Discussion on Numerical Approaches to Dynamics

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Simulating the time evolution of quantum-many body systems far out of equilibrium

Quantum Quenches

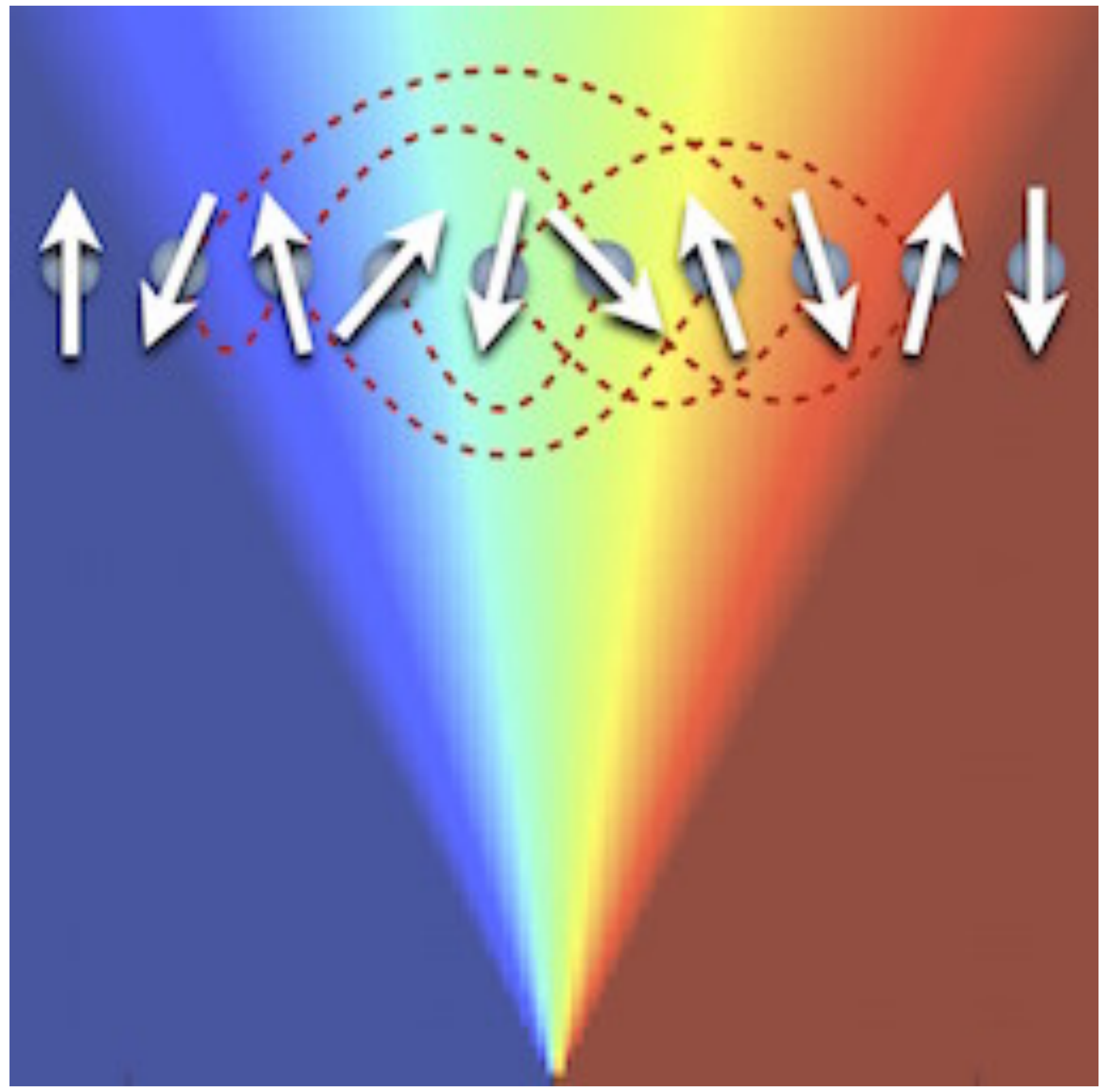
Dynamical phase transitions

Thermalization / Localization

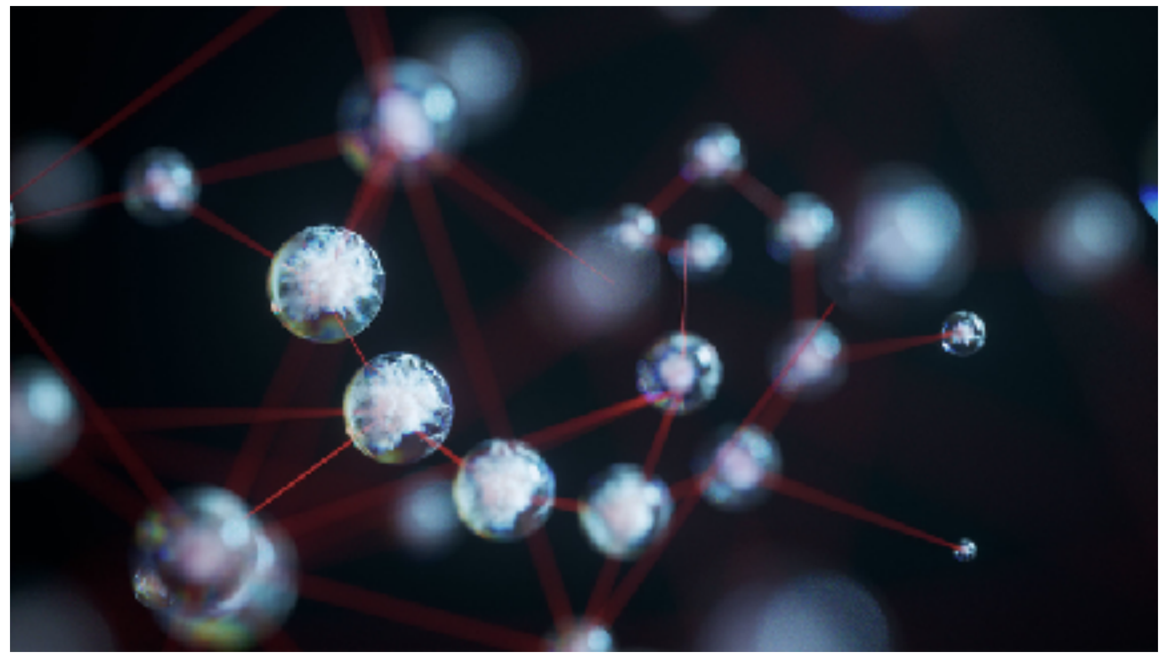
Floquet systems

Circuit models

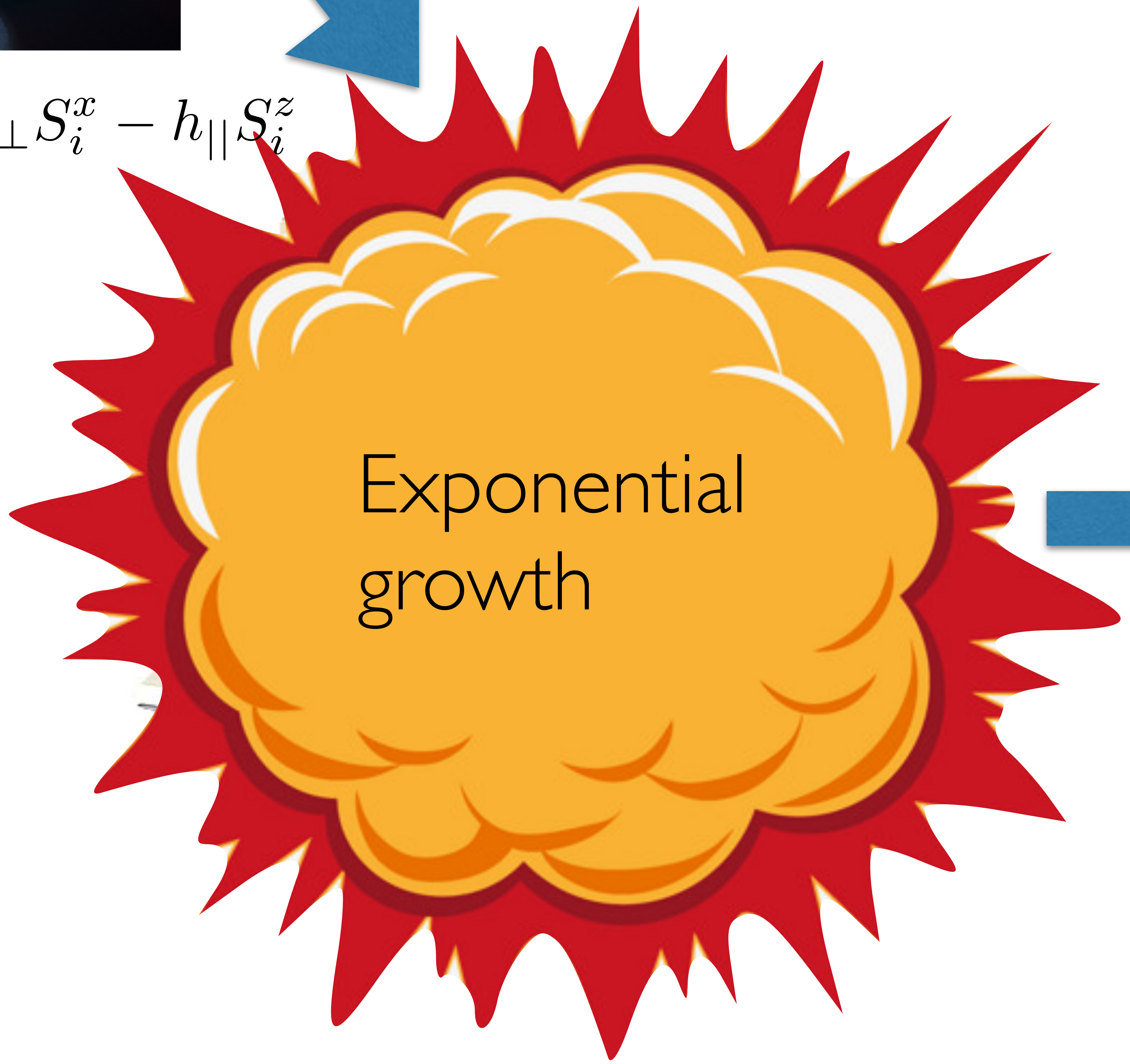
…



Quantum dynamics on a classical computer



$$H = \sum_i J S_i^z S_{i+1}^z - h_\perp S_i^x - h_{||} S_i^z$$



Correlations

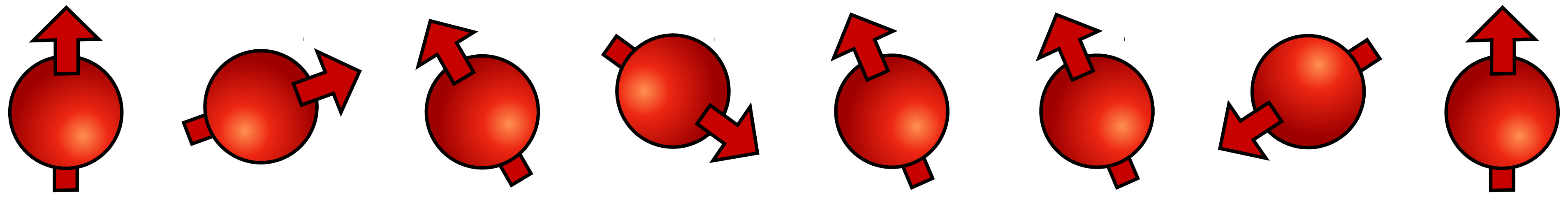
Entanglement

Universality

…

Quantum dynamics on a classical computer

Directly simulate the time evolution within the full many-body Hilbert space

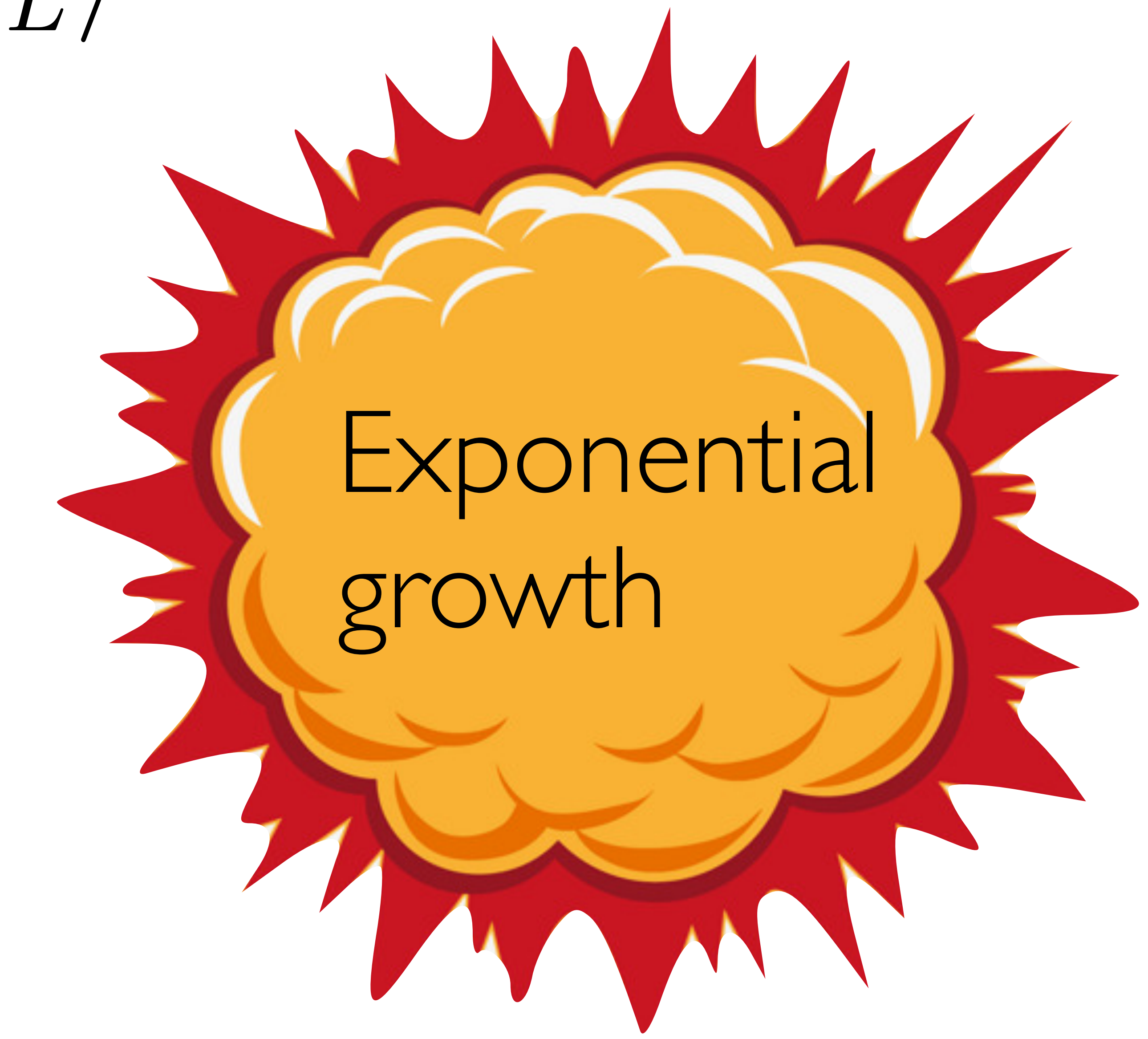


$$|\psi(t)\rangle = e^{-itH}|\psi(0)\rangle$$

$$= \sum_{j_1,\ldots,j_L} \psi_{j_1,\ldots,j_L}(t)|j_1,\ldots,j_L\rangle$$

➡ Full diagonalization up to ~20 sites for spin-1/2

