MPS III: Diagonalization, fermionic signs

1. Iterative diagonalization

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

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

$$\hat{S}_z \equiv \hat{S}^{\dagger z} = \hat{S}_z\,, \qquad \hat{S}_\pm \equiv \tfrac{1}{\sqrt{2}}(\hat{S}_x \pm i\hat{S}_y)\,, \qquad \hat{S}^{\dagger\pm} \equiv \tfrac{1}{\sqrt{2}}(\hat{S}_x \mp i\hat{S}_y) \quad (= \hat{S}_\pm^\dagger) \tag{2}$$

and the operator triplet $\hat{S}_a \in \{\hat{S}_+, \hat{S}_-, \hat{S}_z\}$, $\quad \hat{S}^{\dagger a} \in \{\hat{S}^{\dagger +}, \hat{S}^{\dagger -}, \hat{S}^{\dagger z}\}$ (3)

$a \in \{+,-,z\}$ $\qquad$ $\hat{S}^{\dagger +} = \hat{S}_-$, $\hat{S}^{\dagger -} = \hat{S}_+$, $\hat{S}^{\dagger z} = \hat{S}_z$

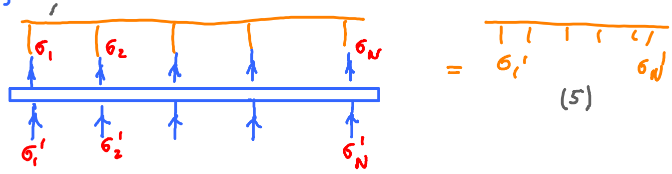
Then
$$\hat{\vec{S}}_\ell \cdot \hat{\vec{S}}_{\ell-1} = \hat{S}^x_\ell \hat{S}^x_{\ell-1} + \hat{S}^y_\ell \hat{S}^y_{\ell-1} + \hat{S}^z_\ell \hat{S}^z_{\ell-1}$$
$$= \underbrace{\hat{S}^{\dagger +}_\ell \hat{S}_{+\ell-1}}_{\hat{S}_- \hat{S}_+} + \underbrace{\hat{S}^{\dagger -}_\ell \hat{S}_{-\ell-1}}_{\hat{S}_+ \hat{S}_-} + \underbrace{\hat{S}^{\dagger z}_\ell \hat{S}_{z\,\ell-1}}_{S_z \cdot S_z} = \hat{S}^{\dagger a}_\ell \hat{S}_{\ell-1\,a} \tag{4}$$

covariant index combination, sum on a implied!

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

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

'no hat' means 'matrix representation'

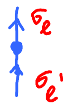


$H^{\vec{\sigma}'}{}_{\vec{\sigma}}$ is a linear map acting on a direct product space: $V^{\otimes N} \equiv V_1 \otimes V_2 \otimes \ldots \otimes V_N$

where V_ℓ is the 2-dimensional representation space of site ℓ. $\quad |\uparrow\rangle \doteq \begin{pmatrix}1\\0\end{pmatrix}$, $\quad |\downarrow\rangle \doteq \begin{pmatrix}0\\1\end{pmatrix}$

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

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



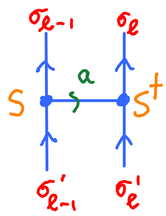
Matrix representation in V_ℓ:
$$(S_a)^{\sigma'_\ell}{}_{\sigma_\ell} = \langle\sigma'_\ell|\hat{S}_{a\ell}|\sigma_\ell\rangle = \begin{pmatrix} (S_a)^\uparrow{}_\uparrow & (S_a)^\uparrow{}_\downarrow \\ (S_a)^\downarrow{}_\uparrow & (S_a)^\downarrow{}_\downarrow \end{pmatrix} \tag{7}$$

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

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

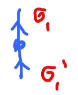
$$\hat{S}_{\ell-1\,a} \otimes \hat{S}^{\dagger a}_\ell = |\sigma'_\ell\rangle|\sigma'_{\ell-1}\rangle \underbrace{(S_a)^{\sigma'_{\ell-1}}{}_{\sigma_{\ell-1}}}_{\equiv\, S^{\sigma'_{\ell-1}}{}_{a\sigma_{\ell-1}}} \underbrace{(S^{\dagger a})^{\sigma'_\ell}{}_{\sigma_\ell}}_{\equiv\, S^{\dagger\sigma'_\ell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

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



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.

