Efficient simulation of 1D quantum many body systems

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Overview:
1. Entanglement & area law
2. Efficient representation: MPS
3. Time evolving block decimation
4. Density-matrix renormalization
5. Dissipation assisted operator evolution

Reviews/Lecture notes:

Hauschild and FP '18
https://arxiv.org/abs/1805.00055

Schollwöck '10
https://arxiv.org/abs/1008.3477

Cirac et al '20
https://arxiv.org/abs/2011.12127

Dissipation assisted operator time evolution:

https://arxiv.org/abs/2004.05177

Tutorials: http://go.tum.de/603150

Many body Hilbert space $\mathcal{H} = \mathbb{C}^{d^N}$ with local dimension d

$\rightsquigarrow$ d^N states $|i_1 i_2 \dots i_N\rangle := |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_N\rangle$, $i_n = 1 \dots d$.

↑ tensor product structure

Example $S = \frac{1}{2}$: $|\uparrow\uparrow\uparrow \dots \uparrow\uparrow\rangle$, $|\downarrow\uparrow\uparrow \dots \uparrow\rangle$ .... $|\downarrow\downarrow\downarrow \dots \downarrow\downarrow\rangle$

Any state in the Hilbert space can be written as

$$|\psi\rangle = \sum_{\{i_n\}} \psi_{i_1 \dots i_L} |i_1 \dots i_N\rangle$$

$\rightsquigarrow$ How to "compress" states to a manageable size?

1. Entanglement and area law

$$\overset{A}{\circ \quad \circ \quad \circ} \; \Big| \; \overset{B}{\circ \quad \circ \quad \circ} \qquad |\psi\rangle \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

Assume that we only have access to A $\quad M_A \otimes 1$

How to characterize measurements?

Reduced density matrix:

$$\rho_A = \sum \psi^*_{i'j} \psi_{ij} \, |i'\rangle\langle i|_A \quad \text{with } \mathrm{Tr}_X(\cdot) = \sum \langle k|\cdot|k\rangle_X$$
$$= \mathrm{Tr}_B \big(\underbrace{|\psi\rangle\langle\psi|}_{\rho} \big)$$

From the def. we find (1) $\rho_A = \rho_A^\dagger$ (2) $\rho_A \geq 0$ (3) $\mathrm{Tr}(\rho_A) = 1$

Entangled state has mixed ρ_A, ρ_B (i.e., $S \neq 0$)

$$\boxed{\text{(von-Neumann) entanglement entropy } S = -\mathrm{Tr}_A\, \rho_A \cdot \log \rho_A}$$

Renyi entropy : $S_\alpha = -\frac{1}{1-\alpha} \ln \mathrm{Tr}\, \rho_A^\alpha$

<u>Schmidt decomposition</u> : ($\hat{=}$ SVD)

Schmidt values Schmidt states

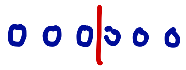
$$|\psi\rangle = \sum_{\alpha=1}^{\min(N_A,N_B)} \lambda_\alpha\, |\phi_\alpha\rangle_A\, |\phi_\alpha\rangle_B\,, \quad \lambda_1 \geq \lambda_2 \geq \cdots \geq 0$$

$\langle \phi_\alpha | \phi_{\alpha'} \rangle = \delta_{\alpha\alpha'}$ (unique up to degeneracies)

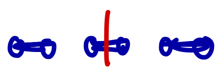
$$\rho_A = \sum_\alpha \lambda_\alpha^2\, |\phi_\alpha\rangle_A {}_A\langle \phi_\alpha|\,, \quad \rho_B = \sum_\alpha \lambda_\alpha^2\, |\phi_\alpha\rangle_B {}_B\langle \phi_\alpha|$$

and thus $S = -\sum \lambda_\alpha^2 \cdot \log \lambda_\alpha^2$. (normalization: $\sum_\alpha \lambda_\alpha^2 = 1$)

Examples: * Product state $\rightsquigarrow \lambda_1 = 1,\ \lambda_{\alpha>1} = 0$ and $S = 0$

