Time Evolution and Locality in Tensor Networks

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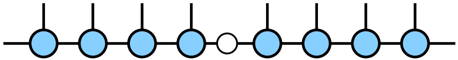
Outline

1. Matrix Product States
2. Time evolution
3. Thermodynamic limit
4. Infinite Boundary Conditions
5. Block-Local decomposition of the time-evolution operator

Matrix Product States

We represent the wavefunction as a Matrix Product State

$$|\Psi\rangle = \mathrm{Tr} \sum_{s_1, s_2, \ldots} A^{s_1} A^{s_2} A^{s_3} A^{s_4} \cdots |s_1\rangle |s_2\rangle |s_3\rangle |s_4\rangle \cdots$$



$$A^{\sigma_1} \; A^{\sigma_2} A^{\sigma_3} \; A^{\sigma_4} \Lambda \; B^{\sigma_5} B^{\sigma_6} B^{\sigma_7} B^{\sigma_8}$$

Λ is the wavefunction in the *Schmidt basis*

$$|\Psi\rangle = \sum_{i=1}^{D} \Lambda_{ii} |i\rangle_L |i\rangle_R$$

This Ansatz restricts the *entanglement* of the wavefunction $S \sim \log D$.
But this is OK for groundstates in 1D!

Time evolution

Real time evolution of a quantum state

$$|\psi(t)\rangle = \exp[iHt]|\psi(0)\rangle$$

Problem: $\exp[iHt]$ is a complicated object! Need an approximation scheme

$$\exp[iHt] = (\exp[iH\Delta t])^N$$

and expand $\exp[iH\Delta t]$ for small Δt.

Two common approaches

- Krylov Subspace - Polynomial approximation

$$\exp[iH\Delta t] \simeq a_0 + a_1 H + a_2 H^2 + \ldots + a_k H^k$$

  and use MPS arithmetic to construct $H|\psi\rangle, H^2|\psi\rangle, \ldots H^k|\psi\rangle$.
- Lie-Trotter-Suzuki decomposition

$$\exp[iH\Delta t] \simeq \exp[iH_{\text{odd}}]\ \exp[iH_{\text{even}}]$$

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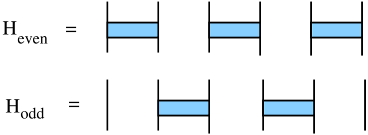
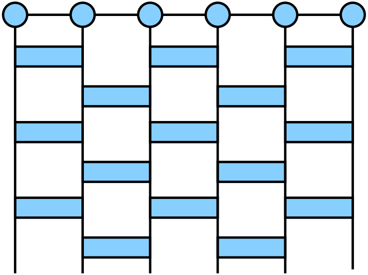
Time Evolving Block Decimation (or T-DMRG)

Each term in $\exp[iH_{\text{odd/even}}]$ is a 2-body unitary gate

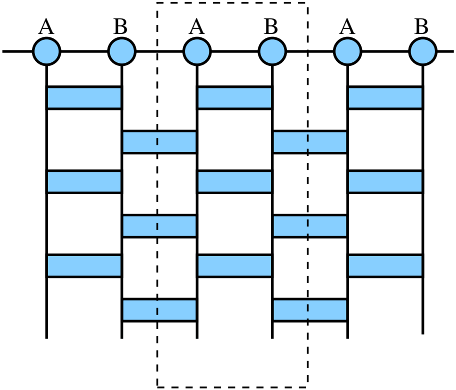


Putting all this together, we have

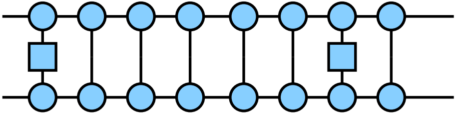


Infinite TEBD (iTEBD, Vidal, 2004)

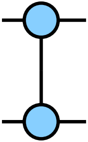
This algorithm also works if we have an infinite system with translational invariance



Correlation functions



The form of correlation functions are determined by the eigenvalues of the *transfer operator*



