What classical resources are required to simulate quantum transport?

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…+related work with Ewan McCulloch, Gabriele Pinna, Srivatsa Prasanna, Oliver Lunt

UK Research and Innovation

Motivation

- Transport properties (e.g., heat, charge and spin diffusion constants) are among the most experimentally accessible and practically important features of quantum materials.

- It is worth improving existing methods for calculating these properties from first principles.

- Existing methods (exact evolution, tensor network evolutions) are strongly limited for such ab into studies.

- Issue: Memory required to story $\psi(t), O(t)$ grows as $e^{\mathcal{O}(t)}$.

Posing the problem

- Class of local (say nearest neighbour) translation invariant Hamiltonians on qubits.
- Generically has only a few local conserved quantities: Energy/charge.
- Generically ergodic.
- Generically exhibits diffusion of energy/charge at high temperature.
- What classical resources (e.g., memory/time) are *typically* required to calculate a diffusion constant within tolerance ϵ?
- How much faster can the same task be accomplished in a quantum simulator?

$$\mathrm{tr}(h_r(t)h_0(0))/\mathrm{tr}(I) \sim \frac{\exp(-r^2/4Dt)}{\sqrt{4\pi Dt}}$$

A slightly simpler problem

- Class of Floquet models where Floquet operator consists of low depth nearest neighbour, translation invariant quantum circuits each of which conserves total z-spin $\sum_j \sigma_j^z$.
- Generically ergodic.
- Generically exhibits diffusion of z-spin at high temperature.
- What classical resources are *typically* required to calculate a diffusion constant within tolerance ϵ?
- How much faster can the same task be accomplished on a quantum computer?

$$\mathrm{tr}(\sigma_r^z(t = nT)\sigma_0^z(0))/\mathrm{tr}(I) \sim \frac{\exp(-r^2/4Dt)}{\sqrt{4\pi Dt}}$$

How hard is it to simulate quantum transport classically?

Brute Force (TEBD/ED/TDVP)

- $|D(t) - D| \leq C/t^{1/2}$ in 1D hydro.
-

$$D = \int_0^\infty d\tau \langle J(\tau) J(0) \rangle / V$$

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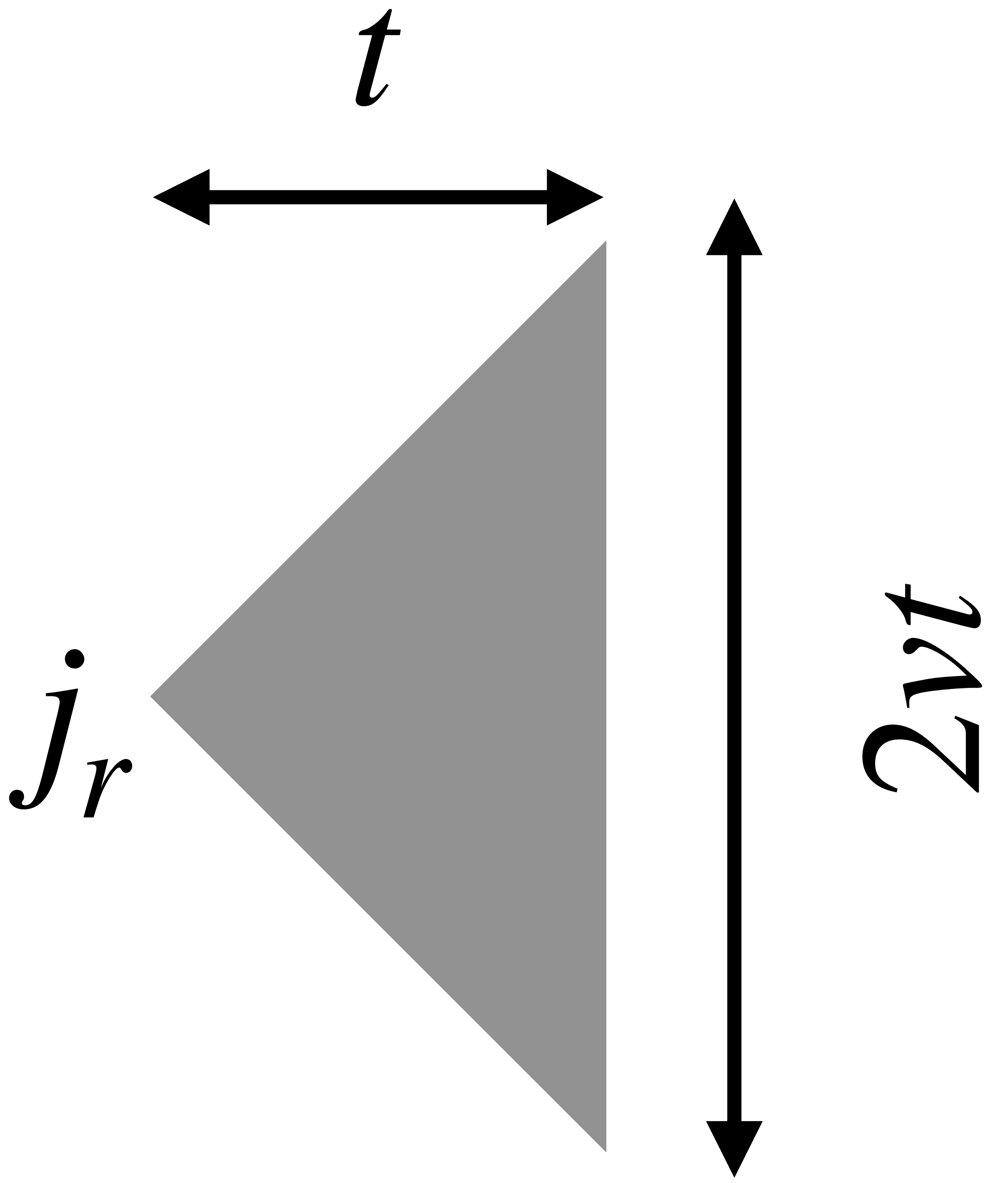

HSD
~Operators on interval length 2vt
$\sim e^{\mathcal{O}(t)}$

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- Operator entanglement grows linearly in time. Guess that required bond dimension grows as

$$\chi \sim e^{\mathcal{O}(t_c)} \sim e^{\mathcal{O}(\text{poly}(\epsilon^{-1}))}$$

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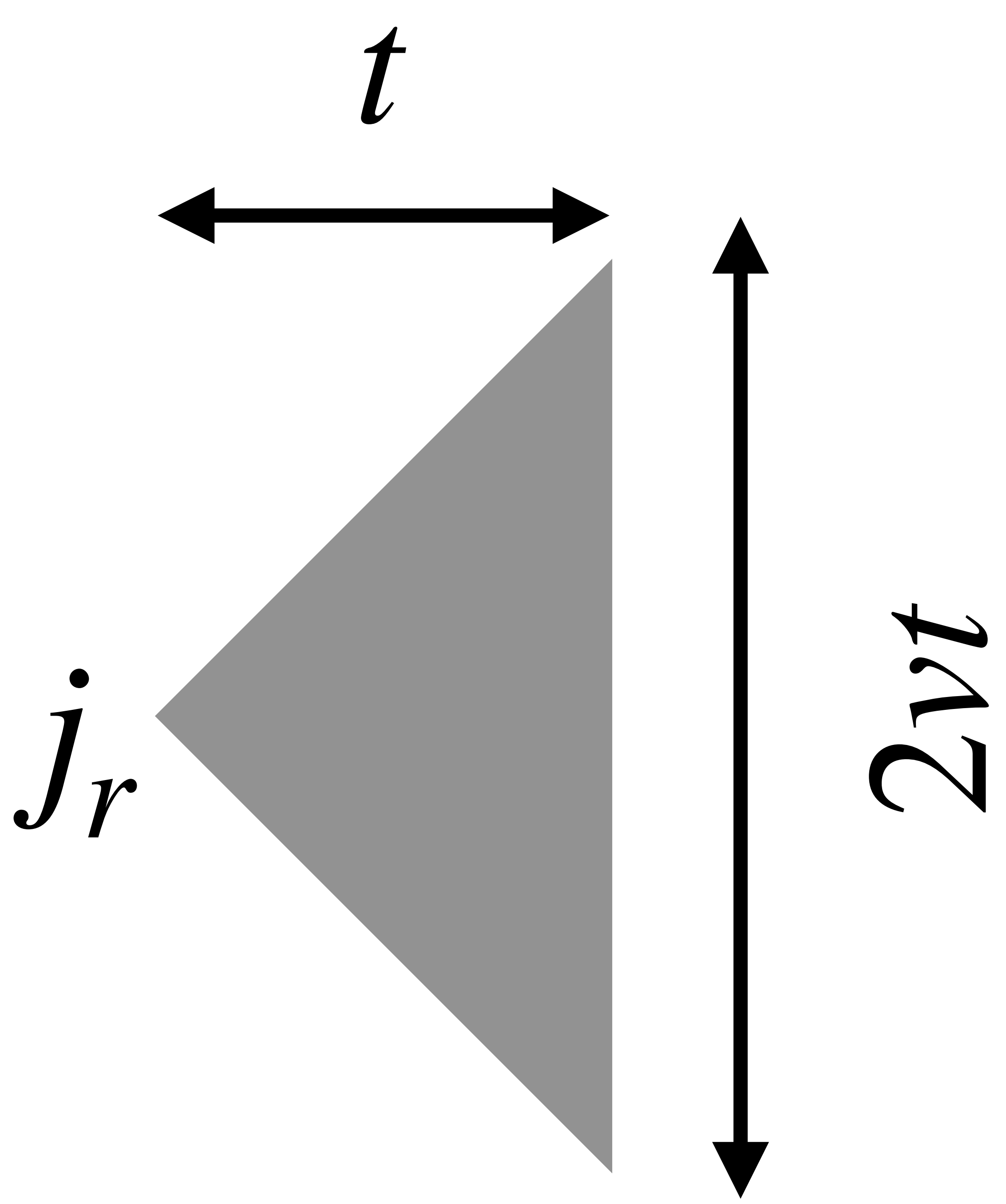

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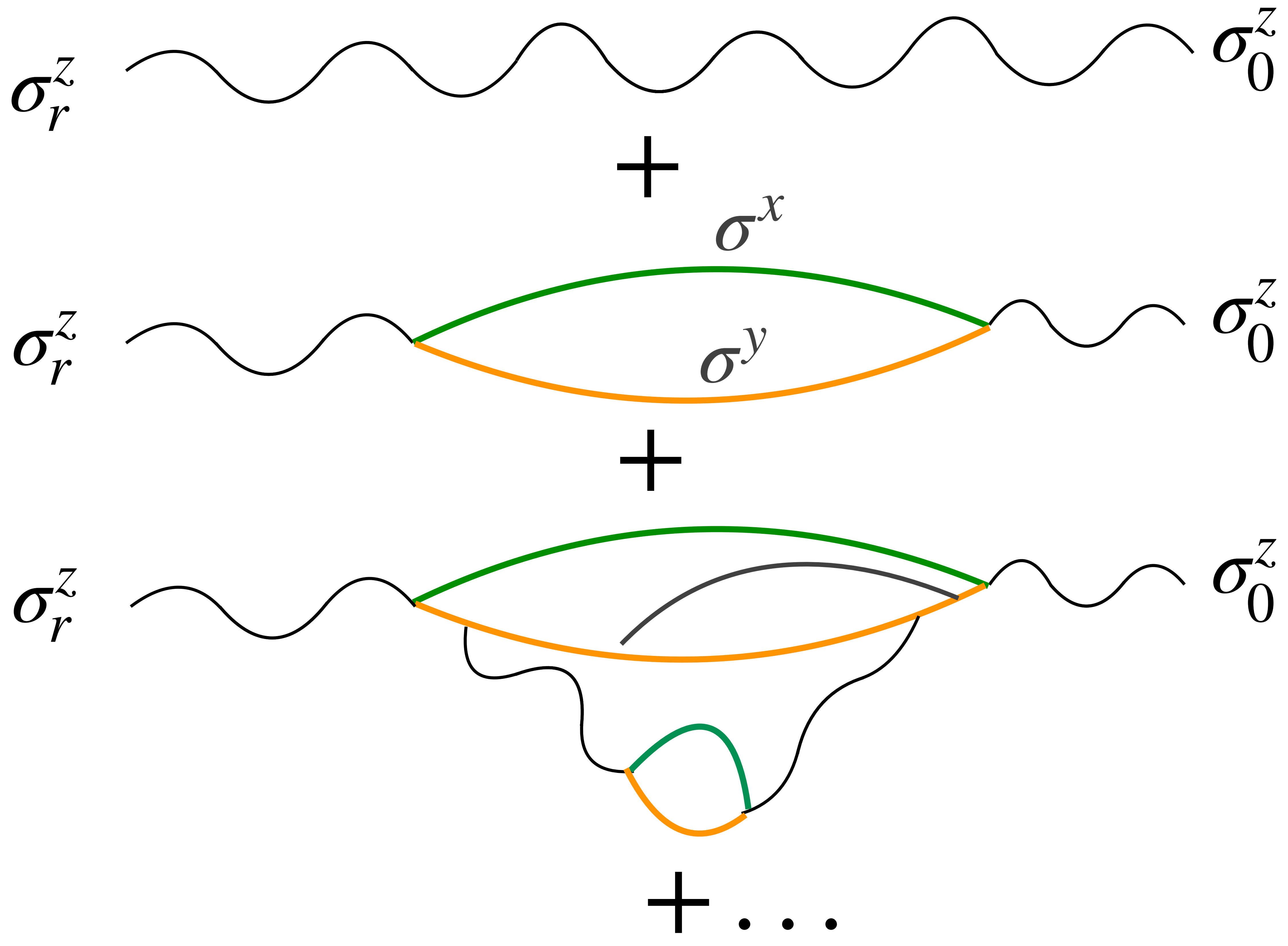
Can we do better?

