Title: Efficient Simulation of Quantum Transport in 1D

Speakers: Frank Pollmann

Series: Quantum Matter

Date: April 18, 2024 - 1:00 PM

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Abstract: Tensor product states are powerful tools for simulating area-law entangled states of many-body systems. The applicability of such methods to the non-equilibrium dynamics of many-body systems is less clear due to the presence of large amounts of entanglement. New methods seek to reduce the numerical cost by selectively discarding those parts of the many-body wavefunction, which are thought to have relatively litte effect on dynamical quantities of interest. We present a theory for the sizes of "backflow corrections", i.e., systematic errors due to these truncation effects and introduce the dissipation-assisted operator evolution (DAOE) method for calculating transport properties of strongly interacting lattice systems in the high temperature regime. In the DAOE method, we represent the observable as a matrix product operator, and show that the dissipation leads to a decay of operator entanglement, allowing us to capture the dynamics to long times. We benchmark this scheme by calculating spin and energy diffusion constants in a variety of physical models and compare to other existing methods.

Zoom link

Efficient Simulation of Quantum Transport in 1D

Frank Pollmann

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T. Rakovszky, Standford **C.v Keyserlingk, Birmingham**

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

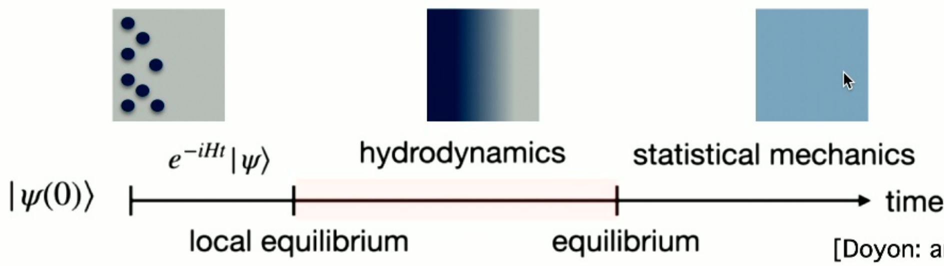
[von Keyserlingk, FP, Rakovszky PRB 105, 245101 (2022)]

[Lloyd, Rakovszky, FP, von Keyserlingk (arXiv:2310.16043)]

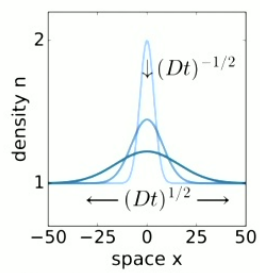
Perimeter Institute
Apr. 18 2024

Characterizing thermalization dynamics

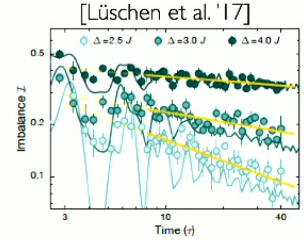
Universal hydrodynamic features tend to emerge in the low-frequency, long-wavelength limit



[Doyon: arXiv 1912.08496]



[Lüschen et al. '17]



Emergent hydrodynamic relaxation:

Diffusion

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

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

Characterizing thermalization dynamics

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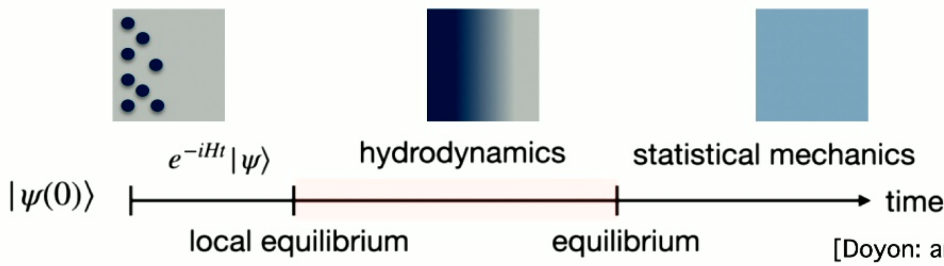

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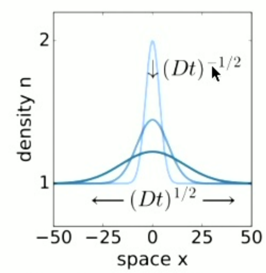

Emergent hydrodynamic relaxation:
Diffusion $\partial_t n = -\partial_x j$ $j = -D\partial_x n$ (Fick's law)

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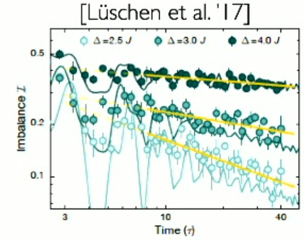


How to numerically extract hydrodynamics for a given microscopic model?

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

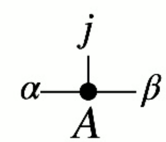
Low entanglement: Matrix-Product States $d^L \to L d \chi^2$

[M. Fannes et al. 92]

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

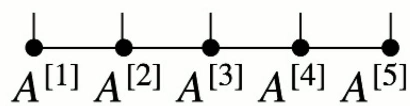
- Efficient representation of ground states of gapped local Hamiltonians [Hastings, Schuch, Verstraete,…]

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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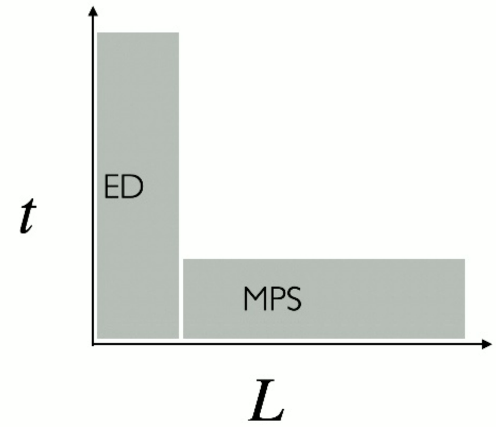