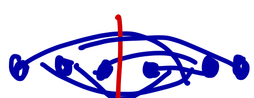


* Dimerized state $\rightsquigarrow \lambda_{\alpha \leq d} = \frac{1}{\sqrt{d}},\ \lambda_{\alpha > d} = 0$ and $S = \ln d$



$\frac{1}{\sqrt{d}} \sum_{\alpha=1}^{d} |\alpha\rangle|\alpha\rangle$

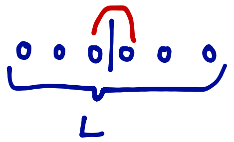
* Random state : Entanglement close to S_{max}



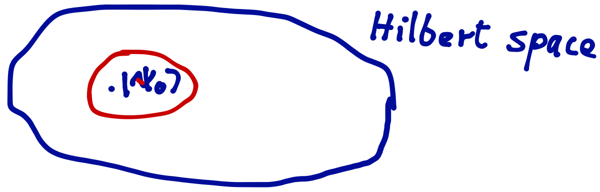
$S = \frac{L}{2} \log d - \frac{1}{2}$ for half chain bipartition. [Page 93]

Area law

Ground states of (gapped) local Hamiltonians fulfill the area law $S \sim L^{D-1}$ [proof exists for 1D, Hastings]

1D  $S(L) = \text{const.} \quad (L > \xi)$

(gapless $S \sim \log L$)



1D area law $\Rightarrow$ Schmidt values decay quickly and thus we can find a good approx. of $|\psi\rangle$ by keeping $\chi = \text{const.}$ Schmidt states: $|\psi\rangle \approx \sum_{\alpha=1}^{\chi \ll 2^L} \lambda_\alpha |\alpha\rangle_L |\alpha\rangle_R$

Ground states are "close" to product states ⇝ efficient representation

2 Matrix-product states

Product states: $\psi_{i_1 \dots i_L} = \phi^{[1],i_1} \cdots \phi^{[L]i_L}, \quad \phi^{[n]i_n} \in \mathbb{C}$

⇝ # parameters $\propto L d$

FM: $|\psi\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$

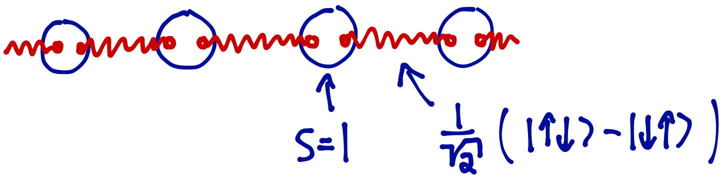
Matrix-product state (MPS): $\psi_{i_1 \dots i_L} = A^{[1]i_1} \cdots A^{[L],i_L}, \quad A^{[n]i_n}$ are $\chi \times \chi$ matrices

⇝ # parameters $\propto L \cdot d \cdot \chi^2 \ll L \cdot d \cdot 2^{L/2}$

GHZ: $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\downarrow\downarrow\rangle)$ has MPS has $\chi = 2$

MPS representation $A^{\uparrow} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad A^{\downarrow} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

AKLT : $S=1$ spin chain $\quad H = \sum P^{S=2}_{j,j+1} = \sum \vec{S}_j \vec{S}_{j+1} + \frac{1}{3}(S_j S_{j+1})^2 + \frac{2}{3}$

$|\Psi_0\rangle$: 

⊙ : $|+\rangle = |\uparrow\uparrow\rangle$, $|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, $|-\rangle = |\downarrow\downarrow\rangle$

The MPS representation is then

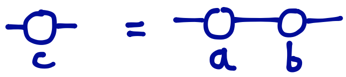
$$A^+ = \sqrt{\tfrac{2}{3}}\,\sigma^+ \;,\quad A^0 = \frac{-1}{\sqrt{3}}\,\sigma^z \;,\quad A^- = -\sqrt{\tfrac{2}{3}}\,\sigma^-$$

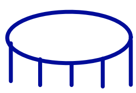
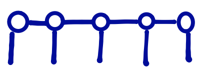
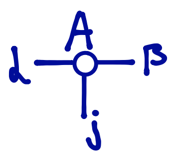
> Key idea : Assume the states we are interested in can be well approximated by MPS.
>
> This is the case for all states that fulfill the area law [Schuch et al. '06].