- Take ergodic system with U(1) conservation law $S^z = \sum_x \sigma^z_x/2 \Longrightarrow \sigma^z$ a hydrodynamical mode.
- Raw ingredient for diffusion constant: correlation functions.

$$\langle \sigma^z_r(t) \mid \sigma^z_0(0) \rangle = \mathrm{tr}(\sigma^z_r(t)\sigma^z_0(0))/\mathrm{tr}(I)$$

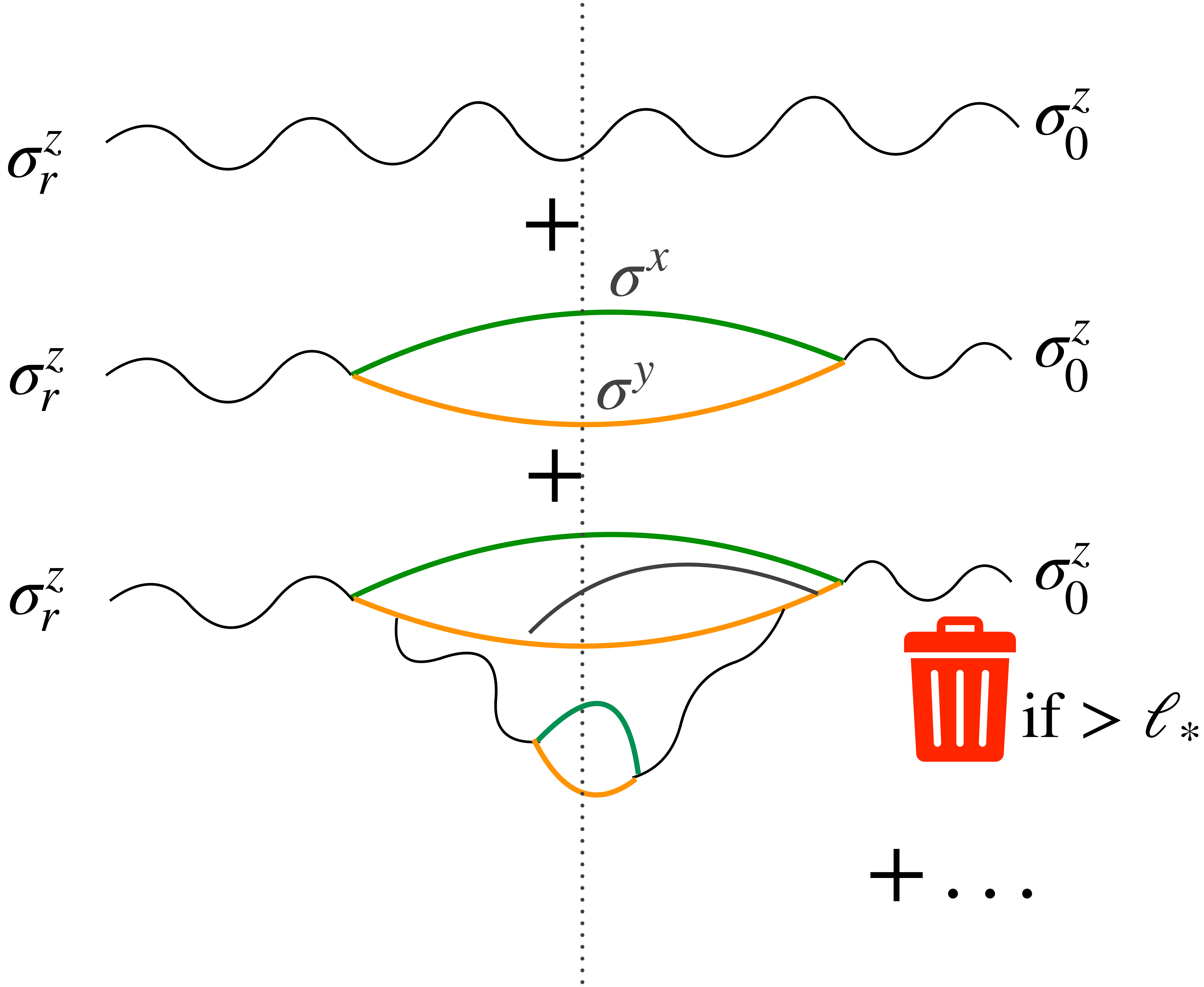
- Hilbert space of operators: On-site basis of operators $\sigma^{0,1,2,3} = I, \sigma^x, \sigma^y, \sigma^z$
- Pauli strings: $\sigma^{\vec{\mu}} = \otimes_r \sigma^{\mu_r}_r$
- Correlation function is a transition amplitude, on space of operators. Express as sum over paths!



- Claim: More complicated diagrams give subleading contributions!!!

DAOE Summary

- Throwing away processes with more than ℓ_* operators incurs $e^{-\mathcal{O}(\ell_*)}$ error in hydrodynamical correlators/coefficients.
- $\Longrightarrow$ Can save much memory with relatively little error!



Phys. Rev. B **105**, 075131

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- Effective Hilbert space reduced! Space of short operators with support in light cone.
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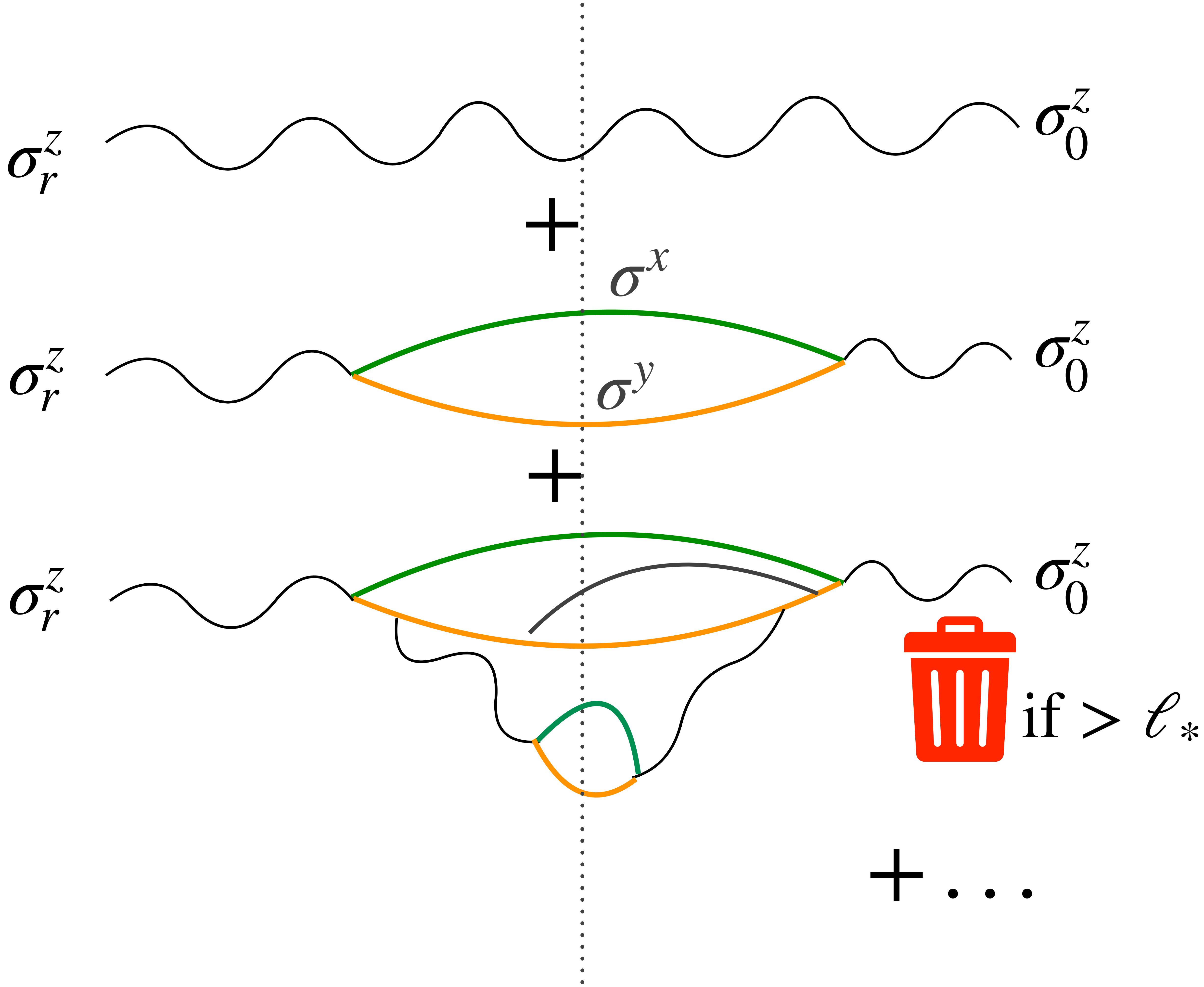

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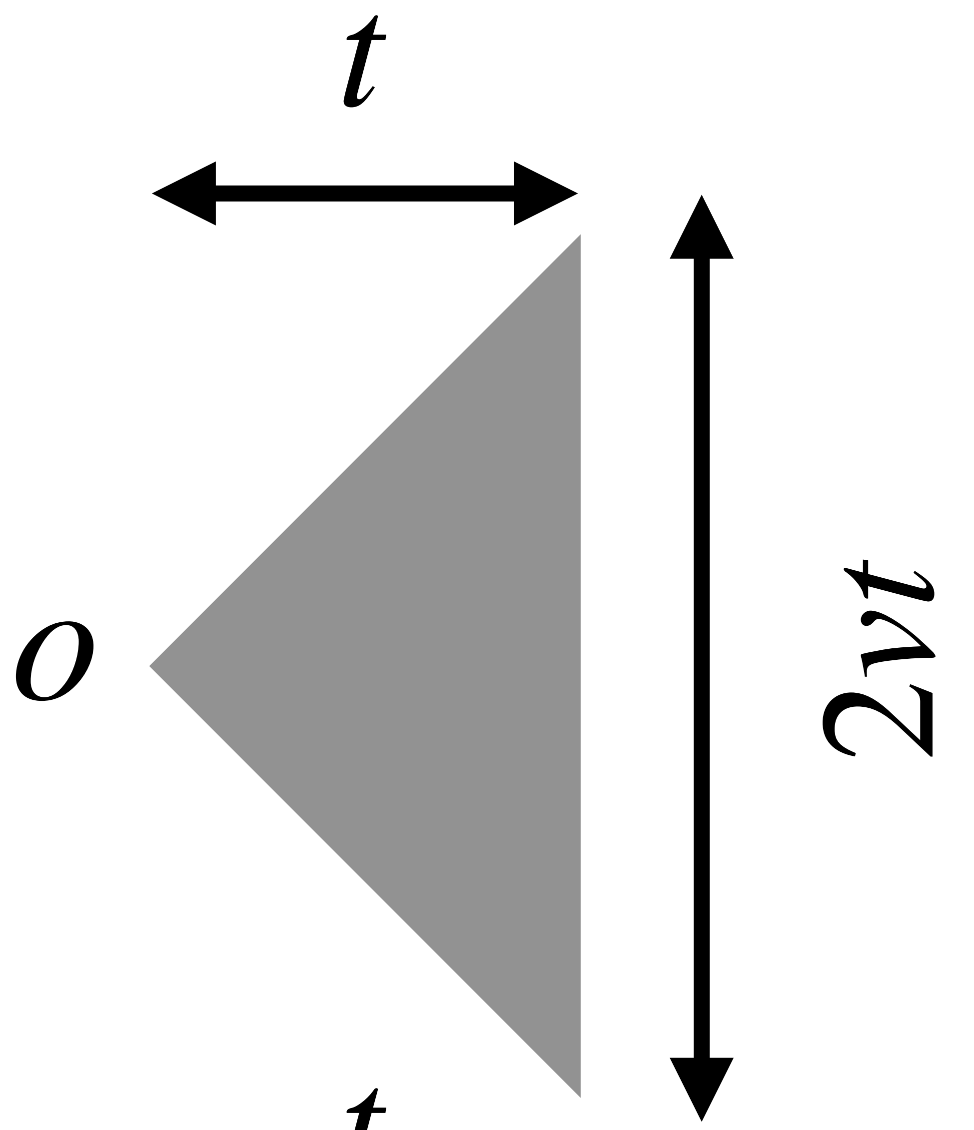
- Effective Hilbert space reduced! Space of short operators with support in light cone.
- Dimension $4^{\ell_*}\binom{2vt_c}{\ell_*}$. Much smaller than 4^{2vt_c}.
- $t_c = \mathcal{O}(\epsilon^{-2})$ gives effective HS required

$$\chi \sim e^{\mathcal{O}(\log(\epsilon^{-1})^2)}$$



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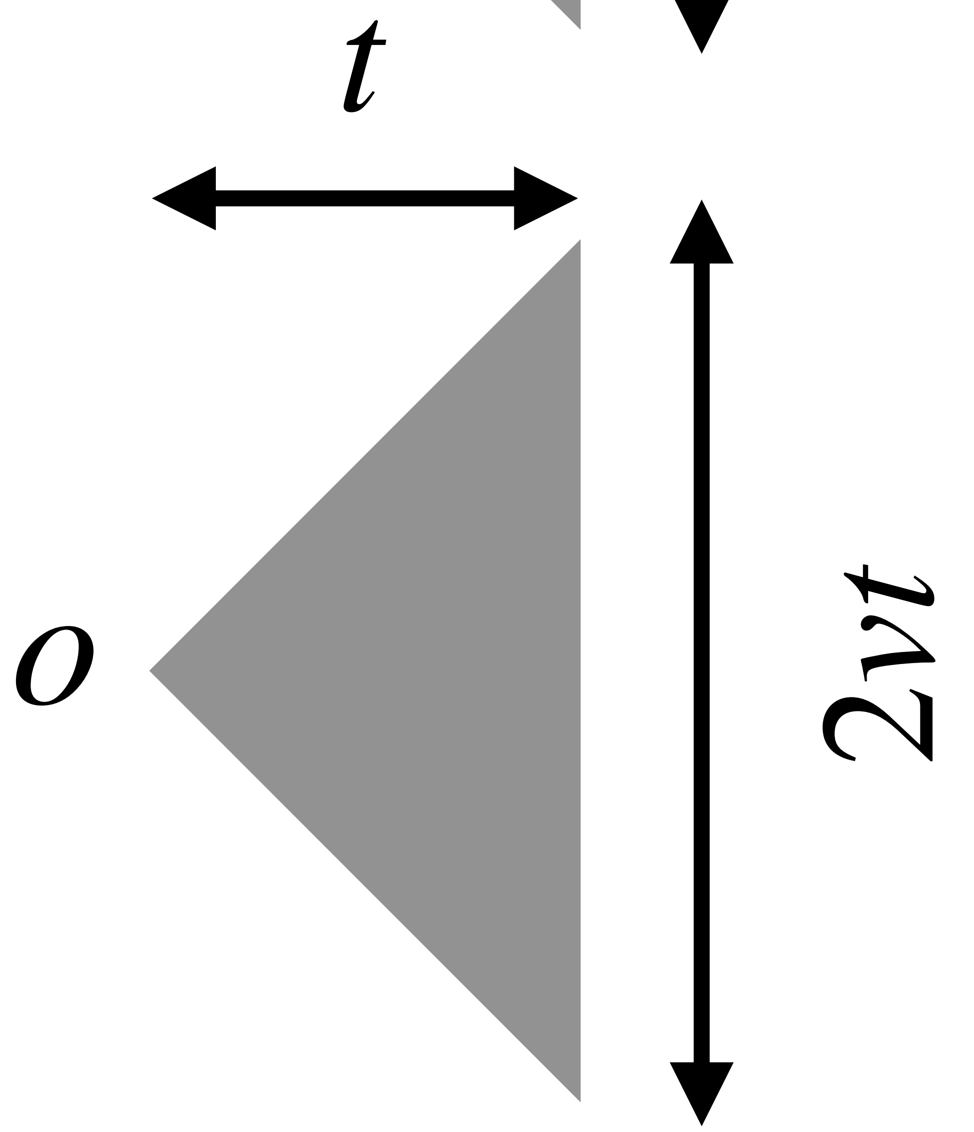

Pick ℓ_* Pauli ops in light cone, $4^{\ell_*}\binom{2vt}{\ell_*} \sim t^{\ell_*}$

Punch-line

- "DAOE": Numerical technique for calculating hydrodynamical correlations/diffusion constants in many-body quantum systems.