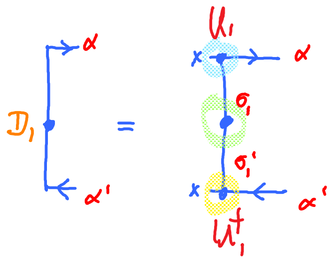
Diagonalize site 1

Matrix acting on V_1 : $\quad H_1 = S^\dagger_{a_1} \cdot h_1^a = U_1 \, D_1 \, U_1^\dagger$  (10)

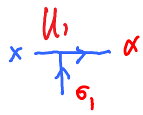
chain of length 1 $\qquad$ site index: $\ell = 1$

$D_1 = U_1^\dagger H_1 U_1$ 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: $\quad |\alpha\rangle = |\sigma_1\rangle (U_1)^{\sigma_1}{}_{\alpha}$  (13)

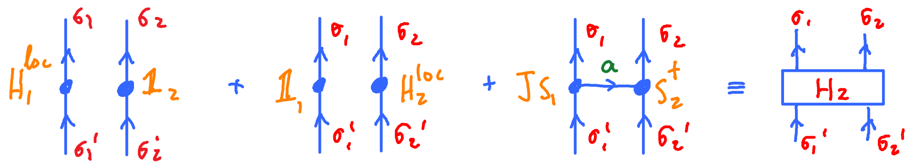
Add site 2

Diagonalize $\hat{H}_2$ in enlarged Hilbert space, $\quad \mathcal{H}_{(2)} = \mathrm{span}\{|\sigma_2\rangle|\sigma_1\rangle\}$ (14)

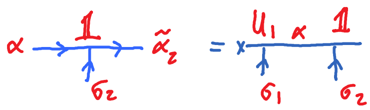
chain of length 2

Matrix acting on $V_1 \otimes V_2$: $\quad H_2 = \underbrace{\vec{S}_1 \cdot \vec{h}_1}_{H_1^{loc}} \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \underbrace{\vec{S}_2 \cdot \vec{h}_2}_{H^{loc}} + \underbrace{J \, S_{a_1} \otimes S_2^{\dagger a}}_{H^{loc}}$ (15)

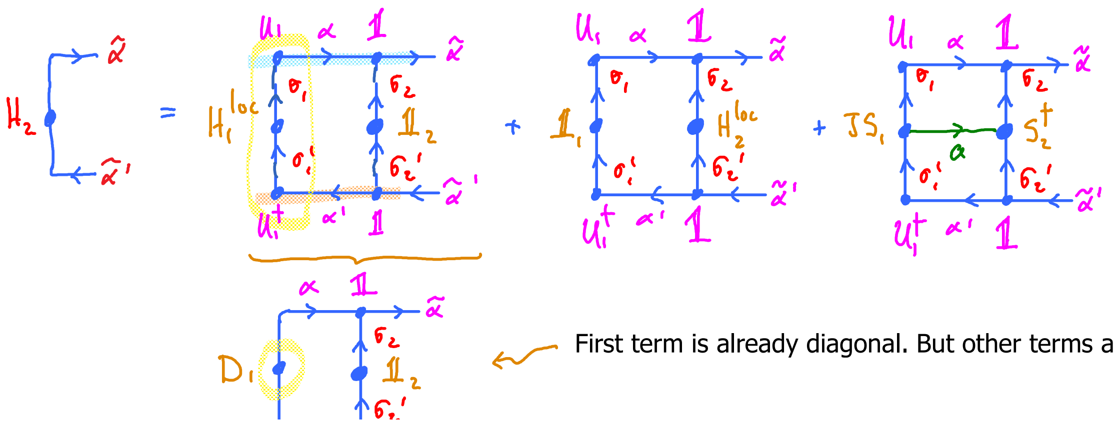
Matrix representation in $V_1 \otimes V_2$ corresponding to 'local' basis, $\{|\sigma_2\rangle|\sigma_1\rangle\}$:

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

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

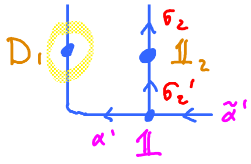
$|\tilde{\alpha}\rangle \equiv |\alpha\,\sigma_2\rangle \equiv |\sigma_2\rangle|\alpha\rangle = |\sigma_2\rangle|\sigma_1\rangle U_1{}^{\sigma_1}{}_{\alpha}$  (17)

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.

