Fermionic tensor networks

Can we use tensor networks (MPS, PEPS, MERA) to simulate fermionic systems?

Setting:

Lattice (1D, 2D, ...) of fermionic modes $a_i^\dagger$, possibly with internal degree of freedom (e.g. spin): $a_{i,s}^\dagger$

Hamiltonian acting on these modes, e.g. Hubbard model

$$H = -\sum_{\langle i,j\rangle,s} a_{i,s}^\dagger a_{j,s} + U a_{i,\uparrow}^\dagger a_{i,\uparrow} a_{i,\downarrow}^\dagger a_{i,\downarrow}$$

Task: Variational ansatz for ground state; eff. evaluation of energies, etc.

Jordan-Wigner trafo: For 1D systems, the J.-W.-trafo allows to map local fermionic theories to local spin theories.
→ not harder than spin systems.

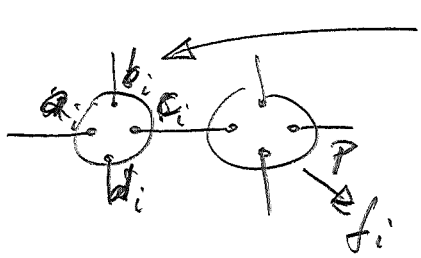
$$a_k^\dagger \longleftrightarrow \sigma_z^1 \otimes \sigma_z^2 \otimes \dots \otimes \sigma_z^{k-1} \otimes \sigma_+^k \qquad \left(\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\right)$$

$$a_k \longleftrightarrow \text{———} u \text{———} \otimes \sigma_-^k \qquad (\sigma_- = (\sigma_+)^\dagger)$$

General ansatz: Fermionic tensor networks.

E.g.: Fermionic PEPS:

Follows PEPS strategy – place max. ent. states & then apply linear maps – using fermionic operators & modes:



creation op. for max. ent. state:

$$h_i^\dagger = 1 + c_i^\dagger a_{i+e_x}^\dagger \quad \leftarrow$$
$$v_i^\dagger = 1 + d_i^\dagger b_{i+e_y}^\dagger \quad \leftarrow \text{fixed parity!}$$

linear map P from auxiliary to physical modes:

$$P = \sum_{\alpha\beta\gamma s} A^s_{\alpha\beta\gamma\delta} \, (f_i^\dagger)^s \, (a_i)^\alpha (b_i)^\beta (c_i)^\gamma (d_i)^\delta$$

↑ constraint: fixed parity of P!

$|\Omega_{aux}\rangle$: vacuum for aux. modes

$|\Omega_{phys}\rangle$: vacuum for ferm. modes

fermionic PEPS (fPEPS):

$$|\Psi\rangle = \langle \Omega_{aux} | \left(P_1 \cdot P_2 \cdot \ldots \cdot P_N\right)\left(h_1^+ h_2^+ \ldots h_N^+\right)\left(v_1^+ v_2^+ \ldots v_N^+\right) |\Omega_{aux}\rangle |\Omega_{phys}\rangle$$

1.) start in vac.

2.) create bonds

3.) apply maps

4.) ensure that aux. modes are left in vac.

... follows usual PEPS construction!

Note: Since both P_i, h_i, and v_i have fixed parity and act on different modes, their order is irrelevant (as long as the P_i are left of the h_i^+, v_i^+, of course!)

This generalizes idea to construct state from local entanglement ($\rightarrow$ area law!), using local maps, to fermionic systems.

We can rewrite

$$|\psi\rangle = \sum_{i_1 \dots i_N} c_{i_1 \dots i_N} \left(f_1^\dagger\right)^{i_1} \cdot \dots \cdot \left(f_N^\dagger\right)^{i_N} |\Omega_{phys}\rangle$$

– what is $c_{i_1 \dots i_N}$?

$$|\psi\rangle = \langle \Omega_{aux}| \underbrace{P_1 \dots P_N \, h_1^\dagger \dots h_N^\dagger \, v_1^\dagger \dots v_N^\dagger} |\Omega_{aux}\rangle |\Omega_{phys}\rangle$$

need to group $a_i a_i^\dagger$, etc., and compute vacuum expectation value: Only $\langle \Omega_{aux}| \mathbb{1} |\Omega_{aux}\rangle$ and $\langle \Omega_{aux}| a_i a_i^\dagger |\Omega_{aux}\rangle$ are non-zero, while $\langle \Omega_{aux}| a_i |\Omega_{aux}\rangle = \langle \Omega_{aux}| a_i^\dagger |\Omega_{aux}\rangle = 0$!

