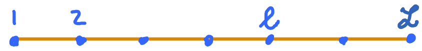
MPS.6 Iterative diagonalization



MPS.6

Consider spin-$\frac12$ 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):

$$[\hat S_i,\hat S_j] = \varepsilon_{ijk}\hat S_k \quad (2a), \qquad \hat S_i^\dagger = \hat S_i, \qquad \hat S_\pm = \tfrac{1}{\sqrt2}(\hat S_x \pm i\hat S_y) = \hat S^\dagger_\mp := \hat S^{\mp\dagger} \qquad (2b)$$

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: $$\overset{(2b)}{=} \hat S_+\hat S^{+\dagger} + \hat S_-\hat S^{-\dagger} + \hat S_z\hat S^{z\dagger} = \hat S_a\hat S^{\dagger a} \qquad (3b)$$

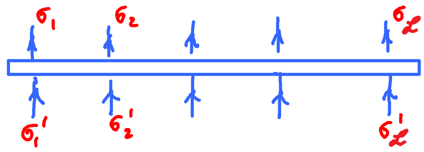
sum on $a\in\{+,z,-\}$ implied!

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'

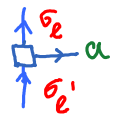


$H^{\vec\sigma'}{}_{\vec\sigma}$ is a linear map acting on a direct product space: $\mathbb V^{\otimes\mathcal L} := \mathbb V_1\otimes\mathbb V_2\otimes\dots\otimes\mathbb V_{\mathcal L}$

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.

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



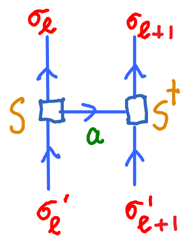
Matrix representation in $\mathbb V_\ell$: $$(S_a)^{\sigma'_\ell}{}_{\sigma_\ell} = \langle\sigma'_\ell|\hat S_{a\ell}|\sigma_\ell\rangle = \begin{pmatrix}[S_a]^\uparrow{}_\uparrow & [S_a]^\uparrow{}_\downarrow\\ [S_a]^\downarrow{}_\uparrow & [S_a]^\downarrow{}_\downarrow\end{pmatrix} \qquad (7)$$

$$S_+ = -\tfrac{1}{\sqrt2}\begin{pmatrix}0&1\\0&0\end{pmatrix}, \qquad S_z = \tfrac12\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \qquad S_- = \tfrac{1}{\sqrt2}\begin{pmatrix}0&0\\1&0\end{pmatrix} \qquad (8)$$

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

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

Matrix representation in $\mathbb V_\ell\otimes\mathbb V_{\ell+1}$: $\quad S^{\sigma'_\ell}{}_{a\sigma_\ell} \qquad S^{\dagger\sigma'_{\ell+1}a}{}_{\sigma_{\ell+1}}$

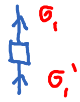


We define the 3-leg tensors S, $S^\dagger$ with index placements matching those of A tensors for wavefunctions:

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

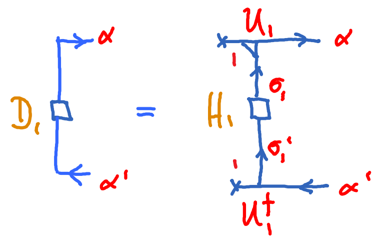
Diagonalize site 1

Matrix acting on $\mathcal{V}_1$:
$$\underbrace{H_1}_{\text{chain of length 1}} = S^\dagger_{a1} \cdot h_1^a = \underbrace{U_1 D_1 U_1^\dagger}_{\text{site index: } \ell = 1} \tag{10}$$



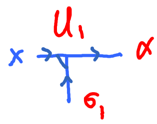
$D_1 = U_1^\dagger H_1 U_1$ is diagonal, with matrix elements

$$[D_1]^{\alpha'}{}_{\alpha'} = [U_1^\dagger]^{\alpha'}{}_{\sigma_1'} [H_1]^{\sigma_1'}{}_{\sigma_1} [U_1]^{\sigma_1}{}_{\alpha} \tag{11}$$



