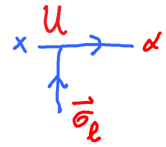
MPS II: Diagonalization, fermionic signs

1. Basis change

It is useful to have a graphical depiction for basis changes.

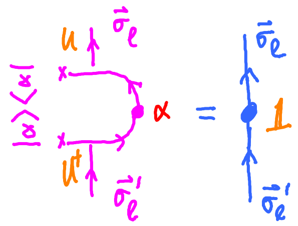
Consider a unitary transformation defined on chain of length ℓ , spanned by basis $\{|\vec\sigma_\ell\rangle\}$:

$$|\alpha\rangle = |\vec\sigma_\ell\rangle\, U^{\vec\sigma_\ell}{}_\alpha \qquad (1)$$



Unitarity guarantees resolution of identity on this subspace:

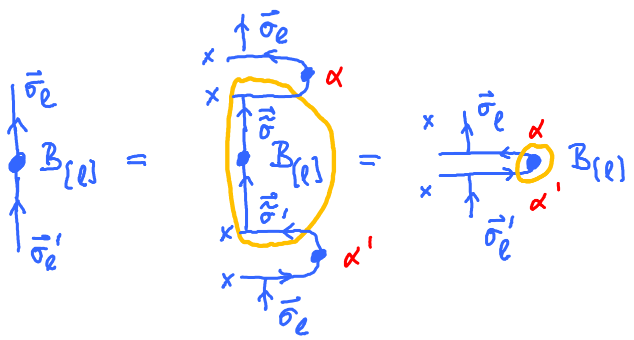
$$\sum_\alpha |\alpha\rangle\langle\alpha| = |\vec\sigma_\ell'\rangle \underbrace{U^{\vec\sigma_\ell'}{}_\alpha\, U^{\dagger\alpha}{}_{\vec\sigma_\ell}}_{\mathbb{1}^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell}} \langle\vec\sigma_\ell| = \sum_{\vec\sigma_\ell} |\vec\sigma_\ell'\rangle\, \mathbb{1}^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell} \langle\vec\sigma_\ell| = \hat{\mathbb{1}} \qquad (2)$$



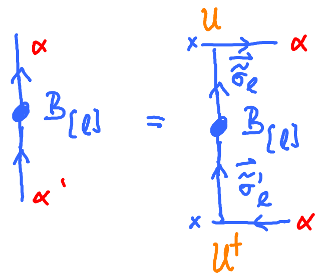
Transformation of an operator defined on this subspace:

$$\hat B = |\vec\sigma_\ell'\rangle B^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell} \langle\vec\sigma_\ell| = \sum_{\alpha'\alpha} |\alpha'\rangle\langle\alpha'|\hat B|\alpha\rangle\langle\alpha| = |\alpha'\rangle B^{\alpha'}{}_\alpha \langle\alpha| \qquad (3)$$

Matrix elements: $B^{\alpha'}{}_\alpha = \langle\alpha'|\vec\sigma_\ell'\rangle B^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell} \langle\vec\sigma_\ell|\alpha\rangle = U^{\dagger\alpha'}{}_{\vec\sigma_\ell'}\, B^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell}\, U^{\vec\sigma_\ell}{}_\alpha$ (4)



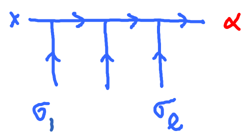
with

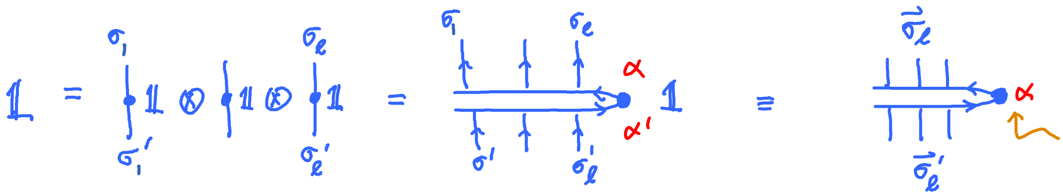


(5)

