Efficient simulation of quantum transport in 1D

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[Rakovszky, von Keyserlingk, FP, PRB 105, 07513 (2022)]
[von Keyserlingk, FP, Rakovszky PRB 105, 245101 (2022)]

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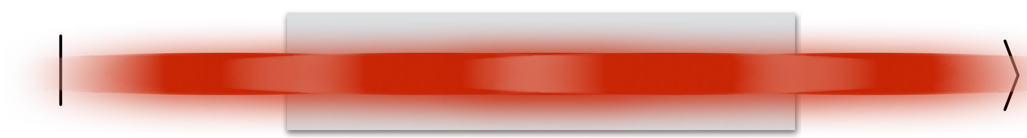
Mathematical results of many-body quantum systems
Herrsching, June 10, 2022

Quantum Thermalization

t

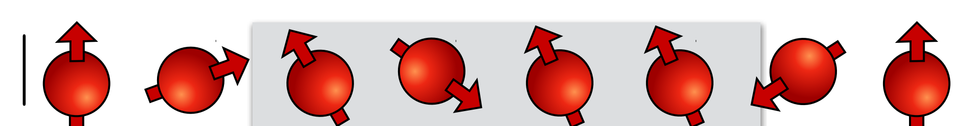
$\rho_{\text{Block}} = \rho_{\text{Thermal}}$



$S = 0$

$U_t = \exp(-itH)$

[non-integrable, local Hamiltonian]



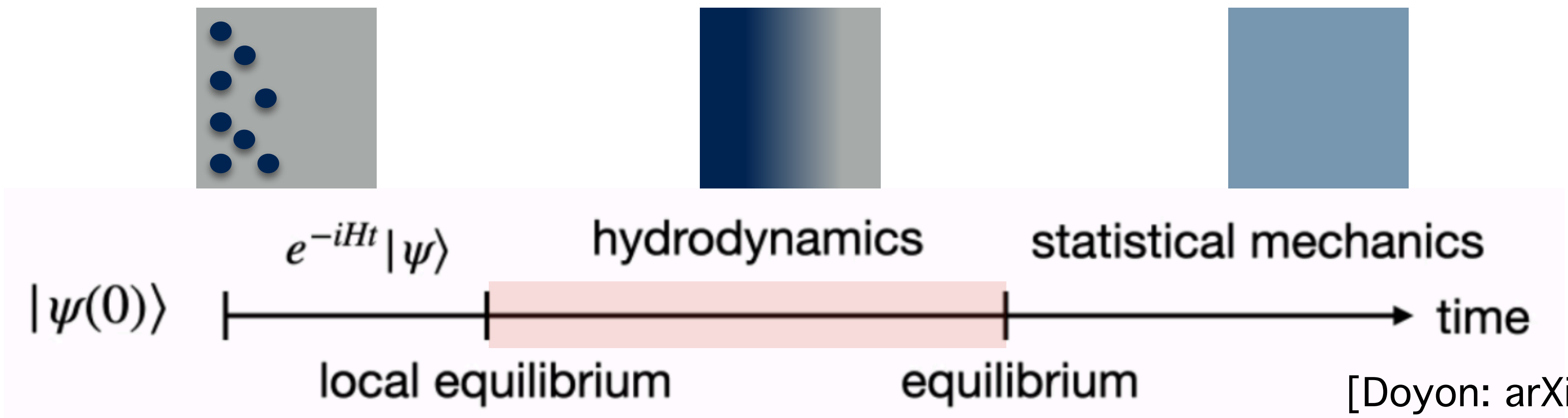
$S = 0$

Closed quantum

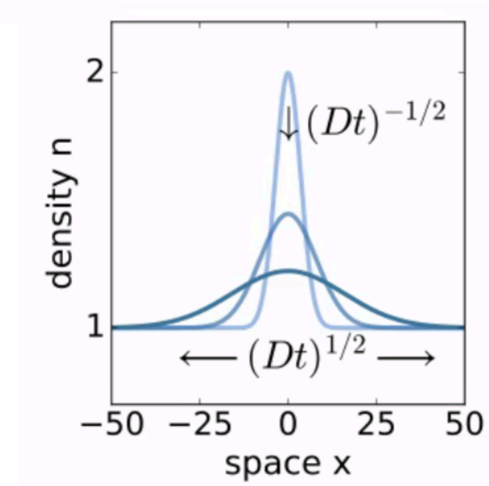
[Srednicki, Deutsch, Rigol]

Characterizing thermalization dynamics

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



[Doyon: arXiv 1912.08496]

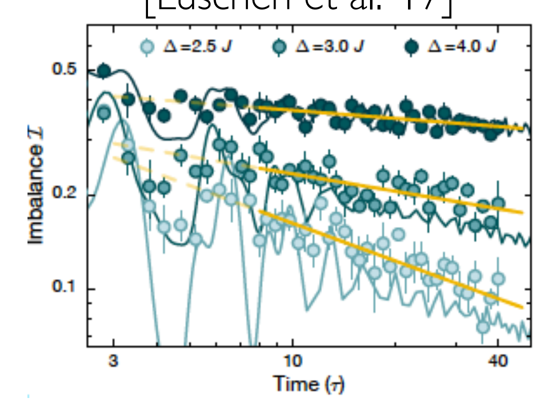


Emergent hydrodynamic relaxation: Diffusion

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

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

[Lüschen 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

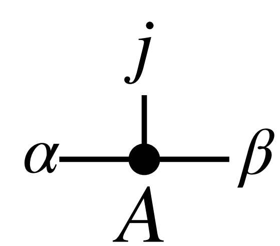
Low entanglement: Matrix-Product States $\quad d^L \to L d\chi^2$

[M. Fannes et al. 92]

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

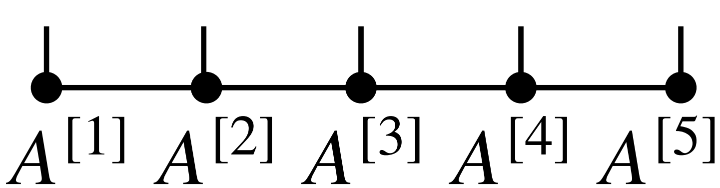
- Efficient representation of ground states of gapped local Hamiltonians [Hastings, Schuch, Verstraete,…]

Diagrammatic representation

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

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

$j = 1\ldots d$

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

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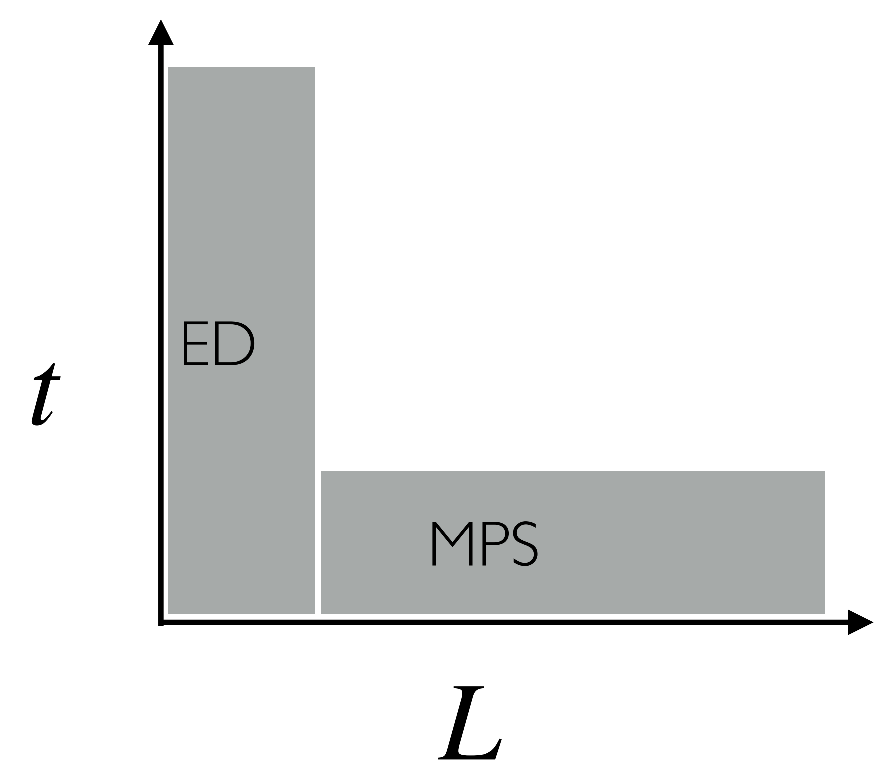
- Complexity $\propto \exp(L)$
- Sparse exact diagonalization methods (dynamical typicality) up to ~30 spins