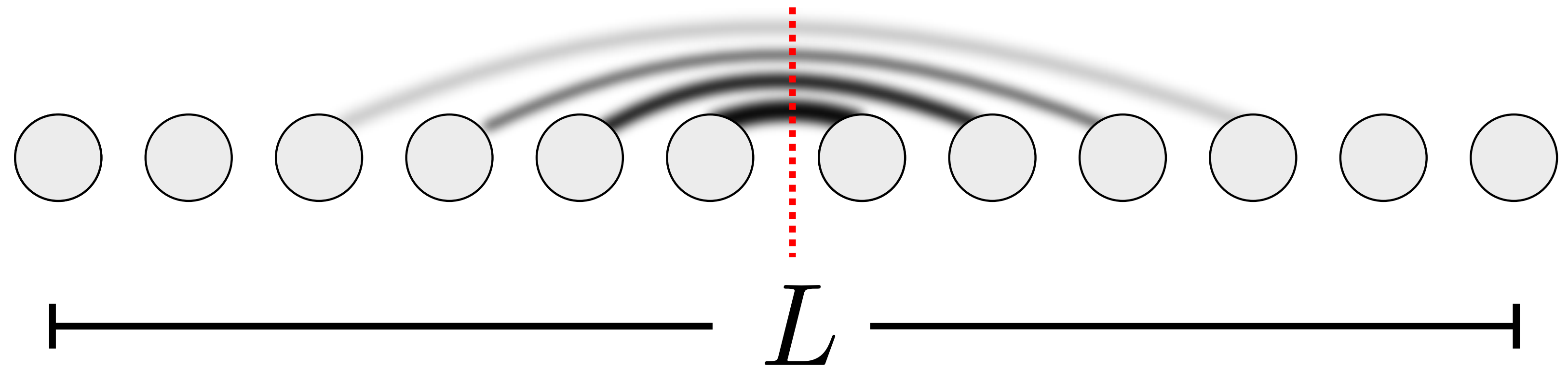
➡ Sparse methods up to ~30 sites for spin-1/2 (dynamical typicality)

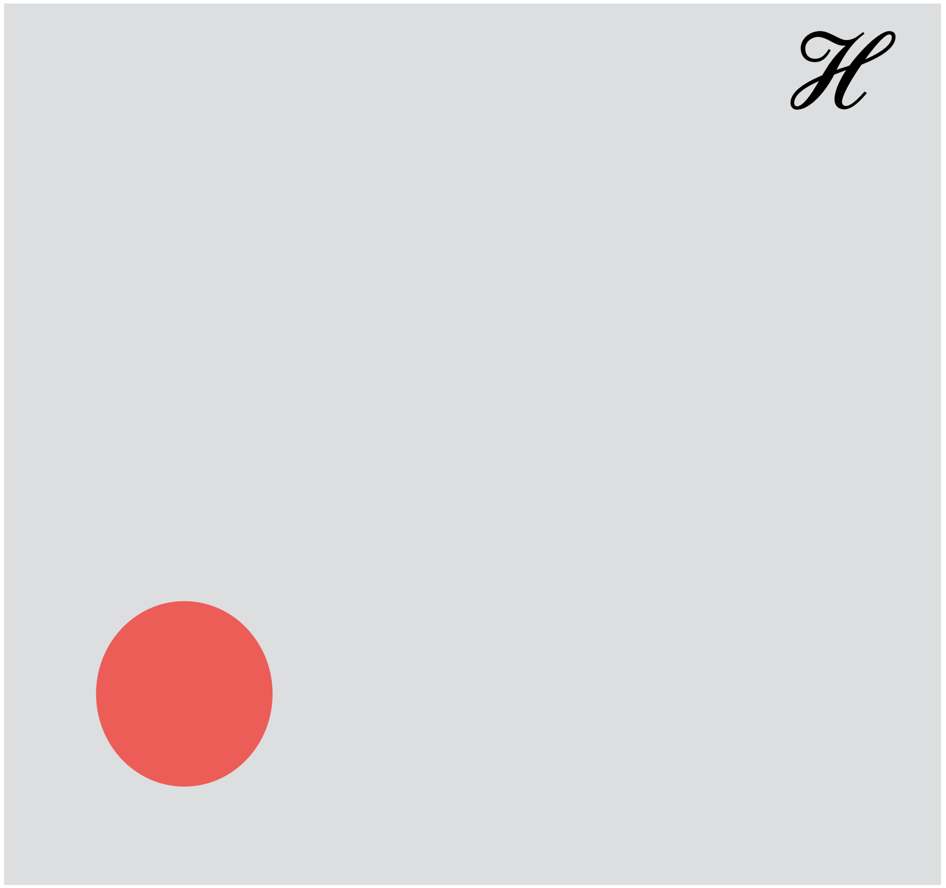


Entanglement

Area law in one dimensional systems: $S(L) = \text{const.}$

[Hastings '07]





All area law states live in a tiny corner of the Hilbert space!

➡ Efficient representation as matrix-product states

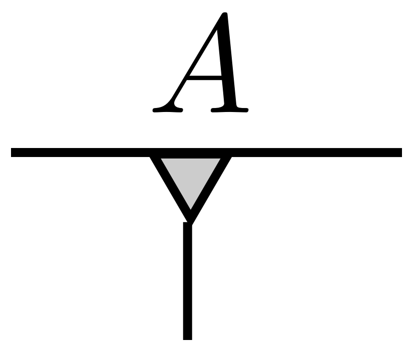
[M. Fannes et al. 92, Schuch et al '08]

Matrix-product states

Matrix-Product States: $d^L \rightarrow L d \chi^2$

[M. Fannes et al. 92, Schuch et al '08]

$$A^{j}_{\alpha\beta} =$$

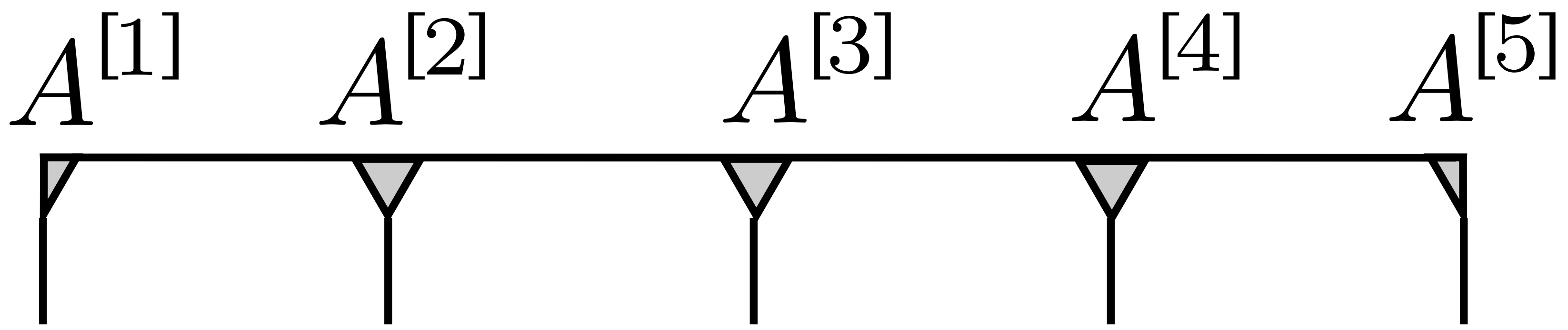


$$\psi_{j_1,j_2,j_3,j_4,j_5} = A^{[1]j_1}_{\alpha} A^{[2]j_2}_{\alpha\beta} A^{[3]j_3}_{\beta\gamma} A^{[4]j_4}_{\gamma\delta} A^{[5]j_5}_{\delta}$$

$$\alpha, \beta, \cdots = 1 \ldots \chi$$

$$j_n = 1 \ldots d$$

$$=$$

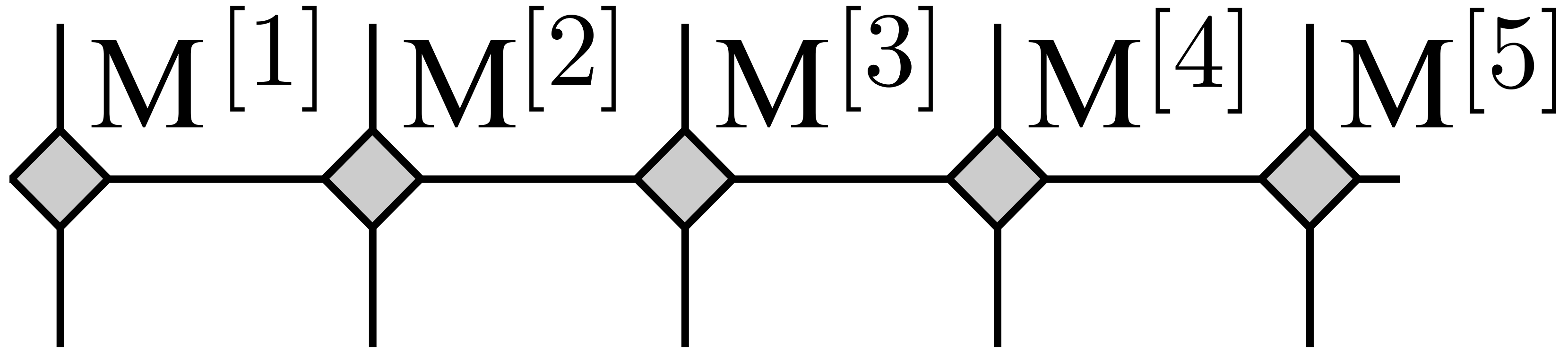


Bond dimension ~ exp(entanglement)

