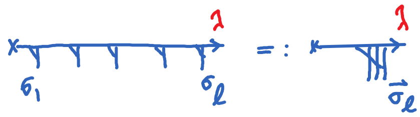
MPS II: Diagonalization, fermionic signs

1. Basis change

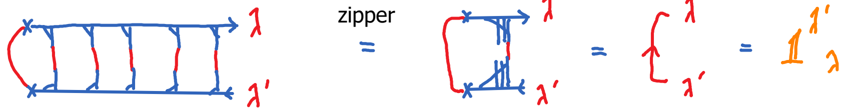
Recall: a set of MPS $|\Psi_\lambda\rangle_\ell = |\vec{\sigma}_\ell\rangle [A^{\sigma_1} \dots A^{\sigma_\ell}]^1{}_\lambda$ =



specified by given left-normalized tensors (1)

defines an orthonormal basis for a state space $\mathbb{V}_\ell = \text{span}\{|\Psi_\lambda\rangle_\ell\} \subseteq \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \dots \otimes \mathbb{V}_\ell =: \mathbb{V}^{\otimes \ell}$ (2)

since ${}_\ell\langle \Psi^{\lambda'} | \Psi_\lambda \rangle_\ell$ =

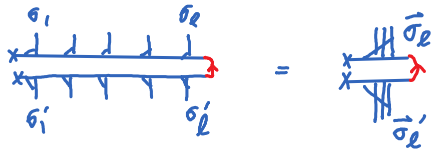


close zipper

$= \mathbb{1}^{\lambda'}{}_\lambda$ (3)

Projector onto $\mathbb{V}_\ell$: $\hat{P}_\ell = |\Psi^\lambda\rangle_\ell\, {}_\ell\langle \Psi_\lambda|$ =

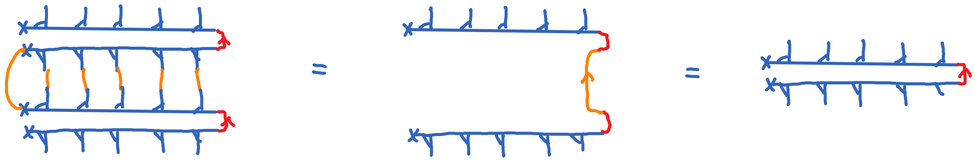
(sum over λ implied)



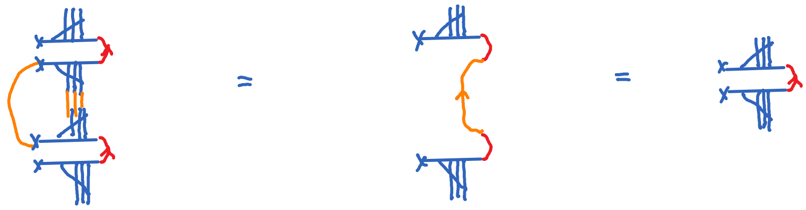
(4)

Indeed:

$$\hat{P}_\ell \hat{P}_\ell = |\Psi^{\lambda'}\rangle_\ell\, \underbrace{{}_\ell\langle \Psi_{\lambda'}| \cdot |\Psi^\lambda\rangle_\ell}_{\mathbb{1}_{\lambda'}{}^{\lambda}}\, {}_\ell\langle \Psi_\lambda| = \hat{P}_\ell \quad ✓ \tag{5}$$



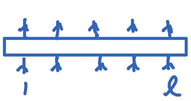
(6a)



(6b)

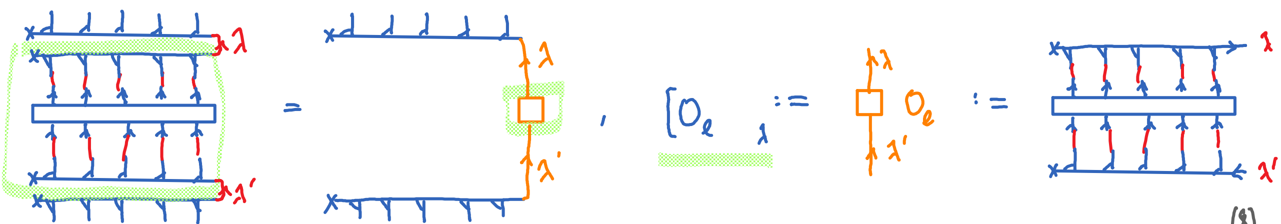
Operators defined on $\mathbb{V}_\ell^{\otimes \ell}$ can be mapped to $\mathbb{V}_\ell$ using these projectors:

