Efficient simulation of quantum transport in 1D

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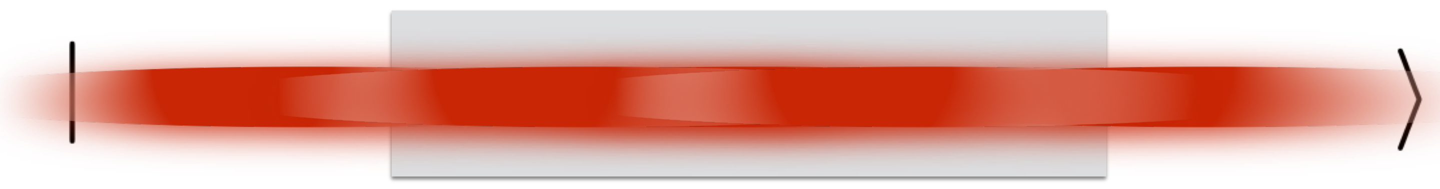
[Rakovszky, von Keyserlingk, FP, PRB **105**, 075137 (2022)]
[von Keyserlingk, FP, Rakovszky, PRB **105**, 245101 (2022)]

Solvay Workshop on 'Quantum Simulation'
Brussels, Aug. 29 2022

Quantum Thermalization

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

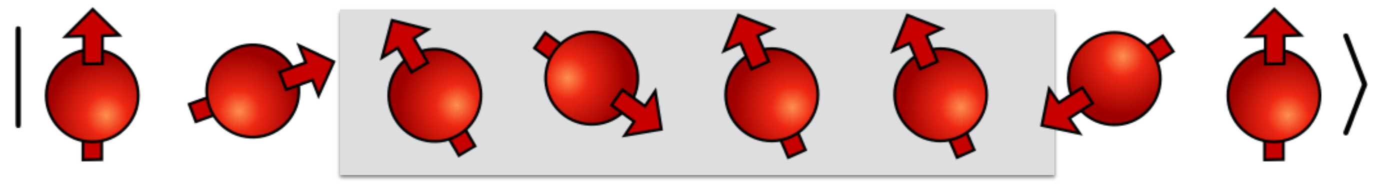
t



$S = 0$

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

[non-integrable, local Hamiltonian]



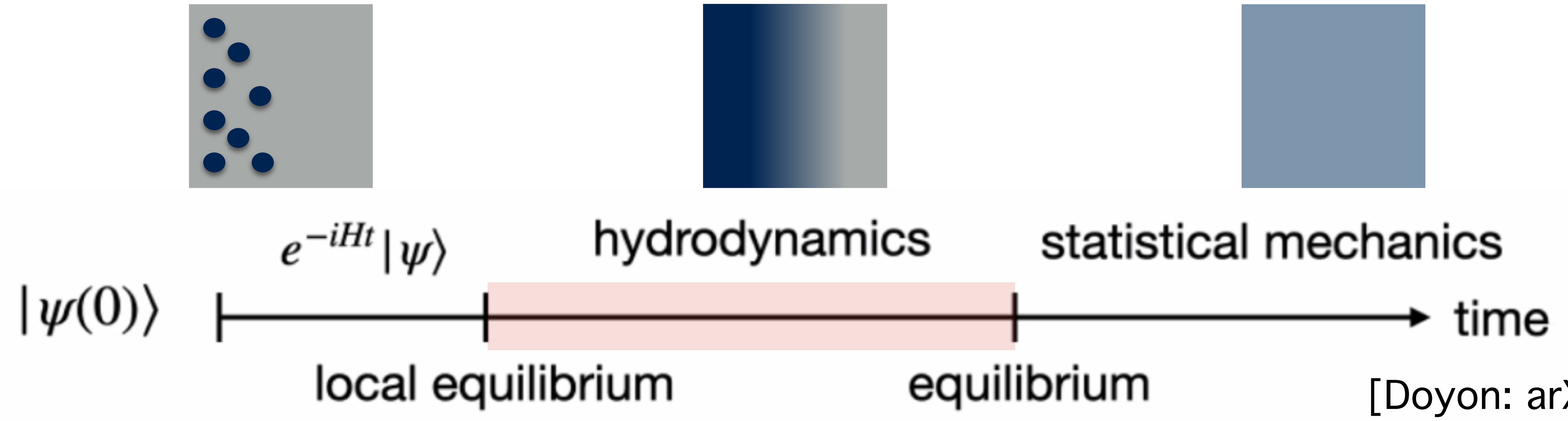
$S = 0$

Closed quantum

[Srednicki, Deutsch, Rigol]

Characterizing thermalization dynamics

Universal hydrodynamic features tend to emerge in the low-frequency, long-wavelength limit

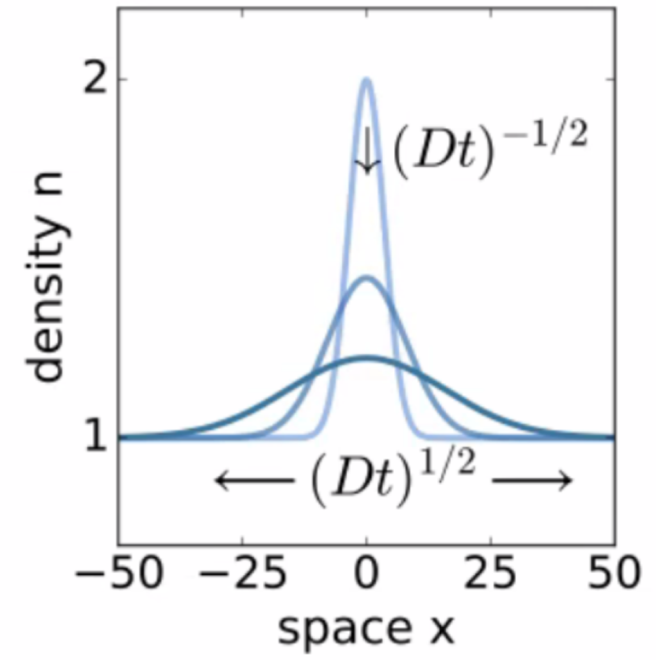


[Doyon: arXiv 1912.08496]

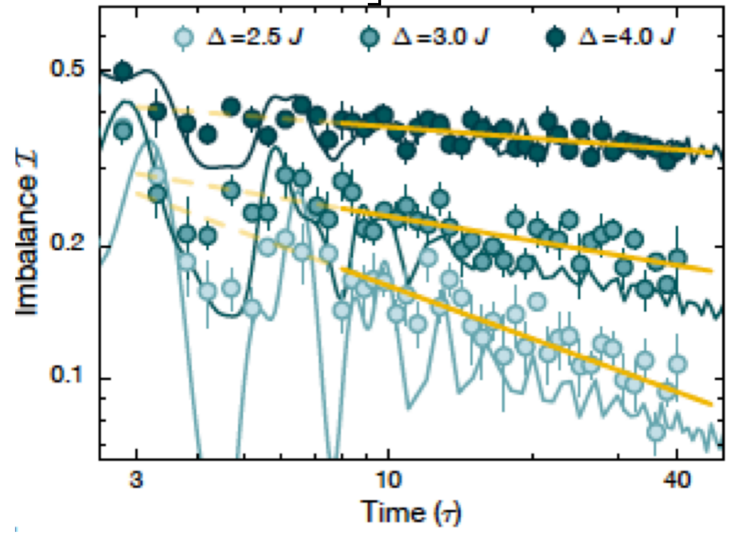
Emergent hydrodynamic relaxation: Diffusion

$$\partial_t n = -\partial_x j \qquad j = -D\partial_x n \quad \text{(Fick's law)}$$

$$\longrightarrow \quad \partial_t n = D\partial_x^2 n \quad \text{(Diffusion)}$$



[I hen et al. '17]



How to numerically extract hydrodynamics for a given microscopic model?

Numerical complexity of many-body dynamics

Directly simulate the time evolution within the full many-body Hilbert space $|\psi(t)\rangle = e^{-itH}|\psi(0)\rangle$

$$|\psi\rangle = \sum_{j_1, j_2, \ldots, j_L} \psi_{j_1, j_2, \ldots, j_L} |j_1\rangle |j_2\rangle \ldots |j_L\rangle \ , \ j_n = 1 \ldots d$$

- Complexity $\propto \exp(L)$
- Exact diagonalization methods (dynamical typicality) up to ~30 spins

Matrix-Product States

Low entanglement: Matrix-Product States

$d^L \to L d \chi^2$

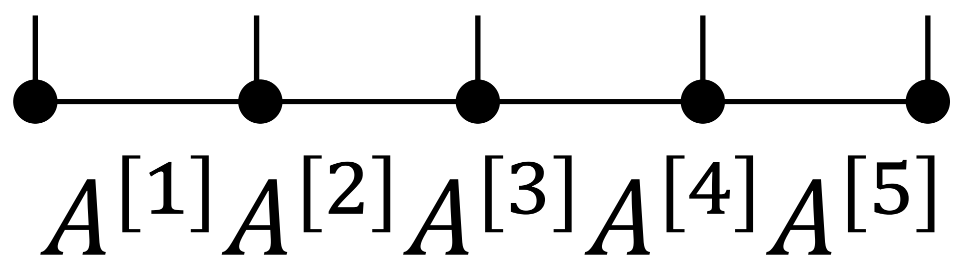
[M. Fannes et al. 92]

$$\psi_{j_1,j_2,\ldots,j_L} \approx \sum_{\alpha_1,\alpha_2,\ldots,\alpha_{L-1}} A^{j_1}_{\alpha_1} A^{j_2}_{\alpha_1,\alpha_2} \ldots A^{j_L}_{\alpha_{L-1}} \quad (\alpha_j = 1 \ldots \chi)$$

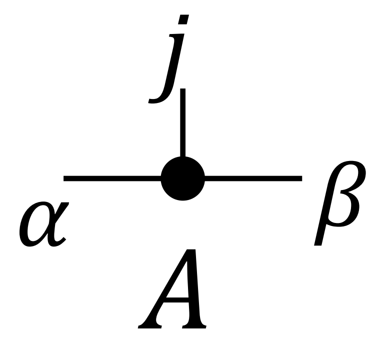
- Efficient representation of ground states of gapped local Hamiltonians [Hastings, Schuch, Verstraete,…]

