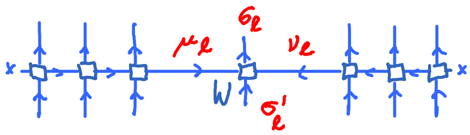
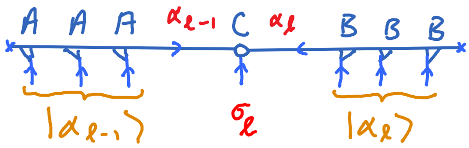
How does MPO act on MPS in mixed-canonical representation with orthogonality center at site ℓ ?
Consider

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



$$|\psi\rangle = \underbrace{|\alpha_\ell\rangle|\sigma_\ell\rangle|\alpha_{\ell-1}\rangle}_{:=|a\rangle} \underbrace{[C_\ell]^{\alpha_{\ell-1}\sigma_\ell\alpha_\ell}}_{C^a_\ell} \qquad (2)$$

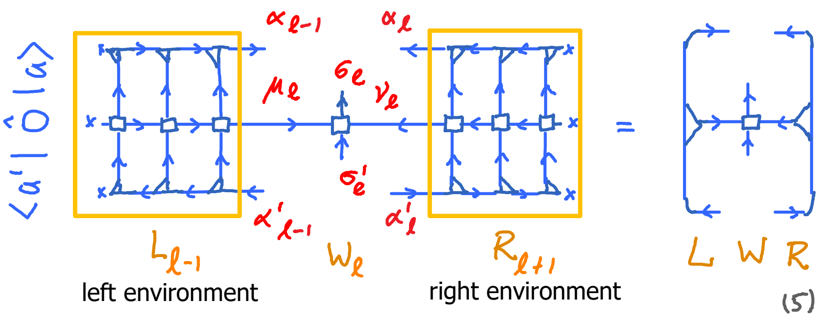


Here $\{|a\rangle\}$ form a basis for the mixed-canonical representation. Express operator in this basis:

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

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

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

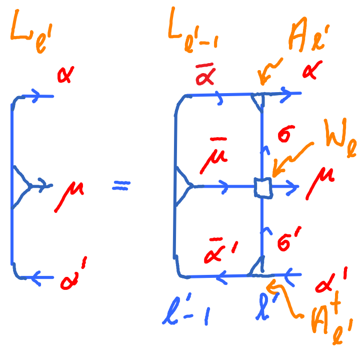


(5)

$$= \underbrace{[L_{\ell-1}]^{\alpha'_{\ell-1}}{}_{\mu_\ell\alpha_{\ell-1}}}_{1}\, [W_\ell]^{\mu_\ell\sigma'_\ell\nu_\ell}{}_{\sigma_\ell}\, \underbrace{[R_{\ell+1}]^{\alpha'_\ell}{}_{\nu_\ell\alpha_\ell}}_{2} \qquad (6)$$

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

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



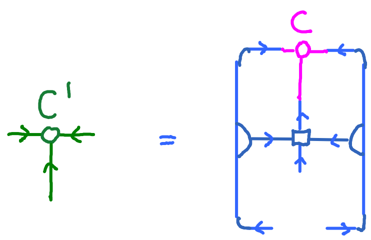
For efficient computation, perform sums in this order:

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

All in all: $\mathcal{O}(D^3dw + D^2d^2w^2)$

The application of MPO to MPS is then represented as:

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



(11)