- Modified evolution: We discard information corresponding to n-point functions with $n > \ell_*$. Saves memory!

- Today's talk: Argue errors induced by truncation ("backflow") are exponentially suppressed in ℓ_*.

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

Resources for ϵ-accurate approximation to diffusion constant:

- **Exact evolution/TEBD requires**

$$t_{\text{cpu}}, \chi_{\text{naive}} = e^{\mathcal{O}(\text{Poly}(\epsilon^{-1}))}.$$

- **DAOE is more efficient**

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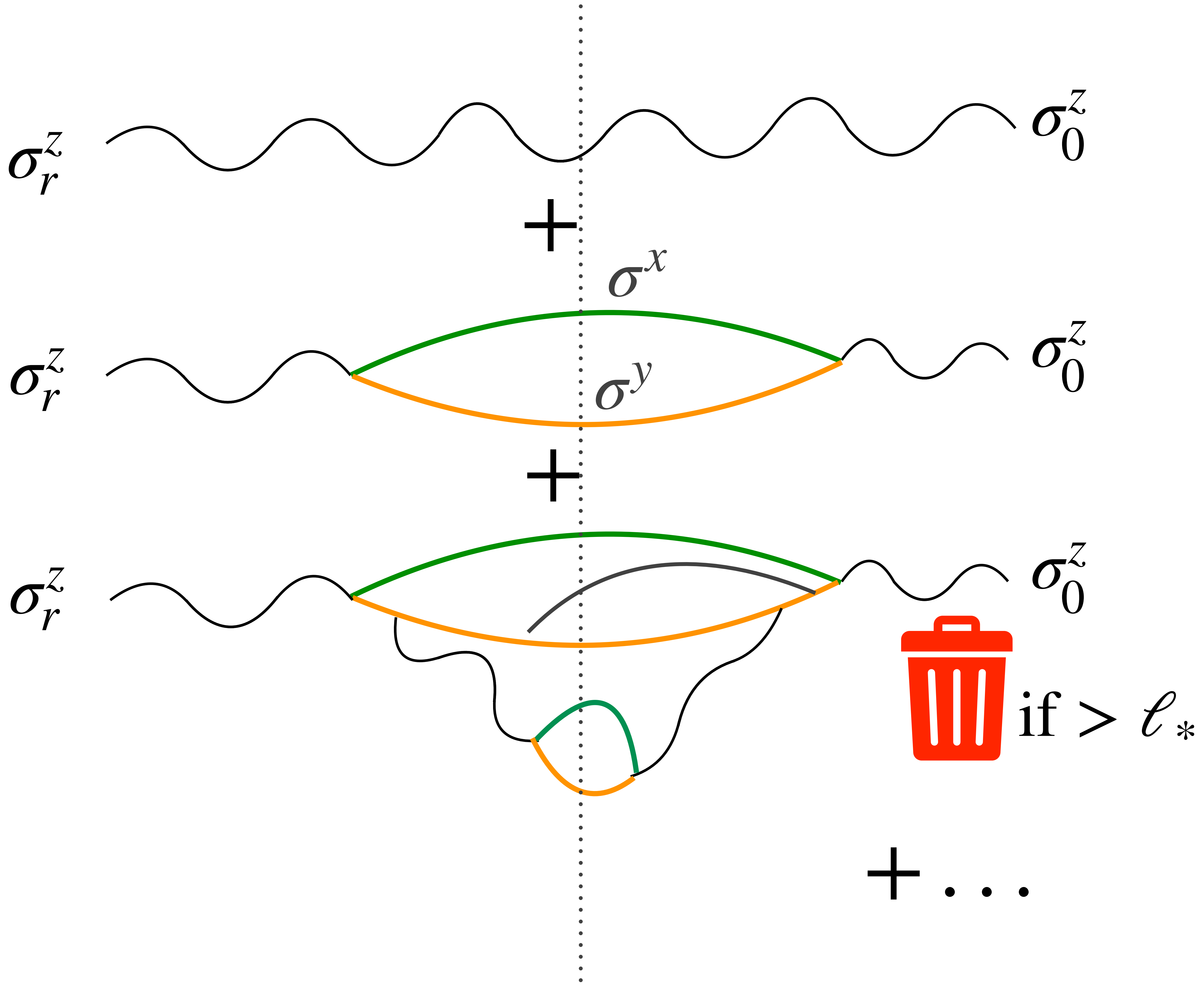
- **Quantum simulators? (Decoherence limited)**

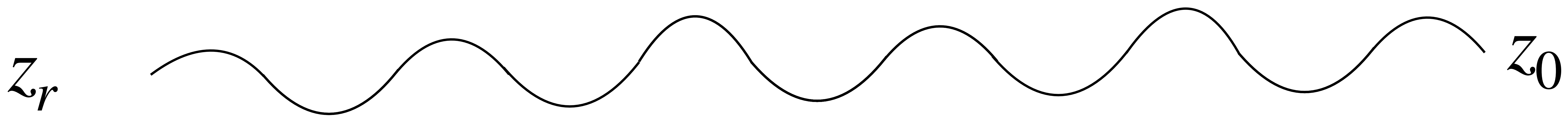
runs x circuit depth = $\text{Poly}(\epsilon^{-1}) = e^{\mathcal{O}(\log(\epsilon^{-1}))}$



- Throwing away processes with more than ℓ_* operators incurs $e^{-\mathcal{O}(\ell_*)}$ error in hydrodynamical correlators/coefficients.
- Some consequences, and then we'll address why.

Consequences for hydrodynamics

$$\langle z_r(t) \mid z_0(0)\rangle = \mathrm{tr}(z_r(t) z_0(0))/\mathrm{tr}(I)$$



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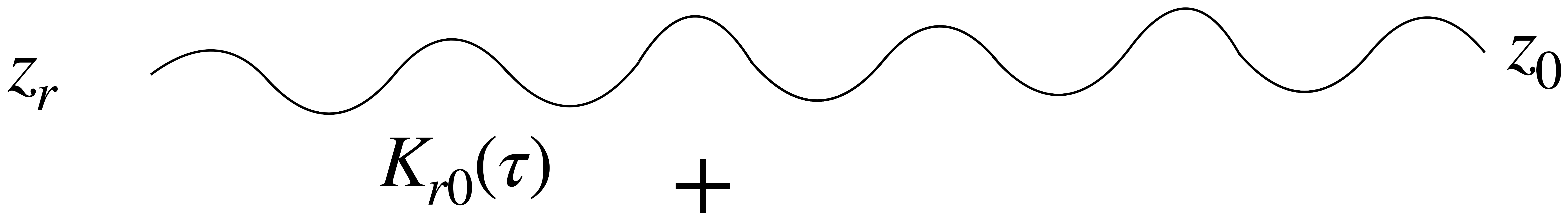

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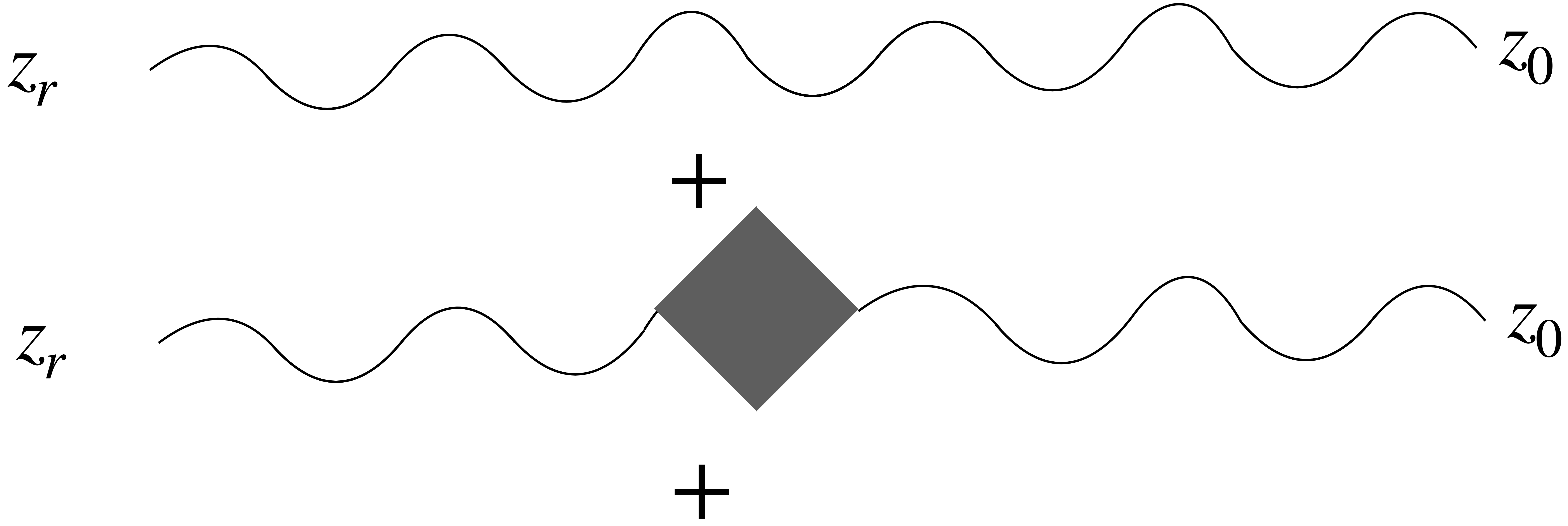

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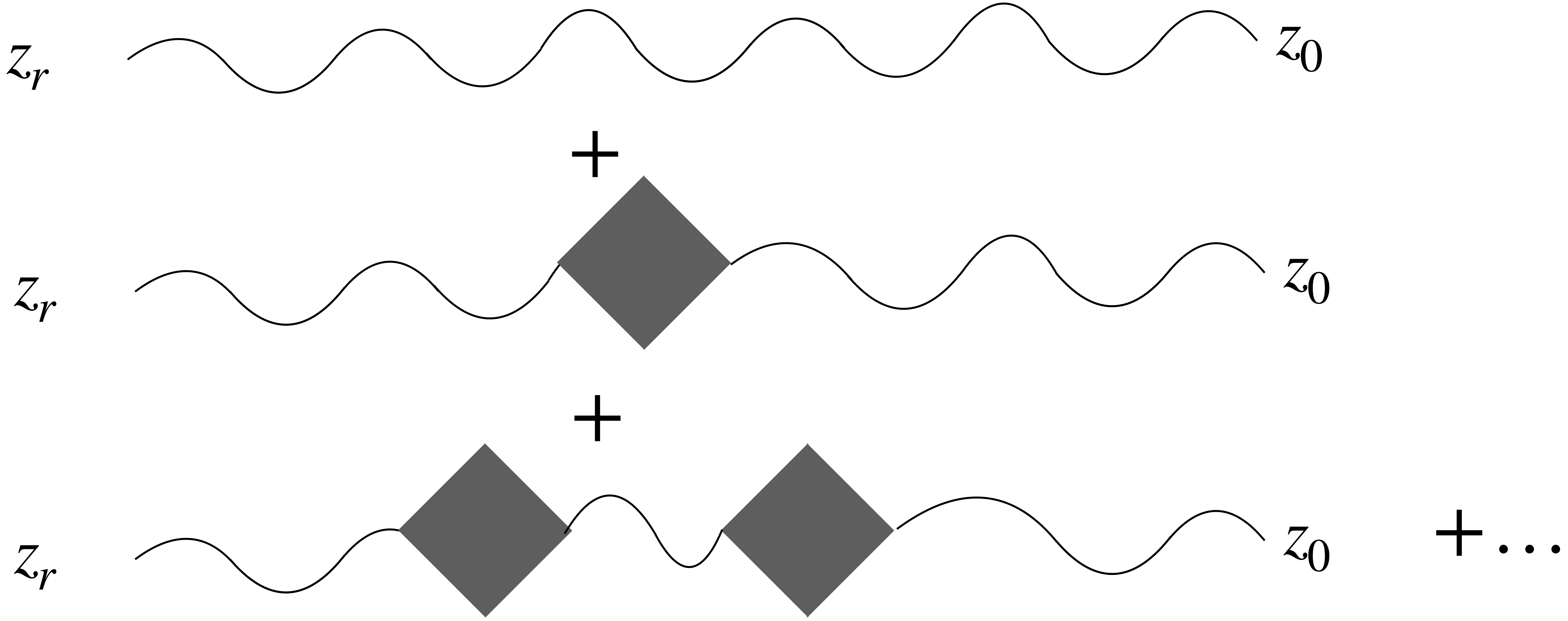
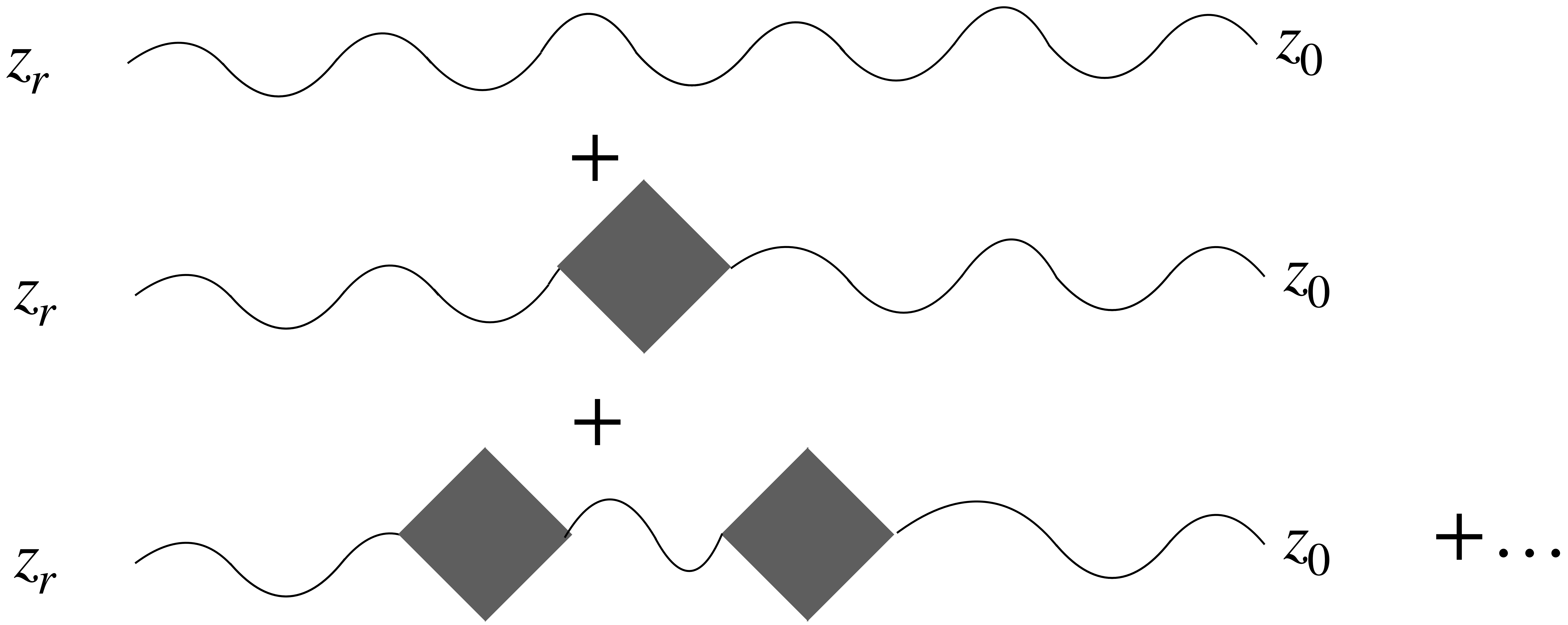
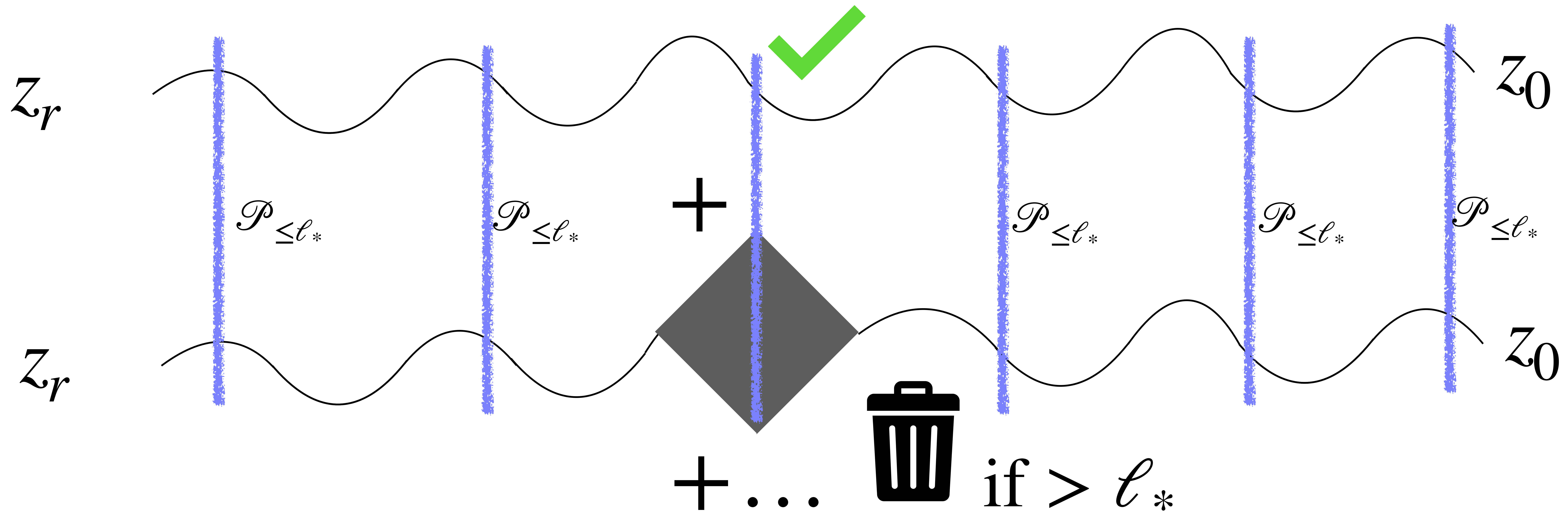


