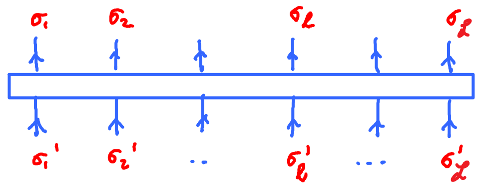
MPS-IV: Matrix product operators

[Schollwöck2011, Sec. 5]

Consider an operator acting on N-site chain:

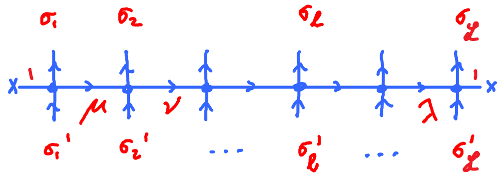
$$\hat O = |\vec\sigma'\rangle O^{\vec\sigma'}{}_{\vec\sigma} \langle \vec\sigma| \quad (1)$$



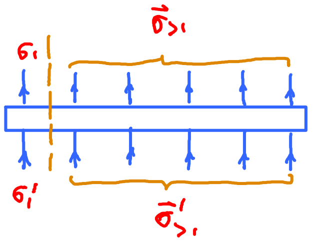
It can always be written as
'matrix product operator' (MPO),

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

$$= |\vec\sigma'\rangle \prod_\ell W^{\sigma_\ell'}{}_{\sigma_\ell} \langle\vec\sigma| \quad (2)$$



using a sequence of QR decompositions:



reshape as matrix
with composite indices

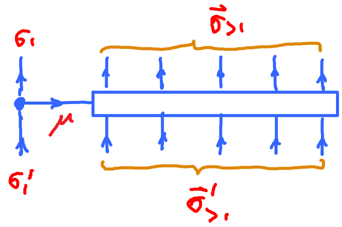
$$=: (\sigma_1', \sigma_1) \rightarrow\bullet\rightarrow (\vec\sigma_{>1}', \vec\sigma_{>1})$$

QR decomposition

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

reshape again

$$=$$



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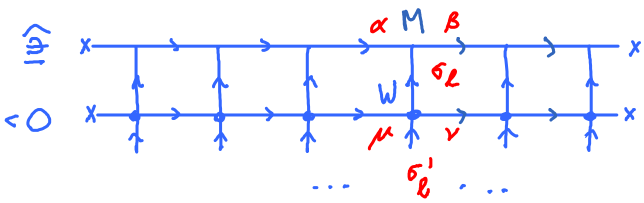
In general, this produces MPO with growing bond dimensions: $d^2, (d^2)^2, (d^2)^3, \ldots$

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

1. Applying MPO to MPS yields MPS

$$|\psi'\rangle = \hat O |\psi\rangle \quad (5)$$



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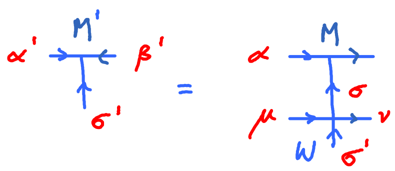
$$|\psi\rangle = |\vec\sigma\rangle \prod_\ell M_{[\ell]}{}^{\alpha_\ell\sigma_\ell}{}_{\beta_\ell} \quad (7)$$

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

$$M'^{\alpha'\sigma'}{}_{\beta'} = W^{\mu\sigma'}{}_{\underbrace{\nu\sigma}} \, \underbrace{M}^{\alpha\sigma}{}_{\beta}$$



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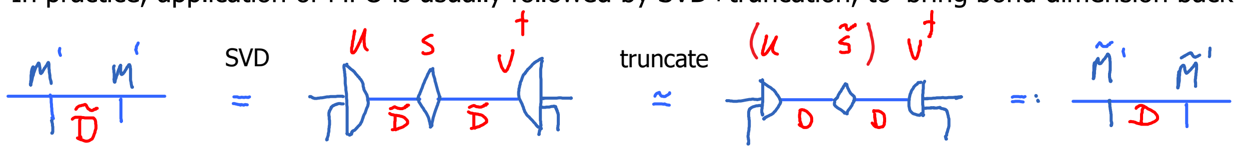
with composite indices, $\alpha_\ell' = (\alpha, \mu)$, $\beta_\ell' = (\beta, \nu)$, of <u>increased</u> dimension: $\tilde D_{M'} = \underline{\underline{D_W}} \cdot D_M$ (10)