Tensor network notation

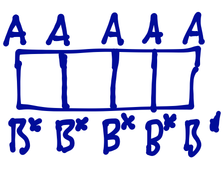
Useful diagramatic representation of tensor networks :

Scalar $a \;\hat{=}\;$ ○ , vector $a_i \;\hat{=}\;$ ○— , matrix $a_{ij} \;\hat{=}\;$ —○—

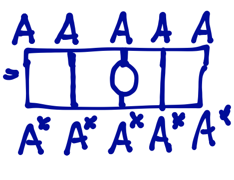
tensor operations : $c_{ik} = \sum_j a_{ij} b_{jk}$ $\rightsquigarrow$ 

MPS :  =  , 

Overlap :

$\langle\psi|\phi\rangle =$ 

Expectation value :

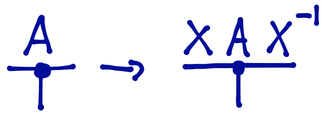
$\langle\psi|O|\psi\rangle =$ 

$\rightsquigarrow$ Scales as $\mathcal{O}(L \cdot \chi^3 d)$

Canonical form of MPS

From now on: $A^{[n]\,i_n} = A^{i_n}$ and $L \to \infty$ / Pure states

MPS are not uniquely defined :



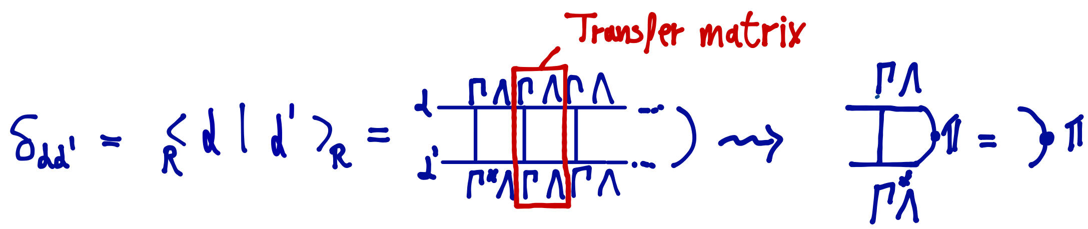
represents same state

Bonds are directly related to the Schmidt decomposition
and $A = \Gamma \cdot \Lambda$ ($\Lambda_{\alpha\alpha} = \lambda_\alpha$) [Vidal '03]

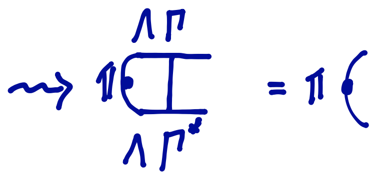
orthonormal basis

$$|\Psi\rangle = \sum_\alpha |\alpha\rangle_L \; \lambda_\alpha \; |\alpha\rangle_R$$

Transfer matrix



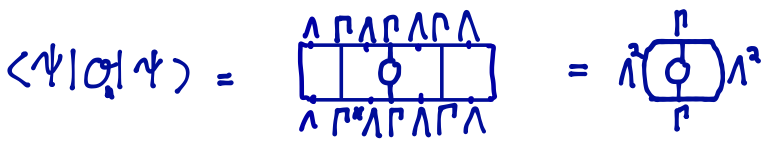
[similar for the left]



⟺ Transfer matrices have left/right eigenvalue 1 with eigenvector 𝟙

Uniquely defines the MPS up to a U(1) phase and dg in λ_α.

- Convenient to evaluate expectation values :



3 Time evolving block decimation (TEBD) [Vidal '03]

We know how to efficiently represent one-dimensional ground states and can calculate expectation values.

