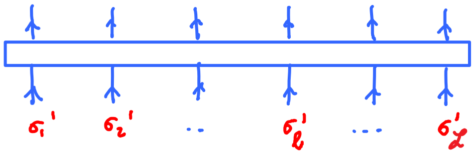
MPS.9-12: Matrix product operators (MPO)

[Schollwöck2011, Sec. 5]

MPS.9

MPS.9: General properties of MPOs

Consider an operator acting on $\mathcal{L}$-site chain: (1)

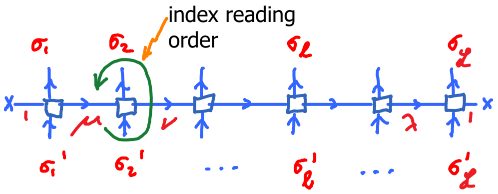


$$\hat O = |\vec\sigma'\rangle O^{\vec\sigma'}{}_{\vec\sigma} \langle\vec\sigma|$$

Goal: express it as a 'matrix product operator' (MPO):

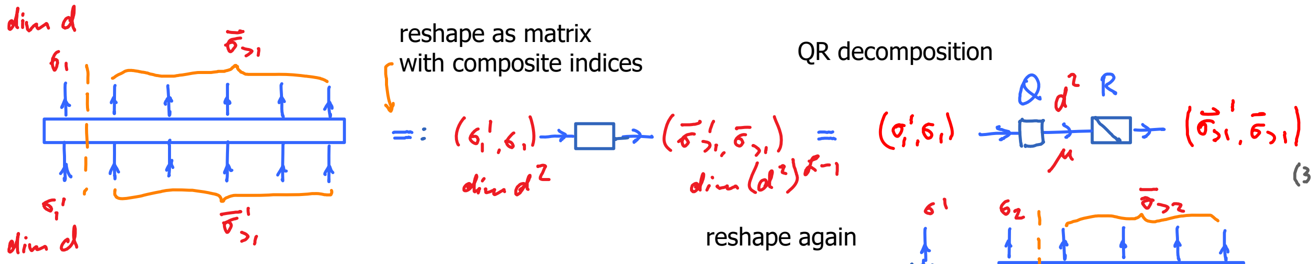
$$\hat O = |\vec\sigma'\rangle [W_1]^{1\sigma_1'}{}_{\mu\sigma_1} [W_2]^{\mu\sigma_2'}{}_{\nu\sigma_2} \cdots [W_{\mathcal L}]^{\lambda\sigma_{\mathcal L}'}{}_{1\sigma_{\mathcal L}} \langle\vec\sigma| \qquad (2)$$

$$:= |\vec\sigma'\rangle \left[\prod_{\ell=1}^{\mathcal L} W_\ell\right]^{\vec\sigma'}{}_{\vec\sigma} \langle\vec\sigma|$$



arrow conventions on virtual MPO bonds
is chosen to be same as for virtual MPS bonds

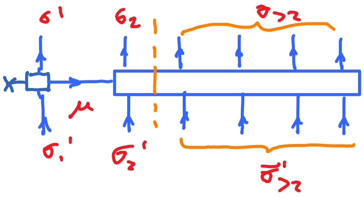
This can always be achieved using a sequence of QR decompositions:



reshape as matrix with composite indices

QR decomposition (3)

reshape again



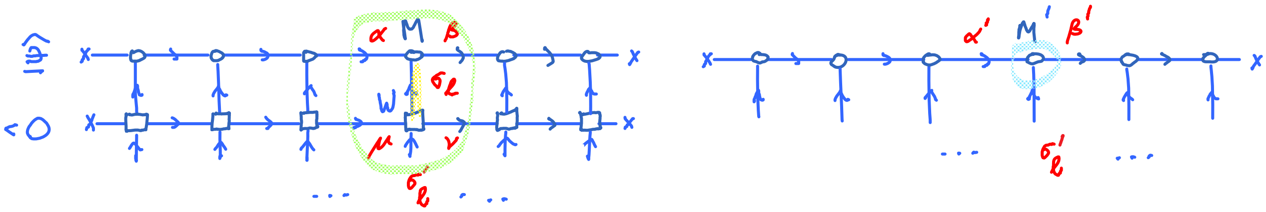
(4)

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

But for short-ranged Hamiltonians, virtual bond dimension of MPO, to be called w, is typically small, $\mathcal{O}(1)$.

Applying MPO to MPS yields MPS

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

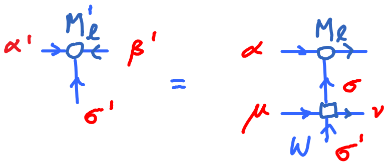


(6)

$$|\psi\rangle = |\vec\sigma\rangle \left[\prod_\ell M_\ell\right]^{\vec\sigma} \qquad (7)$$

$$|\psi'\rangle = \hat O |\psi\rangle = |\vec\sigma'\rangle \left[\prod_\ell M_\ell'\right]^{\vec\sigma'} \qquad (8)$$

$$[M_\ell']^{\alpha'\sigma'}{}_{\beta'} = [W_\ell]^{\mu\sigma'}{}_{\underbrace{\nu\sigma\,[M_\ell]^{\alpha\sigma}}}{}_{\beta}$$

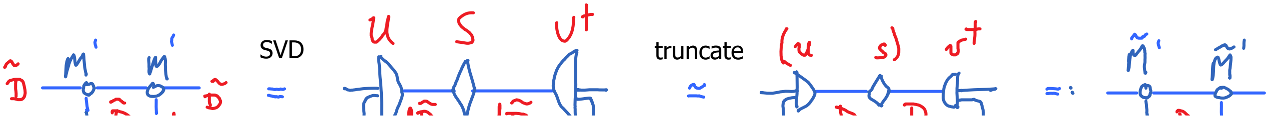


(9)

