Fermionic PEPS

Fermion signs in 2D fermionic tensor networks can be kept track of using two 'fermionization rules'.
[Corboz2009] with Vidal and [Corboz2010b] with Evenbly, Verstrate, Vidal first introduced them, for MERA.
[Corbox2010b] with Orus, Bauer, Vidal adapted them to PEPS context.
This is the approach described in [Bruognolo~~2017~~ 2020] and presented in this lecture.

Key ingredients: (i) use only positive-parity tensors
(ii) replace line crossings by fermion SWAP gates

Equivalent formulations had also been developed by:
[Barthel2009] with Pineda, Eisert, [Pineda2010] with Barthel, Eisert
[Kraus2010] with Schuch, Verstraete, Cirac
[Shi2009] with Li, Zhao, Zhou
[Bultink2017a] with Williamson, Haegeman, Verstraete, building on [Bultinck2017] (same authors); these papers use the mathematical formalism of 'super vector spaces'.

1. Parity conservation

Fermionic Hamiltonians preserve parity of electron number: $\hat{P} = (-1)^{\hat{N}}$ (1)

$$\hat{H} = \hat{c}^\dagger \hat{c} + \hat{c}^\dagger \hat{c}\, \hat{c}^\dagger \hat{c} + \hat{c}^\dagger \hat{c}^\dagger + \hat{c}\hat{c}\,, \qquad [\hat{H}, \hat{P}] = 0 \tag{2}$$

$\Rightarrow$ all energy eigenstates are parity eigenstate, too, hence may be labeled by parity eigenvalue:

$$\hat{H}|\alpha,p\rangle = E_{\alpha,p}|\alpha,p\rangle\,, \quad \hat{P}|\alpha,p\rangle = p|\alpha,p\rangle\,, \quad p = \pm \qquad (\text{'}\mathbb{Z}_2\text{-symmetry'}) \tag{3}$$

So, we may agree to work only with states of well-defined parity.

Example: state space of local fermions, $|n_\uparrow, n_\downarrow; p\rangle$ (4)

$$|0\rangle \equiv |0,0;+\rangle\;; \qquad |\uparrow\downarrow\rangle \equiv c^\dagger_\downarrow c^\dagger_\uparrow|0\rangle \equiv |1,1;+\rangle$$
$$|\uparrow\rangle \equiv c^\dagger_\uparrow|0\rangle \equiv |1,0;-\rangle\,, \qquad |\downarrow\rangle \equiv c^\dagger_\downarrow|0\rangle \equiv |0,1;-\rangle\,, \tag{5}$$

Every line in tensor network diagram also carries a parity index.

[When keeping track of abelian symmetries, parity label can be deduced from particle number: $p = (-1)^Q$]

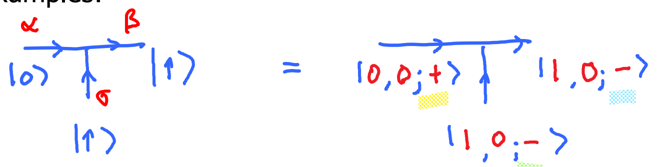
Enforcing $\mathbb{Z}_2$ symmetry [Corboz2010b, Sec.II.F]

To enforce $\mathbb{Z}_2$ symmetry on tensor network: choose all terms to be 'parity preserving'.

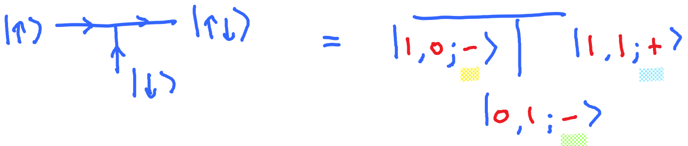
Rule (i): Total parity is positive for all tensors:

n-leg tensor: $A_{\alpha_1 \alpha_2 \ldots \alpha_n} = 0$ if $P_{\alpha_1 \alpha_2 \ldots \alpha_n} \equiv p(\alpha_1) p(\alpha_2) \ldots p(\alpha_n) \neq +1$ (6)