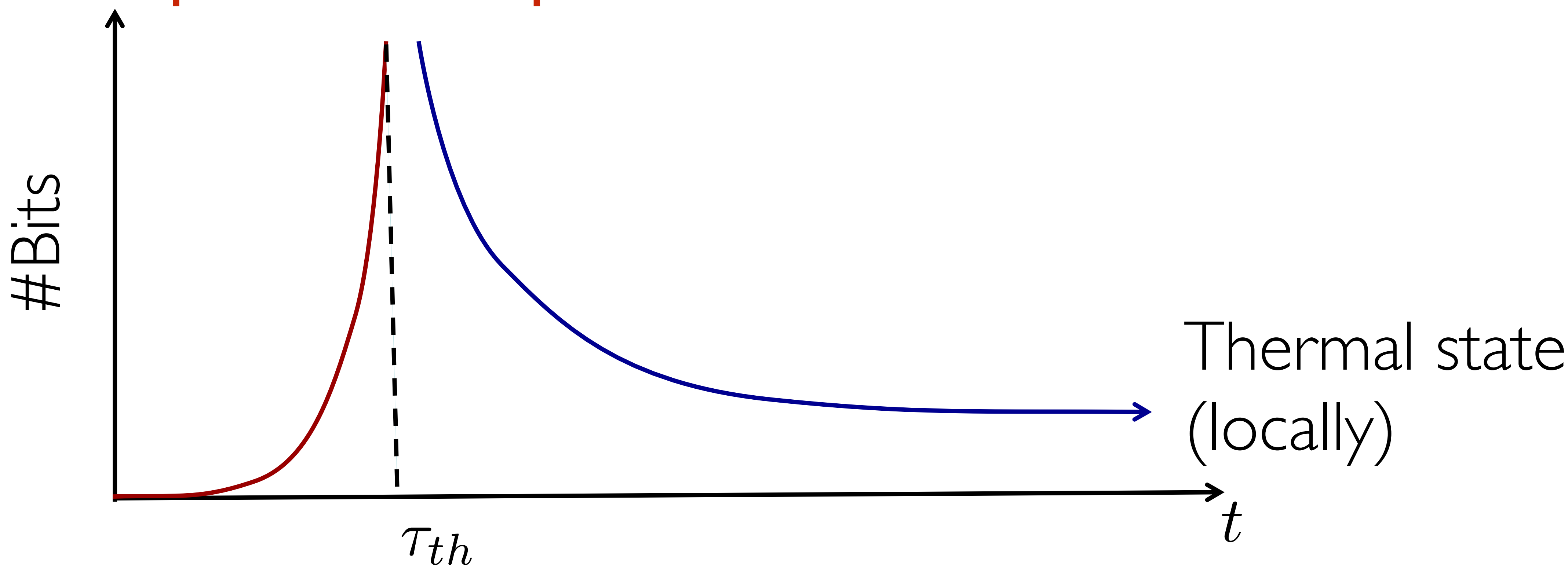
Matrix-Product State based numerics

- 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]

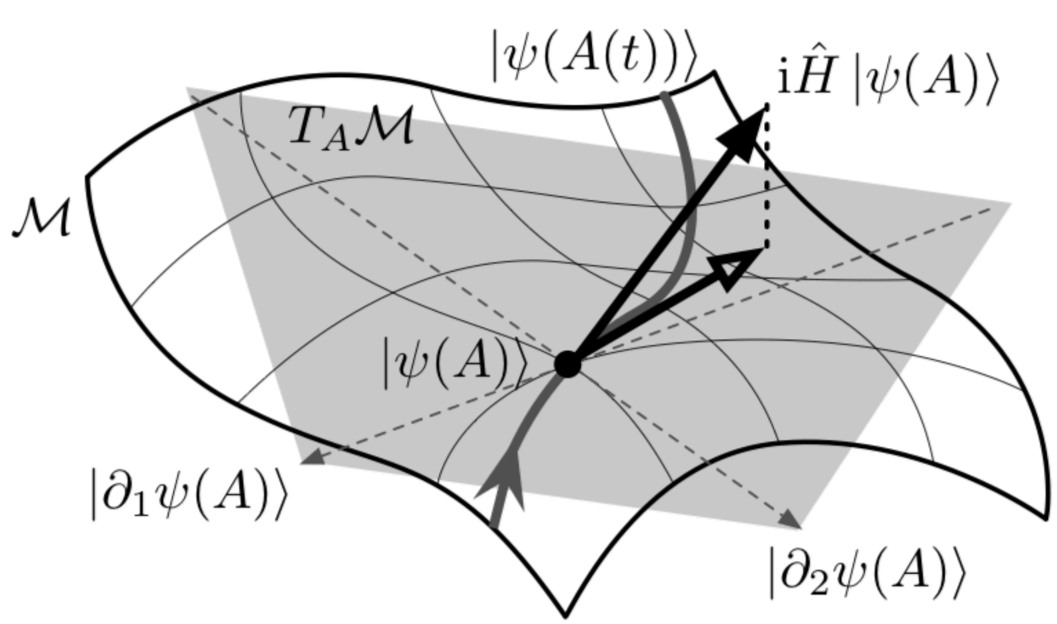
Time-dependent variational principle (TDVP)

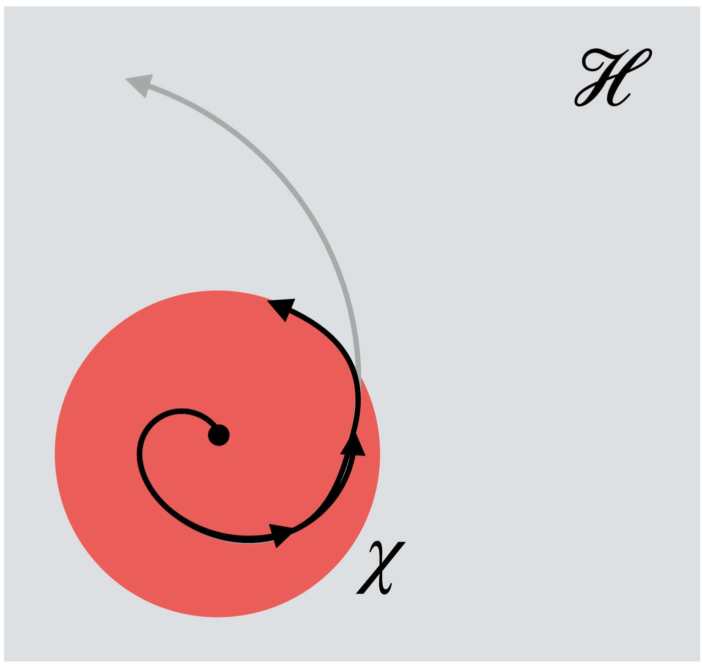
Variational manifold: MPS states with fixed bond dimension

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

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]





