MPS.6 Iterative diagonalization

Consider spin-$1/2$ chain: $$\hat{H}^{\mathcal{L}} = \sum_{\ell=1}^{\mathcal{L}} \hat{\vec{S}}_\ell \cdot \vec{h}_\ell + \sum_{\ell=1}^{\mathcal{L}-1} \hat{\vec{S}}_\ell \cdot \hat{\vec{S}}_{\ell+1} \qquad (1)$$

SU(2) spin algebra for each site ℓ (suppressing site indices in Eqs. (2-4):

$$[\hat{S}_i, \hat{S}_j] = \varepsilon_{ijk} \hat{S}_k \quad (2a), \qquad \hat{S}_i^\dagger = \hat{S}_i, \qquad \hat{S}_\pm = \tfrac{1}{\sqrt{2}}(\hat{S}_x \pm i \hat{S}_y) = \hat{S}_\mp^\dagger := \hat{S}^{\mp\dagger} \qquad (2b)$$

useful convention to achieve covariant notation

$$\overset{(2a,b)}{\Longrightarrow} \quad [\hat{S}_-, \hat{S}_+] = \hat{S}_z, \qquad [\hat{S}_z, \hat{S}_\pm] = \pm \hat{S}_\pm \qquad (2c)$$

$$\hat{\vec{S}} \cdot \hat{\vec{S}} = \hat{S}_x \hat{S}_x + \hat{S}_y \hat{S}_y + \hat{S}_z \hat{S}_z \overset{(2b)}{=} \hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+ + \hat{S}_z \hat{S}_z \qquad (3a)$$

site ℓ, site $\ell+1$

write this covariant notation: $$\overset{(2b)}{=} \hat{S}_+ \hat{S}^{+\dagger} + \hat{S}_- \hat{S}^{-\dagger} + \hat{S}_z \hat{S}^{z\dagger} = \hat{S}_a \hat{S}^{\dagger a} \qquad (3b)$$

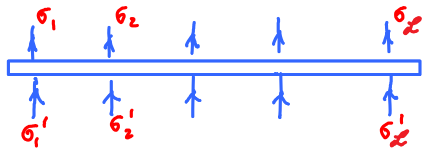
sum on $a \in \{+, z, -\}$ implied!

with operator triplets: $$\hat{S}_a \in \{\hat{S}_+, \hat{S}_z, \hat{S}_-\}, \qquad \hat{S}^{a\dagger} \in \{\hat{S}^{+\dagger}, \hat{S}^{z\dagger}, \hat{S}^{-\dagger}\} \qquad (4)$$

In the basis $\{|\vec{\sigma}_{\mathcal{L}}\rangle\} = \{|\sigma_1\rangle|\sigma_2\rangle \dots |\sigma_{\mathcal{L}}\rangle\}$, the Hamiltonian can be expressed as

$$\hat{H}^{\mathcal{L}} = |\vec{\sigma}'\rangle H^{\vec{\sigma}'}{}_{\vec{\sigma}} \langle \vec{\sigma}| \qquad (5)$$

'no hat' means 'matrix representation'

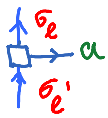


$H^{\vec{\sigma}'}{}_{\vec{\sigma}}$ is a linear map acting on a direct product space: $\mathbb{V}^{\otimes \mathcal{L}} := \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \dots \otimes \mathbb{V}_{\mathcal{L}}$

where $\mathbb{V}_\ell$ is the 2-dimensional representation space of site ℓ .

$\hat{H}^{\mathcal{L}}$ is a sum of single-site and two-site terms.

One-site terms: $$\hat{S}_{a\ell} = |\sigma'_\ell\rangle [S_a]^{\sigma'_\ell}{}_{\sigma_\ell} \langle \sigma_\ell| \qquad (6)$$



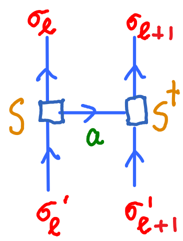
Matrix representation in $\mathbb{V}_\ell$: $$(S_a)^{\sigma'_\ell}{}_{\sigma_\ell} = \langle \sigma'_\ell | \hat{S}_{a\ell} | \sigma_\ell \rangle = \begin{pmatrix} [S_a]^\uparrow{}_\uparrow & [S_a]^\uparrow{}_\downarrow \\ [S_a]^\downarrow{}_\uparrow & [S_a]^\downarrow{}_\downarrow \end{pmatrix} \qquad (7)$$

$$S_+ = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad S_z = \tfrac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad S_- = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad (8)$$

Nearest-neighbor interactions, acting on direct product space, $|\sigma_\ell\rangle \otimes |\sigma_{\ell+1}\rangle$:

$$\hat{S}_{a\ell} \otimes \hat{S}^{a\dagger}_{\ell+1} = |\sigma'_\ell\rangle |\sigma'_{\ell+1}\rangle \underbrace{[S_a]^{\sigma'_\ell}{}_{\sigma_\ell}}_{\substack{!! \\ S^{\sigma'_\ell}{}_{a\sigma_\ell}}} \underbrace{[S^{\dagger a}]^{\sigma'_{\ell+1}}{}_{\sigma_{\ell+1}}}_{\substack{!! \\ S^{\dagger\sigma'_{\ell+1} a}{}_{\sigma_{\ell+1}}}} \langle \sigma_{\ell+1}| \langle \sigma_\ell| \qquad (9)$$

Matrix representation in $\mathbb{V}_\ell \otimes \mathbb{V}_{\ell+1}$:



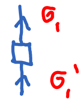
We define the 3-leg tensors S, $S^\dagger$ with index placements matching those of A tensors for wavefunctions:

We define the 3-leg tensors S, $S^\dagger$ with index placements matching those of A tensors for wavefunctions: incoming: high; outgoing: low (fly in high, roll out low), with a (by convention) as middle index.