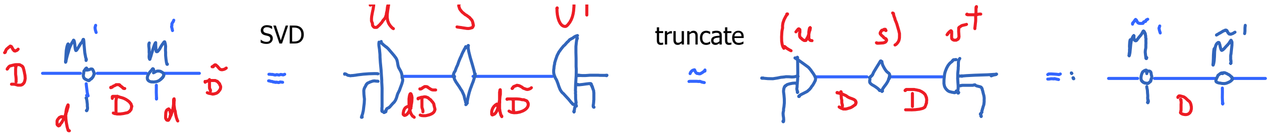
with composite indices, $\alpha_\ell' = (\alpha, \mu)$, $\beta_\ell' = (\beta, \nu)$

of increased dimension: $\tilde D_{M'} = D_M \cdot w$ (10)

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



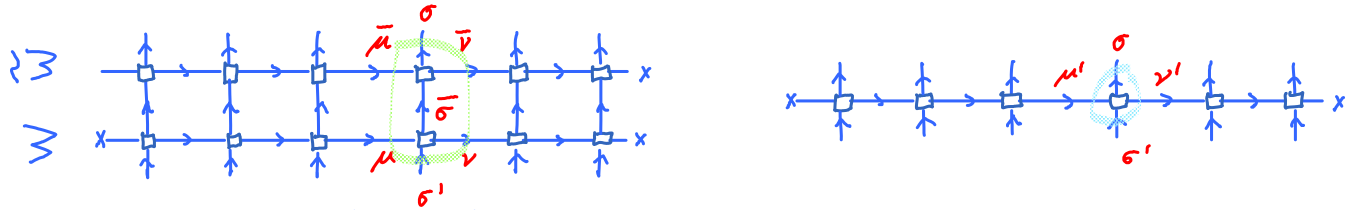
(11)



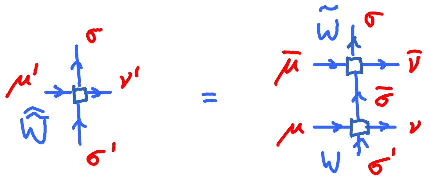
(11)

Multiplication of MPOs

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



$$\underline{[\tilde{\tilde{W}}_\ell]^{\mu'\sigma'}{}_{\nu'\sigma}} = \underline{[W_\ell]^{\mu\sigma'}{}_{\nu\bar{\sigma}} \underbrace{[\tilde{W}_\ell]^{\bar{\mu}\bar{\sigma}}{}_{\bar{\nu}}}_{}}\,{}_{\sigma}$$



(13)

with composite indices, $\mu' = (\mu, \bar{\mu})$, $\nu' = (\nu, \bar{\nu})$ of increased dimension: $\tilde{\tilde{w}} = w \cdot \tilde{w}$ (14)

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

Addition of MPOs

$$\hat{O} + \hat{\tilde{O}}$$

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

$$\hat{\tilde{\tilde{O}}} = \hat{O} + \hat{\tilde{O}} = |\vec{\sigma}'\rangle \left[W_1 W_2 \cdots W_{\ell-1} W_\ell + \tilde{W}_1 \tilde{W}_2 \cdots \hat{W}_{\ell-1} \tilde{W}_\ell \right]^{\vec{\sigma}'}{}_{\vec{\sigma}} \langle\vec{\sigma}| \tag{16}$$

$$= |\vec{\sigma}'\rangle \left[\begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} W_1 W_2 \cdots W_\ell & 0 \\ 0 & \hat{W}_1 \hat{W}_2 \cdots \tilde{W}_\ell \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right]^{\vec{\sigma}'}{}_{\vec{\sigma}} \langle\vec{\sigma}|$$

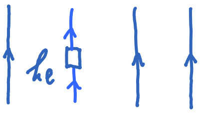
$$= |\vec{\sigma}'\rangle \left[\begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} W_1 & \\ & \tilde{W}_1 \end{pmatrix} \begin{pmatrix} W_2 & \\ & \hat{W}_2 \end{pmatrix} \cdots \begin{pmatrix} W_{\ell-1} & \\ & \tilde{W}_{\ell-1} \end{pmatrix} \begin{pmatrix} W_\ell & \\ & \tilde{W}_\ell \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right]^{\vec{\sigma}}{}_{\vec{\sigma}} \langle\vec{\sigma}|$$

$$= |\vec{\sigma}'\rangle \left[\begin{pmatrix} W_1 & \tilde{W}_1 \end{pmatrix} \begin{pmatrix} W_2 & \\ & \hat{W}_2 \end{pmatrix} \cdots \begin{pmatrix} W_{\ell-1} & \\ & \tilde{W}_{\ell-1} \end{pmatrix} \begin{pmatrix} W_\ell \\ \hat{W}_\ell \end{pmatrix} \right]^{\vec{\sigma}}{}_{\vec{\sigma}} \langle\vec{\sigma}| \tag{17}$$

= MPO in enlarged virtual space, with bond dimension $\hat{\tilde{w}} = w + \tilde{w}$

Sum of single-site operators

Let $\hat{H}_\ell = \sum_{\ell=1}^{\ell} \hat{h}_\ell$ with single-site operators $\hat{h}_\ell \overset{\text{(MPS-I.1.22)}}{=}$



(18)

$$= \hat{h}_1 \otimes \hat{1}_2 \otimes \hat{1}_3 \otimes \cdots \otimes \hat{1}_\ell + \hat{1}_1 \otimes \hat{h}_2 \otimes \hat{1}_3 \otimes \cdots \otimes \hat{1}_\ell + \hat{1} \otimes \hat{1}_2 \otimes \hat{h}_3 \otimes \cdots \otimes \hat{1}_\ell + \cdots \tag{19}$$

Goal: represent sum as product of matrices, constructed such that each $\hat{h}_\ell$ is sandwiched between unity operators.