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



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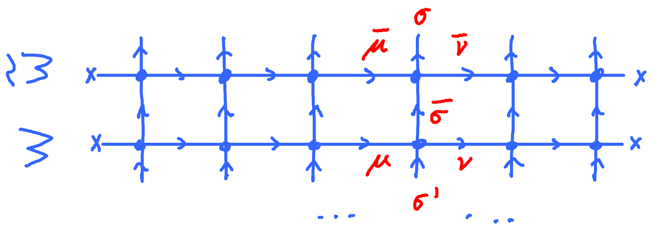
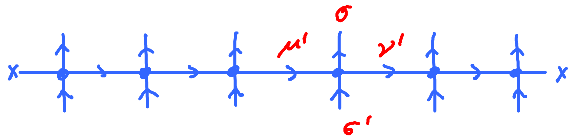
$\sim$ $\approx$

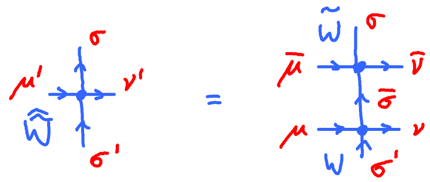
Multiplication of MPOs

$$W \tilde{W} = \tilde{\tilde{W}} \tag{12}$$





$$\tilde{\tilde{W}}^{\mu'\sigma'}{}_{\nu'\sigma} = W^{\mu\sigma'}{}_{\nu\bar{\sigma}} \, \tilde{W}^{\bar{\mu}\bar{\sigma}}{}_{\bar{\nu}\sigma} \tag{13}$$



with composite indices, $\mu' = (\mu, \bar{\mu})$, $\nu' = (\nu, \bar{\nu})$ of <u>increased</u> dimension: $D_{\tilde{\tilde{W}}} = D_W \cdot D_{\tilde{W}}$ (14)

In practice, such a multiplication is typically followed by SVD+truncation.

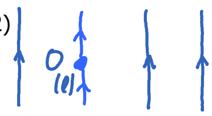
Addition of MPOs $\hat{O} + \hat{\tilde{O}}$

Let $\hat{O} = |\vec{\sigma}'\rangle \prod_\ell W^{\sigma'_\ell}{}_{\sigma_\ell} \langle \vec{\sigma}|$ $\qquad \hat{\tilde{O}} = |\vec{\sigma}'\rangle \prod_\ell \tilde{W}^{\sigma'_\ell}{}_{\sigma_\ell} \langle \vec{\sigma}|$ (15)

$$\hat{O} + \hat{\tilde{O}} = |\vec{\sigma}'\rangle \left[W W \dots W \; + \; \tilde{W}\tilde{W}\dots\tilde{W} \right] \langle \vec{\sigma}| \tag{16}$$

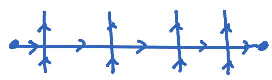
$$= |\vec{\sigma}'\rangle \, \mathrm{Tr} \begin{pmatrix} W & \\ & \tilde{W} \end{pmatrix} \begin{pmatrix} W & \\ & \tilde{W} \end{pmatrix} \dots \begin{pmatrix} W & \\ & \tilde{W} \end{pmatrix} \langle \vec{\sigma}| \quad = \text{MPO in enlarged space} \tag{17}$$

Sum of single-site operators

Let $\hat{O} = \sum_\ell \hat{O}_{[\ell]}$ with single-site operators $\hat{O}_{[\ell]} \overset{\text{(MPS-I.1.22)}}{=}$  (18)

MPO representation:

$$= (0 \;\; 1) \prod_{\ell=1}^{N} \hat{W}_{[\ell]} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \hat{W}_{[\ell]} = \begin{pmatrix} \hat{\mathbb{1}}_{[\ell]} & 0 \\ \hat{O}_{[\ell]} & \hat{\mathbb{1}}_{[\ell]} \end{pmatrix} \tag{19}$$