Matrix-Product Operators: $d^{2L} \rightarrow L d^2 \chi^2$

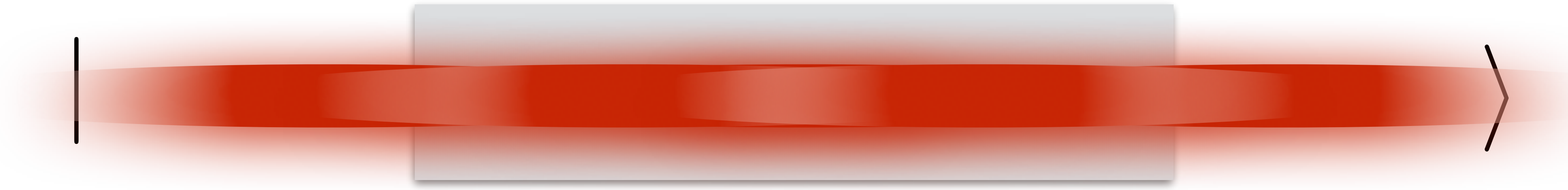
[Verstraete et al '04]

$$O^{j'_1,j'_2,j'_3,j'_4,j'_5}_{j_1,j_2,j_3,j_4,j_5} =$$



Thermalization: Loss of initial local informations

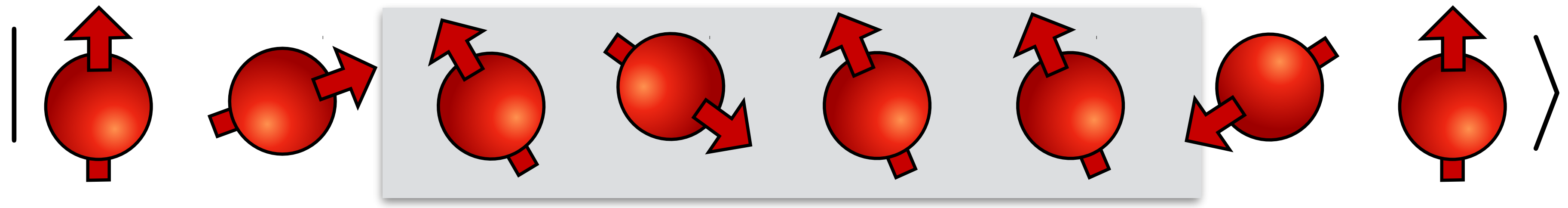
$$\rho_{\text{Block}} = \rho_{\text{Thermal}}$$



$S = 0$

$$U_t = \exp(-itH)$$

[non-integrable]

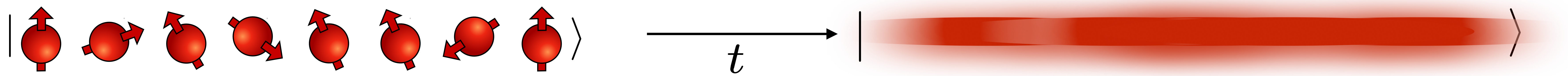


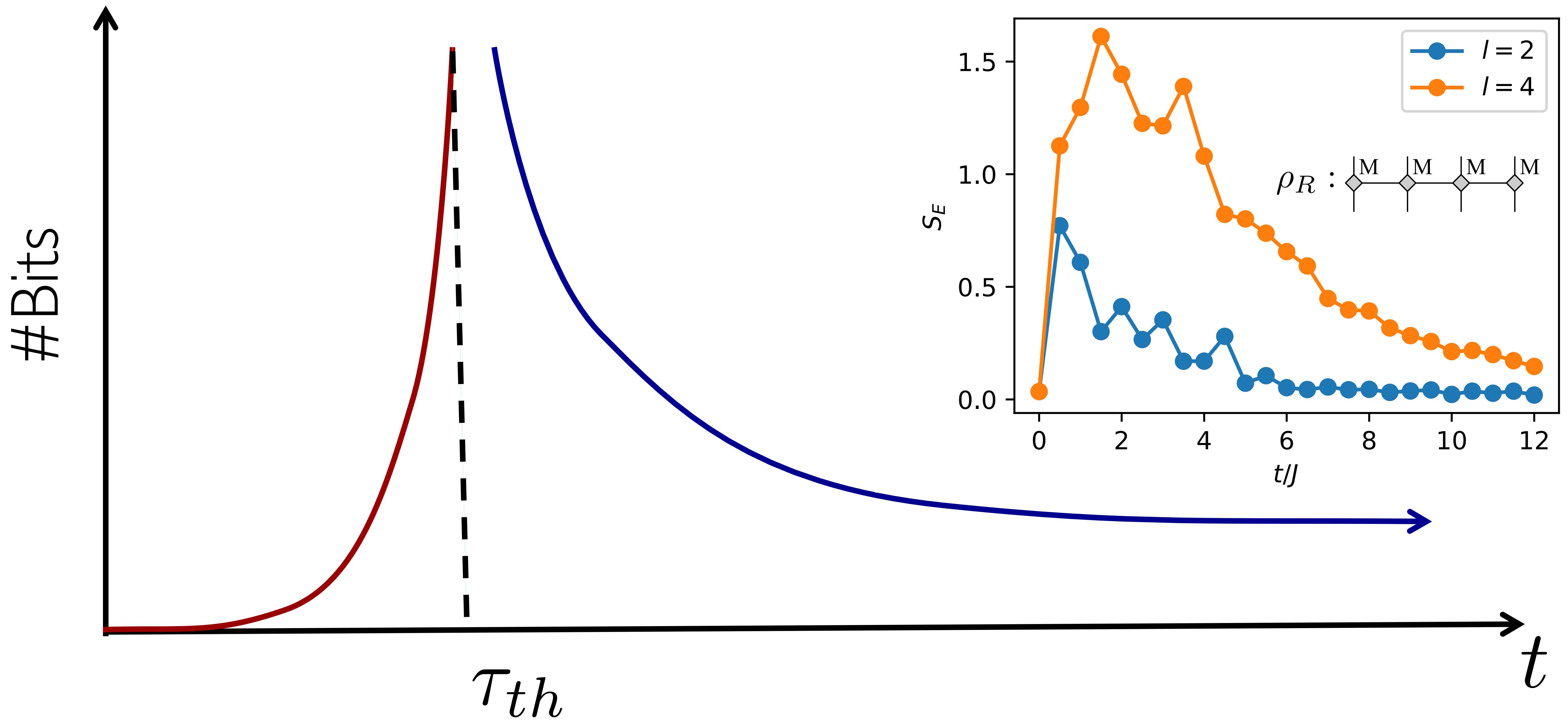
$S = 0$

[Srednicki, Deutsch, Rigol]

“Information paradox"

Quantum quench from product state





How to truncate entanglement (bond dimension) without sacrificing crucial information on physical (local) observables?

Time evolving block decimation

Consider a Hamiltonian $H = \sum_j h^{[j,j+1]}$

Decompose the Hamiltonian as $\mathrm{H{=}F{+}G}$

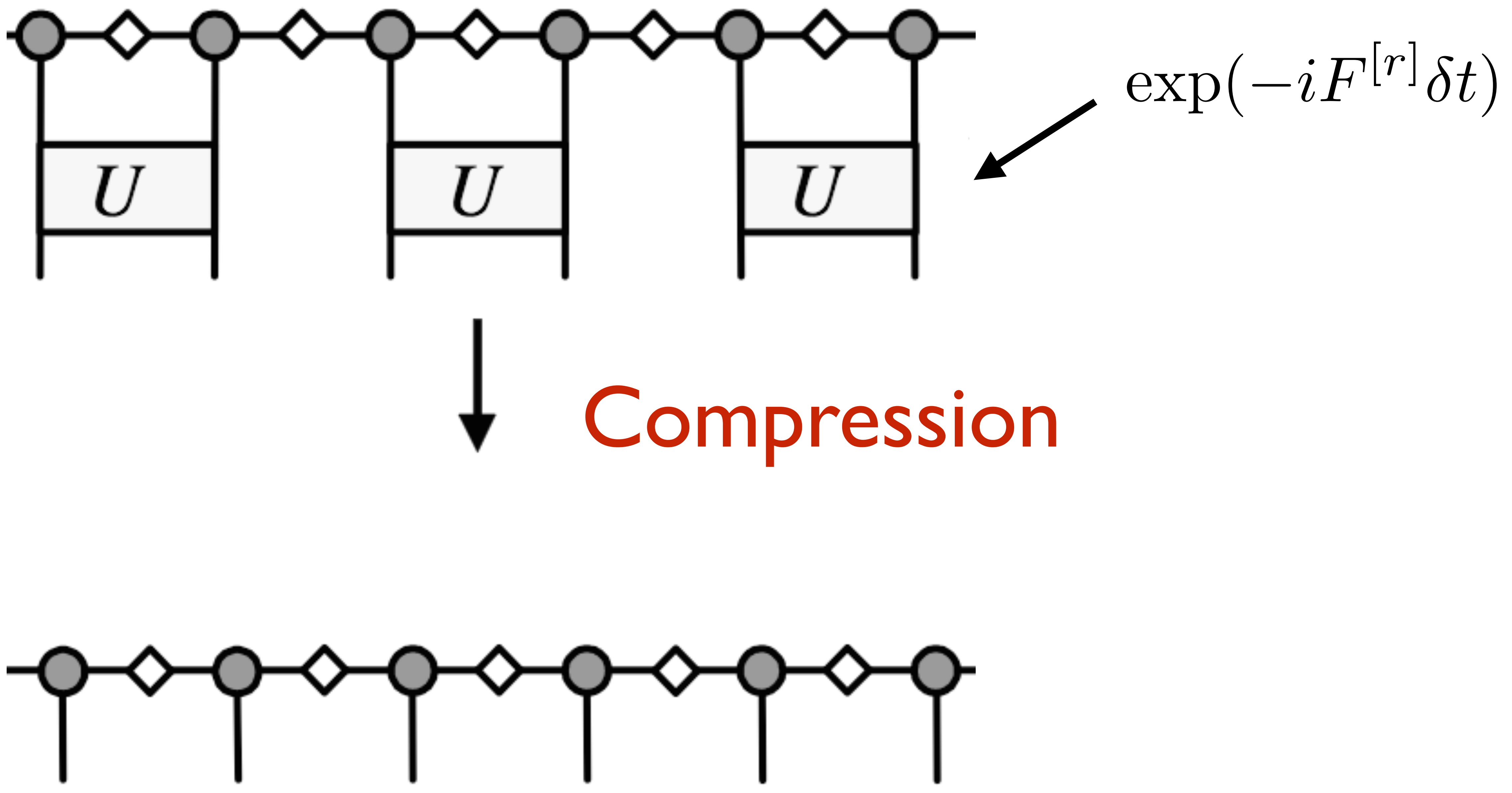
$$F \equiv \sum_{\text{even } j} F^{[j]} \equiv \sum_{\text{even } j} h^{[j,j+1]}$$

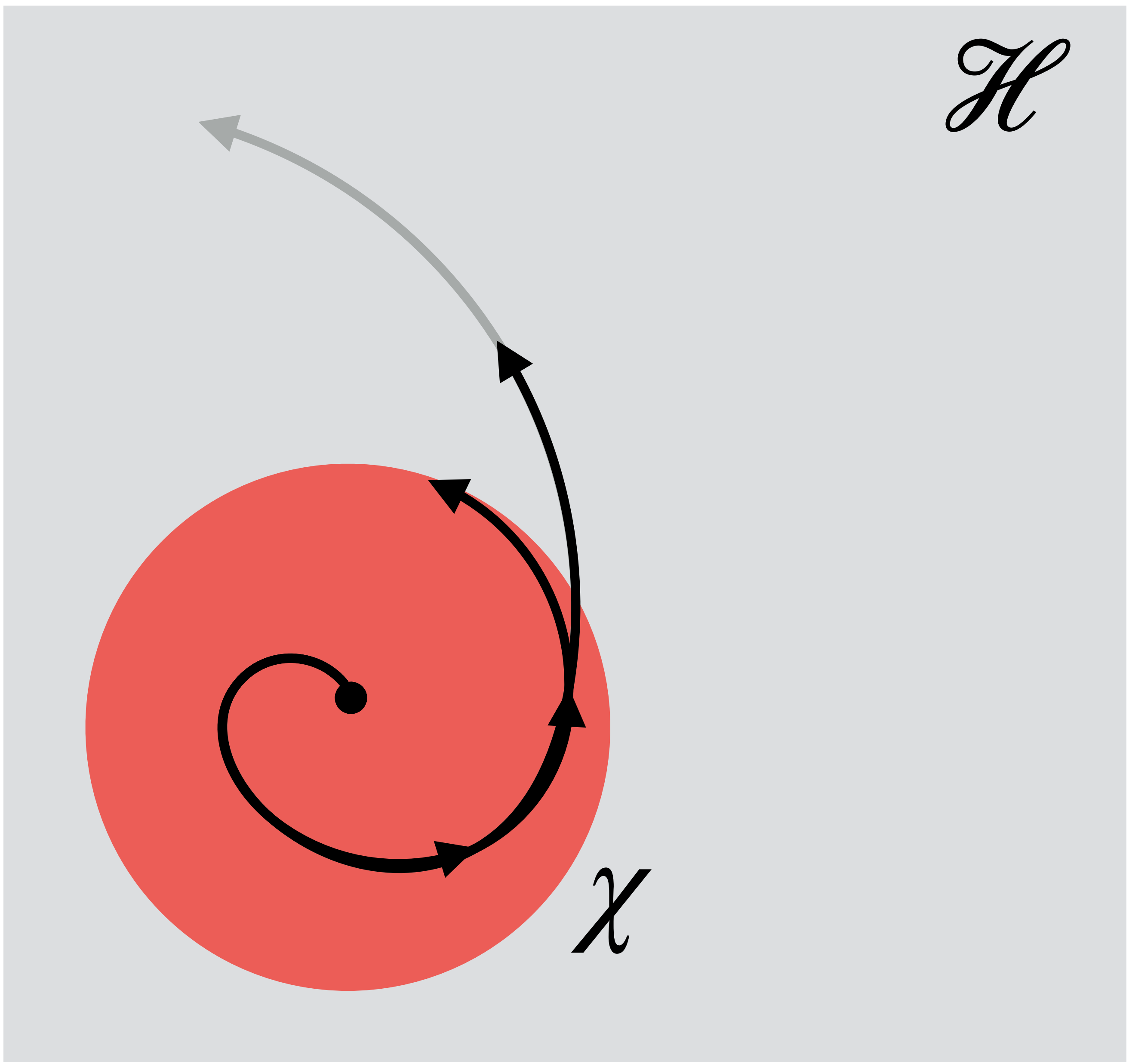
$$G \equiv \sum_{\text{odd } j} G^{[j]} \equiv \sum_{\text{odd } j} h^{[j,j+1]}$$