$\hat{O}$ =



$\xrightarrow{\hat{P}_\ell}$ $\hat{O}_\ell =: \hat{P}_\ell\, \hat{O}\, \hat{P}_\ell =: |\Psi_{\lambda'}\rangle_\ell [O_\ell]^{\lambda'}{}_\lambda\, {}_\ell\langle \Psi^\lambda|$ (7)

$\hat{O}_\ell$ =

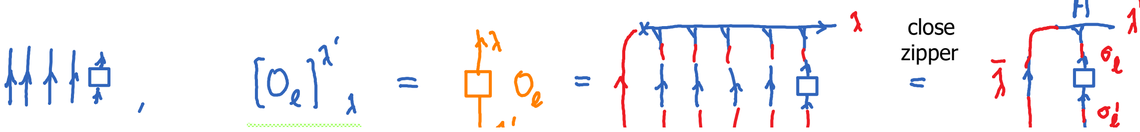


$[O_\ell]^{\lambda'}{}_\lambda :=$ O_ℓ $:=$

(8)

Simplest case: 1-site operator acting only on site ℓ :

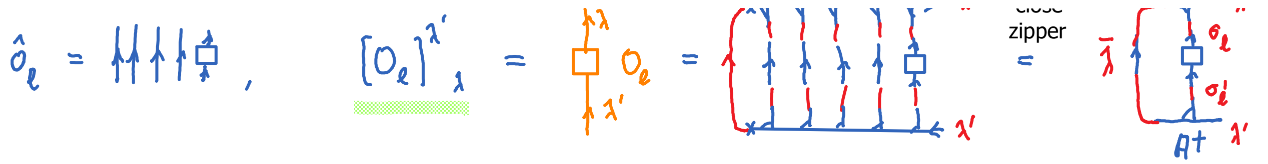
$\hat{O}_\ell$ =



$[O_\ell]^{\lambda'}{}_\lambda$ = O_ℓ =

close zipper

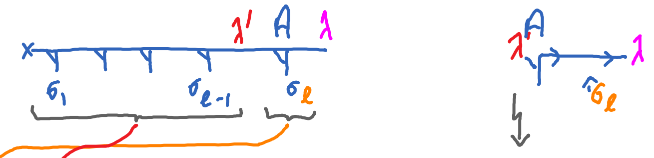
(9)



(9)

During iterative diagonalization, the space $\mathbb{V}_\ell$ is constructed through a sequence of isometric maps:
(possibly involving truncation)

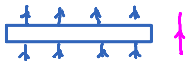
Each A defines an isometric map to a new (possibly smaller) basis:

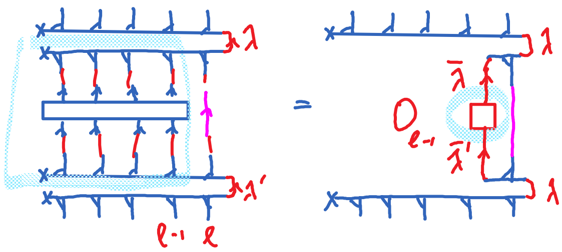
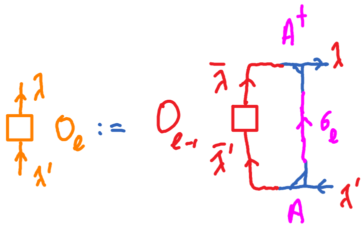


$$A_\ell : V_\ell \otimes \mathbb{V}_{\ell-1} \to \mathbb{V}_\ell , \qquad \underbrace{|\sigma_\ell\rangle |\Psi_{\lambda'}\rangle_{\ell-1}}_{\text{old basis}} \mapsto \underbrace{|\Psi_\lambda\rangle_\ell}_{\text{new basis}} = |\sigma_\ell\rangle |\Psi_{\lambda'}\rangle_{\ell-1} \, A^{\lambda'\sigma_\ell}{}_{\lambda} \qquad (10)$$

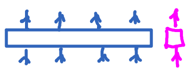
Each such map also induces a transformation of operators defined on its domain of definition.
It is useful to have a graphical depiction for how operators transform under such maps.