Consequences for hydrodynamics

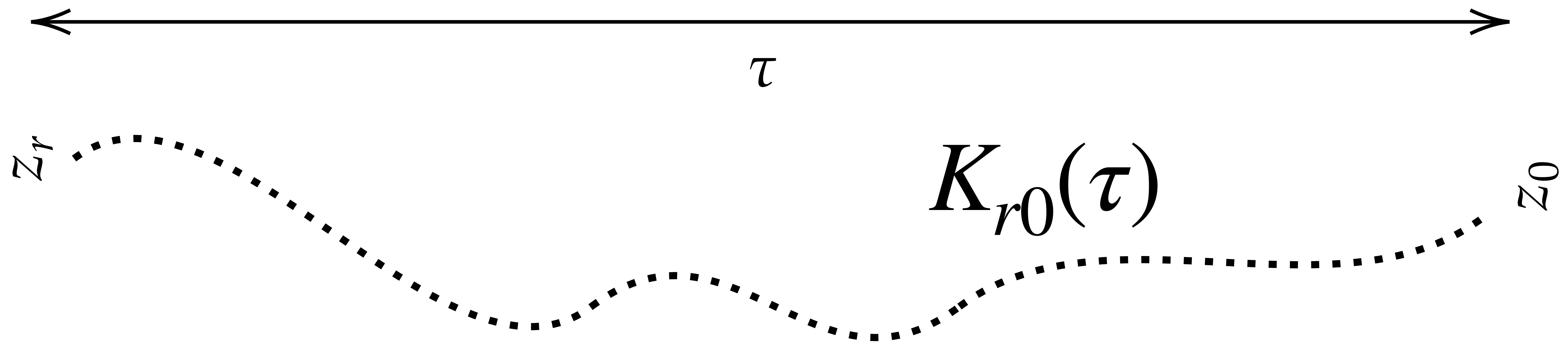
Physical hypothesis: Contributions are suppressed in size and # of grey boxes



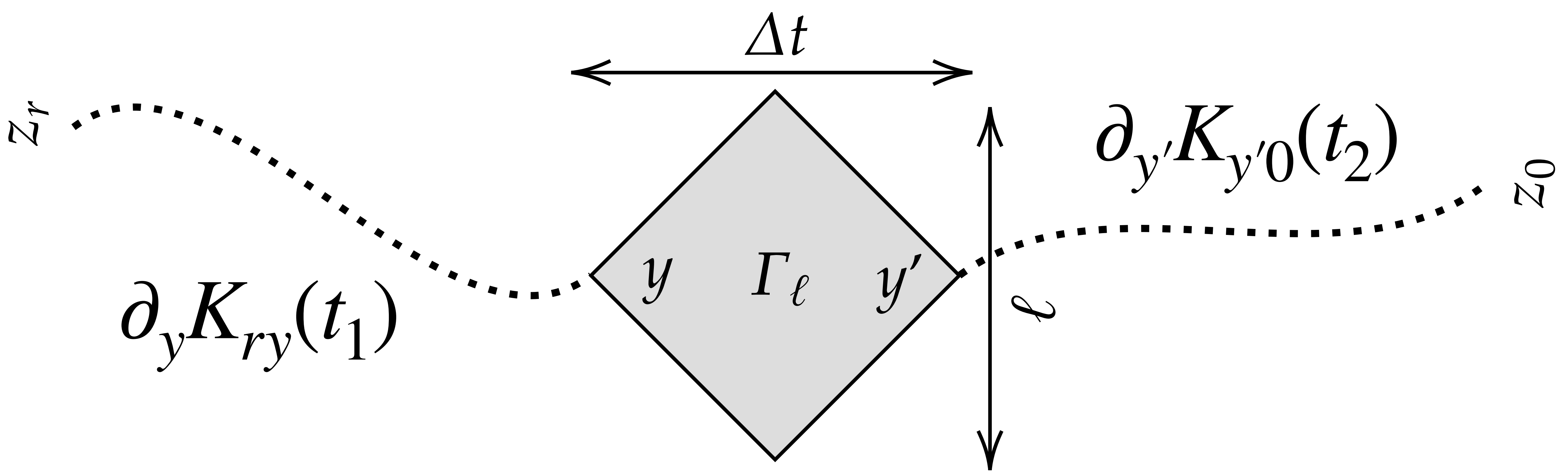
If that's valid, then ignoring processes with large boxes should introduce small error. This is a the principle behind "DAOE", a numerical method we've recently proposed for calculating hydrodynamical correlations in many-body systems.



Operator Feynman Diagrams



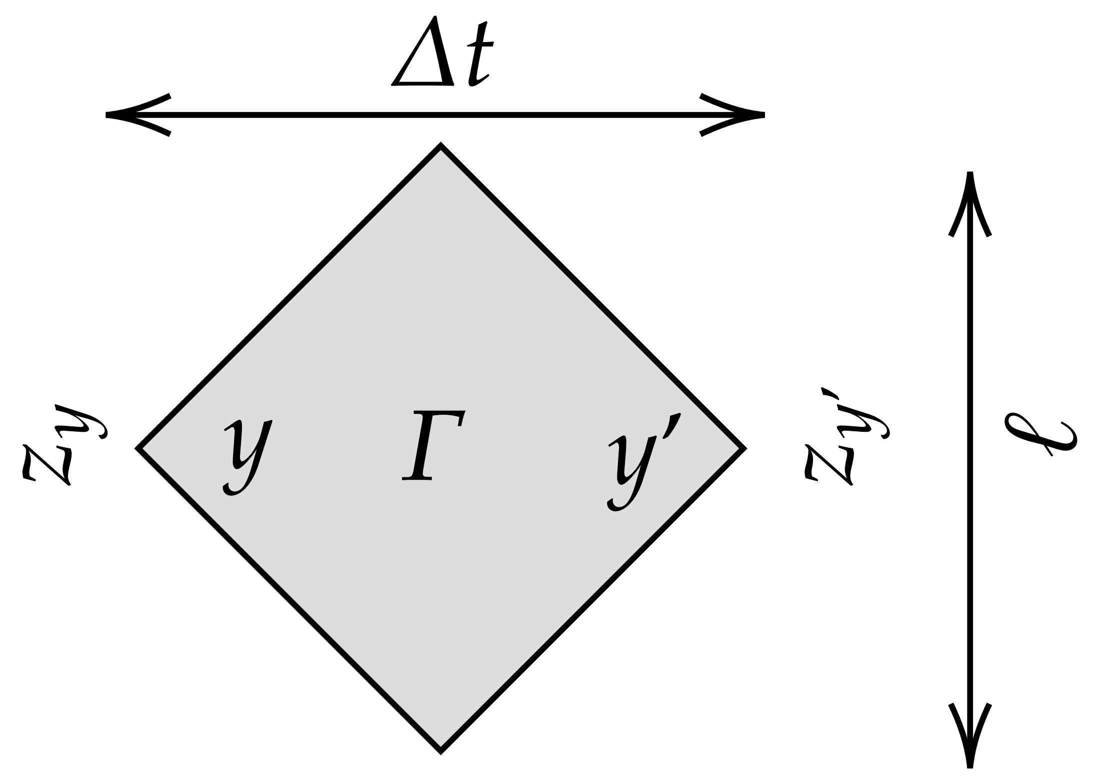
$$K_{r0}(\tau) \sim e^{-r^2/(4D_0t)}/\sqrt{4\pi D_0 t}$$



$$\to \int_{y,y'}\int_{t_1,t_2,\Delta t} \partial_y K_{ry}(t_1)\partial_{y'}K_{y'0}(t_2)\Gamma_\ell(y,y',\Delta t)$$

Backflow associated with all such diagrams with $\ell > \ell_*$

Boxes?



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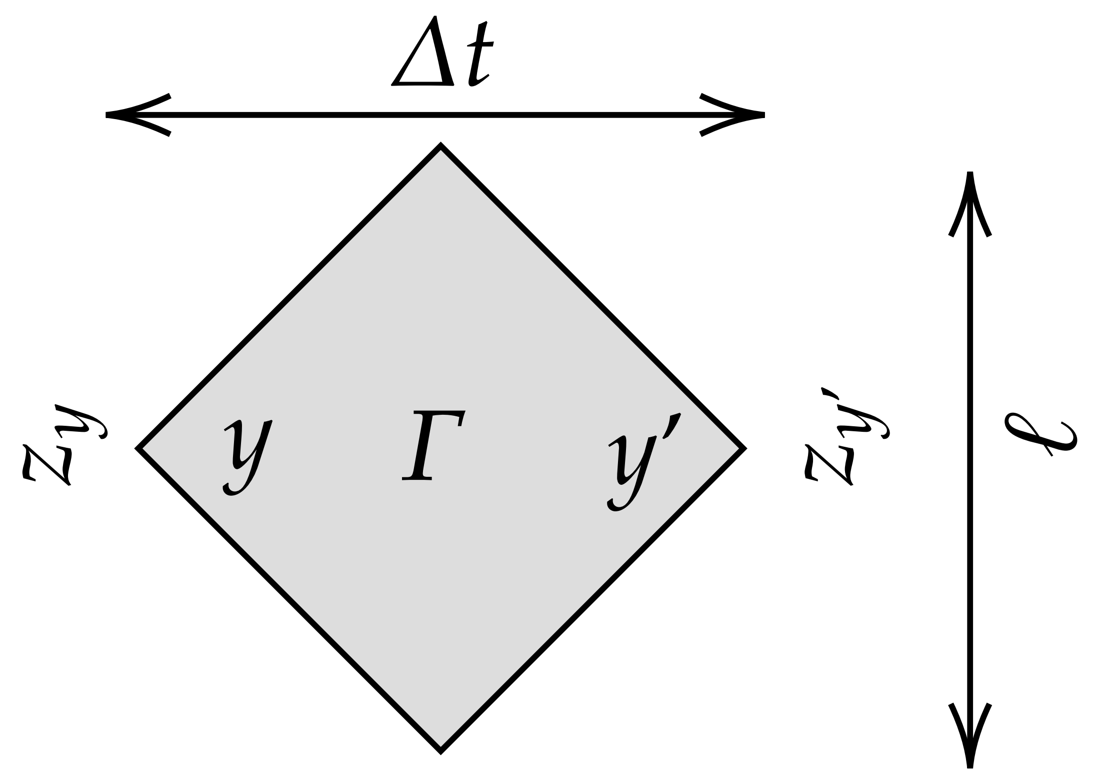

