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, Verstraete, Vidal first introduced them, for MERA.
[Corboz2010b] with Orus, Bauer, Vidal adapted them to PEPS context.
This is the approach described in [Bruognolo2020] 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
[Bultinck2017a] 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:

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

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)

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

Every line in tensor network diagram represents a state space, hence also carries a parity index.

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

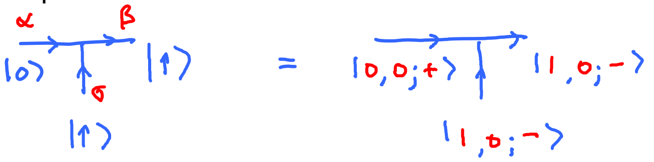
Enforcing $\mathbb{Z}_2$ symmetry [Corboz2010b, Sec.II.F]

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

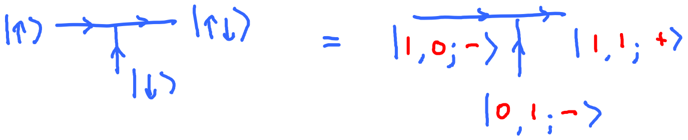
Rule (i): For every tensor, the total parity is positive:

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

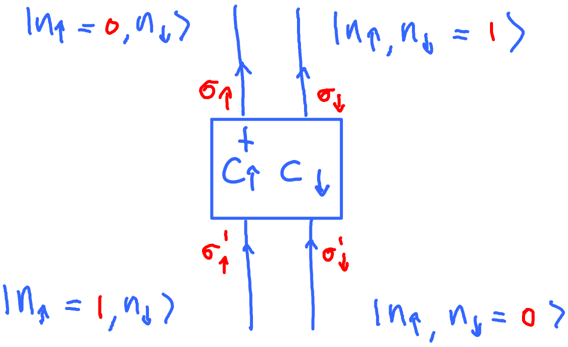
Examples:



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



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



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

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

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

2. Fermionic signs

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

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 $N = 3$:

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

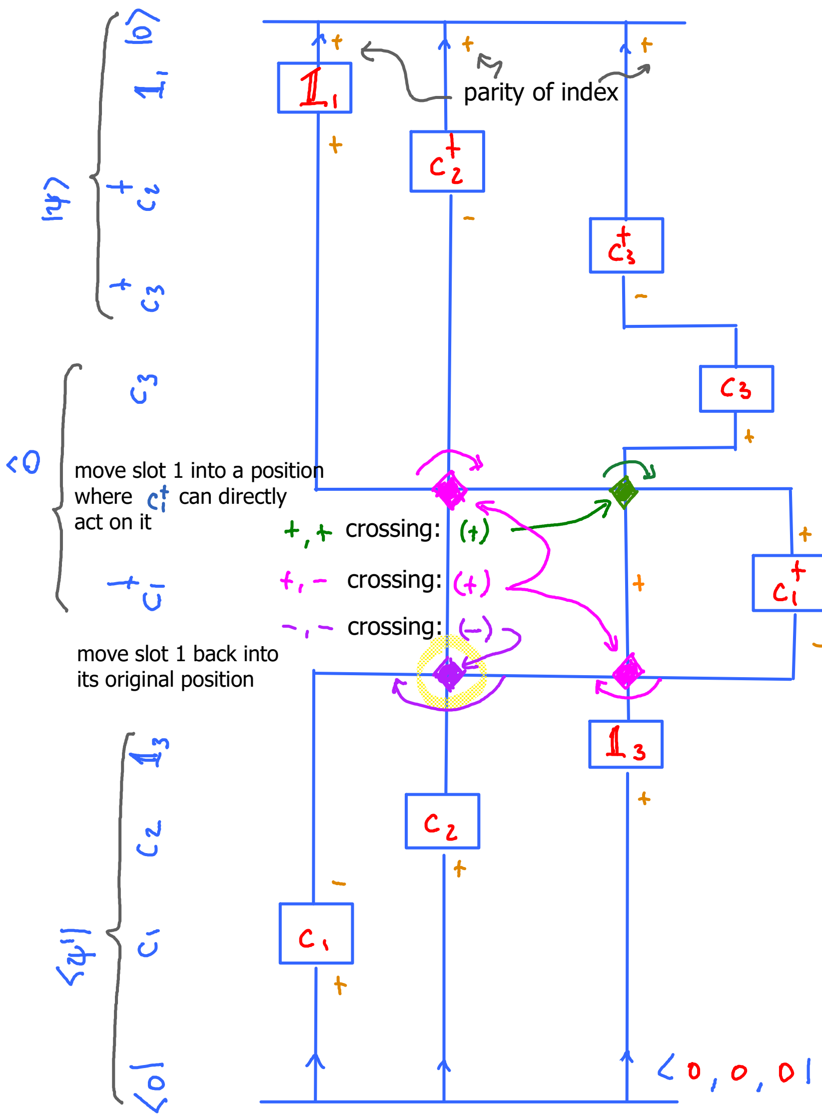
$$\langle\psi'|\underbrace{c_1^\dagger c_3}_{\hat{O}}|\psi\rangle = \langle 0| c_1 c_2 \overbrace{c_1^\dagger \underbrace{c_3 c_3^\dagger}_{=\mathbb{1}_3} c_2^\dagger}^{(-)} |0\rangle = - \underbrace{\langle 0| c_1 \underbrace{c_2 c_2^\dagger}_{\mathbb{1}_2} c_1^\dagger |0\rangle}_{\mathbb{1}_1} = -1$$