Diagonalize site 1

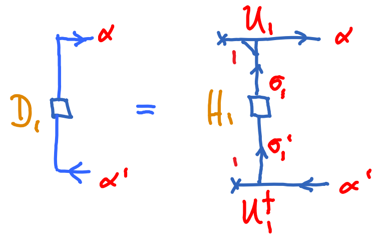
Matrix acting on $\mathbb{V}_1$:

$$\underbrace{H_1}_{\text{chain of length 1}} = S^\dagger_{a1} \cdot h_1^a = \mathcal{U}_1 D_1 \mathcal{U}_1^\dagger \qquad \text{site index: } \ell = 1 \tag{10}$$



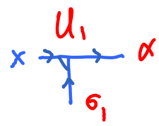
$D_1 = \mathcal{U}_1^\dagger H_1 \mathcal{U}_1$ is diagonal, with matrix elements

$$[D_1]^{\alpha'}{}_{\alpha'} = [\mathcal{U}_1^\dagger]^{\alpha'}{}_{\sigma_1'} [H_1]^{\sigma_1'}{}_{\sigma_1} [\mathcal{U}_1]^{\sigma_1}{}_{\alpha} \tag{11}$$



Eigenvectors of the matrix H_1 are given by column vectors of the matrix $[\mathcal{U}_1]^{\sigma_1}{}_{\alpha}$:

Eigenstates of operator $\hat{H}_1$ are given by: $|\alpha\rangle = |\sigma_1\rangle [\mathcal{U}_1]^{\sigma_1}{}_{\alpha}$ (13)



Add site 2

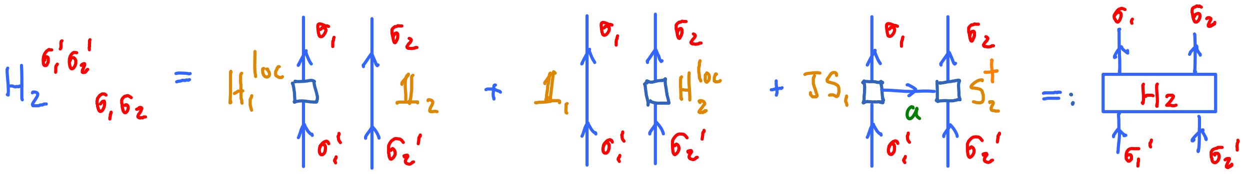
Diagonalize H_2 in enlarged Hilbert space, $\mathcal{H}_{(2)} = \mathrm{span}\{|\sigma_1\rangle|\sigma_2\rangle\}$ (14)

chain of length 2

Matrix acting on $\mathbb{V}_1 \otimes \mathbb{V}_2$:

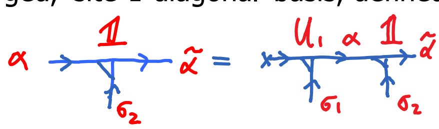
$$H_2 = \underbrace{\vec{S}_1 \cdot \vec{h}_1}_{H_1^{loc}} \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \underbrace{\vec{S}_2 \cdot \vec{h}_2}_{H_2^{loc}} + \underbrace{J\, S_{a1} \otimes S_2^{\dagger a}}_{H_{12}^{loc}} \tag{15}$$

Matrix representation in $\mathbb{V}_1 \otimes \mathbb{V}_2$ corresponding to 'local' basis, $\{|\sigma_1\rangle|\sigma_2\rangle\}$:



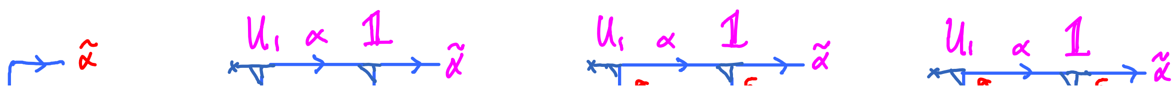
We seek matrix representation in $\mathbb{V}_1 \otimes \mathbb{V}_2$ corresponding to enlarged, 'site-1-diagonal' basis, defined as