Useful identities: $\begin{pmatrix} 1 & 0 \\ a & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ b & 1 \end{pmatrix} = \begin{pmatrix} 1 \cdot 1 & 1 \cdot 0 \\ a \cdot 1 + 1 \cdot b & 1 \cdot 1 \end{pmatrix}$, $\quad \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ a & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = a$ (20)

Useful identities:

$$\begin{pmatrix}1&0\\a&1\end{pmatrix}\begin{pmatrix}1&0\\b&1\end{pmatrix} = \begin{pmatrix}1\cdot1 & 1\cdot0\\ a\cdot1+1\cdot b & 1\cdot1\end{pmatrix}, \qquad (0\ \ 1)\begin{pmatrix}1&0\\a&1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = a \qquad (20)$$

product generates sum of 12-elements, pre- or post-multiplied by unity

extract 12-element of 2x2 matrix

MPO representation with $w = 2$:

zero operator

$$\boxed{\hat O = (0\ \ 1)\prod_{\otimes\ell=1}^{\mathscr{L}}\hat W_\ell\begin{pmatrix}1\\0\end{pmatrix}, \qquad \text{with} \qquad \hat W_\ell = \begin{pmatrix}\hat{\mathbb{1}}_\ell & \hat 0\\ \hat h_\ell & \hat{\mathbb{1}}_\ell\end{pmatrix}} \qquad (21)$$

"opening row vector"

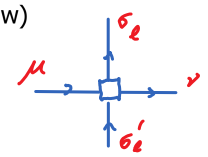
"closing column vector"

single-particle operator for site ℓ

Matrix elements of W have direct-product structure:

zero (suppressed below)

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



(22)

Check for $\mathscr{L}=3$:

$$\hat O = (0\ \ 1)\begin{pmatrix}\hat{\mathbb{1}}_1 & \hat 0_1\\ \hat h_1 & \hat{\mathbb{1}}_1\end{pmatrix}\otimes\begin{pmatrix}\hat{\mathbb{1}}_2 & \hat 0_2\\ \hat h_2 & \hat{\mathbb{1}}_2\end{pmatrix}\otimes\begin{pmatrix}\hat{\mathbb{1}}_3 & \hat 0_3\\ \hat h_3 & \hat{\mathbb{1}}_3\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} \qquad (23a)$$

zeros

$$= (0\ \ 1)\begin{pmatrix}\hat{\mathbb{1}}_1\otimes\hat{\mathbb{1}}_2\otimes\hat{\mathbb{1}}_3 & \hat 0_1\otimes\hat 0_2\otimes\hat 0_3\\ \hat h_1\otimes\hat{\mathbb{1}}_2\otimes\hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1\otimes\hat h_2\otimes\hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1\otimes\hat{\mathbb{1}}_2\otimes\hat h_3 & \hat{\mathbb{1}}_1\otimes\hat{\mathbb{1}}_2\otimes\hat{\mathbb{1}}_3\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} \qquad (23b)$$

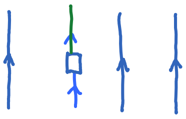
$$= \hat h_1\otimes\hat{\mathbb{1}}_2\otimes\hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1\otimes\hat h_2\otimes\hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1\otimes\hat{\mathbb{1}}_2\otimes\hat h_3 \qquad \checkmark \qquad \text{[matches (19)]} \qquad (23c)$$

(21) can also be expressed as

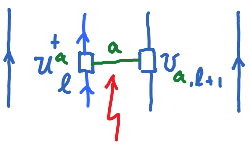
$$\hat O = \prod_{\otimes\ell=1}^{\mathscr{L}}\hat W_\ell, \quad \hat W_1 = (\hat h_1\ \ \hat{\mathbb{1}}_1), \quad \underset{\ell=2,\dots,\mathscr{L}-1}{\hat W_\ell = \begin{pmatrix}\hat{\mathbb{1}}_\ell & \hat 0_\ell\\ \hat h_\ell & \hat{\mathbb{1}}_\ell\end{pmatrix}}, \quad \hat W_{\mathscr{L}} = \begin{pmatrix}\hat{\mathbb{1}}_{\mathscr{L}}\\ \hat h_{\mathscr{L}}\end{pmatrix} \qquad (24)$$

Sum of single-site and two-site operators

Let
$$\hat H_{\mathscr{L}} = \underbrace{\sum_{\ell=1}^{\mathscr{L}}\hat h_\ell}_{\text{single-site operators}} + \underbrace{\sum_{\ell=1}^{\mathscr{L}-1}\hat h_{\ell,\ell+1}}_{\text{nearest-neighbor operators}} = \sum_{\ell=1}^{\mathscr{L}}$$



$$+\sum_{\ell=1}^{\mathscr{L}}$$



(25)

horizontal line indicates summation over a

with

$$\hat h_{\ell,\ell+1} = \underset{\text{row vector}}{\vec u^{\dagger}_\ell}\cdot\underset{\text{column vector}}{\vec v_{\ell+1}} = \sum_a \hat u^{a\dagger}_\ell\,\hat v_{a,\ell+1} = \hat{\mathbb{1}}_1\otimes\hat{\mathbb{1}}_2\otimes\dots\otimes\hat{\mathbb{1}}_{\ell-1}\otimes\vec u^{\dagger}_\ell\otimes\vec v_{\ell+1}\otimes\hat{\mathbb{1}}_{\ell+2}\otimes\dots\otimes\hat{\mathbb{1}}_{\mathscr{L}} \qquad (26)$$

$$(\cdot\ \cdot\ \cdot)\begin{pmatrix}\vdots\end{pmatrix}$$

For example:

(dropping site indices)

$$\underset{\ell}{\hat S_+}\,\underset{\ell+1}{\hat S_-} + \underset{\ell}{\hat S_-}\,\underset{\ell+1}{\hat S_+} = \hat S^{-\dagger}\hat S_- + \hat S^{+\dagger}\hat S_+ = (\hat S^{-\dagger}\ \ \hat S^{+\dagger})\begin{pmatrix}\hat S_-\\ \hat S_+\end{pmatrix} \qquad (27)$$

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!

to be found!

$$\hat H = |\vec\sigma'\rangle H^{\vec\sigma'}{}_{\vec\sigma}\langle\vec\sigma| =: (0,\dots,1)\prod\hat W_\ell\,(1\ \ ) \quad = \text{matrix product of one-site operators}$$

to be found!