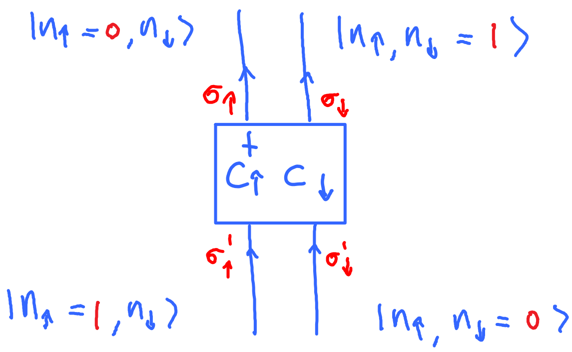
Examples:



$$P^{\alpha\sigma}{}_{\beta} = P_\alpha P_\sigma P_\beta = (+)(-)(-) = +1$$



$$P^{\alpha\sigma}{}_{\beta} = (-)(-)(+) = +1$$



$$P^{\sigma'_\uparrow \sigma'_\downarrow}{}_{\sigma_\uparrow \sigma_\downarrow} = \Big(\underbrace{P_{\sigma'_\uparrow} P_{\sigma_\uparrow}}_{(-1)}\Big)\Big(\underbrace{P_{\sigma'_\downarrow} P_{\sigma_\downarrow}}_{(-1)}\Big) =$$

$c^\dagger_\uparrow$ and $c_\downarrow$ both change parity by (-1)

so overall change is $(-)^2 = +$

2. Fermionic signs

$$c_i c_j = - c_j c_i \,, \quad c_i^\dagger c_j^\dagger = - c_j^\dagger c_i^\dagger \,, \quad c_i c_j^\dagger = \delta_{ij} - c_j^\dagger c_i$$

To keep track of these signs, we choose an ordering convention, say $1, 2, \dots, N$, and define:

$$|1_1, 1_2, \dots, 1_N\rangle = + c_N^\dagger \cdots c_2^\dagger c_1^\dagger \underbrace{|0_1, 0_2, \dots, 0_N\rangle}_{|0\rangle}$$

We have to keep this order in mind when evaluating matrix elements. Example: consider $N = 3$:

$$|\psi\rangle = |0,1,1\rangle = c_3^\dagger c_2^\dagger \mathbb{1}_1 |0\rangle, \qquad |\psi'\rangle = |1,1,0\rangle = \mathbb{1}_3 c_2^\dagger c_1^\dagger |0\rangle$$