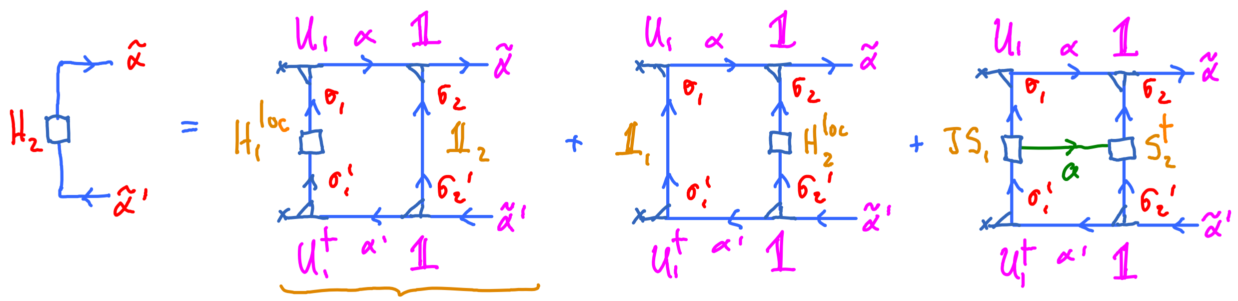
$$|\tilde{\alpha}\rangle \equiv |\alpha, \sigma_2\rangle \equiv |\alpha\rangle|\sigma_2\rangle = |\sigma_1\rangle|\sigma_2\rangle \mathcal{U}^{\sigma_1}{}_{\alpha} \tag{17}$$



$$\hat{H}_2 = |\tilde{\alpha}'\rangle H_2{}^{\tilde{\alpha}'}{}_{\tilde{\alpha}} \langle\tilde{\alpha}| , \qquad H_2{}^{\tilde{\alpha}'}{}_{\tilde{\alpha}} = \langle\tilde{\alpha}'|\hat{H}_2|\tilde{\alpha}\rangle = \langle\tilde{\alpha}'|\sigma_1',\sigma_2'\rangle H_2{}^{\sigma_1'\sigma_2'}{}_{\sigma_1,\sigma_2} \langle\sigma_1,\sigma_2|\tilde{\alpha}\rangle$$

To this end, attach $\mathcal{U}_1^\dagger$, $\mathcal{U}_1$ to in/out legs of site 1, and $\mathbb{1}$, $\mathbb{1}$ to in/out legs of site 2:





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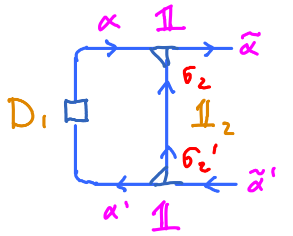


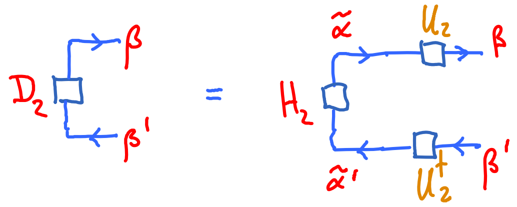
First term is already diagonal. But other terms are not.

Note: the 'triangles' on ⊤, ⊥ suffice to fully specify all arrow direction, hence arrows can be omitted (will often be done in later lectures).

Now diagonalize H_2 in this enlarged basis: $H_2 = U_2 D_2 U_2^\dagger$ (19)

$D_2 = U_2^\dagger H_2 U_2$ is diagonal, with matrix elements

$$[D_2]^{\beta'}{}_{\beta} = [U_2^\dagger]^{\beta'}{}_{\tilde{\alpha}'} [H_2]^{\tilde{\alpha}'}{}_{\tilde{\alpha}} [U_2]^{\tilde{\alpha}}{}_{\beta}$$

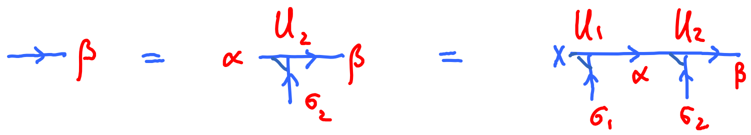


(20)

Eigenvectors of matrix H_2 are given by column vectors of the matrix $[U_2]^{\tilde{\alpha}}{}_{\beta} = [U_2]^{\alpha\sigma_2}{}_{\beta}$:

Eigenstates of the operator $\hat{H}_2$:

$$|\beta\rangle = |\tilde{\alpha}\rangle [U_2]^{\tilde{\alpha}}{}_{\beta} = |\alpha\rangle|\sigma_2\rangle [U_2]^{\alpha\sigma_2}{}_{\beta} = |\sigma_1\rangle|\sigma_2\rangle [U_1]^{\sigma_1}{}_{\alpha} [U_2]^{\alpha\sigma_2}{}_{\beta} \qquad (21)$$

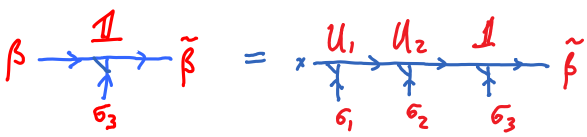


(22)

<u>Add site 3</u>

Transform each term involving new site into the 'enlarged, site-12-diagonal basis', defined as

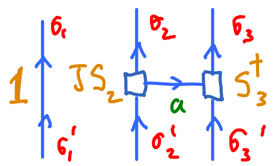
$$|\tilde{\beta}\rangle \equiv |\beta,\sigma_3\rangle \equiv |\beta\rangle|\sigma_3\rangle$$



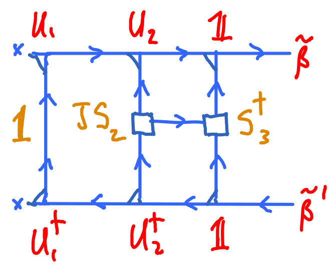
(23)

For example, spin-spin interaction, H_{23}^{int} :

Local basis:



enlarged, site-12-diagonal basis:



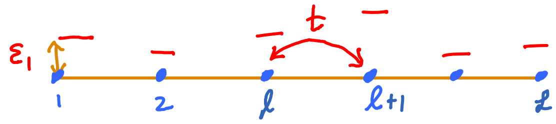
(24)

Then diagonalize in this basis: $H_3 = U_3 D_3 U_3^\dagger$, etc. (25)

At each iteration, Hilbert space grows by a factor of 2. Eventually, truncations will be needed...!