$$\hat H_\mathcal{L} = |\vec\sigma'\rangle H^{\vec\sigma'_\mathcal{L}}{}_{\vec\sigma_\mathcal{L}}\langle\vec\sigma| =: (0,\dots,1)\prod \hat W_\ell \begin{pmatrix}1\\0\\\vdots\\0\end{pmatrix} \tag{28}$$

= matrix <u>product</u> of <u>one</u>-site operators

each matrix has dimensions $w \times w$

"opening row vector"
dimension = w

"closing column vector"
dimension = w

$$=: \left(\hat W_1\right)^{w}{}_{\mu} \otimes \left(\hat W_2\right)^{\mu}{}_{\nu} \otimes \dots \otimes \left(\hat W_\mathcal{L}\right)^{\eta}{}_{1} \tag{29}$$

$$=: \left(|\sigma_1'\rangle [W_1]^{1\sigma_1'}{}_{\mu\sigma_1}\langle\sigma_1|\right) \otimes \left(|\sigma_2'\rangle [W_2]^{\mu\sigma_2'}{}_{\nu\sigma_2}\langle\sigma_2|\right) \otimes\dots\otimes \left(|\sigma_\mathcal{L}'\rangle [W_\mathcal{L}]^{\eta\sigma_\mathcal{L}'}{}_{1\sigma_\mathcal{L}}\langle\sigma_\mathcal{L}|\right) \tag{30}$$

Each $\hat W_\ell$ acts only on site ℓ ; their matrix product gives the full MPO.

Let us construct MPO for Hamiltonian of 2 sites, then 3 sites, then 4 sites, and seek to recognize a pattern.

Start with sites 1 and 2:

$$\hat H_2 = \hat h_1 \otimes \hat 1_2 + \vec u_1^\dagger \otimes \vec v_2 + \hat 1_1 \otimes \hat h_2 = \begin{pmatrix}\hat h_1 & \vec u_1^\dagger & \hat 1_1\end{pmatrix} \otimes \begin{pmatrix}\hat 1_2\\ \vec v_2\\ \hat h_2\end{pmatrix} \tag{31}$$

Here, $\otimes$ denotes direct product of matrix elements, not entire matrices, to reproduce left side

Add site 3:

$$\hat H_3 = \hat H_2 \otimes \hat 1_3 + \hat 1_1 \otimes \vec u_2^\dagger \times \vec v_3 + \hat 1_1 \otimes \hat 1_2 \otimes \hat h_3 = \begin{pmatrix}\hat h_1 & \vec u_1^\dagger & \hat 1_1\end{pmatrix} \otimes \begin{pmatrix}\hat 1_2 & \hat 0 & \hat 0\\ \vec v_2 & \hat 0 & \hat 0\\ \hat h_2 & \vec u_2^\dagger & \hat 1_2\end{pmatrix} \otimes \begin{pmatrix}\hat 1_3\\ \vec v_3\\ \hat h_3\end{pmatrix} \tag{32}$$

zero operators

Add site 4:

$$\hat H_4 = \hat H_3 \otimes \hat 1_4 + \hat 1_1 \otimes \hat 1_2 \otimes \vec u_3^\dagger \times \vec v_4 + \hat 1_1 \otimes \hat 1_2 \otimes \hat 1_3 \otimes \hat h_4 \tag{33}$$

$$= \begin{pmatrix}\hat h_1 & \vec u_1^\dagger & \hat 1_1\end{pmatrix} \otimes \begin{pmatrix}\hat 1_2 & & \\ \vec v_2 & & \\ \hat h_2 & \vec u_2^\dagger & \hat 1_2\end{pmatrix} \otimes \begin{pmatrix}\hat 1_3 & & \\ \vec v_3 & & \\ \hat h_3 & \vec u_3^\dagger & \hat 1_3\end{pmatrix} \otimes \begin{pmatrix}\hat 1_4\\ \vec v_4\\ \hat h_4\end{pmatrix} \tag{34}$$

Useful identity:

$$\begin{pmatrix}\hat 1_\ell & & \\ \vec v_\ell & & \\ \hat h_\ell & \vec u_\ell^\dagger & \hat 1_\ell\end{pmatrix} \otimes \begin{pmatrix}\hat 1_{\ell+1} & & \\ \vec v_{\ell+1} & & \\ \hat h_{\ell+1} & \vec u_{\ell+1}^\dagger & \hat 1_{\ell+1}\end{pmatrix} = \begin{pmatrix}\hat 1_\ell \otimes \hat 1_{\ell+1} & & \\ \vec v_\ell \otimes \hat 1_{\ell+1} & & \\ \underbrace{\left(\hat h_\ell \otimes \hat 1_{\ell+1} + \vec u_\ell^\dagger \otimes \vec v_{\ell+1} + \hat 1_\ell \otimes \hat h_{\ell+1}\right)} & \hat 1_\ell \otimes \vec u_{\ell+1}^\dagger & \hat 1_\ell \otimes \hat 1_{\ell+1}\end{pmatrix} \tag{35}$$

product generates terms from sites ℓ and $\ell+1$

Hence, we conclude: $\hat H_\mathcal{L}$ has an MPO representation with $w = 2 + \dim(\vec v) = 2 + \dim(\vec u^\dagger)$ (36)

Define: $\boxed{\hat W_\ell = \begin{pmatrix}\hat 1_\ell & & \\ \vec v_\ell & & \\ \hat h_\ell & \vec u_\ell^\dagger & \hat 1_\ell\end{pmatrix}}$ then $\left[\hat W_\ell\right]^{w}{}_{\mu} \otimes \left[\hat W_{\ell+1}\right]^{\mu}{}_{1} = \hat h_\ell \otimes \hat 1_{\ell+1} + \vec u_\ell^\dagger \otimes \vec v_{\ell+1} + \hat 1_\ell \otimes \hat h_{\ell+1}$ (37)