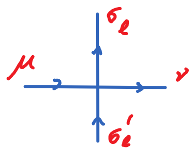
Check for N=2:

$$= (0 \;\; 1) \begin{pmatrix} \hat{\mathbb{1}}_{[1]} & 0 \\ \hat{O}_{[1]} & \hat{\mathbb{1}}_{[1]} \end{pmatrix} \begin{pmatrix} \hat{\mathbb{1}}_{[2]} & 0 \\ \hat{O}_{[2]} & \hat{\mathbb{1}}_{[2]} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{20}$$

$$= (0 \;\; 1) \begin{pmatrix} \hat{\mathbb{1}}_{[1]} \otimes \hat{\mathbb{1}}_{[2]} & 0 \\ \hat{O}_{[1]} \otimes \hat{\mathbb{1}}_{[2]} + \hat{\mathbb{1}}_{[1]} \otimes \hat{O}_{[2]} & \hat{\mathbb{1}}_{[1]} \otimes \hat{\mathbb{1}}_{[2]} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hat{O}_{[1]} \otimes \hat{\mathbb{1}}_{[2]} + \hat{\mathbb{1}}_{[1]} \otimes \hat{O}_{[2]} \tag{21}$$

Matrix elements of W have direct-product structure:

$$W_{[\ell]}{}^{\mu\sigma'_\ell}{}_{\nu\sigma_\ell} = \begin{pmatrix} (\hat{\mathbb{1}}_{[\ell]})^{\sigma'_\ell}{}_{\sigma_\ell} & 0 \\ (\hat{O}_{[\ell]})^{\sigma'_\ell}{}_{\sigma_\ell} & \hat{\mathbb{1}}_{[\ell]}{}^{\sigma'_\ell}{}_{\sigma_\ell} \end{pmatrix}^{\mu}{}_{\nu} \tag{22}$$



2. MPO representation of Heisenberg Hamiltonian

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

is shorthand for

$$= J^z \hat{S}^z_1 \otimes \hat{S}^z_2 \otimes \hat{\mathbb{1}} \otimes \dots \otimes \hat{\mathbb{1}}$$
$$+ J^z \mathbb{1}_1 \otimes \hat{S}^z_2 \otimes \hat{S}^z_3 \otimes \dots \otimes \hat{\mathbb{1}} \qquad + \dots$$

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!

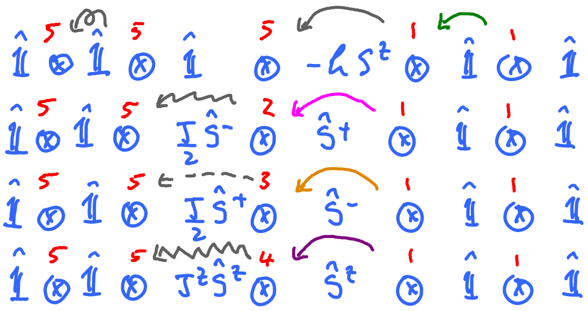
$$\hat{H} = |\vec{\sigma}'\rangle H^{\vec{\sigma}'_\ell}{}_{\vec{\sigma}_\ell} \langle \vec{\sigma}| =: \prod_\ell \hat{W}_{[\ell]}$$ = matrix product of one-site operators

$$=: (\hat{W}_{[1]})^1{}_\mu (\hat{W}_{[2]})^\mu{}_\nu \otimes \dots \otimes (\hat{W}_{[N]})^\eta{}_1$$

$$=: \left(|\sigma'_1\rangle W_{[1]}{}^{1\sigma'_1}{}_{\mu\sigma_1} \langle\sigma_1|\right) \otimes \left(|\sigma'_2\rangle W_{[2]}{}^{\mu\sigma'_2}{}_{\nu\sigma_2} \langle\sigma_2|\right) \otimes \dots \otimes \left(|\sigma'_N\rangle W_{[N]}{}^{\eta\sigma'_N}{}_{1\sigma_N} \langle\sigma_N|\right)$$

Each $\hat{W}_{[\ell]}$ acts only on site ℓ ; their matrix product gives the full MPO. $\quad W_{[\ell]}{}^{\sigma'_\ell}{}_{\sigma_\ell}$

Viewed from any given bond, the string of operators in each term of $\hat{H}$ can be in one of 5 'states':
(mutually exclusive)



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: only $\mathbb{1}$ to the left
(i.e. 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:

Site 1: $\hat{W}_{[1]}$ row vector

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

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

Sites $1 < \ell < \mathcal{L}$: $W_{[\ell]}$

$$\begin{array}{c|ccccc} & 1 & 2 & 3 & 4 & 5 \\ \hline 1 & \hat{\mathbb{1}} & 0 & & & \\ 2 & \hat{S}^+ & 0 & & & \\ 3 & \hat{S}^- & 0 & & & \\ 4 & \hat{S}^z & 0 & 0 & 0 & 0 \\ 5 & -h\hat{S}^z & \tfrac{J}{2}\hat{S}^- & \tfrac{J}{2}\hat{S}^+ & J^z\hat{S}^z & \hat{\mathbb{1}} \end{array}$$

Site $\mathcal{L}$: $\hat{W}_{[\mathcal{L}]} =$ column vector

$$\begin{array}{c} \left[\begin{array}{c} \hat{\mathbb{1}} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -hS_z \end{array}\right] \end{array} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}$$

first column of $\hat{W}_{[\ell]}$

$$\hat{W}_{[1]}{}^1{}_\mu W_{[2]}{}^\nu{}_1 =$$

Key properties:

$$\hat W^{1}_{[1]\,\mu}\,\hat W^{\mu}_{[2]\,1} = \hat H_1 \otimes 1_2 + \hat H_{12} + 1_1 \otimes \hat H_2$$

$$\hat W^{1}_{[\ell-1]\,\mu}\,\hat W^{\mu}_{[\ell]\,1} = \hat H_{\ell-1} \otimes 1_\ell + \hat H_{\ell-1,\ell} + 1_{\ell-1} \otimes \hat H_\ell$$

$$\hat W^{1}_{[\ell]\,\mu}\,\hat W^{\mu}_{[\ell+1]\,1} = \hat H_{\ell} \otimes 1_{\ell+1} + \hat H_{\ell,\ell+1} + 1_{\ell} \otimes \hat H_{\ell+1}$$

Check: multiplying out a product of such $\hat W_{[\ell]}$'s yields desired result:

$$\hat W_{[1]}\,\hat W_{[2]}\,\hat W_{[3]}\,\hat W_{[4]} =$$

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

elements 1,2 and 1,3 and 1,4, couple to site 1, building the interaction between sites 1 and 2

$$= \hat W_{[1]} \begin{bmatrix} \hat 1 \otimes \hat 1 & & & & \\ \hat S^+ \otimes \hat 1 & & & & \\ \hat S^- \otimes \hat 1 & & & & \\ \hat S^z \otimes \hat 1 & & & & \\ \left(-h\hat S^z \otimes \hat 1 + \frac{J}{2}\hat S^- \otimes \hat S^+ + \frac{J}{2}\hat S^+ \otimes \hat S^- + J^z \hat S^z \otimes \hat S^z + \hat 1 \otimes (-h\hat S^z)\right) & \hat 1 \otimes \frac{J}{2}\hat S^- & \hat 1 \otimes \frac{J}{2}\hat S^+ & \hat 1 \otimes J^z \hat S^z & \hat 1 \otimes \hat 1 \end{bmatrix} \hat W_{[4]}$$

element 5,1 contains the full Hamiltonian for sites 2 and 3, excluding terms involving sites 1 and 4.

elements 5,2 and 5,3 and 5,4 couple to site 4, building the interaction between sites 3 and 4

$$= \left[-h\hat S^z,\ \frac{J}{2}\hat S^-,\ \frac{J}{2}\hat S^+,\ J^z\hat S^z,\ \hat 1\right] \left[\quad\cdots\quad\right] \begin{bmatrix} \hat 1 \\ \hat S^+ \\ \hat S^- \\ \hat S^z \\ -h\hat S_z \end{bmatrix}$$

$$= \left[-h\hat S^z \otimes \hat 1 \otimes \hat 1 + \frac{J}{2}\hat S^- \otimes \hat S^+ \otimes \hat 1 + \frac{J}{2}\hat S^+ \otimes \hat S^- \otimes \hat 1 + J^z \hat S^z \otimes \hat S^z \otimes \hat 1\right] \otimes \hat 1$$

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

$$+ \hat 1 \otimes \left[\hat 1 \otimes \frac{J}{2}\hat S^- \otimes \hat S^+ + \hat 1 \otimes \frac{J}{2}\hat S^+ \otimes \hat S^- + \hat 1 \otimes J^z \hat S^z \otimes \hat S^z + \hat 1 \times \hat 1 \otimes (-h\hat S^z_z)\right]$$

