# Relaxation timescales in the dynamics of quantum Ising spin chains

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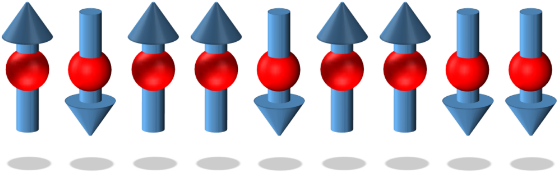
# Problem setting

We consider quantum Ising spin chain in external magnetic field:

$$H = -\sum_i \sigma_z^{(i)} \sigma_z^{(i+1)} + h \sum_i \sigma_z^{(i)} + g \sum_i \sigma_x^{(i)}$$

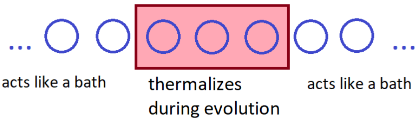


# Thermalization

We are particularly interested in **thermalization**. This is the process when every finite subsystem relaxes to the thermal equilibrium as a result of evolution (the complement of this subsystem plays a role of a thermal bath). Mathematically it can be expressed as follows

$$\langle\psi(t)|\, A\, |\psi(t)\rangle \to \mathrm{Tr}(\rho_{th} A)$$

where $A$ is a local operator, $\rho_{th} = \frac{1}{Z_{th}} e^{-\beta H}$ - thermal Gibbs ensemble.




In other words, at the end of evolution, the system **looks** thermal for any local part of the system and, in this part, the system loses information about initial state, but globally no information is lost, initial pure state transforms into final pure state.

# Integrable and non-integrable systems

- **Integrable systems**

  The system has an extensive number of conserved quantities: $\{Q_i\}, \ \ [H, Q_i] = 0$. **They constrain the dynamics of a system.**

  The system equilibrates to Generalized Gibbs Ensemble (GGE) instead of the Gibbs ensemble:

  $$\langle\psi(t)|\, A \,|\psi(t)\rangle \rightarrow \mathrm{Tr}(\rho_{GGE} A)$$

  where $\rho_{GGE} = \frac{1}{Z_{GGE}} e^{\sum_i \mu_i Q_i}$.

- **Non-integrable systems**

  The system thermalizes to the Gibbs ensemble:

  $$\langle\psi(t)|\, A \,|\psi(t)\rangle \rightarrow \mathrm{Tr}(\rho_{th} A)$$

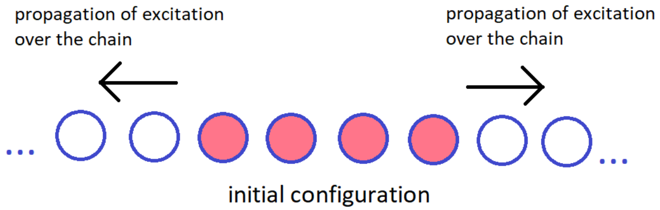
We are interested in the vicinity of an integrable point, and we aim to observe how the system changes its behavior.

$$H = -\sum_i \sigma_z^{(i)}\sigma_z^{(i+1)} + h\sum_i \sigma_z^{(i)} + g\sum_i \sigma_x^{(i)}$$

For our system, it happens for the following sets of parameters in Hamiltonian:

- $g \neq 0$ fixed, $h \to 0$
- $h \neq 0$ fixed, $g \to 0$

Imagine an initial configuration (flux) in some local area of a chain.



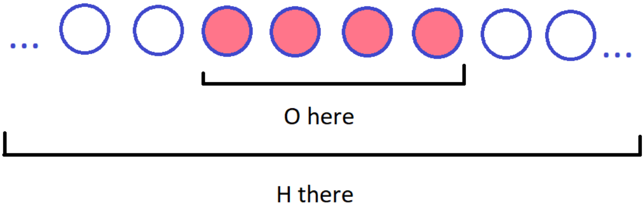

This flux thermalizes, but there are different processes and they happen at different timescales. We concentrate on the slowest one. As the system has only one conserved quantity - energy, one can easily construct local operator with slow dynamics - it is energy flux.
Thus, the slowest timescale is believed to correspond to energy propagation.

Different processes happening at different timescales are described by local operators in the area of initial configuration.