We observe $[F^{[r]}, F^{[r']}] = 0$ $([G^{[r]}, G^{[r']}] = 0)$
but $[G, F] \neq 0$

Time evolving block decimation

Time Evolving Block Decimation algorithm (TEBD) [Vidal '03]





➡ Destroys conservation laws of the microscopic model (e.g., energy conservation)

Time-dependent variational principle (TDVP)

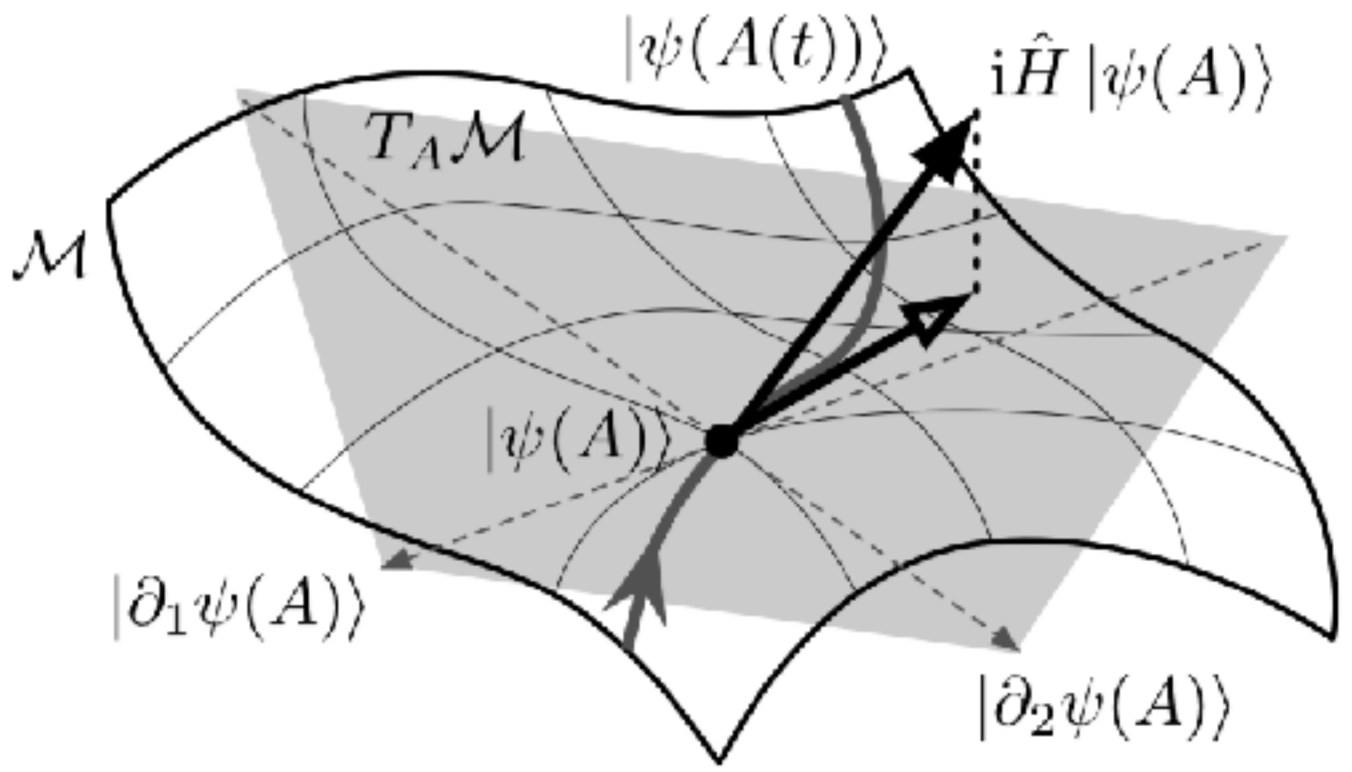
Variational manifold: MPS states with fixed bond dimension

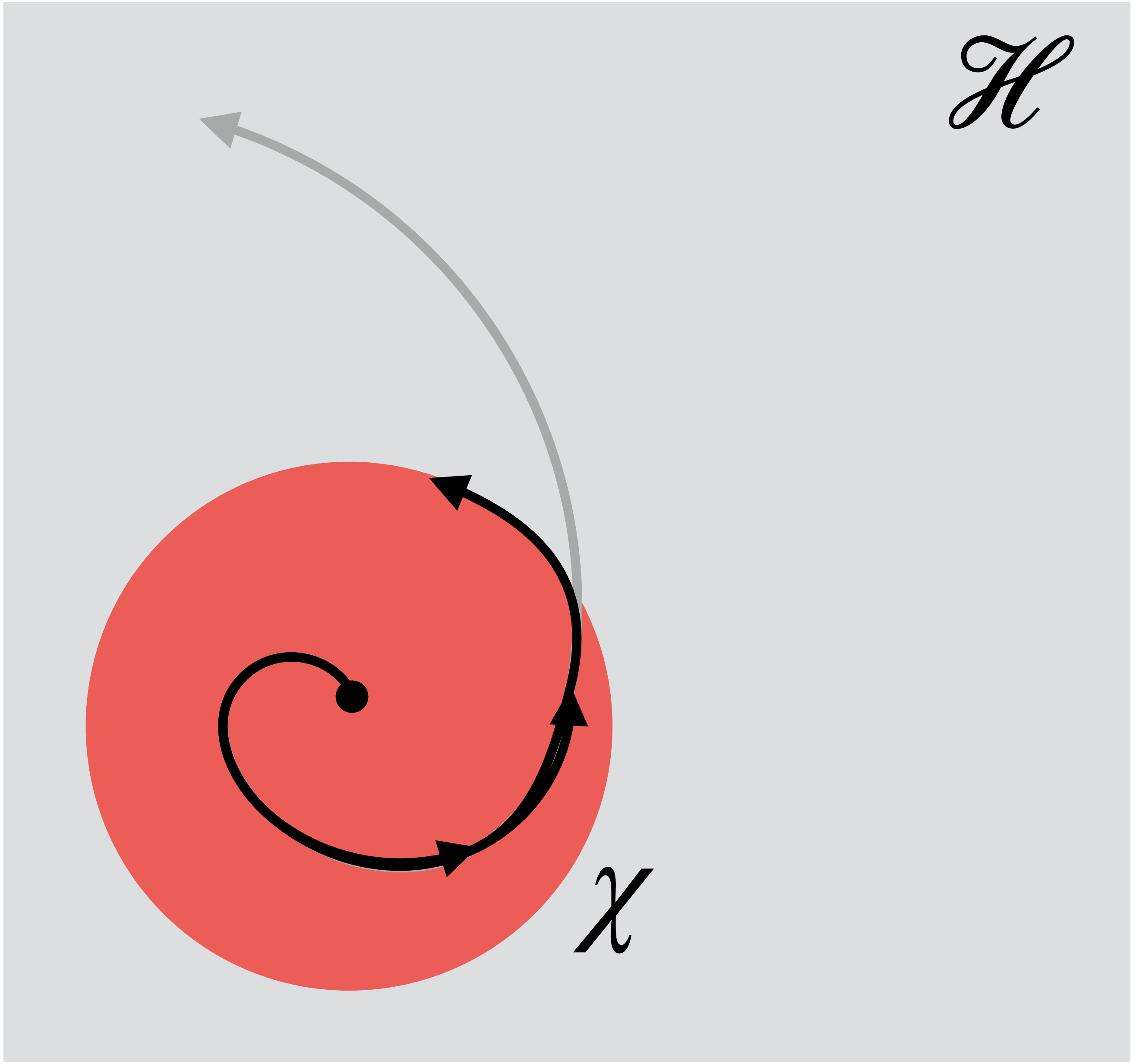
$$\psi_{j_1,j_2,j_3,j_4,j_5} = A^{[1]j_1}_{\alpha} A^{[2]j_2}_{\alpha\beta} A^{[3]j_3}_{\beta\gamma} A^{[4]j_4}_{\gamma\delta} A^{[5]j_5}_{\delta}$$

Classical Lagrangian $\mathcal{L}[\alpha,\dot{\alpha}] = \langle \psi[\alpha] \,|\, i\partial_t \,|\, \psi[\alpha] \rangle - \langle \psi[\alpha] \,|\, H \,|\, \psi[\alpha] \rangle$

Efficient evolution using a projected Hamiltonian

[Haegeman et al. '11, Dorando et al. '09]





➡ Does not violate global conservation laws (energy, particle number,…)

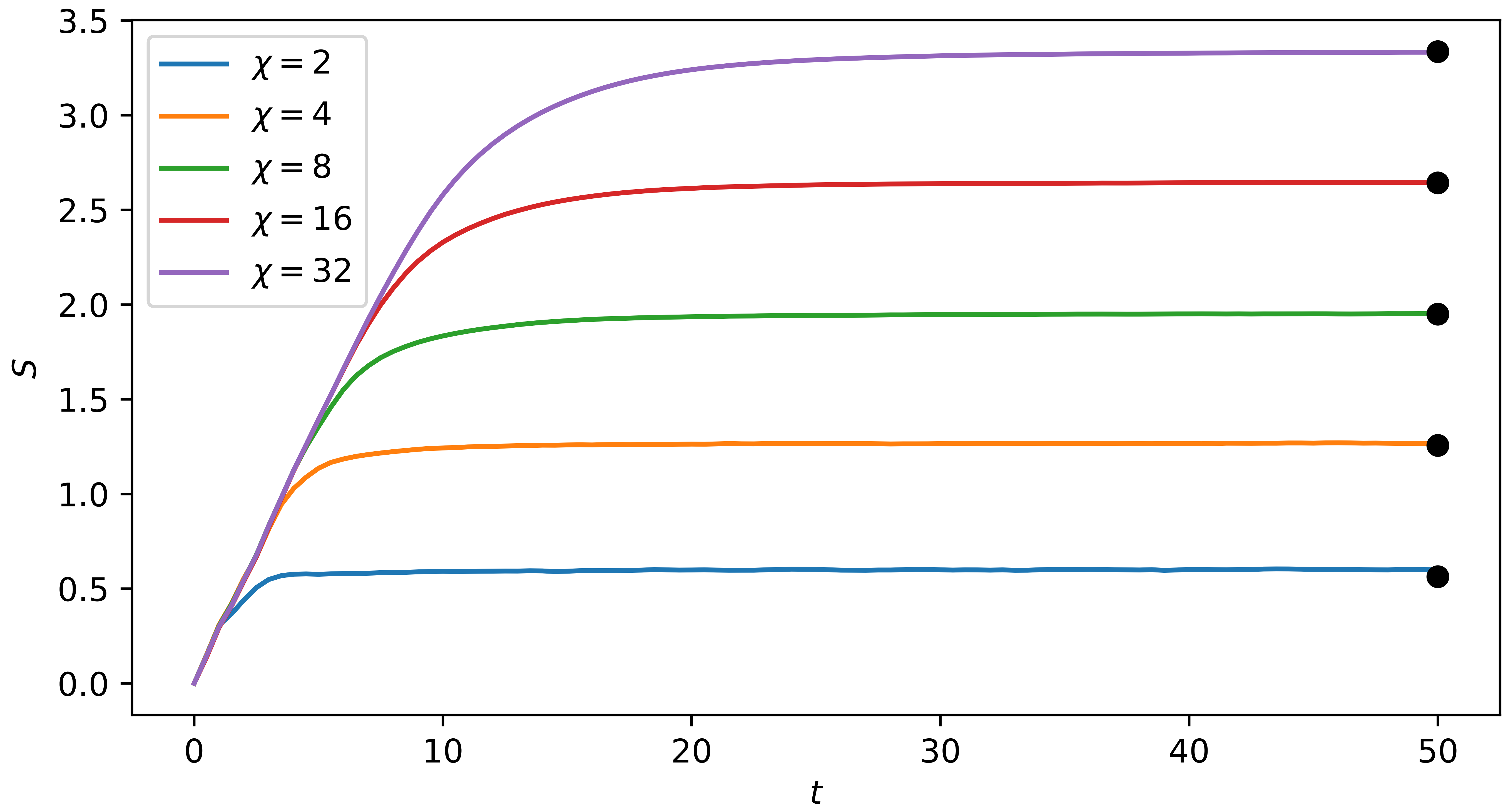
Leviatan, FP, Bardarson, Huse, Altman, arXiv:1702.08894