Diagrammatic representation

$\psi_{j_1,j_2,j_3,j_4,j_5} \approx$



$A^j_{\alpha,\beta} =$



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

$j = 1 \ldots d$

Numerical complexity of many-body dynamics

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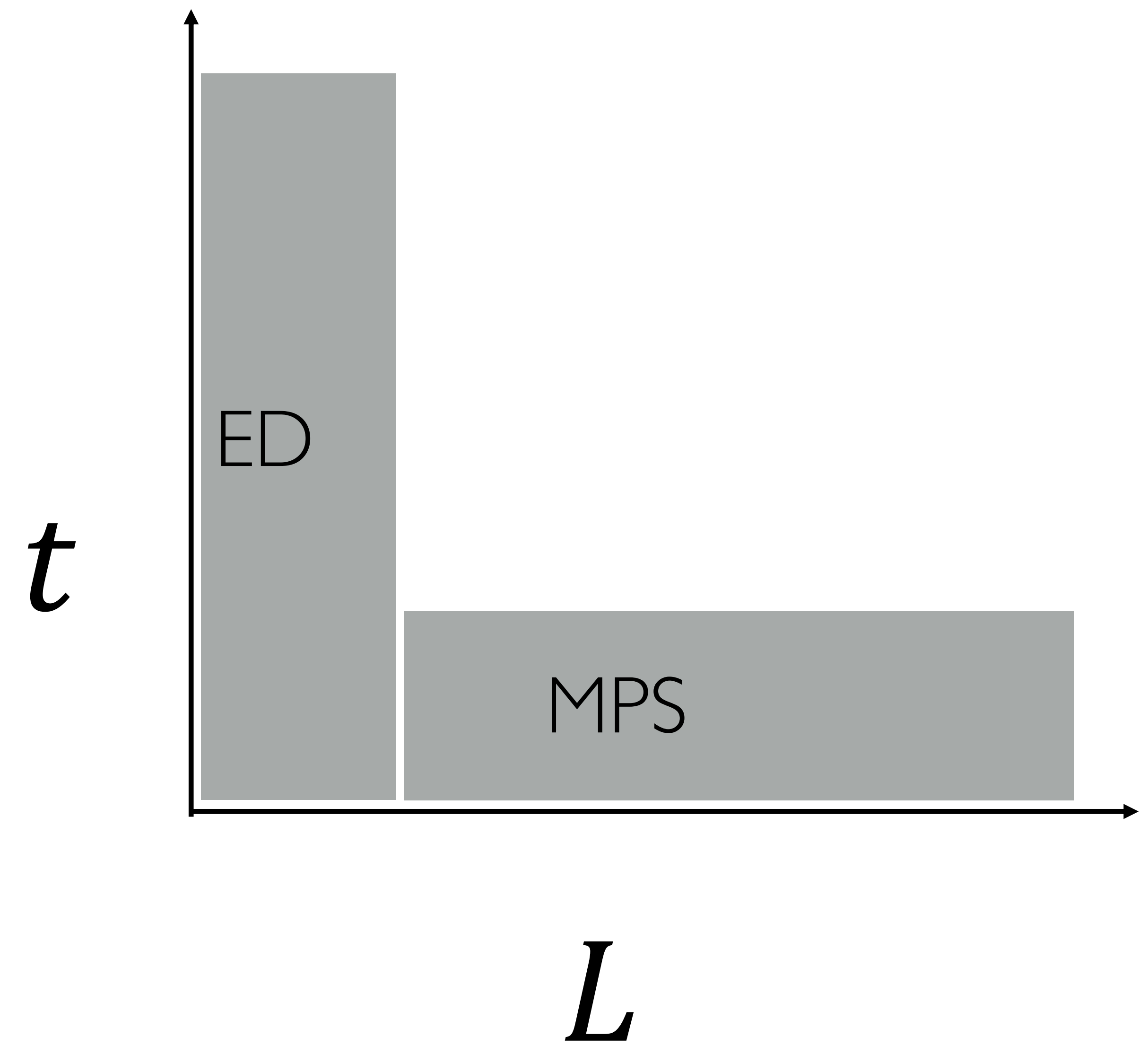
- Complexity $\propto \exp(L)$
- Sparse exact diagonalization methods (dynamical typicality) up to ~30 spins



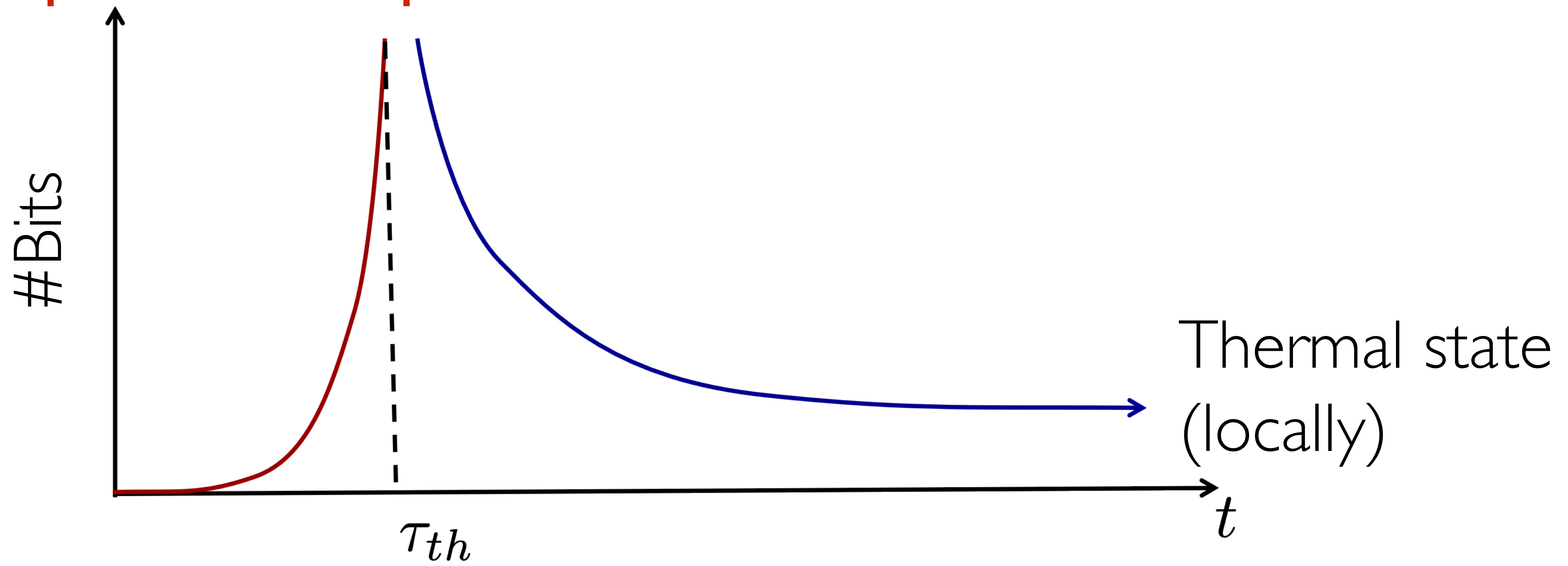
Matrix-Product State based numerics

- Complexity $\propto \exp(t)$ because of linear entanglement growth

[P. Calabrese and J. Cardy, Huse, Nahum]

"Information paradox"

Quantum quench from product state



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

Various approaches to address this problem:

[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]

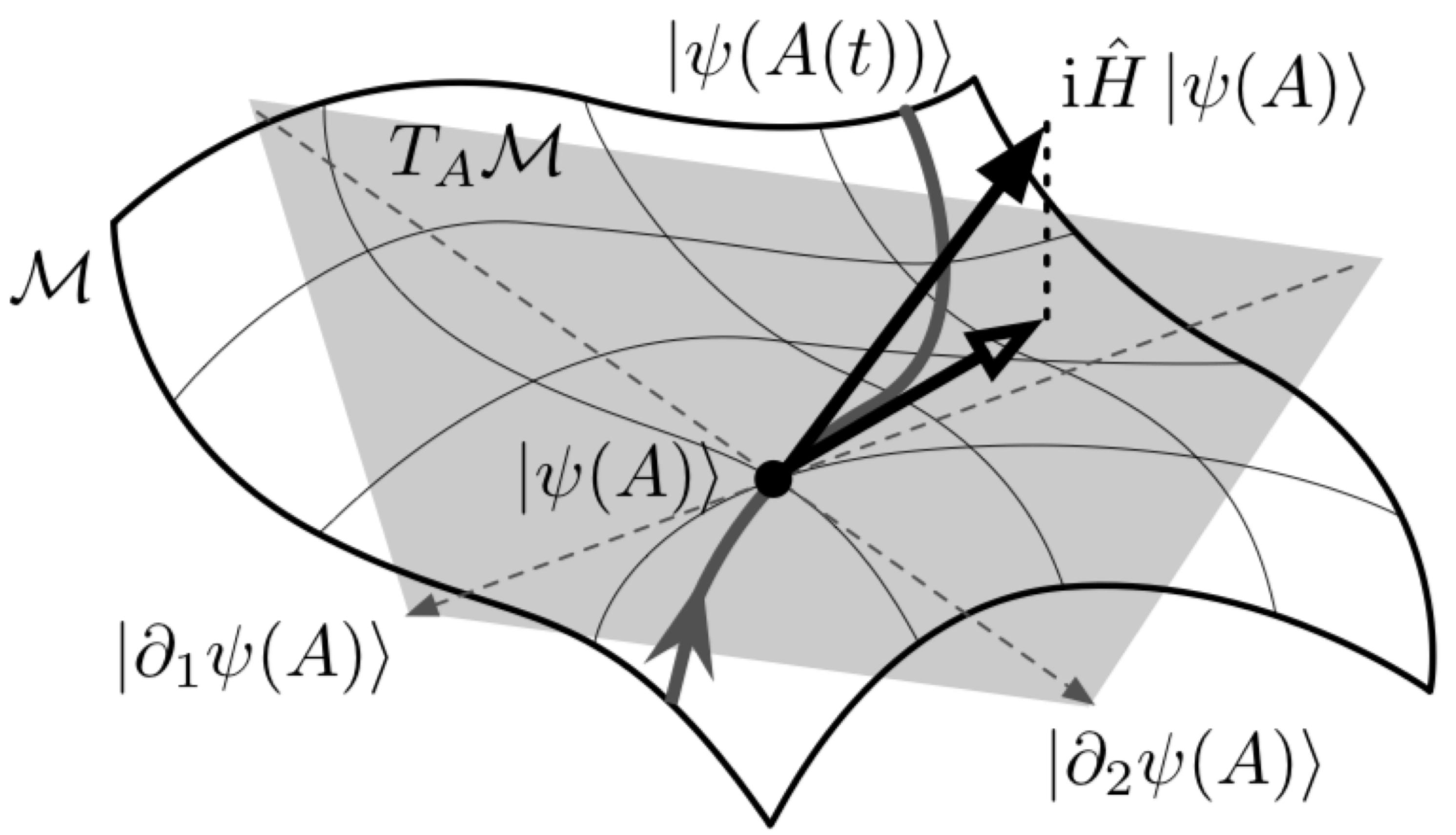
Time-dependent variational principle (TDVP)