→ fermionic max. ent. states enforce the indices of adjacent sites to be equal: $\langle ij|$,

$$(*) = \left(\sum_s A^s_{\alpha\beta\gamma\delta} \left(f_1^\dagger\right)^s q_1^\alpha s_1^\beta c_1^\gamma d_1^\delta\right)\left(\sum_r B^r_{\alpha'\beta'\gamma'\delta'} \left(f_2^\dagger\right)^r q_2^{\alpha'} s_2^{\beta'} c_2^{\gamma'} d_2^{\delta'}\right)\left(1 + c_1^\dagger q_2^\dagger\right)$$

→ leads to $\boxed{\gamma = \alpha'}$!

But: We have to reorder the fermionic operators:

For $\gamma = \alpha' = 0 \longrightarrow$ no phase.

For $\gamma = \alpha' = 1$: fixed parity (w.l.o.g. even!)

phases $(-1)^{\overbrace{\delta' + \gamma' + \beta' + \alpha' + r}^{\text{fixed parity (w.l.o.g. even!)}} + \delta'}$

$(-1)^{\delta' + \gamma' + \beta'} = (-1)^{\delta'}$ (for e_1^+)

$= (-1)^{r+1}$

$\| \quad r + \alpha' = r+1$

$\Rightarrow$ total phase $(-1)^{\delta' + r + 1}$

$\Rightarrow$ contraction w/ this Sund gives

$$(*) \neq \sum_{\gamma=0,1} \left(\sum_s A^s_{\alpha\beta\gamma\delta} \left(f_1^+\right)^s a_1^\alpha b_1^\beta d_1^\delta \right) \left(\sum_r A_{\gamma\beta'\gamma'\delta'} b_2^{\beta'} c_2^{\delta'} d_2^{\delta'} \right) \phi_\gamma \,,$$

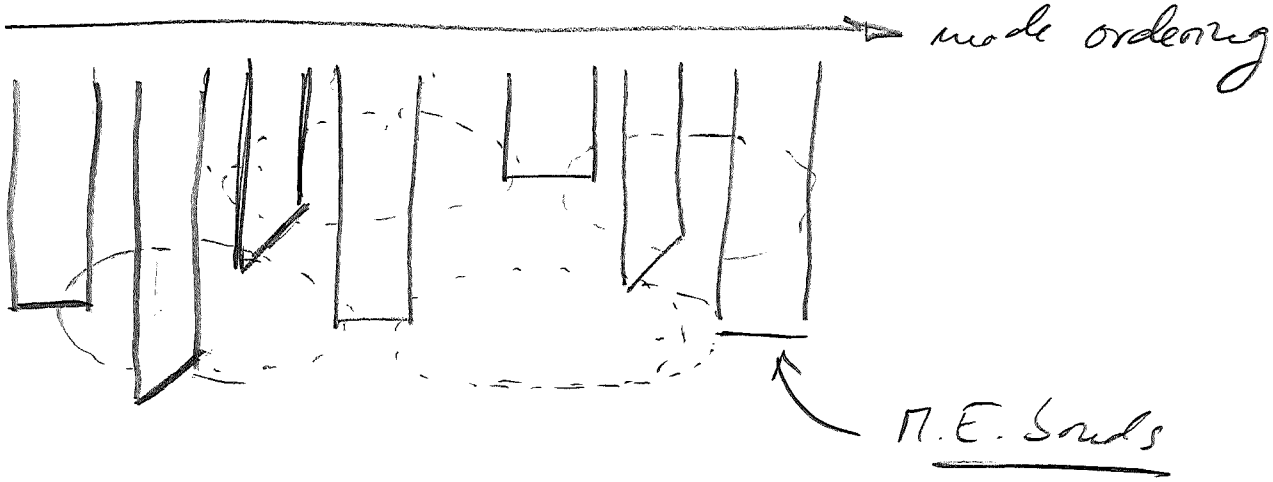
with $\phi_\gamma = \begin{cases} 1 \,, & \gamma = 0 \\ (-1)^{\delta' + r + 1} \,, & \gamma = 1 \end{cases}$

Is there a simple way to keep track of these phases?