MPS.7 Spinless fermions

Consider tight-binding chain of spinless fermions:



$$\hat H = \sum_{\ell=1}^{\mathscr{L}} \varepsilon_\ell \, \hat c_\ell^\dagger \hat c_\ell + \sum_{\ell=1}^{\mathscr{L}-1} t_\ell \left(\hat c_\ell^\dagger \hat c_{\ell+1} + \hat c_{\ell+1}^\dagger \hat c_\ell \right) \qquad (1)$$

Goal: find matrix representation for this Hamiltonian, acting in direct product space $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \dots \otimes \mathbb{V}_{\mathscr{L}}$, while respecting fermionic minus signs:

$$\{\hat c_\ell, \hat c_{\ell'}\} = 0 , \qquad \{\hat c_\ell^\dagger, \hat c_{\ell'}^\dagger\} = 0 , \qquad \{\hat c_\ell^\dagger, \hat c_{\ell'}\} = \delta_{\ell\ell'} \qquad (2)$$

First consider a single site (dropping the site index ℓ):

Hilbert space: $\mathrm{span}\{|0\rangle, |1\rangle\}$, local index: $n = \sigma \in \{0, 1\}$ local occupancy

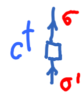
Operator action: $\hat c^\dagger |0\rangle = |1\rangle$, $\quad \hat c^\dagger |1\rangle = 0$ (3a)

$\hat c |0\rangle = 0$, $\quad \hat c |1\rangle = |0\rangle$ (3b)

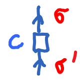
The operators $\hat c^\dagger = |\sigma'\rangle C^{\dagger\sigma'}{}_{\sigma} \langle \sigma|$ and $\hat c = |\sigma'\rangle C^{\sigma'}{}_{\sigma} \langle \sigma|$

have matrix representations in $\mathbb{V}$:

$$C^{\dagger\sigma'}{}_{\sigma} = \langle \sigma' | \hat c^\dagger | \sigma \rangle = \begin{array}{c|cc} & |0\rangle & |1\rangle \\ \hline \langle 0| & 0 & 0 \\ \langle 1| & 1 & 0 \end{array} \qquad (4a)$$



$$C^{\sigma'}{}_{\sigma} = \langle \sigma' | \hat c | \sigma \rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad (4b)$$



Shorthand: we write $\hat c^\dagger \doteq C^\dagger$, $\quad \hat c \doteq C$ where $\doteq$ means 'is represented by'

lower case denotes operator in Fock space

upper case denotes matrix in 2-dim space $\mathbb{V}$

Check: $$C^\dagger C + C C^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1} \ \checkmark \qquad (5)$$

$$C^\dagger C^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \checkmark , \qquad C C = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \checkmark \qquad (6)$$

For the number operator, $\hat n := \hat c^\dagger \hat c$ the matrix representation in $\mathbb{V}$ reads:

$$n := C^\dagger C = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \tfrac{1}{2}(1 - Z) \qquad = \text{"charge"} \qquad (7)$$

where $Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is representation of $\hat z = 1 - 2\hat n = (-1)^{\hat n}$ (8)

Useful relations: $\hat c \hat z = -\hat z \hat c$, $\quad \hat c^\dagger \hat z = -\hat z \hat c^\dagger$ (9)

'commuting $\hat{c}$ or $\hat{c}^\dagger$ past $\hat{z}$ produces a sign' [exercise: check this algebraically, using matrix representations!]

Intuitive reason: $\hat{c}$ and $\hat{c}^\dagger$ both change $\hat{n}$ -eigenvalue by one, hence change sign of $(-1)^{\hat{n}}$.

For example:
$$\hat{c}^\dagger \underbrace{(-1)^{\hat{n}}}_{=(-1)^0=1} = \hat{c}^\dagger = -\underbrace{(-1)^{\hat{n}}}_{=(-1)^1=-1} \hat{c}^\dagger \tag{10a}$$
non-zero only when acting on $|0\rangle$

Similarly:
$$\hat{c}\, \underbrace{(-1)^{\hat{n}}}_{=(-1)^1=-1} = -\hat{c} = -\underbrace{(-1)^{\hat{n}}}_{=(-1)^0=1} \hat{c} \tag{10b}$$
non-zero only when acting on $|1\rangle$

Now consider a <u>chain</u> of spinless fermions:

Complication: fermionic operators on different sites <u>anti</u>commute: $c_\ell c^\dagger_{\ell'} = -c^\dagger_{\ell'} c_\ell$ for $\ell \neq \ell'$