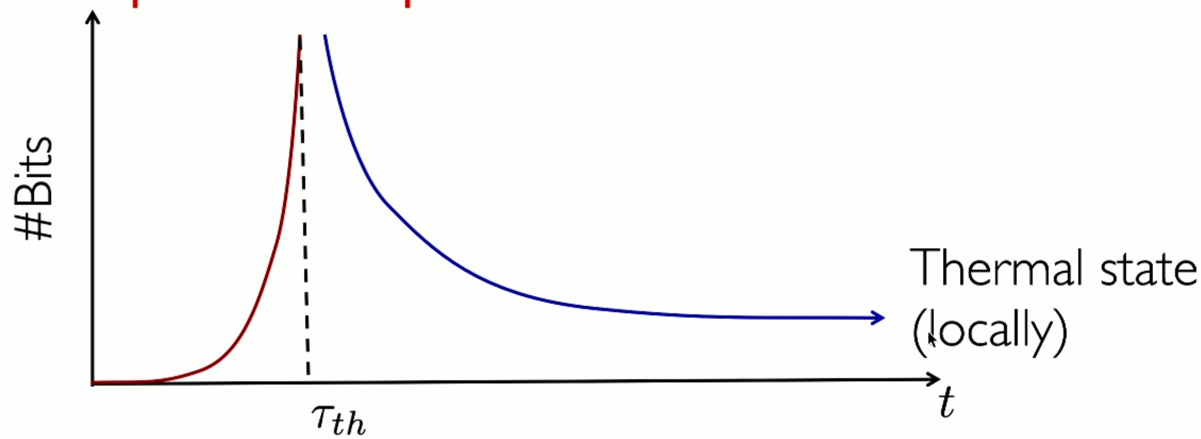
Matrix-Product State based numerics

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

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

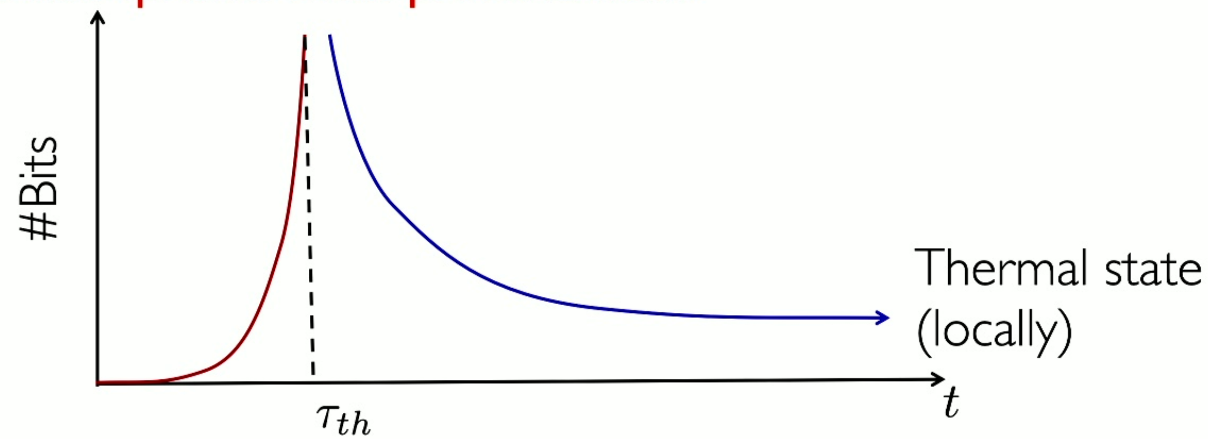
“Information paradox"

Quantum quench from product state



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

“Information paradox"



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]
[Frías-Pérez, et al., arXiv:2308.0429]
[Krumnow et al.: arXiv:1904.11999]
[Leviatan et al., arXiv:1702.08894]

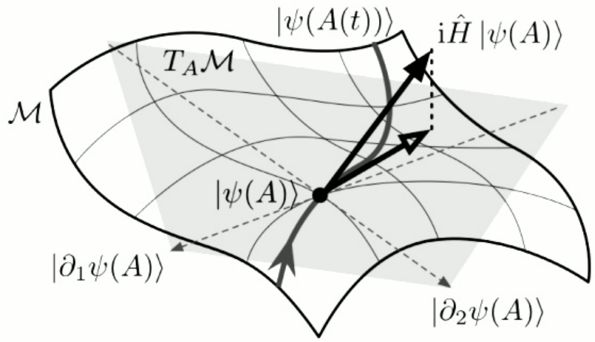
Time-dependent variational principle (TDVP)

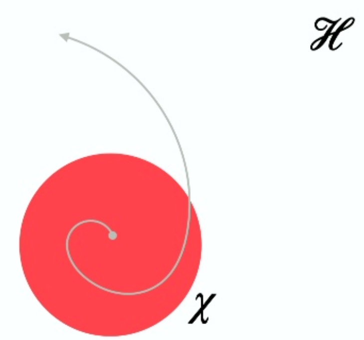
Variational manifold: MPS states with fixed bond dimension

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

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]





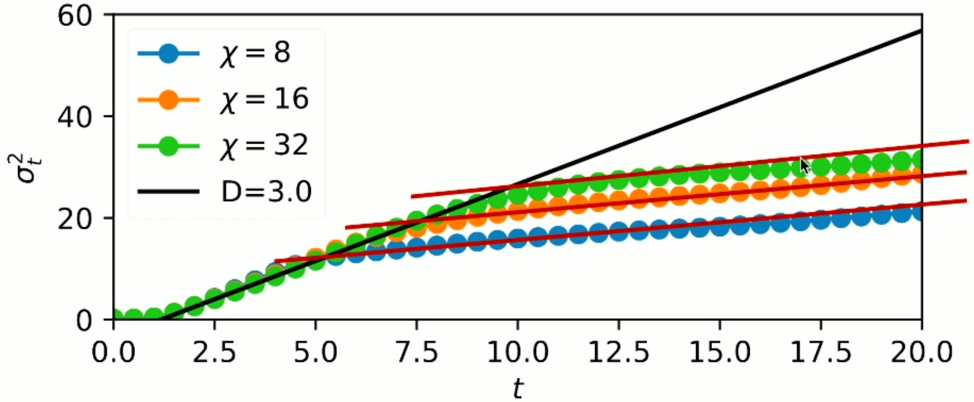
- Global conservation laws (energy, particles,…)