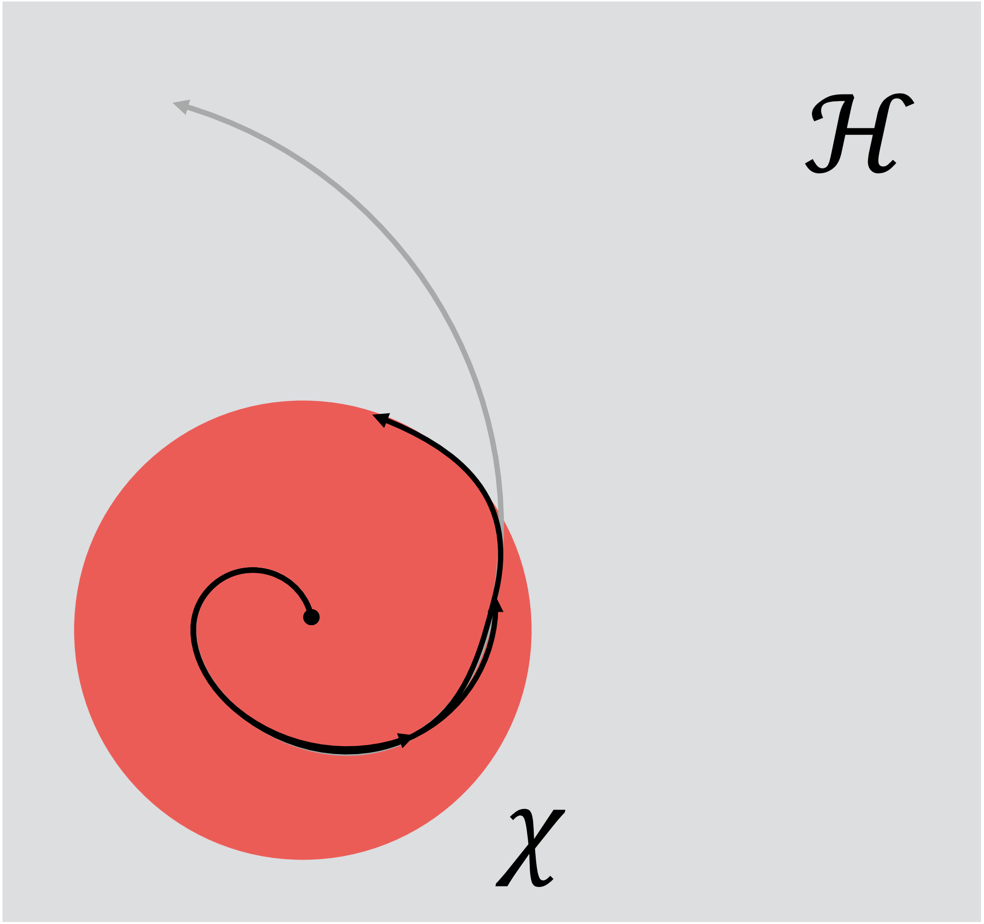
Variational manifold: MPS states with fixed bond dimension

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

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]





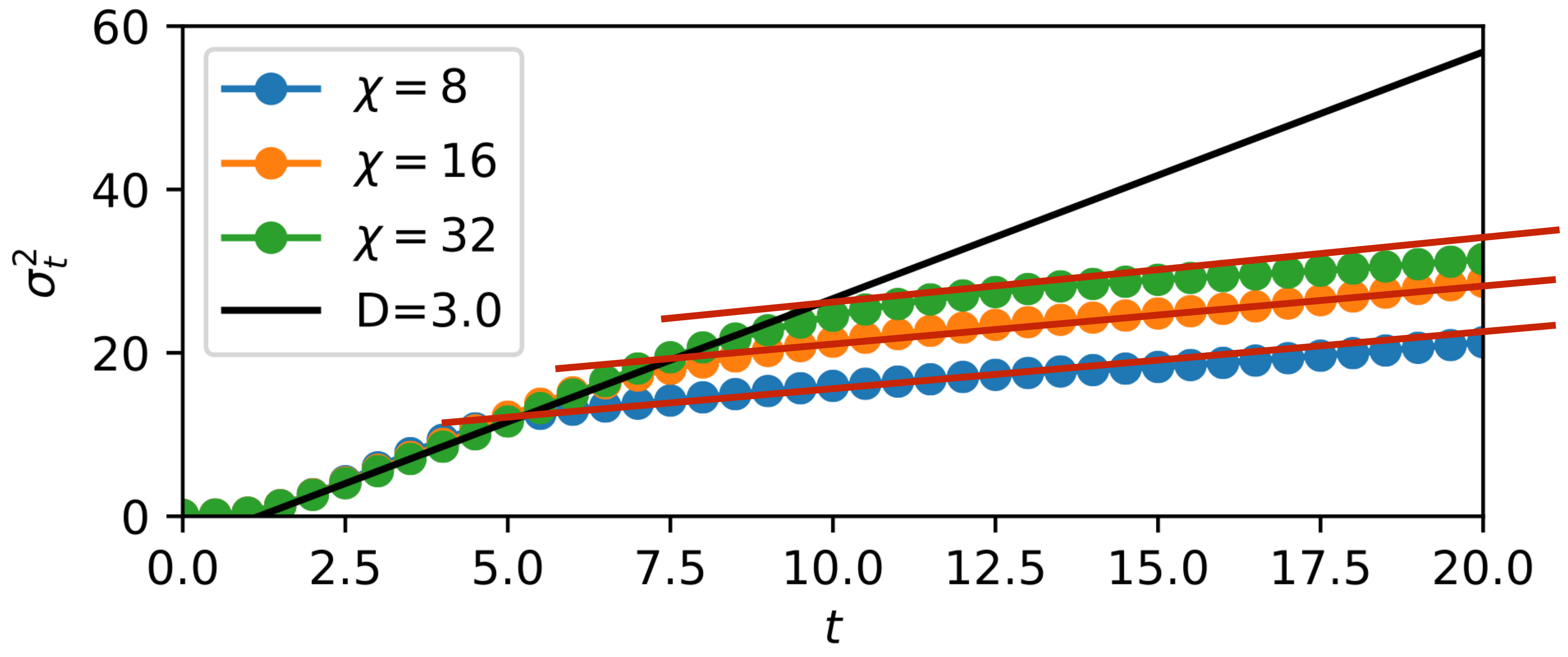
- Global conservation laws (energy, particles,…)

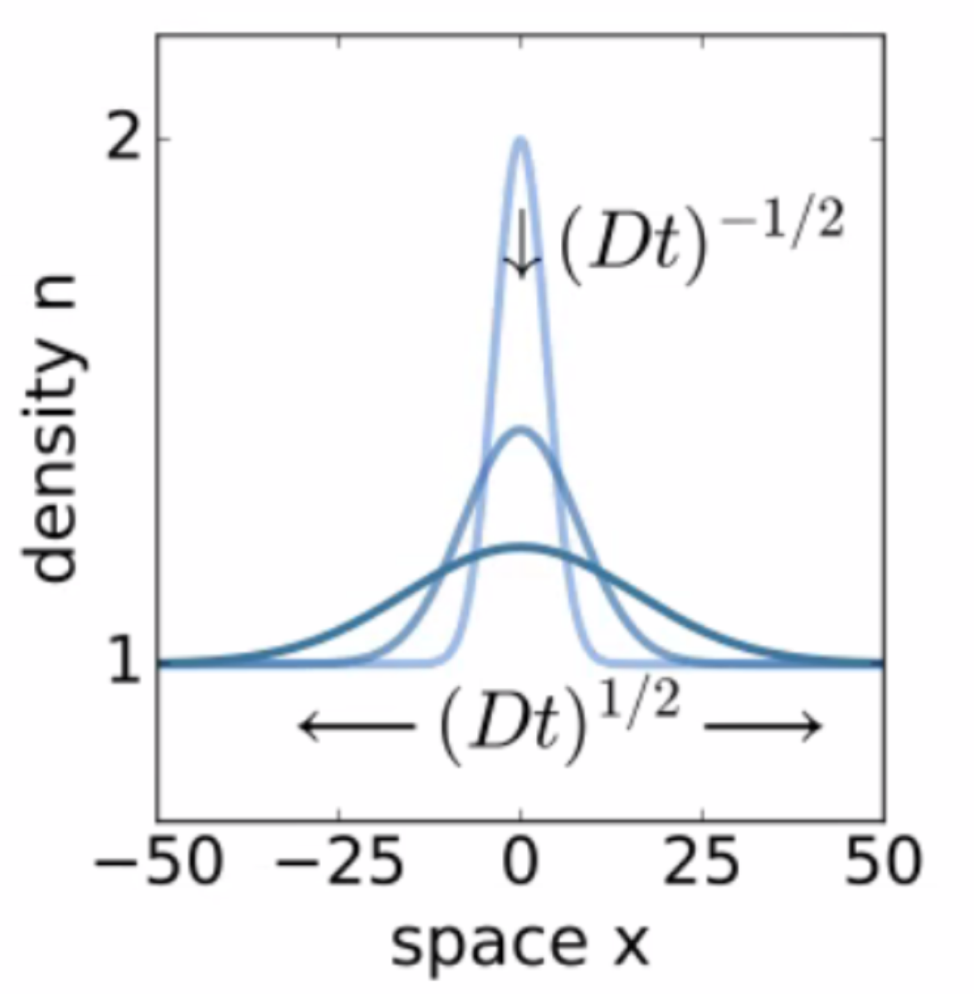
[Leviatan, FP, Bardarson, Huse, Altman, arXiv:1702.08894]

Time-dependent variational principle (TDVP)

XXZ Model with longer range interactions

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





- Diffusion constant changes when truncation kicks it!