Eigenvectors of the matrix H_1 are given by column vectors of the matrix $[U_1]^{\sigma_1}{}_{\alpha}$:

Eigenstates of operator $\hat{H}_1$ are given by: $|\alpha\rangle = |\sigma_1\rangle [U_1]^{\sigma_1}{}_{\alpha}$ (13)



Add site 2

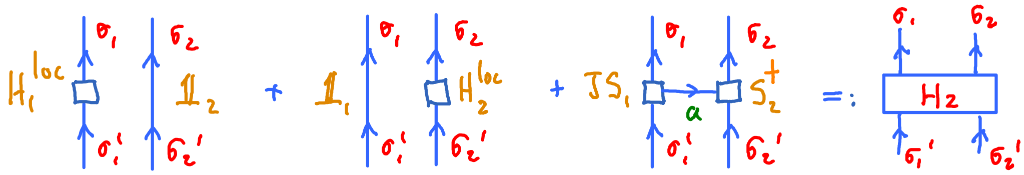
Diagonalize H_2 in enlarged Hilbert space, $\mathcal{H}_{(2)} = \mathrm{span}\{|\sigma_1\rangle|\sigma_2\rangle\}$ (14)

chain of length 2

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

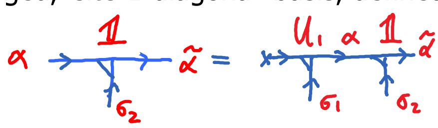
Matrix representation in $\mathbb{V}_1 \otimes \mathbb{V}_2$ corresponding to 'local' basis, $\{|\sigma_1\rangle|\sigma_2\rangle\}$:

$$H_2{}^{\sigma_1'\sigma_2'}{}_{\sigma_1\sigma_2} = \tag{16}$$



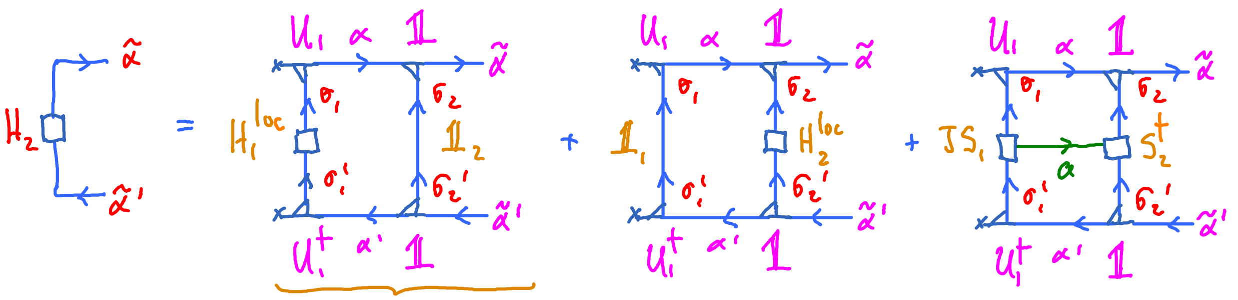
We seek matrix representation in $\mathcal{V}_1 \otimes \mathcal{V}_2$ corresponding to enlarged, 'site-1-diagonal' basis, defined as

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



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

To this end, attach $U_1^\dagger$, 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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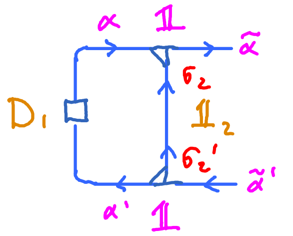


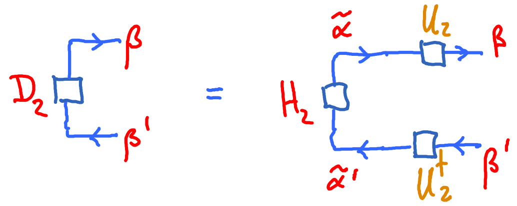
First term is already diagonal. But other terms are not.