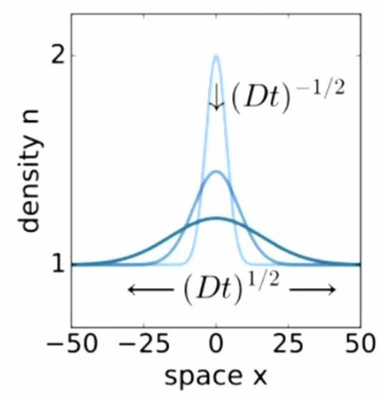
[Leviatan, FP, Bardarson, Huse, Altman, arXiv:1702.08894]

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]

Time-dependent variational principle (TDVP)

Variational manifold: MPS states with fixed bond dimension

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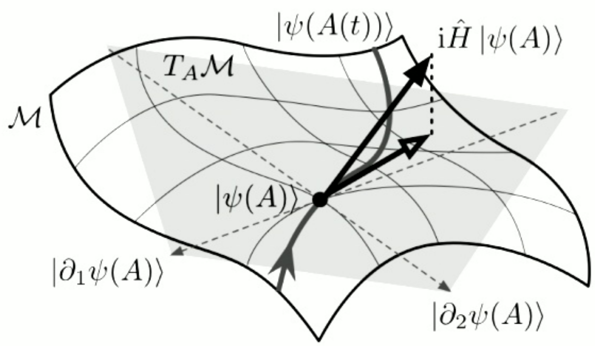

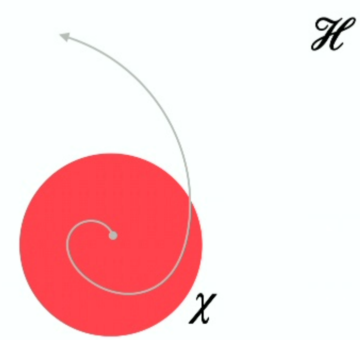

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Dissipation-assisted operator evolution method

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 $n > \ell_*$.

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

Artificial dissipation that not affects hydrodynamics

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

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

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

Artificial Dissipator:

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

$$\mathbb{1}\mathbb{1}\mathbb{1}\mathbb{1}X\mathbb{1}\mathbb{1} \quad \ell_{\mathcal{S}} = 1$$
$$Y\mathbb{1}\mathbb{1}\mathbb{1}X\mathbb{1}\mathbb{1} \quad \ell_{\mathcal{S}} = 2$$
$$Y\mathbb{1}Z\mathbb{1}X\mathbb{1}\mathbb{1} \quad \ell_{\mathcal{S}} = 3$$

- 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

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

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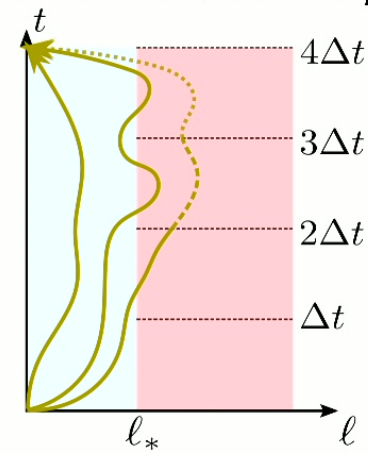

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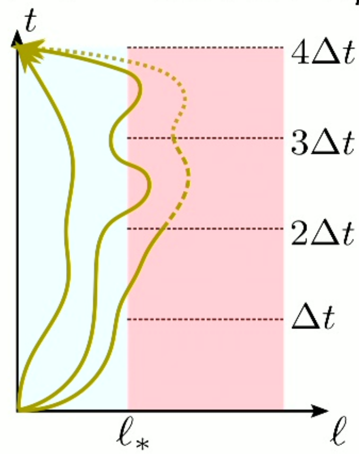
- Key assumption: **backflow** from long to short operators is weak

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

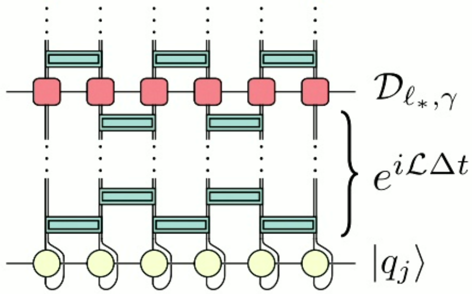
$$C(x,t) \equiv \langle q_x(t) q_0(0)\rangle_{\beta=0}$$



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

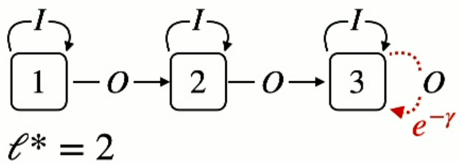
Dissipation stops growth of operator entanglement

Represent dissipative evolution as tensor network

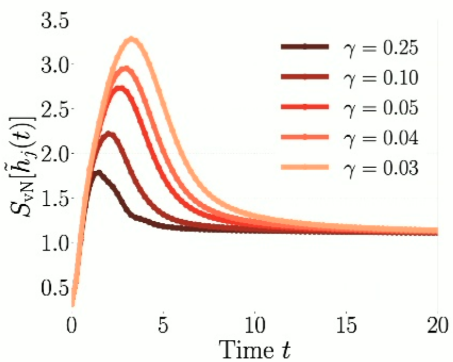


← Low-dimensional Matrix-Product Operator

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



Test on quantum Ising chain:



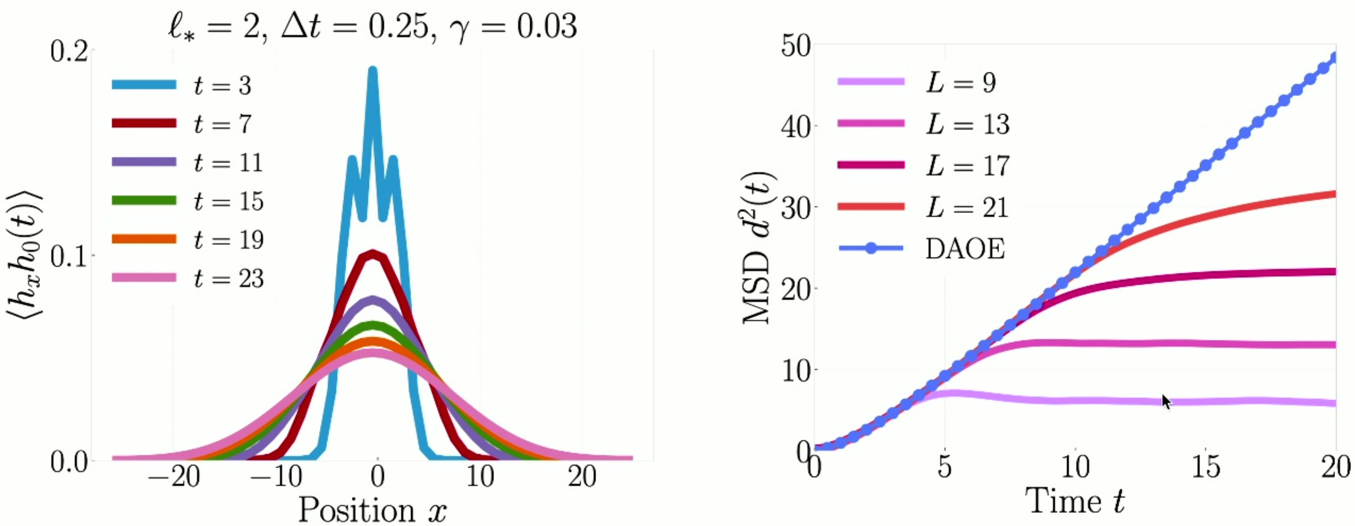
$$H = \sum_j h_j \equiv \sum_j g_x X_j + g_z Z_j + (Z_{j-1} Z_j + Z_j Z_{j+1})/2$$

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

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

Diffusion constant from mean-square displacement

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



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

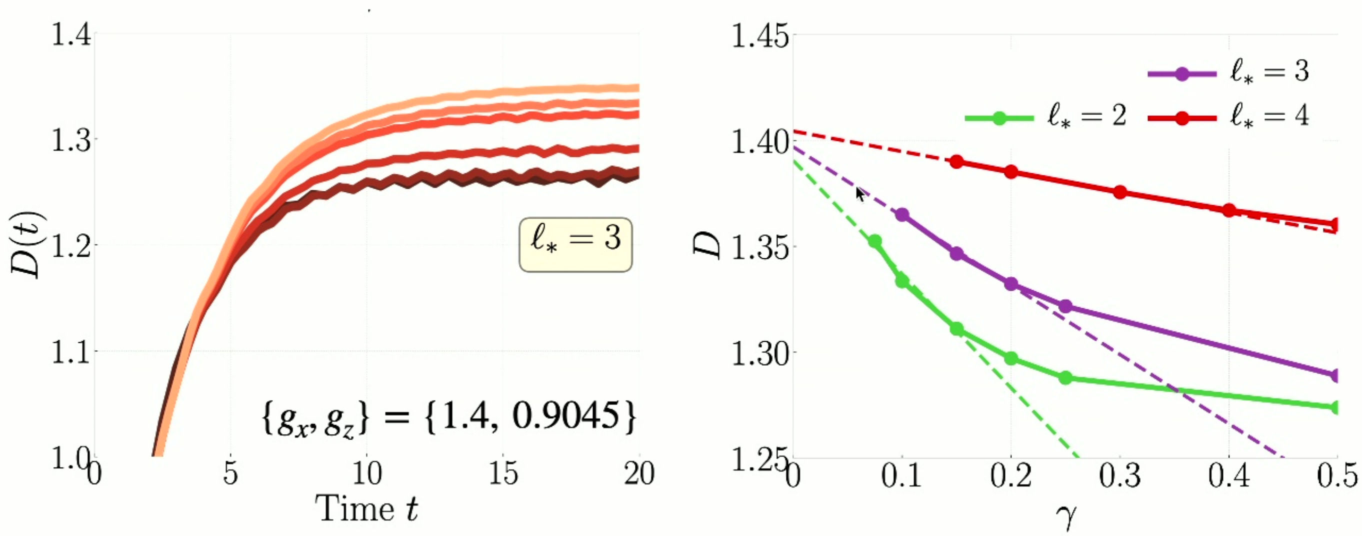
Diffusive transport: $D \equiv \lim_{t \to \infty} D(t)$

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

High precision in various models

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

$q_x \equiv h_j$



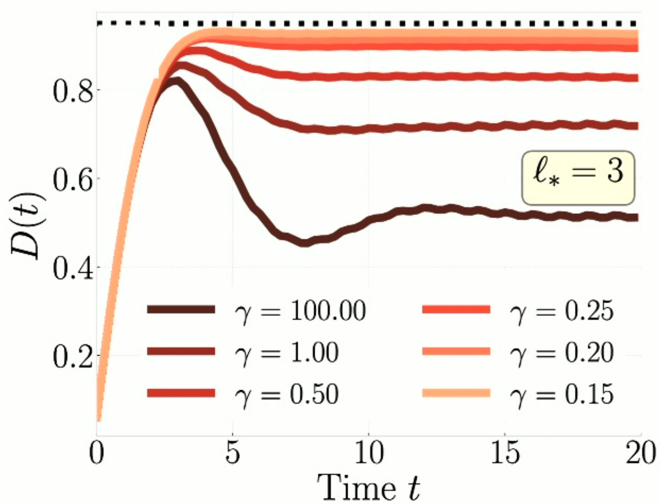
[Rakovszky, von Keyserlingk, FP, PRB **105**, 07513 (2022)]