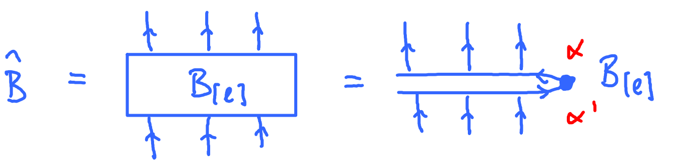
If the states $|\alpha\rangle$ are MPS:

$$|\alpha\rangle = |\sigma_\ell\rangle \ldots |\sigma_1\rangle \left(A^{\sigma_1} \ldots A^{\sigma_\ell}\right)^1{}_\alpha \qquad (6)$$

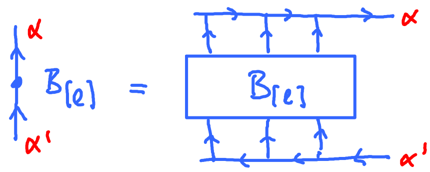




shorthand for unit matrix (7)



with



(8)

2. Iterative diagonalization

Consider spin-½ chain: $$\hat H^N = \sum_{\ell=1}^{N} \hat{\vec S}_\ell \cdot \vec h_\ell + J \sum_{\ell=2}^{N} \hat{\vec S}_\ell \cdot \hat{\vec S}_{\ell-1} \qquad (1)$$

For later convenience, we write the spin-spin interaction in covariant (up/down index) notation:

$$\hat{\vec S}_\ell \cdot \hat{\vec S}_{\ell-1} = \hat S^x_\ell \hat S^x_{\ell-1} + \hat S^y_\ell \hat S^y_{\ell-1} + \hat S^z_\ell \hat S^z_{\ell-1}$$

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

$$= \hat S^{\dagger +}_\ell \hat S_{+\ell-1} + \hat S^{\dagger -}_\ell \hat S_{-\ell-1} + \hat S^{\dagger z}_\ell \hat S_{z\ell-1} = \hat S^{\dagger a}_\ell \hat S_{\ell-1\,a} \qquad (2)$$

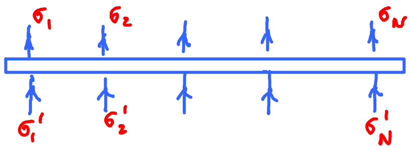
where we defined the operator triplets $$\hat S_a \in \{\hat S_+, \hat S_-, \hat S_z\}, \quad \hat S^{\dagger a} \in \{\hat S^{\dagger +}, \hat S^{\dagger -}, \hat S^{\dagger z}\} \qquad (2)$$

with components $$\hat S_z := \hat S^{\dagger z} = \hat S^z, \quad \hat S_\pm := \tfrac{1}{\sqrt 2}(\hat S^x \pm i \hat S^y) =: \hat S^{\dagger \mp} \qquad (4)$$

In the basis $\{|\vec\sigma\rangle_N\} = \{|\sigma_N\rangle \dots |\sigma_2\rangle|\sigma_1\rangle\}$, the Hamiltonian can be expressed as

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

'no hat' means 'matrix representation'

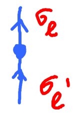


$H^{\vec\sigma'}{}_{\vec\sigma}$ is a linear map acting on a direct product space: $V^{\otimes N} \equiv V_1 \otimes V_2 \otimes \dots \otimes V_N$

where V_ℓ is the 2-dimensional representation space of site ℓ.

$\hat H^N$ is a sum of single-site and two-site terms.

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



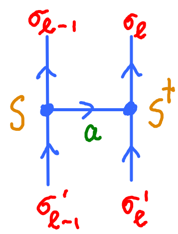
Matrix representation in V_ℓ: $$(S_a)^{\sigma'_\ell}{}_{\sigma_\ell} = \langle\sigma'_\ell|\hat S_{a\ell}|\sigma_\ell\rangle = \begin{pmatrix} (S_a)^\uparrow{}_\uparrow & (S_a)^\uparrow{}_\downarrow \\ (S_a)^\downarrow{}_\uparrow & (S_a)^\downarrow{}_\downarrow \end{pmatrix} \qquad (7)$$

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

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

$$\hat S^{\dagger a}_\ell \otimes \hat S_{a\ell-1} = |\sigma'_\ell\rangle|\sigma'_{\ell-1}\rangle \underbrace{(S_a)^{\sigma'_{\ell-1}}{}_{\sigma_{\ell-1}}}_{\parallel \; S^{\sigma'_{\ell-1}}{}_{a\,\sigma_{\ell-1}}} \underbrace{(S^{\dagger a})^{\sigma'_\ell}{}_{\sigma_\ell}}_{\parallel \; S^{\dagger\sigma'_\ell a}{}_{\sigma_\ell}} \langle\sigma_{\ell-1}|\langle\sigma_\ell| \qquad (9)$$