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: $\quad H_2 = U_2 D_2 U_2^\dagger$ (19)

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

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

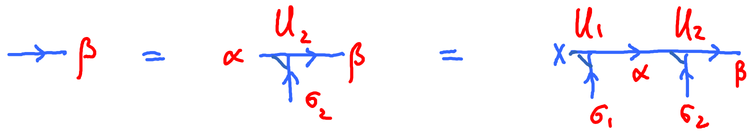


(20)

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 $\hat H_2$:

$$|\beta\rangle = |\tilde\alpha\rangle [U_2]^{\tilde\alpha}{}_{\beta} = |\alpha\rangle|\sigma_2\rangle [U_2]^{\alpha\sigma_2}{}_{\beta} = |\sigma_1\rangle|\sigma_2\rangle\, [U_1]^{\sigma_1}{}_{\alpha}\, [U_2]^{\alpha\sigma_2}{}_{\beta} \tag{21}$$



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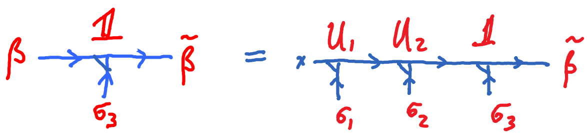
<u>Add site 3</u>

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

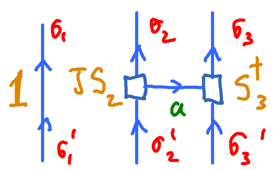
$$|\tilde\beta\rangle \equiv |\beta\sigma_3\rangle \equiv |\beta\rangle|\sigma_3\rangle$$



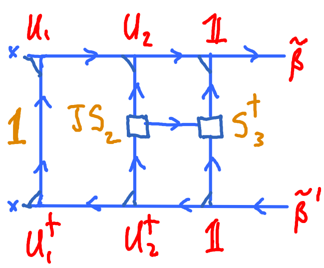
(23)

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

Local basis:



enlarged,
site-12-diagonal
basis:



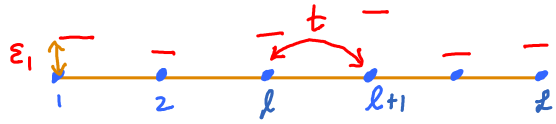
(24)

Then diagonalize in this basis: $\quad H_3 = U_3 D_3 U_3^\dagger$, 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:



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

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

$$\{\hat{c}_\ell, \hat{c}_{\ell'}\} = 0 \, , \quad \{\hat{c}^\dagger_\ell, \hat{c}^\dagger_{\ell'}\} = 0 \, , \quad \{\hat{c}^\dagger_\ell, \hat{c}_{\ell'}\} = \delta_{\ell\ell'} \qquad (2)$$

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

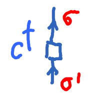
Hilbert space: $\mathrm{span}\{|0\rangle, |1\rangle\}$, local index: $n = \sigma \in \{0, 1\}$ local occupancy

Operator action:
$$\hat{c}^\dagger |0\rangle = |1\rangle \, , \qquad \hat{c}^\dagger |1\rangle = 0 \qquad (3a)$$
$$\hat{c} |0\rangle = 0 \, , \qquad \hat{c} |1\rangle = |0\rangle \qquad (3b)$$

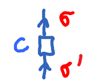
The operators $\hat{c}^\dagger = |\sigma'\rangle C^{\dagger\sigma'}{}_{\sigma} \langle \sigma|$ and $\hat{c} = |\sigma'\rangle C^{\sigma'}{}_{\sigma} \langle \sigma|$