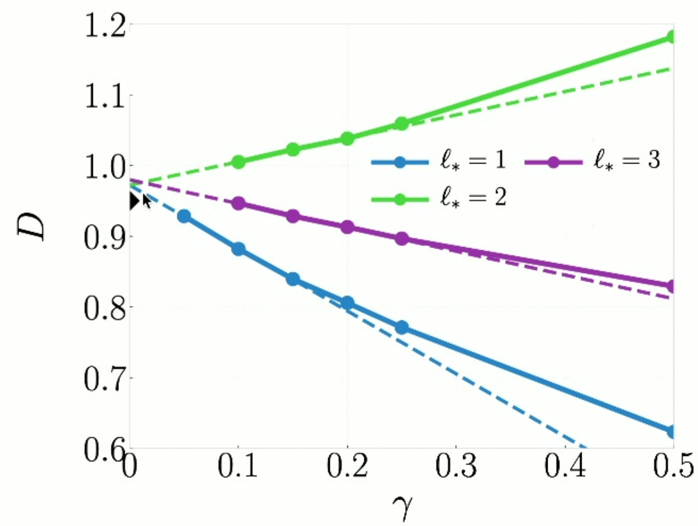
High precision in various models

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]

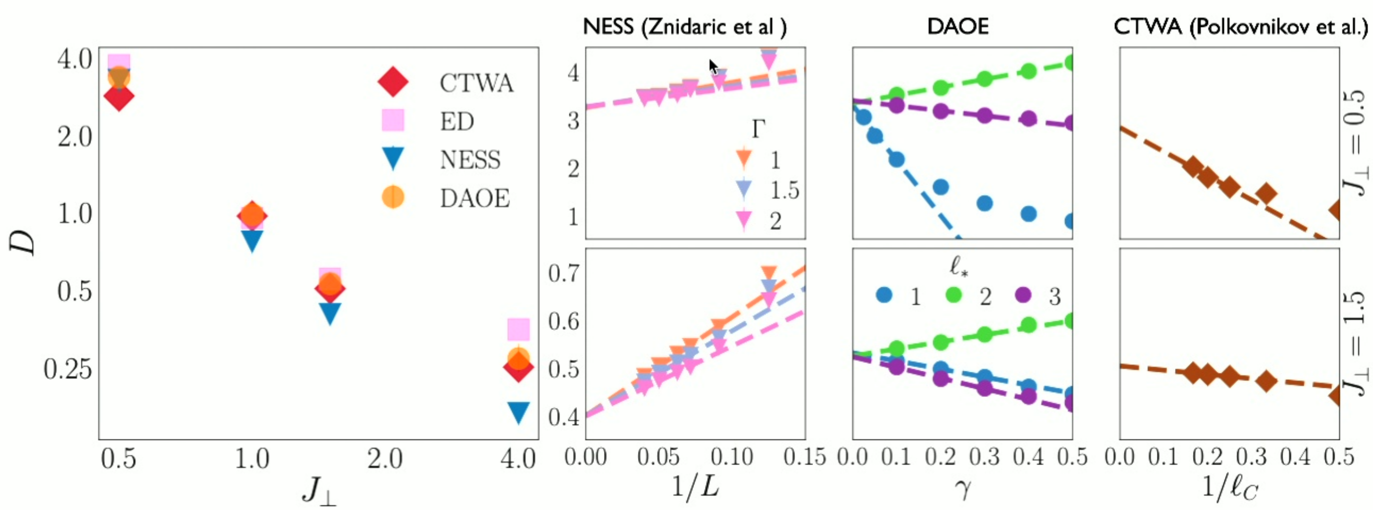




[Rakovszky, von Keyserlingk, FP, PRB **105**, 07513 (2022)]

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)]

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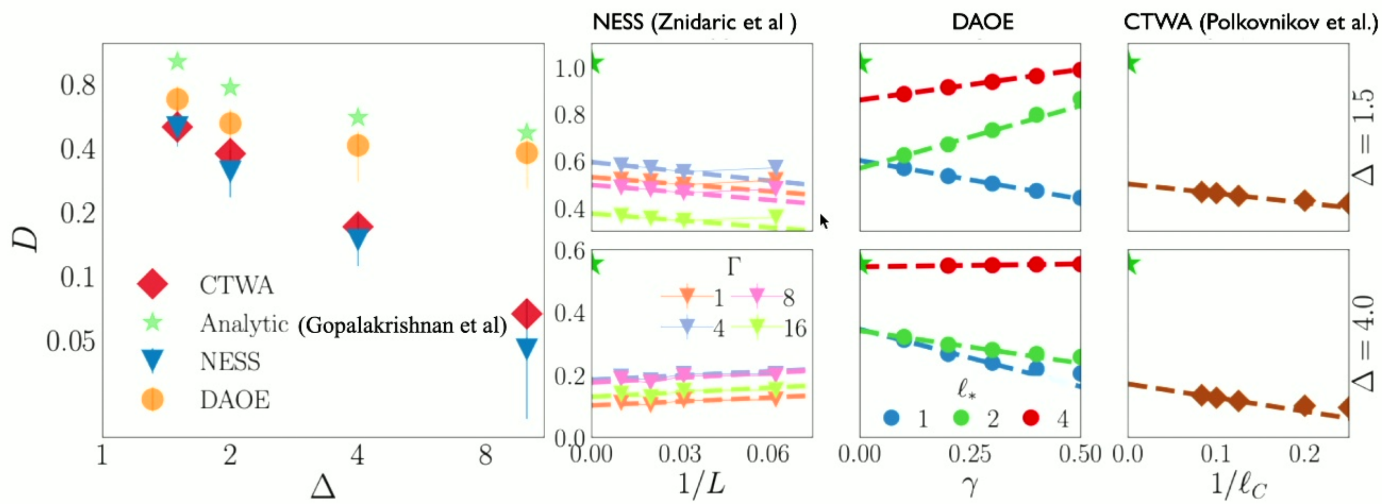
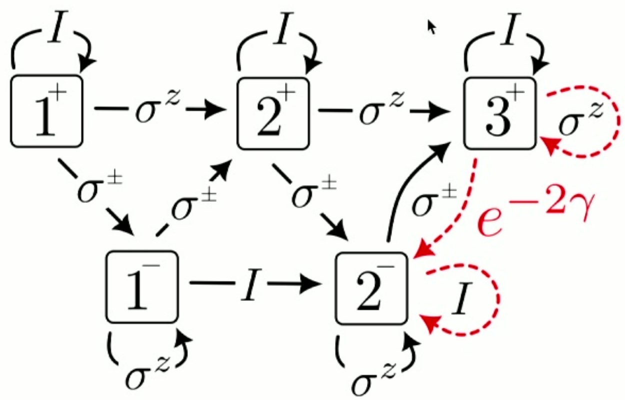