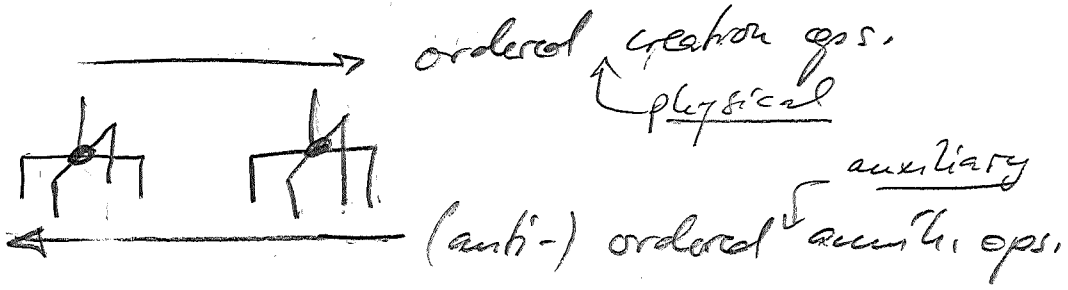
Various possibilities!

Graphical calculus:

Mode ordering: left to right:

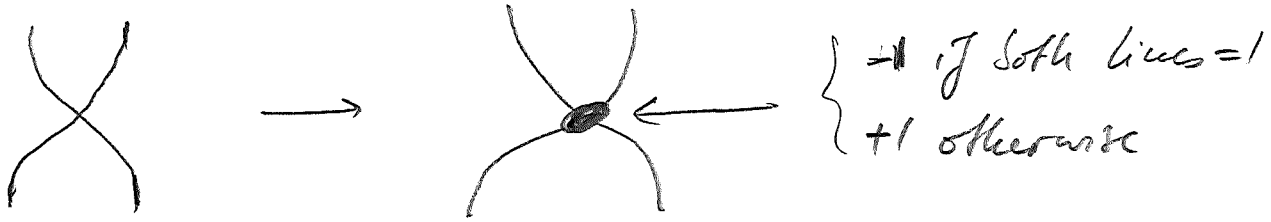


Linear maps:

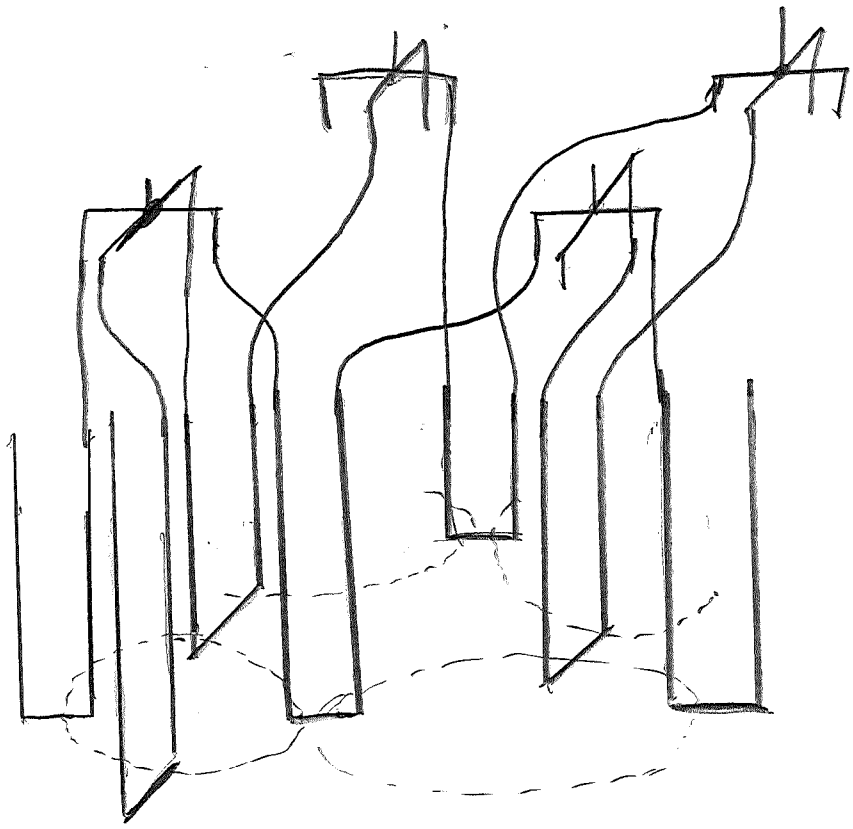


(Note: separating aux and phys. like this gives only closed phases!)

