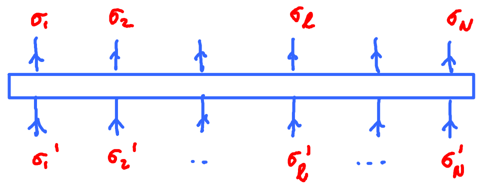
MPS-IV: Matrix product operators

[Schollwöck2011, Sec. 5]

Consider an operator acting on N-site chain:

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

(1)

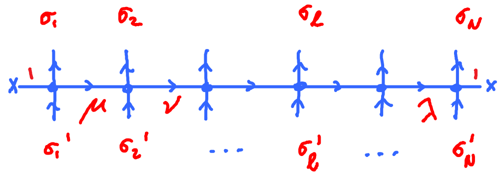


It can always be written as
'matrix product operator' (MPO),

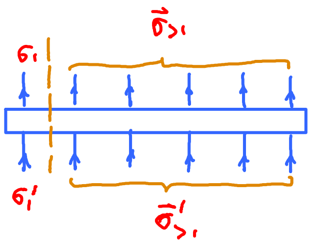
$$\hat{O} = |\vec{\sigma}'\rangle W^{1\sigma_1'}{}_{\mu\sigma_1} W^{\mu\sigma_2'}{}_{\nu\sigma_2} \ldots W^{\lambda\sigma_N'}{}_{1\sigma_N} \langle\vec{\sigma}|$$

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

(2)



using a sequence of QR decompositions:



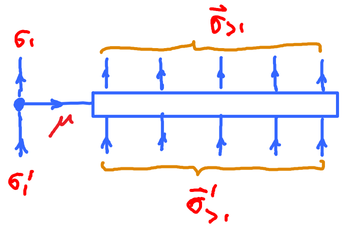
reshape as matrix
with composite indices

QR decomposition

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

reshape again

$=$



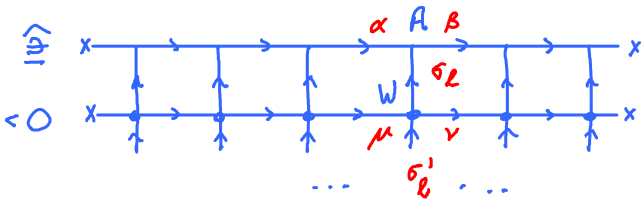
(4)

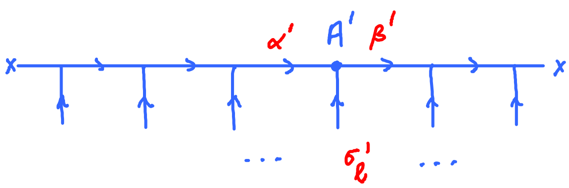
In general, this produces MPO
with growing bond dimensions: $d^2, (d^2)^2, (d^2)^3, \ldots$

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

1. Applying MPO to MPS yields MPS

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



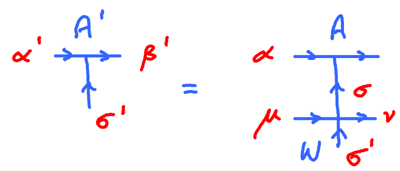


(6)

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

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

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



(9)

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

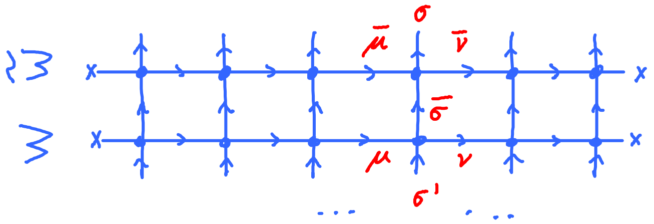
In practice, application of MPO is usually followed by SVD+truncation, to 'bring bond dimension back down':

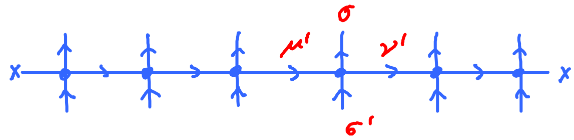
(11)

