z + \mathbb{1}\cdot(-h\hat S^z) \end{bmatrix}$$

$$= \left[-h\hat S^z, \tfrac{J}{2}\hat S^-, \tfrac{J}{2}\hat S^+, J^z\hat S^z, \mathbb{1}\right]\begin{bmatrix} \mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} \\ \hat S^+\otimes\mathbb{1}\otimes\mathbb{1} \\ \hat S^-\otimes\mathbb{1}\otimes\mathbb{1} \\ \hat S^z\otimes\mathbb{1}\otimes\mathbb{1} \\ \begin{aligned}&(-h\hat S^z\otimes\mathbb{1}\otimes\mathbb{1} + \tfrac{J}{2}\hat S^-\otimes\hat S^+\otimes\mathbb{1} + \tfrac{J}{2}\hat S^+\otimes\hat S^-\otimes\mathbb{1} + J^z\hat S^z\otimes\hat S^z\otimes\mathbb{1} \\ &+ \mathbb{1}\otimes(-h\hat S^z)\otimes\mathbb{1} + \mathbb{1}\otimes\tfrac{J}{2}\hat S^-\otimes\hat S^+ + \mathbb{1}\otimes\tfrac{J}{2}\hat S^+\otimes\hat S^- + \mathbb{1}\otimes J^z\hat S^z\otimes\hat S^z \\ &+ \mathbb{1}\otimes\mathbb{1}\otimes(-h\hat S^z))\end{aligned} \end{bmatrix}$$

$$\begin{aligned} = &-h\hat S^z\otimes\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} + \tfrac{J}{2}\hat S^-\otimes\hat S^+\otimes\mathbb{1}\otimes\mathbb{1} + \tfrac{J}{2}\hat S^+\otimes\hat S^-\otimes\mathbb{1}\otimes\mathbb{1} + J^z\hat S^z\otimes\hat S^z\otimes\mathbb{1}\otimes\mathbb{1} \\ &+ \mathbb{1}\otimes(-h\hat S^z)\otimes\mathbb{1}\otimes\mathbb{1} + \mathbb{1}\otimes\tfrac{J}{2}\hat S^-\otimes\hat S^+\otimes\mathbb{1} + \mathbb{1}\otimes\tfrac{J}{2}\hat S^+\otimes\hat S^-\otimes\mathbb{1} + \mathbb{1}\otimes J^z\hat S^z\otimes\hat S^z\otimes\mathbb{1} \\ &+ \mathbb{1}\otimes\mathbb{1}\otimes(-h\hat S^z)\otimes\mathbb{1} + \mathbb{1}\otimes\mathbb{1}\otimes\tfrac{J}{2}\hat S^-\otimes\hat S^+ + \mathbb{1}\otimes\mathbb{1}\otimes\tfrac{J}{2}\hat S^+\otimes\hat S^- + \mathbb{1}\otimes\mathbb{1}\otimes J^z\hat S^z\otimes\hat S^z \\ &+ \mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1}\otimes(-h\hat S^z) \end{aligned}$$

= full Hamiltonian for 4 sites! ✓

Longer-ranged interactions

$$\hat{H} = J_1 \sum_\ell \hat{S}^z_\ell \hat{S}^z_{\ell+1} + J_2 \sum_\ell \hat{S}^z_\ell \hat{S}^z_{\ell+2}$$

$$\hat{\mathbb{1}} \overset{4}{\otimes} \hat{\mathbb{1}} \overset{4}{\otimes} J_1 \hat{S}^z \overset{2}{\otimes} \hat{S}^z \overset{1}{\otimes} \hat{\mathbb{1}} \overset{1}{\otimes} \hat{\mathbb{1}}$$

$$\hat{\mathbb{1}} \overset{4}{\otimes} \hat{\mathbb{1}} \overset{4}{\otimes} J_2 \hat{S}^z \overset{3}{\otimes} \mathbb{1} \overset{2}{\otimes} \hat{S}^z \overset{1}{\otimes} \hat{\mathbb{1}}$$