Hilbert space: $$\mathrm{span}\{|\vec{\sigma}\rangle_{\mathscr{L}} = |n_1, n_2, \dots, n_{\mathscr{L}}\rangle\}, \quad n_\ell \in \{0,1\} \tag{11}$$

Define canonical ordering: fill states from right to left:
$$|n_1, \dots, n_\ell, \dots, n_{\mathscr{L}}\rangle = (\hat{c}^\dagger_1)^{n_1} \dots (\hat{c}^\dagger_\ell)^{n_\ell} \dots (\hat{c}^\dagger_{\mathscr{L}})^{n_{\mathscr{L}}} |\mathrm{Vac}\rangle \tag{12}$$

Now consider:
$$c^\dagger_\ell |n_1, \dots, 0, \dots, n_{\mathscr{L}}\rangle = (-1)^{n_1+\dots+n_{\ell-1}} (\hat{c}^\dagger_1)^{n_1} \dots \underbrace{c^\dagger_\ell (\hat{c}^\dagger_\ell)^0}_{(\hat{c}^\dagger_\ell)^1} \dots (\hat{c}^\dagger_{\mathscr{L}})^{n_{\mathscr{L}}} |\mathrm{Vac}\rangle \tag{13}$$
$$= (-1)^{n^<_\ell} |n_1, \dots, 1, \dots, n_{\mathscr{L}}\rangle, \quad n^<_\ell = \sum_{\ell'=1}^{\ell-1} n_{\ell'} \tag{14}$$

$$c_\ell |n_1, \dots, 1, \dots, n_{\mathscr{L}}\rangle = (-1)^{n_1+\dots+n_{\ell-1}} (\hat{c}^\dagger_1)^{n_1} \dots \underbrace{c_\ell (\hat{c}^\dagger_\ell)^1}_{(\hat{c}^\dagger_\ell)^0} \dots (\hat{c}^\dagger_{\mathscr{L}})^{n_{\mathscr{L}}} |\mathrm{Vac}\rangle \tag{15}$$
$$= (-1)^{n^<_\ell} |n_1, \dots, 0, \dots, n_{\mathscr{L}}\rangle \tag{16}$$

To keep track of such signs, matrix representations in $\mathbb{V}^{\otimes \mathscr{L}} = \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \dots \otimes \mathbb{V}_{\mathscr{L}}$ need extra 'sign counters', tracking fermion numbers:

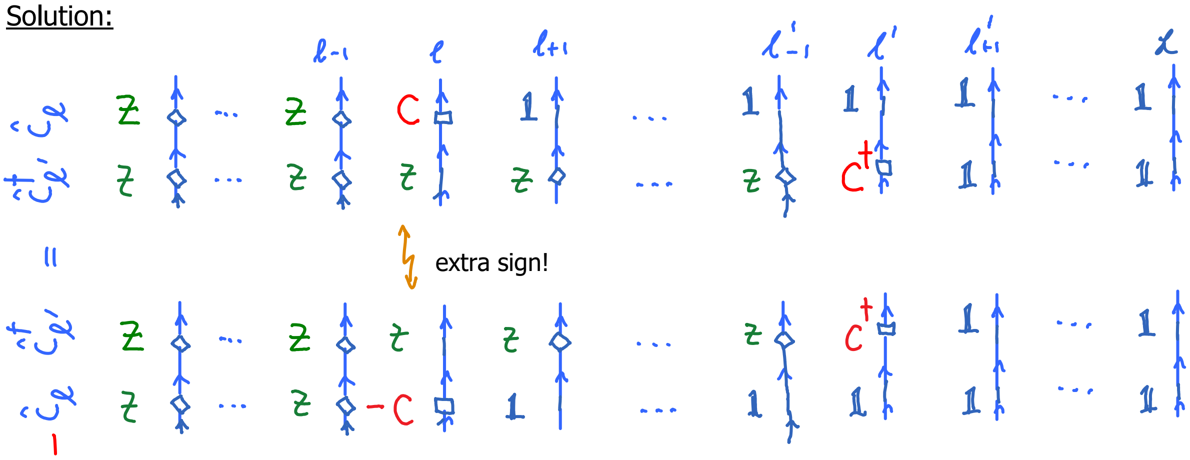
$$\hat{c}^\dagger_\ell \doteq Z_1 \otimes \dots Z_{\ell-1} \otimes C^\dagger_\ell \otimes \mathbb{1}_{\ell+1} \otimes \dots \otimes \mathbb{1}_{\mathscr{L}} =: Z^<_\ell C^\dagger_\ell \tag{21}$$
$$\hat{c}_\ell \doteq Z_1 \otimes \dots Z_{\ell-1} \otimes C_\ell \otimes \mathbb{1}_{\ell+1} \otimes \dots \otimes \mathbb{1}_{\mathscr{L}} =: Z^<_\ell C_\ell \tag{22}$$
'Jordan-Wigner transformation'

with $$Z^<_\ell := \prod_{\otimes \ell'<\ell} Z_{\ell'}$$ 'Z-string' (23)

$\otimes\ \ell' < \ell$

<u>Exercise:</u> verify graphically that $\hat{c}^\dagger_{\ell'} \hat{c}_\ell = - \hat{c}_\ell \hat{c}^\dagger_{\ell'}$ for $\ell' > \ell$.