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, because then two fermion operators are exchanged.



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

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

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

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

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

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

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

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

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

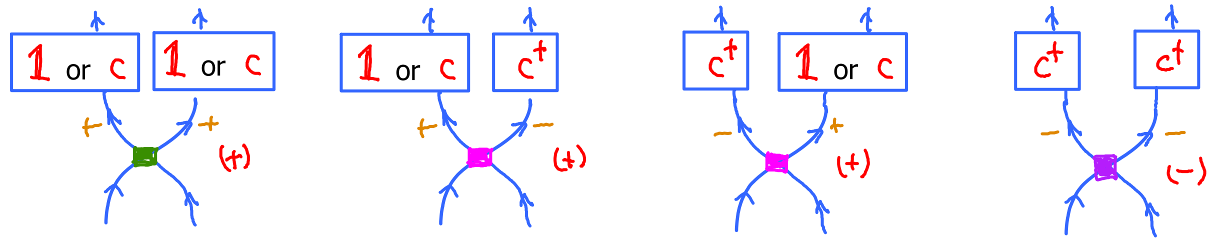
$$- \underbrace{c_2 c_2^\dagger}_{=\mathbb{1}_2} c_1^\dagger |0\rangle = -|1,0,0\rangle$$

$$- \underbrace{c_1 c_1^\dagger}_{=\mathbb{1}_1} |0\rangle = -|0,0,0\rangle$$

$$\langle 0,0,0|$$

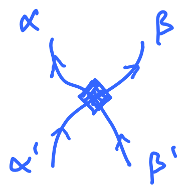
SWAP gates

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):



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

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

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

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

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 $(i<j)$

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

Examples:

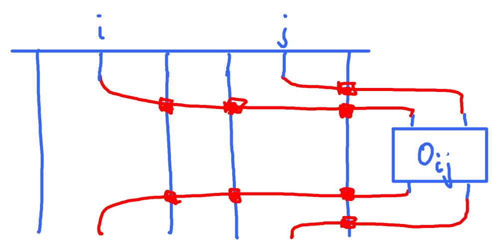
only non-zero element:

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

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

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

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

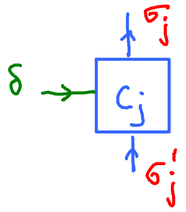


Parity changing tensors

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

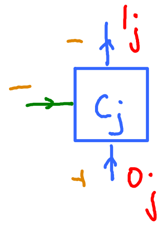
Remedy: add additional leg, with index taking just a single value, $\delta := 1$ with parity $p(\delta) := (-)$