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

Dissipation-assisted operator evolution method

Heisenberg Picture: Artificial dissipation leads to a decay of operator entanglement, allowing us to capture the dynamics to long times

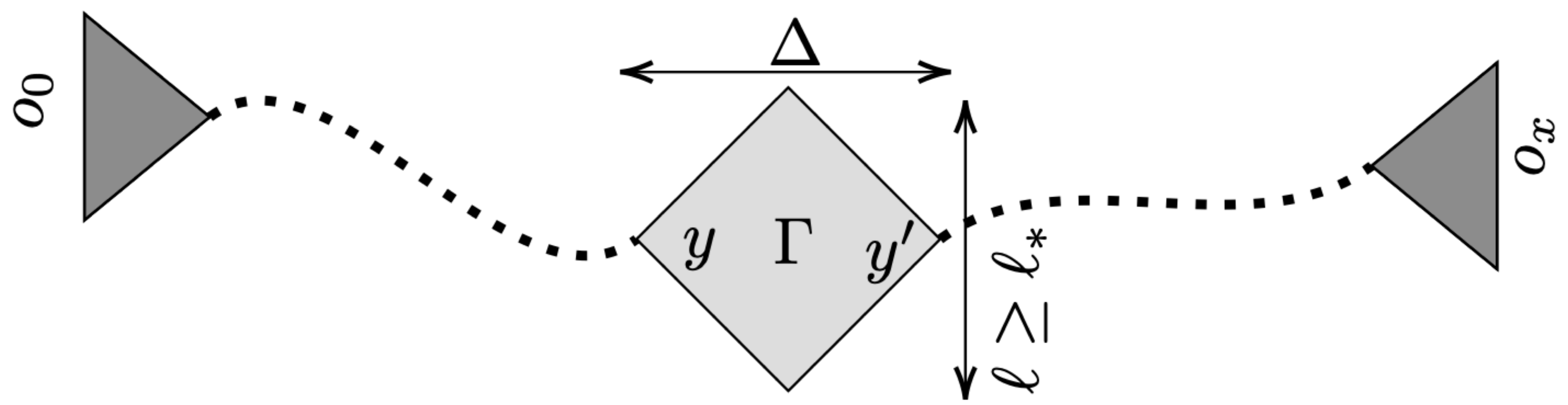
- Discard information corresponding to n-point functions with $n > \ell_*$.
- Errors induced by truncation (“backflow”) are exponentially suppressed in ℓ_*

[Rakovszky, von Keyserlingk, FP, PRB **105**, 075137 (2022)]
[von Keyserlingk, FP, Rakovszky, PRB **105**, 245101 (2022)]

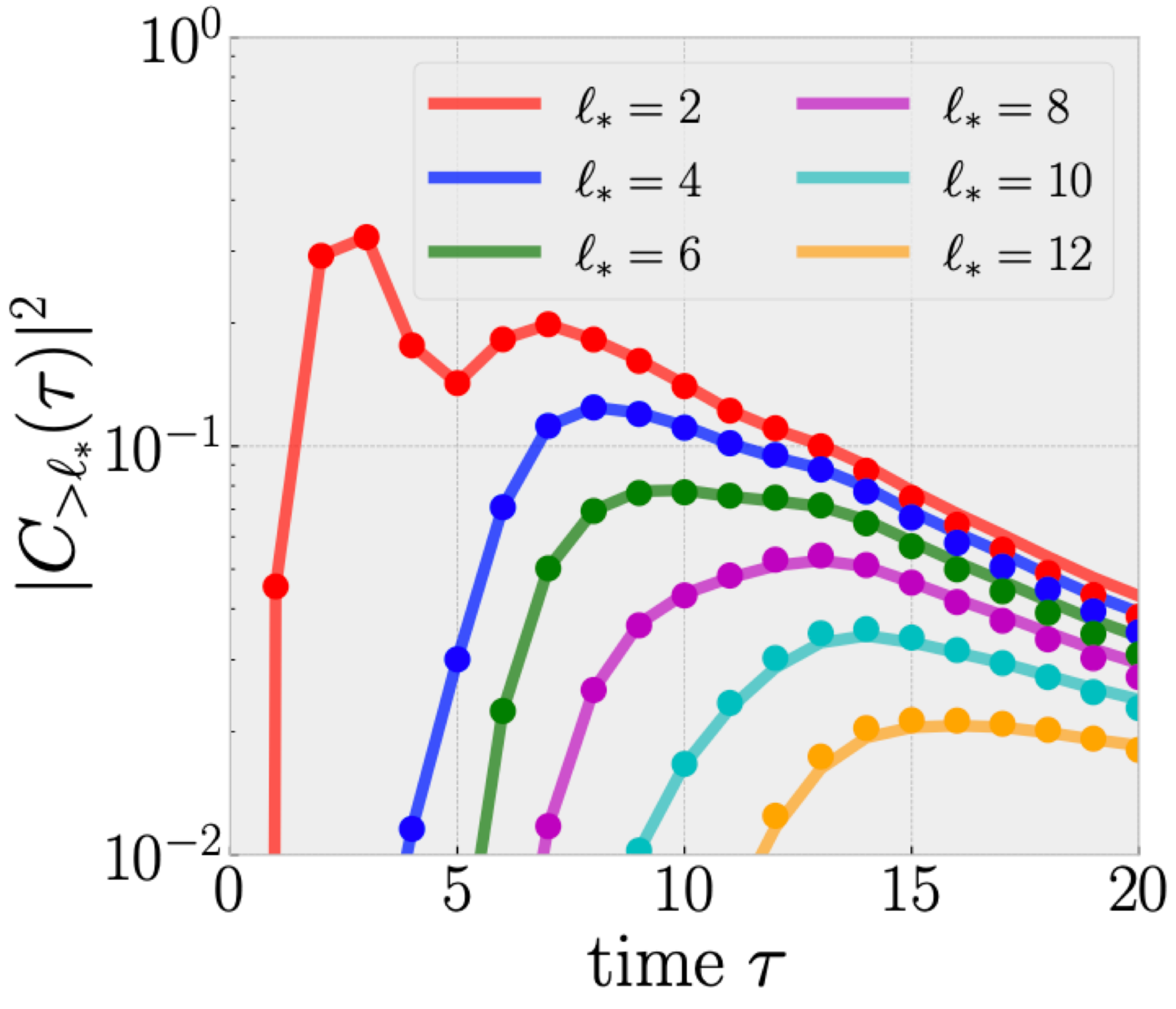
Non rigorous theory of “backflow” corrections

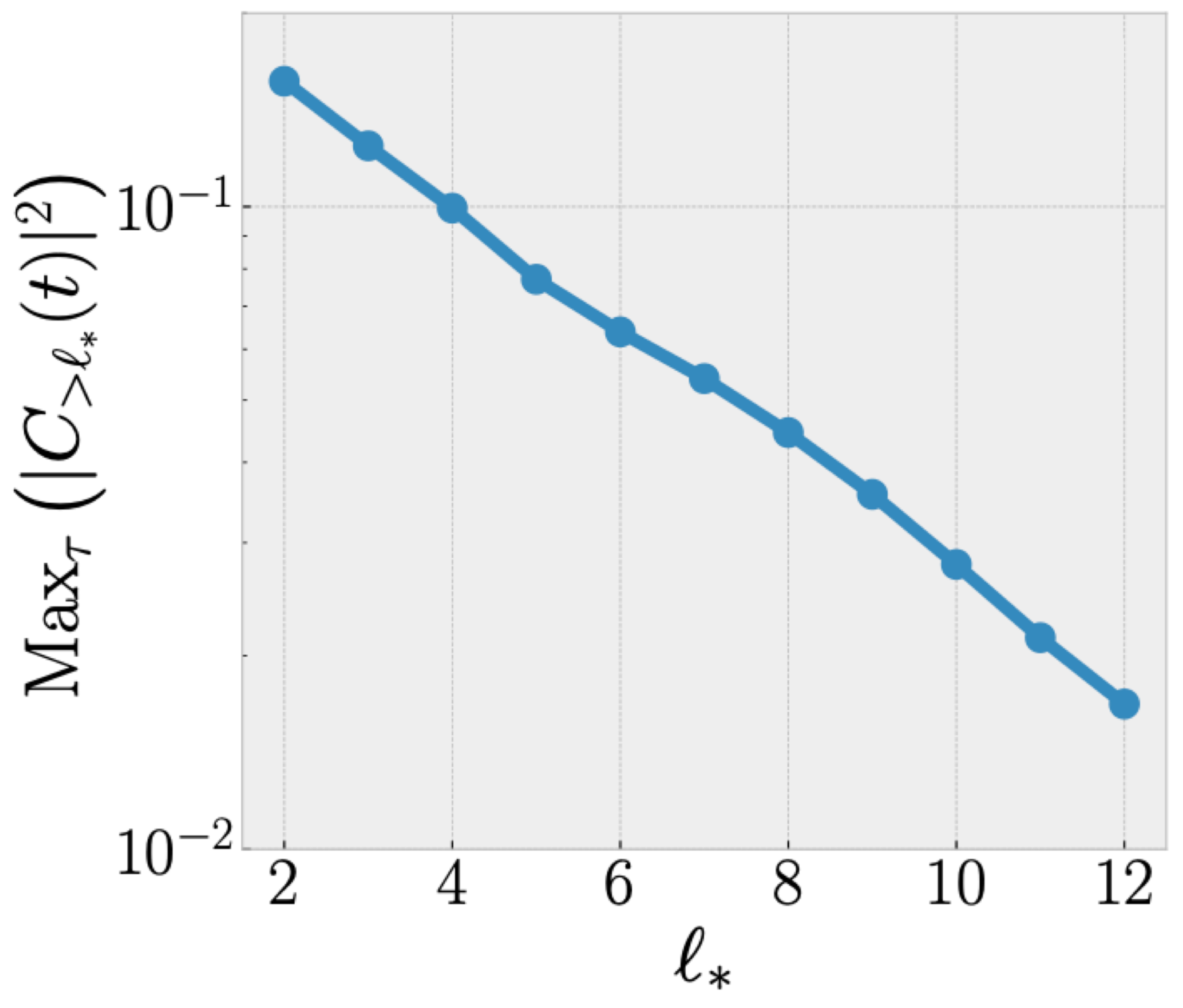
Dynamical correlations

$$C(\tau, x) \equiv \langle o_0(\tau) | o_x \rangle$$



Contributions from “backflow” exponentially small in ℓ_*: $C_{>\ell_*}(\tau, x) \equiv \langle o_0 | \mathcal{U}(\tau = 2t, t) \mathcal{P}_{>\ell_*} \mathcal{U}(t, 0) | o_x \rangle$

