

# Mixing time of local Hamiltonians:

## Rapid state preparation via dissipative dynamics

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- Background (Existing result and current challenges)
- Our results
- Outlook

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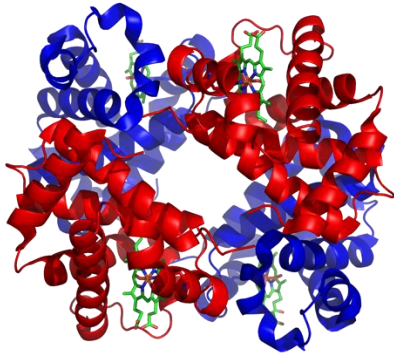
# Motivation

- Ground state and low-temperature Gibbs state are among the most important problems in many-body physics and quantum chemistry.



# How does the Nature prepare low energy states?

Proteins function in a thermal bath at temperature  $T=310\text{K}$



High Temperature superconducting materials can be cooled down to superconducting phase by putting into liquid Nitrogen ( $T=77\text{K}$ )

# Simulating Nature

Recently, a series of quantum algorithm simulating the dissipative dynamics in Nature has been proposed to prepare Gibbs state and ground state of quantum systems

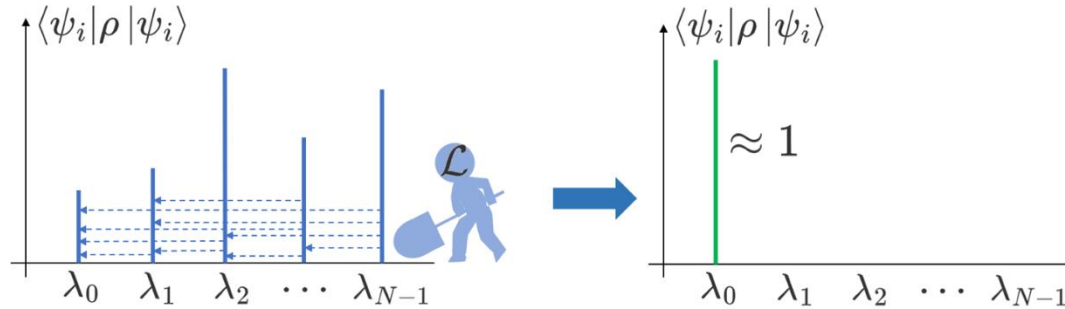
$$\frac{d\rho}{dt} = -i[G, \rho] + \mathcal{L}(\rho)$$

They have ground state or Gibbs state as their fixed points

They are efficiently implementable on a quantum circuit.

# Simulating Nature

The ground state preparation algorithm proposed by [DCL 23]



$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k K_k \rho K_k^\dagger - \frac{1}{2} \{K_k^\dagger K_k, \rho\}.$$

$$K_k := \sum_{i,j} \hat{f}(\lambda_i - \lambda_j) |\psi_i\rangle \langle \psi_i| A_k |\psi_j\rangle \langle \psi_j|$$

# Simulating Nature

- Correctness
- Implementable
- Efficient



# Simulating Nature

- Correctness 

(Ground state or Gibbs state is the fixed point)

- Implementable 

(can be efficiently implemented on a quantum circuit)

- Efficient 

(Converge to the fixed point in polynomial time, i.e.  $T_{mix} = O(poly N)$ )

# Mixing time of quantum systems: Existing results on Gibbs samplers

- Gap of Gibbs samplers implies fast mixing.

Inverse polynomial gap implies  $O(\text{poly } N)$  mixing time. Constant gap implies  $O(N)$  mixing time.

- Log Sobolev constant implies rapid mixing.

Positive log Sobolev constant implies  $O(\log N)$  mixing time.

# Mixing time of quantum systems: Existing results

	Commuting	Non-Commuting	
Gibbs state	1D commuting Local Hamiltonian: $O(N) \rightarrow O(\log N)$ 2D toric code: $O(N)$	?	High temperature: $O(N)$
Ground state	?	?	