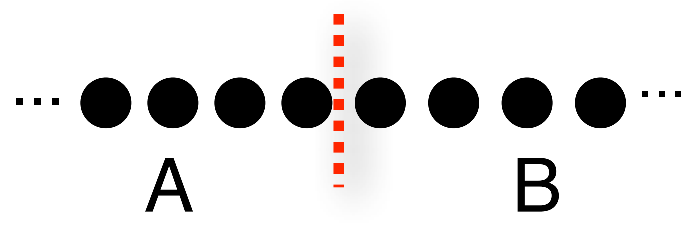
Time-dependent variational principle (TDVP)

Tilted field Ising model $$H = \sum_i J S_i^z S_{i+1}^z - h_\perp S_i^x - h_{||} S_i^z$$

Ensemble of random product states

Entanglement growth

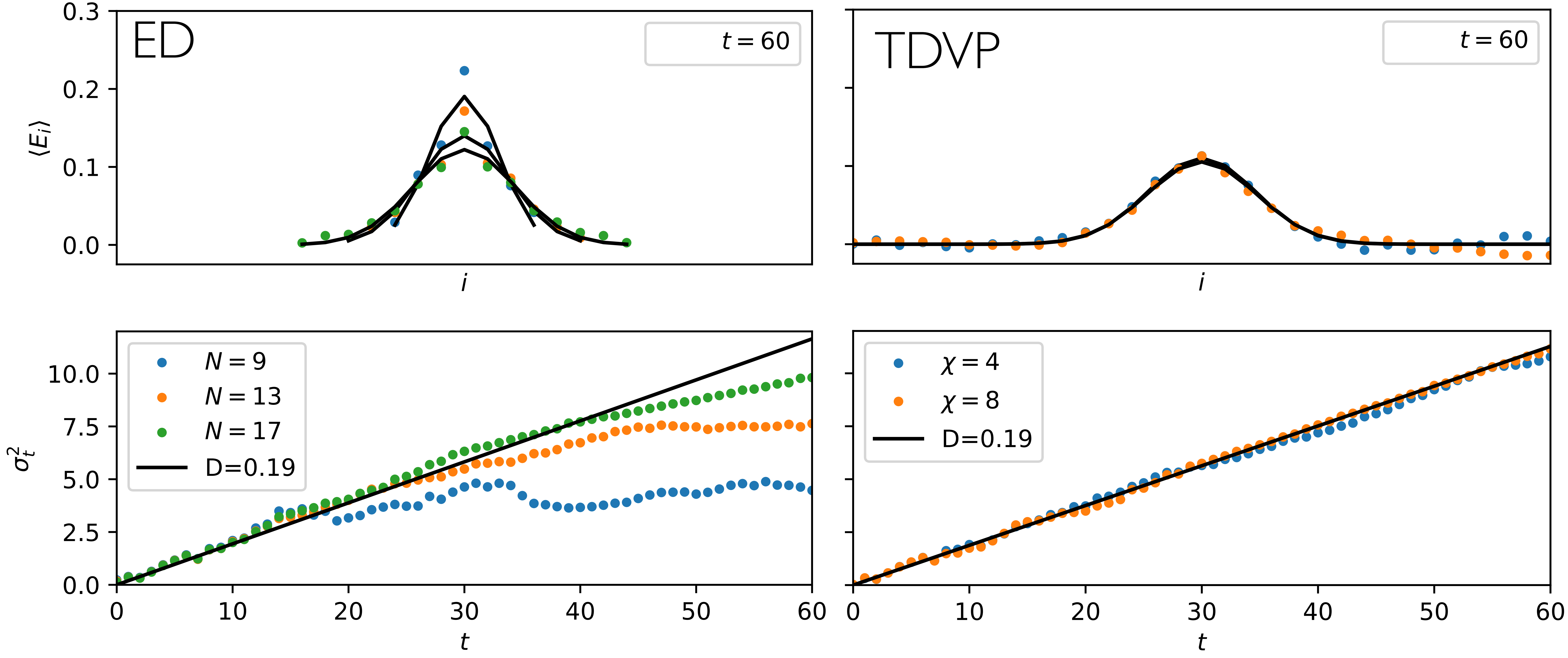




Time-dependent variational principle (TDVP)

Tilted field Ising model $H = \sum_i J S_i^z S_{i+1}^z - h_\perp S_i^x - h_{||} S_i^z$

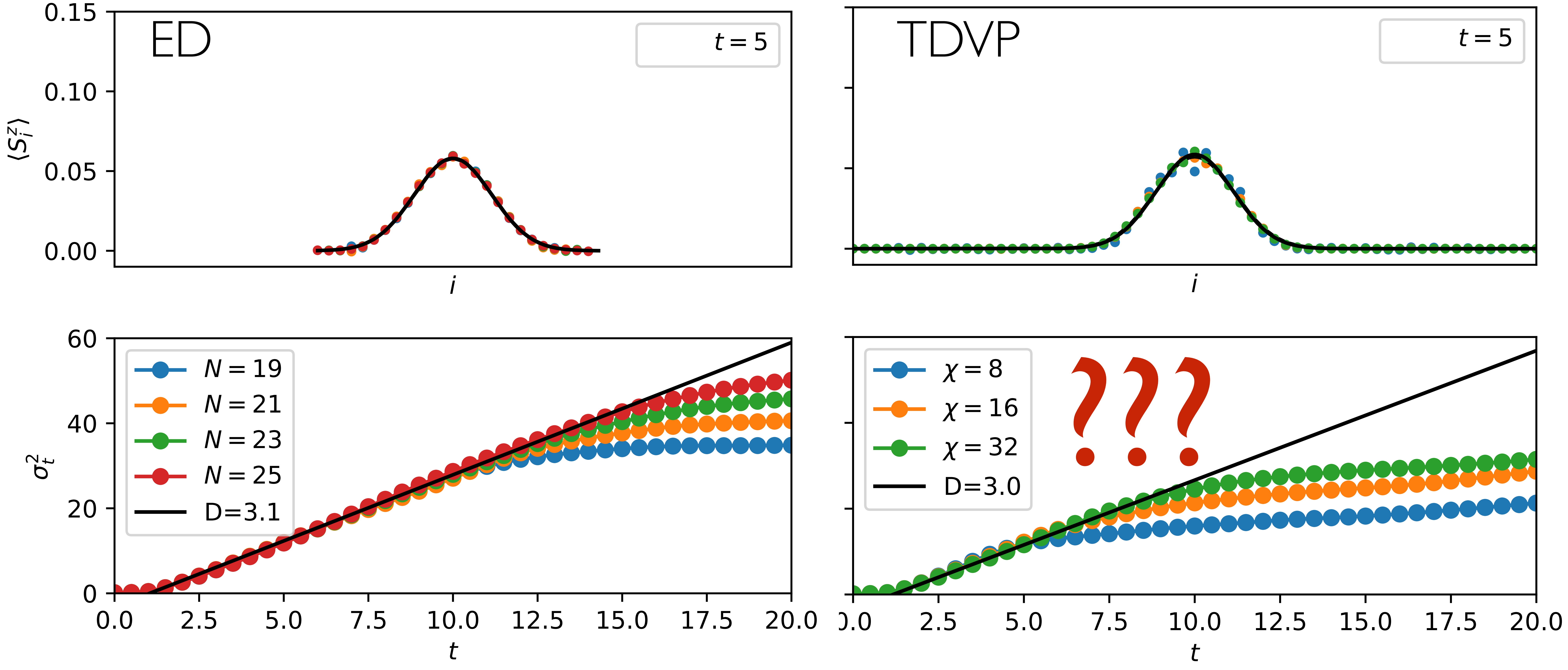
Ensemble of initial states: $S_{L/2}^+ |\psi(0)\rangle$ **Energy relaxation**



Time-dependent variational principle (TDVP)

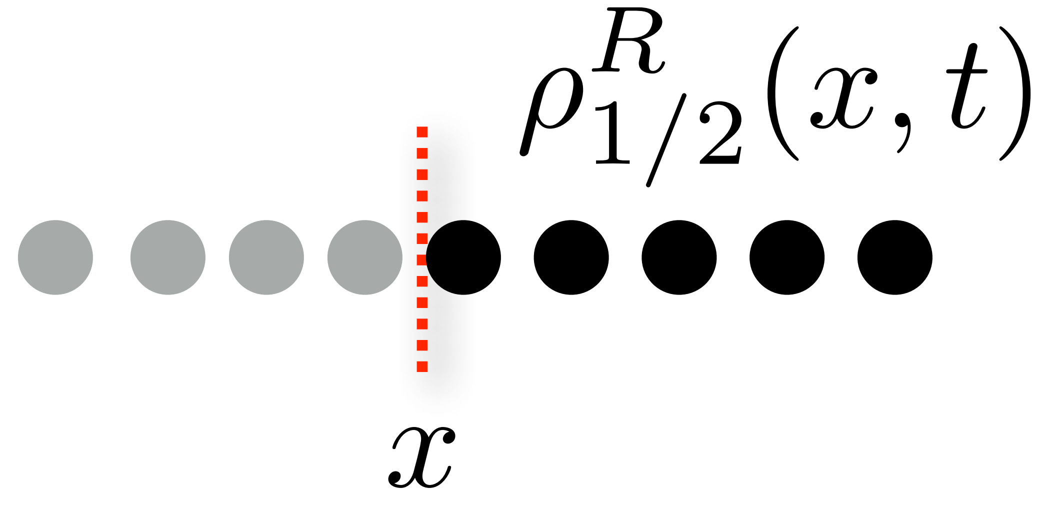
XXZ model $$H = \sum_{i>j} \xi^{i-j} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z)$$

Ensemble of initial states: $S^+_{L/2}|\psi(0)\rangle$ **Sz relaxation**



Diagnostics of chaos

Measure divergence between reduced density matrices



$$|\psi_1(t)\rangle = e^{-iHt}|\bullet\bullet\bullet\bullet\bullet\bullet\bullet\bullet\rangle$$

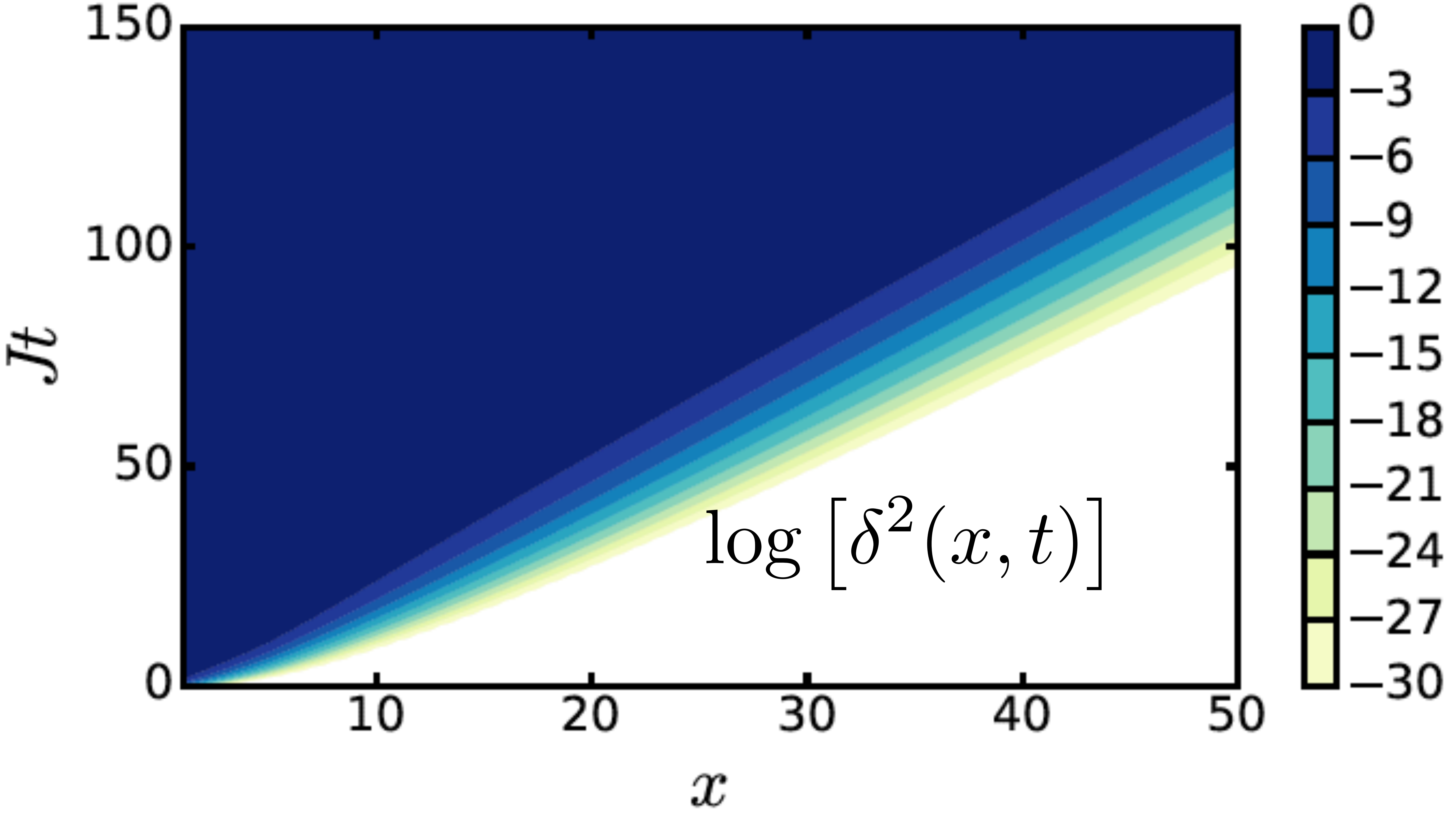
$$|\psi_2(t)\rangle = e^{-iHt}|{\color{red}\bullet}\bullet\bullet\bullet\bullet\bullet\bullet\bullet\rangle$$