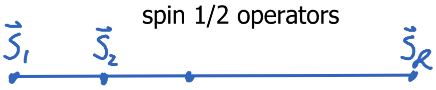
and $$\hat{H}_{\mathcal{L}} = \left[\hat{W}_1\right]^{w}{}_{\mu} \left[\prod_{\ell=2}^{\mathcal{L}-1} \hat{W}_\ell\right]^{\mu}{}_{\nu} \left[\hat{W}_{\mathcal{L}}\right]^{\nu}{}_{1} = \boxed{\begin{pmatrix} 0 & \vec{0} & 1 \end{pmatrix} \prod_{\ell=1}^{\mathcal{L}} \hat{W}_\ell \begin{pmatrix} 1 \\ \vec{0} \\ 0 \end{pmatrix}} \qquad (38)$$

compare (29)

compare (28)

MPS.10 MPO for Heisenberg Hamiltonian

MPS.10



$$\hat{H}_\mathcal{L} = \sum_{\ell=1}^{\mathcal{L}} \hat{h}_\ell + \sum_{\ell=1}^{\mathcal{L}-1} \hat{h}_{\ell,\ell+1} \qquad (1)$$

$$\hat{h}_\ell = -h\hat{S}^z_\ell , \qquad \hat{h}_{\ell,\ell+1} = J\hat{S}^+_\ell \hat{S}^-_{\ell+1} + J\hat{S}^-_\ell \hat{S}^+_{\ell+1} + J^z \hat{S}^z_\ell \hat{S}^z_{\ell+1} \qquad (2)$$

$$= \begin{pmatrix} J\hat{S}^-_\ell & J\hat{S}^+_\ell & J_z\hat{S}^z_\ell \end{pmatrix} \begin{pmatrix} \hat{S}^+_{\ell+1} \\ \hat{S}^-_{\ell+1} \\ \hat{S}^z_{\ell+1} \end{pmatrix} =: \vec{u}^{\,T}_\ell \cdot \vec{v}_{\ell+1} \qquad (3)$$

MPO bond dimension: $w = 2 + 3 = 5$ (4)

(MPS.13.36)

$$H_\mathcal{L} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \end{pmatrix} \prod_{\ell=1}^{\mathcal{L}} \hat{W}_\ell \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{with} \quad \hat{W}_\ell = \begin{array}{c|ccccc} & 1 & 2 & 3 & 4 & 5 \\ \hline 1 & \hat{\mathbb{1}}_\ell & 0 & & & \\ 2 & \hat{S}^+_\ell & 0 & & & \\ 3 & \hat{S}^-_\ell & 0 & & & \\ 4 & \hat{S}^z_\ell & 0 & 0 & 0 & 0 \\ 5 & -h\hat{S}^z_\ell & J\hat{S}^-_\ell & J\hat{S}^+_\ell & J^z\hat{S}^z_\ell & \hat{\mathbb{1}}_\ell \end{array} \qquad (5)$$

(MPS.13.38) (MPS.13.37)

Rationalization of this matrix structure:

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

The matrix element $\mu\nu$ of $\hat{W}_\ell$ implements 'transition' from 'state' ν to μ on its left: $(\mu, \nu \in \{1, \dots, 5\})$

$$\hat{\mathbb{1}}_1 \overset{5}{\otimes} \hat{\mathbb{1}}_2 \overset{5}{\otimes} \hat{\mathbb{1}}_3 \overset{5}{\otimes} -h\hat{S}^z_4 \overset{1}{\otimes} \hat{\mathbb{1}}_5 \overset{1}{\otimes} \hat{\mathbb{1}}_6$$

$$\hat{\mathbb{1}}_1 \overset{5}{\otimes} \hat{\mathbb{1}}_2 \overset{5}{\otimes} J\hat{S}^-_3 \overset{2}{\otimes} \hat{S}^+_4 \overset{1}{\otimes} \hat{\mathbb{1}}_5 \overset{1}{\otimes} \hat{\mathbb{1}}_6$$

$$\hat{\mathbb{1}}_1 \overset{5}{\otimes} \hat{\mathbb{1}}_2 \overset{5}{\otimes} J\hat{S}^+_3 \overset{3}{\otimes} \hat{S}^-_4 \overset{1}{\otimes} \hat{\mathbb{1}}_5 \overset{1}{\otimes} \hat{\mathbb{1}}_6$$

$$\hat{\mathbb{1}}_1 \overset{5}{\otimes} \hat{\mathbb{1}}_2 \overset{5}{\otimes} J^z\hat{S}^z_3 \overset{4}{\otimes} \hat{S}^z_4 \overset{1}{\otimes} \hat{\mathbb{1}}_5 \overset{1}{\otimes} \hat{\mathbb{1}}_6$$

state 1: only $\hat{\mathbb{1}}$ to the right (6a)

state 2: one $\hat{S}^+$ just to the right (6b)

state 3: one $\hat{S}^-$ just to the right (6c)

state 4: one $\hat{S}^z$ just to the right (6d)

state 5: only $\hat{\mathbb{1}}$ to the left (6e)

(i.e. one $-h\hat{S}^z$ or completed interaction somewhere to the right)

Key property: $$\left[\hat{W}_\ell\right]^5{}_\mu \otimes \left[\hat{W}_{\ell+1}\right]^\mu{}_1 = \hat{H}_\ell \otimes \hat{\mathbb{1}}_{\ell+1} + \hat{H}_{\ell,\ell+1} + \hat{\mathbb{1}}_\ell \otimes \hat{H}_{\ell+1} \qquad (7)$$