As we are interested in the slowest timescale, the corresponding operator $O$ is the one which best commutes with Hamiltonian:

$$\min \mathrm{Tr}[H, O]^{\dagger}[H, O]$$

where $H$ lives in the whole chain
$O$ has some local support at $N$ consecutive spins



As $O$ is almost conserved, it modifies the thermalization process. One observes an extra prethermalization stage, and all operators first relax to it, and only after completely thermalize.

1. **Initial period of prethermalization** when all operators equilibrate to $\widetilde{GGE}$:

$$\langle\psi(t)|\, A \,|\psi(t)\rangle \to \mathrm{Tr}(\rho_{\widetilde{GGE}} A)$$

   where $\rho_{\widetilde{GGE}} = e^{-\beta H + \mu O_0}$.

2. **Period of final thermalization**:

$$\mathrm{Tr}(\rho_{\widetilde{GGE}} A) \to \mathrm{Tr}(\rho_{th} A)$$

# Objectives (part 1/2)

We aim to answer the following questions:

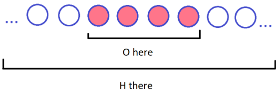
- Does $O$ really correspond to the energy propagation?
- What is the speed of propagation of $O$?
- Does $O$ become one of the integrals of motion, when one approaches an integrable point?
  We check the validity of prethermalization stage description.
- What are the changes in the dynamics of $O$ when one approaches an integrable point?

# Relaxation timescales

We construct the slowest operator $O_0$ as the one, which best commutes with Hamiltonian:

$$\min \operatorname{Tr}[H, O_0]^\dagger [H, O_0]$$

where $H$ lives in the whole chain. $O_0$ has some local support at $N$ consecutive spins.




The faster operators are constructed in a similar way. The next operator $O_1$ is defined as: $\operatorname{Tr}[H, O_1]^\dagger [H, O_1]$ is minimal, provided $\operatorname{Tr} O_0 O_1 = 0$ (orthogonality). Then, one can define other operators $O_2, O_3, \ldots$ by minimizing $\operatorname{Tr}[H, O_i]^\dagger [H, O_i]$, with the condition that $O_i$ is orthogonal to all the previous operators.

# Objectives (part 2/2)

We aim to answer the following questions:

- What is the physical meaning of all these operators? Do they correspond to propagation of some conserved quantities?
- How do they change their dynamics when one approaches an integrable point?
- Do they become integrals of motion?

# Construction

We construct the slowest operator in a tensor network form:

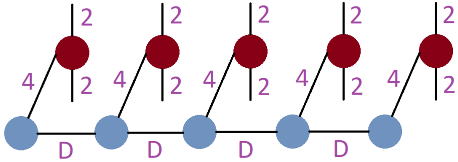
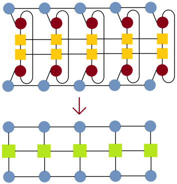


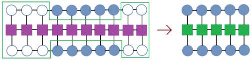

Figure 1: Tensor network representation of the slowest operator. The dark red circles correspond to Pauli matrices $\sigma^{(i)}$, blue ones - to the tensor coefficients $A^{(i)}$ in front of them. Numbers correspond to dimensions of the edges.

$$O = \sum_{\substack{l,m,n,\ldots \\ k_0\ldots k_{N-1}}} A_l^{(0),k_0} A_{lm}^{(1),k_1} \ldots A_n^{(N-1),k_{N-1}} \times$$

$$\times \sigma_{k_0}^{(0),i_0,j_0} \otimes \sigma_{k_1}^{(1),i_1,j_1} \ldots \otimes \sigma_{k_{N-1}}^{(N-1),i_{N-1},j_{N-1}}$$



(a) Transformation of the term $\mathrm{Tr}(O^\dagger H_{loc}^2 O)$. After combining the resulting tensor networks for all the terms, DMRG algorithm can be applied.



(b) Reduction of the tensor network, corresponding to $-\mathrm{Tr}[H,O]^2$. DMRG algorithm can be applied to the network on the right.