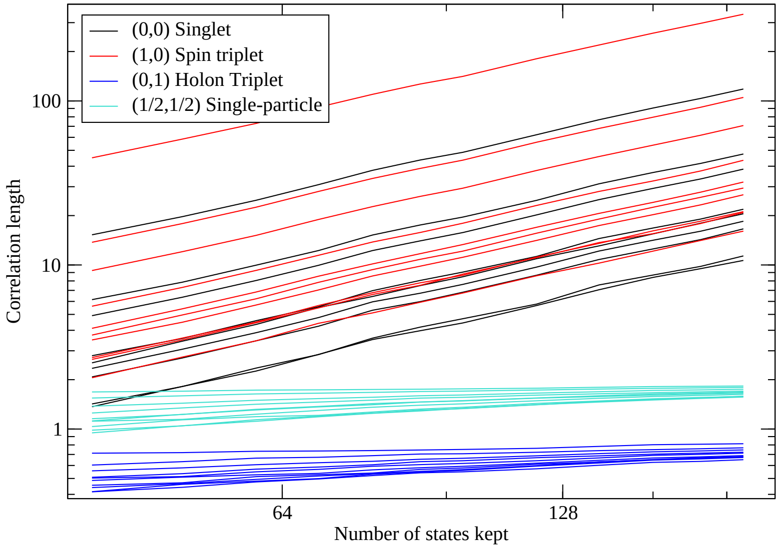
- All eigenvalues magnitude ≤ 1
- One eigenvalue equal to 1, corresponding to the identity operator
- Eigenvalues may be complex only if parity symmetry is broken

Expansion in terms of eigenspectrum λ_i:

$$\langle O(x) O(y) \rangle = \sum_i a_i \, \lambda_i^{|y-x|}$$

Hubbard model transfer matrix spectrum

Half-filling, U/t=4



CFT Parameters

For a critical mode, the correlation length increases with number of states m as a power law,

$$\xi \sim m^{\kappa}$$

[T. Nishino, K. Okunishi, M. Kikuchi, Phys. Lett. A **213**, 69 (1996)
M. Andersson, M. Boman, S. Östlund, Phys. Rev. B **59**, 10493 (1999)
L. Tagliacozzo, Thiago. R. de Oliveira, S. Iblisdir, J. I. Latorre, Phys. Rev. B **78**, 024410 (2008)]

This exponent is a function *only* of the central charge,

$$\kappa = \frac{6}{\sqrt{12c} + c}$$

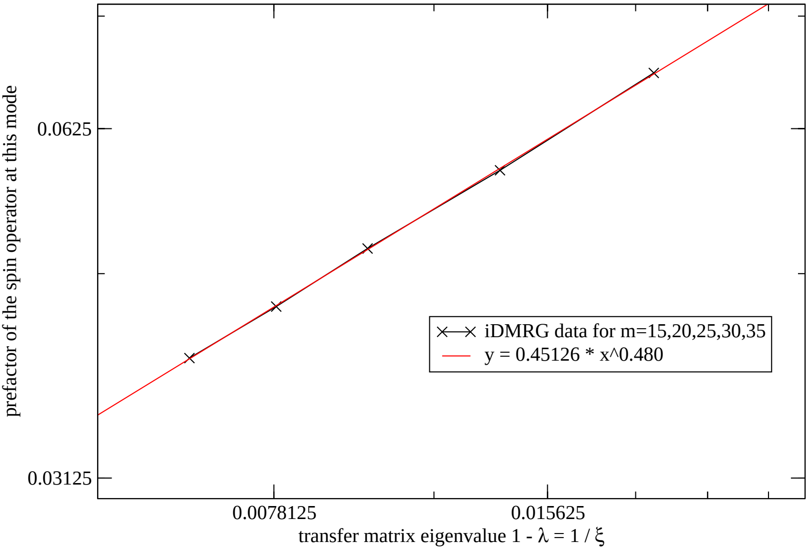
[Pollmann et al, PRL 2009]

Even better, we can directly calculate the scaling dimension

$$a = (1 - \lambda)^{\Delta}$$

(And CFT operator product expansion?...)

Heisenberg model fit for the scaling dimension

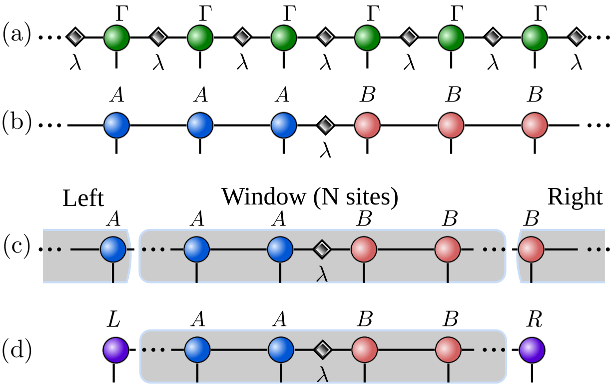


Infinite boundary conditions

H.N. Phien, G. Vidal, IPM, Phys. Rev. B 86, 245107 (2012), Phys. Rev. B 88, 035103 (2013)

(see also Zauner et al 1207.0862, Milsted et al 1207.0691)