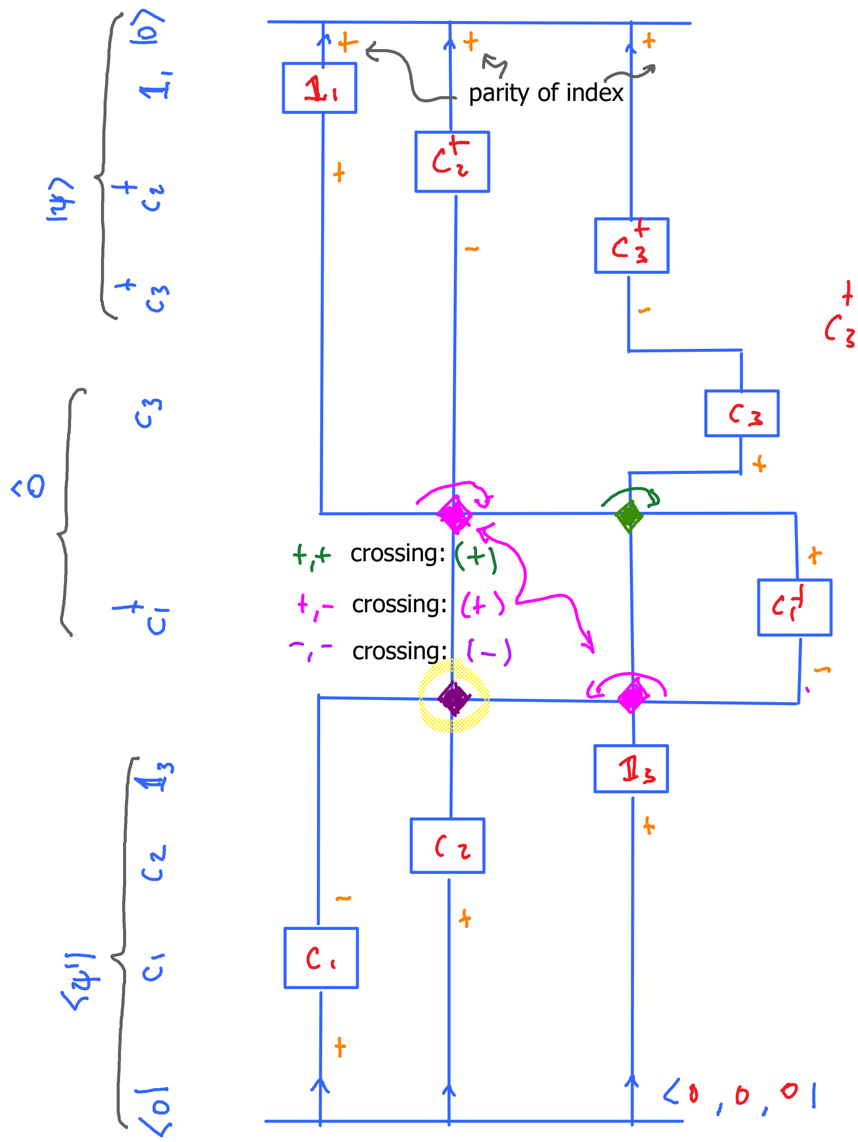
$$\langle\psi'|\underbrace{c_1^\dagger c_3}_{\hat{O}}|\psi\rangle = \langle 0| c_1 c_2 c_1^\dagger \underbrace{c_3 c_3^\dagger}_{=\mathbb{1}_3} c_2 |0\rangle = - \langle 0| \underbrace{c_1 \underbrace{c_2 c_2^\dagger}_{\mathbb{1}_2} c_1^\dagger}_{\mathbb{1}_1} |0\rangle = -1$$

Let us repeat this computation in MPS language: [Corboz2009, App. A]

Order of vertical lines, from left to right, indicates order of operators acting on $|0\rangle$, from right to left.

Horizontal lines show how to move operators in $\hat{O}$ (here $c_1^\dagger c_3$) into appropriate 'slots' in $|\psi\rangle$ or $|\psi'\rangle$.

Line crossings indicate operator swaps. An overall minus sign arises whenever two odd-parity lines cross.



$$|0\rangle = |0,0,0\rangle$$

$$\mathbb{1}_1 |0\rangle = |0,0,0\rangle$$

$$c_2^\dagger \mathbb{1}_1 |0\rangle = |0,1,0\rangle$$

$$c_3^\dagger c_2^\dagger \mathbb{1}_1 |0\rangle = |0,1,1\rangle$$

$$\underbrace{c_3 c_3^\dagger}_{\mathbb{1}_3} c_2^\dagger \mathbb{1}_1 |0\rangle = |0,1,0\rangle$$