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



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

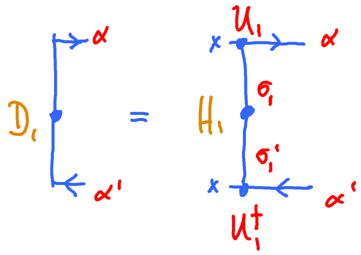
Matrix acting on V_1 :

$$H_1 = S^{\dagger}_{a1} \cdot h^a_1 = U_1 D_1 U_1^{\dagger} \qquad (10)$$

chain of length 1 site index: $\ell = 1$

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

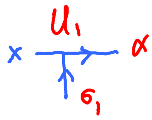
$$(D_1)^{\alpha'}{}_{\alpha'} = (U_1^{\dagger})^{\alpha'}{}_{\sigma_1'} (H_1)^{\sigma_1'}{}_{\sigma_1} (U_1)^{\sigma_1}{}_{\alpha}$$



(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

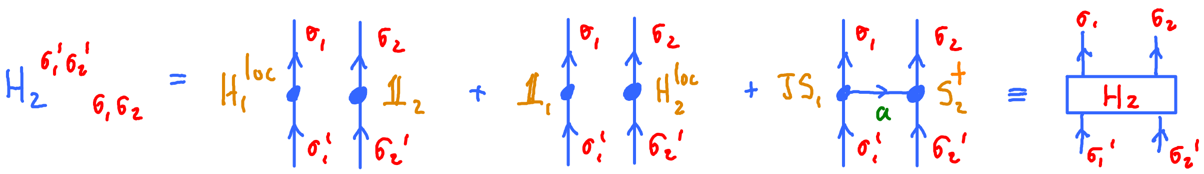
Diagonalize H_2 in enlarged Hilbert space, $\mathcal{H}_{(2)} = \mathrm{span}\{|\sigma_2\rangle|\sigma_1\rangle\}$ (14)

chain of length 2

Matrix acting on $V_1 \otimes V_2$:

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

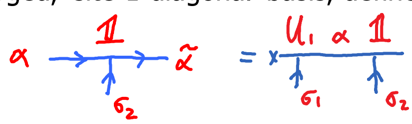
Matrix representation in $V_1 \otimes V_2$ corresponding to 'local' basis, $\{|\sigma_2\rangle|\sigma_1\rangle\}$:



(16)

We seek matrix representation in $V_1 \otimes V_2$ corresponding to enlarged, 'site-1-diagonal' basis, defined as

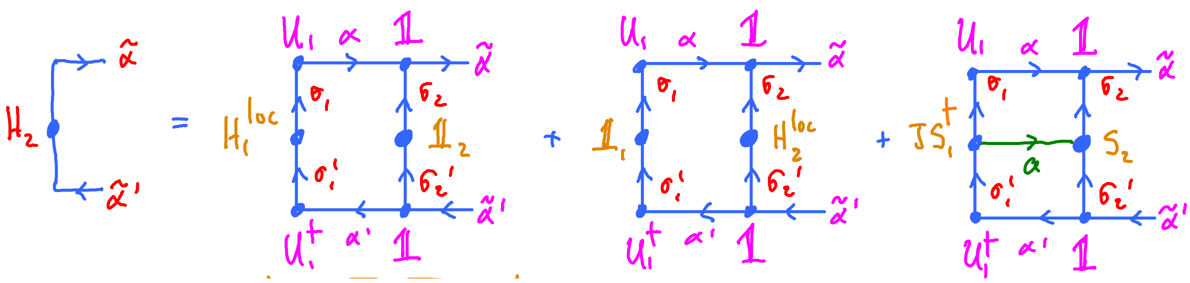
$$|\tilde{\alpha}\rangle \equiv |\alpha\sigma_2\rangle \equiv |\sigma_2\rangle|\alpha\rangle = |\sigma_2\rangle|\sigma_1\rangle U^{\sigma_1}{}_{\alpha}$$