$\hat{H} = |\tilde{\sigma}\rangle H^{\sigma'}{}_{\sigma} \langle\tilde{\sigma}|\tilde{\alpha}\rangle\langle\tilde{\alpha}|$
$|\tilde{\alpha}'\rangle\langle\tilde{\alpha}'|$
$= |\tilde{\alpha}'\rangle H^{\alpha'}{}_{\alpha} \langle\alpha|$

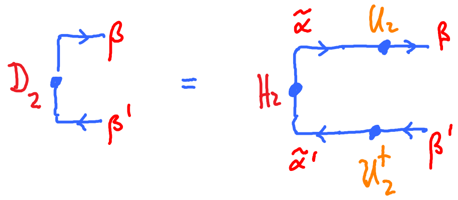


First term is already diagonal. But other terms are not.

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

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

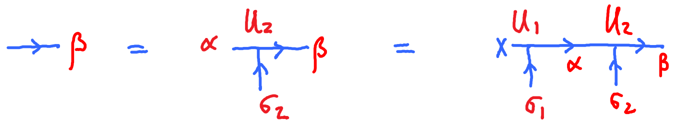


(20)

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 $\hat{H}_2$:

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

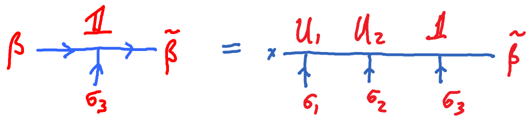


(22)

Add site 3

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

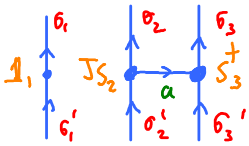
$|\tilde\beta\rangle \equiv |\beta\sigma_3\rangle \equiv |\sigma_3\rangle|\beta\rangle$



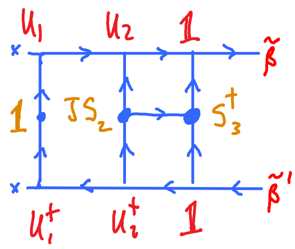
(23)

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)

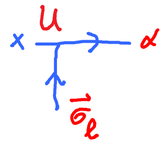
At each iteration, Hilbert space grows by a factor of 2. Eventually, trunctations will be needed...!

2. Graphical notation for 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 $\{|\vec\sigma_\ell\rangle\}$:

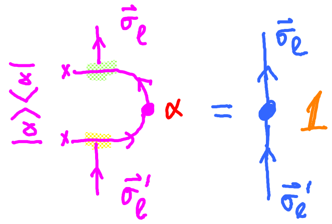
$$|\alpha\rangle = |\vec\sigma_\ell\rangle\, U^{\vec\sigma_\ell}{}_{\alpha}$$



(1)

Unitarity guarantees resolution of identity on this subspace:

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

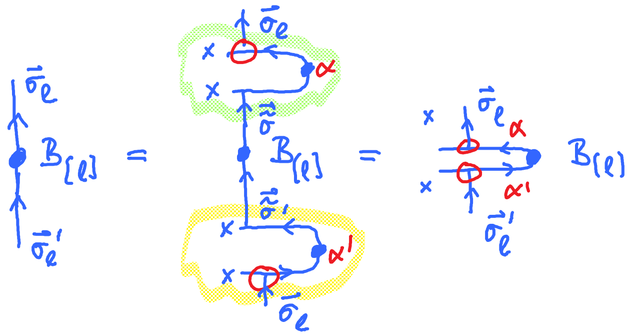


(2)