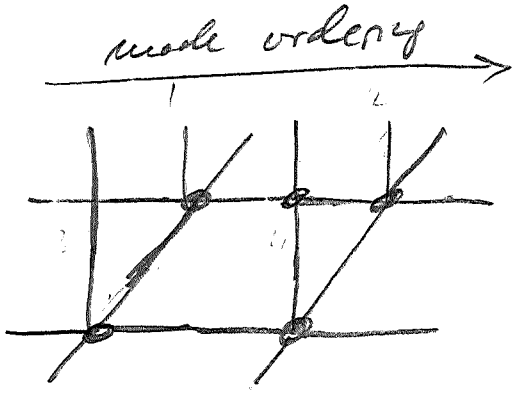
Re-arranging operators in contraction gives rise to sign (from comm. relations) → "swap" tensor



Lines commute w/ objects w/ fixed parity (e.g. )

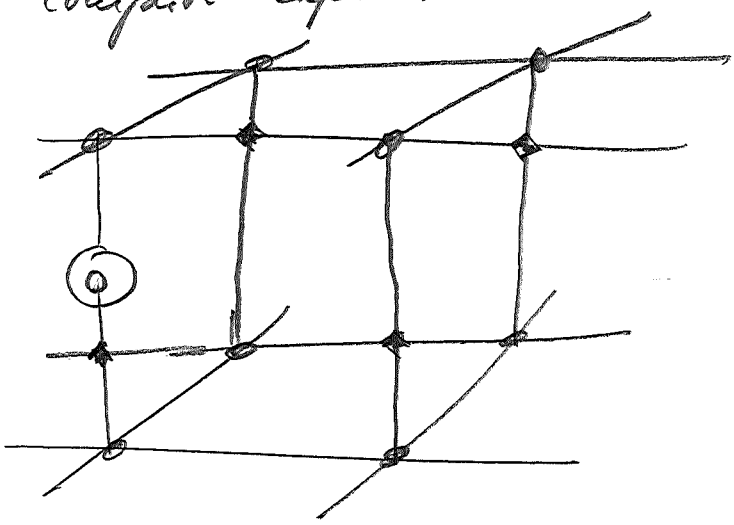


→ diagram can be flattened (up to "self-intersections" such as  : can be incorporated in PI).

⇒ 

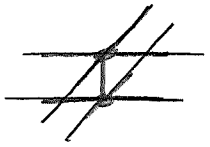
: Tensor network w/ fermionic indices!

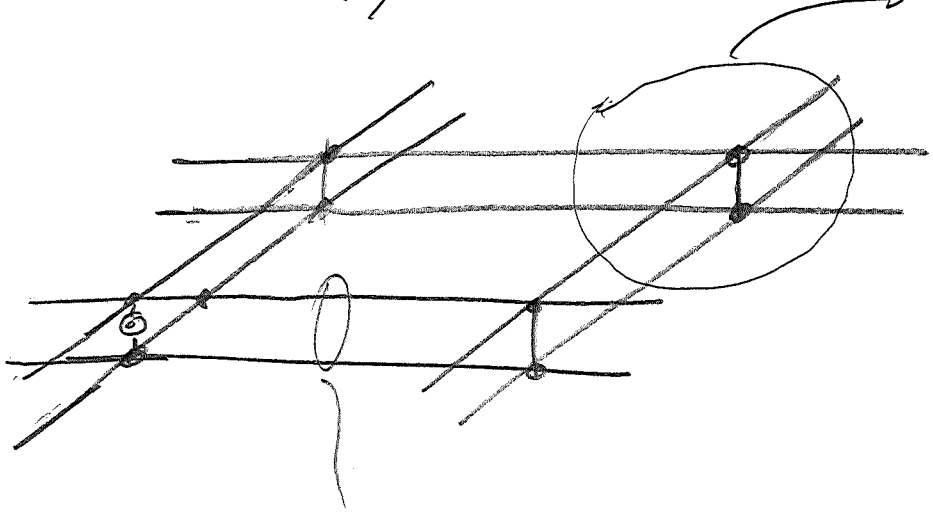
To compute exp. values:



⇒ Fermionic TNs can be evaluated as normal ones — take a bet-bra w/ Op. network — but we need to draw the TN in a 2D plane and put a "swap" tensor at every crossing.

We can contract this network <u>as usual</u> using transfer operators





⇒ Fermionic systems can be simulated at the same cost as spin systems!