[Hemery, Lovas, Mc Culloch, von Keyserlingk, FP, Rakovszky (in progress)]

Fermionic DOAE

Jordan Wigner Transformation: $f_x^\dagger = \left[\prod_{s<x} \sigma_s^z\right] \sigma_x^+$

fDAOE MPO



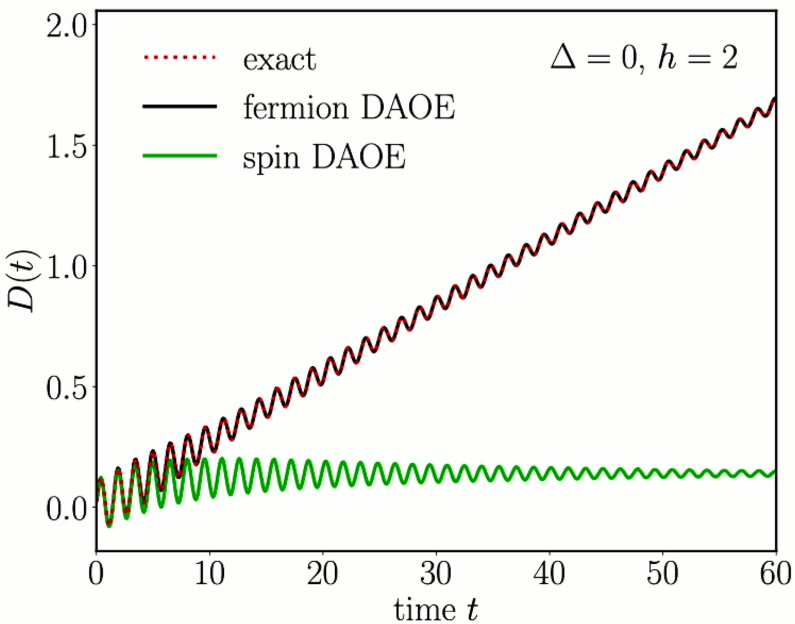
$\lvert o^\mu \rangle$	I	I	$f^\dagger$	I	I	z	f	I	z
$\lvert \sigma^\mu \rangle$	I	I	σ^+	σ^z	σ^z	I	σ^-	I	σ^z
s	1^+	1^+	1^-	1^-	1^-	2^-	3^+	3^+	3^+

[see also Kuo et al., arXiv:2311.17148]

[Lloyd, Rakovszky, FP, von Keyserlingk (arXiv:2310.16043)]

Fermionic DOAE

Model $$H = \underbrace{-\sum_x \left(\frac{J}{2}(f^\dagger_{x+1} f_x + \text{h.c.}) + h(-1)^x (1-2n_x) \right)}_{H_0} + \underbrace{\Delta \sum_x (1-2n_x)(1-2n_{x+1})}_{\Delta \times V}$$



Fermion DAOE agrees with the exact result provided $\ell^* \geq 2$

[see also Kuo et al., arXiv:2311.17148]

[Lloyd, Rakovszky, FP, von Keyserlingk (arXiv:2310.16043)]