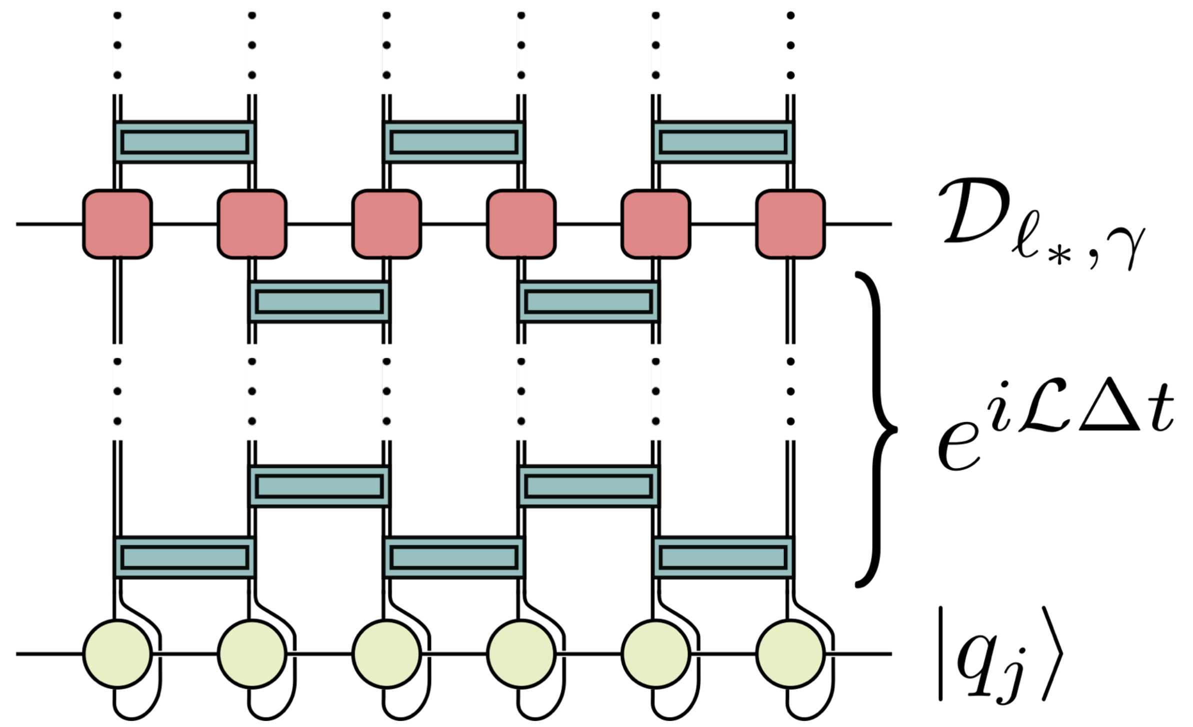




[von Keyserlingk, FP, Rakovszky, PRB **105**, 245101 (2022)]

Dissipation stops growth of operator entanglement

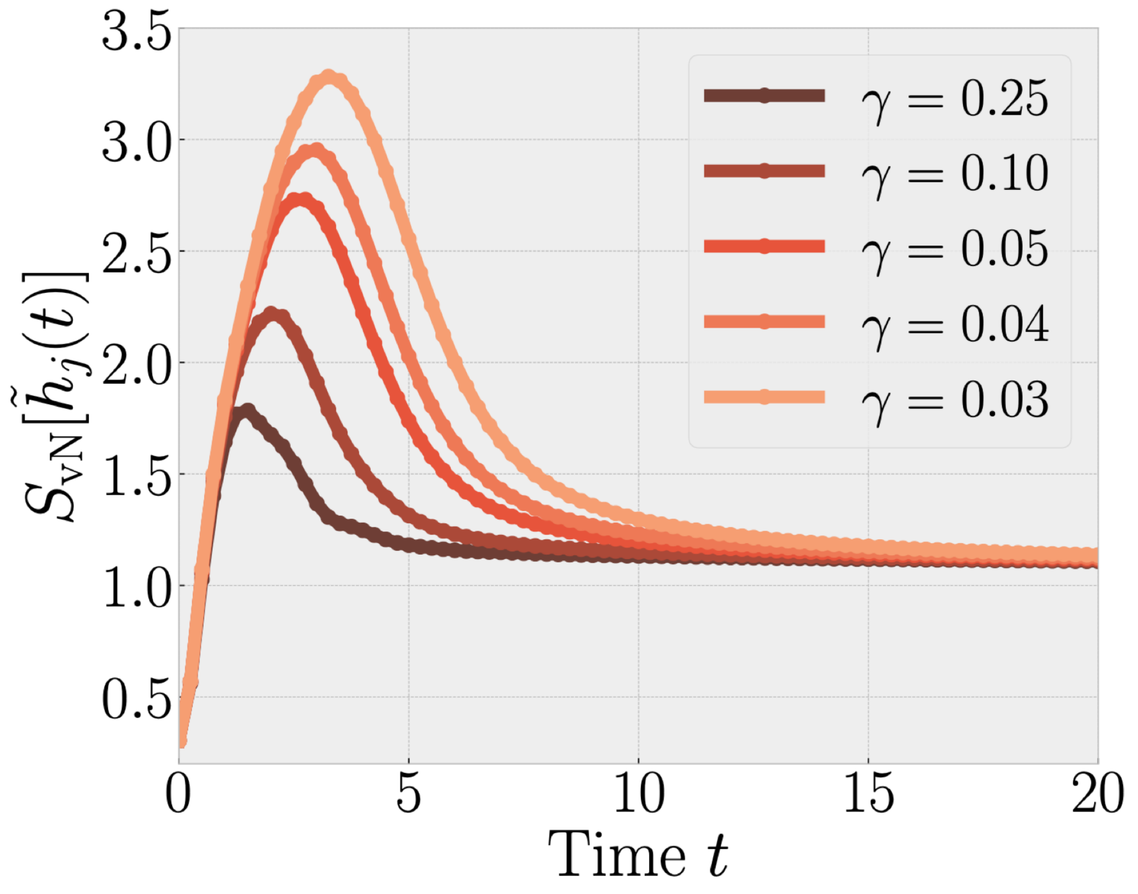
Represent dissipative evolution as tensor network



Low-dimensional Matrix-Product Operator

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

Test on quantum Ising chain:



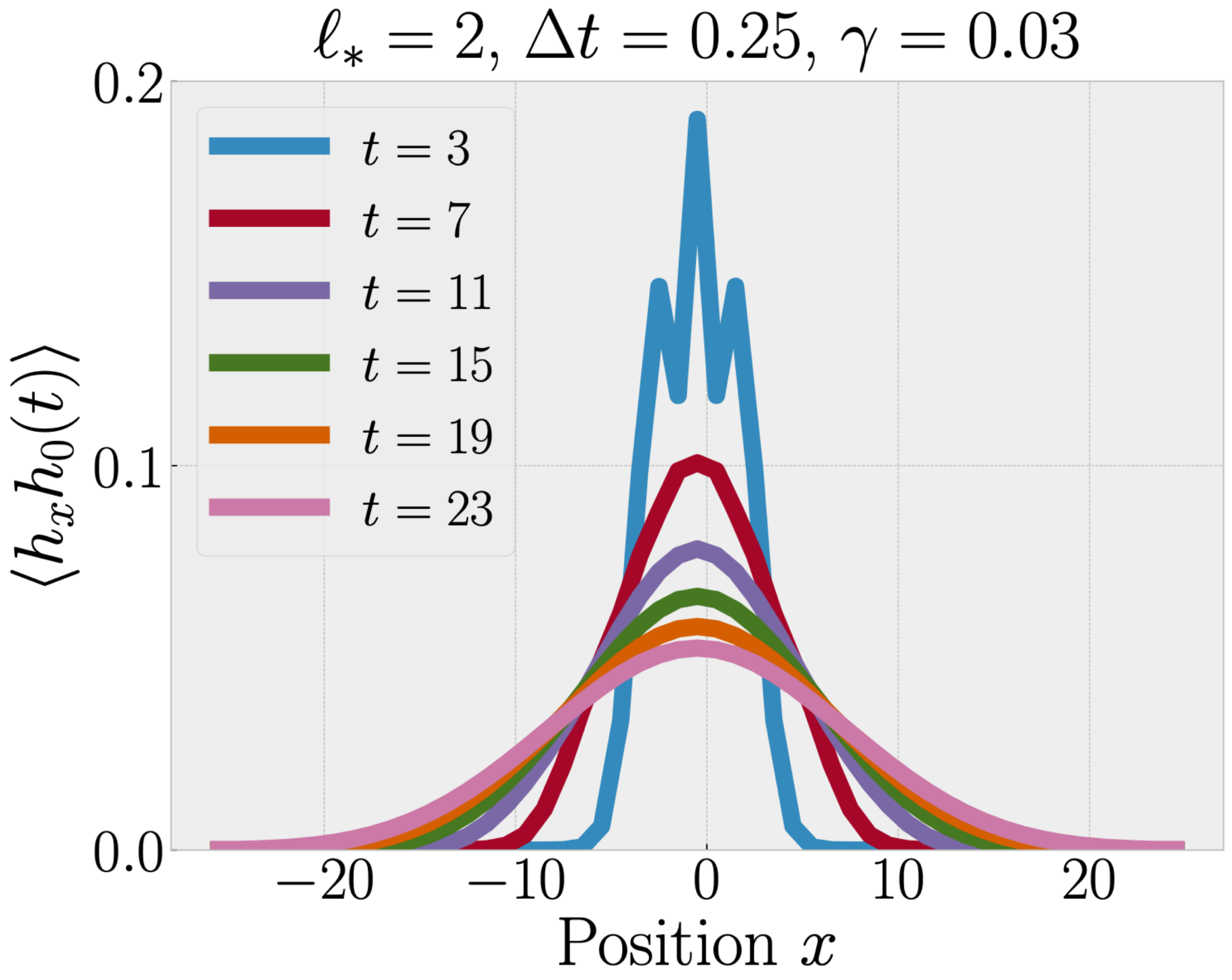
$$H = \sum_j h_j \equiv \sum_j g_x X_j + g_z Z_j + (Z_{j-1}Z_j + Z_j Z_{j+1})/2$$

