2. Other MPS-based algorithms

Brief overview of other MPS-based algorithms

a) Time evolution (real/imaginary)

Can we use MPS to simulate real/imag. time evolution:

$$|\psi(0)\rangle \mapsto |\psi(t)\rangle = e^{-iHt}|\psi\rangle, \text{ or}$$

$$|\psi(0)\rangle \mapsto |\psi(t)\rangle = e^{-H\tau}|\psi\rangle,$$

where $|\psi(0)\rangle$ is some MPS?

Trotter expansion

Consider e.g. NN Ham. $H = \sum h_i$.
N.N. terms

$$H = \sum h_i = \underbrace{\sum_{i \text{ even}} h_i}_{=: H_{even}} + \underbrace{\sum_{i \text{ odd}} h_i}_{=: H_{odd}}$$

$$e^{-iHt} = e^{-i(H_{even} + H_{odd})t}$$

$$= \left(e^{-i(H_{even}+H_{odd})t/K}\right)^K$$

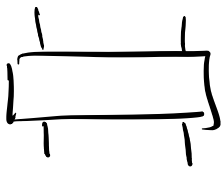
$$\approx \left(e^{-iH_{even}t/K}\, e^{-iH_{odd}t/K}\right)^K$$

Can get better accuracy w/ higher-order expansion!

$$= {\underbrace{\left(\prod_{i\ even} e^{-ih_i t/K} \prod_{i\ odd} e^{-ih_i t/K}\right)}_{\circledast}}^K$$

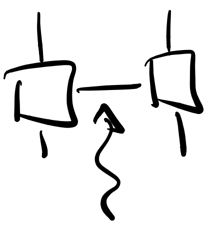
Tensor network formulation

$$e^{-ih_i t/K} =$$



← operator acting on 2 sites

$$=$$

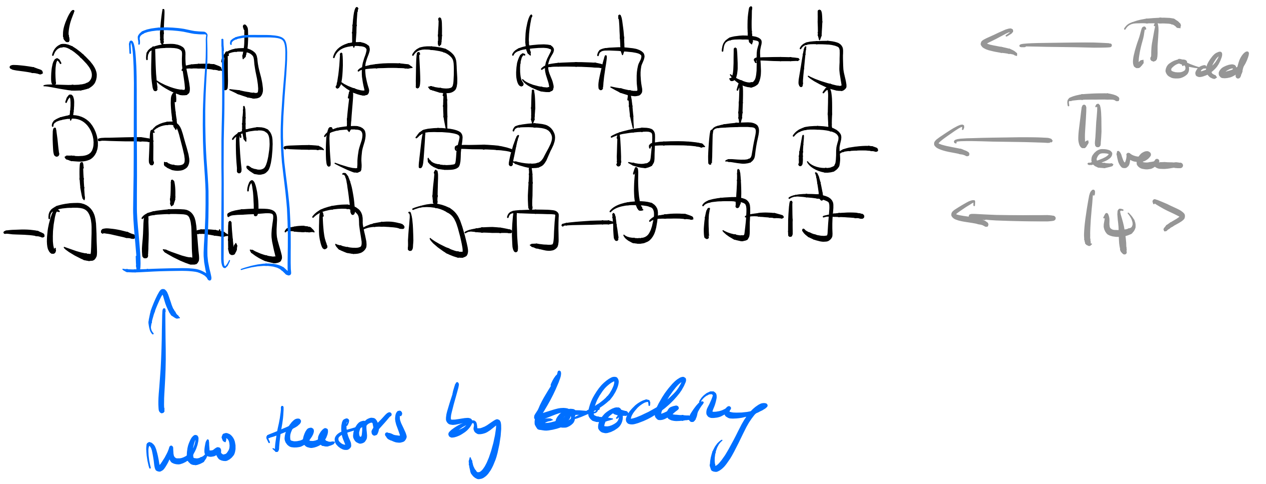


← TN decomposition (via SVD/QR)

dim. χ

$$\Rightarrow |\psi(t/K)\rangle = \left(\prod_{i\ even} e^{-ih_i t/K} \prod_{i\ odd} e^{-ih_i t/K}\right) |\psi(0)\rangle$$

$=$



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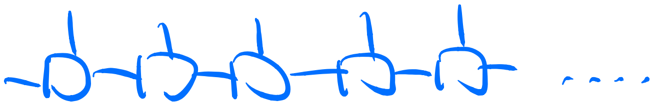


$\Rightarrow$ $|\psi(t/k)\rangle$ is an MPS with an enlarged bond dimension $D\chi$.

$\Rightarrow$ Can now use some truncation scheme (e.g. as in II.1, or by maximizing the overlap with an MPS with bond dim. D – this can be done analogous to DMRG) to get the bond dim. back to D.

Can be used as an alternative method for finding ground states, using $|\psi\rangle \mapsto e^{-H\tau}|\psi\rangle$, or for simulating time evolution.