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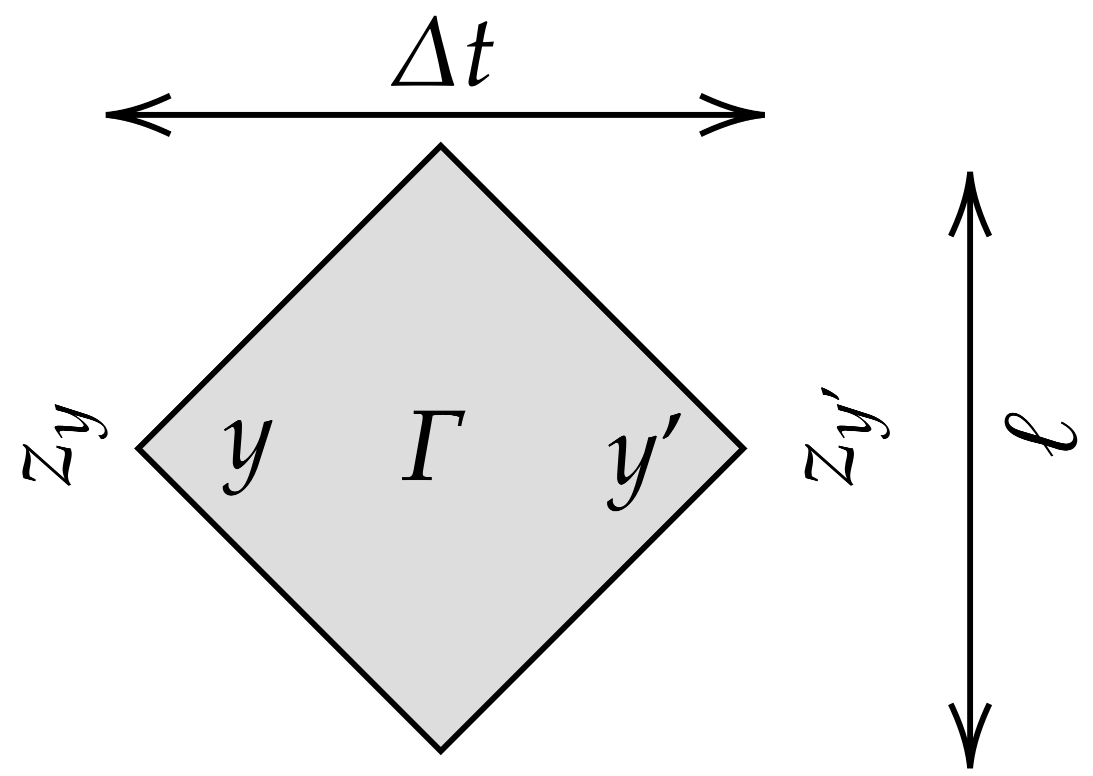

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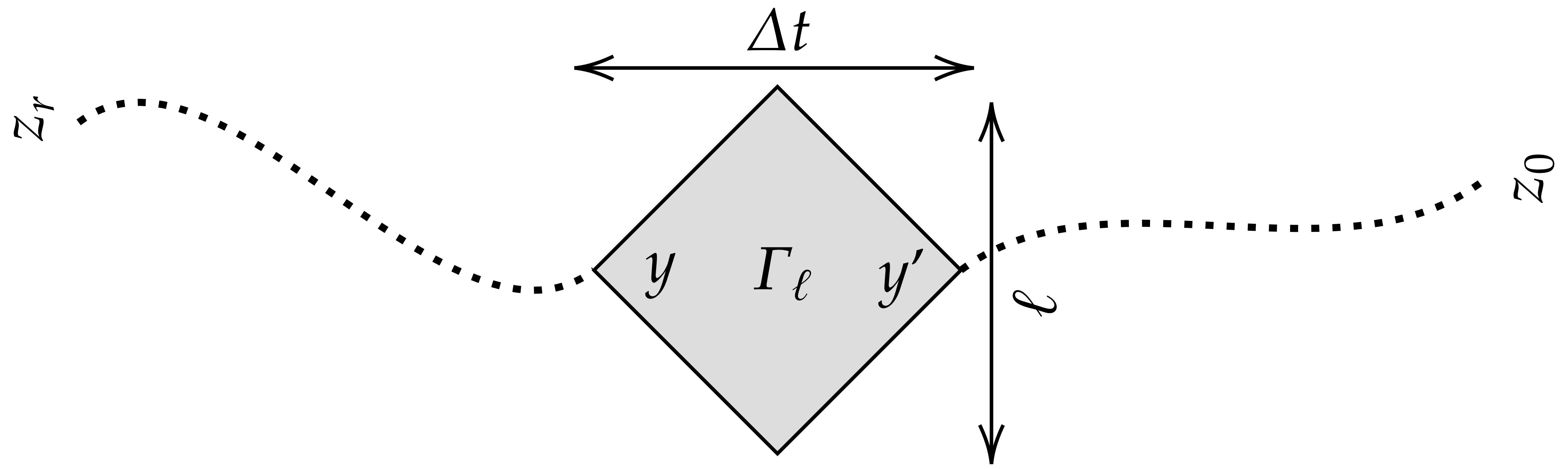

$$|\langle z_r(\tau) z_0(0)\rangle - \langle z_r(\tau) z_0(0)\rangle_{\text{daoe}}| \sim \int_{y,y'} \int_{t_1,t_2,\Delta t} \partial_y K_{ry}(t_1) \partial_{y'} K_{y'0}(t_2) \Gamma_\ell(y, y', \Delta t)$$

$$\sim e^{-\mathcal{O}(\ell)} \tau^{-\alpha}$$

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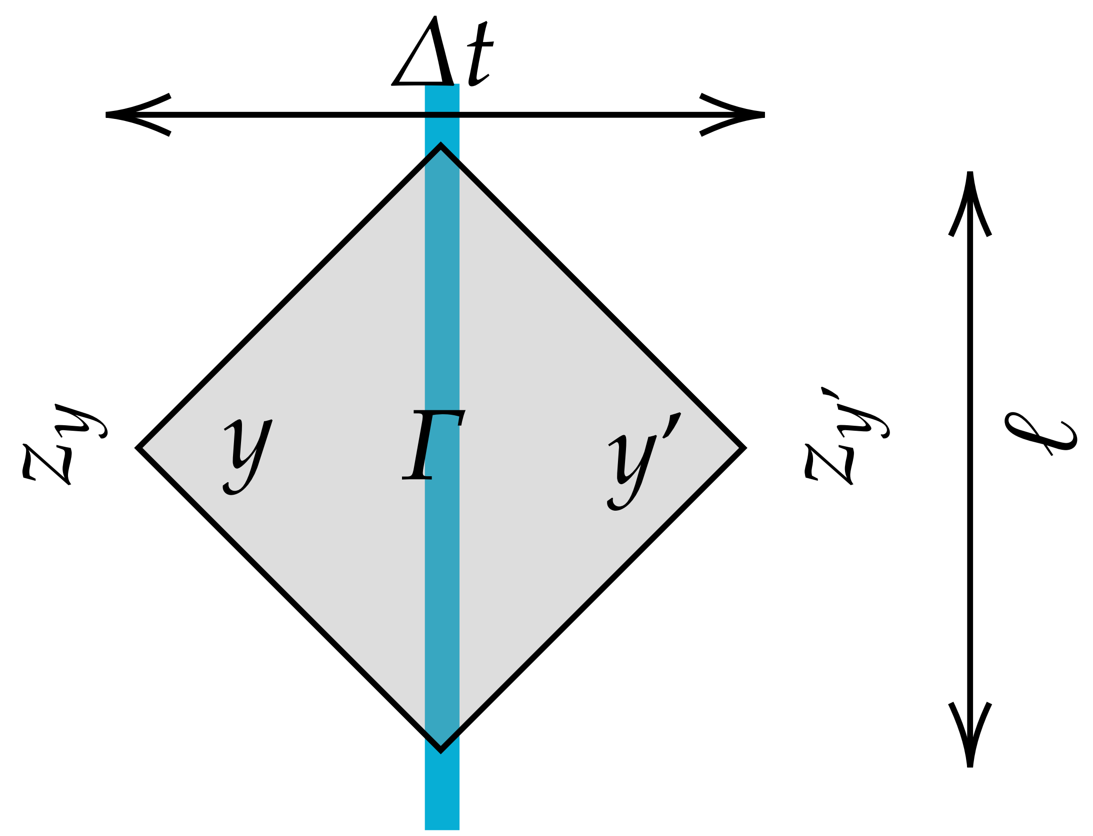
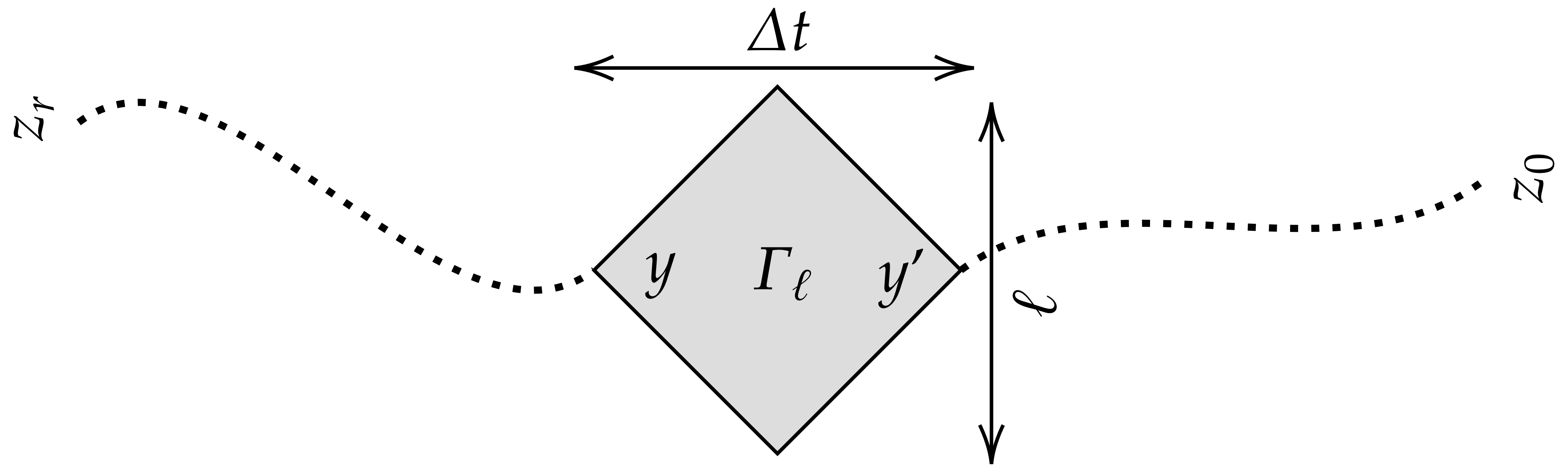


$$\Gamma_\ell = \sum_{\mu:\ell(\mu)=\ell} c_{z_y\to\sigma^\mu}(\Delta t/2)c_{\sigma^\mu\to z_{y'}}(\Delta t/2)$$



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Proof sketch

$$\Gamma = \sum_{\mu:\ell(\mu)=\ell} c_{z\to\mu} c_{\mu\to z}$$

In ergodic systems, phases of c's random and (largely) uncorrelated

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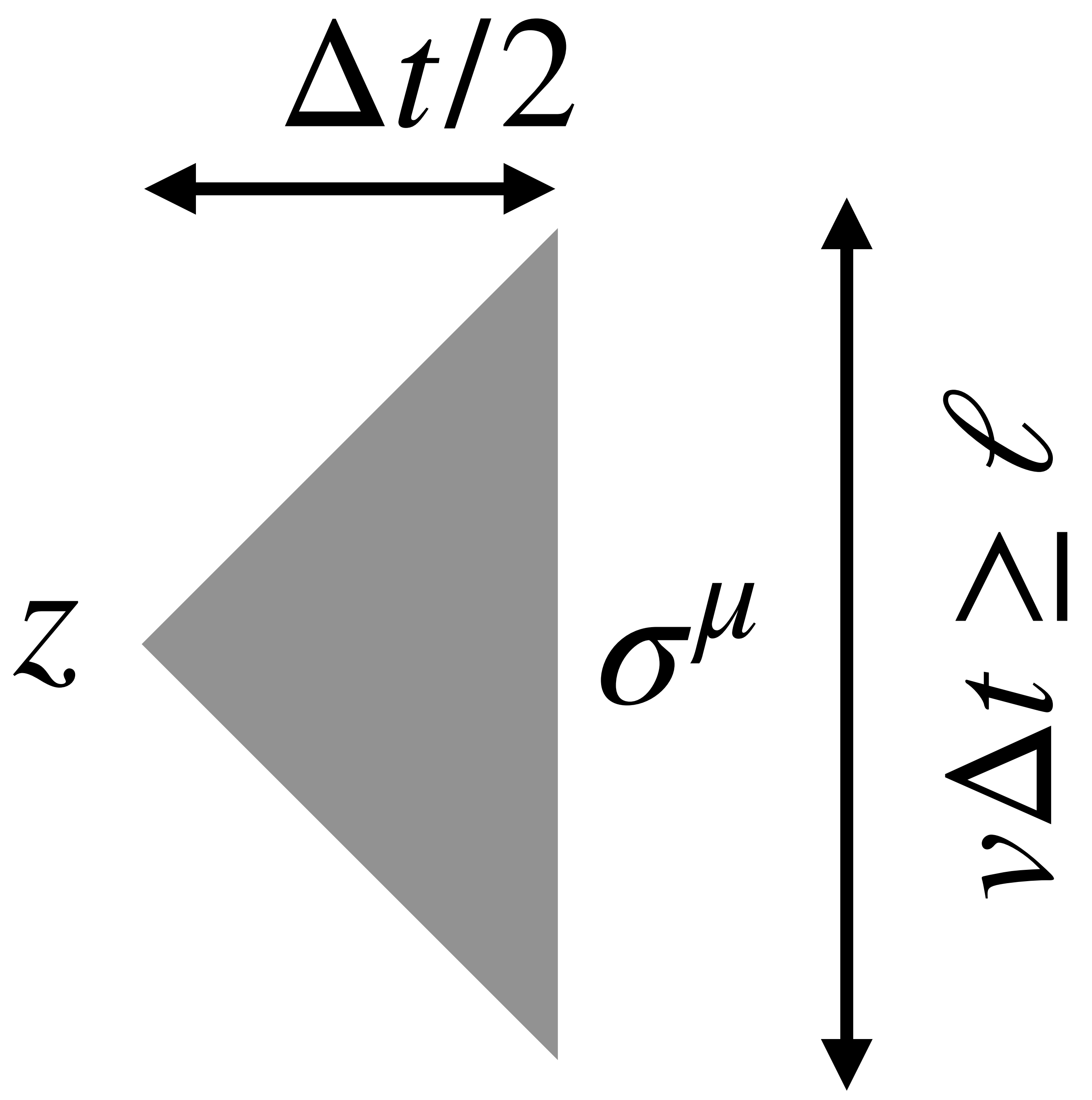
Exp. many operators (in ℓ, Δt) in light cone.