Given a Hamiltonian H, how to obtain the ground state MPS? Time evolution?

Real and imaginary time evolution of MPS

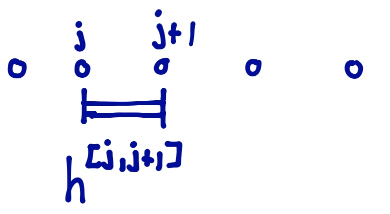
Time evolution in real time :

$$|\Psi(t)\rangle = e^{-iHt}\,|\Psi(t=0)\rangle$$

Time evolution in imaginary time yields GS:

$$|\Psi_0\rangle = \lim_{\tau\to\infty} \frac{e^{-H\tau}\,|\Psi_i\rangle}{\|\, e^{-H\tau}\,|\Psi_i\rangle \|}$$

Assume the Hamiltonian has the form $H = \sum_j h^{[j,j+1]}$



Decompose the Hamiltonian $H = F + G$

$$F = \sum_{\text{even } j} h^{[j,j+1]} \;, \quad G = \sum_{\text{odd } j} h^{[j,j+1]}$$

We observe: $[F^j, F^k] = [G^j, G^k] = 0$

$[G, F] \neq 0$

Baker-Campbell-Hausdorff $\left[e^{\varepsilon A} \cdot e^{\varepsilon B} = e^{\varepsilon(A+B) + \frac{\varepsilon^2}{2}[A,B] + \cdots} \right]$

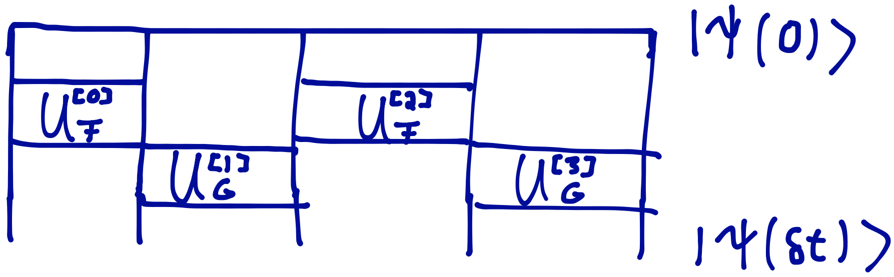
Decompose time evolution $\exp(-iHt) = \left[\exp(-iH \underbrace{t/N}_{=\delta t}) \right]^N$

$$e^{-i\delta t(F+G)} = \underbrace{e^{-i\delta t F}}_{U_F} \cdot \underbrace{e^{-i\delta t G}}_{U_G} + O(\delta t^2)$$

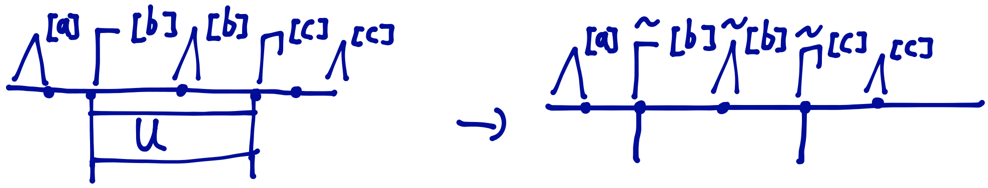
Two chains of two-site gates

$$U_F = \prod_{\text{even } j} e^{-iF^{[j]}\delta t}, \qquad U_G = \prod_{\text{odd } j} e^{-iG^{[j]}\delta t}$$

This is how the evolution of an MPS for one time step looks like:



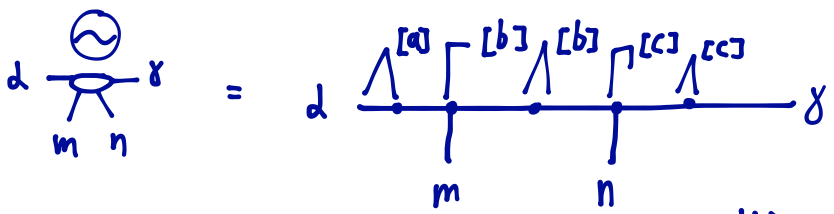
Need an algorithm to project back to MPS form