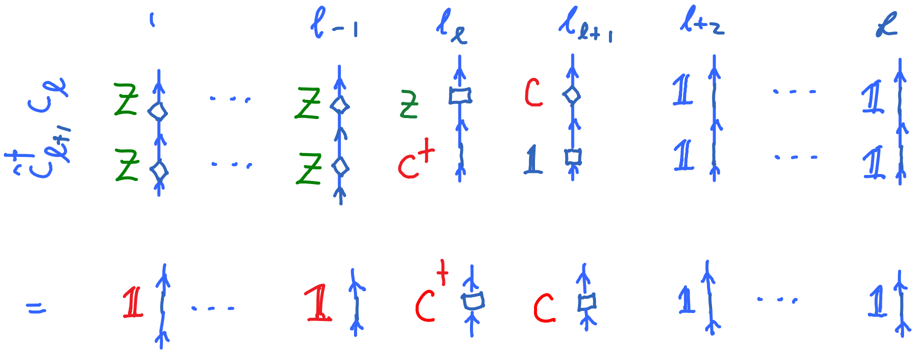
<u>Solution:</u>



(24)

(25)

In bilinear combinations, all(!) of the Z's cancel. Example: hopping term, $\hat{c}^\dagger_\ell \hat{c}_{\ell+1}$:



(26)

(27)

since at sites $\ell' < \ell$ we have $Z_{\ell'} Z_{\ell'} = \mathbb{1}_{\ell'}$, $\quad c^\dagger_\ell Z_\ell \overset{(10a)}{=} c^\dagger_\ell$, (28)

non-zero only when acting on $|\ldots, n_\ell = 0, \ldots\rangle$,

and in this subspace, $Z_\ell = 1$

Conclusion: $\hat{c}^\dagger_\ell c_{\ell+1} \doteq c^\dagger_\ell c_{\ell+1}$ and similarly, [using (10b)] $\hat{c}^\dagger_{\ell+1} \hat{c}_\ell \doteq c^\dagger_{\ell+1} c_\ell$ (29)

Hence, the hopping terms end up looking as though fermions carry no signs at all.

For spinful fermions, this will be different.

MPS.8 Spinful fermions

Consider chain of spinful fermions. Site index: $\ell = 1, \dots, \mathscr{L}$, spin index: $s \in \{\uparrow, \downarrow\} := \{+, -\}$

$$\{\hat c_{\ell s}, \hat c_{\ell' s'}\} = 0 \; , \qquad \{\hat c^\dagger_{\ell s}, \hat c^\dagger_{\ell' s'}\} = 0 \; , \qquad \{\hat c^\dagger_{\ell s}, \hat c_{\ell' s'}\} = \delta_{\ell\ell'}\delta_{ss'} \tag{1}$$

Define canonical order for fully filled state: $\hat c^\dagger_{1\uparrow} \hat c^\dagger_{1\downarrow} \hat c^\dagger_{2\uparrow} \hat c^\dagger_{2\downarrow} \dots \hat c^\dagger_{\mathscr{L}\uparrow} \hat c^\dagger_{\mathscr{L}\downarrow} |\mathrm{Vac}\rangle$ (2)

First consider a single site (dropping the index ℓ):

Hilbert space: $= \mathrm{span}\{|0\rangle, |\downarrow\rangle, |\uparrow\rangle, |\uparrow\downarrow\rangle\}$, local index: $\sigma \in \{0, \downarrow, \uparrow, \uparrow\downarrow\}$ (3)

constructed via: $|0\rangle \equiv |\mathrm{Vac}\rangle , \quad |\downarrow\rangle \equiv \hat c^\dagger_\downarrow |0\rangle ,$ (4)

$$|\uparrow\rangle \equiv \hat c^\dagger_\uparrow |0\rangle , \quad |\uparrow\downarrow\rangle \equiv \hat c^\dagger_\uparrow \hat c^\dagger_\downarrow |0\rangle = \hat c^\dagger_\uparrow |\downarrow\rangle = - \hat c^\dagger_\downarrow |\uparrow\rangle \tag{5}$$

To deal with minus signs, introduce $\hat Z_s := (-1)^{\hat n_s} = \frac{1}{2}(1 - \underbrace{\hat n_s}_{\hat c^\dagger_s \hat c_s}) , \quad s \in \{\uparrow, \downarrow\}$ (6)

We seek a matrix representation of $\hat c^\dagger_s , \; \hat c_s , \; \hat Z_s$ in direct product space $\tilde{\mathbb{V}} := \mathbb{V}_\uparrow \otimes \mathbb{V}_\downarrow$. (7)

(Matrices acting in this space will carry tildes.)