state 1: only $\mathbb{1}$ to the right

state 2: one $\hat{S}^z$ just to the right

state 3: one $\mathbb{1} \otimes \hat{S}^z$ just to the right

state 4: completed interaction somewhere to the right

$$\hat{W}_{[\ell]} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} \hat{\mathbb{1}} & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 \\ 0 & \mathbb{1} & 0 & 0 \\ 0 & J_1 \hat{S}_z & J_2 \hat{S}^z & \hat{\mathbb{1}} \end{pmatrix} \end{array}$$

$$\hat{W}_{[N]} = \begin{pmatrix} \mathbb{1} \\ \hat{S}^z \\ 0 \\ 0 \end{pmatrix} = \text{column } 1 \text{ of } \hat{W}_{[\ell]}$$

$$\hat{W}_{[1]} = (0, J_1 \hat{S}^z, J_2 \hat{S}^z, \hat{\mathbb{1}})$$

$$= \text{row } 4 \text{ of } \hat{W}_{[\ell]}$$

Check:

$$\hat{W}^{[1]} \hat{W}^{[2]} W^{[3]} = \hat{W}^{(1)} \begin{pmatrix} \hat{\mathbb{1}} & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 \\ 0 & \hat{\mathbb{1}} & 0 & 0 \\ 0 & J_1 \hat{S}^z & J_2 \hat{S}^z & \hat{\mathbb{1}} \end{pmatrix} \begin{pmatrix} \hat{\mathbb{1}} \\ \hat{S}^z \\ 0 \\ 0 \end{pmatrix}$$

$$= (0, J_1 \hat{S}^z, J_2 \hat{S}^z, \hat{\mathbb{1}}) \begin{pmatrix} \hat{\mathbb{1}} \otimes \hat{\mathbb{1}} \\ \hat{S}_z \otimes \hat{\mathbb{1}} \\ \hat{\mathbb{1}} \otimes \hat{S}^z \\ 0 + J_1 \hat{S}^z \otimes \hat{S}^z + 0 + 0 \end{pmatrix}$$

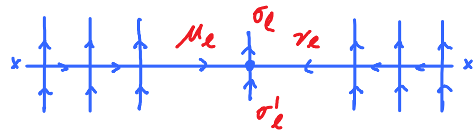
$$= J_1 \hat{S}^z \otimes \hat{S}^z \otimes \hat{\mathbb{1}} + J_2 \hat{S}^z \otimes \hat{\mathbb{1}} \otimes \hat{S}^z + \hat{\mathbb{1}} \otimes J_1 \hat{S}_z \otimes \hat{S}_z \quad \checkmark$$

3. Applying Hamiltonian to mixed-canonical state

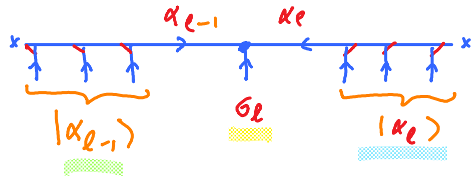
[Schollwöck2011, Sec. 6.2]

How does an MPO act on an MPS in mixed-canonical representation w.r.t. site ℓ ? Consider

$$\hat{O} = |\vec{\sigma}'\rangle \prod_{\ell} W_{[\ell]}{}^{\sigma'_\ell}{}_{\sigma_\ell} \langle \vec{\sigma}| \qquad (1)$$



$$|\psi\rangle = \underbrace{|\alpha_\ell\rangle |\sigma_\ell\rangle |\alpha_{\ell-1}\rangle}_{\equiv |a\rangle} \underbrace{A^{\alpha_{\ell-1}\sigma_\ell\alpha_\ell}}_{A^a} \qquad (2)$$