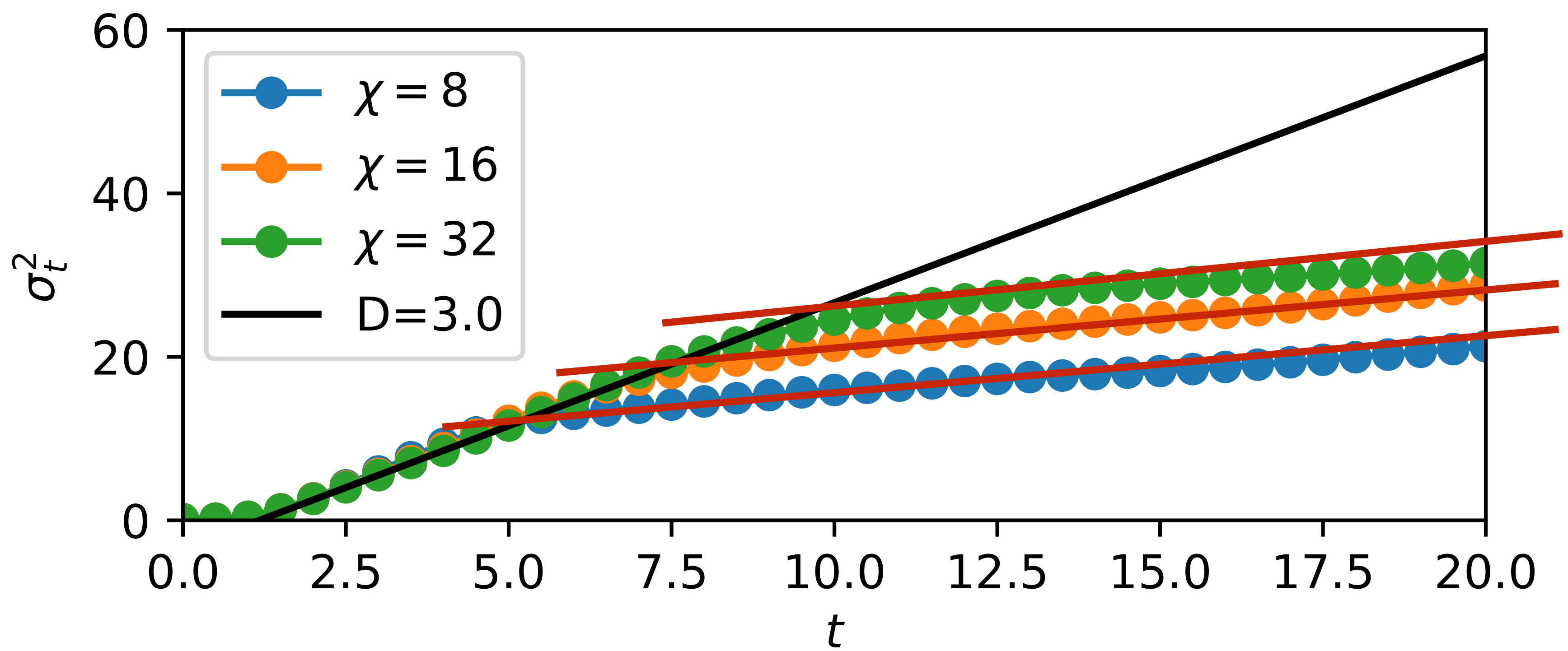
- Global conservation laws (energy, particles,…)

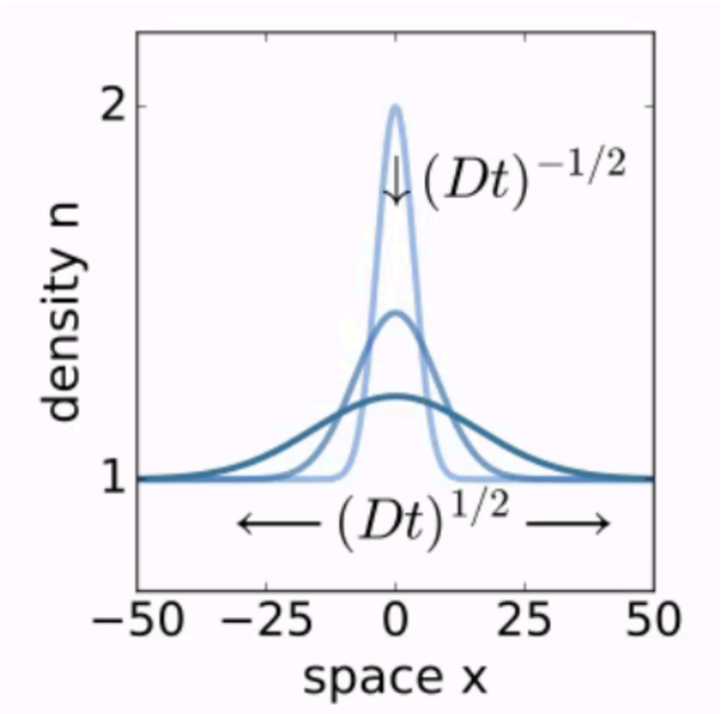
[Leviatan, FP, Bardarson, Huse, Altman, arXiv:1702.08894]

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

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

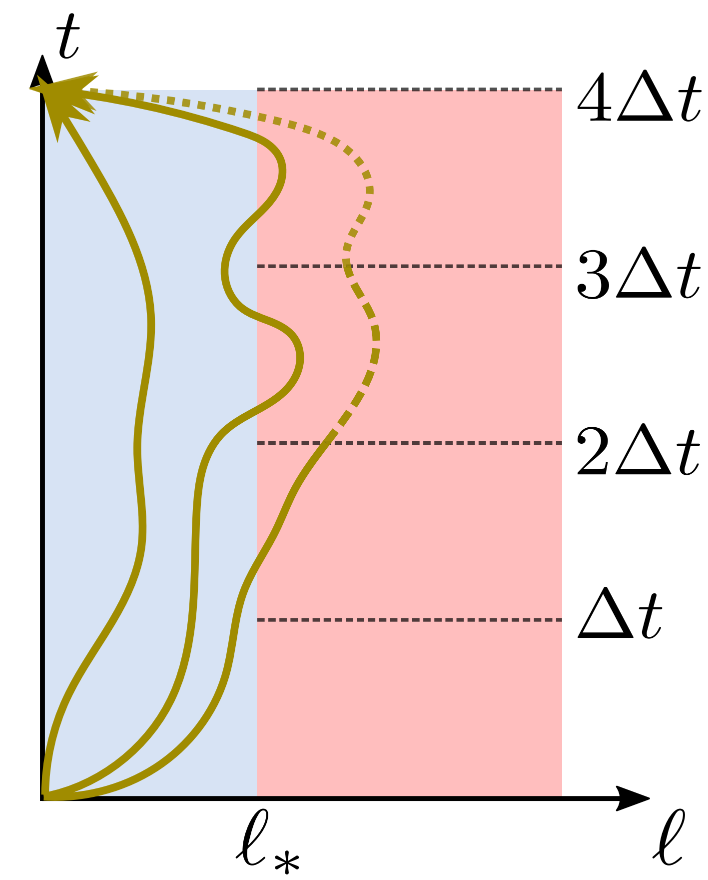
- Discard information corresponding to n-point functions with $n > \ell_*$.

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

- Errors induced by truncation ("backflow") are exponentially suppressed in ℓ_*

$$|D - D_{\mathrm{DAOE}}| \sim e^{-\mathcal{O}(\ell_*)}$$

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



Artificial dissipation that not affects hydrodynamics

$$C(x,t) \equiv \langle q_x(t) q_0(0) \rangle_{\beta=0} = \langle q_x | e^{i\mathcal{L}t} | q_0 \rangle, \quad \mathcal{L} | q_x \rangle \equiv [H, q_x] = -i\partial_t | q_x \rangle$$

Basis of operators: Pauli strings $(\mathbb{1}, X, Y, Z)$

$$\mathcal{S} = \ldots ZX\mathbb{1}YX\mathbb{1}\mathbb{1}Y\ldots \longrightarrow | q_0(t) \rangle = \sum_{\mathcal{S}} a_{\mathcal{S}} | \mathcal{S} \rangle$$

Artificial Dissipator:

$$\mathcal{D}_{\ell_*,\gamma} | \mathcal{S} \rangle = \begin{cases} | \mathcal{S} \rangle & \text{if } \ell_{\mathcal{S}} \leq \ell_* \\ e^{-\gamma(\ell_{\mathcal{S}} - \ell_*)} | \mathcal{S} \rangle & \text{otherwise} \end{cases}$$

$$\begin{array}{ll} \mathbb{1}\mathbb{1}\mathbb{1}\mathbb{1}X\mathbb{1}\mathbb{1} & \ell_{\mathcal{S}} = 1 \\ Y\mathbb{1}\mathbb{1}\mathbb{1}X\mathbb{1}\mathbb{1} & \ell_{\mathcal{S}} = 2 \\ Y\mathbb{1}Z\mathbb{1}X\mathbb{1}\mathbb{1} & \ell_{\mathcal{S}} = 3 \end{array}$$

- Cutoff length $\ell_* =$ #non-trivial Paulis
- Should be larger than support of conserved densities!
- Dissipation strength: γ

