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 eigenstates, too, hence may be labeled by parity eigenvalue:

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

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: $p = (-1)^Q$]

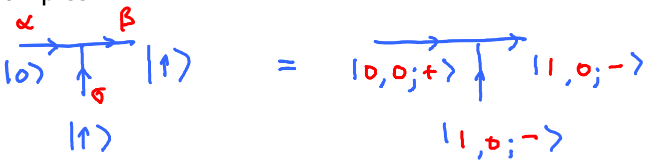
Enforcing $\mathbb{Z}_2$ symmetry [Corboz2010b, Sec.II.F]

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

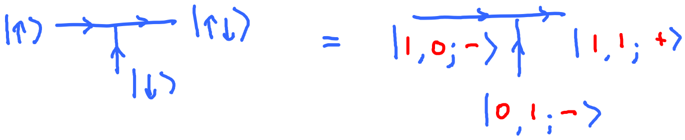
Rule (i): For every tensor, the total parity is positive:

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)

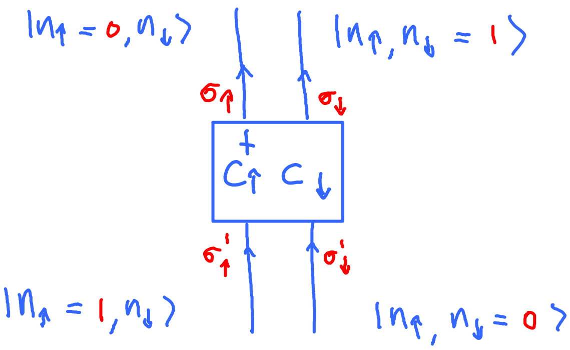
Examples:



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



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



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

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

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

2. Fermionic signs

$$c_\ell c_{\bar\ell} = - c_{\bar\ell} c_\ell \,, \quad c_\ell^\dagger c_{\bar\ell}^\dagger = - c_{\bar\ell}^\dagger c_\ell^\dagger \,, \quad c_\ell c_{\bar\ell}^\dagger = \delta_{\ell\bar\ell} - c_{\bar\ell}^\dagger c_\ell$$

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

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

We have to keep this order in mind when evaluating matrix elements. Example: consider $\mathcal{L} = 3$:

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

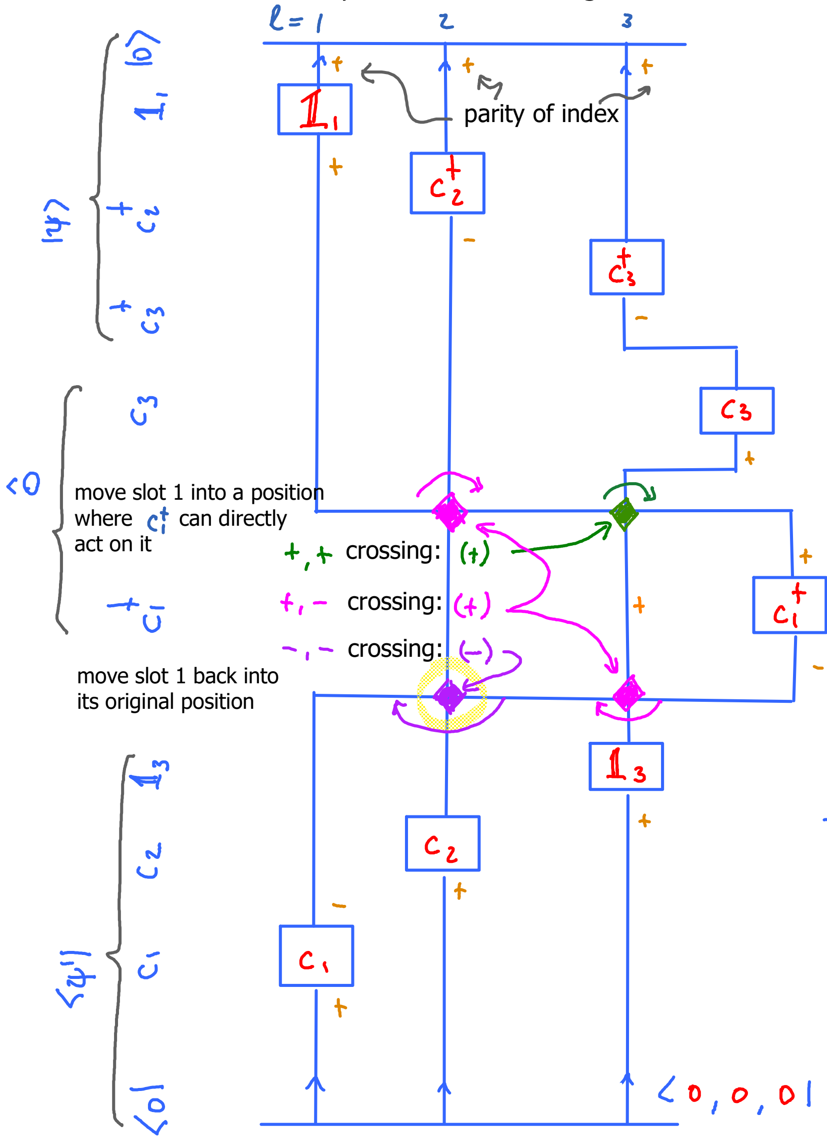
$$\langle\psi'|\underbrace{c_1^\dagger c_3}_{\hat{O}}|\psi\rangle = \langle 0| c_1 c_2 \mathbb{1}_3 \overbrace{c_1^\dagger \underbrace{c_3 c_3^\dagger}_{=\mathbb{1}_3}}^{(-)} c_2^\dagger \mathbb{1}_1 |0\rangle = - \langle 0| \underbrace{c_1 \underbrace{c_2 c_2^\dagger}_{\mathbb{1}_2} c_1^\dagger}_{\mathbb{1}_1}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