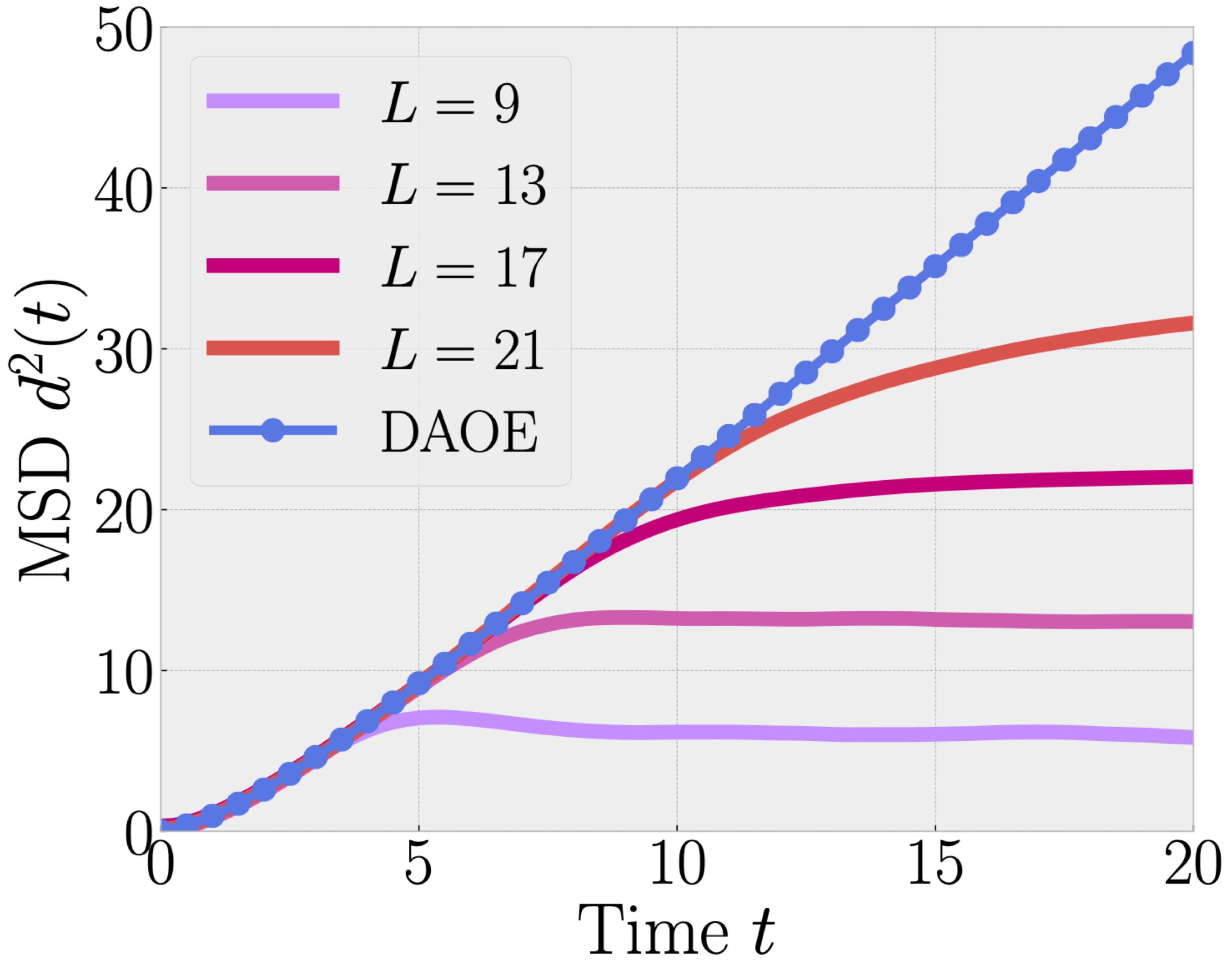
$$g_x = 1.4; g_z = 0.9045$$

[Rakovszky, von Keyserlingk, FP, PRB **105**, 075137 (2022)]

Diffusion constant from mean-square displacement

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





Time-dependent diffusion constant: $2D(t) \equiv \dfrac{\partial d^2(t)}{\partial t}$

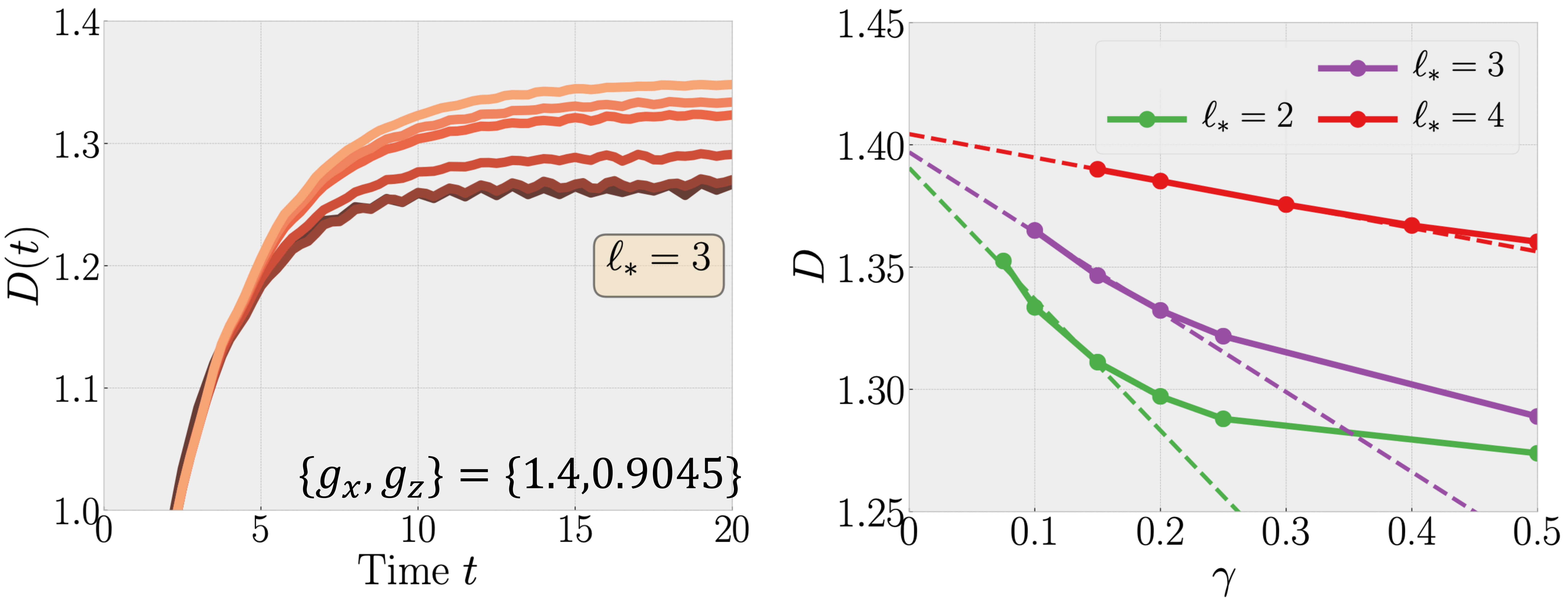
Diffusive transport: $D \equiv \lim\limits_{t\to\infty} D(t)$

[Rakovszky, von Keyserlingk, FP, PRB **105**, 07513 (2022)]

High precision in various models

Ising: $H = \sum_j h_j \equiv \sum_j g_x X_j + g_z Z_j + \frac{1}{2}(Z_{j-1}Z_j + Z_j Z_{j+1})$