$$\hat Z_\uparrow \doteq Z_\uparrow \otimes \mathbb{1}_\downarrow = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} = \left(\begin{array}{c|c} 1\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} & 0\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \\ \hline 0\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} & -1\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \end{array}\right) = \left(\begin{array}{cc|cc} 1 & & & \\ & 1 & & \\ \hline & & -1 & \\ & & & -1 \end{array}\right) =: \tilde Z_\uparrow \tag{8}$$

$$\hat Z_\downarrow \doteq \mathbb{1}_\uparrow \otimes Z_\downarrow = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = \left(\begin{array}{cc|cc} 1 & & & \\ & -1 & & \\ \hline & & 1 & \\ & & & -1 \end{array}\right) =: \tilde Z_\downarrow \tag{9}$$

$$\hat Z_\uparrow \hat Z_\downarrow \doteq Z_\uparrow \otimes Z_\downarrow = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = \left(\begin{array}{cc|cc} 1 & & & \\ & -1 & & \\ \hline & & -1 & \\ & & & 1 \end{array}\right) =: \tilde Z \tag{10}$$

$$\hat c^\dagger_\uparrow \doteq c^\dagger_\uparrow \otimes \mathbb{1} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} = \left(\begin{array}{cc|cc} & & & \\ & & & \\ \hline 1 & & & \\ & 1 & & \end{array}\right) =: \tilde c^\dagger_\uparrow$$

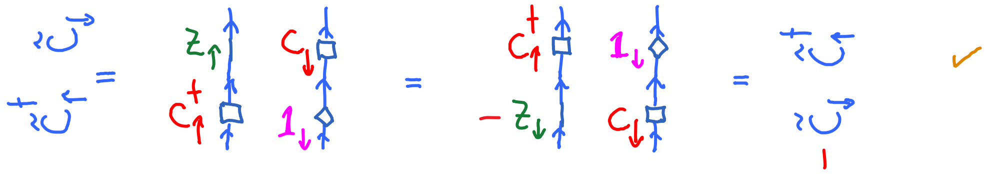
$$\hat c_\uparrow \doteq c_\uparrow \otimes \mathbb{1} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} = \left(\begin{array}{cc|cc} & & 1 & \\ & & & 1 \\ \hline & & & \\ & & & \end{array}\right) =: \tilde c_\uparrow \tag{11}$$

$$\hat c^\dagger_\downarrow \doteq Z_\uparrow \otimes c^\dagger_\downarrow = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \left(\begin{array}{cc|cc} 0 & 0 & & \\ 1 & 0 & & \\ \hline & & 0 & 0 \\ & & -1 & 0 \end{array}\right) =: \tilde c^\dagger_\downarrow \tag{12}$$

$$\hat c_\downarrow \doteq Z_\uparrow \otimes c_\downarrow = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \left(\begin{array}{cc|cc} 0 & 1 & & \\ 0 & 0 & & \\ \hline & & 0 & -1 \\ & & 0 & 0 \end{array}\right) =: \tilde c_\downarrow \tag{12}$$

$$\hat c_\downarrow \doteq Z_\uparrow \otimes c_\downarrow = \begin{pmatrix}1&\\&-1\end{pmatrix}\otimes\begin{pmatrix}0&1\\0&0\end{pmatrix} = \left(\begin{array}{cc|cc} 0&1&&\\ 0&0&&\\ \hline &&0&-1\\ &&0&0\end{array}\right) =: \tilde c_\downarrow \qquad (12)$$

The factors Z_s guarantee correct signs. For example $\tilde c^\dagger_\uparrow \tilde c_\downarrow = -\tilde c_\downarrow \tilde c^\dagger_\uparrow$:
(fully analogous to MPS-II.1.17)



(13)

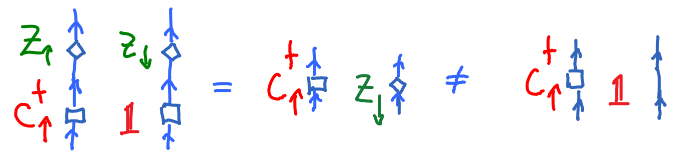
Algebraic check:

$$\left(\begin{array}{cc|cc} &&&\\ &&&\\ \hline 1&&&\\ &1&&\end{array}\right)\left(\begin{array}{cc|cc} 0&1&&\\ 0&0&&\\ \hline &&0&-1\\ &&0&0\end{array}\right) = \left(\begin{array}{cc|cc} 0&1&&\\ 0&0&&\\ \hline &&&\\ &&&\end{array}\right), \qquad \left(\begin{array}{cc|cc} 0&1&&\\ 0&0&&\\ \hline &&0&-1\\ &&0&0\end{array}\right)\left(\begin{array}{cc|cc} &&&\\ &&&\\ \hline 1&&&\\ &1&&\end{array}\right) = \left(\begin{array}{cc|cc} 0&-1&&\\ 0&0&&\\ \hline &&&\\ &&&\end{array}\right) \checkmark \qquad (14)$$

Remark: for spinful fermions (in constrast to spinless fermions, compare MPS-II.28), we have

$$\tilde c^\dagger_s \tilde Z \neq \tilde c^\dagger_s \quad \text{and} \quad \tilde Z \tilde c_s \neq \tilde c_s \qquad (15)$$

For example, consider $s=\uparrow$; action in $\tilde{\mathbb V} = \mathbb V_\uparrow \otimes \mathbb V_\downarrow$:

$\tilde c^\dagger_\uparrow \tilde Z =$  $= \tilde c^\dagger_\uparrow$ (16)

Now consider a <u>chain</u> of spinful fermions (analogous to spinless case, with $\tilde{\mathbb V}_\ell$ instead of $\mathbb V_\ell$).