$$\mathbb{1}_1 \mathbb{1}_3 c_2^\dagger |0\rangle$$

$$c_1^\dagger \mathbb{1}_3 c_2^\dagger |0\rangle$$

$$- \mathbb{1}_3 c_2^\dagger c_1^\dagger |0\rangle$$

$$- \mathbb{1}_3 \mathbb{1}_3 c_2^\dagger c_1^\dagger |0\rangle$$

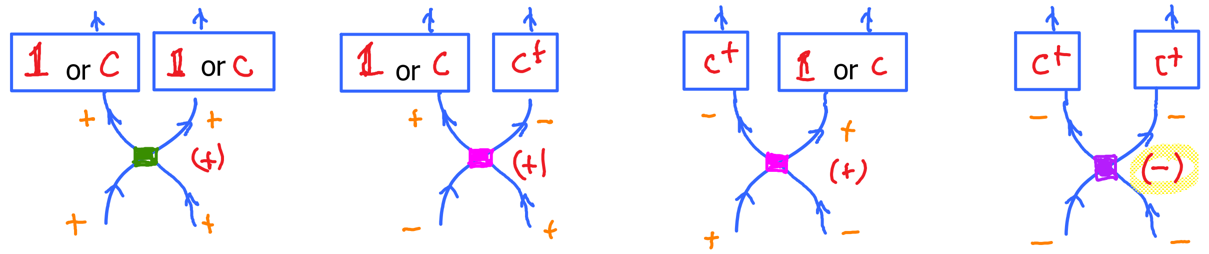
$$- \underbrace{c_2 c_2^\dagger}_{\mathbb{1}_2} c_1^\dagger |0\rangle = -|1,0,0\rangle$$

$$- c_1 c_1^\dagger |0\rangle = -|0,0,0\rangle$$

SWAP gates

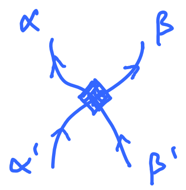
Line crossings keep track of operator orderings.

$(-)$ needed only for exchanging two lines which both host a fermion, i.e. which both have parity $(-)$.



To encode this compactly, introduce SWAP gate whose value depends on parity of incoming lines.

Rule (ii):



$$S^{\beta'\alpha'}{}_{\alpha\beta} = \delta^{\beta'}{}_{\alpha}\,\delta^{\alpha'}{}_{\beta}\,S(\alpha,\beta)$$

$$S(\alpha,\beta) = \begin{cases} -1 & \text{if} \quad p(\alpha) = p(\beta) = -1 \\ +1 & \text{otherwise} \end{cases}$$

Operators

[Corboz2010b, Sec. III.F]

Some matrix elements of operators involving fermions need minus signs.

Example: spinless fermions, consider two sites i, j, with local basis

$$|\sigma_i \sigma_j\rangle = \left(c_j^\dagger\right)^{\sigma_j}\left(c_i^\dagger\right)^{\sigma_i}|0_i,0_j\rangle \quad , \quad \sigma_i \in \{0,1\}$$

Two-site operator: $\hat{O} = \sum |\sigma_i',\sigma_j'\rangle\, O^{\sigma_i'\sigma_j'}{}_{\sigma_i\sigma_j}\,\langle\sigma_i\,\sigma_j|$,

with matrix elements $(i<j)$

$$O^{\sigma_i'\sigma_j'}{}_{\sigma_i\sigma_j} = \langle\sigma_i'\sigma_j'|\hat{O}|\sigma_i,\sigma_j\rangle = \langle 0_i 0_j|\left(c_i\right)^{\sigma_i'}\left(c_j\right)^{\sigma_j'}\hat{O}\left(c_j^\dagger\right)^{\sigma_j}\left(c_i^\dagger\right)^{\sigma_i}|0_i,0_j\rangle$$

Examples:

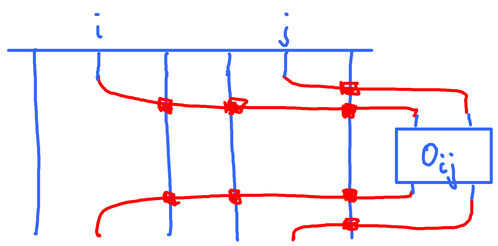
only non-zero element:

Hopping: $\hat{O} = c_i^\dagger c_j$, $\quad O^{1_i 0_j}{}_{0_i 1_j} = \langle 0_i 0_j|\underbrace{c_i\, c_i^\dagger}_{\mathbb{1}_i}\,\underbrace{c_j\, c_j^\dagger}_{\mathbb{1}_j}|0_i 0_j\rangle = +1$