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

$$+ \mathbb{1}\otimes\Big[\mathbb{1}\otimes\tfrac{J}{2}\hat S^-\otimes\hat S^+ + \mathbb{1}\otimes\tfrac{J}{2}\hat S^+\otimes\hat S^- + \mathbb{1}\otimes J^z\hat S^z\otimes\hat S^z + \mathbb{1}\times\mathbb{1}\otimes(-h\hat S^z_z)\Big]$$

= full Hamiltonian for 4 sites! ✓

Longer-ranged interactions

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

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

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

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

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

x

$$\hat W_{[L]} = \begin{pmatrix} \hat{\mathbb{1}} \\ \hat S^z \\ 0 \\ 0 \end{pmatrix}$$ = 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:

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

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

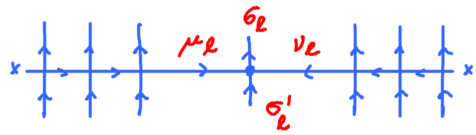
$$= J_1\hat S^z\otimes\hat S^z\otimes\hat{\mathbb{1}} + J_2\hat S^z\otimes\hat{\mathbb{1}}\otimes\hat S^z + \hat{\mathbb{1}}\otimes J_1\hat S_z\otimes\hat S_z$$ ✓

3. Applying MPO to mixed-canonical state

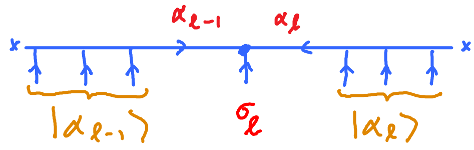
[Schollwöck2011, Sec. 6.2] MPS-IV.3

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

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



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

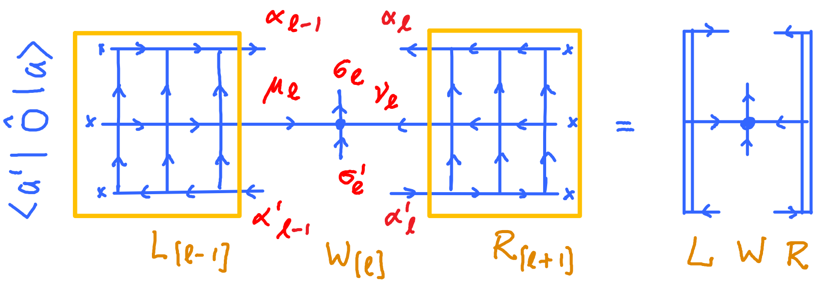


Here $\{|a\rangle\}$ form a basis for the mixed-canonical representation. Express operator in this basis:

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

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

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

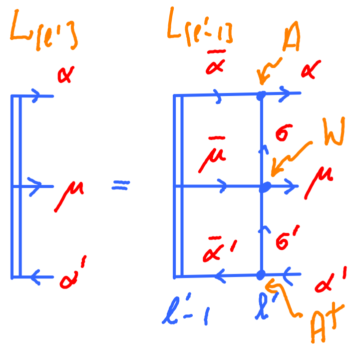


(5)

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

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

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

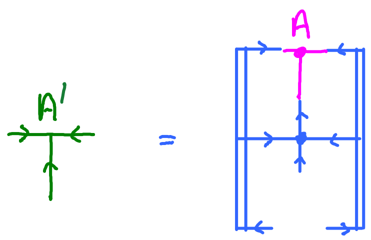


For efficient computation, perform sums in this order:

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

The application of MPO to MPS is then represented as:

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



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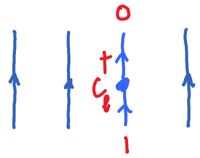
4. MPS representation of Fermi sea

key idea: [Silvi2013]
we follow compact discussion of [Wu2020]
further applications: [Jin2020,Jin2020a]

Consider a system of non-interacting fermions defined on sites $\ell = 1, \dots, N$,

with local basis $|\sigma_\ell\rangle \in \{|0_\ell\rangle, |1_\ell\rangle\}$ (empty, filled) and $|1_\ell\rangle = c^\dagger_\ell |0_\ell\rangle$