Local unitary

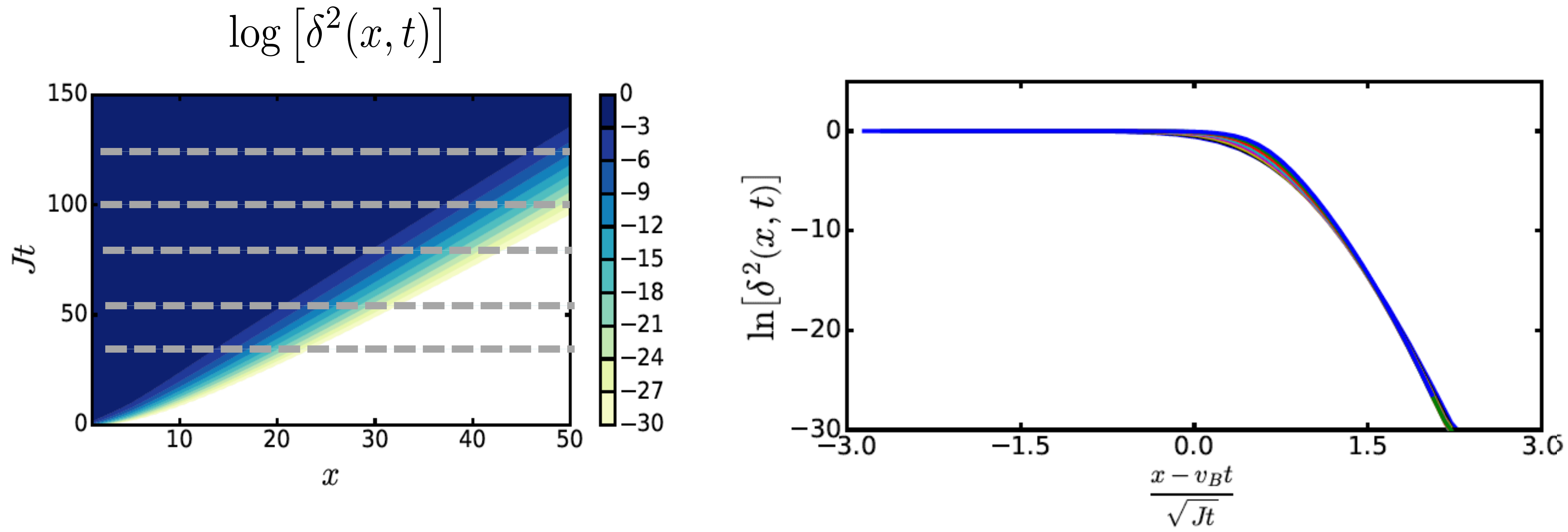
Normalized measure of the distance

$$\delta^2(x,t) = \frac{\mathrm{tr}[(\rho^R_1(x,t) - \rho^R_2(x,t))^2]}{\mathrm{tr}[\rho^R_1(x,t)^2] + \mathrm{tr}[\rho^R_2(x,t)^2]}$$

Diagnostics of chaos



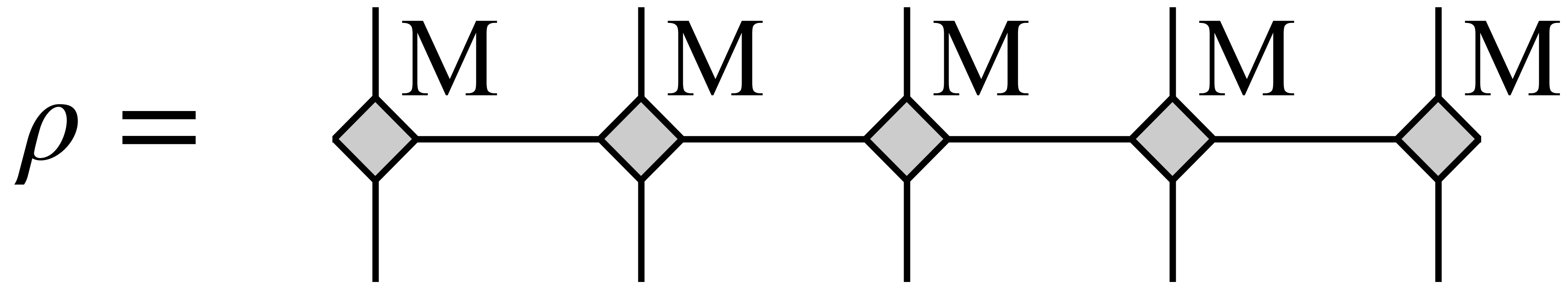
Propagation of chaotic front



Front propagates ballistically and broadens diffusively: $\delta x = \sqrt{D_B t}$

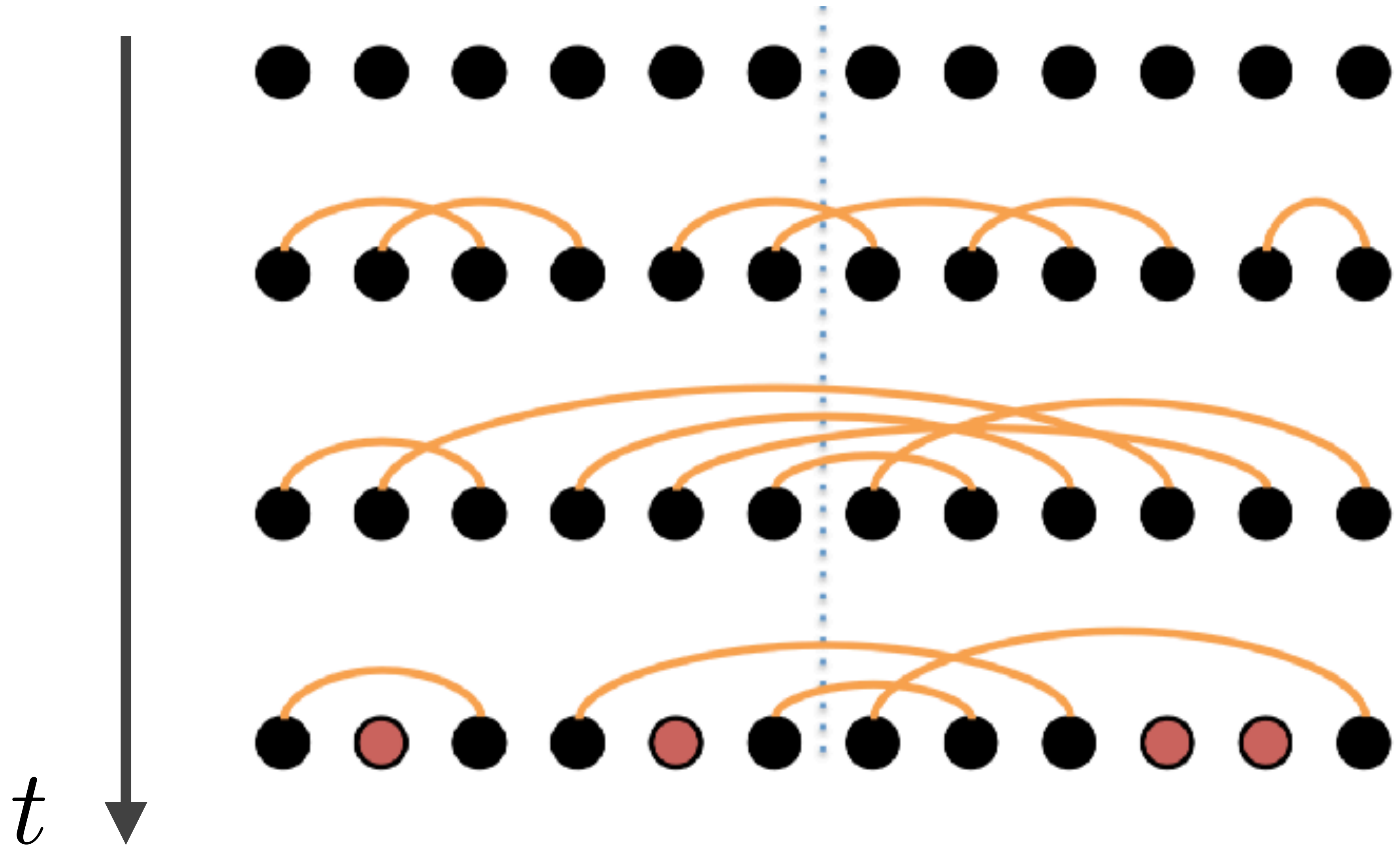
Density matrix truncation (DMT) method

Matrix Product Density Operator



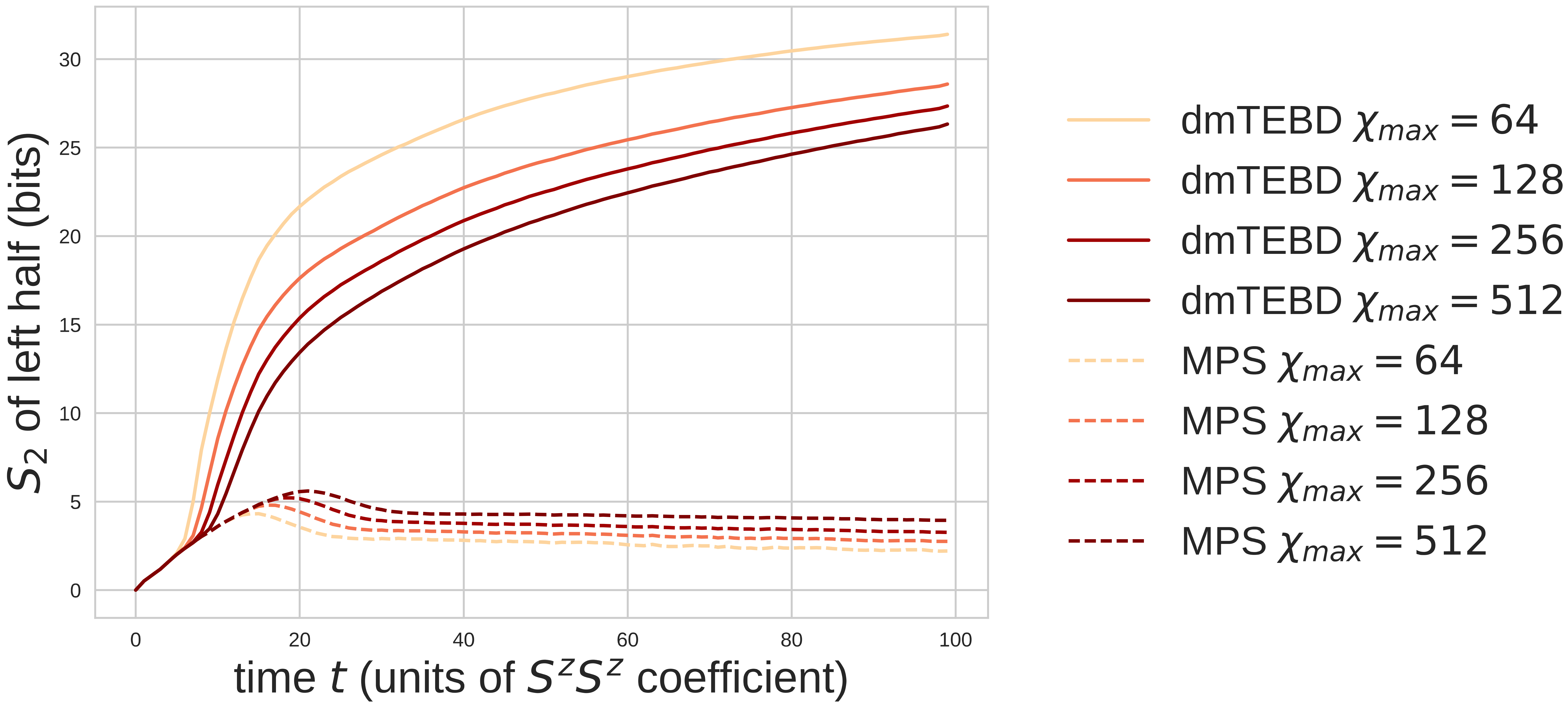
Exactly preserves expectation values of operators on up to three contiguous sites