Local perturbation to a translationally invariant state



Map infinite system onto a finite MPS, with an effective boundary

- Key point: Even if the perturbation is correlated at long range, only the tensors at the perturbation are modified
- Decompose the Hamiltonian

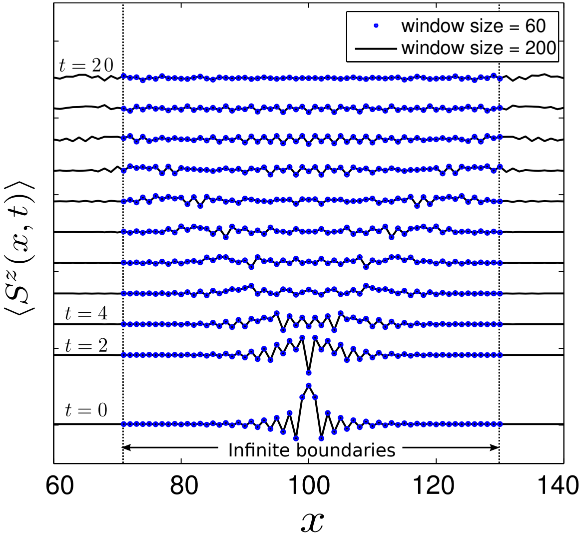
$$H = H_L + H_{LW} + H_W + H_{WR} + H_R$$

- We can calculate H_L and H_R by summing the infinite series of terms from the left and right (see arXiv:0804.2509 and arXiv:1008.4667)
- Away from the perturbation the wavefunction is approximately an eigenstate, so

$$\exp itH_L \sim I$$

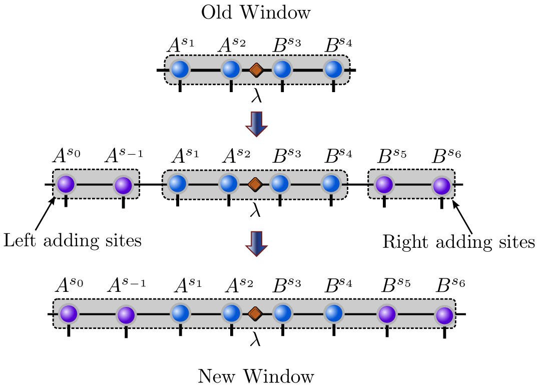
  and we don't leave the Hilbert space of the semi-infinite strip

Spin-1 Heisenberg chain, S^+ initial perturbation

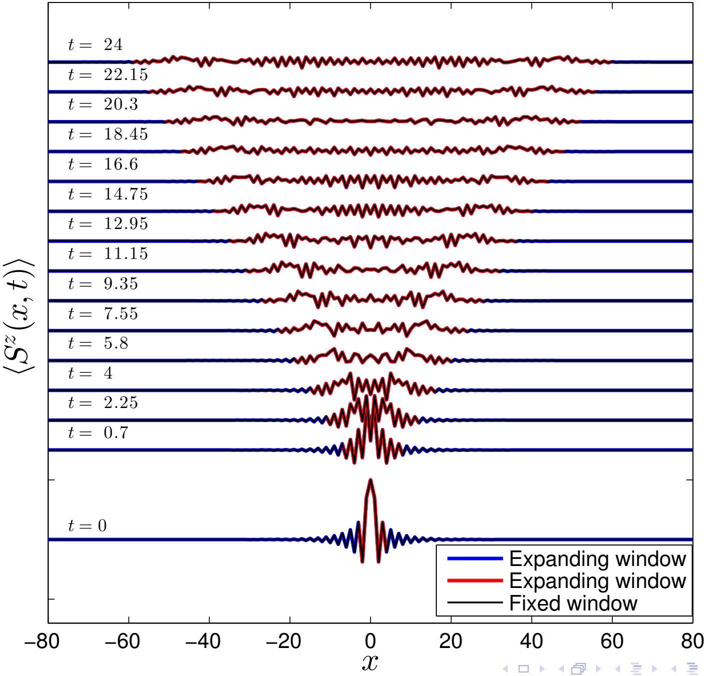


Resize the window

We can do better - why keep the size of the window fixed?
Window expansion - incorporate sites from the translationally-invariant section into the window



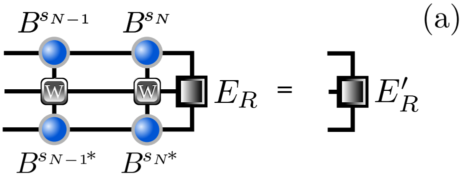
Criteria for expanding: is the wavefront near the boundary?
(Calculate from the fidelity of the wavefunction at the boundary)