$\sim$ $\approx$

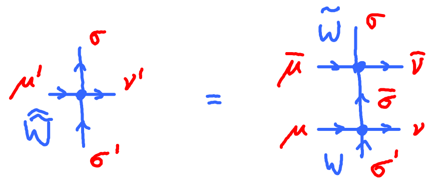
Multiplication of MPOs

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





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



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

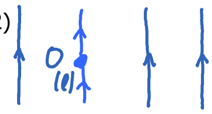
Let $\hat O = |\vec\sigma'\rangle \prod_\ell W^{\sigma'_\ell}{}_{\sigma_\ell} \langle\vec\sigma|$ $\qquad \hat{\tilde O} = |\vec\sigma'\rangle \prod_\ell \tilde W^{\sigma'_\ell}{}_{\sigma_\ell} \langle\vec\sigma|$ (15)

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

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

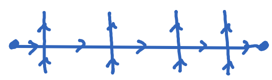
Sum of single-site operators

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



MPO representation:

$$= \begin{pmatrix} 0 & 1 \end{pmatrix} \prod_{\ell=1}^{N} \hat W_{[\ell]} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \hat W_{[\ell]} = \begin{pmatrix} \hat{\mathbb 1}_{[\ell]} & 0 \\ \hat O_{[\ell]} & \hat{\mathbb 1}_{[\ell]} \end{pmatrix} \tag{19}$$

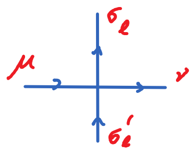


Check for N=2:

$$= \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{\mathbb 1}_{[1]} & 0 \\ \hat O_{[1]} & \hat{\mathbb 1}_{[1]} \end{pmatrix} \begin{pmatrix} \hat{\mathbb 1}_{[2]} & 0 \\ \hat O_{[2]} & \hat{\mathbb 1}_{[2]} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{20}$$

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

Matrix elements of W have direct-product structure: $W_{[\ell]}{}^{\mu\sigma'_\ell}{}_{\nu\sigma_\ell} = \begin{pmatrix} (\hat{\mathbb 1}_{[\ell]})^{\sigma'_\ell}{}_{\sigma_\ell} & 0 \\ (\hat O_{[\ell]})^{\sigma'_\ell}{}_{\sigma_\ell} & \hat{\mathbb 1}_{[\ell]}{}^{\sigma'_\ell}{}_{\sigma_\ell} \end{pmatrix}^{\mu}{}_{\nu}$ (22)



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 $= J^z\,\hat{S}^z_1 \otimes \hat{S}^z_2 \otimes \hat{\mathbb{1}} \otimes \dots \otimes \hat{\mathbb{1}}$

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

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:

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

$1 < \ell < N$

Site N: $\hat{W}_{[N]}$ = first column of $\hat{W}_{[\ell]}$ $= \left[\begin{array}{c} \hat{\mathbb{1}} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -hS_z \end{array}\right]\begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}$

column vector

Site 1: $\hat{W}_{[1]}$ = last row of $\hat{W}_{[\ell]}$

row vector

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

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

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

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

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

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

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

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

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

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

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

= 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

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

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

$$\hat W_{[1]} = \left(0,\ J_1 \hat S^z,\ J_2 \hat S^z,\ \hat{\mathbb{1}}\right)$$

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

Check:

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

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

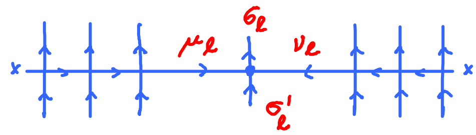
$$= J_1 \hat S^z \otimes \hat S^z \otimes \hat{\mathbb{1}} + J_2 \hat S^z \otimes \hat{\mathbb{1}} \otimes \hat S^z + \hat{\mathbb{1}} \otimes J_1 \hat S_z \otimes \hat S_z \quad \checkmark$$

3. Applying MPO to mixed-canonical state

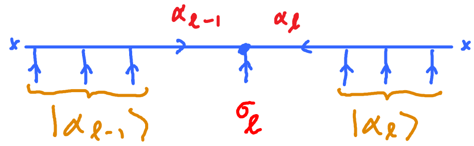
[Schollwöck2011, Sec. 6.2] MPS-IV.3

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

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



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

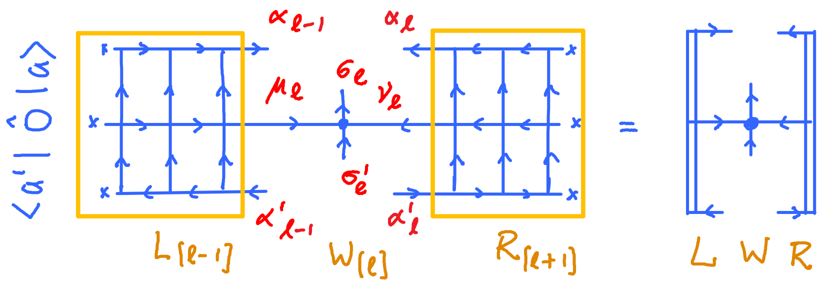


Here $\{|a\rangle\}$ form a basis for the mixed-canonical representation. Express operator in this basis:

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

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

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

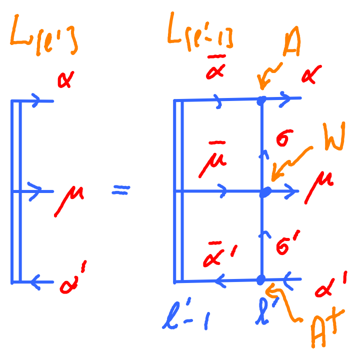


(5)

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

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

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

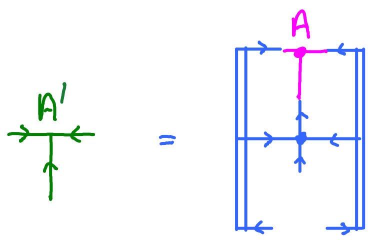


For efficient computation, perform sums in this order:

1. Sum over $\bar\alpha'$ 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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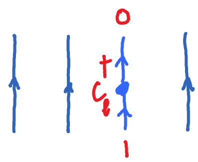
4. MPS representation of Fermi sea

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 $|\sigma_\ell\rangle \in \{ \underbrace{|0_\ell\rangle, |1_\ell\rangle}_{\text{empty, filled}} \}$ and $|1_\ell\rangle = c^\dagger_\ell |0_\ell\rangle$



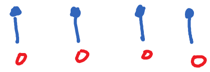
described by a quadratic Hamiltonian,

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

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

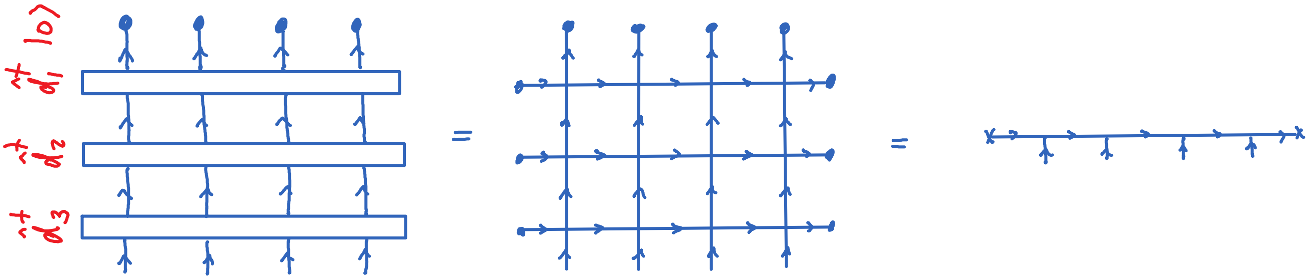
Filled Fermi sea of M particles: $|F\rangle = \prod_{\alpha=1}^{M} \hat{d}^\dagger_\alpha |0\rangle$

vacuum state $|0_1\rangle \otimes |0_2\rangle \otimes \dots \otimes |0_N\rangle$
(all sites empty)
bond dim. = 1



Goal: express this state as an MPS!

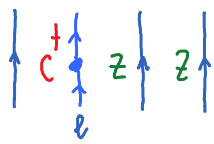
Strategy: express each $\hat{d}^\dagger_\alpha$ as an MPO, sequentially apply these to vacuum state.



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

$$\hat{d}^\dagger_\alpha = \sum_\ell \hat{c}^\dagger_\ell u^\ell{}_\alpha$$

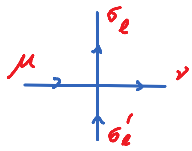
with single-site operators $\hat{c}^\dagger_\ell \overset{\text{(MPS-I.1.22)}}{=}$



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

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

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

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 $d^\dagger_\alpha = f^\dagger_r B^{\dagger r}{}_\alpha$

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

$$= \underbrace{B^{\dagger r_1}{}_M \dots B^{\dagger r_2}{}_2 B^{\dagger r_1}{}_1\, \varepsilon_{r_M \dots r_2 r_1}}_{\det B^\dagger = 1} \; f^\dagger_M \dots f^\dagger_2 f^\dagger_1 |0\rangle$$