Check: multiplying out a product of such $\hat{W}_\ell$'s yields desired result: an MPO with bond dimension $w = 5$:

$$\hat{W}_1 \otimes \hat{W}_2 \otimes \hat{W}_3 \otimes \hat{W}_4 = \qquad (11)$$

$$\hat{W}_1 \otimes \begin{bmatrix} \hat{\mathbb{1}}_2 & 0 & & & \\ \hat{S}_2^+ & 0 & & & \\ \hat{S}_2^- & 0 & & & \\ \hat{S}_2^z & 0 & & & \\ -h\hat{S}_2^z & J\hat{S}_2^- & J\hat{S}_2^+ & J^z\hat{S}_2^z & \hat{\mathbb{1}}_2 \end{bmatrix} \otimes \begin{bmatrix} \hat{\mathbb{1}}_3 & 0 & & & \\ \hat{S}_3^+ & 0 & & & \\ \hat{S}_3^- & 0 & & & \\ \hat{S}_3^z & 0 & & & \\ -h\hat{S}_3^z & J\hat{S}_3^- & J\hat{S}_3^+ & J^z\hat{S}_3^z & \hat{\mathbb{1}}_3 \end{bmatrix} \otimes \hat{W}_4 \tag{12}$$

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

$$= \hat{W}_1 \otimes \begin{bmatrix} \hat{\mathbb{1}}_1 \otimes \hat{\mathbb{1}}_2 & & & & \\ \hat{S}_1^+ \otimes \hat{\mathbb{1}}_2 & & & & \\ \hat{S}_1^- \otimes \hat{\mathbb{1}}_2 & & & & \\ \hat{S}_1^z \otimes \hat{\mathbb{1}}_2 & & & & \\ \underbrace{\left(-h\hat{S}_1^z \otimes \hat{\mathbb{1}}_2 + J\hat{S}_1^- \otimes \hat{S}_2^+ + J\hat{S}_1^+ \otimes \hat{S}_2^- + J^z\hat{S}_1^z \otimes \hat{S}_2^z + \hat{\mathbb{1}}_1 \otimes (-h\hat{S}_2^z)\right)} & \underbrace{\hat{\mathbb{1}}_1 \otimes J\hat{S}_2^- \quad \hat{\mathbb{1}}_1 \otimes J\hat{S}_2^+ + \hat{\mathbb{1}}_1 \otimes J^z\hat{S}_2^z} + \hat{\mathbb{1}}_1 \otimes \hat{\mathbb{1}}_2 \end{bmatrix} \otimes \hat{W}_4$$

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

(13)

$$= \left[-h\hat{S}_1^z,\ J\hat{S}_1^-,\ J\hat{S}_1^+,\ J^z\hat{S}_1^z,\ \hat{\mathbb{1}}_1\right] \otimes \begin{bmatrix} & \downarrow & \end{bmatrix} \otimes \begin{bmatrix} \hat{\mathbb{1}}_4 \\ \hat{S}_4^+ \\ \hat{S}_4^- \\ \hat{S}_4^z \\ -h\hat{S}_4^z \end{bmatrix} \tag{14}$$

$$\begin{aligned} = &\left[-h\hat{S}_1^z \otimes \hat{\mathbb{1}}_2 \otimes \hat{\mathbb{1}}_3 + J\hat{S}_1^- \otimes \hat{S}_2^+ \otimes \hat{\mathbb{1}}_3 + J\hat{S}_1^+ \otimes \hat{S}_2^- \otimes \hat{\mathbb{1}}_3 + J^z S_1^z \otimes S_2^z \otimes \hat{\mathbb{1}}_3\right] \otimes \hat{\mathbb{1}}_4 \\ &+ \hat{\mathbb{1}}_1 \otimes \left((-h\hat{S}_2^z) \otimes \hat{\mathbb{1}}_3 + J\hat{S}_2^- \otimes \hat{S}_3^+ + J\hat{S}_2^+ \otimes \hat{S}_3^- + J^z\hat{S}_2^z \otimes \hat{S}_3^z + \hat{\mathbb{1}}_2 \otimes (-h\hat{S}_3^z)\right) \otimes \hat{\mathbb{1}}_4 \\ &+ \hat{\mathbb{1}}_1 \otimes \left[\hat{\mathbb{1}}_2 \otimes J\hat{S}_3^- \otimes \hat{S}_4^+ + \hat{\mathbb{1}}_2 \otimes J\hat{S}_3^+ \otimes \hat{S}_4^- + \hat{\mathbb{1}}_2 \otimes J^z\hat{S}_3^z \otimes \hat{S}_4^z + \hat{\mathbb{1}}_2 \times \hat{\mathbb{1}}_3 \otimes (-h\hat{S}_4^z)\right] \end{aligned} \tag{15}$$

= full Hamiltonian for 4 sites! ✓

Longer-ranged interactions

$$\hat{H} = J_1 \sum_\ell \hat{S}_\ell^z \hat{S}_{\ell+1}^z + J_2 \sum_\ell \hat{S}_\ell^z \hat{S}_{\ell+2}^z \tag{16}$$

$$\hat{\mathbb{1}}_1 \overset{4}{\otimes} \hat{\mathbb{1}}_2 \overset{4}{\otimes} J_1\hat{S}_3^z \overset{2}{\otimes} \hat{S}_4^z \overset{1}{\otimes} \hat{\mathbb{1}}_5 \overset{1}{\otimes} \hat{\mathbb{1}}_6$$

$$\hat{\mathbb{1}}_1 \overset{6}{\otimes} \hat{\mathbb{1}}_2 \overset{4}{\otimes} J_2\hat{S}_3^z \overset{3}{\otimes} \hat{\mathbb{1}}_4 \overset{2}{\otimes} \hat{S}_5^z \overset{1}{\otimes} \hat{\mathbb{1}}_6$$