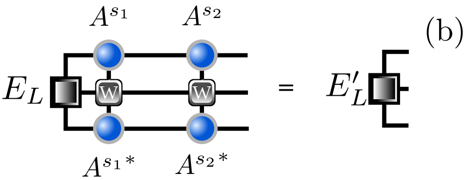


t = 24
t = 22.15
t = 20.3
t = 18.45
t = 16.6
t = 14.75
t = 12.95
t = 11.15
t = 9.35
t = 7.55
t = 5.8
t = 4
t = 2.25
t = 0.7
t = 0
$\langle S^z(x,t) \rangle$
Expanding window
Expanding window
Fixed window
–80
–60
–40
–20
0
20
40
60
80
x

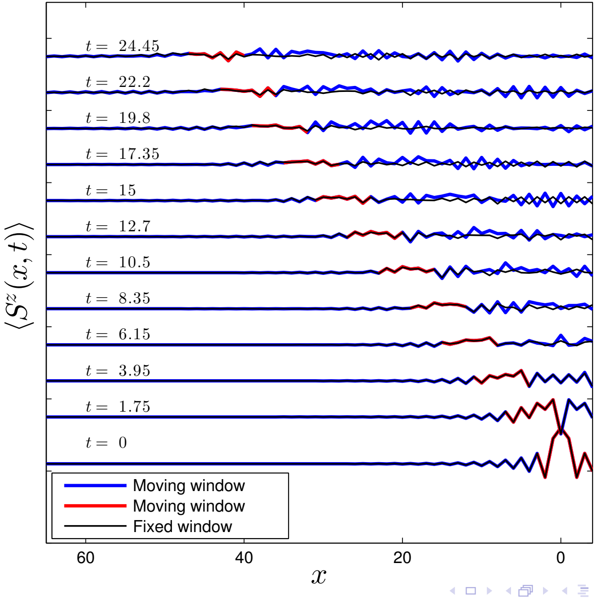
Window contraction

Window contraction - incorporate tensors from the window into the boundary
Contract the MPS and Hamiltonian MPO



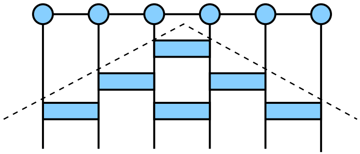


Follow the wavefront



Locality of time evolution

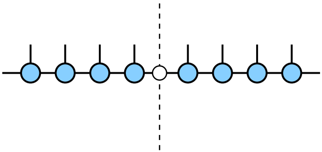
- Although the time evolution operator is complicated, evolution itself is *purely local*
- Lieb-Robinson bound: the 'quantum speed limit' on the rate that information can flow
- Existing algorithms don't really capture this
- Light cone in Lie-Trotter-Suzuki expands way too fast



- What about longer range interactions?

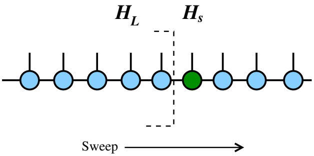
Stop decomposing H into 2-body gates!

Partition a quantum system (anything, doesn't have to be MPS):



The surface states form an almost-complete Hilbert space for some depth (at least a few lattice sites)

- Basic idea: Decompose the time-evolution operator into terms that are local to a block



Accumulate $H_L \leftarrow H_L + H_s$

$H_s =$ components of H acting on site s (and to the left)

- H_L and H_s act on the left-half of the system, $D \times D$ matrices
- Decompose the evolution operator into a product of terms:

$$\exp[-it(H_L + H_s)] = \exp[-itH_L] \exp[-itH'_s]$$

What is H'_s?

$$itH'_s = itH_s + t^2[H_L, H_s] + \frac{t^3}{6}[2H_L + H_s, [H_L, H_s]] + i\frac{t^4}{24}[H_L + H_s, [H_L, [H_L, H_s]]] + \dots$$

- H'_s is more complicated, but acts on a *finite* range (if H is finite range), and decays rapidly
- Easy to calculate - similar complexity to one iteration of DMRG.
- High order algorithm with *one pass* through the system (compare 4th order Lie-Trotter-Suzuki)
- Can do long(er) range interactions - as long as they decay sufficiently quickly

Conclusions

- MPS in the infinite size limit has many advantages
- Infinite Boundary Conditions - solve a finite section of a lattice embedded in an infinite system
- Expanding window - ‘light cone‘ evolution
- Moving window - follow the wavefront
- Decompositions of the time evolution operator are efficient if they are *block local*