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

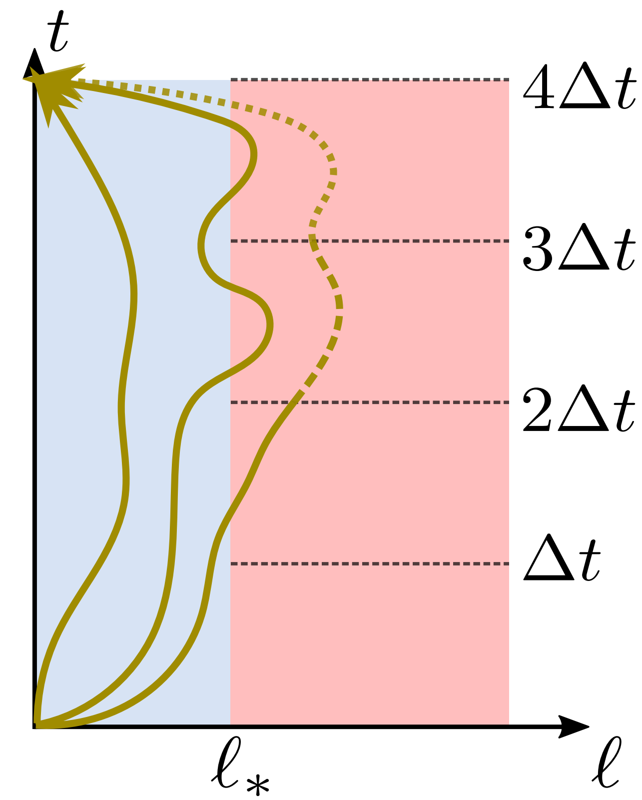
Artificial dissipation that not affects hydrodynamics

Modified evolution: dissipate after every Δt

$$|\tilde{q}_x(N\Delta t)\rangle \equiv \left(\mathscr{D}_{\ell_*,\gamma} e^{i\mathscr{L}\Delta t}\right)^N |q_x\rangle$$

$$\mathscr{D}_{\ell_*,\gamma}|\mathcal{S}\rangle = \begin{cases} |\mathcal{S}\rangle & \text{if } \ell_{\mathcal{S}} \leq \ell_* \\ e^{-\gamma(\ell_{\mathcal{S}}-\ell_*)}|\mathcal{S}\rangle & \text{otherwise} \end{cases}$$

$$C(x,t) \equiv \langle q_x(t) q_0(0) \rangle$$



- Key assumption: **backflow** from long to short operators is weak

(Cf.: **Short memory time** in Zwanzig-Mori memory matrix)

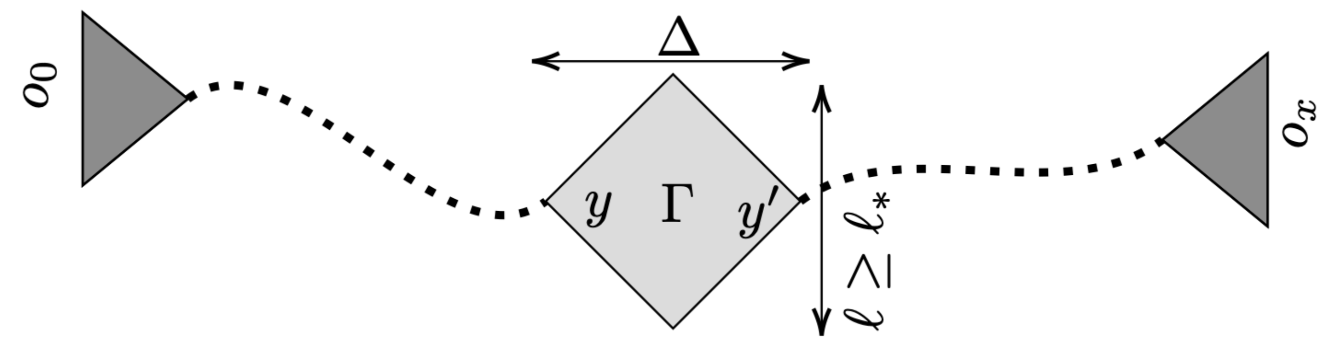
Reduction of operator entanglement: Efficient MPS representation!

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

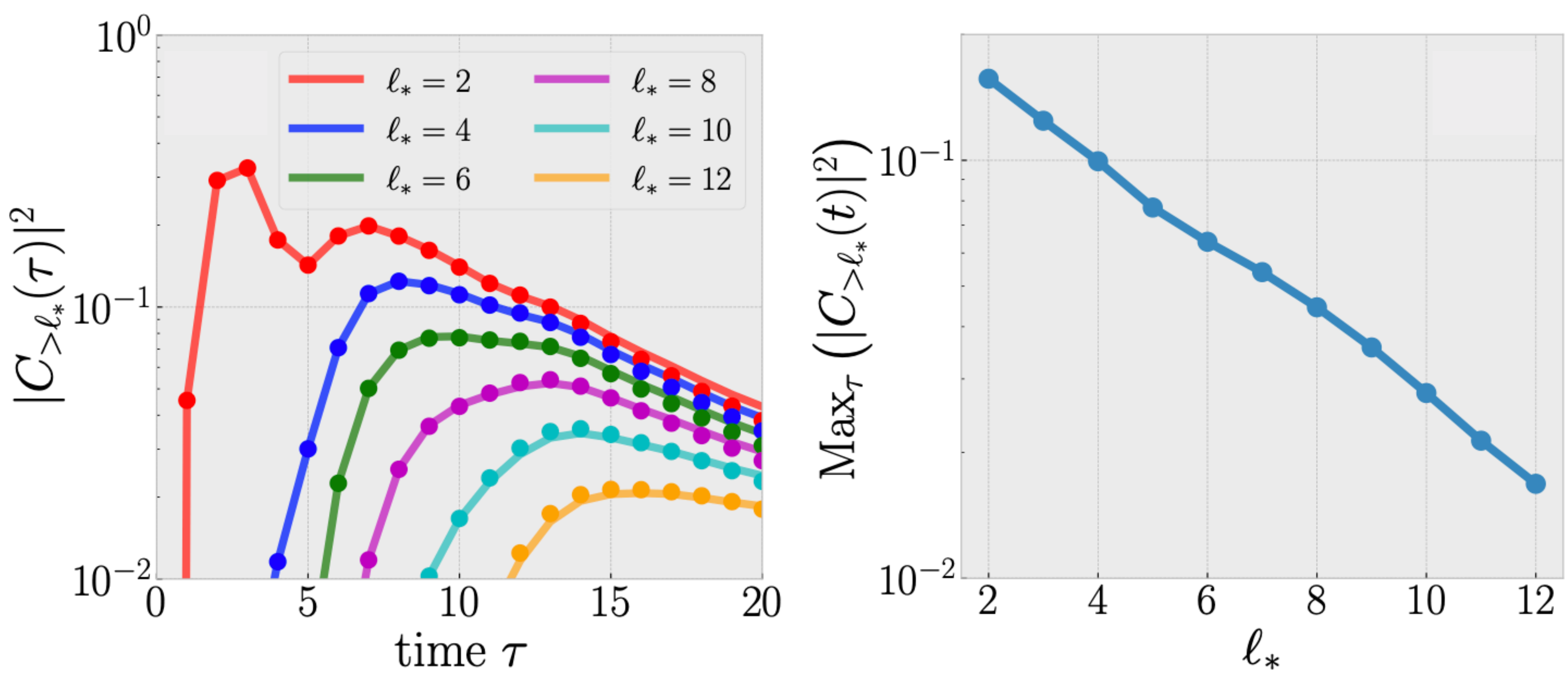
Non rigorous theory of "backflow" corrections

Dynamical correlations

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



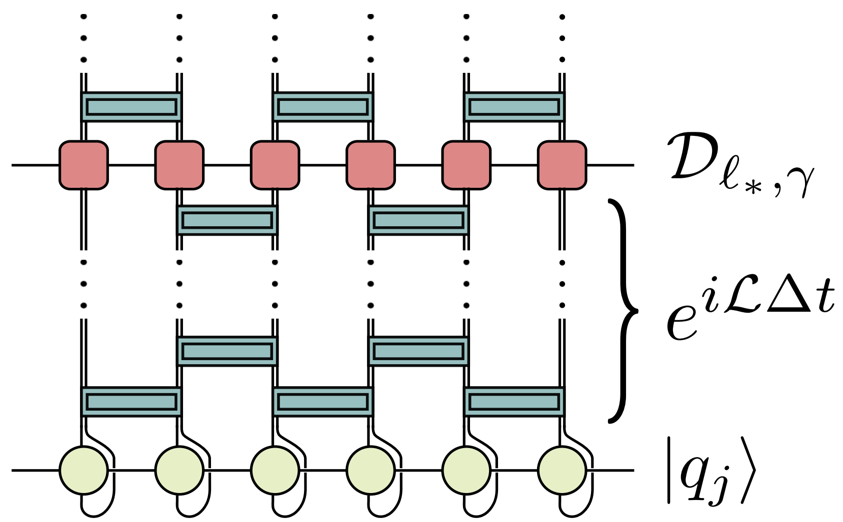
Contributions from "backflow" exponentially small in ℓ_*: $C_{>\ell_*}(\tau, x) \equiv \langle o_0 | \mathcal{U}(\tau = 2t, t) \mathcal{P}_{>\ell_*} \mathcal{U}(t, 0) | o_x \rangle$