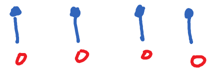


described by a quadratic Hamiltonian,

$$\hat{H} = \hat{c}^\dagger_{\ell'} h^{\ell'}{}_{\ell}\, \hat{c}_\ell = \hat{c}^\dagger_{\ell'} (\underbrace{U D U^\dagger}_{D \text{ diagonal}})^{\ell'}{}_{\ell}\, \hat{c}_\ell = \sum_\alpha \varepsilon_\alpha \hat{d}^\dagger_\alpha \hat{d}_\alpha$$

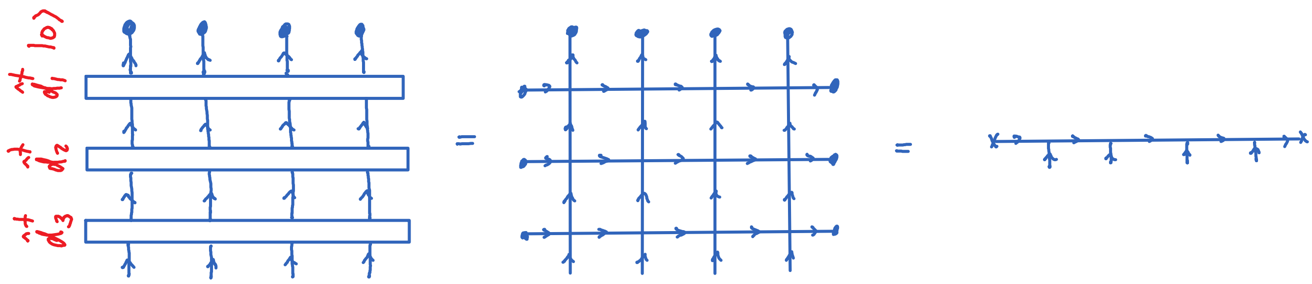
with eigenenergies ε_α and eigenmodes $\hat{d}^\dagger_\alpha = \hat{c}^\dagger_{\ell'} U^{\ell'}{}_{\alpha}$.

Filled Fermi sea of M particles: $|F\rangle = \prod_{\alpha=1}^{M} \hat{d}^\dagger_\alpha |0\rangle$ vacuum state (all sites empty) bond dim. = 1 $\quad |0_1\rangle \otimes |0_2\rangle \otimes \dots \otimes |0_N\rangle$



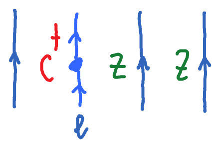
Goal: express this state as an MPS!

Strategy: express each $\hat{d}^\dagger_\alpha$ as an MPO, sequentially apply these to vacuum state.



MPO representation of $d^\dagger_\alpha$: (similar to MPS-IV.1.19)

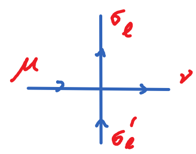
$$\hat{d}^\dagger_\alpha = \sum_\ell \hat{c}^\dagger_\ell U^\ell{}_\alpha$$ with single-site operators $\hat{c}^\dagger_\ell \overset{\text{(MPS-I.1.22)}}{=}$



$$= \begin{pmatrix} 0 & 1 \end{pmatrix} \prod_{\ell=1}^{M} \hat{W}_{[\ell]} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \hat{W}_{[\ell]} = \begin{pmatrix} \hat{Z}_{[\ell]} & 0 \\ \hat{c}^\dagger_\ell U^\ell{}_\alpha & \hat{\mathbb{1}}_{[\ell]} \end{pmatrix}$$

Matrix elements:

$$W_{[\ell]}^{\mu\sigma'_\ell}{}_{\nu\sigma_\ell} = \begin{pmatrix} (Z)^{\sigma'_\ell}{}_{\sigma_\ell} & 0 \\ (c^\dagger)^{\sigma'_\ell}{}_{\sigma_\ell} U^\ell{}_\alpha & (\mathbb{1})^{\sigma'_\ell}{}_{\sigma_\ell} \end{pmatrix}^{\mu}{}_{\nu} = \begin{pmatrix} \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} & 0 \\ \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} U^\ell{}_\alpha & \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \end{pmatrix}$$



When computing $d^\dagger_M \cdots d^\dagger_2 d^\dagger_1 |0\rangle$ a truncation is needed after each application of an MPO to an MPS.
If the $U^\ell{}_\alpha$ coefficients have similar magnitudes throughout the chain (i.e. when varying ℓ for fixed α),
then application of $d^\dagger_\alpha$ substantially modifies the matrices of the MPS on all lattice sites, hence subsequent

truncation is likely to introduce considerable errors.