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 $\hat{c}^\dagger \doteq C^\dagger$, $\hat{c} \doteq C$ where $\doteq$ means 'is represented by'

lower case denotes operator in Fock space

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

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

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

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

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

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: $\hat{c} \, \hat{z} = - \hat{z} \, \hat{c}$, $\hat{c}^\dagger \hat{z} = - \hat{z} \, \hat{c}^\dagger$ (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:
$$\hat{c}^\dagger \underbrace{(-1)^{\hat{n}}}_{=(-1)^0=1} = \hat{c}^\dagger = -\underbrace{(-1)^{\hat{n}}}_{=(-1)^1=-1}\hat{c}^\dagger \qquad (10a)$$

non-zero only when acting on $|0\rangle$

Similarly:
$$\hat{c}\underbrace{(-1)^{\hat{n}}}_{=(-1)^1=-1} = -\hat{c} = -\underbrace{(-1)^{\hat{n}}}_{=(-1)^0=1}\hat{c} \qquad (10b)$$

non-zero only when acting on $|1\rangle$

Now consider a chain of spinless fermions:

Complication: fermionic operators on different sites anticommute: $c_\ell c^\dagger_{\ell'} = -c^\dagger_{\ell'} c_\ell$ for $\ell \neq \ell'$

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

Define canonical ordering: fill states from right to left:

$$|n_1,\dots,n_\ell,\dots,n_{\mathscr{L}}\rangle = (\hat{c}_1^\dagger)^{n_1}\dots(\hat{c}_\ell^\dagger)^{n_\ell}\dots(\hat{c}_{\mathscr{L}}^\dagger)^{n_{\mathscr{L}}}|\mathrm{Vac}\rangle \qquad (12)$$

Now consider:

$$c_\ell^\dagger|n_1,\dots,0,\dots,n_{\mathscr{L}}\rangle = (-1)^{n_1+\dots+n_{\ell-1}}(\hat{c}_1^\dagger)^{n_1}\dots\underbrace{c_\ell^\dagger(\hat{c}_\ell^\dagger)^0}_{(\hat{c}_\ell^\dagger)^1}\dots(\hat{c}_{\mathscr{L}}^\dagger)^{n_{\mathscr{L}}}|\mathrm{Vac}\rangle \qquad (13)$$

$$= (-1)^{n_\ell^<}|n_1,\dots,1,\dots,n_{\mathscr{L}}\rangle \quad , \quad n_\ell^< = \sum_{\ell'=1}^{\ell-1} n_{\ell'} \qquad (14)$$

$$c_\ell|n_1,\dots,1,\dots,n_{\mathscr{L}}\rangle = (-1)^{n_1+\dots+n_{\ell-1}}(\hat{c}_1^\dagger)^{n_1}\dots\underbrace{c_\ell(\hat{c}_\ell^\dagger)^1}_{(\hat{c}_\ell^\dagger)^0}\dots(\hat{c}_{\mathscr{L}}^\dagger)^{n_{\mathscr{L}}}|\mathrm{Vac}\rangle \qquad (15)$$

$$= (-1)^{n_\ell^<}|n_1,\dots,0,\dots,n_{\mathscr{L}}\rangle \qquad (16)$$

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:

$$\hat{c}_\ell^\dagger \doteq Z_1\otimes\dots Z_{\ell-1}\otimes C_\ell^\dagger\otimes \mathbb{1}_{\ell+1}\otimes\dots\otimes\mathbb{1}_{\mathscr{L}} =: Z_\ell^< C_\ell^\dagger \qquad (21)$$

$$\hat{c}_\ell \doteq Z_1\otimes\dots Z_{\ell-1}\otimes C_\ell\otimes \mathbb{1}_{\ell+1}\otimes\dots\otimes\mathbb{1}_{\mathscr{L}} =: Z_\ell^< C_\ell \qquad (22)$$