We find $O$ by minimization of $\mathrm{Tr}[H,O]^\dagger[H,O]$. For this, we represent $\mathrm{Tr}[H,O]^\dagger[H,O]$ in a form $\langle O|\,\mathcal{H}\,|O\rangle$ and apply DMRG algorithm.

$$\mathrm{Tr}([H,O]^\dagger[H,O]) = \mathrm{Tr}(O^\dagger H_{loc}^2 O) + \mathrm{Tr}(O^\dagger O H_{loc}^2) - 2\,\mathrm{Tr}(O^\dagger H_{loc} O H_{loc}) +$$
$$2 - 2\,\mathrm{Tr}(O^\dagger \sigma_z^{(0)} O \sigma_z^{(0)}) + 2 - 2\,\mathrm{Tr}(O^\dagger \sigma_z^{(N-1)} O \sigma_z^{(N-1)})$$

Each one of these terms can be represented in a tensor network form $\langle O|\ldots|O\rangle$.

# Quantities we calculate

1. **Scaling of** $\mathrm{Tr}([H, O]^\dagger [H, O])$ **with** $h$ - to see if the operators become integrals of motion, how many of them are significantly slower than others.
2. **Overlap** $\mathrm{Tr}\, OP$ **of an operator** $O$ **with probe operators** $P$ **(energy flux, diffusion mode, magnetization1,2,3)** - to see if obtained operators do correspond to any known quantities.
3. **Time evolution of** $\mathrm{Tr}\, O(t)O(0)$ - to estimate the rate of propagation of operators over the chain (recall Kubo relations: transport coefficients are proportional to 2-point correlation functions).
4. **Out-Of-Time-Ordered Commutator (OTOC)** $\mathrm{Tr}([O(t), \sigma^{(i)}_{x,y,z}(0)]^\dagger [O(t), \sigma^{(i)}_{x,y,z}(0)])$ - also to estimate the rate of propagation of operators (different method).

## Overlap with probe operators

We calculate overlap (Tr $OP$) of both slowest operators with diffusion mode, energy flux and magnetization to find their physical meaning.

- Diffusion mode

$$E^{(0)} = \sum_{i=0}^{N-2} \cos\left(-\frac{\pi}{2} + \frac{i+\frac{1}{2}}{N}\pi\right)(-\sigma_z^{(i)}\sigma_z^{(i+1)}) + \sum_{i=0}^{N-1} \cos\left(-\frac{\pi}{2} + \frac{i}{N}\pi\right)(h\sigma_z^{(i)} + g\sigma_x^{(i)})$$

(energy flux with density gradually vanishing to the boundaries of its support - bell shape)

- Energy flux

$$\sum_{i=0}^{N-2}(-\sigma_z^{(i)}\sigma_z^{(i+1)}) + \sum_{i=0}^{N-1}(h\sigma_z^{(i)} + g\sigma_x^{(i)}) + (-\sigma_z^{(N-1)}\sigma_z^{(0)})$$

(Hamiltonian terms + extra cyclic boundary terms)

- Magnetization

$$M_{x,y,z}^{(0)} = \sum_{i=0}^{N-1} \sigma_{x,y,z}^{(i)}$$

# Time evolution

We calculate 2-point correlation function $\mathrm{Tr}\, O(t)O(0)$ in a spirit of Kubo relations (transport coefficients are connected to correlation functions of operators).

We use **random vector** approximation (for the trace) to simplify the calculation:

$$\frac{1}{2^L}\,\mathrm{Tr}\, O(t)O(0) = \frac{1}{2^L}\,\mathrm{Tr}\left(O(0)e^{-iHt}O(0)e^{iHt}\right) \sim \frac{1}{K}\sum_{k=1}^{K}\langle\psi_k|\,O(0)e^{-iHt}O(0)e^{iHt}\,|\psi_k\rangle = \frac{1}{K}\sum_{k=1}^{K}\langle\phi_k(-t)|\,O(0)\,|\chi_k(-t)\rangle$$

We calculate time evolution of vectors $|\phi_k(-t)\rangle$ and $|\chi_k(-t)\rangle$ using the method of **Chebyshev polynomials**:

$$|\psi(t)\rangle = e^{-iHt}\,|\psi\rangle = J_0(2\bar{E}t)\,|\psi\rangle + 2\sum_{n=1}^{\infty}(-i)^n J_n(2\bar{E}t)\,T_n\left(\frac{\bar{H}}{2}\right)|\psi\rangle$$