(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 $f^\dagger_r$'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:

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

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

5. Application to spin models

[Wu2020]

MPS-IV.5

Parton representation of spin models

Models involving spin-1/2 degrees of freedom can be expressed through fermions (sometimes called 'pseudofermions' or 'partons' in this context), using the 'Abrikosov representation':

$$S^a_{[\ell]} = c^\dagger_{\ell s}\, \tfrac{1}{2}\underbrace{(\tau^a)}_{\text{Pauli matrices}}{}^{s'}{}_{s}\, c_{\ell s}, \quad a \in \{x,y,z\}$$

with constraint $\sum_{s=\uparrow\downarrow} d^\dagger_{\ell s} d_{\ell s} = 1$

with $\{c_{\ell' s'}, c^\dagger_{\ell s}\} = \delta_{\ell\ell'}\delta_{ss'}$, $\{c_{\ell' s'}, c_{\ell s}\} = 0$, $\{c_{\ell' s'}, c_{\ell s}\} = 0$.

The constraint forbids unphysical states:

$$|n_\uparrow, n_\downarrow\rangle \in \{ \underbrace{\overset{|\uparrow\rangle}{|1,0\rangle}, \overset{|\downarrow\rangle}{|0,1\rangle}}_{\text{physical}}, \underbrace{\cancel{|0,0\rangle}, \cancel{|1,1\rangle}}_{\text{unphysical}} \}$$

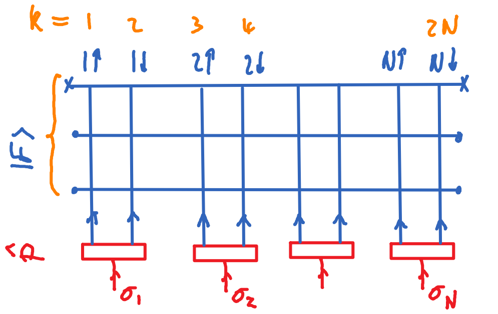
Exercise: verify that $[\hat S^a, \hat S^b] = i\,\varepsilon^{abc}\,\hat S^c$ holds, by using the fermionic anti-commutators

Spin-spin interaction: $\hat H = \sum_\ell \vec S_\ell \cdot \vec S_{\ell+1} = \sum_\ell \left(c^\dagger_{\ell s}\vec\sigma^{s'}{}_s c_{\ell s}\right)\left(c^\dagger_{\ell+1\, \bar s'}\vec\sigma^{\bar s'}{}_{\bar s}\, c_{\ell+1\, \bar s}\right)$

The quartic interaction is often treated in mean-field approximation. The resulting quadratic model is diagonalized, then a half-filled Fermi sea of eigenmodes is constructed, and in the end, a single-occupancy projector is applied to enforce the constraint.

The MPO approach allows us to do this explicitly using tensor network methodology [Wu2020].
Use a chain of 2N fermionic sites, labeled by composite index $k = (\ell, s)$, $\ell = 1, \dots, N$, $s = \uparrow, \downarrow$:
Build Fermi sea of Wannier orbitals built from mean-field parton eigenstates, then apply single-occupancy projector:

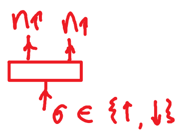
$|F\rangle = \prod_r d^\dagger_r |0\rangle$ $\quad f^\dagger_r = d^\dagger_\alpha \overline{B^\alpha{}_r}$ $\quad d^\dagger_\alpha = c^\dagger_k U^k{}_\alpha$ $\quad \hat P$



$$\hat P = \prod_{\ell=1}^N \hat P_{[\ell]},$$ yields 0 when acting on $|1,1\rangle_\ell$ or $|0,0\rangle_\ell$

$$\hat P_{[\ell]} = (1 - \hat n_{\ell\uparrow}\hat n_{\ell\downarrow})\,\hat n_{\ell\uparrow}\hat n_{\ell\downarrow}$$

$$= |\uparrow\rangle_{\ell\,\ell}\langle 1,0| + |\downarrow\rangle_{\ell\,\ell}\langle 0,1|$$



'single-occupancy projector'