Each $\hat c_{\ell s}$ or $\hat c^\dagger_{\ell s}$ must produce sign change when moved past any $\hat c_{\ell' s'}$ or $\hat c^\dagger_{\ell' s'}$, with $\ell' > \ell$.
So, define the following matrix representations in $\tilde{\mathbb V}^{\otimes \mathscr L} = \tilde{\mathbb V}_1 \otimes \tilde{\mathbb V}_2 \otimes \dots \otimes \tilde{\mathbb V}_{\mathscr L}$:

$$\hat c^\dagger_\ell \doteq \tilde Z_1 \otimes \dots \otimes \tilde Z_{\ell-1} \otimes \tilde c^\dagger_\ell \otimes \mathbb 1_{\ell+1} \otimes \dots \mathbb 1_{\mathscr L} \equiv \tilde Z^<_\ell \tilde c^\dagger_\ell \qquad (17)$$

$$\hat c_\ell \doteq \tilde Z_1 \otimes \dots \otimes \tilde Z_{\ell-1} \otimes \tilde c_\ell \otimes \mathbb 1_{\ell+1} \otimes \dots \mathbb 1_{\mathscr L} \equiv \tilde Z^<_\ell \tilde c_\ell \qquad (18)$$

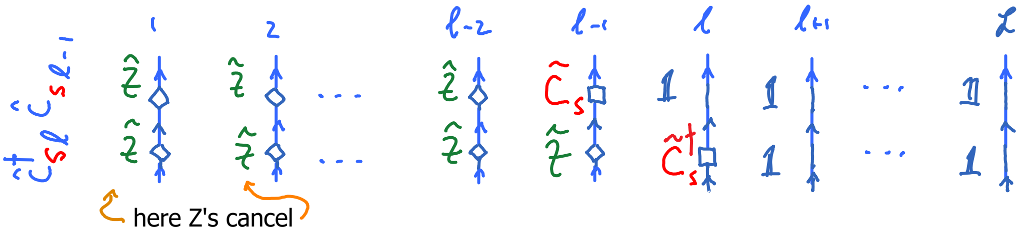
'Jordan-Wigner transformation'

with $$\tilde Z^<_\ell \equiv \prod_{\otimes \ell' < \ell} \tilde Z_{\ell'} = \prod_{\otimes \ell' < \ell} Z_{\uparrow \ell'} \otimes Z_{\downarrow \ell'}$$ 'Z-string' (19)

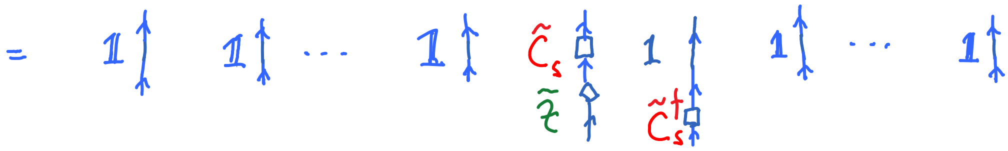
In <u>bilinear combinations</u>, most (but not all!) of the Z 's cancel.

Example: hopping term $\hat c^\dagger_{\ell s} \hat c_{\ell-1 s}$: (sum over s impied)

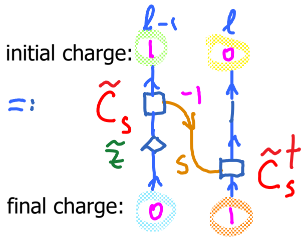
1 2 $\ell-2$ $\ell-1$ ℓ $\ell+1$ $\mathscr L$



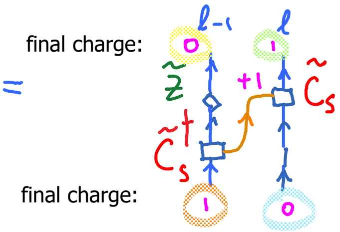
(20)



(21)



Similarly: $\hat{c}^{\dagger}_{\ell-1\,s}\,\hat{c}_{\ell s} =$



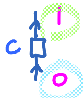
(22)

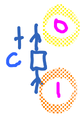
bond → indicates spin sum $\sum_s$

How does action of operators change quantum numbers?

$$c^{\sigma'}{}_{\sigma} = \begin{array}{c|cc} & |0\rangle & |1\rangle \\ \hline \langle 0| & c^{0}{}_{0} & c^{0}{}_{1} \\ \langle 1| & c^{1}{}_{0} & c^{1}{}_{1} \end{array} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$c^{\dagger\,\sigma'}{}_{\sigma} = \begin{array}{c|cc} & |0\rangle & |1\rangle \\ \hline \langle 0| & c^{\dagger 0}{}_{0} & c^{\dagger 0}{}_{1} \\ \langle 1| & c^{\dagger 1}{}_{0} & c^{\dagger 1}{}_{1} \end{array} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

only non-zero element: 

only non-zero element: 

Arrow convention for <u>virtual bonds</u> of creation/annihilation operators: (23)

'charge conservation' holds for each operator, i.e. total charge in = total charge out.

Annihilation operator: outgoing -1 or incoming $+1$

Creation operator: incoming -1 or outgoing $+1$