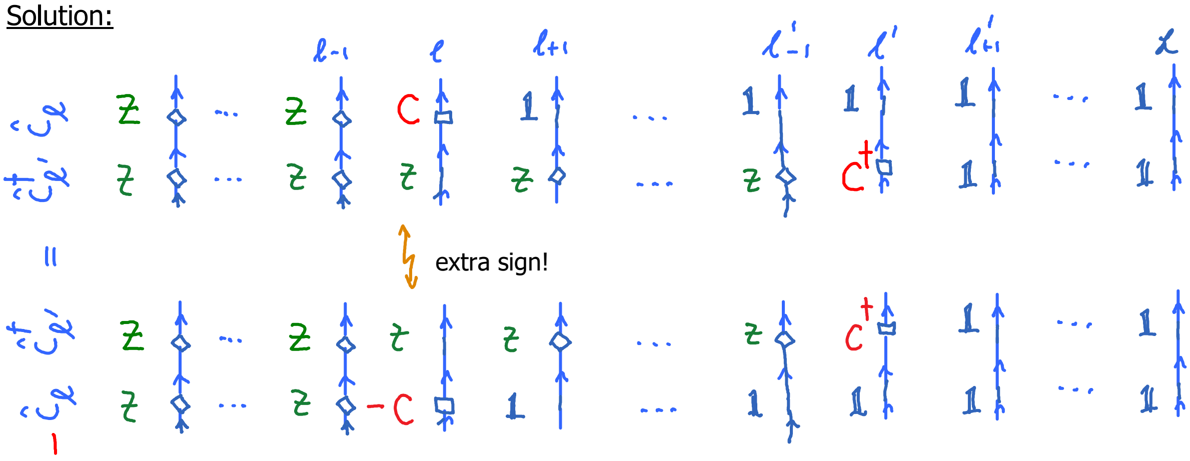
'Jordan-Wigner transformation'

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 $\ell' > \ell$.

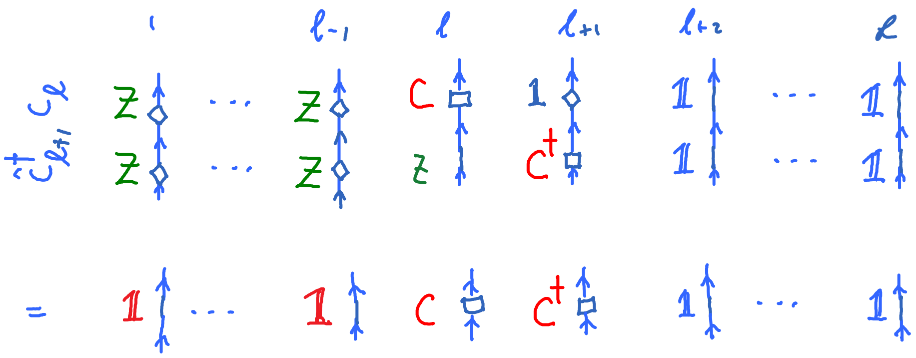
<u>Solution:</u>



(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 site ℓ 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 $|\dots, n_\ell = 0, \dots\rangle$,

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

Conclusion: $\hat{c}^\dagger_{\ell+1} c_\ell \doteq C^\dagger_{\ell+1} C_\ell$ and similarly, [using (10b)] $\hat{c}^\dagger_\ell \hat{c}_{\ell+1} \doteq C^\dagger_\ell C_{\ell+1}$ (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: $s \in \{\uparrow, \downarrow\} := \{+, -\}$

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

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

$|\uparrow\rangle \equiv \hat c^\dagger_\uparrow |0\rangle$, $|\uparrow\downarrow\rangle \equiv \hat c^\dagger_\uparrow \hat c^\dagger_\downarrow |0\rangle = \hat c^\dagger_\uparrow |\downarrow\rangle = - \hat c^\dagger_\downarrow |\uparrow\rangle$ (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.)

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

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

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

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

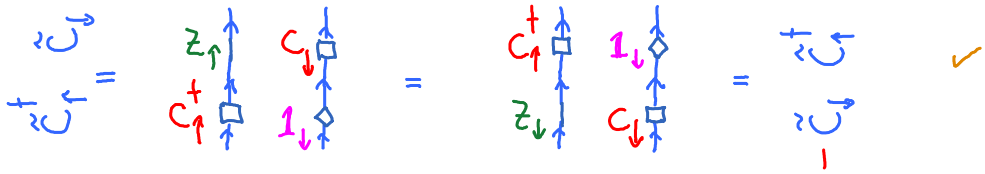
$$\hat c_\uparrow \doteq c_\uparrow \otimes \mathbb{1} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} = \left(\begin{array}{cc|cc} & & 1 & \\ & & & 1 \\ \hline & & & \\ & & & \end{array}\right) =: \tilde c_\uparrow \tag{11}$$