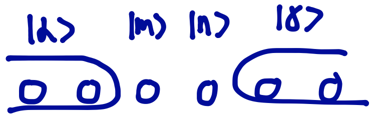
TEBD algorithm [Vidal '03]

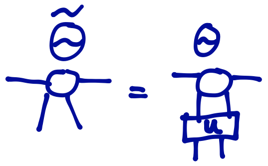
① „Apply U"

$d\chi \times d\chi$



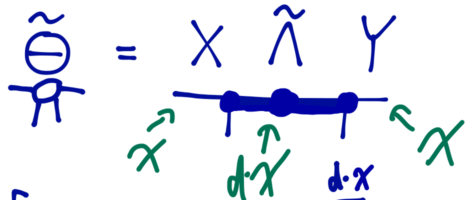
$$|\psi\rangle = \sum \Theta^{mn}_{\alpha\gamma} \, |\alpha\rangle |m\rangle |n\rangle |\gamma\rangle$$

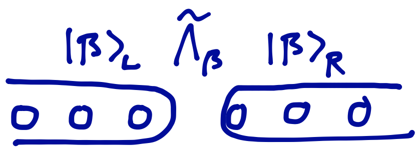




$$\left[\tilde{\Theta}^{mn}_{\alpha\gamma} = U^{mn}_{m'n'} \, \Theta^{m'n'}_{\alpha\gamma} \right]$$

② „SVD" ($d\chi \times d\chi$ matrix)

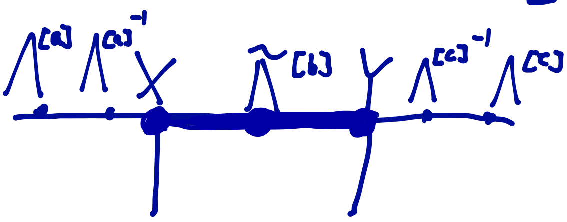




$$\left[\tilde{\Theta}_{(\alpha m)(n\gamma)} = \sum_{\beta=1}^{d\cdot\chi} X_{(\alpha m),\beta} \, \tilde{\Lambda}_\beta \, Y_{\beta,(n\gamma)} \right]$$

③ „Obtain new MPS"

insert identity



④ „Truncate"

Discard smallest Schmidt values / states: $d\chi \rightarrow \chi$
(i.e., keep only χ rows / columns of the tensors)

Applying this algorithm iteratively to even / odd bonds, we obtain the time evolution!

Computational time scales as $O(L \cdot d^3 \chi^3)$

Computational errors:
* truncation error: exponential growth of χ when doing real time evolution
* Trotter error (relatively harmless): Smaller δt and higher order expansions
* Instabilities for small Λ_β (as we need to invert it): fix by [Hastings '09]
* Canonical form for imaginary time evolution only when $\delta\tau \to 0$.
* Generalization to 2D: Isometric tensor networks [Zaletel & FP '20]

4 Density-matrix renormalization group (DMRG) [White '92]

Variational method to find ground states of a one-dimensional Hamiltonian within the manifold of MPS.

Original motivation: Improvement of RG (thus the name)

Here we will discuss the DMRG algorithm in the framework of MPS.

Matrix-Product Operators (MPOs)

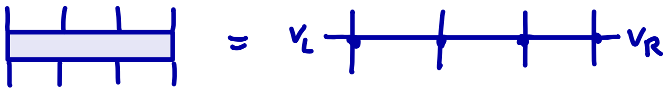
Recall: MPS

$$\psi_{i_1 \dots i_L} = A^{[1] i_1} \cdots A^{[L], i_L}, \quad A^{[n] i_n} \text{ are } \chi \times \chi \text{ matrices}$$

