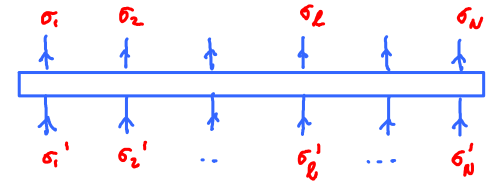
Consider an operator acting on N-site chain:

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

(1)

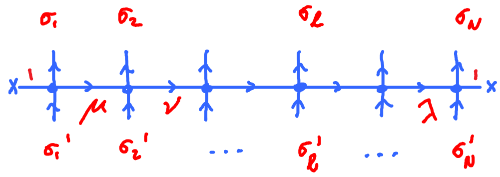


It can always be written as
'matrix product operator' (MPO),

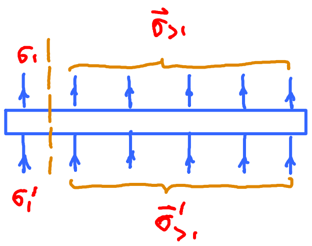
$$\hat{O} = |\vec{\sigma}'\rangle W^{1\sigma_1'}{}_{\mu\sigma_1} W^{\mu\sigma_2'}{}_{\nu\sigma_2} \cdots W^{\lambda\sigma_N'}{}_{\sigma_N 1} \langle\vec{\sigma}|$$

$$\equiv |\vec{\sigma}'\rangle \prod_\ell W^{\sigma_\ell'}{}_{\sigma_\ell} \langle\vec{\sigma}|$$

(2)



using a sequence of QR decompositions:



reshape as matrix
with composite indices

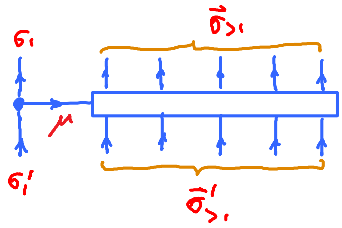
$$\equiv (\sigma_1', \sigma_1) \rightarrow\bullet\rightarrow (\vec{\sigma}_{>1}', \vec{\sigma}_{>1})$$

QR decomposition

$$= (\sigma_1', \sigma_1) \rightarrow \overset{Q}{\bullet} \xrightarrow{\mu} \overset{R}{\bullet} \rightarrow (\vec{\sigma}_{>1}', \vec{\sigma}_{>1}) \qquad (3)$$

reshape again

$$= \qquad (4)$$

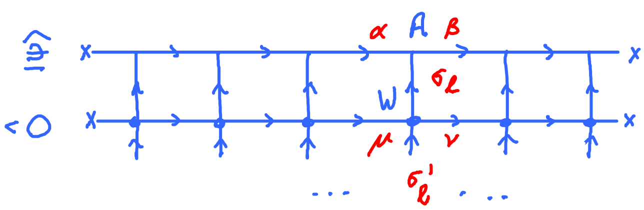


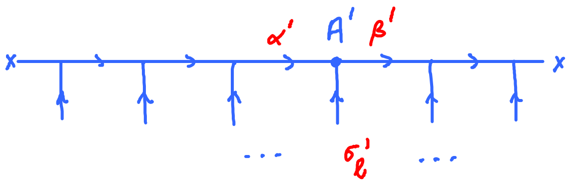
In general, this produces MPO
with growing bond dimensions: $d^2, \ (d^2)^2, \ (d^2)^3, \ \ldots$

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

1. Applying MPO to MPS yields MPS

$$|\psi'\rangle = \hat{O}|\psi\rangle \qquad (5)$$



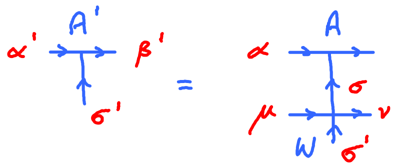


(6)

$$|\psi\rangle = |\vec{\sigma}\rangle \prod_\ell A^{\alpha_\ell \sigma_\ell}_{[\ell]}{}_{\beta_\ell} \qquad (7)$$

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

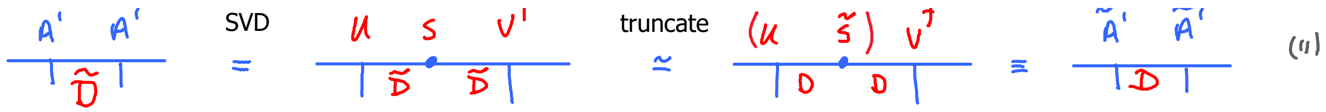
$$A'^{\alpha'\sigma'}{}_{\beta'} = W^{\mu\sigma'}{}_{\nu\sigma} \underbrace{A^{\alpha\sigma}{}_{\beta}} \qquad (9)$$



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

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

(11)