Consider an operator defined on $\mathbb{V}^{\otimes(\ell-1)}$, represented on $\mathbb{V}_{\ell-1}$ by $\hat{O}_{\ell-1} = \hat{P}_{\ell-1}\hat{O}\hat{P}_{\ell-1}$ (11)

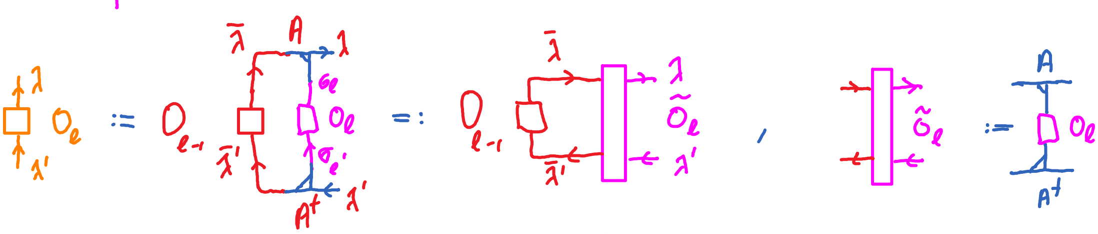
What is its representation on $\mathbb{V}_\ell$? $\hat{O} = \hat{O}_{\ell-1} \otimes \mathbb{1}_\ell =$  (12)

$\hat{O}_\ell =$  , $[O_\ell]^{\lambda'}{}_{\lambda} :=$  (13)

Explicitly: $$[O_\ell]^{\lambda'}{}_{\lambda} = A^{\dagger\lambda'}{}_{\sigma_\ell \bar\lambda'} \, [O_{\ell-1}]^{\bar\lambda'}{}_{\bar\lambda} \, A^{\bar\lambda \sigma_\ell}{}_{\lambda} \qquad (14)$$

Similarly, for operator with non-trivial action also on site : $\hat{O}_\ell = \hat{O}_{\ell-1} \otimes \hat{o}_\ell =$  (15)

Just replace  by  in (9):

$[O_\ell]^{\lambda'}{}_{\lambda} :=$  (16)

$$= A^{\dagger\lambda'}{}_{\sigma_\ell'\bar\lambda'} \, [O_{\ell-1}]_{\lambda} \, [o_\ell]^{\sigma_\ell'}{}_{\sigma_\ell} \, A^{\bar\lambda\sigma_\ell}{}_{\lambda} = [O_{\ell-1}]^{\bar\lambda'}{}_{\bar\lambda} \, [\tilde{o}_\ell]_{\bar\lambda'}{}^{\bar\lambda}{}_{\lambda} \qquad (17)$$

Thus, the isometry A maps the local operator into an effective basis associated with $\mathbb{V}_{\ell-1}$, and $\mathbb{V}_\ell$

2. Iterative diagonalization

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

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!

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

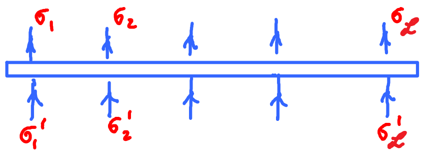
where we defined the operator triplets
$$\hat{S}_a \in \{\hat{S}_+, \hat{S}_-, \hat{S}_z\}, \quad \hat{S}^{\dagger a} \in \{\hat{S}^{\dagger +}, \hat{S}^{\dagger -}, \hat{S}^{\dagger z}\} \qquad (3)$$

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 $\{|\vec{\sigma}_{\mathcal{L}}\rangle\} = \{|\sigma_{\mathcal{L}}\rangle \dots |\sigma_2\rangle|\sigma_1\rangle\}$, 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'