$q_x \equiv h_j$

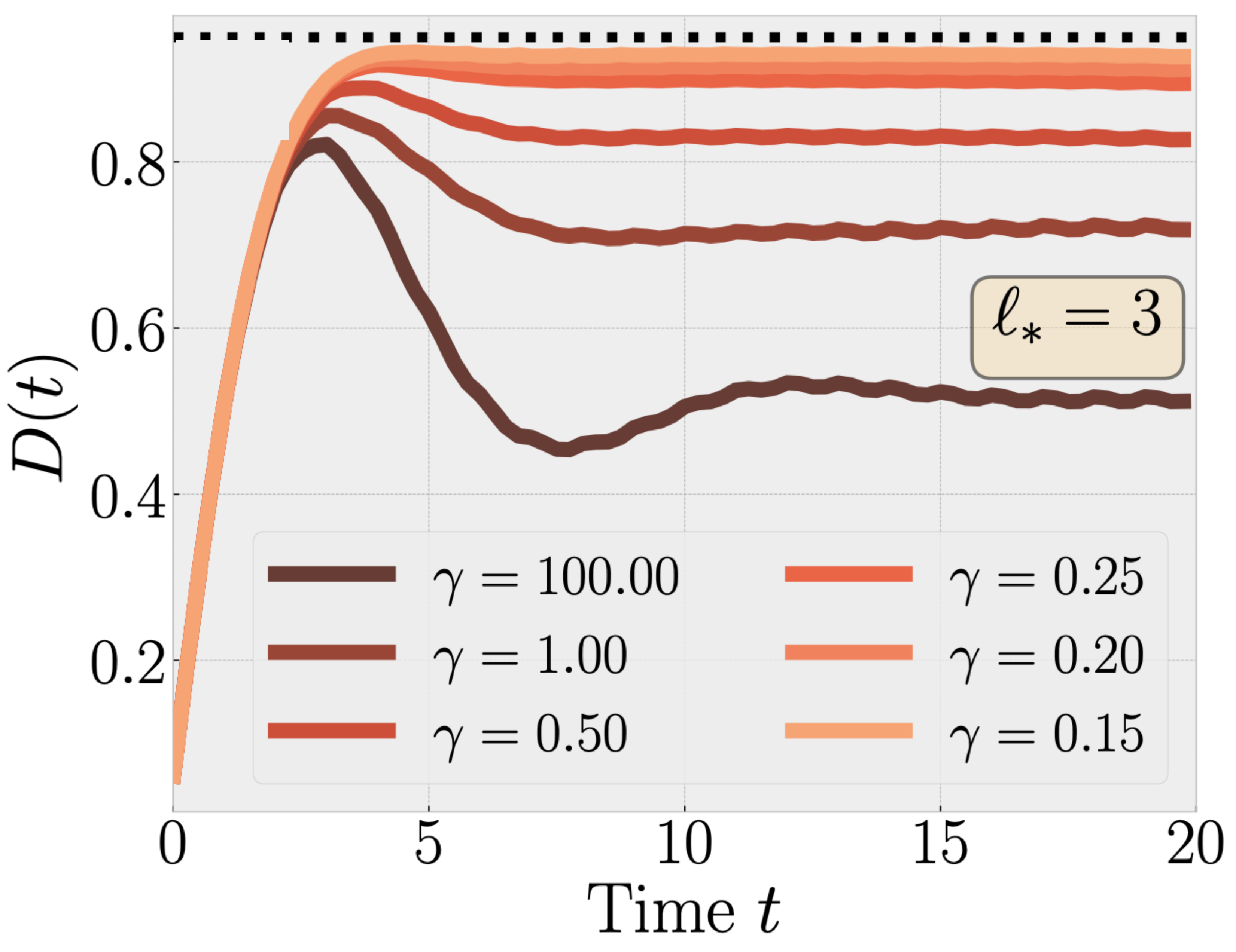


[Rakovszky, von Keyserlingk, FP, PRB **105**, 075137 (2022)]

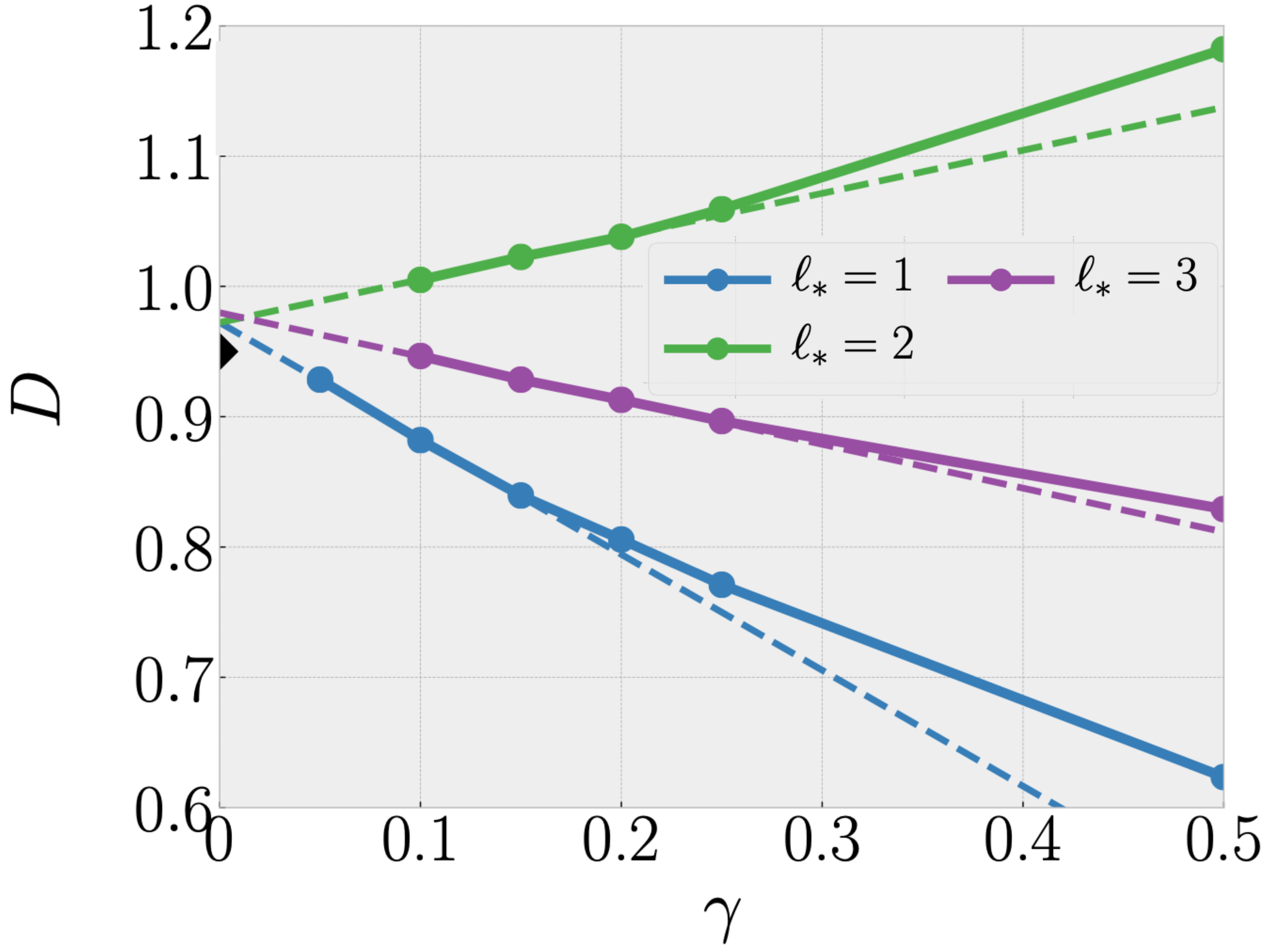
High precision in various models

XX ladder: $$H = \sum_{j=1}^{L} \sum_{a=1,2} \left(X_{j,a} X_{j+1,a} + Y_{j,a} Y_{j+1,a} \right) + \sum_{j=1}^{L} \left(X_{j,1} X_{j,2} + Y_{j,1} Y_{j,2} \right)$$

$q_x \equiv (Z_{j,1} + Z_{j,2})/2$



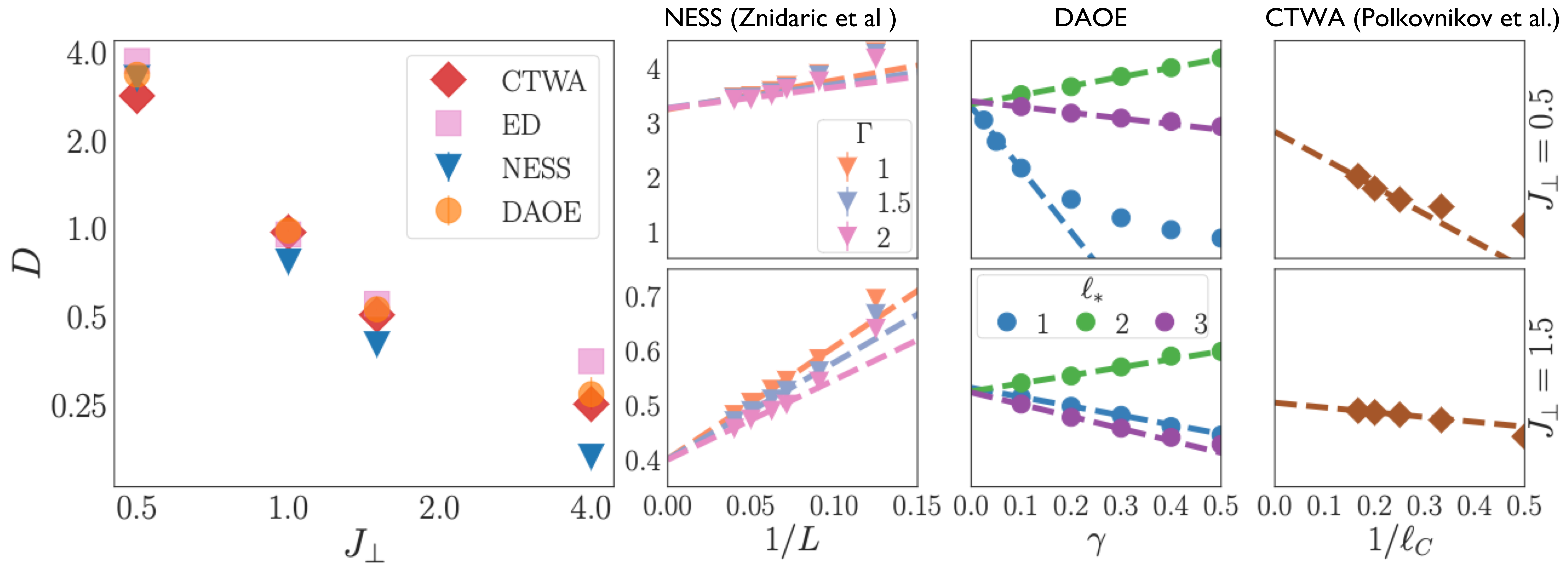
$D \approx 0.95$ [Steinigeweg et al., '14]



[Rakovszky, von Keyserlingk, FP, PRB **105**, 075137 (2022)]

Benchmark to other methods (work in progress)