Similarly, an operator $\hat{O}$ can be expressed as an MPO

$$O_{i_1 i_2 \dots i_L,\, i_1' i_2' \dots i_L'} = M^{[1] i_1 i_1'} \cdots M^{[L], i_L i_L'}, \quad M^{[n] i_n i_n'} \text{ are } \chi\times\chi \text{ matrices}$$

Graphically this looks like:



Example:

Pauli matrices

$$H = -J\sum_i \sigma^z_i \sigma^z_{i+1} + g\sum_i \sigma^x_i \rightsquigarrow M = \begin{pmatrix} \mathbb{1} & \sigma^z & g\sigma^x \\ 0 & 0 & -J\sigma^z \\ 0 & 0 & \mathbb{1} \end{pmatrix}$$

$$L=3:\ \underset{v_L}{(1,0,0)} \begin{pmatrix} \mathbb{1} & \sigma^z & g\sigma^x \\ 0 & 0 & -J\sigma^z \\ 0 & 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} \mathbb{1} & \sigma^z & g\sigma^x \\ 0 & 0 & -J\sigma^z \\ 0 & 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} \mathbb{1} & \sigma^z & g\sigma^x \\ 0 & 0 & -J\sigma^z \\ 0 & 0 & \mathbb{1} \end{pmatrix} \underset{v_R}{\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}$$

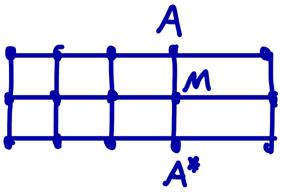
$$= (\mathbb{1}, \sigma^z, g\sigma^x) \begin{pmatrix} \mathbb{1} & \sigma^z & g\sigma^x \\ 0 & 0 & -J\sigma^z \\ 0 & 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} \mathbb{1} & \sigma^z & g\sigma^x \\ 0 & 0 & -J\sigma^z \\ 0 & 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= (\mathbb{1}\otimes\mathbb{1},\ \mathbb{1}\otimes\sigma^z,\ g\,\mathbb{1}\otimes\sigma^x - J\sigma^z\otimes\sigma^z + g\sigma^x\otimes\mathbb{1}) \begin{pmatrix} \mathbb{1} & \sigma^z & g\sigma^x \\ 0 & 0 & -J\sigma^z \\ 0 & 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= g\left(\mathbb{1}\otimes\mathbb{1}\otimes\sigma^x + \mathbb{1}\otimes\sigma^x\otimes\mathbb{1} + \sigma^x\otimes\mathbb{1}\otimes\mathbb{1}\right)$$
$$-J\left(\mathbb{1}\otimes\sigma^z\otimes\sigma^z + \sigma^z\otimes\sigma^z\otimes\mathbb{1}\right) \ \checkmark$$

The expectation value of an MPO is given by:

$\langle H \rangle =$



Now we have all the tools to introduce the DMRG algorithm!

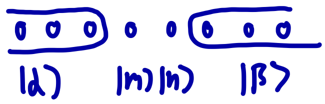
⇝ Sequencially optimize the matrices A^{i_n}.

⇝ The DMRG algorithm proceeds similarly to TEBD.

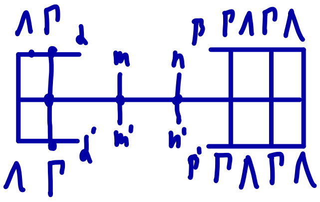
2-site DMRG algorithm:

① "2-site optimization"

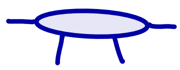
First project the Hamiltonian onto an effective basis in terms of physical states on adjacent sites $|m\rangle|n\rangle$ and Schmidt states left/right of the two sites:

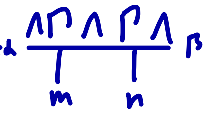


$$H^{eff}_{\alpha i j \beta, \alpha' i' j' \beta'} =$$

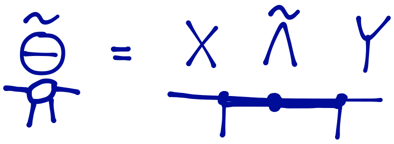


Use an iterative eigensolver to find the ground state of H^{eff} ⇝ $H^{eff}|\tilde{\Theta}\rangle = E_0|\tilde{\Theta}\rangle$ ⇝ $\tilde{\Theta} =$