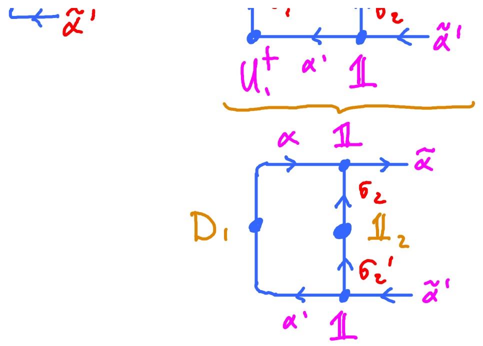
(17)

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

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:



(18)

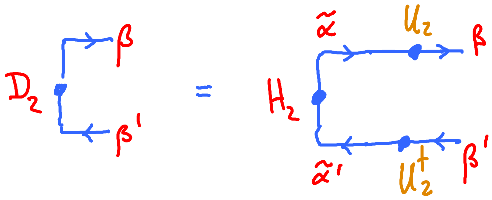


First term is already diagonal. But other terms are not.

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

$$D_2{}^{\beta'}{}_{\beta} = (U_2^\dagger)^{\beta'}{}_{\tilde\alpha'} (H_2)^{\tilde\alpha'}{}_{\tilde\alpha} (U_2)^{\tilde\alpha}{}_{\beta}$$

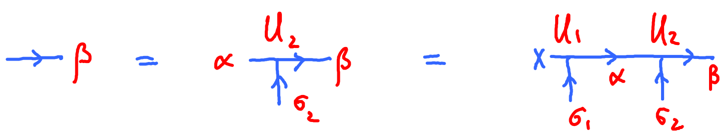


(20)

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 $\hat H_2$:

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

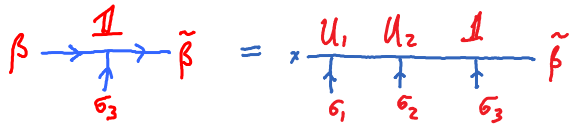


(22)

<u>Add site 3</u>

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

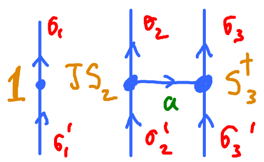
$$|\tilde\beta\rangle \equiv |\beta\sigma_3\rangle \equiv |\sigma_3\rangle|\beta\rangle$$



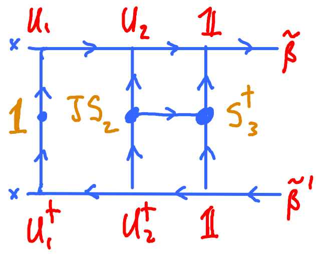
(23)

For example, spin-spin interaction, H^{int}_{32} :

Local basis:



enlarged, site-12-diagonal basis:



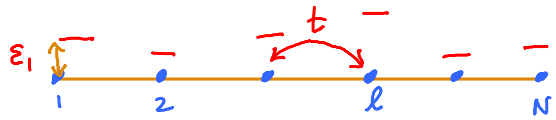
(24)

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, trunctations will be needed...!

3. Spinless fermions

Consider tight-binding chain of spinless fermions:



$$\hat{H} = \sum_{\ell=1}^{N} \varepsilon_\ell \, \hat{c}^\dagger_\ell \hat{c}_\ell + \sum_{\ell=2}^{N} t_\ell \left(\hat{c}^\dagger_\ell \hat{c}_{\ell-1} + \hat{c}^\dagger_{\ell-1} \hat{c}_\ell \right) \tag{1}$$

Goal: find matrix representation for this Hamiltonian, acting in direct product space $V_1 \otimes V_2 \otimes \dots \otimes V_N$, while respecting fermionic minus signs:

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

First consider a <u>single site</u> (dropping the site index ℓ):

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

Operator action:

$$\hat{c}^\dagger |0\rangle = |1\rangle \,, \qquad \hat{c}^\dagger |1\rangle = 0 \tag{3a}$$

$$\hat{c}\,|0\rangle = 0 \,, \qquad \hat{c}\,|1\rangle = |0\rangle \tag{3b}$$

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 V:

$$c^{\dagger\sigma'}{}_{\sigma} = \langle \sigma' | \hat{c}^\dagger | \sigma \rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad c^{\dagger}\,{}^{\sigma}_{\sigma'} \tag{4a}$$

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

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 V

Check:

$$C^\dagger C + C C^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1} \ \checkmark \tag{5}$$