$\hat{O} = c_j^\dagger c_i$, $\quad O^{0_i 1_j}{}_{1_i 0_j} = \langle 0_i 0_j|\, c_j\, c_j^\dagger\, c_i\, c_i^\dagger|0_i 0_j\rangle = +1$

Pairing: $\hat{O} = c_j c_i$, $\quad O = \langle 0_i 0_j|\, c_j c_i\, c_j^\dagger c_i^\dagger|0_i 0_j\rangle = -1$

When applying such an operator
to a generic state, line crossings appear.
These yield additional signs, which
can be tracked using rule (ii).

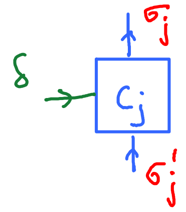


Parity changing tensors

$c^\dagger$ and c change parity; but rule (i) demands: use only parity-conserving tensors!

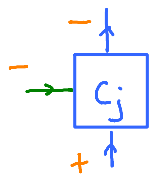
Remedy: add additional leg, with index taking just a single value, $\delta \equiv 1$ with parity $p(\delta) \equiv -1$

which compensates for parity change induced by $c^\dagger$ or c :



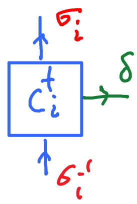
$$= (c_j)^{\delta\sigma_j'}{}_{\sigma_j}$$

only nonzero element:



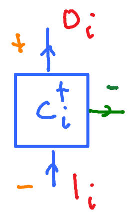
$$= \langle 0_j | c_j \, c_j^\dagger | 0_j \rangle = 1$$

Total parity: $P^{\delta\sigma_j'}{}_{\sigma_j} = p(\delta)\, p(\sigma_j')\, p(\sigma_j) = (-)(+)(-) = +1$ ✓



$$= (c_i^\dagger)^{\sigma_i'}{}_{\sigma_i\delta}$$

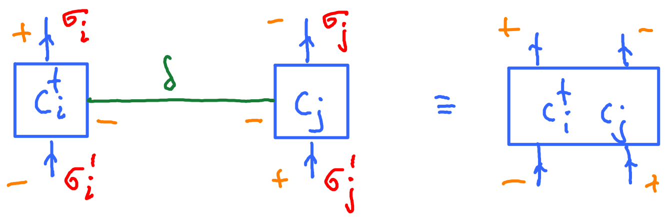
only nonzero element:



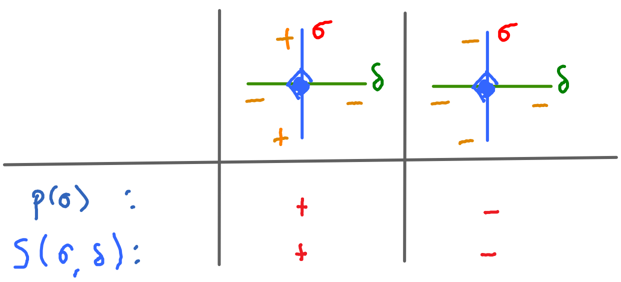
$$= \langle 0_i | c_i \, c_i^\dagger | 0_i \rangle = 1$$

Total parity: $P^{\sigma_i'}{}_{\sigma_i\delta} = p(\sigma_i')\, p(\sigma_i)\, p(\delta) = (-)(+)(-) = +1$ ✓

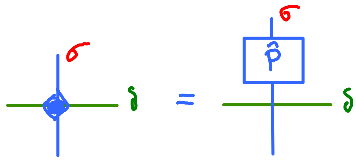
Two-site operator is represented as $c_i^\dagger c_j =$



Since δ carries just a single value, a SWAP gate involving crossing of δ -line and physical σ -line can be simplified to a parity operator acting on latter:



$\Rightarrow$



$$\hat{P}(\sigma) = p(\sigma)$$

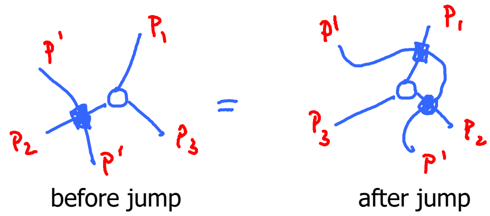
3. Jump move

[Corboz2009, App. C], [Corboz2010b, p. 9]

F-PEPS.3

Because all tensors by construction preserve parity, lines can be 'dragged over tensors':

(Shorthand: $p(\sigma_i) = p_i$)



This is trivially true for $p' = +1$

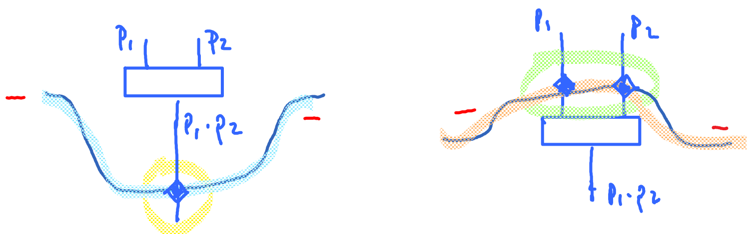
since then all swap signs are $+1$: $S(p_i, +) = +1$ for all p_i

Consider $p' = -1$:

2-leg tensor:

SWAP sign: $S(p,-)$ = $S(p,-)$

3-leg tensor:



SWAP sign:

(p_1,p_2)	$S(p_1 \cdot p_2, -)$	$S(p_1,-)\,S(p_2,-)$
$+,-$	$S(-,-) = -1$	$S(+,-)\,S(-,-) = (+)(-) = -1$
$-,+$	$S(-,-) = -1$	$S(-,-)\,S(+,-) = (-)(+) = -1$
$+,+$	$S(+,-) = (+)$	$S(+,-)\,S(+,-) = (+)(+) = (+)$
$-,-$	$S(+,-) = (+)$	$S(-,-)\,S(-,-) = (-)(-) = (+)$

General argument: parity-preserving tensor has <u>even</u> number of minus-parity lines:

$$(\text{sign})_{\text{before}} \cdot (\text{sign})_{\text{after}} = \prod_{\alpha \in \text{before}} S(p_\alpha, -) \prod_{\beta \in \text{after}} S(p_\beta, -) = (-)^{\text{even}} = (+)$$

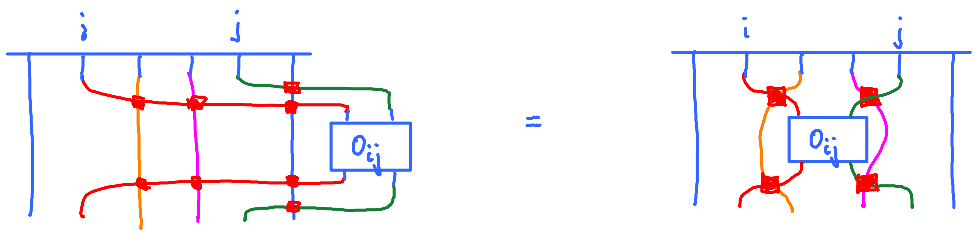
all minus-parity legs cut by before line

all minus-parity legs cut by after line

total number of minus-parity lines, which is even

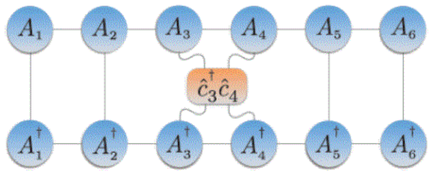
$\Longrightarrow$ $(\text{sign})_{\text{before}} = (\text{sign})_{\text{after}}$ ✓

Jump move allows tensor network diagrams to be rearranged according to convenience:



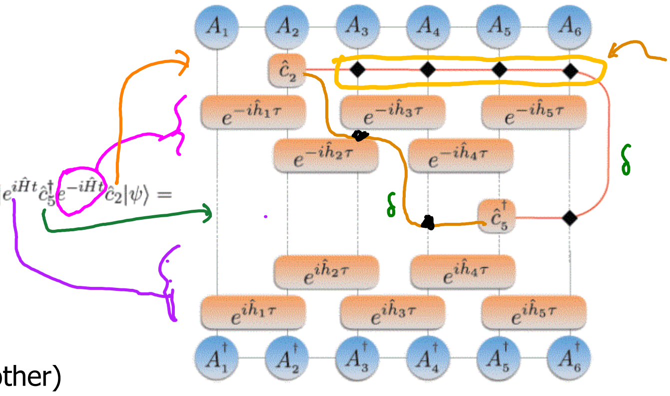
Nearest-neighbor
expectation value
needs no swap gates:

$\langle\psi|\hat{c}_3^\dagger \hat{c}_4|\psi\rangle =$



Time evolution of
non-nearest-neighbor
hopping operator:

$\langle\psi|e^{i\hat{H}t}\hat{c}_5^\dagger e^{-i\hat{H}t}\hat{c}_2|\psi\rangle =$