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



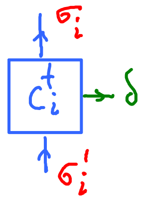
$= (c_j)^{\delta\,\sigma_j'}{}_{\sigma_j}$

only nonzero element:



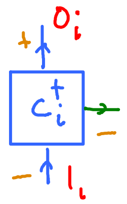
$= \langle 0_j | c_j \, c_j^\dagger | 0_j \rangle = 1$

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



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

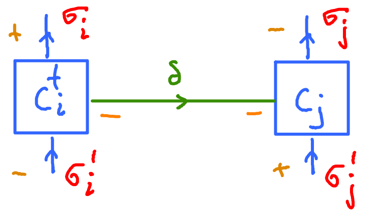
only nonzero element:



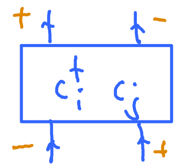
$= \langle 0_i | c_i \, c_i^\dagger | 0_i \rangle = 1$

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

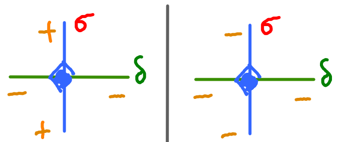
Two-site operator is represented as $c_i^\dagger c_j$ =



:=

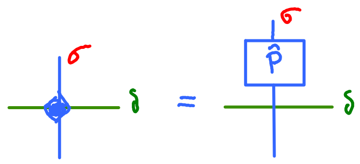


Since δ carries just a single value, a SWAP gate involving crossing of δ-line and physical σ-line can be simplified to a parity operator acting on latter:



σ	+	−
$S(\sigma,\delta)$:	+	−
$p(\sigma)$:	+	−

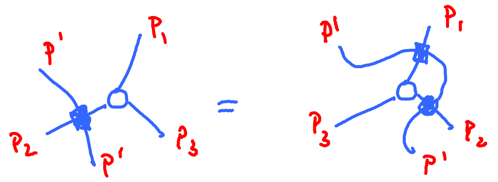
$\Rightarrow$



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

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

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



before jump after jump

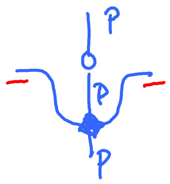
This is trivially true for $p' = (+)$

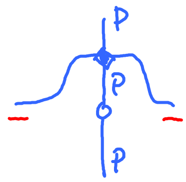
since then all swap signs are $+$: $S(p_i, +) = (+)$ for all p_i

Consider $p' = (-)$:

2-leg tensor:

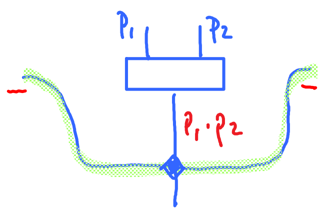
both legs have same parity

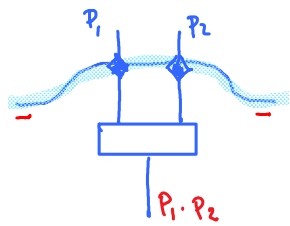




SWAP sign: $S(p, -) = S(p, -)$

3-leg tensor:





SWAP sign:

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

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

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

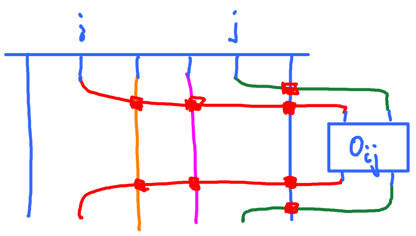
all minus-parity legs cut by 'before' line

all minus-parity legs cut by 'after' line

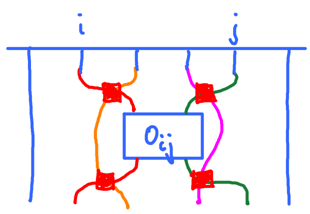
total number of minus-parity lines, which is even