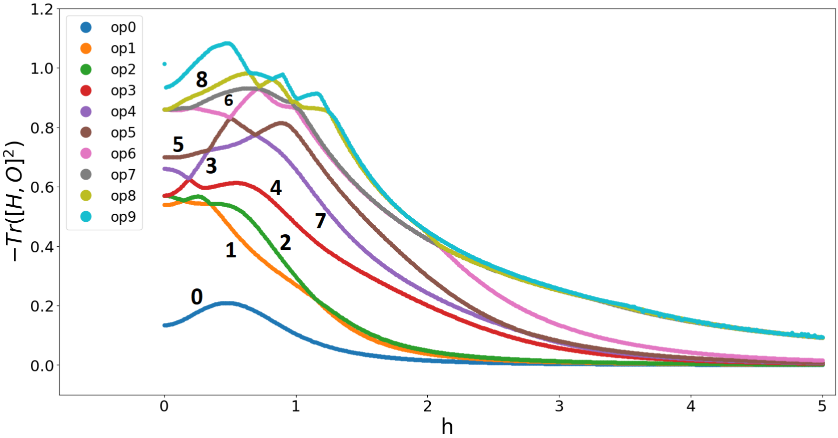
where $T_n$ are Chebyshev polynomials of the first kind, and $J_n$ are Bessel functions of the first kind.

# Time evolution: OTOC

We also calculate Out-Of-Time-Ordered Commutator (OTOC) with Pauli matrices fixed at various positions over the chain. In this way we see how the slowest operator propagates over the chain.

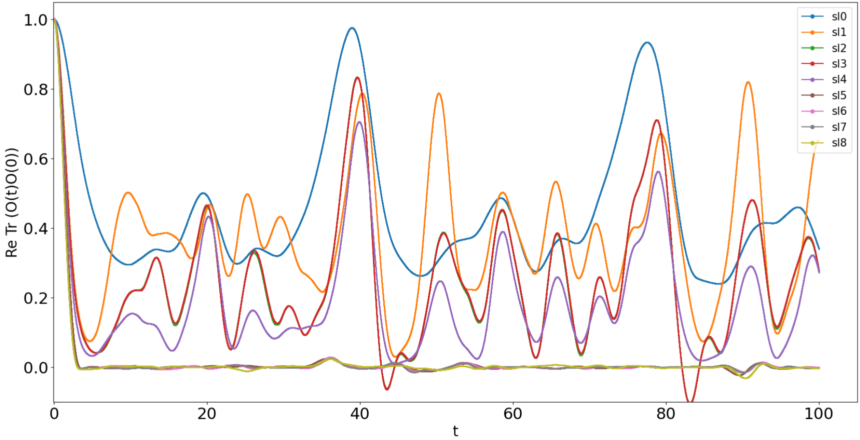
$$\mathrm{Tr}([O(t), \sigma_{x,y,z}^{(i)}(0)]^\dagger [O(t), \sigma_{x,y,z}^{(i)}(0)])$$

# Results: scaling of $\mathrm{Tr}([H,O]^\dagger[H,O])$ with $h$



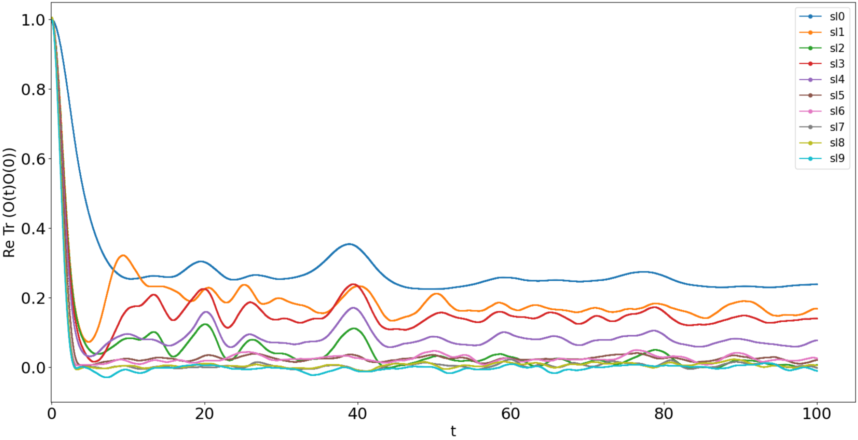

(a) Scaling of $\mathrm{Tr}([H,O]^\dagger[H,O])$ with $h$, $g = 1.05$

# Results: time evolution of $\mathrm{Tr}\, O(t) O(0)$




(a) Time evol., g=1.05, h=0.0 (integrable)