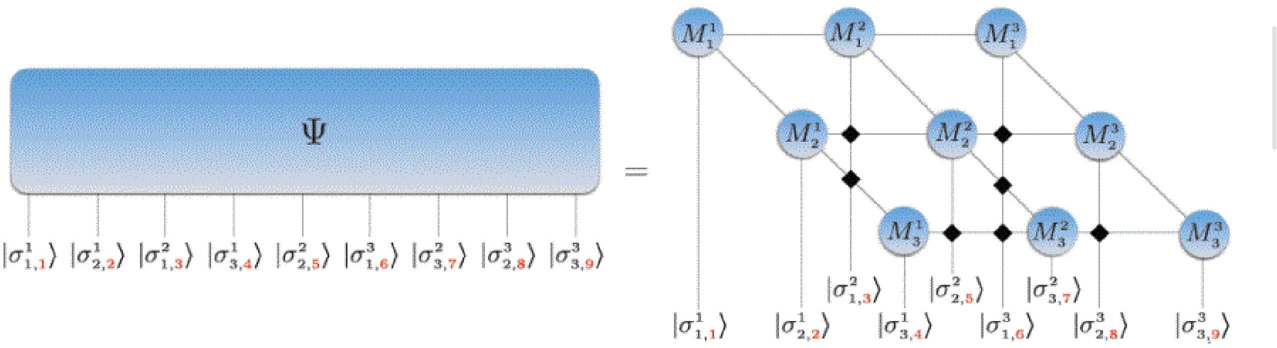


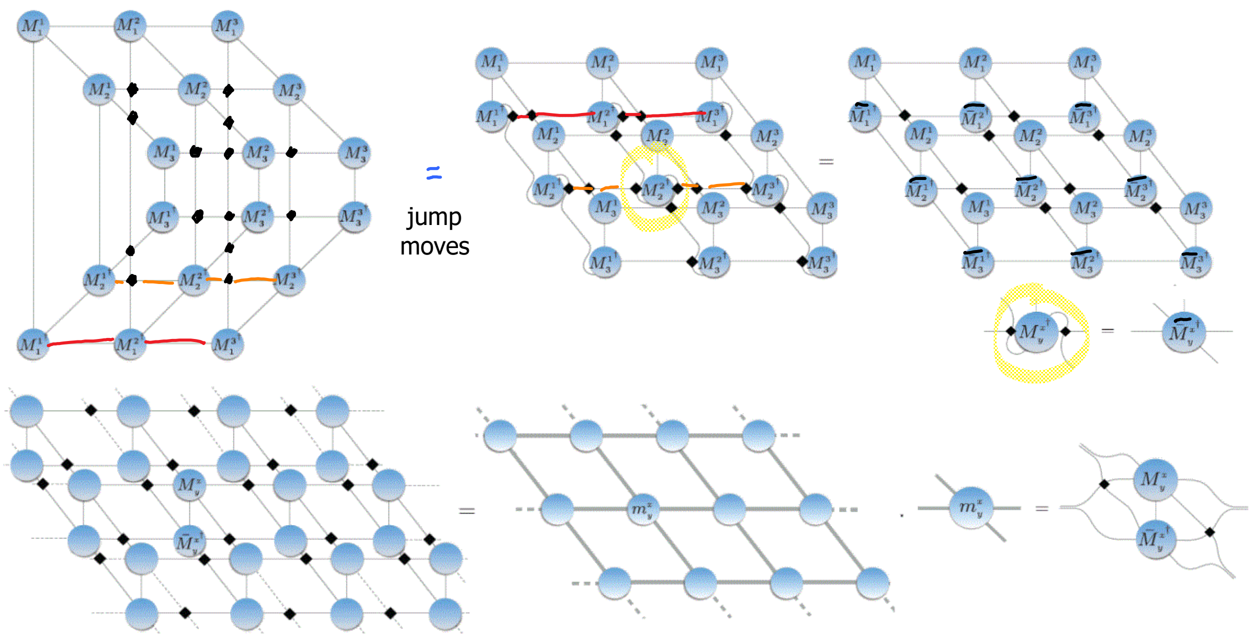
has same effect
as Jordan-Wigner
string

Due to jump moves, the
red line and light brown lines
connecting c_2 and c_5^+
are equivalent (use one or the other)

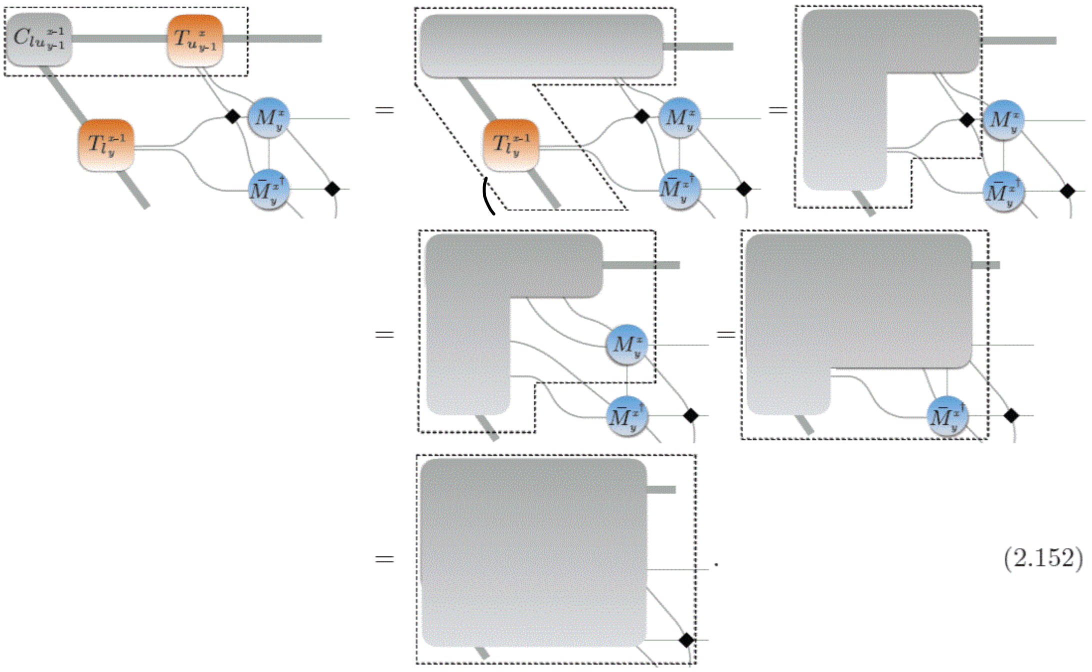
Fermionic order in a PEPS

Choose some ordering for open indices and stick to it!





Absorbing SWAP gates



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