- ➡ Trace preserving $\rho \to \rho'$
- ➡ Matching reduced density matrices
- ➡ All 3-site density matrices are preserved



[White, Zaletel, Mong, Refael '18]

Density matrix truncation (DMT) method

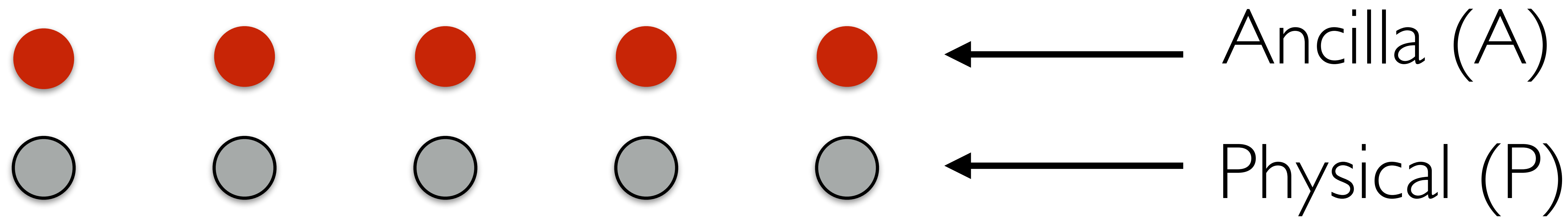


[White, Zaletel, Mong, Refael '18]

Purification of mixed states

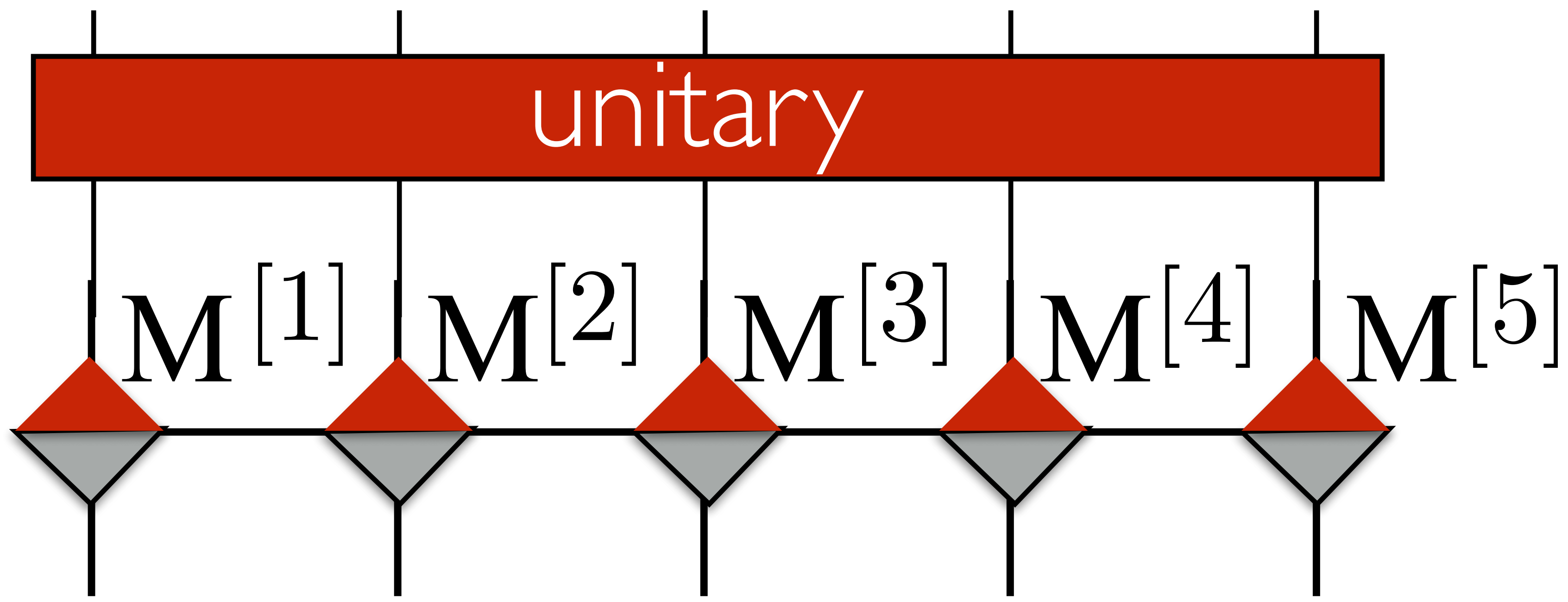
Purification of a mixed state ρ on system P:
$|\tilde{\psi}\rangle\langle\tilde{\psi}|$ on $P \cup A$, such that $\rho = \mathrm{Tr}_A|\tilde{\psi}\rangle\langle\tilde{\psi}|$

$|\tilde{\psi}\rangle$:



Purified states can be expressed and manipulated using
Matrix-Product State techniques [Verstraete et al '05, Feiguin and White '05, Barthel et al. '09]

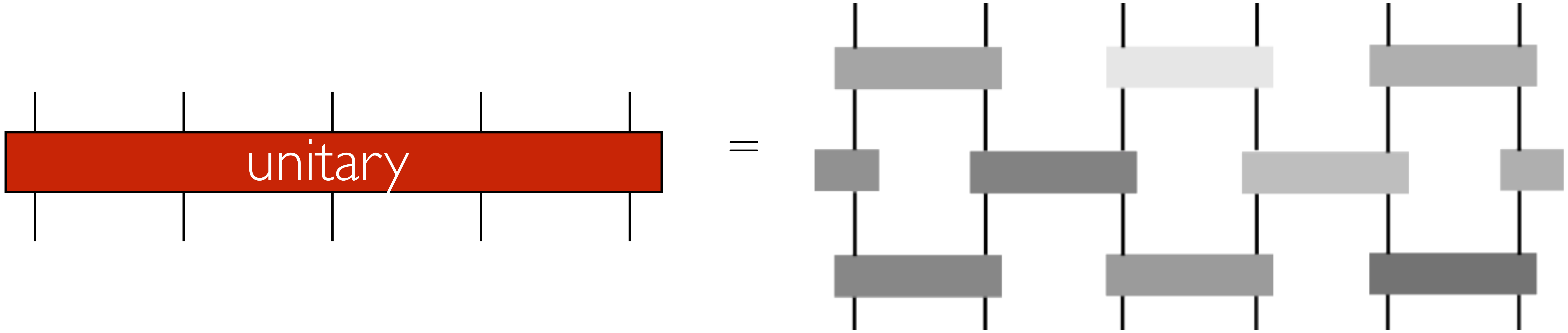
$|\tilde{\psi}\rangle$:



➡ Backwards evolution on ancilla optimal at infinite temperatures
[Karrasch, Bardarson, Moore '12]
[Barthel '13]

Purification of mixed states

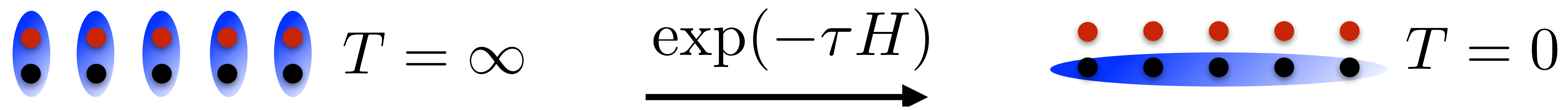
Find variational a unitary minimizing the spacial entanglement of $|\tilde{\psi}\rangle$:



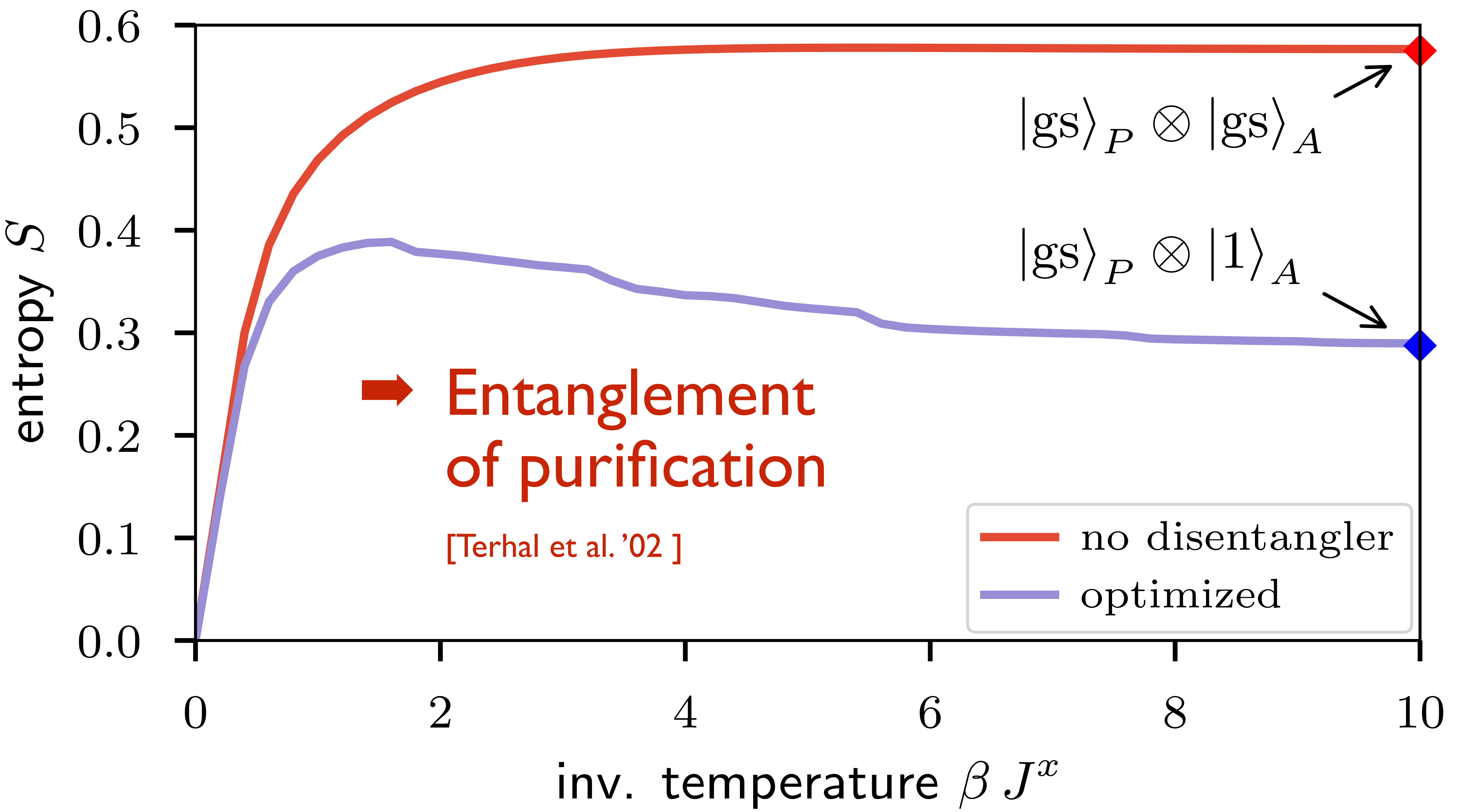
Alternatively, other networks are possibly to minimize the entanglement (e.g., MERA)

Cooling a purified state

Obtain **minimally entangled purified state** as we cool down

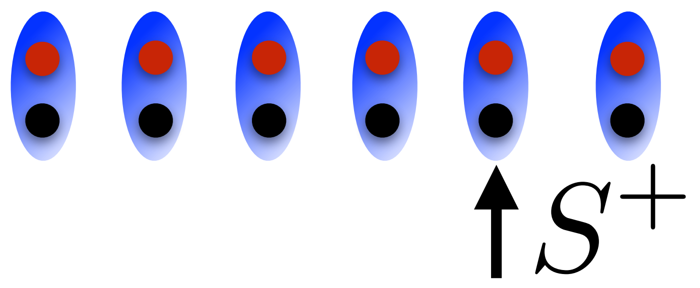


$$\hat{H} = -J^x \sum_i \sigma_i^x \sigma_{i+1}^x - J^z \sum_i \sigma_i^z \sigma_{i+1}^z - h^z \sum_i \sigma_i^z$$