# Results: time evolution of Tr $O(t)O(0)$

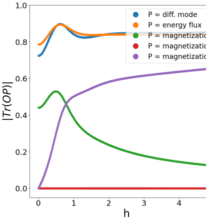



(a) Time evol., g=1.05, h=0.1 (non-integrable)

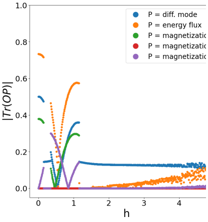
# Results

- Different physical operators intertwine between integrable points ($g >> h$ and $h >> g$).
- For $g >> h$, there is one operator much slower than others, while for $h >> g$, there is a degenerate space of slowest operators.
- Operators form groups.
- Near an integrable point $g >> h$, operators <u>do not</u> become integrals of motion, but near $h >> g$ - they do.
- The quantity $\mathrm{Tr}[H, O]^\dagger [H, O]$ defines overall time evolution of an operator (op2 and op3 have identical $\mathrm{Tr}\, O(t)O(0)$, see Fig. (b)).
- Hierarchy between quantities $\mathrm{Tr}[H, O_i]^\dagger [H, O_i]$ does not correspond to the hierarchy between thermalization times (op2 thermalizes faster than op3 and op4, see Fig. (c)).
- Revivals of all operators get suppressed when one goes away from an integrable point.

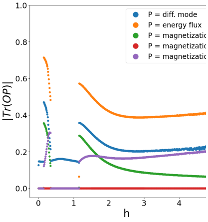
# Overlap



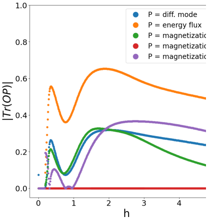

(a) op0



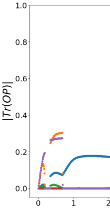

(b) op1



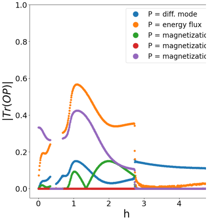

(c) op2



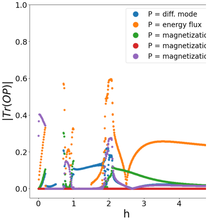

(d) op3



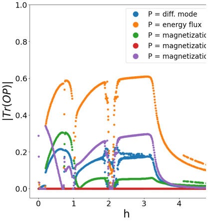

(e) op4



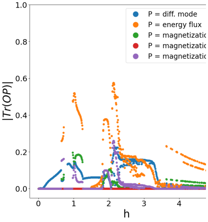

(f) op5



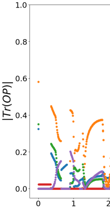

(g) op6




(h) op7

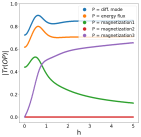



(i) op8

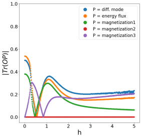



(j) op9

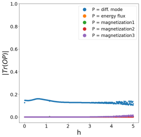
From these figures, one can construct the **physical modes**, enumerated above.



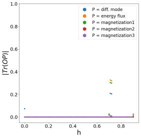

(a) phys.0



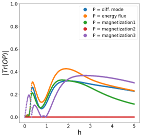

(b) phys.1



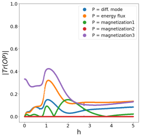

(c) phys.2



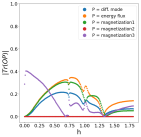

(d) phys.3



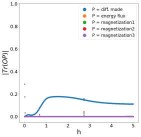

(e) phys.4



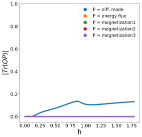

(f) phys.5




(g) phys.6



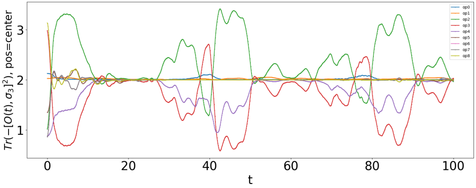

(h) phys.7



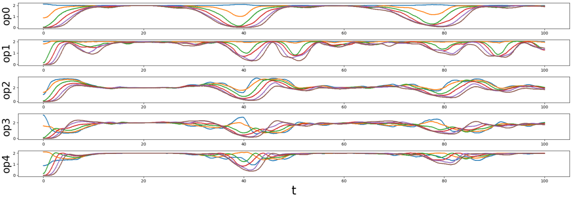

(i) phys.8

- There is a significant portion of energy dynamics at fast timescales. There are also signs of diffusion transport.