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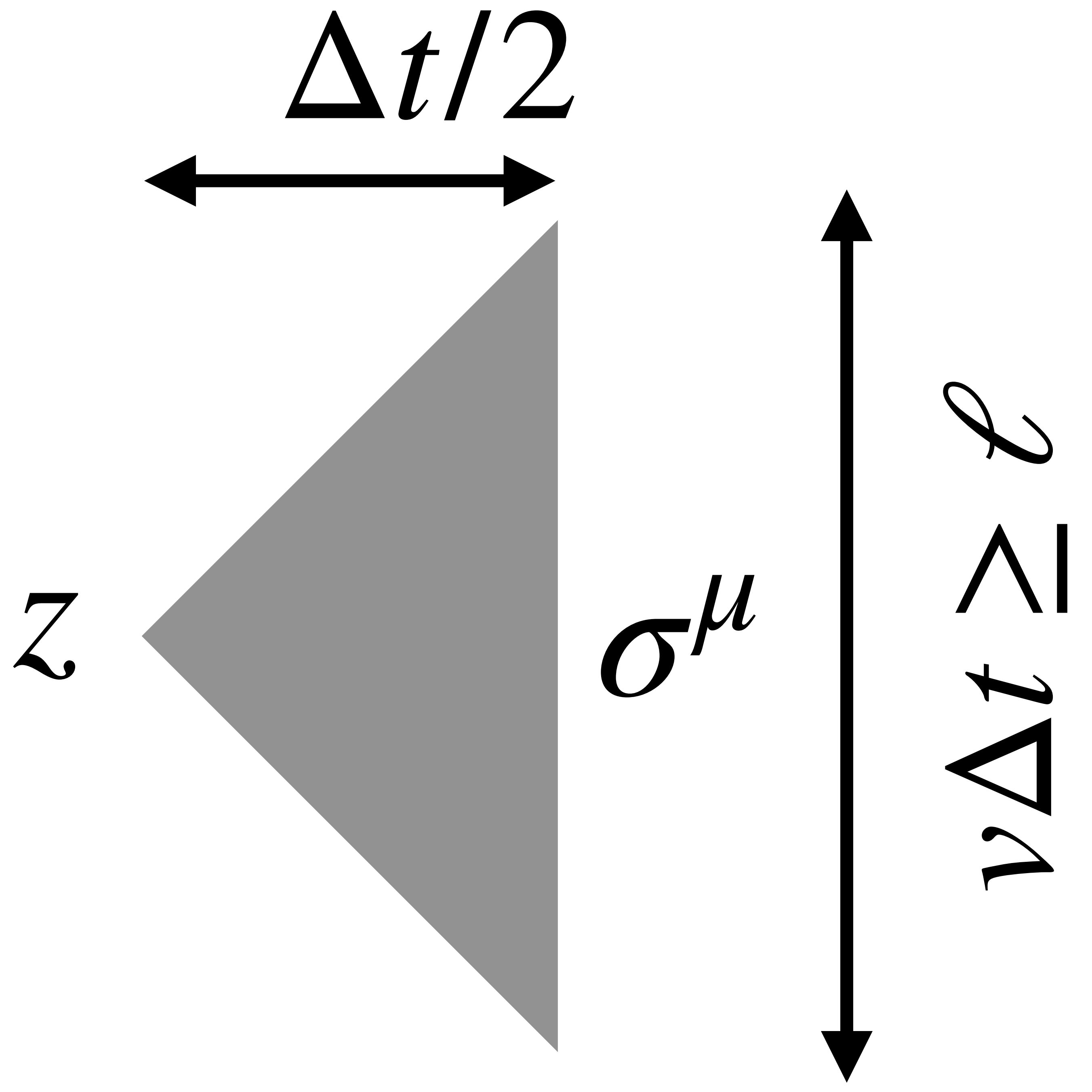

Exp. many operators (in ℓ, Δt) in light cone.

$$\sum_{\mu:\ell(\mu)=\ell} |c_{z\to\mu}|^2 \leq 1$$

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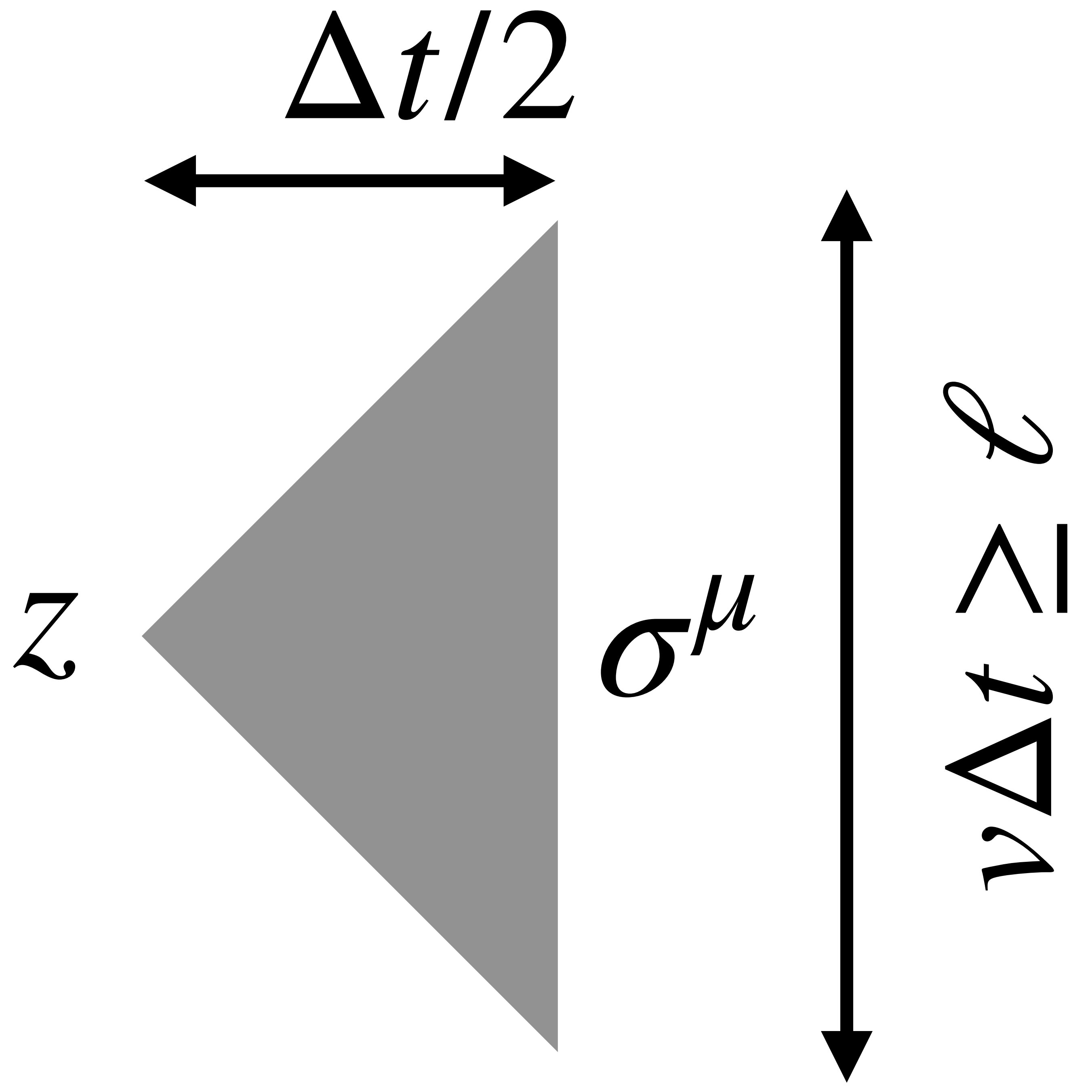

$$\sum_{\mu:\ell(\mu)=\ell} |c_{z\to\mu}|^2 \leq 1$$

$$\to \quad |\Gamma|^2 \sim \exp(-\mathcal{O}(\ell))$$

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$$\leq \sup_{\mu:\ell(\mu)=\ell} |c_{z\to\mu}|^2 = \exp(-\mathcal{O}(\ell))$$

Moral: Use sum rule + random phase assumption.

Problem

- Strong assumption of random phases

$$|\Gamma|^2 = \sum_{\mu,\mu':\ell(\mu)=\ell} c_{z\to\mu} c^*_{z\to\mu'} c_{\mu\to z} c^*_{\mu'\to z} \quad \sim \sum_{\mu:\ell(\mu)=\ell} |c_{z\to\mu}|^2 |c_{\mu\to z}|^2$$

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- Change of Pauli-string basis. Let μ represent strings of I, σ^+, σ^-, z operators.

Case with symmetry

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$\mu_\perp$ is the $\sigma^\pm$ part of μ

Exact in U(1) RUC

$$\sim \sum_{\mu,\mu':\ell(\mu)=\ell} c_{z\to\mu} c^*_{z\to\mu'} c_{\mu\to z} c^*_{\mu'\to z} \delta(\mu_\perp = \mu'_\perp)$$

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Exact in U(1) RUC

$$\sigma^{\mu} = \sigma_1^+ z_3 \sigma_9^- \to \sigma^{\mu_\perp} = \sigma_1^+ \sigma_9^-$$

$$\sigma^{\mu'} = \sigma_1^+ z_1 z_7 \sigma_9^- \to \sigma^{\mu'_\perp} = \sigma_1^+ \sigma_9^-$$

✅

Case with symmetry

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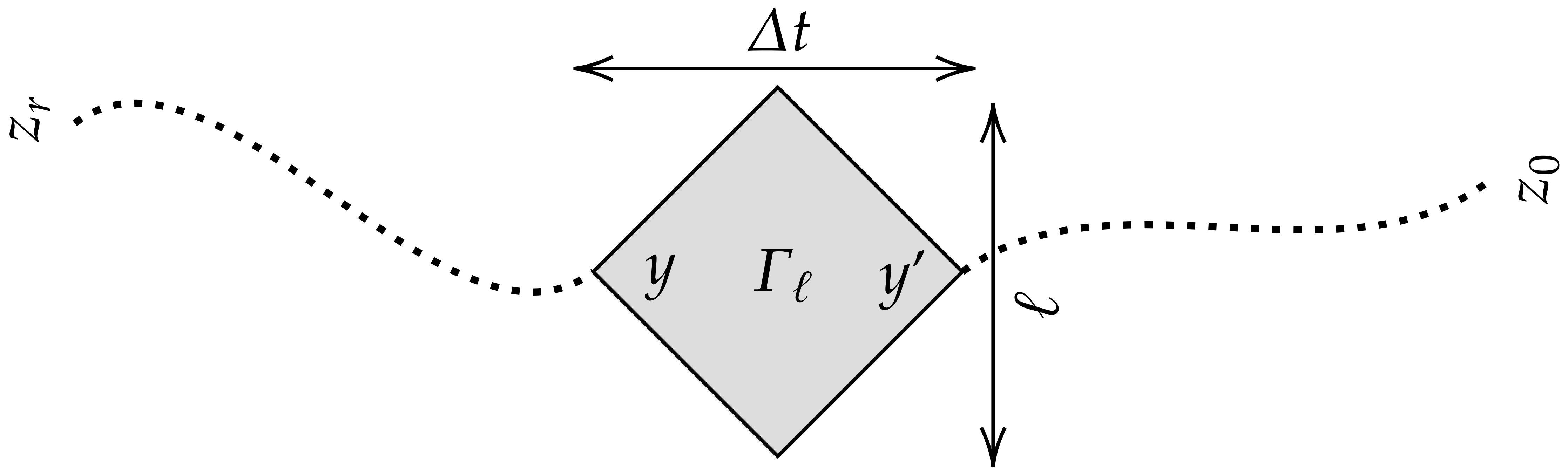
…some work… $\lesssim e^{-\mathcal{O}(\ell)}$

Predictions

$$|\Gamma_\ell|^2 \lesssim e^{-\mathcal{O}(\ell)}$$

$$\int_{y,y'}\int_{t_1,t_2,\Delta t} \partial_y K_{ry}(t_1)\partial_{y'}K_{y'0}(t_2)\Gamma_\ell(y,y',\Delta t)$$



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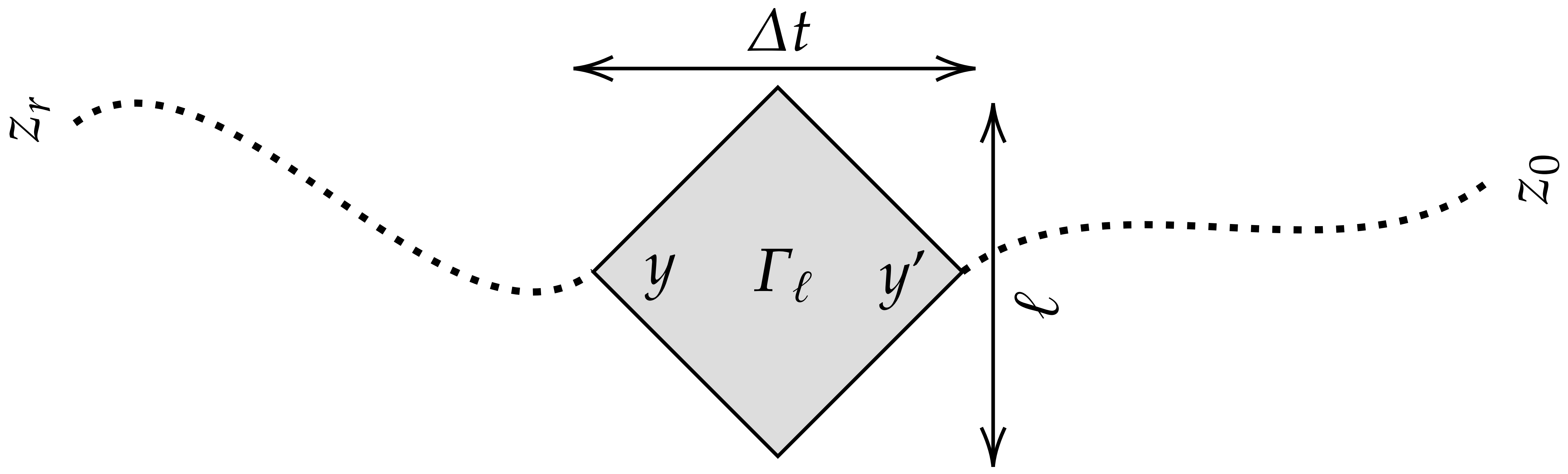
$$|\Gamma_\ell|^2 \lesssim e^{-\mathcal{O}(\ell)}$$

$$\int_{y,y'}\int_{t_1,t_2,\Delta t} \partial_y K_{ry}(t_1)\partial_{y'}K_{y'0}(t_2)\Gamma_\ell(y,y',\Delta t)$$



$$|\langle z_r(\tau)z_0(0)\rangle - \langle z_r(\tau)z_0(0)\rangle_{\text{daoe}}| \sim \begin{cases} \tau^{-1/2}e^{-\mathcal{O}(\ell)} & \text{deterministic} \\ \tau^{-5/4}e^{-\mathcal{O}(\ell)} & \text{stochastic/RUC} \end{cases}$$

$$|D(\tau) - D_{\text{daoe}}(\tau)| \sim \begin{cases} e^{-\mathcal{O}(\ell)} & \text{deterministic} \\ \tau^{-3/4}e^{-\mathcal{O}(\ell)} & \text{stochastic/RUC} \end{cases}$$

Evidence

- Picture supported by numerics, discussed next.
- We also have an independent (but also non-rigorous) diagrammatic argument specific to the U(1) RUC. See paper.