<u>Addition of MPOs</u> $\hat{O} + \hat{\tilde{O}}$

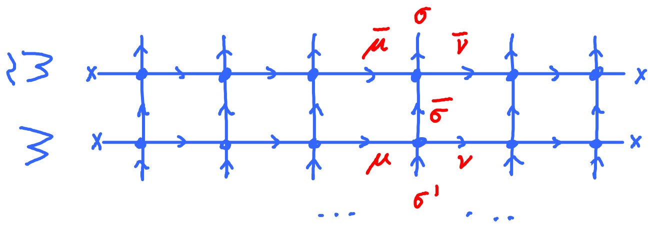
Let $\hat{O} = |\vec{\sigma}'\rangle \prod_\ell W^{\sigma'_\ell}{}_{\sigma_\ell} \langle\vec{\sigma}|$ $\qquad \hat{\tilde{O}} = |\vec{\sigma}'\rangle \prod_\ell \tilde{W}^{\sigma'_\ell}{}_{\sigma_\ell} \langle\vec{\sigma}|$

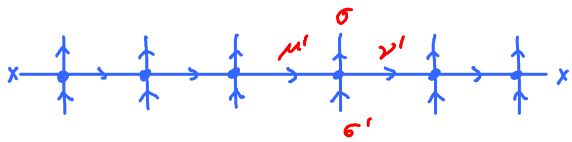
$$\hat{O} + \hat{\tilde{O}} = |\vec{\sigma}'\rangle \left[W W \dots W + \tilde{W}\tilde{W} \dots \tilde{W} \right] \langle\vec{\sigma}|$$

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

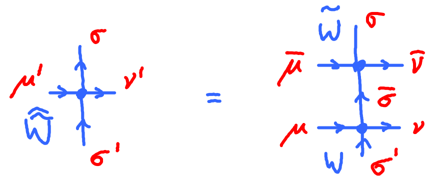
= MPO in enlarged space

<u>Multiplication of MPOs</u> $\qquad W\tilde{W} = \tilde{\tilde{W}}$





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



with composite indices, $\begin{array}{l} \mu' = (\mu, \bar{\mu}), \\ \nu' = (\nu, \bar{\nu}) \end{array}$ of <u>increased</u> dimension: $D_{\tilde{\tilde{W}}} = D_W \cdot D_{\tilde{W}}$

2. MPO representation of Heisenberg Hamiltonian

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

is shorthand for $\quad = J^z \hat{S}^z_1 \otimes \hat{S}^z_2 \otimes \hat{\mathbb{1}} \otimes \dots \otimes \hat{\mathbb{1}}$

$$+ J^z \mathbb{1} \otimes \hat{S}^z_2 \otimes \hat{S}^z_3 \otimes \dots \otimes \hat{\mathbb{1}} \qquad + \dots$$

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 5 '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 on its left:

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

On site N: $\hat{W}_{[N]} =$

and also column 1 of $\hat{W}_{[\ell]}$

$$\begin{bmatrix} \hat{\mathbb{1}} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -hS_z \end{bmatrix} \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix}$$

One site 1 (= row 1 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:

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

$$= \hat{W}_{[1]}\begin{bmatrix} \hat{\mathbb{1}} & 0 & & & \\ \hat{S}^+ & 0 & & & \\ \hat{S}^- & 0 & & & \\ \hat{S}^z & 0 & & & \\ -h\hat{S}^z & \frac{J}{2}\hat{S}^- & \frac{J}{2}\hat{S}^+ & J^z\hat{S}^z & \hat{\mathbb{1}} \end{bmatrix}\begin{bmatrix} \hat{\mathbb{1}}\otimes\hat{\mathbb{1}} \\ \hat{S}^+\otimes\hat{\mathbb{1}} \\ \hat{S}^-\otimes\hat{\mathbb{1}} \\ \hat{S}^z\otimes\hat{\mathbb{1}} \\ \left(-h\hat{S}^z\otimes\hat{\mathbb{1}} + \frac{J}{2}\hat{S}^-\otimes\hat{S}^+ + \frac{J}{2}\hat{S}^+\otimes\hat{S}^- + J^z\hat{S}^z\otimes\hat{S}^z + \hat{\mathbb{1}}\otimes(-h\hat{S}^z)\right) \end{bmatrix}$$