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

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

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

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

Useful relations: $\hat{c}\,\hat{z} = -\hat{z}\,\hat{c} \,, \qquad \hat{c}^\dagger \hat{z} = -\hat{z}\,\hat{c}^\dagger$ (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 <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: $\mathrm{span}\{|\vec{\sigma}\rangle_N = |n_1, n_2, \dots, n_N\rangle\}$, $n_i \in \{0,1\}$ (11)

Define canonical ordering for fully filled state:

$$|n_1 = 1, n_2 = 1, \dots, n_N = 1\rangle = c^\dagger_N \dots c^\dagger_1 c^\dagger_1 |\mathrm{Vac}\rangle \qquad (12)$$

Now consider:

$$\hat{c}^\dagger_1 |n_1 = 0, n_2 = 1\rangle = \hat{c}^\dagger_1 \hat{c}^\dagger_2 |\mathrm{Vac}\rangle = -\hat{c}^\dagger_2 \hat{c}^\dagger_1 |\mathrm{Vac}\rangle = -|n_1 = 1, n_2 = 1\rangle \qquad (13)$$

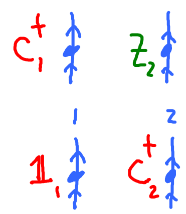
To keep track of such signs, matrix representations in $V_1 \otimes V_2$ need extra 'sign counters', tracking fermion numbers:

$$\hat{c}^\dagger_1 \doteq c^\dagger_1 \otimes (-1)^{n_2} = c^\dagger_1 \otimes z_2 \qquad (14)$$

subscripts denote site numbers

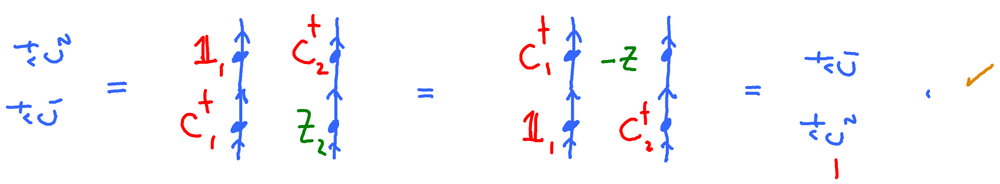
$$\hat{c}^\dagger_2 \doteq \mathbb{1}_1 \otimes c^\dagger_2 \equiv c^\dagger_2 \qquad (15)$$

(shorthand: omit unity)



Here $\otimes$ denotes a direct product operation; the order (space 1, space 2, ...) matches that of the indices on the corresponding tensors: $A^{\sigma_1 \sigma_2 \dots}$

Check whether $\hat{c}^\dagger_1 \hat{c}^\dagger_2 = -\hat{c}^\dagger_2 \hat{c}^\dagger_1$? (16)



(17)

Algebraically:

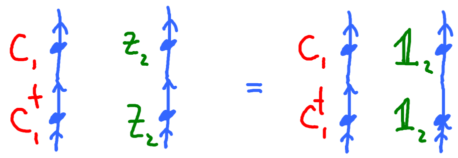
(14) (9)

Algebraically:

$$\hat{c}_1^\dagger \hat{c}_2^\dagger \doteq (C_1^\dagger \otimes Z_2)(\mathbb{1}_1 \otimes C_2^\dagger) \overset{(14)}{=} C_1^\dagger \mathbb{1}_1 \otimes (Z_2 C_2^\dagger) \overset{(9)}{=} -\mathbb{1}_1 C_1^\dagger \otimes C_2^\dagger Z_2 \tag{18}$$

$$= -(\mathbb{1}_1 \otimes C_2^\dagger)(C_1^\dagger \otimes Z_2) \doteq -\hat{c}_2^\dagger \hat{c}_1^\dagger \quad ✓ \tag{19}$$

Similarly:

$$\hat{n}_1 = \hat{c}_1^\dagger \hat{c}_1 \doteq$$  $$\doteq C_1^\dagger C_1 \otimes \mathbb{1}_2 \tag{20}$$