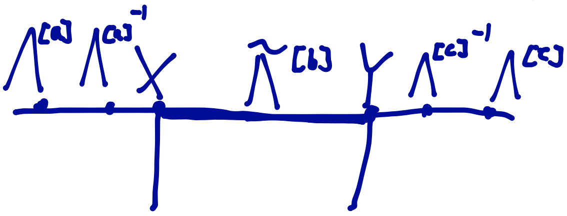


(use $\Theta_{\alpha m n \beta} =$  to initiate the iteration).

② „SVD" (dχ × dχ matrix)



③ „Obtain new MPS" ↙ insert identity



④ „Truncate"

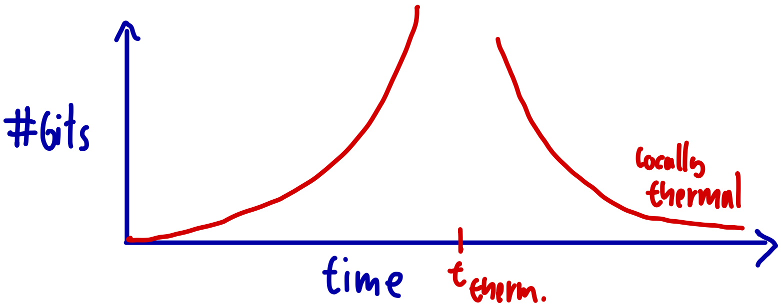
Discard smallest Schmidt values / states: $d\chi \to \chi$
(i.e., keep only χ rows/columns of the tensors)

... move to the next bond and repeat.

5 Dissipation assisted operator evolution (DAOE)

Time evolution following a global quench is exponentially hard due to the fast growth of entanglement.

In termalizing systems there is a paradox:



⇝ How to truncate the entanglement w/o loosing crucial information? (e.g., physical observables).

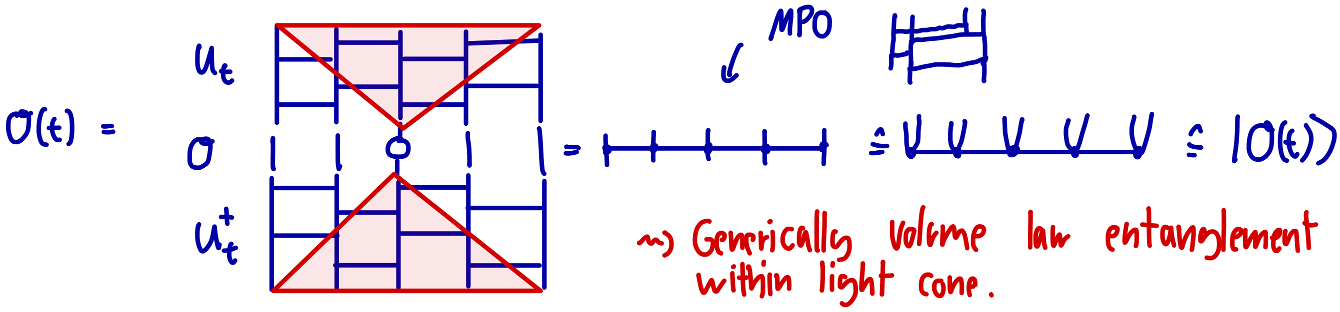
⇝ Various approaches

[White et al.: PRB 2018]
[Wurtz et al.: Ann. Phys. 2018]
[Klein Kvorning, arXiv:2105.11206]
[Schmitt, Heyl: SciPost 2018]
[Parker et al., PRX 2019]
[Krumnow et al.: arXiv:1904.11999]
[Leviatan et al., arXiv:1702.08894]

DOAE: The goal is to obtain $\langle O_2(t)\, O_1(0)\rangle_{\beta=0}$ (one dimension).