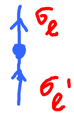


$H^{\vec{\sigma}'}{}_{\vec{\sigma}}$ is a linear map acting on a direct product space: $\mathbb{V}^{\otimes \mathcal{L}} := \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \dots \otimes \mathbb{V}_{\mathcal{L}}$

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:
$$\hat{S}_{a\ell} = |\sigma'_\ell\rangle (S_a)^{\sigma'_\ell}{}_{\sigma_\ell} \langle \sigma_\ell| \qquad (6)$$



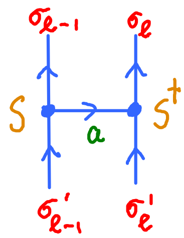
Matrix representation in $\mathbb{V}_\ell$:
$$(S_a)^{\sigma'_\ell}{}_{\sigma_\ell} = \langle \sigma'_\ell | \hat{S}_{a\ell} | \sigma_\ell \rangle = \begin{pmatrix} (S_a)^{\uparrow}{}_{\uparrow} & (S_a)^{\uparrow}{}_{\downarrow} \\ (S_a)^{\downarrow}{}_{\uparrow} & (S_a)^{\downarrow}{}_{\downarrow} \end{pmatrix}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

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

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

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

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



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

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.

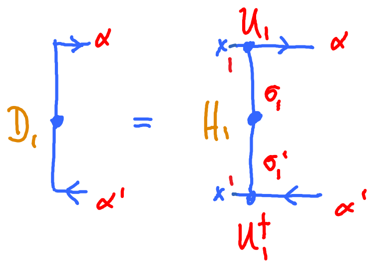
Diagonalize site 1

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

$$\underbrace{H_1}_{\text{chain of length 1}} = S^\dagger_{a1}\cdot h^a_1 = U_1 D_1 U_1^\dagger \qquad \text{site index: } \ell = 1 \tag{10}$$

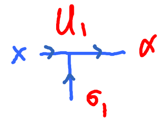
$D_1 = U_1^\dagger H_1 U_1$ is diagonal, with matrix elements

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



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, $\mathcal{H}_{(2)} = \mathrm{span}\{|\sigma_2\rangle|\sigma_1\rangle\}$ (14)

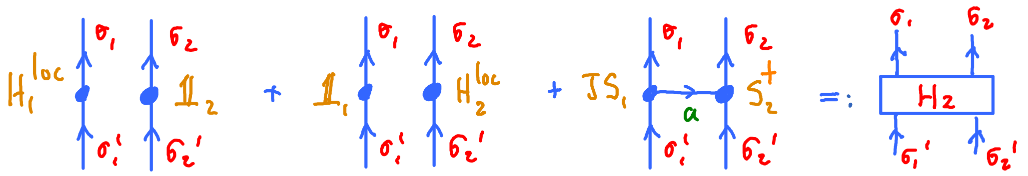
chain of length 2

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

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

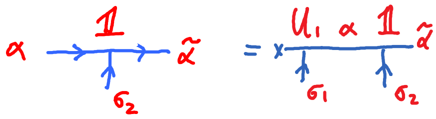
Matrix representation in $\mathcal{V}_1\otimes\mathcal{V}_2$ corresponding to 'local' basis, $\{|\sigma_2\rangle|\sigma_1\rangle\}$:

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



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

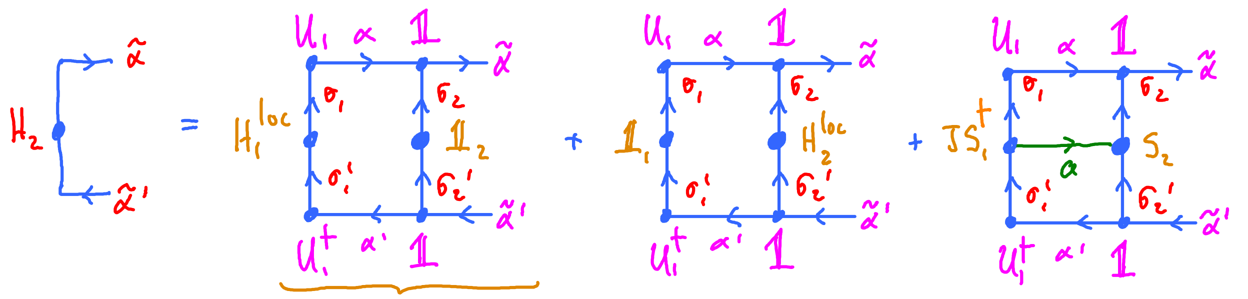
$$|\tilde{\alpha}\rangle \equiv |\alpha\sigma_2\rangle \equiv |\sigma_2\rangle|\alpha\rangle = |\sigma_2\rangle|\sigma_1\rangle U^{\sigma_1}{}_{\alpha} \tag{17}$$