More generally: each $\hat{c}_\ell$ or $\hat{c}_\ell^\dagger$ must produce sign change when moved past any $\hat{c}_{\ell'}$ or $\hat{c}_{\ell'}^\dagger$, with $\ell' > \ell$. So, define the following matrix representations in $V^{\otimes N} = V_1 \otimes V_2 \otimes \dots \otimes V_N$:

$$\hat{c}_\ell^\dagger \doteq \mathbb{1}_1 \otimes \dots \mathbb{1}_{\ell-1} \otimes C_\ell^\dagger \otimes Z_{\ell+1} \otimes \dots Z_N \equiv C_\ell^\dagger Z_\ell^> \tag{21}$$

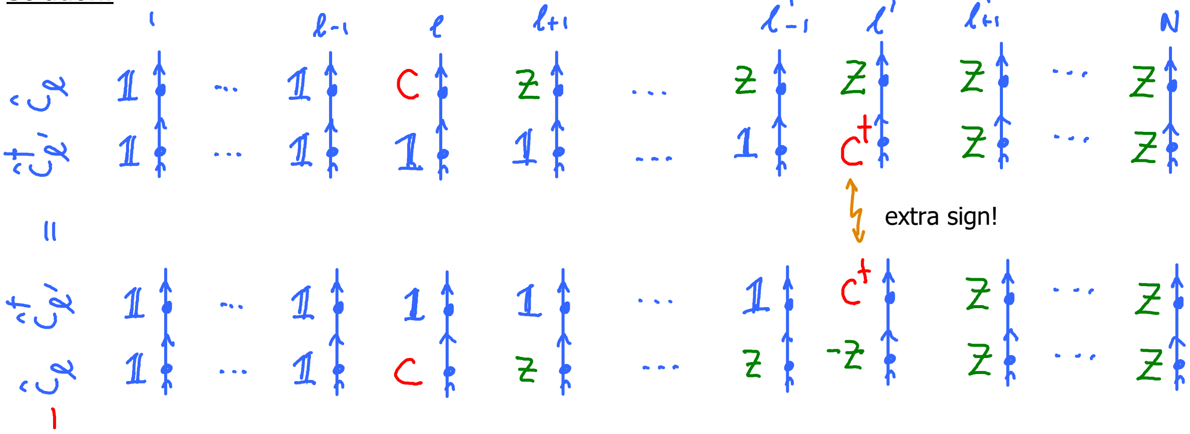
$$\hat{c}_\ell \doteq \mathbb{1}_1 \otimes \dots \mathbb{1}_{\ell-1} \otimes C_\ell \otimes Z_{\ell+1} \otimes \dots Z_N \equiv C_\ell Z_\ell^> \tag{22}$$

'Jordan-Wigner transformation'

with $$Z_\ell^> \equiv \prod_{\otimes \ell' > \ell} Z_{\ell'}$$ 'Z-string' (23)

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

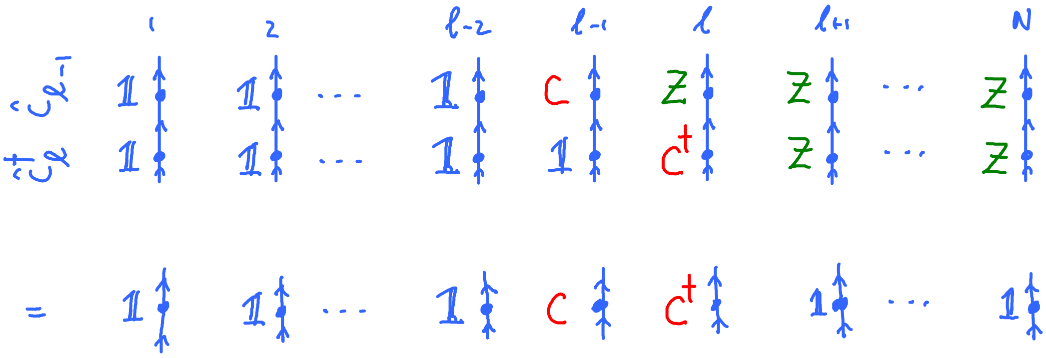
<u>Solution:</u>



(24)

(25)

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



(26)

(27)

$$= \mathbb{1} \quad \mathbb{1} \cdots \mathbb{1} \quad c \quad c^{\dagger} \quad \mathbb{1} \cdots \mathbb{1} \tag{27}$$

since at site ℓ we have $\quad Z_\ell Z_\ell = \mathbb{1}_\ell, \qquad c^{\dagger}_\ell Z_\ell \overset{(10a)}{=} c^{\dagger}_\ell \quad , \qquad (28)$

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

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

Conclusion: $\quad \hat{c}^{\dagger}_\ell \hat{c}_{\ell-1} \doteq c^{\dagger}_\ell c_{\ell-1}$ and similarly, $\quad \hat{c}^{\dagger}_{\ell-1} \hat{c}_\ell \doteq c^{\dagger}_{\ell-1} c_\ell \qquad (29)$

[using (10b)]

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

For spinful fermions, this will be different.