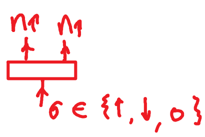
In practice, doubly-occupied sites can be removed after each application of $f^\dagger_r$, because they don't survive the final projection anyway. Advantage: local state space dimension is reduced from 4 to 3:

$$\hat P|F\rangle = \hat P \underbrace{\prod_{r=1}^N f^\dagger_r |0\rangle}_{\text{half-filled Fermi sea}} = \hat P \prod_{r=1}^N (\hat G f^\dagger_r)|0\rangle,$$

$$\hat G = \prod_{\ell=1}^N \hat G_{[\ell]}, \qquad \hat G_{[\ell]} = (1 - \hat n_{\ell\uparrow}\hat n_{\ell\downarrow})$$ yields 0 when acting on $|1,1\rangle_\ell$

'Gutzwiller projector', eliminates double occupancies

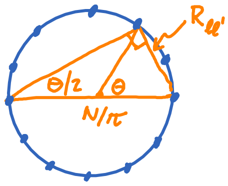
$$= |\uparrow\rangle_{\ell\,\ell}\langle 1,0| + |\downarrow\rangle_{\ell\,\ell}\langle 0,1| + |0\rangle_{\ell\,\ell}\langle 0,0|$$



Haldane-Shastry model [Haldane1988], [Shastry1988]

Haldane and Shastry (HS) independently studied a spin-1/2 chain with periodic boundary conditions, for a Hamiltonian fine-tuned such that the parton construction yields the exact ground state:

Hamiltonian: $H_{HS} = \sum_{l<l'} \frac{\vec{S}_l \cdot \vec{S}_{l'}}{R^2_{ll'}}$ $\quad l, l' = 1, \dots, N$ = even



$\theta = \frac{2\pi}{N}(l-l')$

$R_{ll'} = \frac{N}{\pi} \sin\frac{\theta}{2}$

$R_{ll'} = \frac{N}{\pi} \sin\left[\frac{\pi}{N}(l-l')\right]$ = cord length for circle of diameter N/π

It can be shown analytically that ground state has following form:

'position parton' creator

$|g\rangle = \hat{P} \prod_\alpha \prod_{s=\uparrow,\downarrow} d^\dagger_{\alpha s} |0\rangle$ with $d^\dagger_{\alpha s} = \frac{1}{N^{1/2}} \sum_{l=1}^{N} e^{-i\alpha 2\pi l/N} c^\dagger_{l s}$,

creates a parton with 'momentum' $\frac{2\pi\alpha}{N}$

where the occupied states are labeled $\alpha = \begin{cases} 0, \pm 1, \dots \pm\left(\frac{N}{4} - 1\right), \frac{N}{4} & \text{if } N \bmod 4 = 0 \\ 0, \pm 1, \dots, \pm \frac{N-2}{4} & \text{if } N \bmod 4 = 2 \end{cases}$

Exact ground state energy: $E_g = -\frac{\pi^2}{24}\left(N + 5/N\right)$

Exact spin-spin correlator: $\langle \vec{S}_{l'} \cdot \vec{S}_{l'+l} \rangle = \dfrac{\sum_{n=1}^{N/2} \frac{3(-1)^l}{2n-1} \sin\left[\frac{\pi}{N}(2n-1)\,l\right]}{2N \sin\left[\frac{\pi}{N} l\right]}$

Numerical benchmark test of the MPS representation of parton ground state: the difference between its results for the spin-spin correlator and the exact analytical expression is very small.

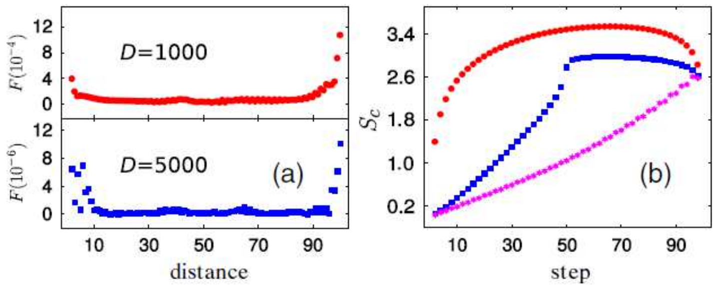


FIG. 2. (a) The absolute difference F between the numerical and exact values of the spin-spin correlation function in the $N = 100$ system. (b) The evolution of the von Neumann entanglement entropy S_c at the center of the $N = 100$ system during the calculation. Three methods are compared: (1) the original modes in $|\Psi_{HS}\rangle$ (red dots), (2) the Wannier transformed modes from left to right (blue squares), and (3) the Wannier transformed modes and the left-meet-right strategy (magenta hexagons).

From [Wu2020].