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

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

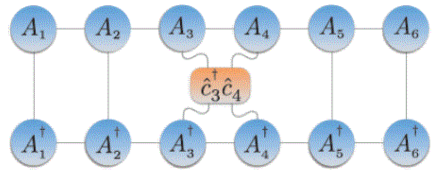


=



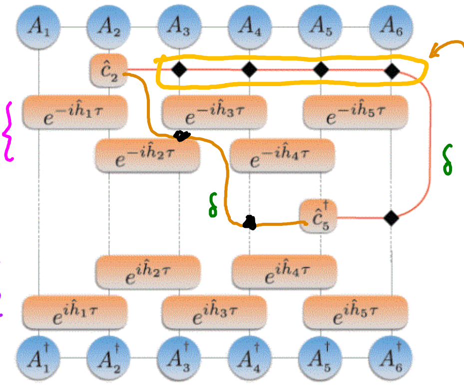
Nearest-neighbor expectation value needs no swap gates:

$\langle\psi| c_3^\dagger c_4 |\psi\rangle =$



Time evolution of non-nearest-neighbor hopping operator:

$\langle\psi| e^{iHt} c_5^\dagger e^{-iHt} c_2 |\psi\rangle =$

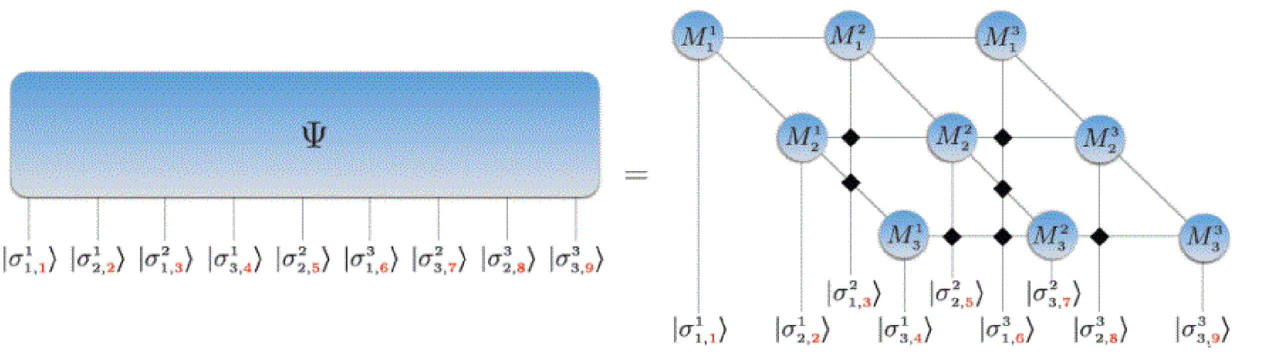


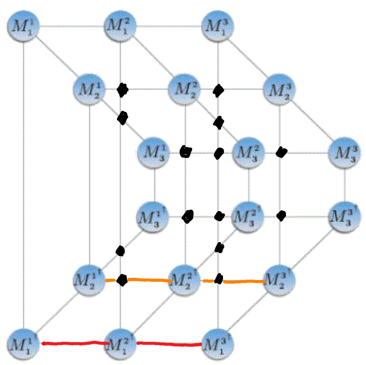
has same effect as Jordan-Wigner string

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

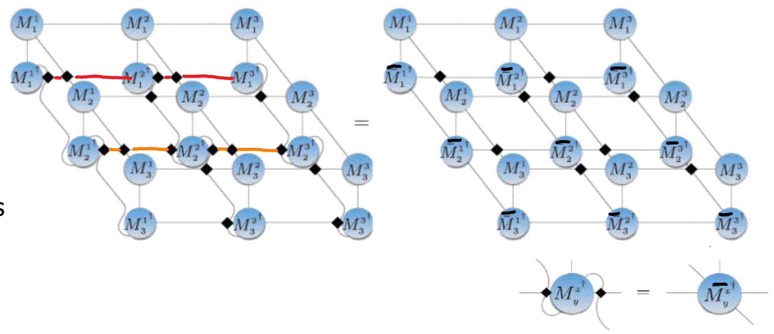
Fermionic order in a PEPS

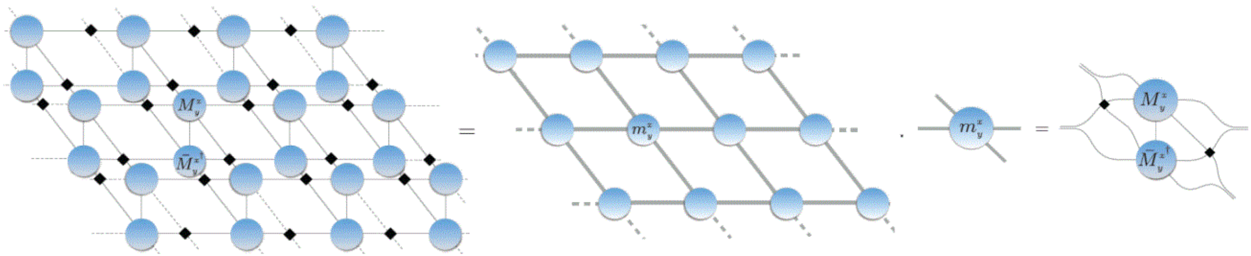
Choose some ordering for open indices and stick to it!



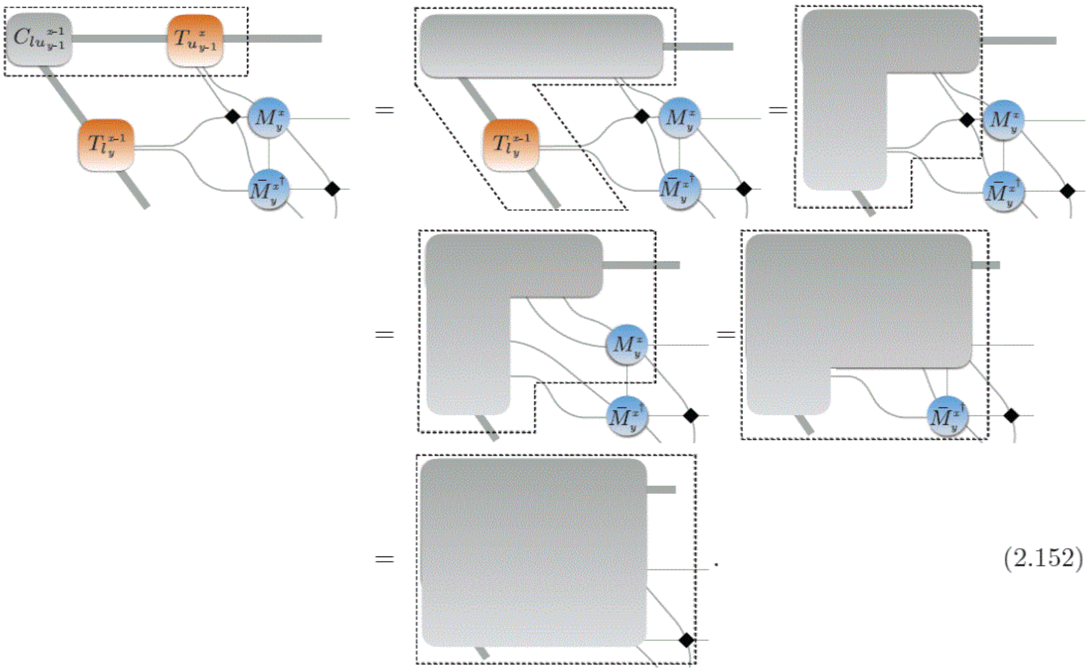


= jump moves





Absorbing SWAP gates



(2.152)