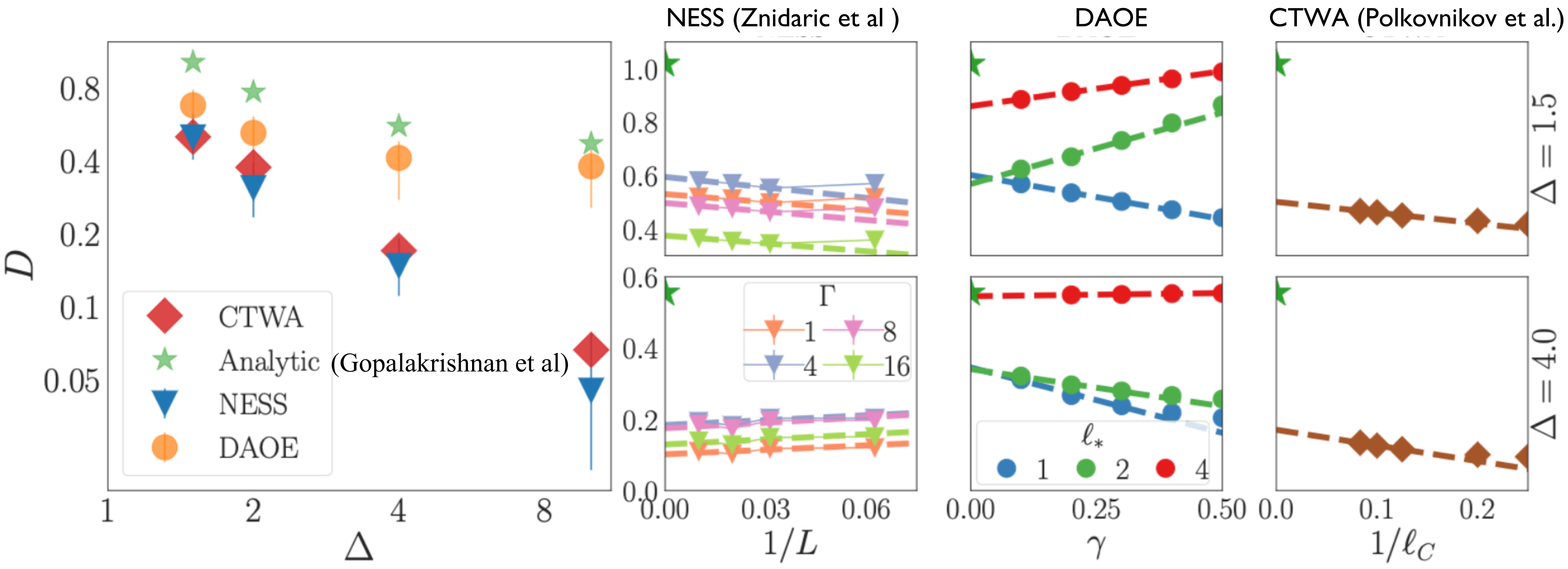
XX ladder: $H = \sum_{j=1}^{L} \sum_{a=1,2} \left(X_{j,a}X_{j+1,a} + Y_{j,a}Y_{j+1,a}\right) + J_\perp \sum_{j=1}^{L} \left(X_{j,1}X_{j,2} + Y_{j,1}Y_{j,2}\right)$



[Hemery, Lovas, Mc Culloch, von Keyserlingk, FP, Rakovszky (in progress)]

Benchmark to other methods (work in progress)

XXZ chain $H = \sum_{j=1}^{L} \left(X_j X_{j+1} + Y_j Y_{j+1} + \Delta Z_j X_{j+1} \right)$



[Hemery, Lovas, Mc Culloch, von Keyserlingk, FP, Rakovszky (in progress)]

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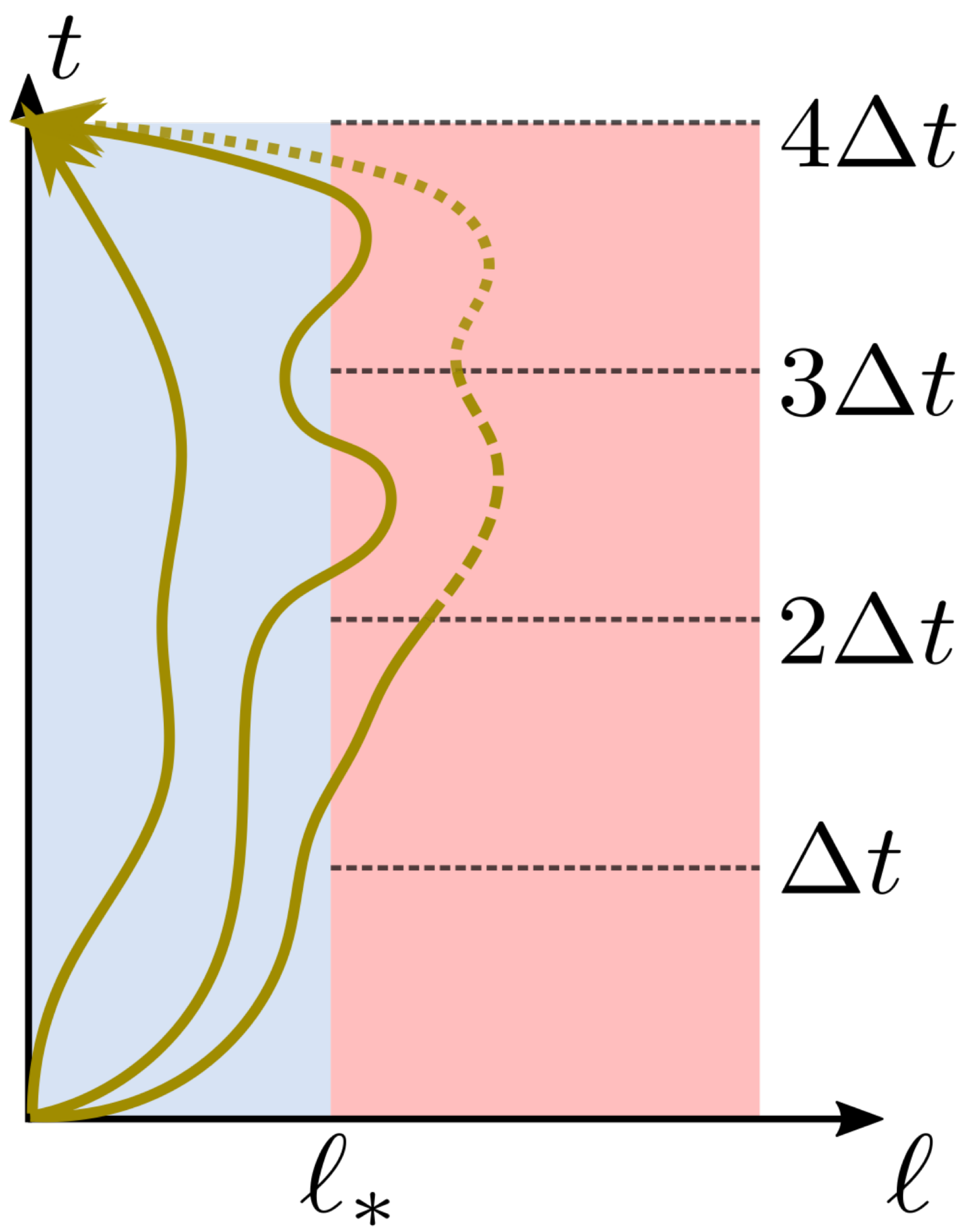

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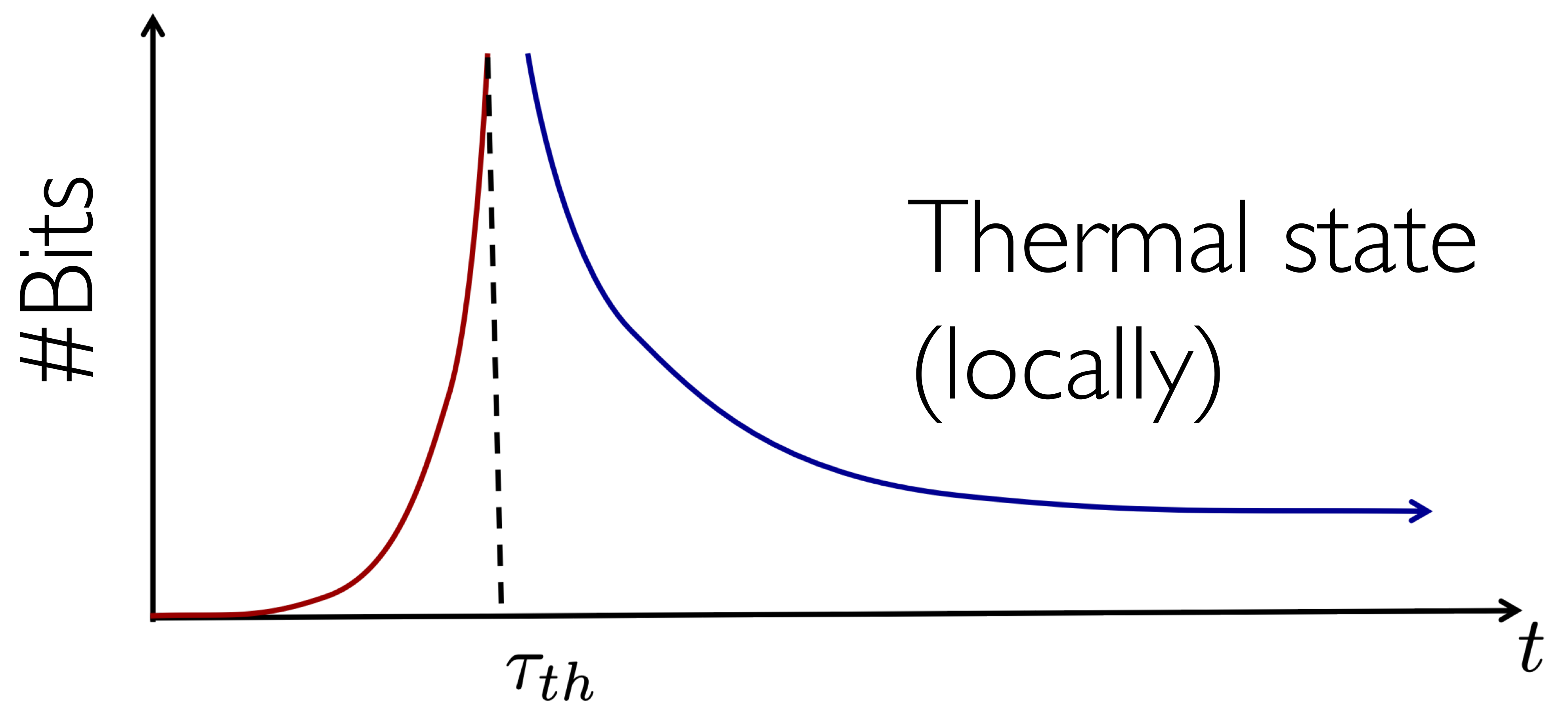
Thank you!

Open questions and challenges

(1) What is the optimal way to truncate entanglement without sacrificing crucial information on physical (local) observables?



(2) What are the problems for which we do actually require a quantum computer to simulate physical (local) observables?