## Current challenges in proving mixing time

- The Lindbladians of non-commuting Hamiltonians are quasi-local. Their mixing times are widely open. ❌
- Current mathematical tools for proving mixing time do not apply to Lindbladians for ground state preparation. ❌
- It is difficult to improve  $O(\text{poly } N)$  mixing time to  $O(\log N)$ . ❌

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# Quasi-free systems

Consider a quadratic fermionic Hamiltonian with annihilation and creation operators as the jump operator.

$$H = \sum_{i,j} a_{ij} c_i c_j^\dagger, \quad A_k = c_k, c_k^\dagger$$

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k K_k \rho K_k^\dagger - \frac{1}{2} \{K_k^\dagger K_k, \rho\}.$$

We show that the one-body density matrix  $P_{ij} = \text{Tr}(\rho c_i c_j^\dagger)$  is exponentially converging to the ground state distribution  $P_f$ .

$$\frac{dP}{dt} = -(P - P_f)$$

# Quasi-free systems

Consider a quadratic fermionic Hamiltonian with annihilation and creation operators as the jump operator.

$$H = \sum_{i,j} a_{ij} c_i c_j^\dagger, \quad A_k = c_k, c_k^\dagger$$

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k K_k \rho K_k^\dagger - \frac{1}{2} \{K_k^\dagger K_k, \rho\}.$$

Using Wick's Theorem, all k-body density matrices can be derived from one-body density matrix, so all local density matrices are exponentially converging at a constant rate.

# Quasi-free systems

Consider a transverse field Ising model with coupling operators  $A = X_1, X_n, Y_1, Y_n$ .

$$\hat{H}_{\text{TFIM}} = -g \sum_{i=1}^n Z_i - J \sum_{i=1}^{n-1} X_i X_{i+1},$$

$$K = \sum_{i,j \in [N]} \tilde{f}(\lambda_i - \lambda_j) |\psi_i\rangle \langle \psi_i| X_1 |\psi_j\rangle \langle \psi_j|,$$

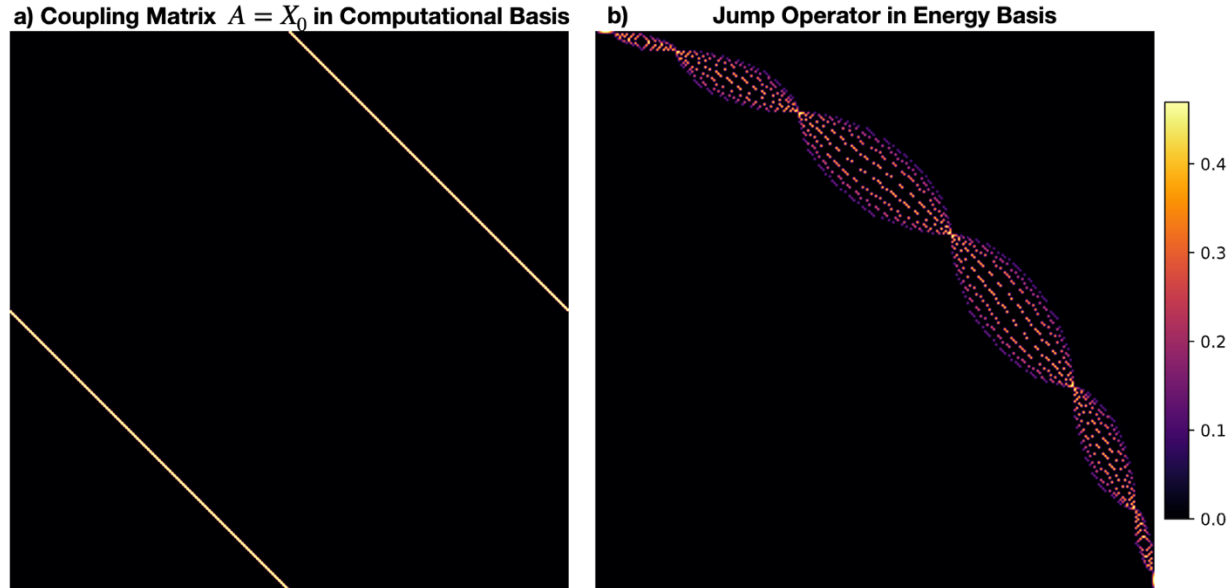
$$\tilde{f}(\omega) = \begin{cases} 0 & : \omega \geq 0 \\ 1 & : \omega < 0 \end{cases}.$$

Using J-W transformation, we can convert the Lindbladian to the quasi-free form.