To avoid this, it is advisable to express the $d^\dagger_\alpha$ through 'Wannier orbitals' that are more localized in space, in that they diagonalize the projection, $\tilde{X}$, of the position operator $\hat{X}$ into the space of occupied orbitals [Kivelson1982] :

position operator: $\hat{X} = \sum_{\ell=1}^{N} j \, c^\dagger_j c_j$ its projection: $\tilde{X}^{\alpha'}{}_{\alpha} = \langle 0 | d^\dagger_{\alpha'} \hat{X} d_\alpha | 0 \rangle$

Diagonalize: $\underbrace{\tilde{D}}_{\text{diagonal}} = B^\dagger \hat{X} B$, define Wannier orbitals
$$\begin{cases} f_r = d_\alpha B^\alpha{}_r \\ f^\dagger_r = d^\dagger_\alpha \underbrace{\overline{B^\alpha{}_r}}_{B^{\dagger r}{}_\alpha} = c^\dagger_\ell U^\ell{}_\alpha \overline{B^\alpha{}_r} \end{cases}$$

with $B^{-1} = B^\dagger$ unitary

(then $\langle 0 | f^\dagger_{r'} \hat{X} f_r | 0 \rangle = B^{\dagger r'}{}_{\alpha'} \langle 0 | d^\dagger_{\alpha'} \hat{X} d_\alpha | 0 \rangle B^\alpha{}_r = B^{\dagger r}{}_{\alpha'} \tilde{X}^{\alpha'}{}_\alpha B^{\alpha r} = D^{r'}{}_r$ is diagonal)

Now, express the Fermi sea through Wannier orbitals, using $d^\dagger_\alpha = f^\dagger_r B^{\dagger r}{}_\alpha$

$$|F\rangle = d^\dagger_M \dots d^\dagger_2 d^\dagger_1 |0\rangle = \left(f^\dagger_{r_M} B^{\dagger r_M}{}_M \right) \dots \left(f^\dagger_{r_2} B^{\dagger r_2}{}_2 \right) \left(f^\dagger_{r_1} B^{\dagger r_1}{}_1 \right) |0\rangle$$

$$= \underbrace{B^{\dagger r_1}{}_M \dots B^{\dagger r_2}{}_2 B^{\dagger r_1}{}_1 \, \varepsilon_{r_M \dots r_2 r_1}}_{\det B^\dagger = 1} \, f^\dagger_M \dots f^\dagger_2 f^\dagger_1 |0\rangle \quad \text{(since B is unitary)}$$

$$= \prod_{r=1}^{M} f^\dagger_r |0\rangle = \prod_{r=1}^{M} c^\dagger_\ell (U \bar{B})^\ell{}_r |0\rangle$$

due to Pauli principle, only those terms survive for which all r-indices are different. In each surviving term, rearrange all $f^\dagger$'s into canonical N,...,2,1 order, keeping track of minus signs using a fully antisymmetric Levi-Civita symbol, $\varepsilon_{\dots i \dots j \dots} = - \varepsilon_{\dots j \dots i \dots}$

Truncation errors are much reduced when using an MPO representation for the f operators:

$$f^\dagger_r = \begin{pmatrix} 0 & 1 \end{pmatrix} \prod_{\ell=1}^{M} \hat{W}_{[\ell]} \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \qquad \hat{W}_{[\ell]} = \begin{pmatrix} \hat{Z}_{[\ell]} & 0 \\ \hat{c}^\dagger_\ell (U \bar{B})^\ell{}_r & \hat{1}_{[\ell]} \end{pmatrix}$$

In practice, truncation errors have been found to be smallest [Wu2020] if the parton operators are applied in an 'left-meets-right' order (first apply left-most , then right-most, then proceed inwards):

e.g. for even N: $|F\rangle = f^\dagger_{N/2} f^\dagger_{N/2-1} \dots f^\dagger_{N-1} f^\dagger_2 f^\dagger_N f^\dagger_1 |0\rangle$