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, because then two fermion operators are exchanged.



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

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

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

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

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

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

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

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

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

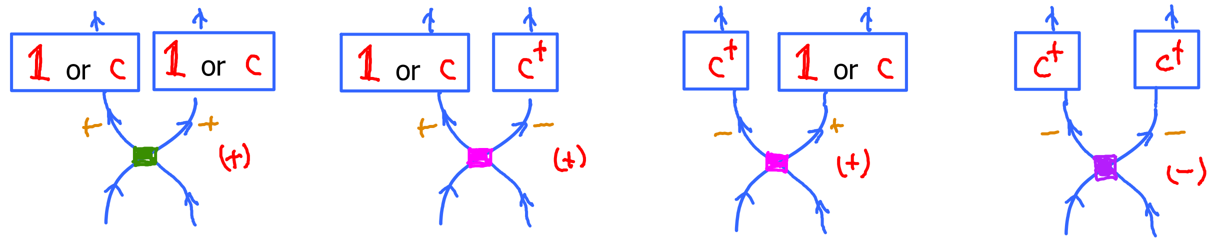
$$- \underbrace{c_2 c_2^\dagger}_{=\mathbb{1}_2} c_1^\dagger |0\rangle = -|1,0,0\rangle$$

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

SWAP gates

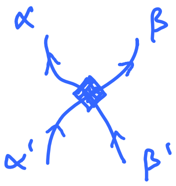
Line crossings keep track of operator orderings.

$(-)$ 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 $\ell, \bar\ell$, with local basis

$$|\sigma_\ell\,\sigma_{\bar\ell}\rangle = (c^\dagger_{\bar\ell})^{\sigma_{\bar\ell}}(c^\dagger_\ell)^{\sigma_\ell}|0_\ell, 0_{\bar\ell}\rangle \quad , \quad \sigma_\ell \in \{0,1\}$$

Two-site operator: $\hat O = \sum |\sigma'_\ell, \sigma'_{\bar\ell}\rangle\, O^{\sigma'_\ell\,\sigma'_{\bar\ell}}_{\sigma_\ell\,\sigma}\,\langle \sigma_\ell\,\sigma_{\bar\ell}|$,

with matrix elements $(\ell < \bar\ell)$

$$O^{\sigma'_\ell\,\sigma'_{\bar\ell}}_{\sigma_\ell\,\sigma_{\bar\ell}} = \langle \sigma'_\ell\,\sigma'_{\bar\ell}|\hat O|\sigma_\ell\,\sigma_{\bar\ell}\rangle = \langle 0_\ell 0_{\bar\ell}|(c^\dagger_\ell)^{\sigma'_\ell}(c^\dagger_{\bar\ell})^{\sigma'_{\bar\ell}}\,\hat O\,(c^\dagger_{\bar\ell})^{\sigma_{\bar\ell}}(c^\dagger_\ell)^{\sigma_\ell}|0_\ell, 0_{\bar\ell}\rangle$$