Numerical evidence

$$D(\tau) = \sum_x \frac{x^2}{2\tau} \langle z_x \mid \mathcal{U}(\tau,0) \mid z_0 \rangle \,. \quad D(\ell_*, \tau) = \sum_x \frac{x^2}{2\tau} \langle z_x \mid \prod_{k=0}^{n} [\mathcal{U}(t_{k+1}, t_k) P_{\leq \ell_*}] \mid z_0 \rangle,$$

- Error due to regular dissipation

$$\delta D(\ell_*, \tau) = D(\ell_*, \tau) - D(\tau)$$

Numerical evidence

$$D(\tau) = \sum_x \frac{x^2}{2\tau} \langle z_x \mid \mathcal{U}(\tau,0) \mid z_0 \rangle \,. \quad D(\ell_*, \tau) = \sum_x \frac{x^2}{2\tau} \langle z_x \mid \prod_{k=0}^{n} [\mathcal{U}(t_{k+1}, t_k) P_{\leq \ell_*}] \mid z_0 \rangle,$$

- Error due to regular dissipation

$$\delta D(\ell_*, \tau) = D(\ell_*, \tau) - D(\tau)$$

- Error in D due to single dissipation event

$$\delta_1 D(\ell_*, \tau) \equiv \sum_x \frac{x^2}{2\tau} \langle z_x \mid \mathcal{U}(\tau = 2t, t) P_{>\ell_*} \mathcal{U}(t,0) \mid z_0 \rangle$$

Numerical evidence

$$D(\tau) = \sum_x \frac{x^2}{2\tau} \langle z_x \mid \mathcal{U}(\tau,0) \mid z_0 \rangle \,. \quad D(\ell_*, \tau) = \sum_x \frac{x^2}{2\tau} \langle z_x \mid \prod_{k=0}^{n} [\mathcal{U}(t_{k+1}, t_k) P_{\leq \ell_*}] \mid z_0 \rangle,$$

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- Error in corr. function due to single dissipation event

$$C_{>\ell_*}(\tau) \equiv \langle z_0 | \mathcal{U}(\tau = 2t, t) P_{>\ell_*} \mathcal{U}(t,0) | z_0 \rangle$$

Numerical evidence

$$D(\tau) = \sum_x \frac{x^2}{2\tau}\langle z_x \mid \mathcal{U}(\tau,0) \mid z_0\rangle\,. \quad D(\ell_*,\tau) = \sum_x \frac{x^2}{2\tau}\langle z_x \mid \prod_{k=0}^{n}[\mathcal{U}(t_{k+1},t_k)P_{\leq \ell_*}] \mid z_0\rangle,$$

PREDICTIONS

- Error due to regular dissipation

$$\delta D(\ell_*,\tau) = D(\ell_*,\tau) - D(\tau)$$

$$\sim \begin{cases} e^{-\mathcal{O}(\ell)} & \text{deterministic} \\ \tau^{-3/4}e^{-\mathcal{O}(\ell)} & \text{stochastic/RUC} \end{cases}$$

- Error in D due to single dissipation event

$$\delta_1 D(\ell_*,\tau) \equiv \sum_x \frac{x^2}{2\tau}\langle z_x \mid \mathcal{U}(\tau=2t,t)P_{>\ell_*}\mathcal{U}(t,0) \mid z_0\rangle$$

$$\sim \begin{cases} \tau^{-1}e^{-\mathcal{O}(\ell)} & \text{deterministic} \\ \tau^{-5/4}e^{-\mathcal{O}(\ell)} & \text{stochastic/RUC} \end{cases}$$

- Error in corr. function due to single dissipation event

$$C_{>\ell_*}(\tau) \equiv \langle z_0 | \mathcal{U}(\tau=2t,t)P_{>\ell_*}\mathcal{U}(t,0) | z_0\rangle$$

$$\sim \begin{cases} \tau^{-3/2}e^{-\mathcal{O}(\ell)} & \text{deterministic} \\ \tau^{-7/4}e^{-\mathcal{O}(\ell)} & \text{stochastic/RUC} \end{cases}$$

Deterministic

$$C_{>\ell_*}(t) \equiv \langle o \mid \mathscr{U}(2t,t)\mathscr{P}_{>\ell_*}\mathscr{U}(t,0) \mid o\rangle$$

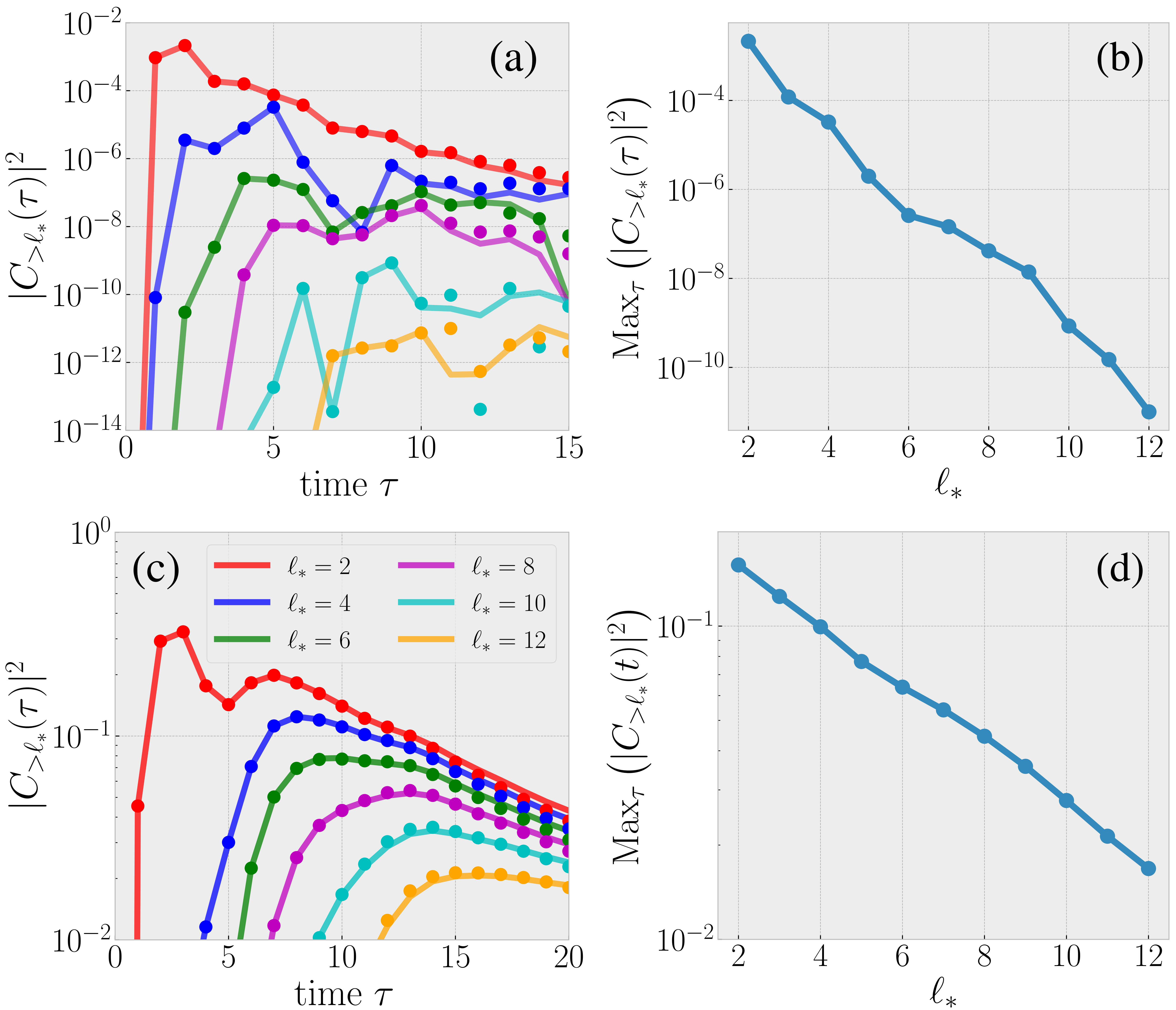
$$H \equiv \sum_j \left(g_x X_j + g_z Z_j + Z_{j-1}Z_j\right)$$