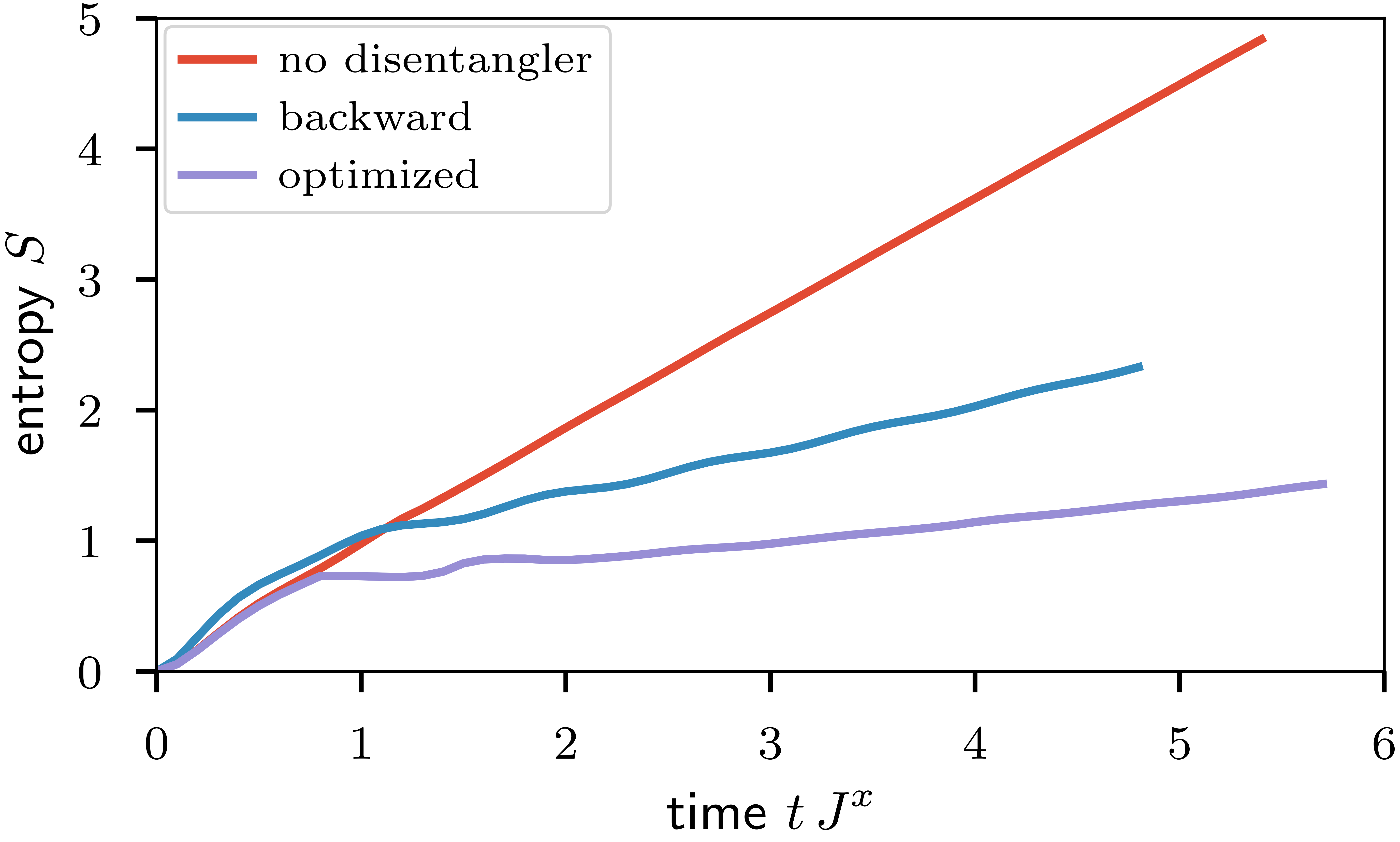


Time evolution of a purified state

Real time evolution

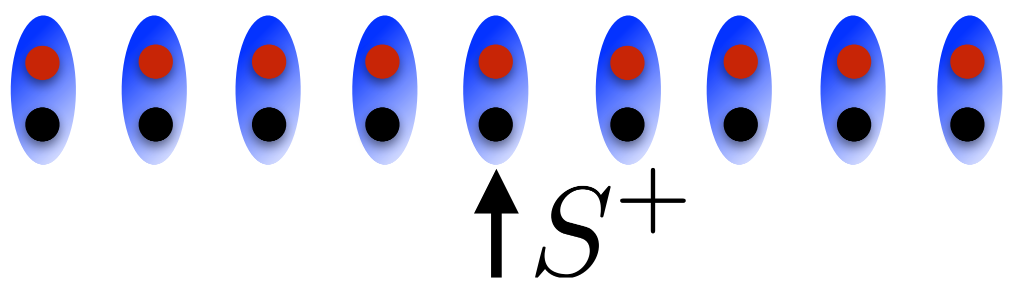


$$\hat{H} = -J^x \sum_i \sigma_i^x \sigma_{i+1}^x - J^z \sum_i \sigma_i^z \sigma_{i+1}^z - h^z \sum_i \sigma_i^z$$

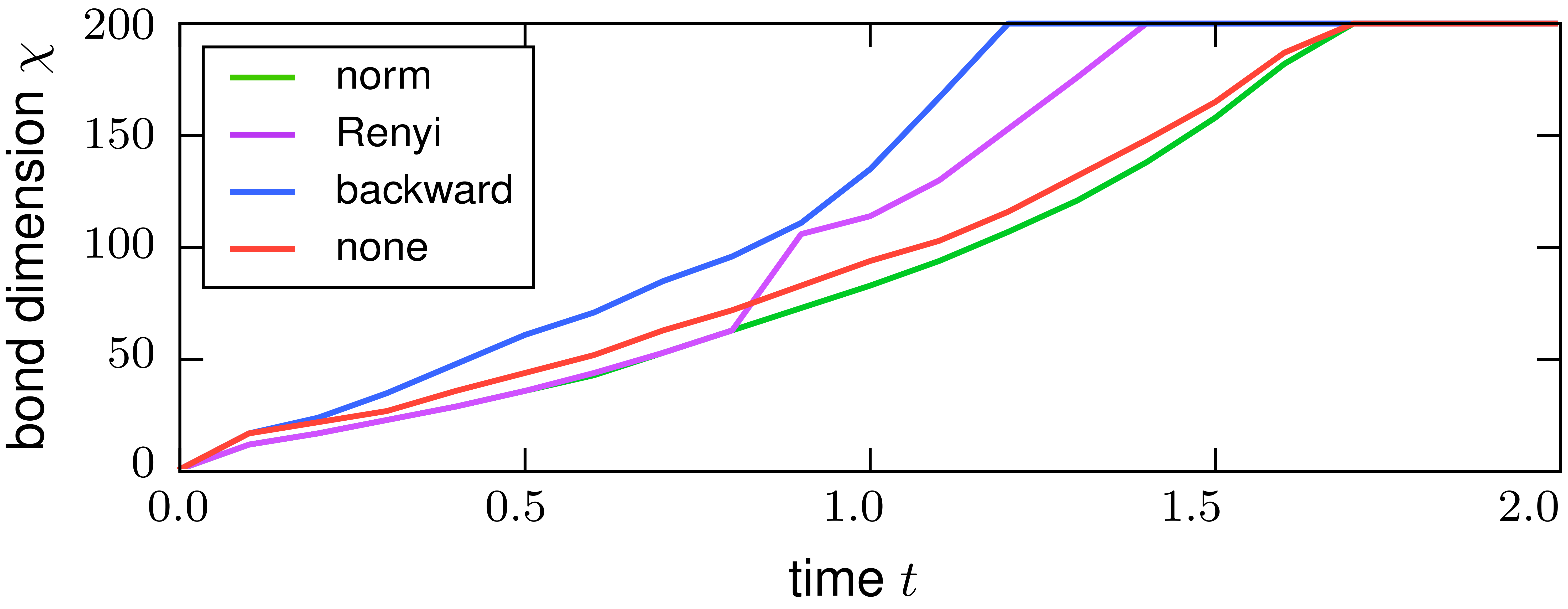


Time evolution of a purified state

Real time evolution



$$\hat{H} = -J^x \sum_i \sigma_i^x \sigma_{i+1}^x - J^z \sum_i \sigma_i^z \sigma_{i+1}^z - h^z \sum_i \sigma_i^z$$



➡ Tails in the Schmidt spectrum

➡ Better cost function?

TDVP for Thermofield Double

Thermofield Double

$$\hat{\rho} = \sum_{\alpha} \gamma_\alpha |\alpha\rangle\langle\alpha| \quad \Leftrightarrow \quad |\boldsymbol{\psi}\rangle = \sum_{\alpha} \gamma_\alpha^{1/2} |\alpha, \alpha\rangle$$

- Evolve $|\boldsymbol{\psi}\rangle$ with $\boldsymbol{\mathcal{H}} = \mathcal{H} \otimes \mathbf{1} + \mathbf{1} \otimes \mathcal{H}$
- Expectations same on two subspaces – Numerical errors

  => Symmetrize $\boldsymbol{A}^{\sigma\delta}_{i\otimes i', j\otimes j'} = \boldsymbol{A}^{\delta\sigma}_{i'\otimes i, j'\otimes j}$

  => Additional constraint on null space

  [Haegeman et al PRL107, 070601 (2011)]

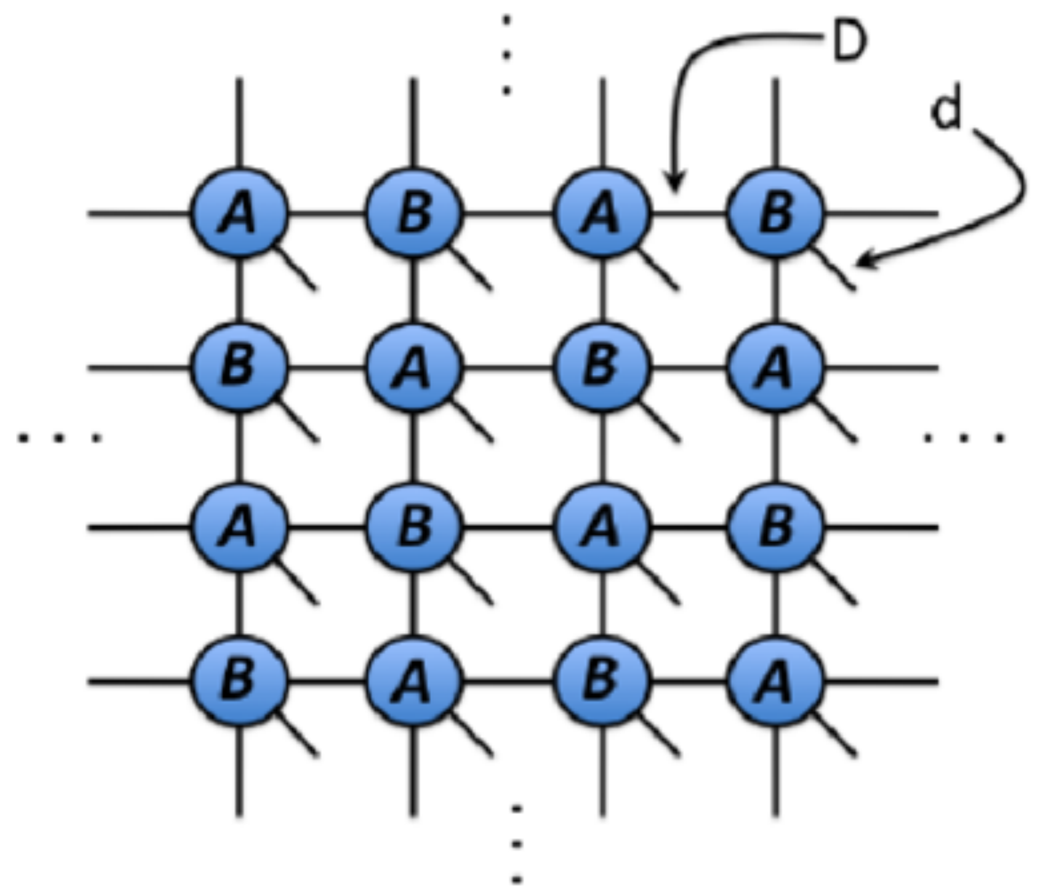
  [Hallam,Morley, Green arXiv:1806.05204]

Discussion on Numerical Approaches to Dynamics

MPS based Lindblad dynamics

$$\dot{\rho}(t) = \mathcal{L}[\rho] = -\frac{i}{\hbar}[H, \rho] + \gamma \sum_i \left[L_i^\dagger L_i \rho - \frac{1}{2}\left\{ \rho, L_i L_i^\dagger \right\} \right]$$

2D Tensor-Product States



Numerical Linked-Cluster Expansions

Truncated Wigner Approximation

Discussion on Numerical Approaches to Dynamics

Hauschild, Leviatan, Bardarson, Altman, Zaletel, FP
arXiv:1711.01288

Leviatan, FP, Bardarson, Huse, Altman
arXiv:1702.08894