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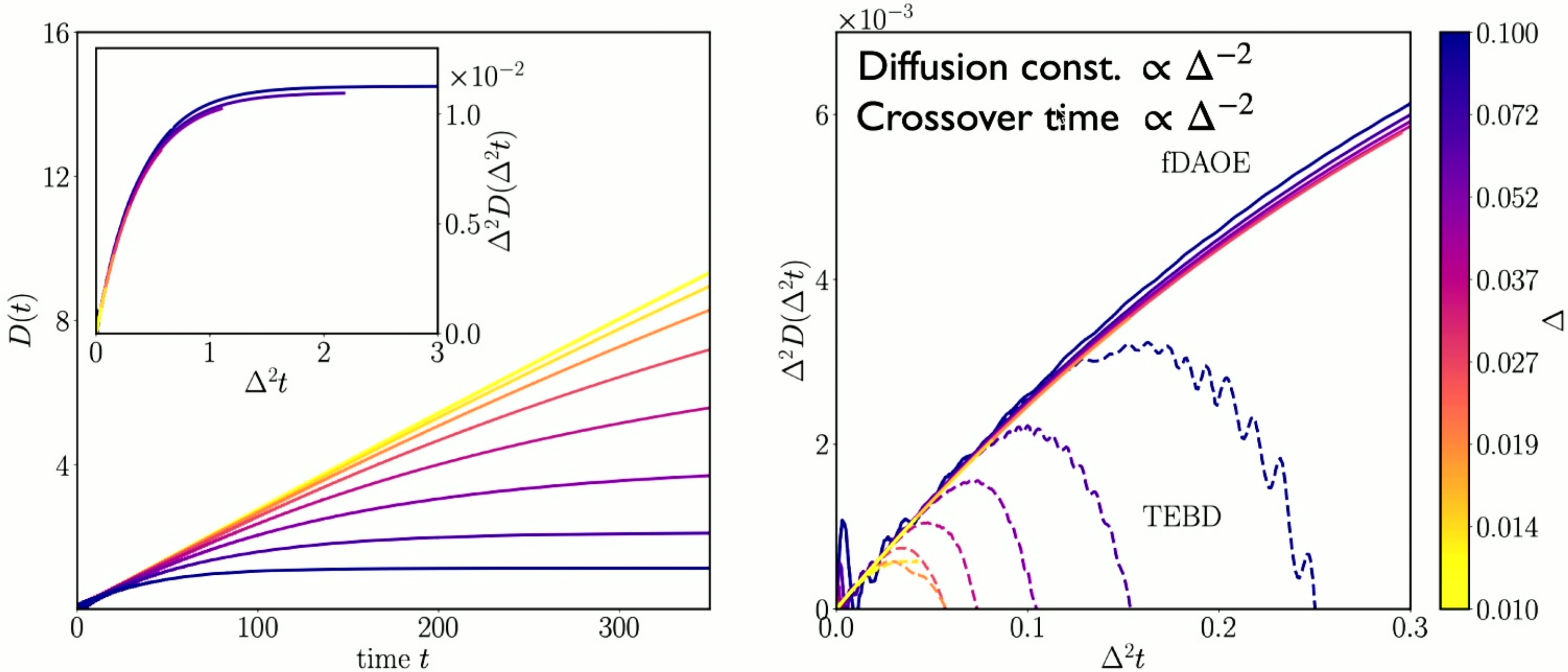

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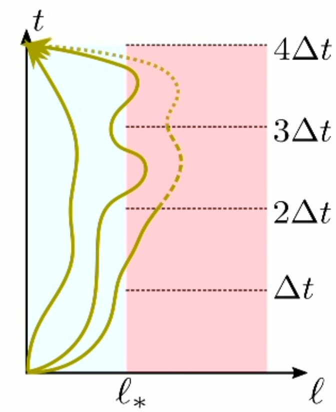


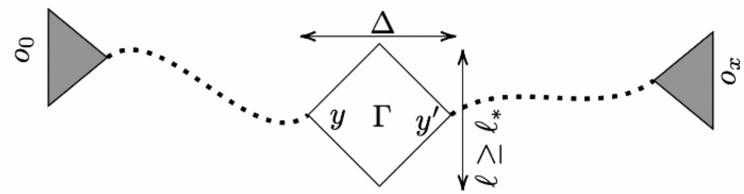
[Rakovszky, von Keyserlingk, FP, PRB **105**, 07513 (2022)]
[von Keyserlingk, FP, Rakovszky PRB **105**, 245101 (2022)]

Thank you!

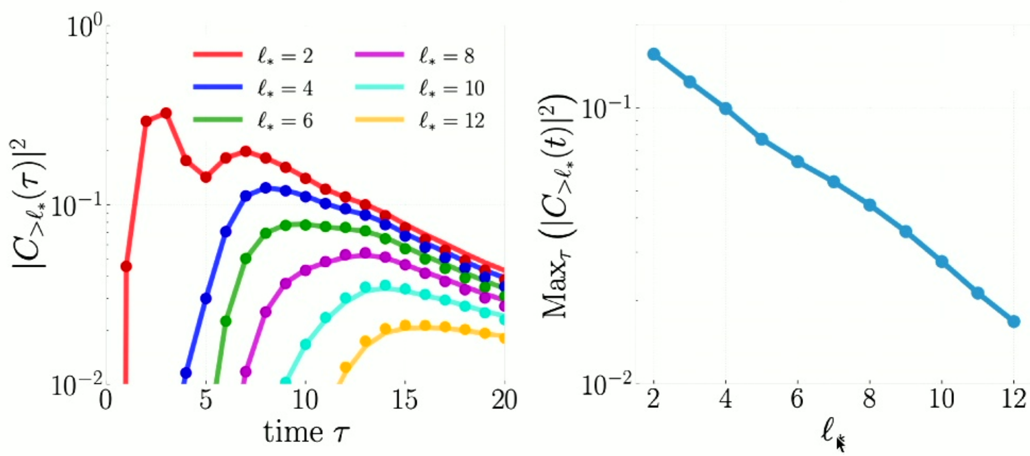
“Backflow” corrections

Dynamical correlations

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



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



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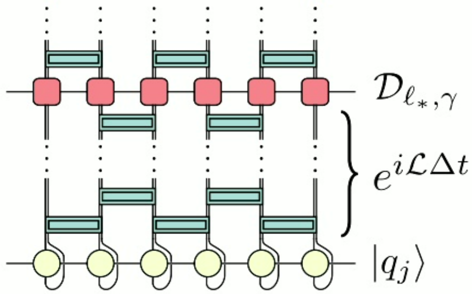
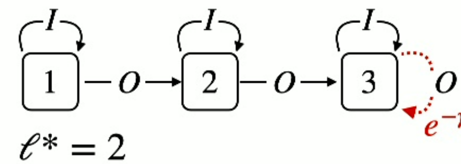
Dissipation stops growth of operator entanglement