4. Spinful fermions

Consider chain of <u>spinful</u> fermions. Site index: $\ell = 1, \dots, N$, spin index: $s \in \{\uparrow, \downarrow\} := \{+, -\}$

$$\{\hat c_{\ell s}, \hat c_{\ell' s'}\} = 0 \, , \quad \{\hat c^\dagger_{\ell s}, \hat c^\dagger_{\ell' s'}\} = 0 \, , \quad \{\hat c^\dagger_{\ell s}, \hat c_{\ell' s'}\} = \delta_{\ell \ell'} \delta_{s s'} \qquad (1)$$

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

First consider a <u>single</u> 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)

$$|\uparrow\rangle \equiv \hat c^\dagger_\uparrow |0\rangle , \quad |\uparrow\downarrow\rangle \equiv \hat c^\dagger_\downarrow \hat c^\dagger_\uparrow |0\rangle = \hat c^\dagger_\downarrow |\uparrow\rangle = - \hat c^\dagger_\uparrow |\downarrow\rangle \qquad (5)$$

To deal 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 $\tilde V \equiv V_\uparrow \otimes V_\downarrow$. (7)

(Matrices acting in this space will carry tildes.)

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

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

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

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

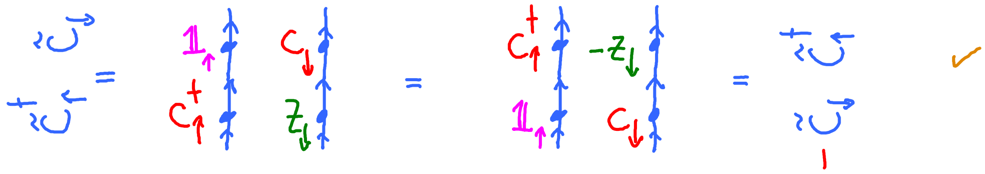
$$\hat c_\uparrow \doteq c_\uparrow \otimes Z_\downarrow = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = \left(\begin{array}{cc|cc} & & 1 & \\ & & & -1 \\ \hline & & & \\ & & & \end{array}\right) \equiv \tilde c_\uparrow \qquad (11)$$

$$\hat c^\dagger_\downarrow \doteq \mathbb{1}_\uparrow \otimes c^\dagger_\downarrow = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \left(\begin{array}{cc|cc} 0 & 0 & & \\ 1 & 0 & & \\ \hline & & 0 & 0 \\ & & 1 & 0 \end{array}\right) \equiv \tilde c^\dagger_\downarrow \qquad (12)$$

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

$$\hat{c}_\downarrow \doteq \mathbb{1}_\uparrow \otimes c_\downarrow = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \left(\begin{array}{cc|cc} 0 & 1 & & \\ 0 & 0 & & \\ \hline & & 0 & 1 \\ & & 0 & 0 \end{array}\right) \equiv \tilde{C}_\downarrow \qquad (12)$$

The factors Z_s guarantee correct signs. For example $\tilde{C}^\dagger_\uparrow \hat{\tilde{C}}_\downarrow = - \tilde{C}_\downarrow \tilde{C}^\dagger_\uparrow$:
(fully analogous to MPS-II.1.17)


(13)

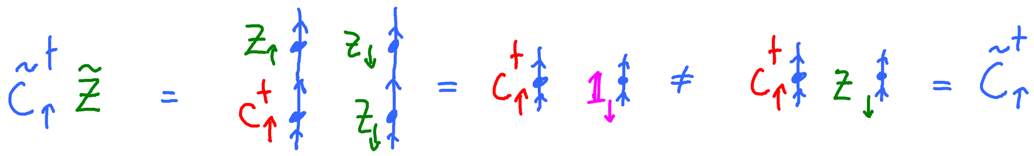
Algebraic check:

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

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

$$\tilde{C}^\dagger_s \tilde{Z} \neq \tilde{C}^\dagger_s \qquad \text{and} \qquad \tilde{Z}\,\tilde{C}_s \neq \tilde{C}_s \qquad (15)$$

For example, consider $s = \uparrow$; action in $V_\uparrow \otimes V_\downarrow$:


(16)

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

Each $\hat{c}_\ell$ or $\hat{c}^\dagger_\ell$ must produce sign change when moved past any $\hat{c}_{\ell'}$ or $\hat{c}^\dagger_{\ell'}$, with $\ell' > \ell$.