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

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

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

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)

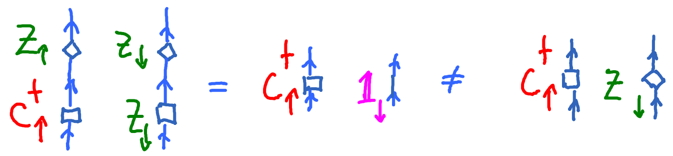
Algebraic check:

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

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 $\tilde{\mathbb{V}}^{\otimes \mathcal{L}} = \tilde{\mathbb{V}}_1 \otimes \tilde{\mathbb{V}}_2 \otimes \ldots \otimes \tilde{\mathbb{V}}_{\mathcal{L}}$:

$$\hat{c}^\dagger_\ell \doteq \tilde{Z}_1 \otimes \ldots \otimes \tilde{Z}_{\ell-1} \otimes \tilde{C}^\dagger_\ell \otimes \mathbb{1}_{\ell+1} \otimes \ldots \mathbb{1}_{\mathcal{L}} \equiv \tilde{Z}^<_\ell \tilde{C}^\dagger_\ell \qquad (17)$$

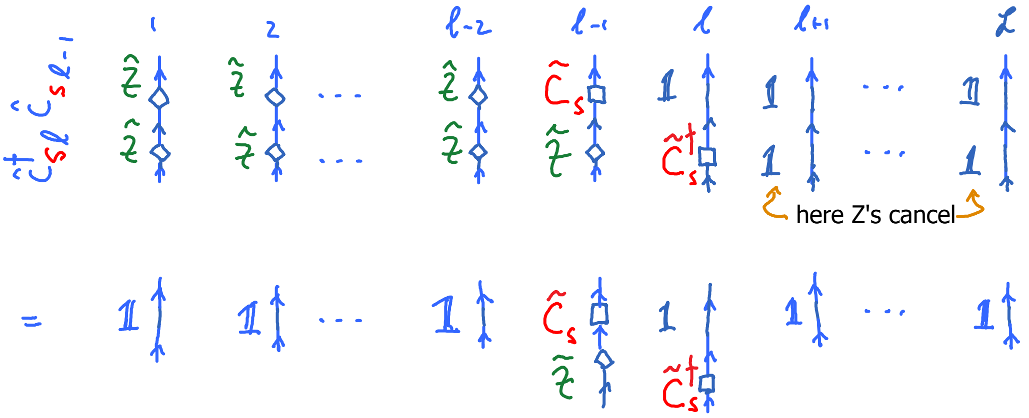
'Jordan-Wigner transformation'

$$\hat{c}_\ell \doteq \tilde{Z}_1 \otimes \ldots \otimes \tilde{Z}_{\ell-1} \otimes \tilde{C}_\ell \otimes \mathbb{1}_{\ell+1} \otimes \ldots \mathbb{1}_{\mathcal{L}} \equiv \tilde{Z}^<_\ell \tilde{C}_\ell \qquad (18)$$

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)

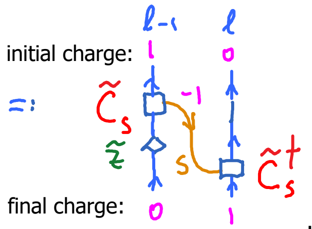
In <u>bilinear combinations</u>, most (but not all!) of the Z 's cancel.

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

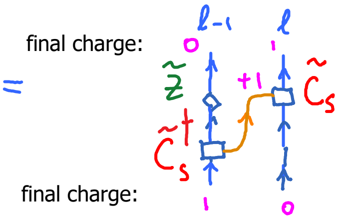


(20)

(21)



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



(22)

bond → indicates spin sum $\sum_s$

Arrow convention for virtual bonds of creation/annihilation operators:

'charge conservation' holds for each operator, i.e. total charge in = total charge out. (23)

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

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