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

Dissipation stops growth of operator entanglement

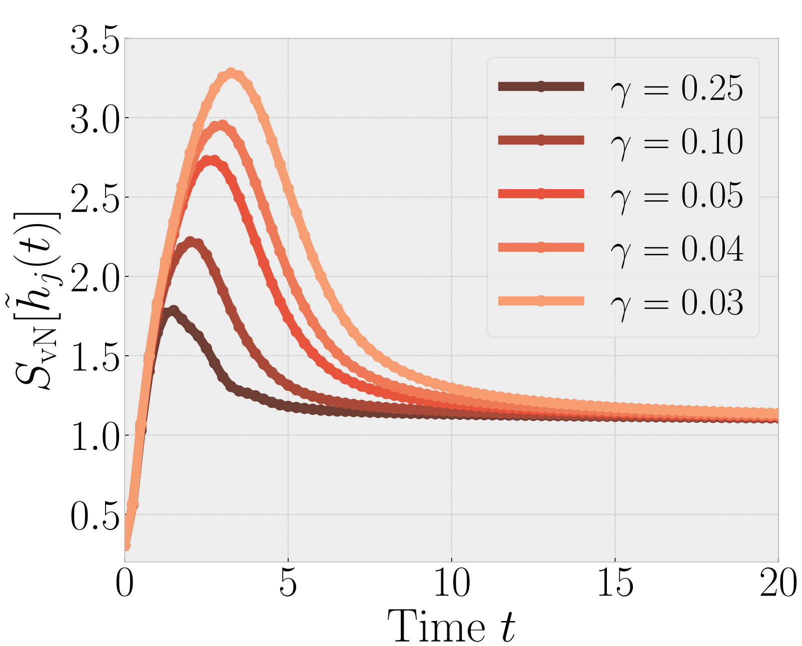
Represent dissipative evolution as tensor network



← Low-dimensional Matrix-Product Operator

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

Test on quantum Ising chain:



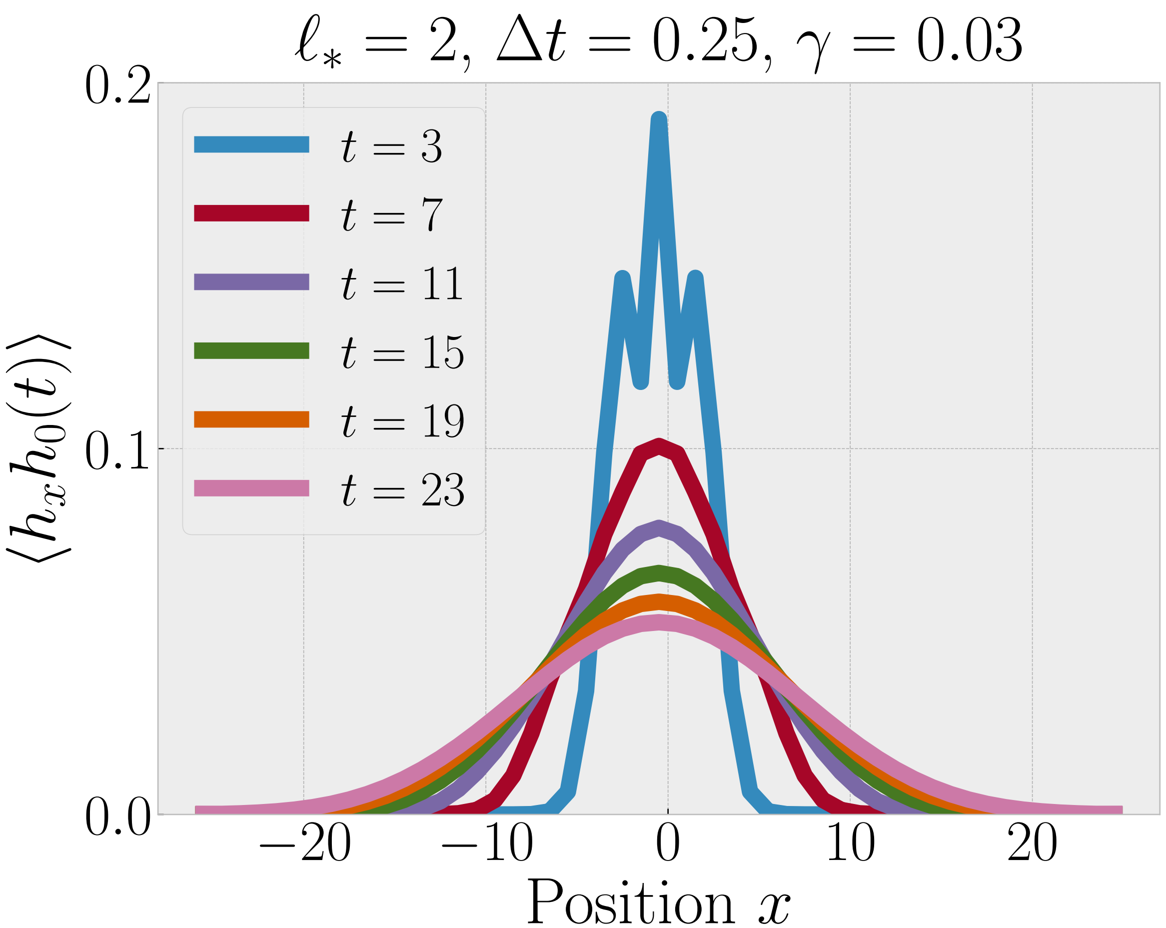
$$H = \sum_j h_j \equiv \sum_j g_x X_j + g_z Z_j + (Z_{j-1}Z_j + Z_j Z_{j+1})/2$$