$g_x = 1.4,\ \ g_z = 0.9045$

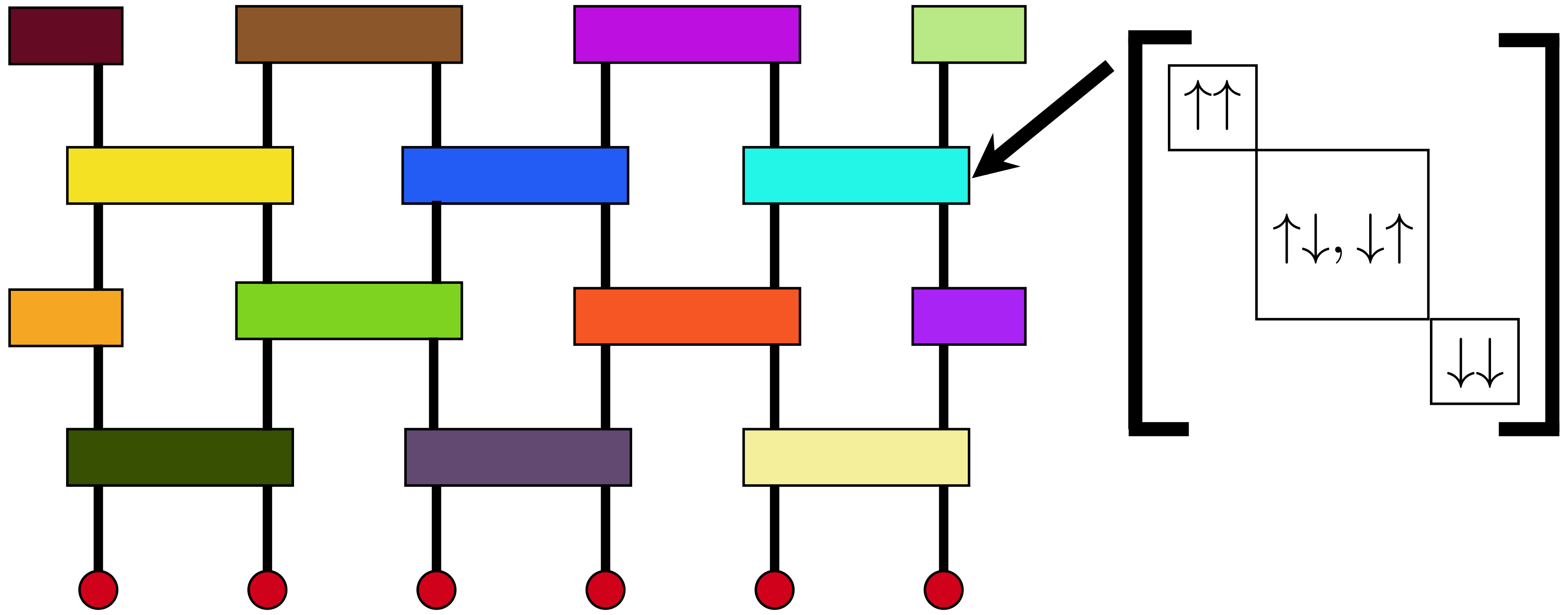
$o = h_j$

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

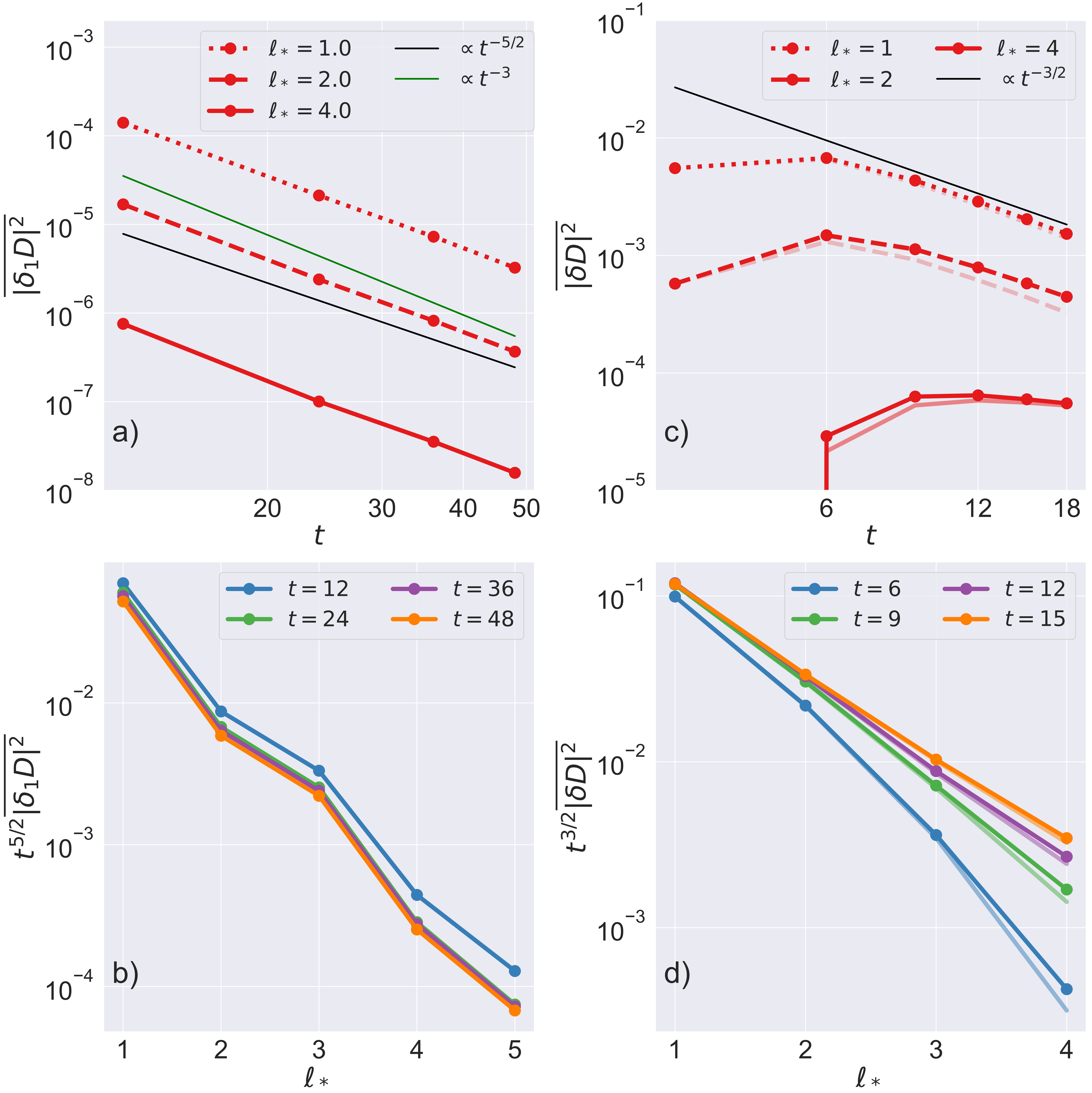
$o = Z_{j,1} + Z_{j,2}$



U(1) RUC



↑↑
↑↓, ↓↑
↓↓



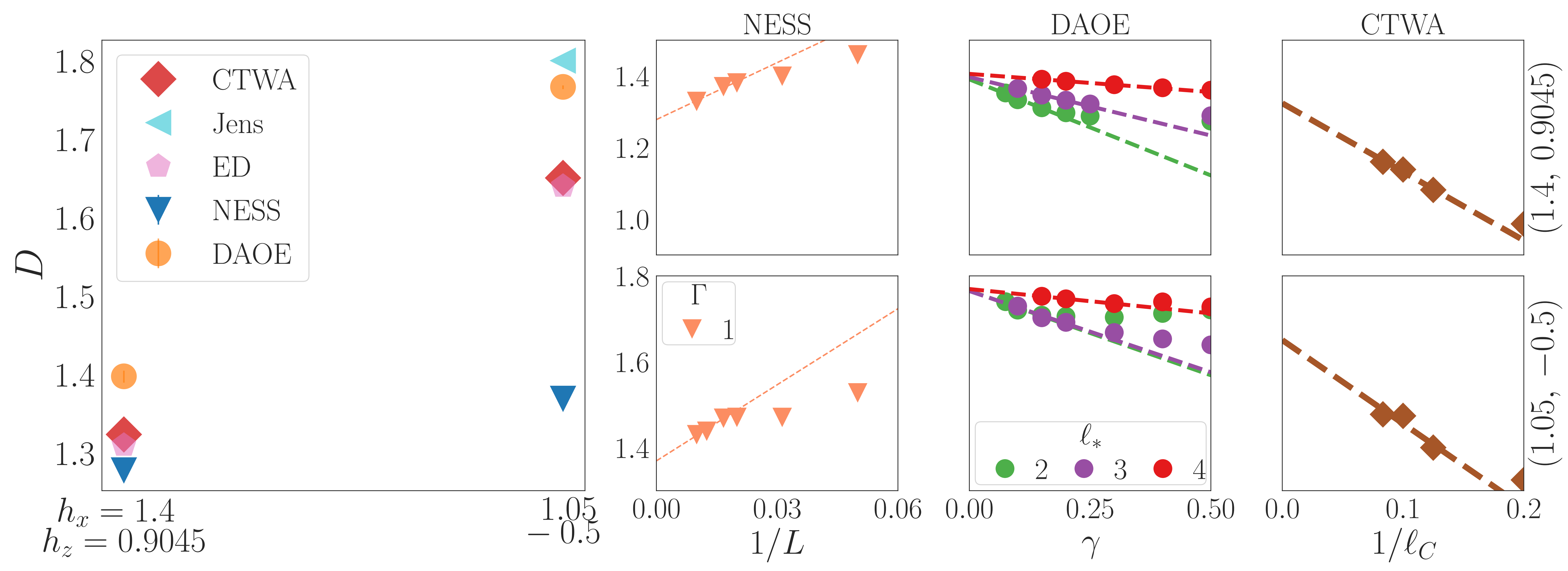
a)
b)
c)
d)
$\ell_* = 1.0$
$\ell_* = 2.0$
$\ell_* = 4.0$
$\propto t^{-5/2}$
$\propto t^{-3}$
$\overline{|\delta_1 D|^2}$
t
$\ell_* = 1$
$\ell_* = 2$
$\ell_* = 4$
$\propto t^{-3/2}$
$\overline{|\delta D|^2}$
$t = 12$
$t = 24$
$t = 36$
$t = 48$
$t^{5/2}\overline{|\delta_1 D|^2}$
ℓ_*
$t = 6$
$t = 9$
$t = 12$
$t = 15$
$t^{3/2}\overline{|\delta D|^2}$

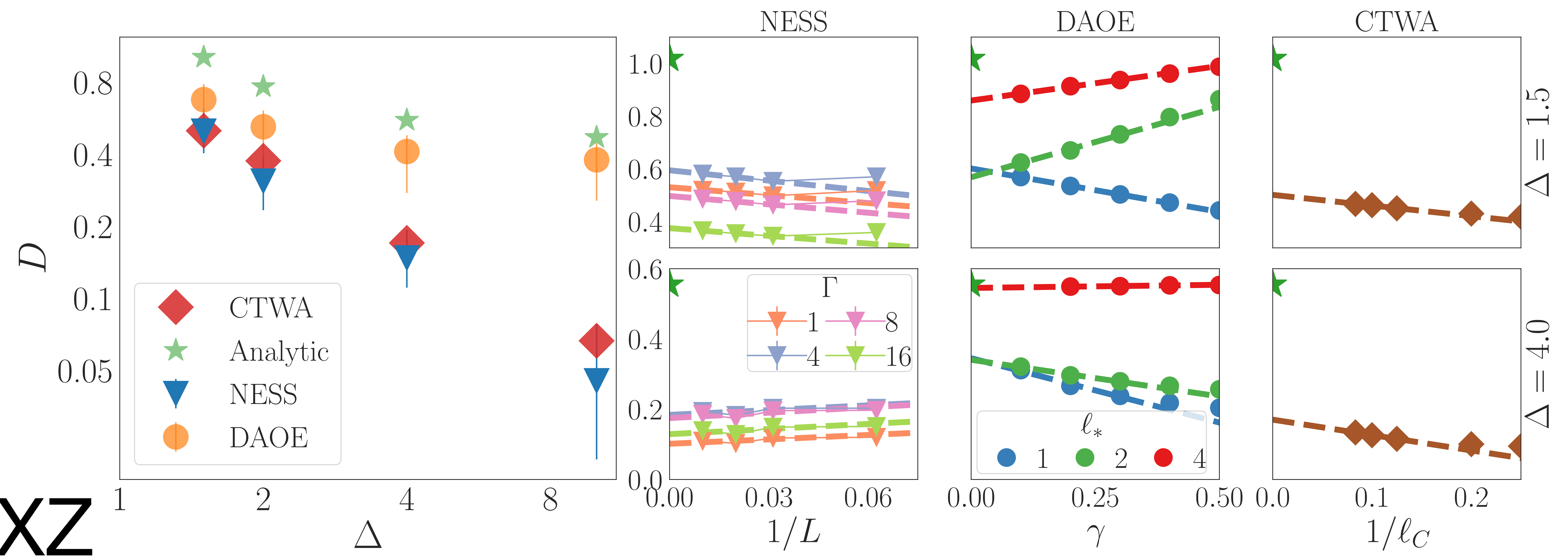
Advertisements

- How does DAOE compare to other methods? Hard to tell for sure! Unfortunately, there are few exact results to benchmark against, and exact results only available in finely tuned models for which most numerical methods are pathological.

- What happens if you throw away on basis of operator diameter rather than length? $\delta D \sim \mathrm{Poly}(1/\ell_*)$. Best guess $\delta D \sim \mathcal{O}(1/\ell_*^4)$, and $\chi \sim e^{\mathcal{O}(\epsilon^{-1/4})}$.

Tilted Field Ising





XXZ

Advertisements

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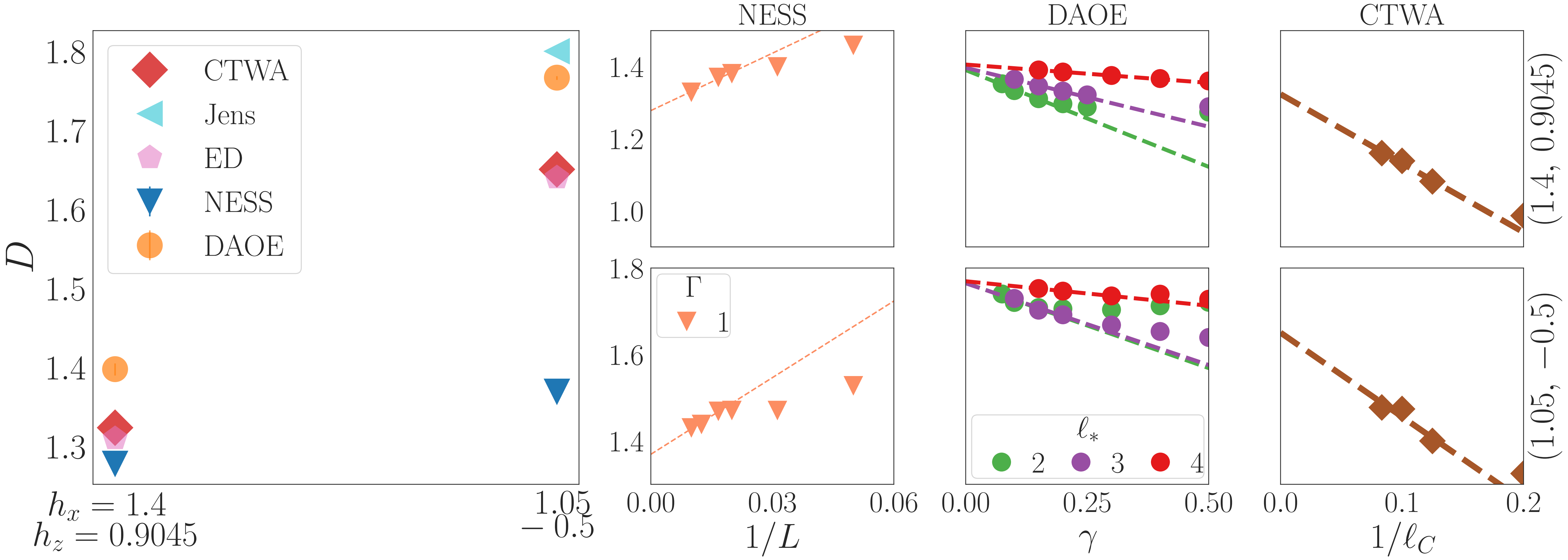
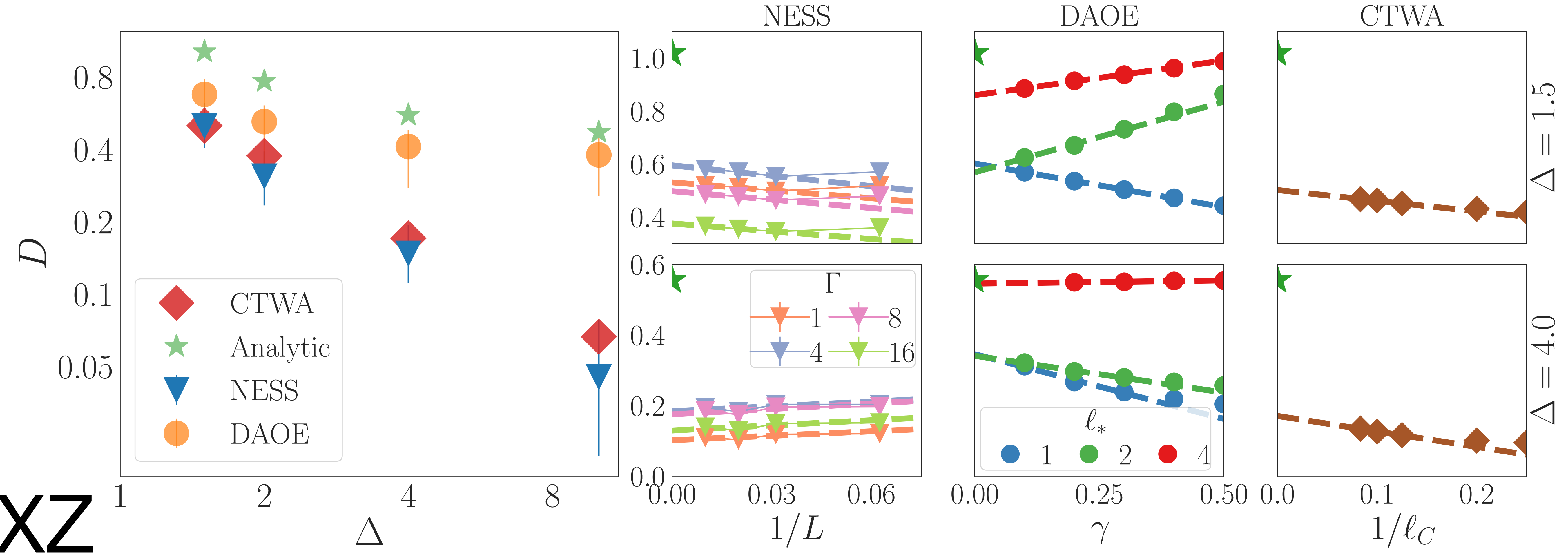
Benchmark against quantum simulators???

Tilted Field Ising





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Conclusion

- Truncation on operator length leads to $e^{-\mathcal{O}(\ell_*)}$ systematic error.

- In region size R, #operators length ℓ_* is $\mathcal{O}(R^{\ell_*})$. Much smaller than 4^R! Much less memory required.

Error analysis relevant to other methods on the market. CD White et al. (2018), Kvorning (2021).

- Some conjectured upper bounds on classical resources required for ϵ-accurate simulation of D:

$$\chi_{\text{naive}} = e^{\mathcal{O}(\text{poly}(\epsilon^{-1}))}.$$

- For our new method:

$$\chi_{\text{DAOE}} = e^{\mathcal{O}(|\log \epsilon|^2)}.$$

- Quantum simulators. (Decoherence limited)

runs x circuit depth = $\text{Poly}(\epsilon^{-1}) = e^{\mathcal{O}(\log(\epsilon^{-1}))}$

Rigorous results lacking!!!

UK Research and Innovation

Thank you!

Curt von Keyserlingk
KCL

with Tibor Rakovszky & Frank Pollmann

…+related work with Ewan McCulloch, Gabriele Pinna, Srivatsa Prasanna, Oliver Lunt

Useful discussions: V. Oganesyan, S. Choi

UK Research and Innovation

Quantum simulator vs DAOE

- Suppose you have an analogue simulation of an ergodic diffusing quantum spin-chain. How many runs and what run time is required to get ϵ-accurate diffusion constants?
- **Time:** $t > t_c = \mathrm{Poly}(1/\epsilon)$**. Limited by decoherence!** $\epsilon_{\mathrm{min}} = \mathrm{Poly}(t_{\mathrm{dec}}^{-1})$

$$\left\langle \sigma_i^z(t)\sigma_j^z(0) \right\rangle \to D(t) \qquad |D(t) - D| \leq C/t^a$$

Quantum simulator vs DAOE

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- Number of measurement runs?

$$\left\langle \sigma_0^z(t)\sigma_0^z(0) \right\rangle_{\mathrm{est},M} = \left\langle \sigma_0^z(t)\sigma_0^z(0) \right\rangle + \frac{\xi}{\sqrt{M}}$$

$$\frac{1}{\sqrt{D_{\mathrm{est}} t_c}} \sim \frac{1}{\sqrt{D t_c}} + \frac{\xi}{\sqrt{M}}$$

$$\overline{\xi} = 0, \overline{\xi^2} = 1$$

Quantum simulator vs DAOE

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$\overline{\xi} = 0, \overline{\xi^2} = 1$

Accurate D_{est} requires: $\left| \frac{\sqrt{t_c}\xi}{\sqrt{M}} \right|^2 < \epsilon^2$

$$\implies M \times t_c = \mathrm{Poly}(1/\epsilon) \sim e^{\mathcal{O}(\log(\epsilon^{-1}))}$$

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$$t_{\text{cpu}}, \chi_{\text{DAOE}} = e^{\mathcal{O}(\log(\epsilon^{-1})^2)} .$$

Can we do better classically?
Can we use simulators more intelligently?