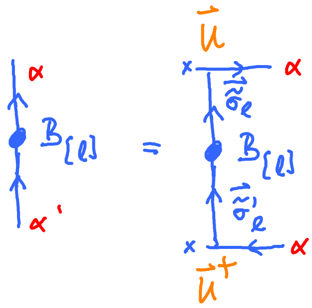
Transformation of an operator defined on this subspace:

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

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



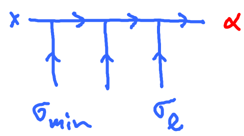
with



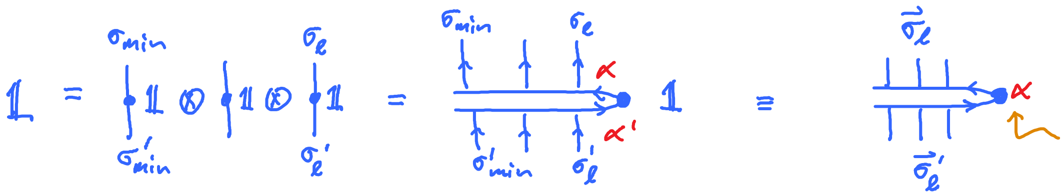
(5)

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

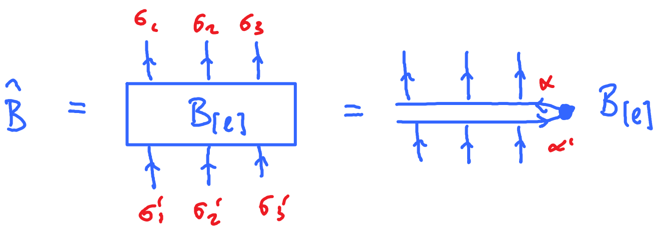
$$|\alpha\rangle = |\sigma_\ell\rangle \dots |\sigma_{min}\rangle \left(A^{\sigma_{min}} \dots A^{\sigma_\ell}\right)^{1}{}_{\alpha}$$



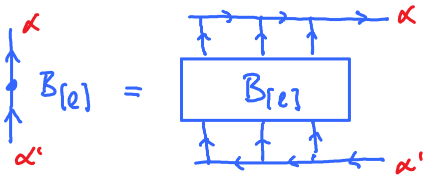
(6)



shorthand for unit matrix (7)



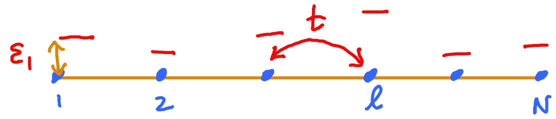
with



(8)

3. Spinless fermions

Consider tight-binding chain of spinless fermions:



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

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

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

$$c_\ell c_{\ell'} = - c_{\ell'} c_\ell$$

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

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

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

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

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 V :

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

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

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

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

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

Useful relations: $$\boxed{\hat{c}\,\hat{z} = -\hat{z}\,\hat{c} \, , \qquad \hat{c}^\dagger \hat{z} = -\hat{z}\,\hat{c}^\dagger} \qquad (9)$$

'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: $$\text{span}\{|\vec{\sigma}\rangle_N = |n_1, n_2, \dots, n_N\rangle\} \qquad (11)$$

Define canonical ordering for fully filled state: $|\sigma_N\rangle \dots |\sigma_2\rangle|\sigma_1\rangle$

$$|n_1=1, n_2=1, \dots, n_N=1\rangle = c^\dagger_N \dots c^\dagger_2 c^\dagger_1 |Vac\rangle \qquad (12)$$

Now consider:

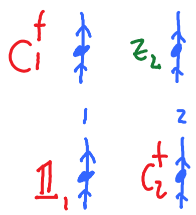
$$\hat{c}^\dagger_1 |n_1=0, n_2=1\rangle = c^\dagger_1 \hat{c}^\dagger_2 |Vac\rangle = -\hat{c}^\dagger_2 c^\dagger_1 |Vac\rangle = -|n_1=1, n_2=1\rangle \qquad (13)$$