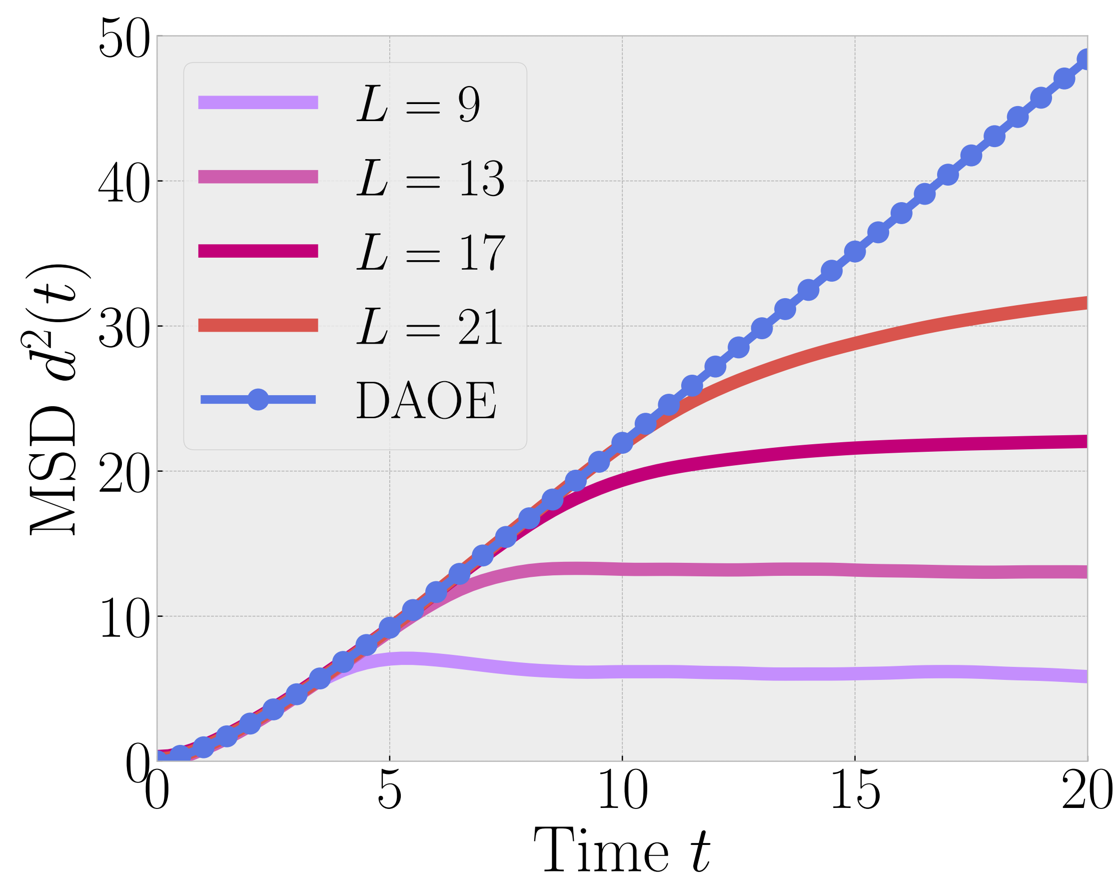
$$g_x = 1.4; \;\; g_z = 0.9045$$

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

Diffusion constant from mean-square displacement

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





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

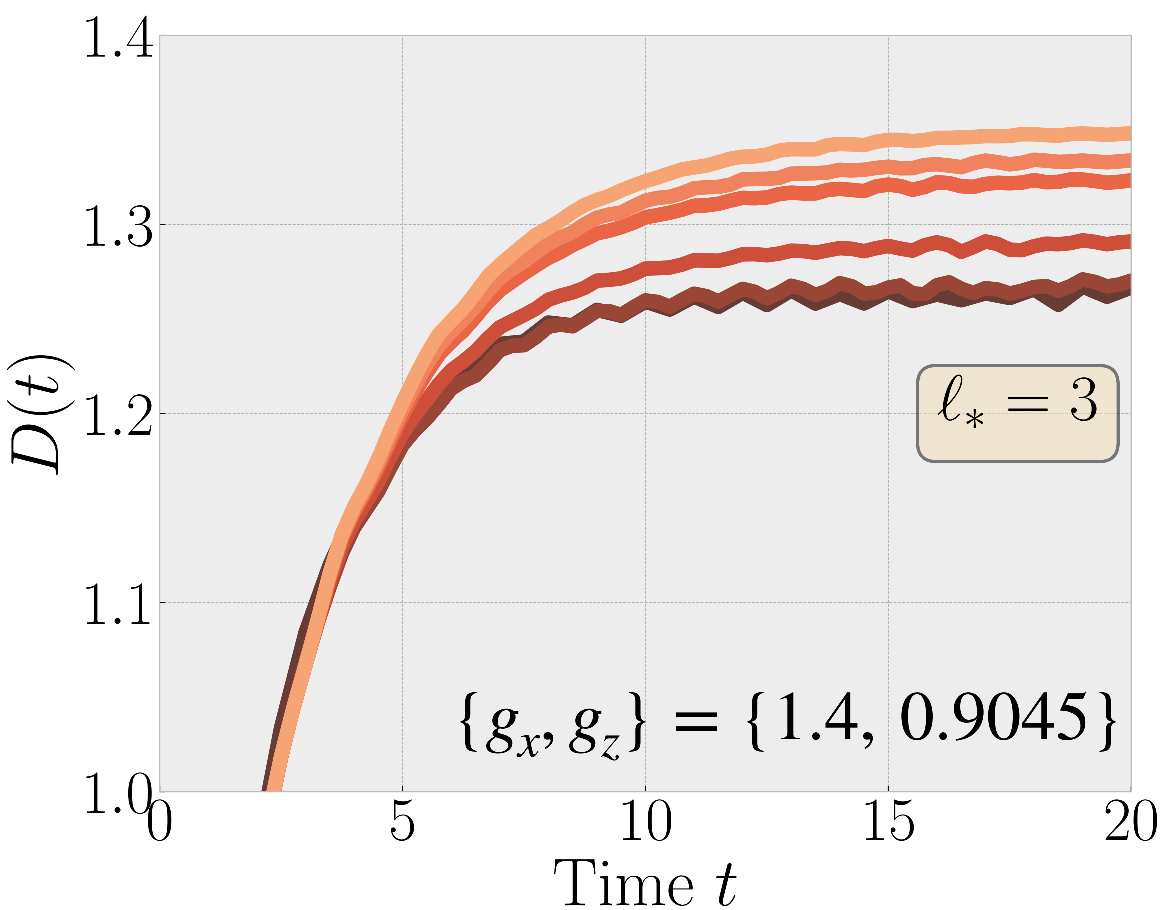
Diffusive transport: $D \equiv \lim\limits_{t \to \infty} D(t)$

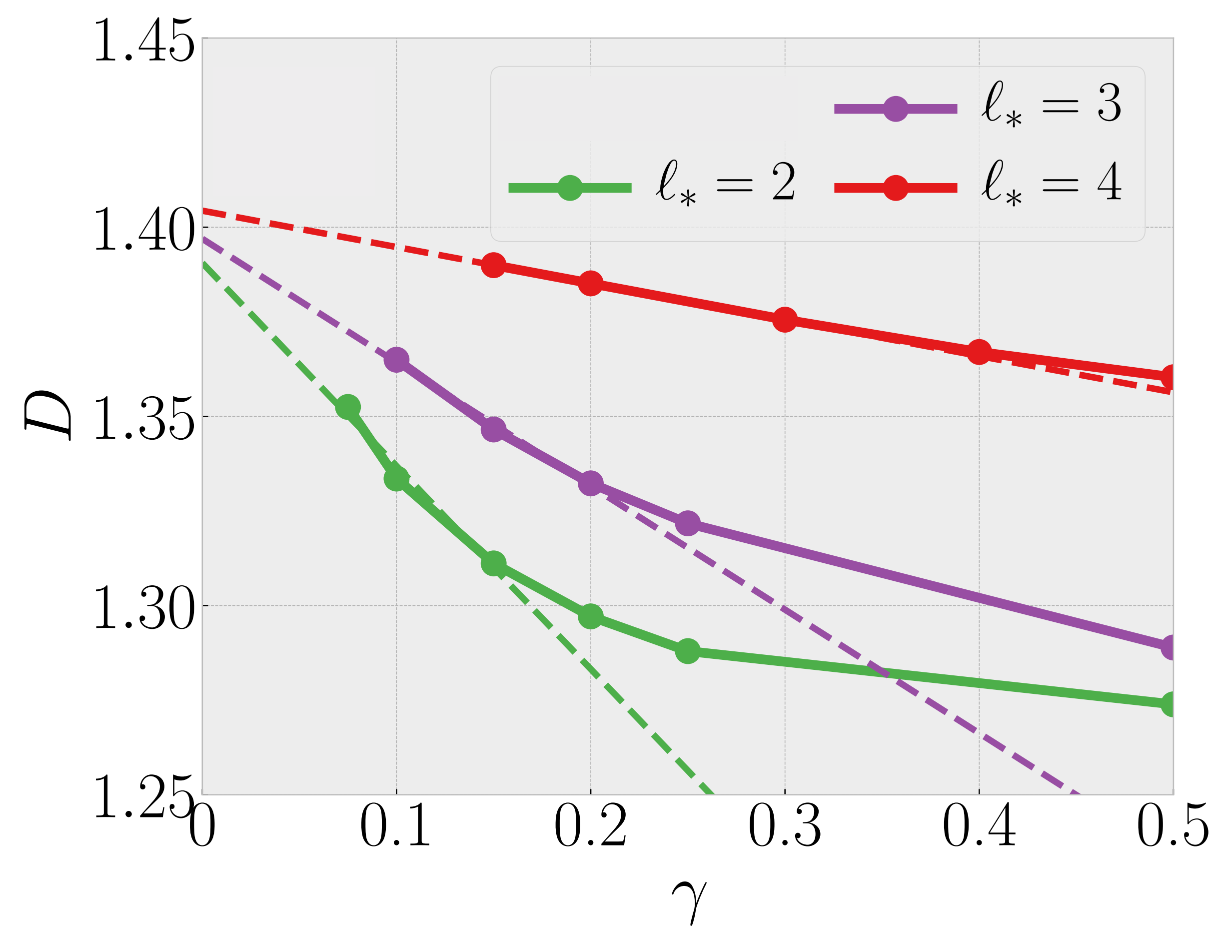
[Rakovszky, von Keyserlingk, FP, PRB **105**, 07513 (2022)]