# Results: OTOC $\mathrm{Tr}([O(t), \sigma^{(i)}_{x,y,z}(0)]^\dagger [O(t), \sigma^{(i)}_{x,y,z}(0)])$




(a) OTOC, g=1.05, h=0.0 (integrable), different operators, position of sigma3=center

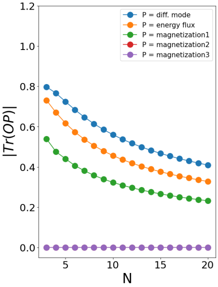



(b) OTOC, g=1.05, h=0.0 (integrable), different positions of sigma3

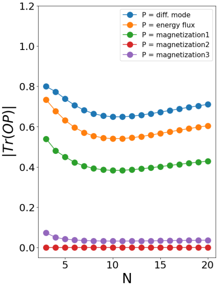
- The operators from the same group transform one into another during the evolution.
- OTOCs for different operators have various shapes of dynamics.
- OTOC also shows the suppression of revivals when one goes away from an integrable point.

# Results

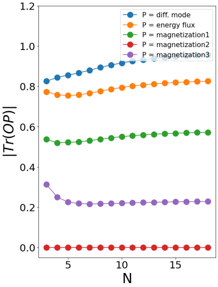
There is a transient behavior of the local slowest operator when one goes away from the integrable point:




(a) Loc. ($g = 1.05, h = 0.0$)




(b) Loc. ($g = 1.05, h = 0.1$)




(c) Loc. ($g = 1.05, h = 0.4$)

Figure 9: Overlap $\mathrm{Tr}(OP)$ of the slowest operator $O$ and a probe operator $P$ as a function of support size $N$ of the slowest operator. We take $P$ as diffusion mode, energy flux, magnetization1,2,3.