<u>Caveat</u>: The entanglement in time evol. can grow <u>linearly</u> in time (i.e., D grows <u>exponentially</u> in time), if initial state has finite energy density

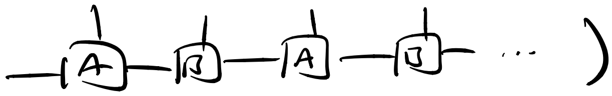
$\Rightarrow$ simulation becomes quickly inaccurate (can be seen from truncation error, or by evolving back again & checking for consistency).

<u>Note</u>: Truncation errors don't matter for imag. time evol., in case we want to read the ground state!

b) Infinite systems

Can we simulate <u>infinite</u> systems (with a transl. inv. Hamiltonian $H = \sum h_i$)?
all equal.

<u>Ansatz:</u> tr. inv. MPS (possibly with larger unit cell,

e.g.  ...).

– also termed iMPS ("infinite MPS") in this context.

Can again either use <u>variational methods</u> (as DMRG) or real/imag. <u>time evolution</u> methods.

<u>Variational methods:</u>

<u>iDMRG</u>: Start with 2 sites, optimize, and add a site in the middle, which is optimized next, and so on.
No sweeps – the "old" tensors are pushed to the outside. The tensors in the

center should converge to the iMPS tensor.

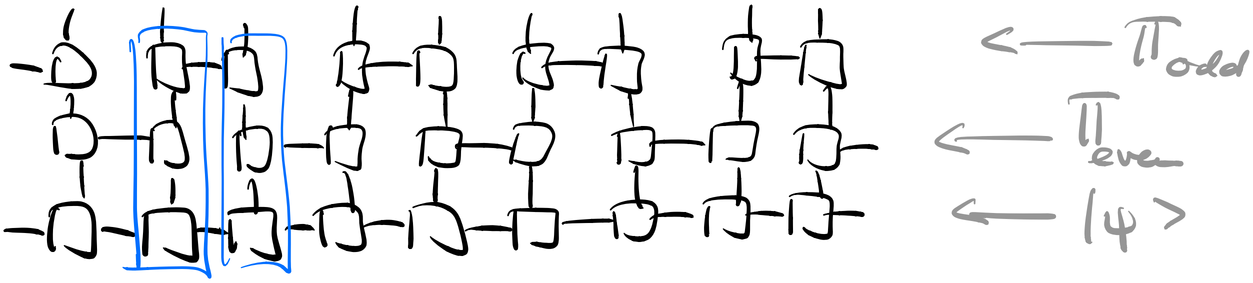
<u>VUMPS</u> (variational uniform MPS): Formulate the energy optimization problem directly in the thdyn. limit, by using a <u>canonical form</u> for the iMPS around a working site.

In essence, the problem is <u>linearized</u> by keeping all but the central tensor fixed — this gives a quadratic problem, which is then solved. The new tensor is updated everywhere in a neat way (respecting the canonical form).

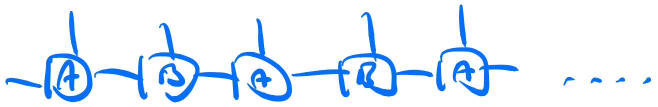
<u>Time evolution:</u>

<u>TEBD</u> (time evolving block decimation):

Similar to the time evolution in the prev. section, but now we cut everywhere:

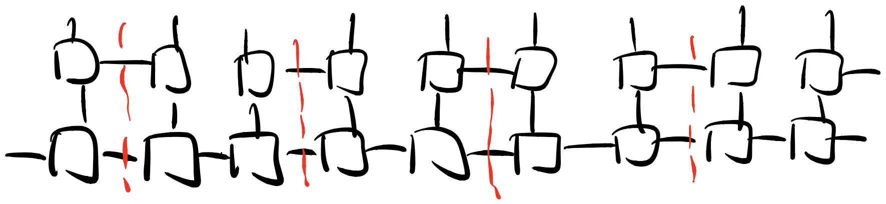


new tensors by blocking ← But: Diff. tensor on odd/even sites: 2-site unit cell!



option 1: cut everywhere

option 2: only apply 1 layer



and cut every 2nd site.

For <u>real</u> time evol., working in a suitable can. form allows to determine the optimal cut <u>locally</u> & keep the can. form: very simple & efficient.

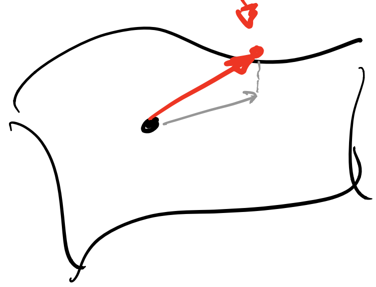
TDVP (time-dependent variational principle)

Consider the space of iMPS w/ bond dim. D

as a manifold.

Consider evolution

$$|\psi(t+\delta t)\rangle = e^{-iH\delta t} |\psi(t)\rangle$$



evolution leads out

of manifold

$\Downarrow$

find best projection

back onto manifold.