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

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

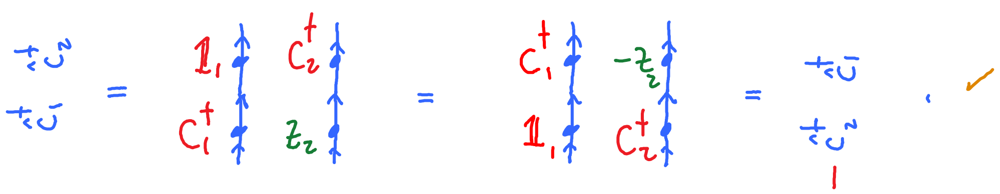
$$\hat{c}^\dagger_2 \doteq \mathbb{1}_1 \otimes c^\dagger_2 \equiv c^\dagger_2 \qquad (15)$$

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: $A^{\sigma_1 \sigma_2 \dots}$

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



(17)

Algebraically:

(14) (9)

Algebraically:

$$\hat c_1^\dagger \hat c_2 \doteq (c_1^\dagger \otimes Z_2)(\mathbb{1}_1 \otimes c_2) \overset{(14)}{=} c_1^\dagger \mathbb{1} \otimes (Z_2 c_2) \overset{(9)}{=} -\mathbb{1}\, c_1^\dagger \otimes c_2 Z_2 \tag{18}$$

$$= -(\mathbb{1}_1 \otimes c_2)(c_1^\dagger \otimes Z_2) \doteq -\hat c_2 \hat c_1^\dagger \quad ✓ \tag{19}$$

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 $V^{\otimes N} = V_1 \otimes V_2 \otimes \dots \otimes V_N$:

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

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

'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>

$$\begin{array}{c|cccccccccccc} & 1 & & \ell-1 & \ell & \ell+1 & & \ell'-1 & \ell' & \ell'+1 & & N \\ \hat c_\ell & \mathbb{1} & \cdots & \mathbb{1} & c & Z & \cdots & Z & Z & Z & \cdots & Z \\ \hat c_{\ell'}^\dagger & \mathbb{1} & \cdots & \mathbb{1} & \mathbb{1} & \mathbb{1} & \cdots & \mathbb{1} & c^\dagger & Z & \cdots & Z \end{array} \tag{24}$$

extra sign!

$$= \begin{array}{c|cccccccccccc} \hat c_{\ell'}^\dagger & \mathbb{1} & \cdots & \mathbb{1} & \mathbb{1} & & \cdots & \mathbb{1} & c^\dagger & Z & \cdots & Z \\ \hat c_\ell & \mathbb{1} & \cdots & \mathbb{1} & c & & \cdots & Z & -Z & Z & \cdots & Z \end{array} \tag{25}$$

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

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

$$= \begin{array}{cccccccc} \mathbb{1} & \mathbb{1} & \cdots & \mathbb{1} & c & c^\dagger & \mathbb{1} & \cdots & \mathbb{1} \end{array} \tag{27}$$

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

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

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 spinful fermions. Site index: $\ell = 1, \dots, N$, spin index: $s \in \{\uparrow, \downarrow\} \equiv \{+, -\}$

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

Define canonical order for fully filled state: $\hat{c}^\dagger_{N\downarrow}\hat{c}^\dagger_{N\uparrow} \dots \hat{c}^\dagger_{2\downarrow}\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{1\uparrow}|Vac\rangle$ (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: $|0\rangle \equiv |Vac\rangle$, $\quad |\downarrow\rangle \equiv \hat{c}^\dagger_\downarrow|0\rangle$, (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 minus signs, introduce $\hat{Z}_s = (-1)^{\hat{n}_s} = \frac{1}{2}(1 - \hat{n}_s) \qquad s \in \{\uparrow, \downarrow\}$ (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.)