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

$w = 4$

state 4: completed interaction somewhere to the right

$$\hat{W}_\ell = \begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & \underline{\hat{\mathbb{1}}_\ell} & 0 & 0 & 0 \\ 2 & \underline{\hat{S}^z_\ell} & 0 & 0 & 0 \\ 3 & 0 & \underline{\hat{\mathbb{1}}_\ell} & 0 & 0 \\ 4 & 0 & \underline{J_1 \hat{S}^z_\ell} & \underline{J_2 \hat{S}^z_\ell} & \underline{\hat{\mathbb{1}}_\ell} \end{array}$$

x

$$\hat{W}_\mathcal{L} = \begin{pmatrix} \hat{\mathbb{1}}_\mathcal{L} \\ \hat{S}^z_\mathcal{L} \\ 0 \\ 0 \end{pmatrix} = \text{column } 1 \text{ of } \hat{W}_{\ell=\mathcal{L}} \qquad (17)$$

$$\hat{W}_1 = (0, J_1 \hat{S}^z_1, J_2 \hat{S}^z_1, \hat{\mathbb{1}}_1)$$

$$= \text{row } 4 \text{ of } \hat{W}_{\ell=1}$$

Check:

$$\hat{W}_1 \otimes \hat{W}_2 \otimes W_3 = \hat{W}_1 \otimes \begin{pmatrix} \hat{\mathbb{1}}_2 & 0 & 0 & 0 \\ \hat{S}^z_2 & 0 & 0 & 0 \\ 0 & \hat{\mathbb{1}}_2 & 0 & 0 \\ 0 & J_1 \hat{S}^z_2 & J_2 \hat{S}^z_2 & \hat{\mathbb{1}}_2 \end{pmatrix} \otimes \begin{pmatrix} \hat{\mathbb{1}}_3 \\ \hat{S}^z_3 \\ 0 \\ 0 \end{pmatrix} \qquad (18)$$

$$= (0, J_1 \hat{S}^z_1, J_2 \hat{S}^z_1, \hat{\mathbb{1}}_1) \otimes \begin{pmatrix} \hat{\mathbb{1}}_2 \otimes \hat{\mathbb{1}}_3 \\ \hat{S}^z_2 \otimes \hat{\mathbb{1}}_3 \\ \hat{\mathbb{1}}_2 \otimes \hat{S}^z_3 \\ 0 + J_1 \hat{S}^z_2 \otimes \hat{S}^z_3 + 0 + 0 \end{pmatrix} \qquad (19)$$

$$= J_1 \hat{S}^z_1 \otimes \hat{S}^z_2 \otimes \hat{\mathbb{1}}_3 + J_2 \hat{S}^z_1 \otimes \hat{\mathbb{1}}_2 \otimes \hat{S}^z_3 + \hat{\mathbb{1}}_1 \otimes J_1 \hat{S}^z_2 \otimes \hat{S}^z_3 \quad ✓ \qquad (20)$$

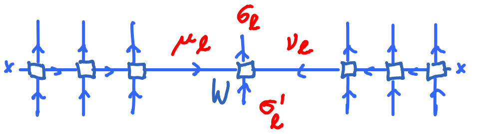
MPS.11 Applying MPO to Site - mixed-canonical state

[Schollwöck2011, Sec. 6.2]

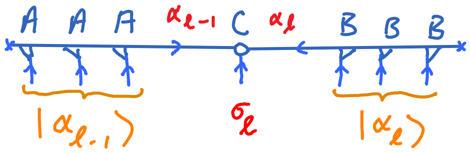
MPS.11

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

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



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

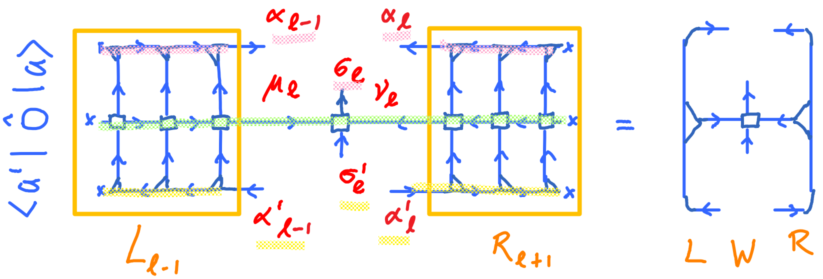


Here $\{|a\rangle\}$ form a basis for the mixed-canonical representation. Express operator in this basis:

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

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

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



left environment

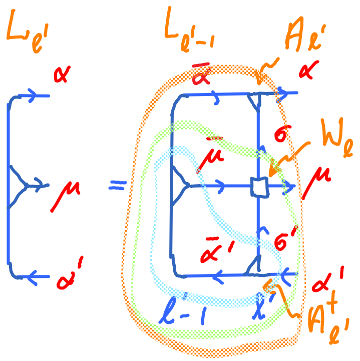
right environment

(5)

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

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

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



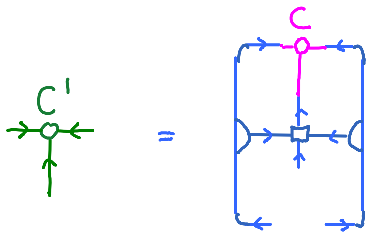
For efficient computation, perform sums in this order:

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

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

The application of MPO to MPS is then represented as:

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



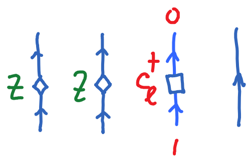
(11)

MPS.12 MPO representation of Fermi sea

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

Consider a system of (spinless) non-interacting fermions defined on sites $\ell = 1, \dots, \mathcal{L}$,

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



(1)

described by a quadratic Hamiltonian,

$$\hat H = \hat c^\dagger_{\ell'} h^{\ell'}{}_{\ell} \hat c^\ell = \underbrace{\hat c^\dagger_{\ell'} (U}_{d^\dagger_\alpha} \overset{\text{diagonal}}{\underbrace{D}_{\varepsilon_\alpha}} \underbrace{U^\dagger)^{\ell'}{}_{\ell} \hat c^\ell}_{d_\alpha} = \sum_\alpha \varepsilon_\alpha \hat d^\dagger_\alpha \hat d_\alpha \qquad (2)$$

[$\hat c^\ell$ is conjugate of $\hat c^\dagger_\ell$, hence index upstairs]