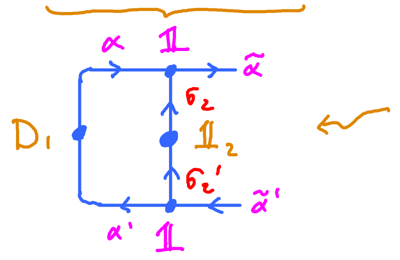
$$\hat{H}_2 = |\tilde{\alpha}'\rangle H_2{}^{\tilde{\alpha}'}{}_{\tilde{\alpha}}\langle\tilde{\alpha}| , \qquad H_2{}^{\tilde{\alpha}'}{}_{\tilde{\alpha}} = \langle\tilde{\alpha}'|\hat{H}_2|\tilde{\alpha}\rangle = \langle\tilde{\alpha}'|\sigma_1'\sigma_2'\rangle H_2{}^{\sigma_1'\sigma_2'}{}_{\sigma_1\sigma_2}\langle\sigma_1\sigma_2|\tilde{\alpha}\rangle$$

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:

To this end, attach U_1, $U_1^\dagger$ to in/out legs of site 1, and $\mathbb{1}$, $\mathbb{1}$ to in/out legs of site 2.



(18)

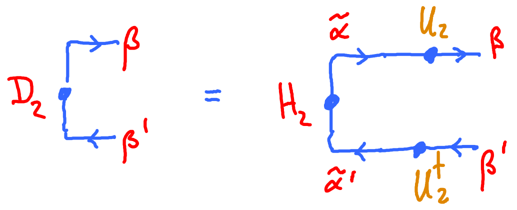


First term is already diagonal. But other terms are not.

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

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

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

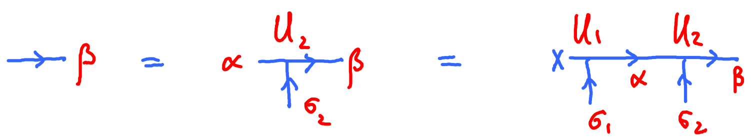


(20)

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 $\hat H_2$:

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

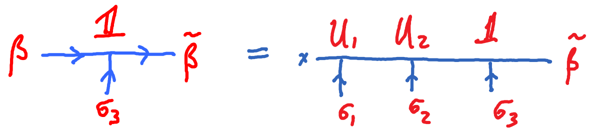


(22)

Add site 3

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

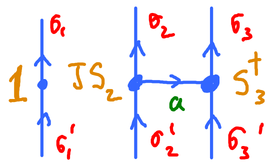
$$|\tilde\beta\rangle \equiv |\beta\sigma_3\rangle \equiv |\sigma_3\rangle|\beta\rangle$$



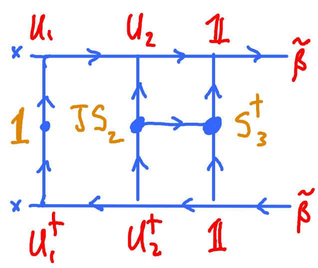
(23)

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

Local basis:



enlarged,
site-12-diagonal
basis:



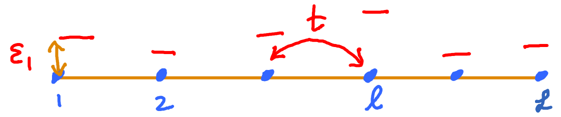
(24)

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:



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

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

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

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

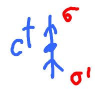
Operator action: $\hat{c}^\dagger |0\rangle = |1\rangle$, $\quad \hat{c}^\dagger |1\rangle = 0$ (3a)

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

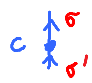
The operators $\hat{c}^\dagger = |\sigma'\rangle c^{\dagger\sigma'}{}_\sigma \langle\sigma|$ and $\hat{c} = |\sigma'\rangle c^{\sigma'}{}_\sigma \langle\sigma|$

have matrix representations in V :

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



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



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

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

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

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

where $Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ 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: $\mathrm{span}\{ |\vec{\sigma}\rangle_{\mathscr{L}} = |n_1, n_2, \ldots, n_{\mathscr{L}}\rangle \}$, $n_i \in \{0,1\}$ (11)

Define canonical ordering for fully filled state:

$$|n_1 = 1, n_2 = 1, \ldots, n_{\mathscr{L}} = 1\rangle = c^\dagger_{\mathscr{L}} \ldots c^\dagger_2 c^\dagger_1 |\mathrm{Vac}\rangle \tag{12}$$

Now consider:

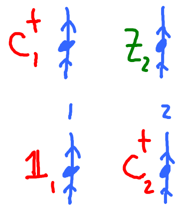
$$\hat{c}^\dagger_1 |n_1 = 0, n_2 = 1\rangle = \hat{c}^\dagger_1 \hat{c}^\dagger_2 |\mathrm{Vac}\rangle = -\hat{c}^\dagger_2 \hat{c}^\dagger_1 |\mathrm{Vac}\rangle = -|n_1 = 1, n_2 = 1\rangle \tag{13}$$

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

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

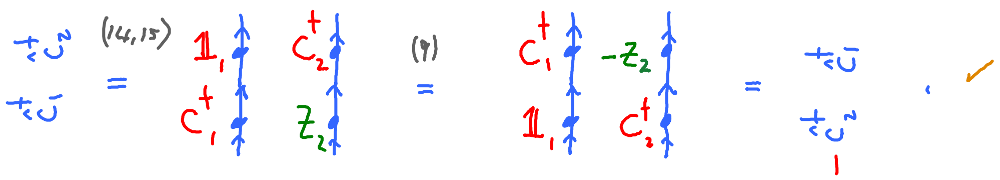
$$\hat{c}^\dagger_2 \doteq \mathbb{1}_1 \otimes c^\dagger_2 =: c^\dagger_2 \tag{15}$$

subscripts denote site numbers (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: $A^{\sigma_1 \sigma_2 \ldots}$

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



(17)

Algebraically:

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:

$$\hat{n}_1 = \hat{c}_1^\dagger \hat{c}_1 \doteq \begin{array}{cc} C_1 & Z_2 \\ C_1^\dagger & Z_2 \end{array} = \begin{array}{cc} C_1 & \mathbb{1}_2 \\ C_1^\dagger & \mathbb{1}_2 \end{array} \doteq C_1^\dagger C_1 \otimes \mathbb{1}_2 \tag{20}$$

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 $V^{\otimes \mathscr{L}} = V_1 \otimes V_2 \otimes \cdots \otimes V_{\mathscr{L}}$:

$$\hat{c}_\ell^\dagger \doteq \mathbb{1}_1 \otimes \cdots \mathbb{1}_{\ell-1} \otimes C_\ell^\dagger \otimes Z_{\ell+1} \otimes \cdots Z_{\mathscr{L}} =: C_\ell^\dagger Z_\ell^> \tag{21}$$

$$\hat{c}_\ell \doteq \mathbb{1}_1 \otimes \cdots \mathbb{1}_{\ell-1} \otimes C_\ell \otimes Z_{\ell+1} \otimes \cdots Z_{\mathscr{L}} =: C_\ell Z_\ell^> \tag{22}$$

'Jordan-Wigner transformation'

with $$Z_\ell^> := \prod_{\otimes \ell' > \ell} Z_{\ell'} \tag{23}$$

'Z-string'