So, define the following matrix representations in $\tilde{V}^{\otimes N} = \tilde{V}_1 \otimes \tilde{V}_2 \otimes \cdots \otimes \tilde{V}_N$:

$$\hat{c}^\dagger_\ell \doteq \tilde{\mathbb{1}}_1 \otimes \cdots \tilde{\mathbb{1}}_{\ell-1} \otimes \tilde{C}^\dagger_\ell \otimes \tilde{Z}_{\ell+1} \otimes \cdots \tilde{Z}_N \equiv \tilde{C}^\dagger_\ell \,\hat{\tilde{Z}}^>_\ell \qquad (17)$$

$$\hat{c}_\ell \doteq \tilde{\mathbb{1}}_1 \otimes \cdots \tilde{\mathbb{1}}_{\ell-1} \otimes \tilde{C}_\ell \otimes \tilde{Z}_{\ell+1} \otimes \cdots \tilde{Z}_N \equiv \tilde{C}_\ell \,\hat{\tilde{Z}}^>_\ell \qquad (18)$$

'Jordan-Wigner transformation'

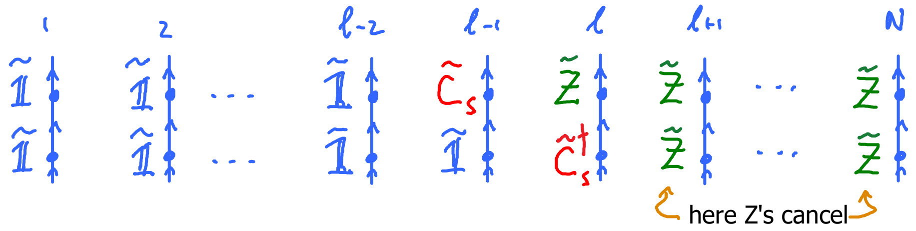
with
$$\hat{\tilde{Z}}^>_\ell \equiv \prod_{\otimes \ell' > \ell} \tilde{Z}_{\ell'} = \prod_{\otimes \ell' > \ell} Z_{\uparrow \ell'} \otimes Z_{\downarrow \ell'} \qquad \text{'Z-string'} \qquad (19)$$

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)

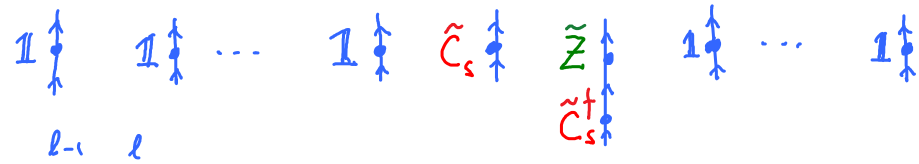
1 2 $\ell-2$ $\ell-1$ ℓ $\ell+1$ N

$$\hat c^\dagger_{s\ell}\,\hat c_{s\ell-1}$$



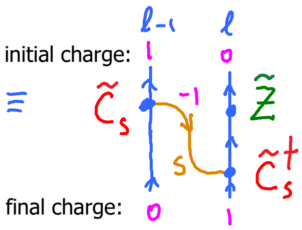
(20)

=



(21)

≡



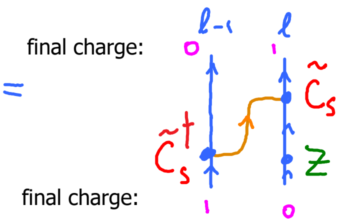
Bond → indicates sum $\sum_s$ (22)

Convention: annihilation: outgoing -1 or incoming $+1$

Creation: outgoing $+1$ or incoming -1

Similarly:

$$\hat c^\dagger_{\ell-1\,s}\;\hat c_{\ell s} =$$



(23)