Examples:

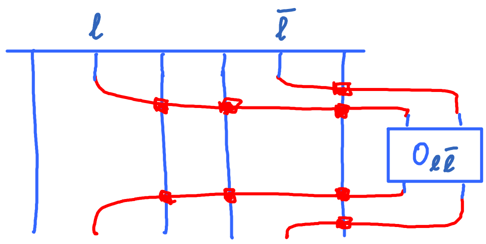
only non-zero element:

Hopping: $\hat O = c^\dagger_\ell\, c_{\bar\ell}$, $\quad O^{1_\ell 0_{\bar\ell}}_{0_\ell 1_{\bar\ell}} = \langle 0_\ell 0_{\bar\ell}|\, c_\ell\, c^\dagger_\ell\, c_{\bar\ell}\, c^\dagger_{\bar\ell}\,|0_\ell 0_{\bar\ell}\rangle = +1$

$\hat O = c^\dagger_{\bar\ell}\, c_\ell$, $\quad O^{0_\ell 1_{\bar\ell}}_{1_\ell 0_{\bar\ell}} = \langle 0_\ell 0_{\bar\ell}|\, c_{\bar\ell}\, c^\dagger_{\bar\ell}\, c_\ell\, c^\dagger_\ell\,|0_\ell 0_{\bar\ell}\rangle = +1$

Pairing: $\hat O = c_{\bar\ell}\, c_\ell$, $\quad O^{0_\ell 0_{\bar\ell}}_{1_\ell 1_{\bar\ell}} = \langle 0_\ell 0_{\bar\ell}|\, c_{\bar\ell}\, c_\ell\, c^\dagger_{\bar\ell}\, c^\dagger_\ell\,|0_\ell 0_{\bar\ell}\rangle = -1$

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

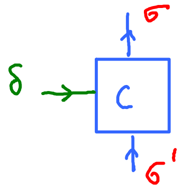


Parity changing tensors

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

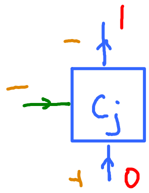
Remedy: add additional leg, with index taking just a single value, $\delta := 1$ with parity $p(\delta) := (-)$

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



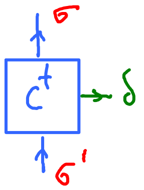
$= (c)^{\delta\sigma'}{}_{\sigma}$

only nonzero element:



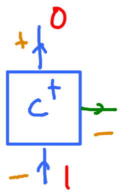
$= \langle 0 | c \, c^\dagger | 0 \rangle = 1$

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



$= (c^\dagger)^{\sigma'}{}_{\sigma\delta}$

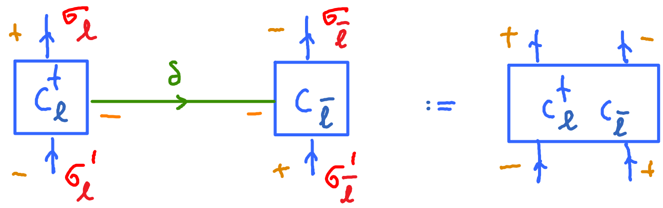
only nonzero element:



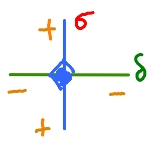
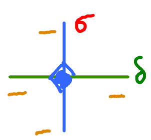
$= \langle 0 | c \, c^\dagger | 0 \rangle = 1$

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

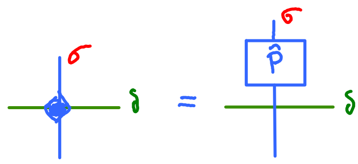
Two-site operator is represented as $c^\dagger_\ell c_{\bar\ell} =$



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

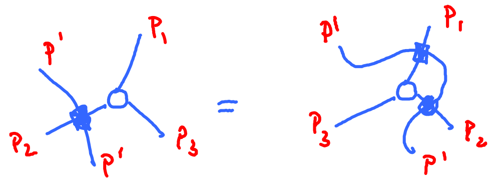
$\Longrightarrow$



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

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

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



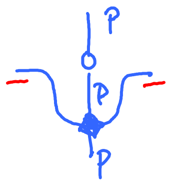
before jump after jump

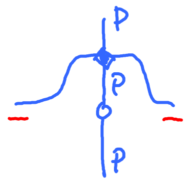
This is trivially true for $p' = (+)$

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

Consider $p' = (-)$:

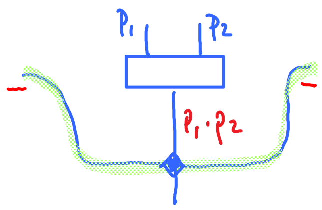
2-leg tensor:
both legs have same parity

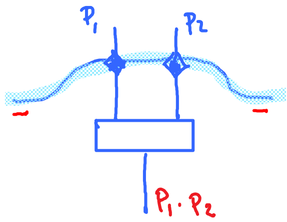




SWAP sign: $S(p, -) = S(p, -)$

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:

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

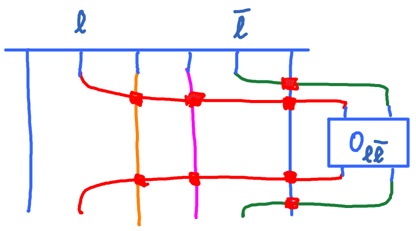
all minus-parity legs cut by 'before' line

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:



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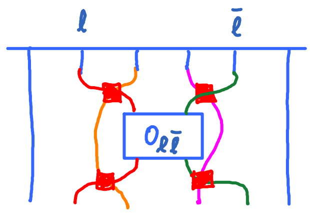
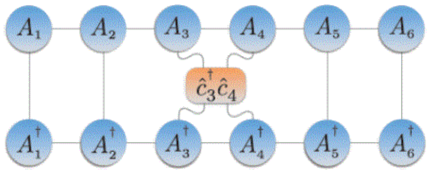


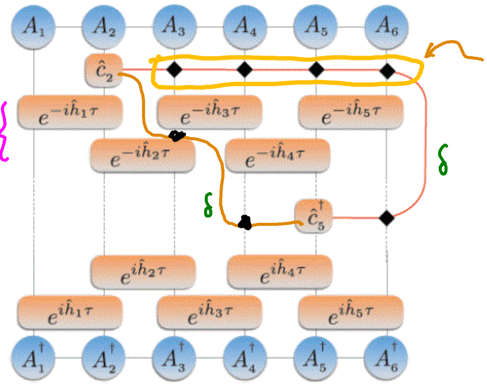
Nearest-neighbor expectation value needs no swap gates:

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



Time evolution of non-nearest-neighbor hopping operator:

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



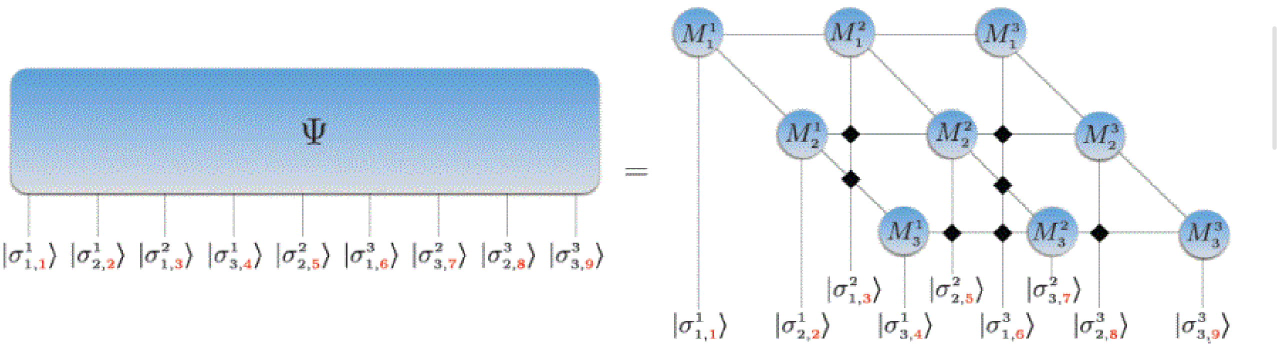
has same effect as Jordan-Wigner string

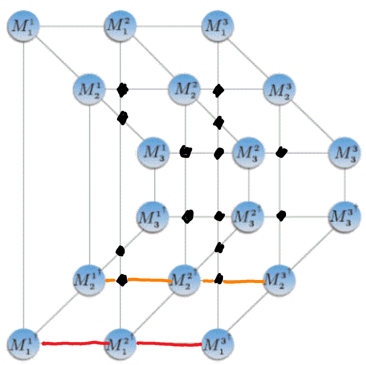
δ

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

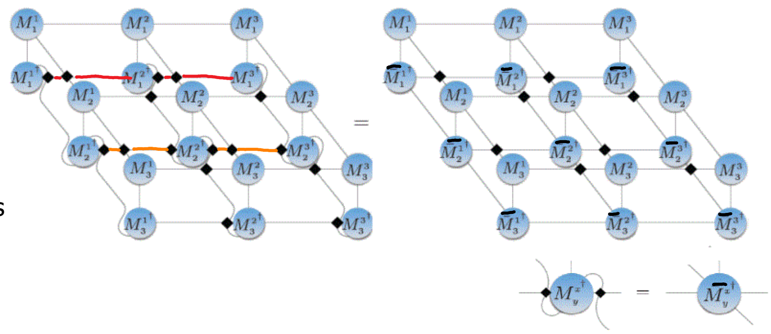
Choose some ordering for open indices and stick to it!

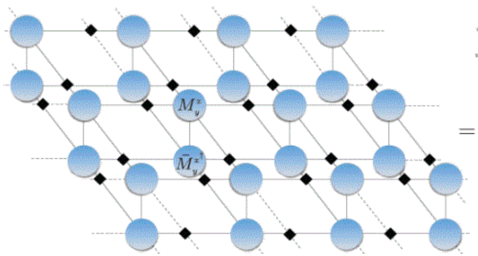


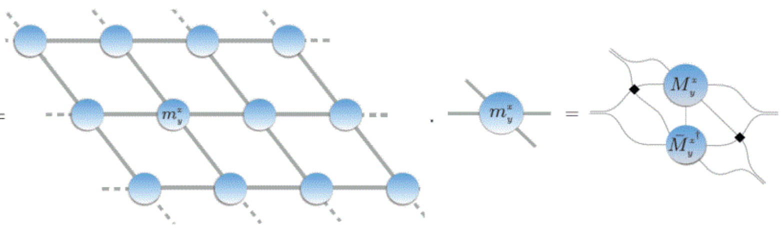


$=$

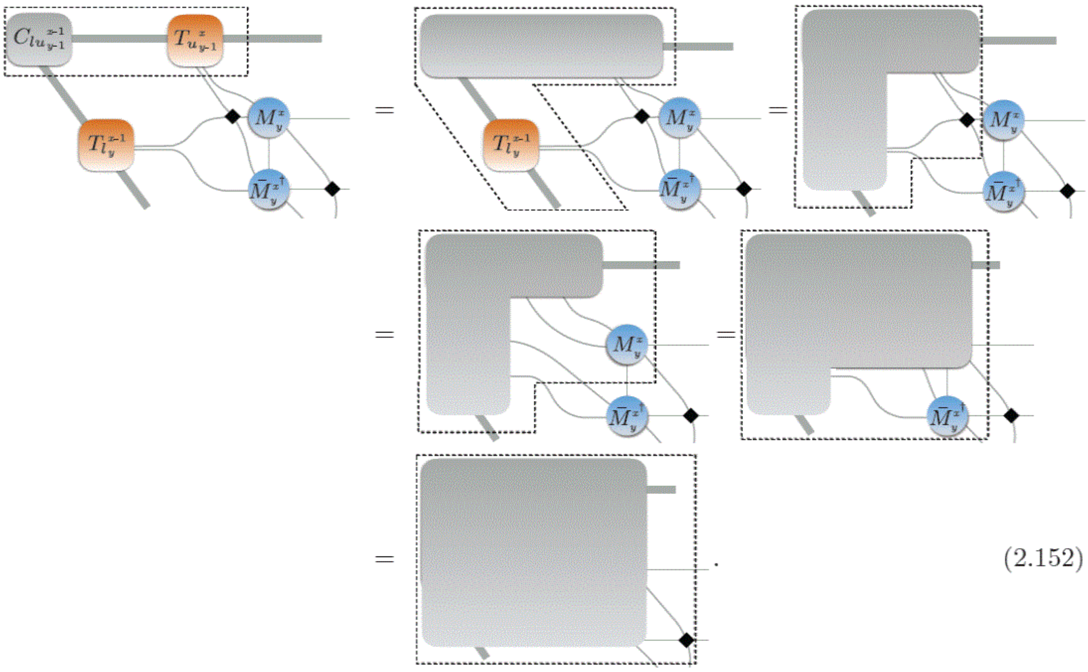
jump moves







Absorbing SWAP gates



(2.152)