Heisenberg picture + truncation of "complicated" contributions

TEBD in the Heisenberg picture:



⇝ Generically volume law entanglement within light cone.

Truncate entanglement using artificial dissipation!

Every operator with local dimension $d=2$ can be expressed as superposition of Pauli strings:

$$|O) = \sum O_{i_1 i_2 \cdots i_L} \underbrace{|\sigma^{i_1}) \otimes |\sigma^{i_2}) \cdots \otimes |\sigma^{i_L})}_{|S)}, \quad i = 1, x, y, z$$

Define ℓ to be the number of non-trivial Pauli operators

$$1\,1\,1\,\sigma^x\,1\,\sigma^y\,1 \quad : \quad \ell = 2$$
$$1\,1\,1\,\sigma^y\,\sigma^z\,1\,\sigma^y \quad : \quad \ell = 3$$

Introduce an artificial dissipation:

$$D_{\ell^*}|S) = \begin{cases} |S) & \text{for } \ell \leq \ell^* \\ e^{-\gamma(\ell-\ell^*)}|S) & \text{for } \ell > \ell^* \end{cases}$$

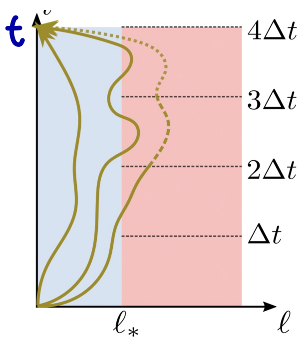
ℓ^* should be larger or equal to the support of conserved quantities.

D_{ℓ^*} can be written as MPO with small bond dimension!

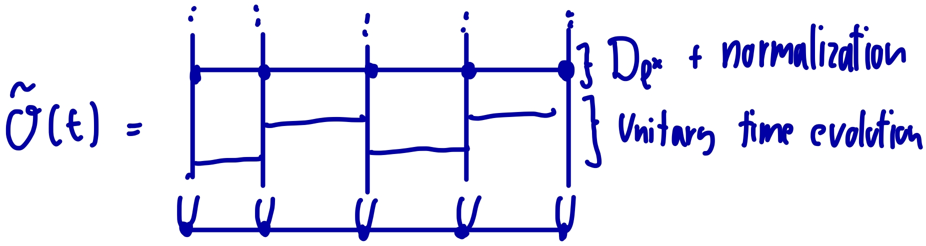
Why is it a promising approach to remove entanglement using D_{ℓ^*} when calculating $\langle O_2(t)|O_1(0)\rangle_{\beta=0}$?

⇝ D_{ℓ^*} removes entanglement by damping complicated operators.

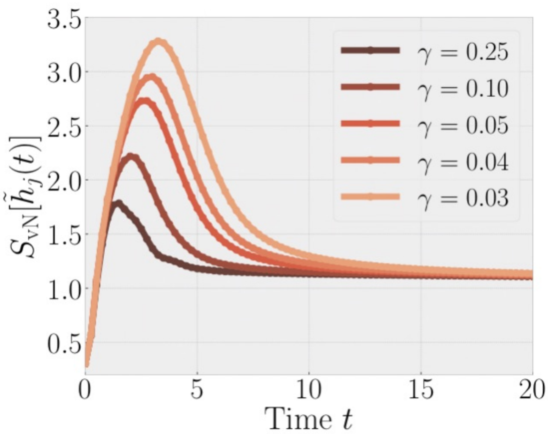
⇝ Key assumption: Backflow from large to small operators is weak!



Time evolution now combines unitary Heisenberg evolution and the application of the dissipator D_{ℓ^*}!



Test on the tilted field Ising chain



Obtain the diffusion constant from the mean square displacement (MSD):

$$C(x,t) \equiv \langle q_x \,|\, \tilde{q}_0(t) \rangle \quad \longrightarrow \quad d^2(t) \equiv \sum_x C(x,t)\, x^2 \quad \text{(MSD)}$$