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

$$= -hS^z\otimes\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} + \frac{J}{2}\hat{S}^-\otimes\hat{S}^+\otimes\mathbb{1}\otimes\mathbb{1} + \frac{J}{2}\hat{S}^+\otimes\hat{S}^-\otimes\mathbb{1}\otimes\mathbb{1} + J^zS^z\otimes S^z\otimes\mathbb{1}\otimes\mathbb{1}$$

$$+ \mathbb{1}\otimes(-h\hat{S}^z)\otimes\mathbb{1}\otimes\mathbb{1} + \mathbb{1}\otimes\frac{J}{2}\hat{S}^-\otimes\hat{S}^+\otimes\mathbb{1} + \mathbb{1}\otimes\frac{J}{2}\hat{S}^+\otimes\hat{S}^-\otimes\mathbb{1} + \mathbb{1}\otimes J^z\hat{S}^z\otimes\hat{S}^z\otimes\mathbb{1}$$

$$+ \mathbb{1}\otimes\mathbb{1}\otimes(-h\hat{S}^z)\otimes\mathbb{1} + \mathbb{1}\otimes\mathbb{1}\otimes\frac{J}{2}\hat{S}^-\otimes\hat{S}^+ + \mathbb{1}\otimes\mathbb{1}\otimes\frac{J}{2}\hat{S}^+\otimes\hat{S}^- + \mathbb{1}\otimes\mathbb{1}\otimes J^z\hat{S}^z\otimes\hat{S}^z$$

$$+ \mathbb{1}\otimes\mathbb{1}\times\mathbb{1}\otimes(-h\hat{S}_z^z)$$

= full Hamiltonian for 4 sites! ✓

Longer-ranged interactions

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

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

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

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

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

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

state 4: completed interaction somewhere to the right

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

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

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

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

Check:

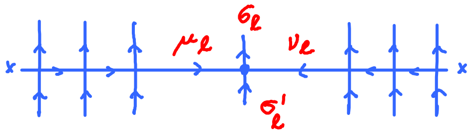
$$\hat{W}^{[1]} \hat{W}^{[2]} W^{[3]} = \hat{W}^{(1)} \begin{pmatrix} \hat{\mathbb{1}} & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 \\ 0 & \hat{\mathbb{1}} & 0 & 0 \\ 0 & J_1 \hat{S}^z & J_2 \hat{S}^z & \hat{\mathbb{1}} \end{pmatrix} \begin{pmatrix} \hat{\mathbb{1}} \\ \hat{S}^z \\ 0 \\ 0 \end{pmatrix}$$

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

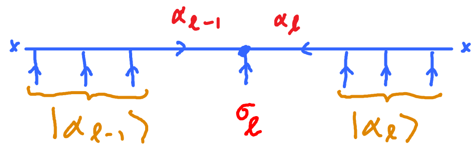
$$= J_1 \hat{S}^z \otimes \hat{S}^z \otimes \hat{\mathbb{1}} + J_2 \hat{S}^z \otimes \hat{\mathbb{1}} \otimes \hat{S}^z + \hat{\mathbb{1}} \otimes J_1 \hat{S}_z \otimes \hat{S}_z \quad \checkmark$$

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

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



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

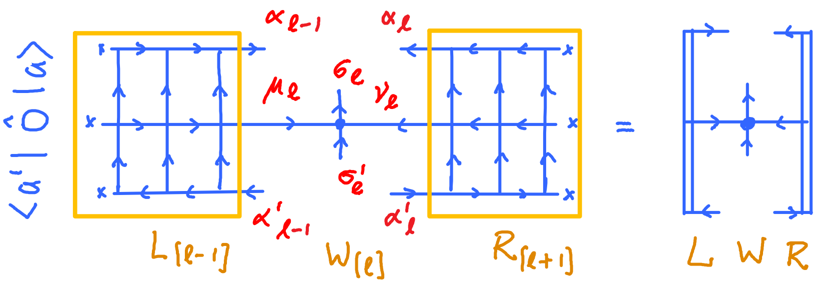


Here $\{|a\rangle\}$ form a basis for the mixed-canonical representation. Express operator in this basis:

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

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

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

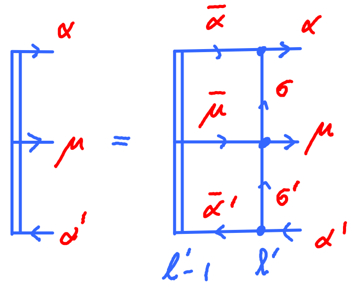


(5)

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

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

$$L^{\alpha'}_{[\ell']\,\mu\alpha} = A^{\dagger\,\alpha'}_{[\ell']\,\sigma'\bar\alpha'}\, L^{\bar\alpha'}_{[\ell'-1]\,\bar\mu\bar\alpha}\, A^{\bar\alpha\sigma}_{[\ell']\,\alpha}\, W^{\bar\mu\sigma'}_{[\ell']\,\mu\sigma} \qquad (7)$$

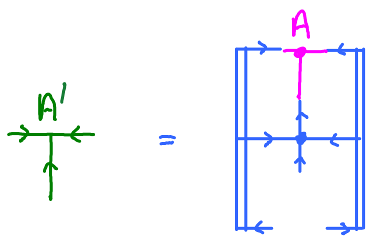


For efficient computation, perform sums in this order:

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

The application of MPO to MPS is then represented as:

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



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