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

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

$$\begin{pmatrix} 1\cdot\begin{pmatrix} 1 & \\ & -1 \end{pmatrix} & 0\begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \\ 0\begin{pmatrix} 1 & \\ & -1 \end{pmatrix} & 1\begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \end{pmatrix}$$

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

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

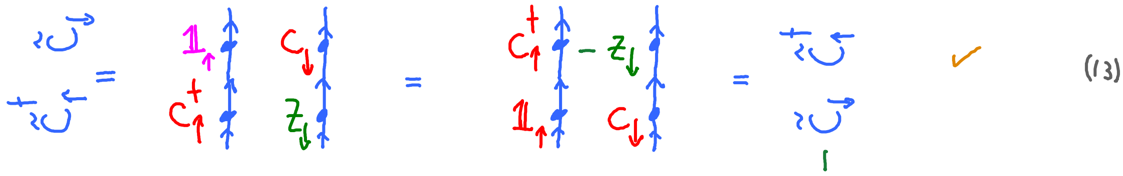
$$\hat{c}_\uparrow \doteq c_\uparrow \otimes Z_\downarrow = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = \left(\begin{array}{cc|cc} & & 1 & \\ & & & -1 \\ \hline & & & \\ & & & \end{array}\right) \equiv \tilde{c}_\uparrow \tag{11}$$

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

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

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

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)



Algebraic check:

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

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 $V_\uparrow \otimes V_\downarrow$:

$$\tilde{c}^\dagger_\uparrow \tilde{Z} = \begin{matrix} z_\uparrow & z_\downarrow \\ c^\dagger_\uparrow & z_\downarrow \end{matrix} = c^\dagger_\uparrow \; \mathbb{1}_\downarrow \neq c^\dagger_\uparrow \; z_\downarrow = \tilde{c}^\dagger_\uparrow \tag{16}$$

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

Each $\hat{c}_{\ell s}$ 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 $\tilde{V}^{\otimes N} = \tilde{V}_1 \otimes \tilde{V}_2 \otimes \cdots \otimes \tilde{V}_N$:

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

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

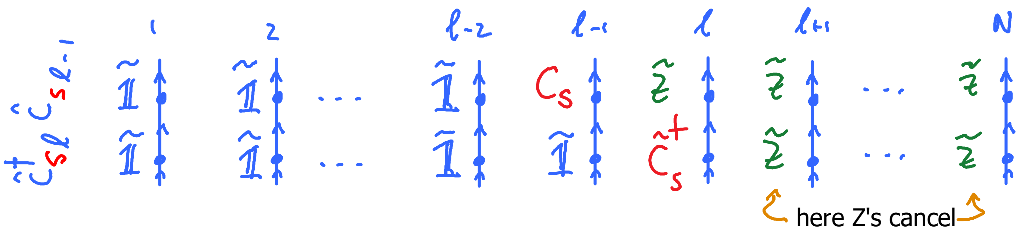
'Jordan-Wigner transformation'

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'

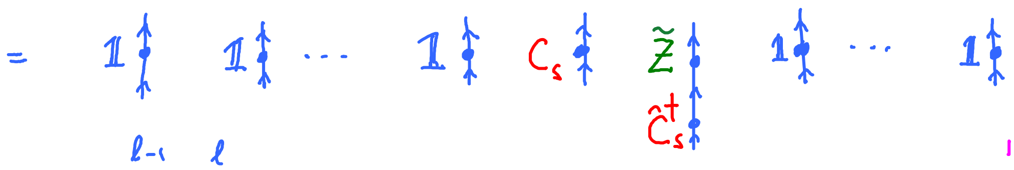
In <u>bilinear combinations</u>, most (but not all!) of the Z 's cancel.

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

1 2 $\ell-2$ $\ell-1$ ℓ $\ell+1$ N



(20)



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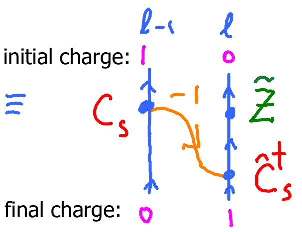
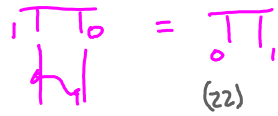


Bond $\longrightarrow$ indicates sum $\sum_s$

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

Creation: outgoing $+1$ or incoming -1



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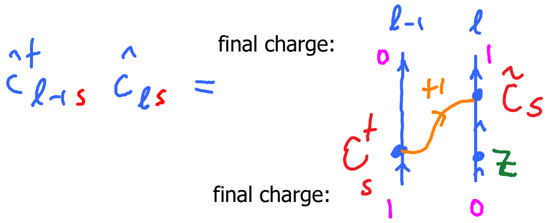
Similarly:



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