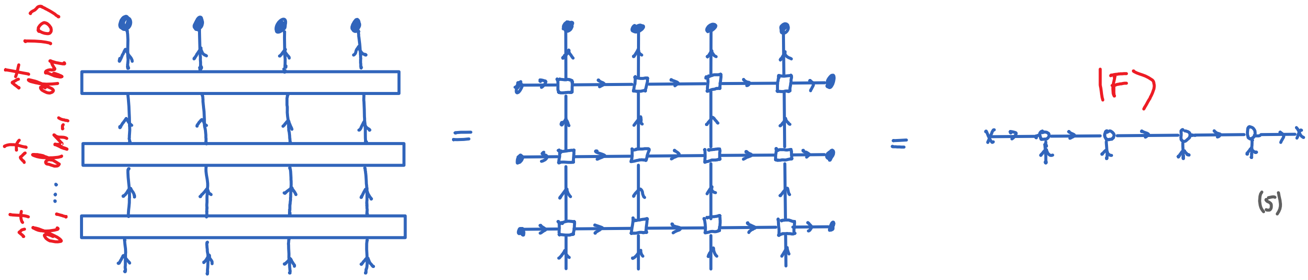
with eigenenergies ε_α and eigenmodes (sometimes called 'partons') $\hat d^\dagger_\alpha = \hat c^\dagger_{\ell'} U^{\ell'}{}_\alpha$, (3)

(4)

Filled Fermi sea of M particles: $|F\rangle = d^\dagger_1 d^\dagger_2 \dots d^\dagger_{M-1} d^\dagger_M |0\rangle$ vacuum state (all sites empty) bond dim. = 1 $|0_1\rangle \otimes |0_2\rangle \otimes \dots \otimes |0_\mathcal{L}\rangle$

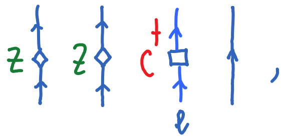
Goal: express this state as an MPS!

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



(5)

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



, (6)

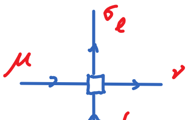
involves a sum over $\hat c^\dagger_\ell$, and has following MPO representation [similar to MPS.13, Eqs. (18-22)]:

$$\hat d^\dagger_\alpha = \begin{pmatrix} 0 & 1 \end{pmatrix} \prod_{\ell=1}^{\mathcal{L}} \hat W_{\ell\alpha} \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \qquad \hat W_{\ell\alpha} = \begin{pmatrix} \mathbb{1}_\ell & \mathbb{0}_\ell \\ \hat c^\dagger_\ell U^\ell{}_\alpha & \hat Z_\ell \end{pmatrix} \qquad (7)$$

this product generates sum on ℓ , see MPS.13, Eqs. (23)

no summation on ℓ here

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



(8)

When computing $d^\dagger_1 d^\dagger_2 \dots d^\dagger_M |0\rangle$, 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 M occupied orbitals [Kivelson1982] :

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 M occupied orbitals [Kivelson1982] :

position operator: $\hat{X} = \sum_{\ell=1}^{\mathcal{L}} \ell \, c^\dagger_\ell c^\ell$ its projection: $\tilde{X}^{\alpha'}{}_{\alpha} = \langle 0| d^{\alpha'} \hat{X} \, d^\dagger_\alpha |0\rangle$, $\alpha, \alpha' = 1, \dots, M$

Diagonalize: $\underset{\text{diagonal}}{\tilde{D}} = \underset{\text{with}}{B^\dagger \tilde{X} B}$, define Wannier orbitals $\underset{\text{unitary}}{}$
$$\begin{cases} f^\dagger_r = d^\dagger_\alpha B^\alpha{}_r \overset{(3)}{=} & (10a) \\ f^r = B^{\dagger r}{}_\alpha d^\alpha , \quad r = 1, \dots, M & (10b) \end{cases}$$

(then $\langle 0| f^{r'} \hat{X} f^\dagger_r |0\rangle \overset{(10)}{=} B^{\dagger r'}{}_{\alpha'} \langle 0| d^{\alpha'} \hat{X} d^\dagger_\alpha |0\rangle B^\alpha{}_r \overset{(9)}{=} B^{\dagger r'}{}_{\alpha'} \tilde{X}^{\alpha'}{}_\alpha B^\alpha{}_r = D^{r'}{}_r$ is diagonal ✓)

Now, express the Fermi sea through Wannier orbitals, using $d^\dagger_\alpha \overset{(10a)'}{=} f^\dagger_r B^r{}_\alpha$

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

$$= f^\dagger_1 f^\dagger_2 \dots f^\dagger_M |0\rangle \underbrace{\varepsilon^{12 \dots M}{}_{r_1 r_2 \dots r_M} B^{\dagger r_1}{}_1 B^{\dagger r_2}{}_2 \dots B^{\dagger r_M}{}_M}_{\det B^\dagger = 1 \text{ (since B is unitary)}}$$

$$= \prod_{r=1}^{M} f^\dagger_r |0\rangle \overset{(10a)}{=} \prod_{r=1}^{M} c^\dagger_\ell (UB)^\ell{}_r |0\rangle$$

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 1,2,...,M order, keeping track of minus signs using a fully antisymmetric Levi-Civita symbol,

$$\varepsilon^{12\dots M}{}_{\dots r \dots r' \dots} = -\varepsilon^{12\dots M}{}_{\dots r' \dots r \dots}$$

Each $f^\dagger_r$ involves a sum over $c^\dagger_\ell$, and has MPO representation analogous to (7) for $d^\dagger_\alpha$:

$$f^\dagger_r = (0 \quad 1) \prod_{\ell=1}^{\mathcal{L}} \hat{W}_{\ell r} \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \qquad \hat{W}_{\ell r} = \begin{pmatrix} \mathbb{1}_\ell & 0 \\ c^\dagger_\ell (UB)^\ell{}_r & \hat{Z}_\ell \end{pmatrix}$$

↑ this product generates sum on ℓ , see MPS.13, Eqs. (23)

↑ no summation on ℓ here

Truncation errors are much reduced when using an MPO representation for the f operators:
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 right-most , then left-most, then proceed inwards):

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

Wannier :