Represent dissipative evolution as tensor network



← Low-dimensional Matrix-Product Operator

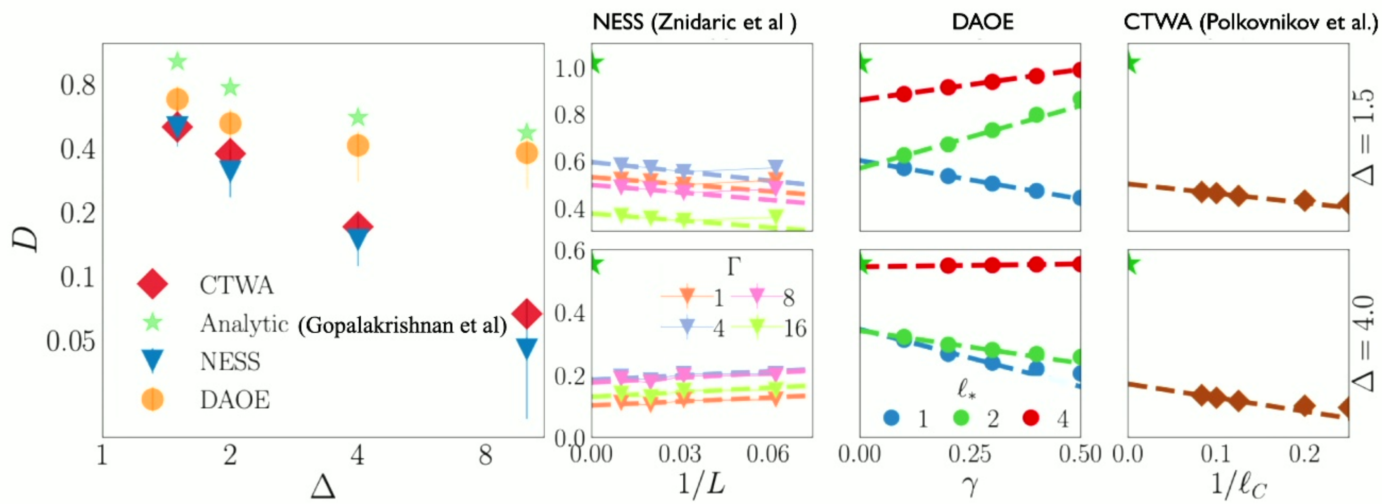
← Time Evolving Block Decimation (TEBD) [Vidal '03]



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

Benchmark to other methods (work in progress)

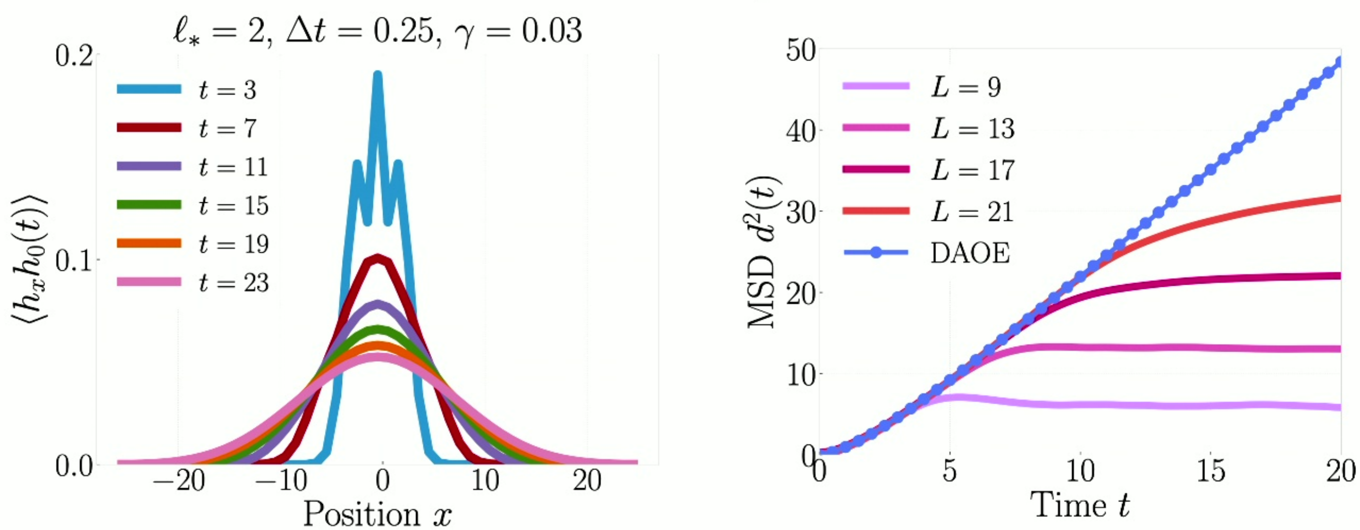
XXZ chain $H = \sum_{j=1}^{L} \left(X_j X_{j+1} + Y_j Y_{j+1} + \Delta Z_j Z_{j+1} \right)$



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

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: $D \equiv \lim_{t\to\infty} D(t)$

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

Artificial dissipation that not affects hydrodynamics

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

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

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

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

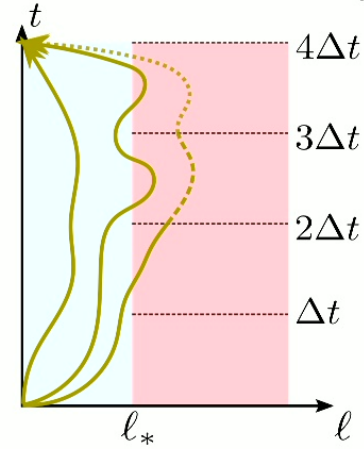
Artificial dissipation that not affects hydrodynamics

Modified evolution: dissipate after every Δt

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

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

$$C(x,t) \equiv \langle q_x(t) q_0(0)\rangle_{\beta=0}$$



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

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Artificial Dissipator:

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

$$\mathbb{1}\mathbb{1}\mathbb{1}\mathbb{1}X\mathbb{1}\mathbb{1} \quad \ell_{\mathcal{S}} = 1$$
$$Y\mathbb{1}\mathbb{1}\mathbb{1}X\mathbb{1}\mathbb{1} \quad \ell_{\mathcal{S}} = 2$$
$$Y\mathbb{1}Z\mathbb{1}X\mathbb{1}\mathbb{1} \quad \ell_{\mathcal{S}} = 3$$

- 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)]