High precision in various models

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

$q_x \equiv h_j$



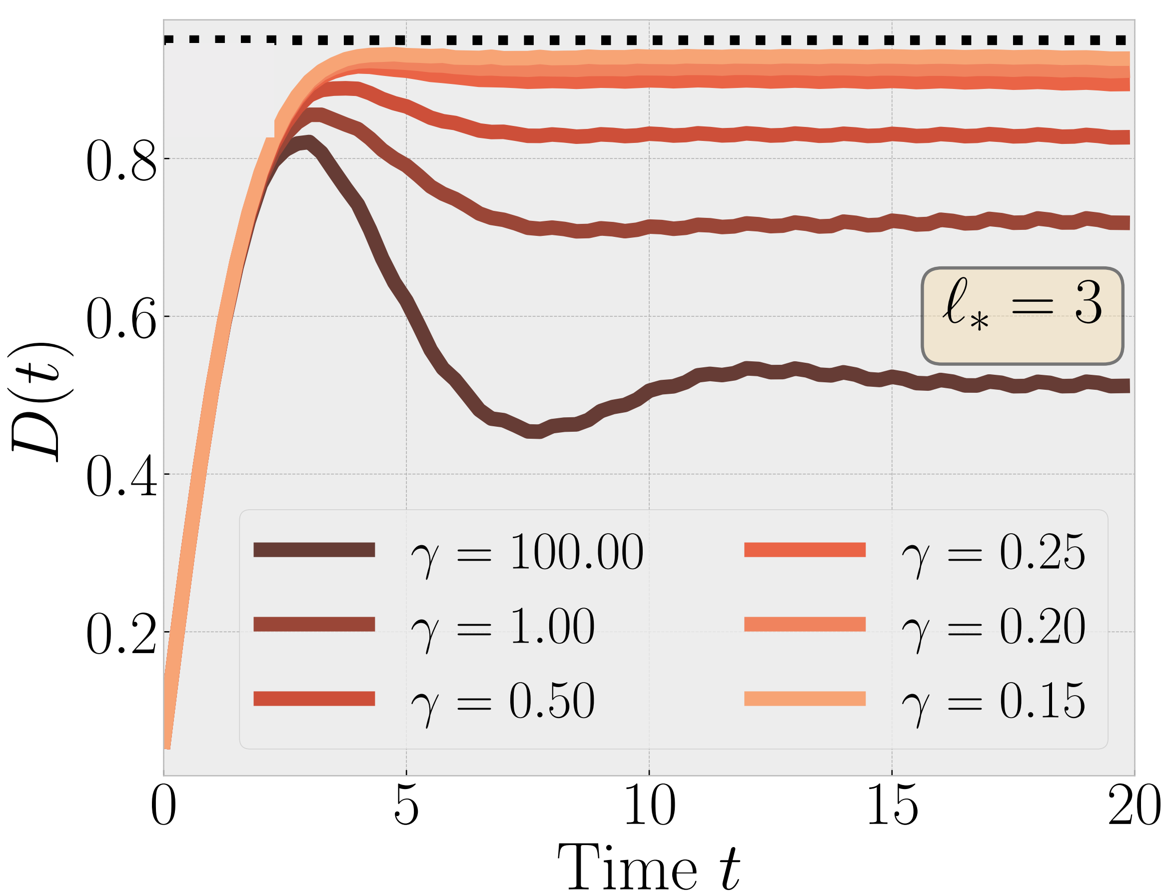


[Rakovszky, von Keyserlingk, FP, PRB **105**, 07513 (2022)]

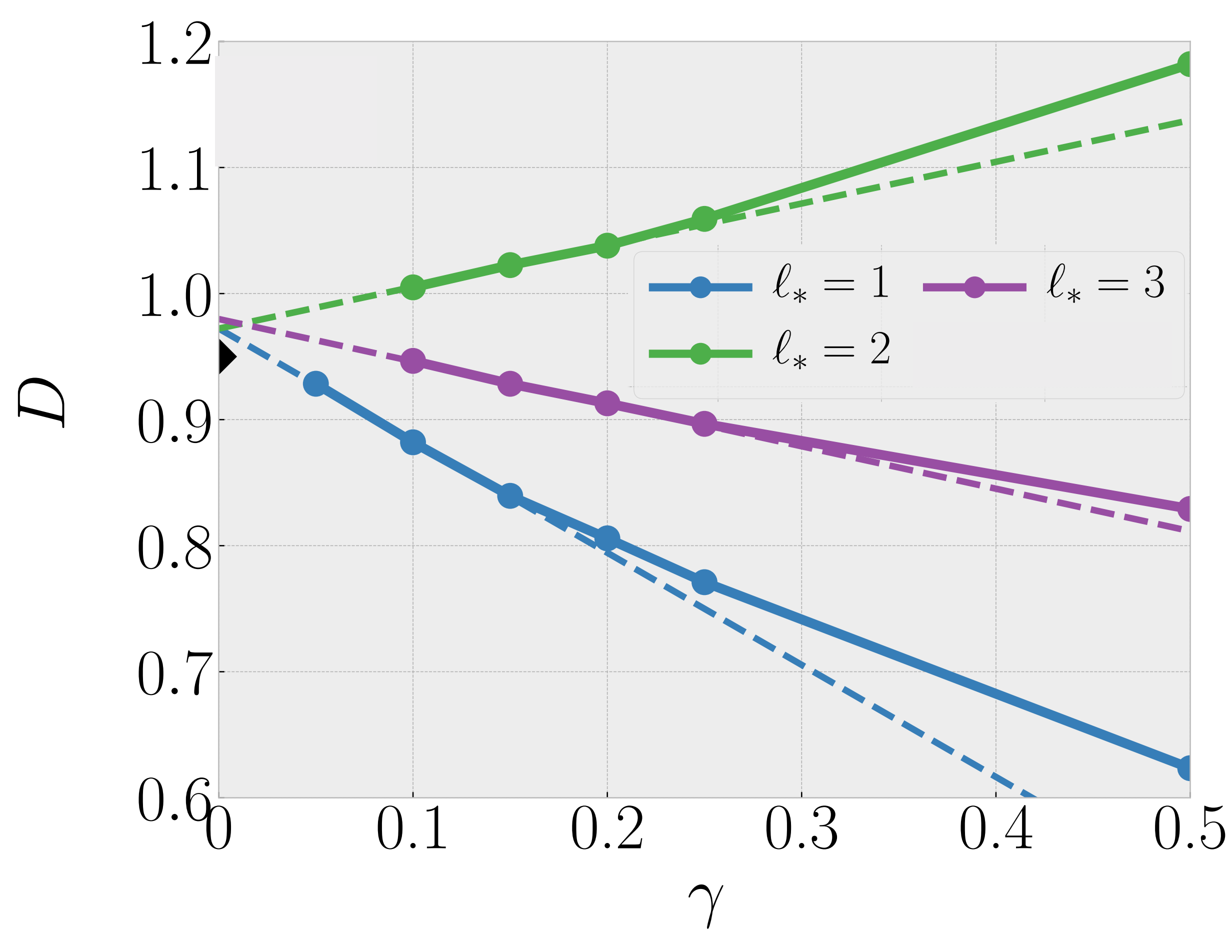
High precision in various models

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]