<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>

$$\begin{array}{c|ccccccccccccc} & 1 & & \ell-1 & \ell & \ell+1 & & \ell'-1 & \ell' & \ell'+1 & & \mathscr{L} \\ \hat{c}_\ell & \mathbb{1} & \cdots & \mathbb{1} & C & Z & \cdots & Z & Z & Z & \cdots & Z \\ \hat{c}_{\ell'}^\dagger & \mathbb{1} & \cdots & \mathbb{1} & \mathbb{1} & \mathbb{1} & \cdots & \mathbb{1} & C^\dagger & Z & \cdots & Z \end{array} \tag{24}$$

extra sign!

$$= \quad \begin{array}{c|ccccccccccc} \hat{c}_{\ell'}^\dagger & \mathbb{1} & \cdots & \mathbb{1} & \mathbb{1} & \mathbb{1} & \cdots & \mathbb{1} & C^\dagger & Z & \cdots & Z \\ -\hat{c}_\ell & \mathbb{1} & \cdots & \mathbb{1} & C & Z & \cdots & Z & -Z & Z & \cdots & Z \end{array} \tag{25}$$

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

$$\begin{array}{c|cccccccccc} & 1 & 2 & & \ell-2 & \ell-1 & \ell & \ell+1 & & \mathscr{L} \\ \hat{c}_{\ell-1} & \mathbb{1} & \mathbb{1} & \cdots & \mathbb{1} & C & Z & Z & \cdots & Z \\ \hat{c}_\ell^\dagger & \mathbb{1} & \mathbb{1} & \cdots & \mathbb{1} & \mathbb{1} & C^\dagger & Z & \cdots & Z \end{array} \tag{26}$$

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

since at site ℓ we have $\quad Z_\ell Z_\ell = \mathbb{1}_\ell, \qquad c^\dagger_\ell Z_\ell \overset{(10a)}{=} c^\dagger_\ell \quad ,$ (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, $\quad \hat{c}^\dagger_{\ell-1} \hat{c}_\ell \doteq c^\dagger_{\ell-1} c_\ell$ (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 spinful fermions. Site index: $\ell = 1, \dots, \mathcal{L}$, spin index: $s \in \{\uparrow, \downarrow\} := \{+, -\}$

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

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 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)

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

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 $\tilde V := V_\uparrow \otimes V_\downarrow$. (7)

(Matrices acting in this space will carry tildes.)

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

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

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

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

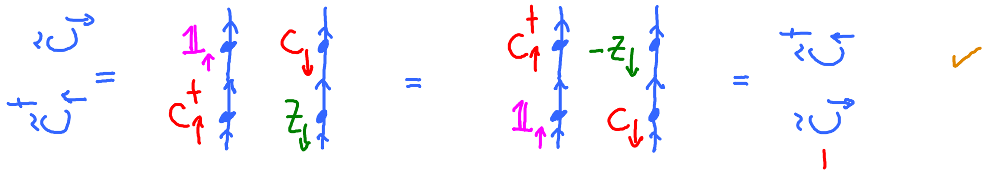
$$\hat c_\uparrow \doteq c_\uparrow \otimes Z_\downarrow = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = \left(\begin{array}{cc|cc} & & 1 & \\ & & & -1 \\ \hline & & & \\ & & & \end{array}\right) =: \tilde c_\uparrow \tag{11}$$

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

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

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

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:

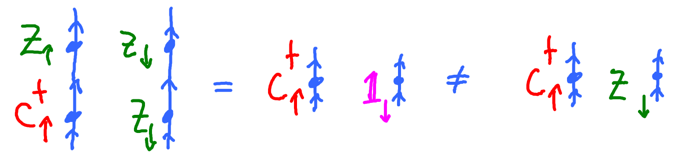
$$\left(\begin{array}{c|c} & \\ \hline \begin{smallmatrix} 1 & \\ & -1 \end{smallmatrix} & \end{array}\right) \left(\begin{array}{c|c} \begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix} & \\ \hline & \begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix} \end{array}\right) = \left(\begin{array}{c|c}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