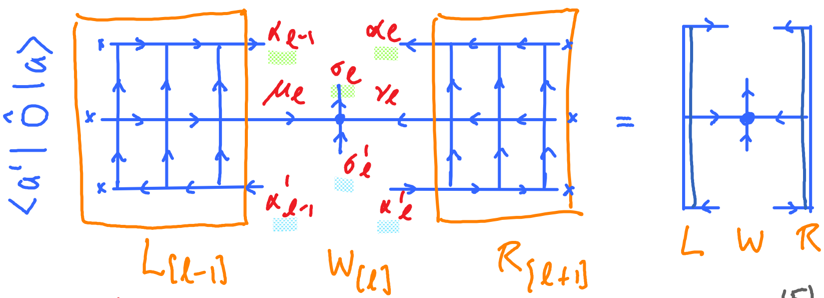


Here $\{ |a\rangle \}$ form a basis for the mixed-canonical representation. Express operator in this basis:

$$\hat{O} = |a'\rangle O^{a'}{}_{a} \langle a| \quad \text{, with matrix elements} \quad O^{a'}{}_{a} = \langle a'|\hat{O}|a\rangle \qquad (3)$$

then $|\psi'\rangle = \hat{O}|\psi\rangle = |a'\rangle A'^{a'}$, with components $A'^{a'} = O^{a'}{}_{a} A^{a}$ (4)

$$O^{a'}{}_{a} = \langle a'|\hat{O}|a\rangle$$

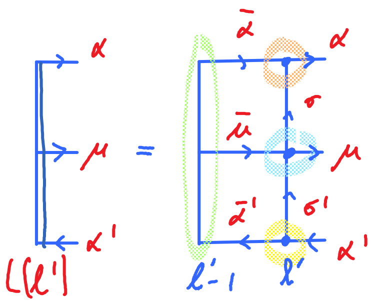


(5)

$$= L_{[\ell-1]}{}^{\alpha'_{\ell-1}}{}_{\mu_\ell \alpha_{\ell-1}} W_{[\ell]}{}^{\mu_\ell \sigma'_\ell \nu_\ell}{}_{\sigma_\ell} R_{[\ell+1]}{}^{\alpha'_\ell}{}_{\nu_\ell \alpha_\ell} \qquad (6)$$

L can be computed iteratively, for $\ell' \le \ell - 1$:
(Similarly for R, for $\ell' \ge \ell + 1$)

$$L_{[\ell']}{}^{\alpha'}{}_{\mu\alpha} = A^{\dagger}_{[\ell']}{}^{\alpha'}{}_{\sigma'\bar{\alpha}'} L_{[\ell'-1]}{}^{\bar{\alpha}'}{}_{\bar{\mu}\bar{\alpha}} A_{[\ell']}{}^{\bar{\alpha}\sigma}{}_{\alpha} W_{[\ell']}{}^{\bar{\mu}\sigma'}{}_{\mu\sigma} \qquad (7)$$



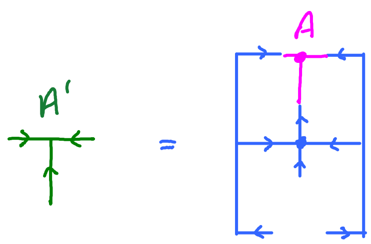
For efficient computation, perform sums in this order:

1. Sum over $\bar{\alpha}', \sigma'$ for fixed $\alpha', \bar{\alpha}, \bar{\mu}, \sigma, \mu$ at cost $(D \cdot d)(D^2 \cdot D_W^2 \cdot d)$ (8)
2. Sum over $\bar{\mu}, \sigma$ for fixed $\alpha', \bar{\alpha}, \mu$ at cost $(D_W d) \cdot (D^2 D_W)$ (9)
3. Sum over $\bar{\alpha}$ for fixed α', α, μ at cost $D \cdot (D^2 D_W)$ (10)

$\Big\} \sim D^3$

The application of MPO to MPS is then represented as:

$$A'^{a'} = O^{a'}{}_{a} A^{a}$$



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