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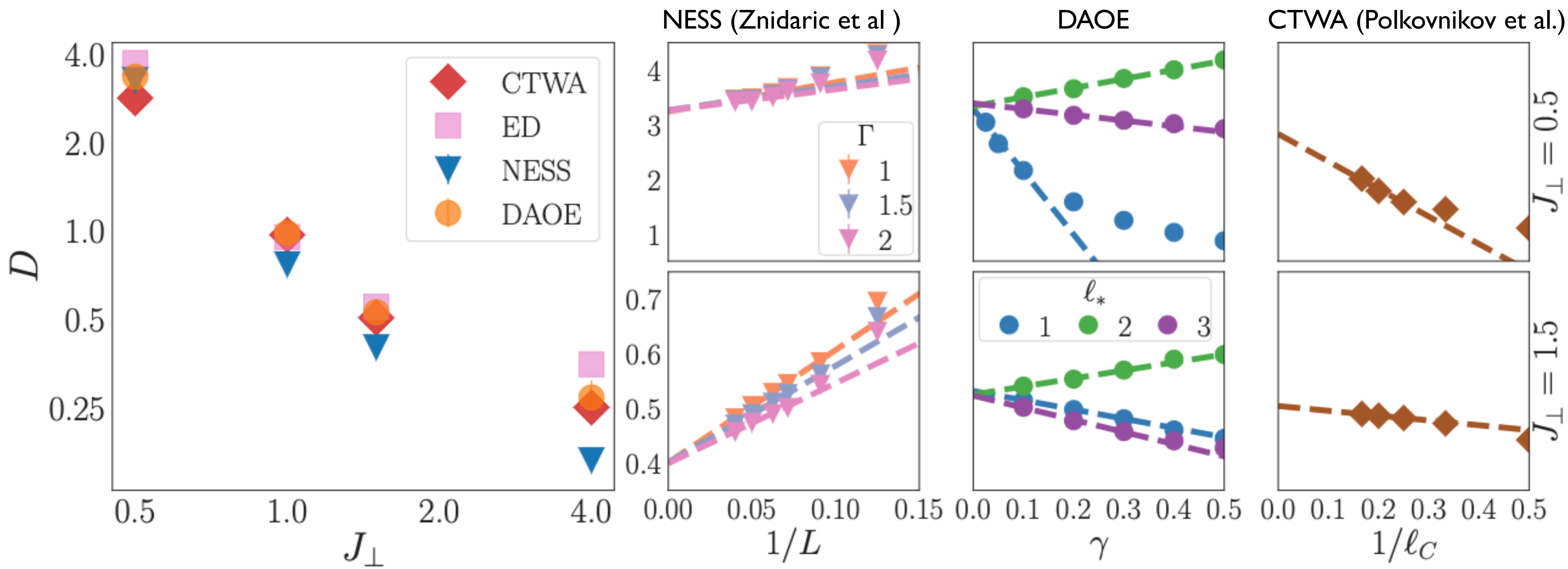
Benchmark to other methods (work in progress)

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)]

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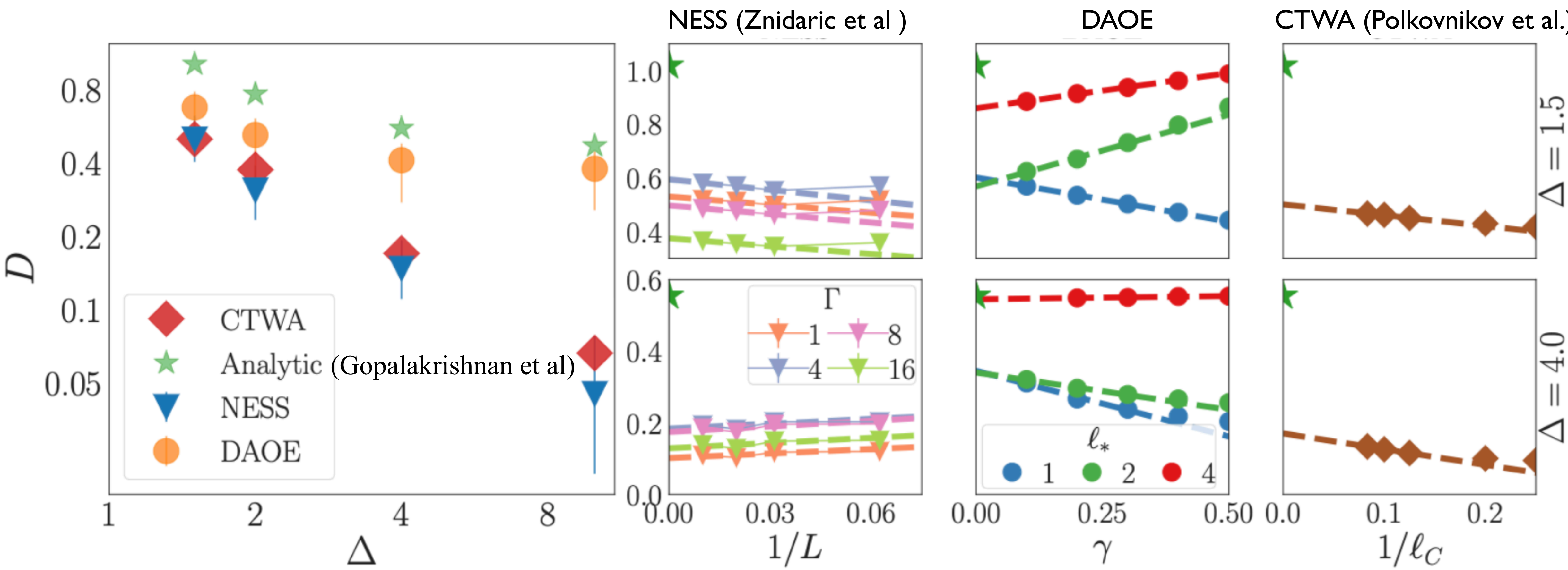

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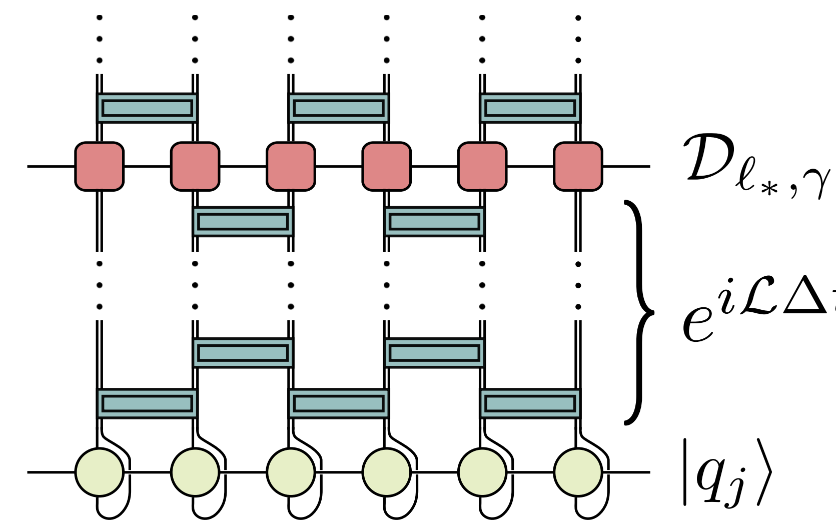

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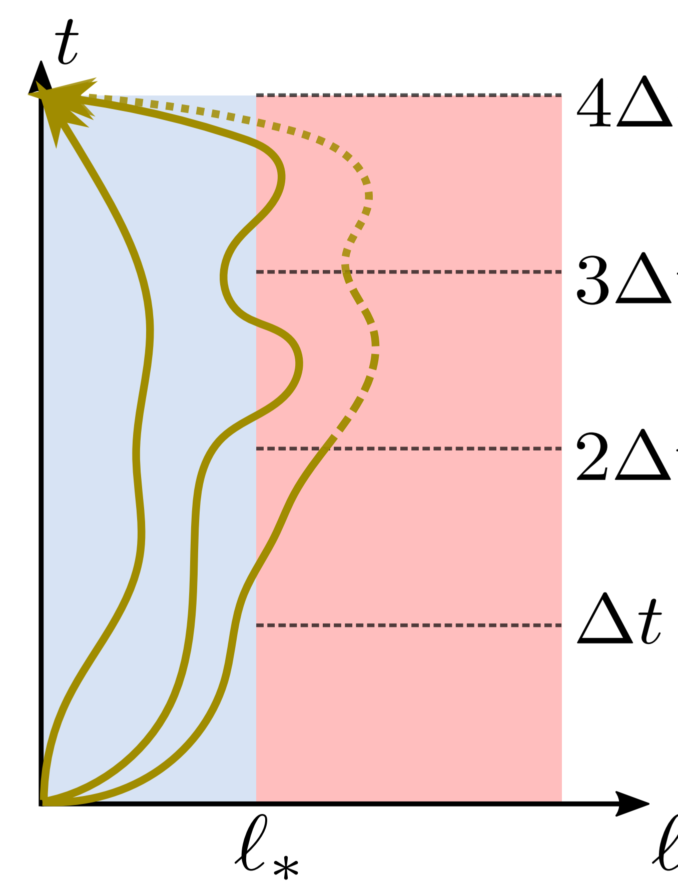

Thank you!