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

$$\tilde{C}^\dagger_s \tilde{Z} \neq \tilde{C}^\dagger_s \quad \text{and} \quad \tilde{Z}\,\tilde{C}_s \neq \tilde{C}_s \tag{15}$$

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

$$\tilde{C}^\dagger_\uparrow \tilde{Z} =$$



$$= \tilde{C}^\dagger_\uparrow \tag{16}$$

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 $\tilde{V}^{\otimes N} = \tilde{V}_1 \otimes \tilde{V}_2 \otimes \cdots \otimes \tilde{V}_\mathcal{L}$:

$$\hat{c}^\dagger_\ell \doteq \tilde{\mathbb{1}}_1 \otimes \cdots \tilde{\mathbb{1}}_{\ell-1} \otimes \tilde{C}^\dagger_\ell \otimes \tilde{Z}_{\ell+1} \otimes \cdots \tilde{Z}_\mathcal{L} \equiv \tilde{C}^\dagger_\ell \,\tilde{Z}^>_\ell \tag{17}$$

$$\hat{c}_\ell \doteq \tilde{\mathbb{1}}_1 \otimes \cdots \tilde{\mathbb{1}}_{\ell-1} \otimes \tilde{C}_\ell \otimes \tilde{Z}_{\ell+1} \otimes \cdots \tilde{Z}_\mathcal{L} \equiv \tilde{C}_\ell \,\tilde{Z}^>_\ell \tag{18}$$

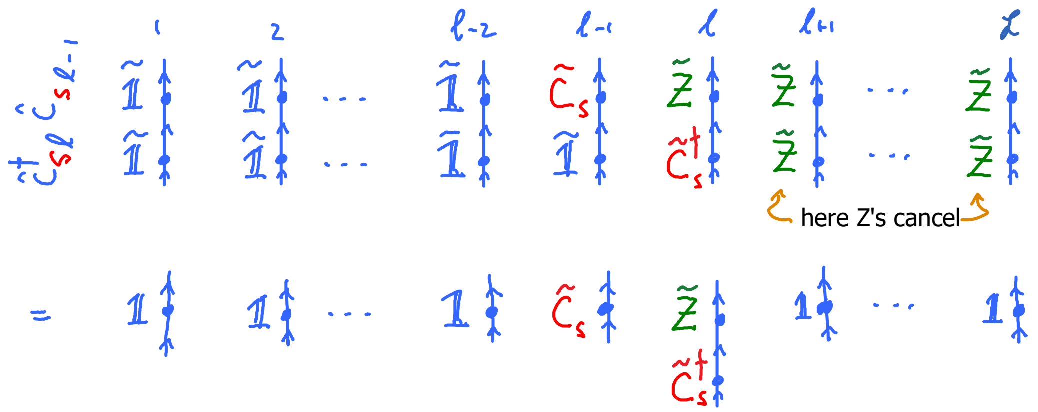
'Jordan-Wigner transformation'

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

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

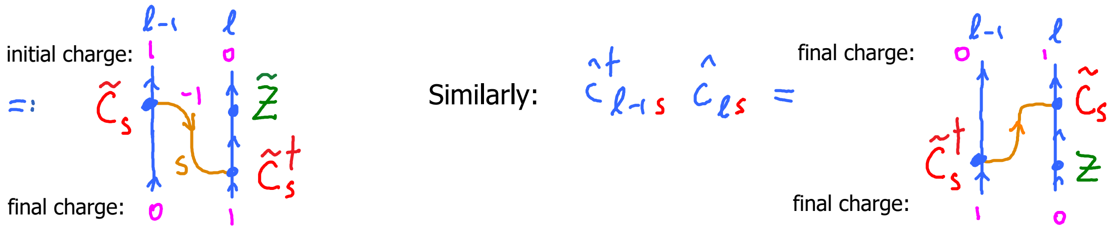
Example: hopping term $\hat{c}^\dagger_{\ell s} \hat{c}_{\ell-1 s}$: (sum over s impied)

1 2 $\ell-2$ $\ell-1$ ℓ $\ell+1$ $\mathcal{L}$



(20)

(21)



(22)

Bond indicates sum $\sum_s$ (23)

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

Creation: outgoing $+1$ or incoming -1