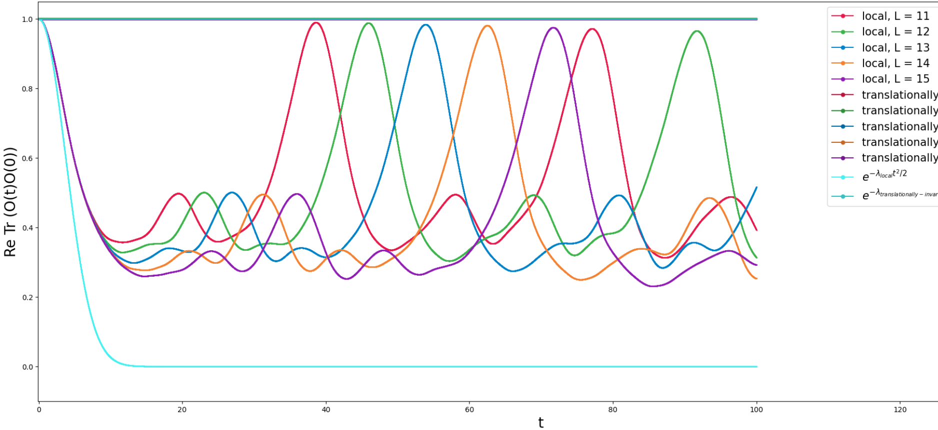



Figure 10: $g = 1.05,\ h = 0.0$

# Results

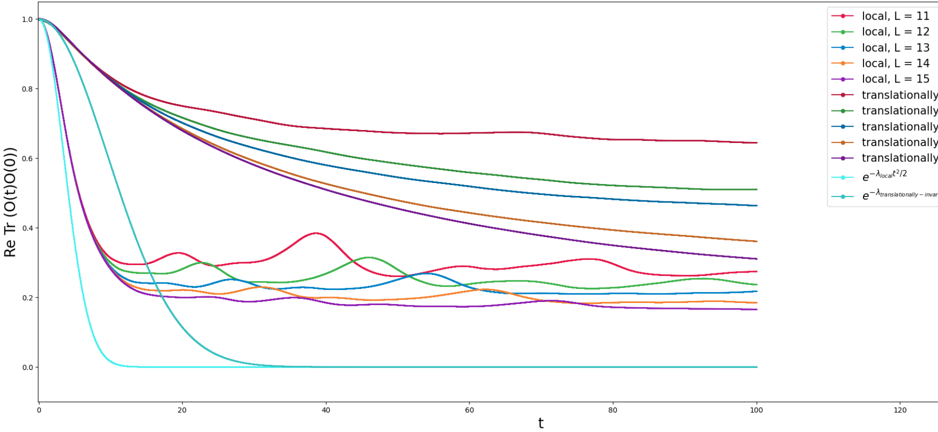



Figure 11: $g = 1.05,\ h = 0.1$

# Results

- For the local slowest operator, there are revivals - they signify that the operator has propagated through the whole chain and has come back.
- There are revivals of half the amplitude.
- Revivals get suppressed when one goes away from an integrable point.
- One can clearly see the moment when the local operator reaches the boundaries of the whole system.
- Translationally-invariant operator does not have revivals and thermalizes slower.

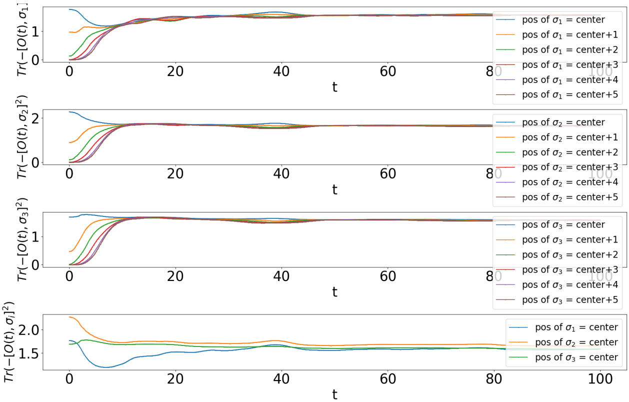



Figure 12: OTOC of the slowest operator with the Pauli matrix at a particular site: $Tr(-[O(t), \sigma_i(0)]^2)$ ($L = 11$, $N = 6$). Local operator, $g = 1.05, h = 0.1$.

Initially, the local operator commutes only with those Pauli matrices that do not have overlap with its support. But, as the system evolves, the commutators at different positions acquire equal values - the operator propagates through the whole chain and settles down equally everywhere.

One can see the suppression of revivals for OTOC, as well:

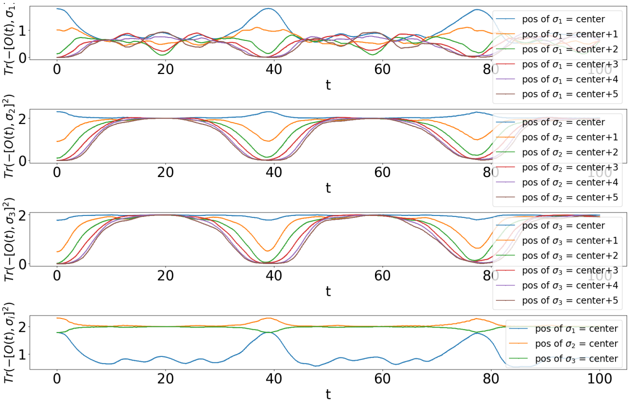



Figure 13: OTOC of the slowest operator with the Pauli matrix at a particular site: $Tr(-[O(t), \sigma_i(0)]^2)$ $(L = 11,\ N = 6)$. Local operator, $g = 1.05, h = 0.0$.

# Conclusion

- Slowest operators correspond to the slowest mode of dynamics of the local flux relaxation.
- Slowest operators appear in the GGE ensemble, to which a system equilibrates at intermediate (prethermalization) stage.
- Local slowest operators are constructed using tensor networks and DMRG algorithm.
- Local operator does not correspond to an integral of motion and does not appear in GGE exponent.
- Local slowest operator has great overlap with energy flux.
- When one goes away from an integrable point, revivals of the local operator get suppressed, while overlap function shows transient behavior.
- OTOC is connected to chaotic behavior, but also describes propagation of operator over the chain.

Thank you