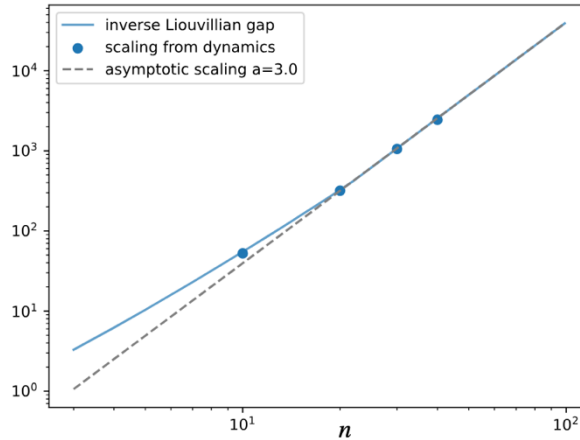
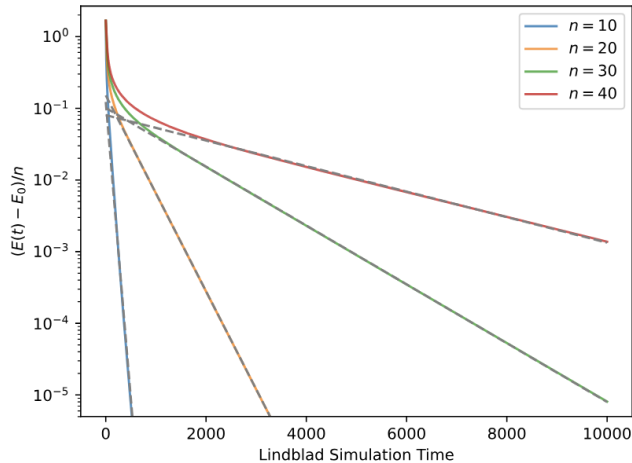
# Quasi-free systems

Matrix element of Pauli operator  $X_1$  in the computational basis and energy basis, allowing energy transitions. ( $g/J = 1.5$ )



# Mixing time of TFIM (boundary dissipation)

Energy decay of Lindbladian dynamics and the loglog plot of mixing time, showing mixing time scales polynomially with system size.  $T_{mix} = O(n^3)$



In quasifree setting, we evaluate the mixing time using the energy decay rate.

# Quasi-free systems

Another quasi-free example is the cluster Hamiltonian.

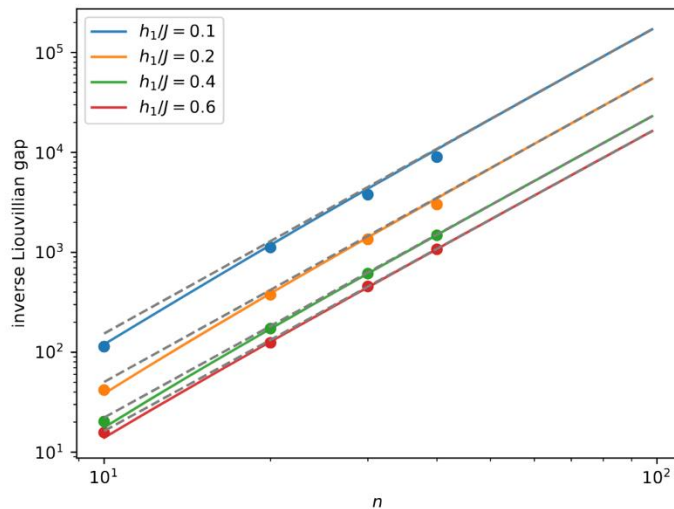
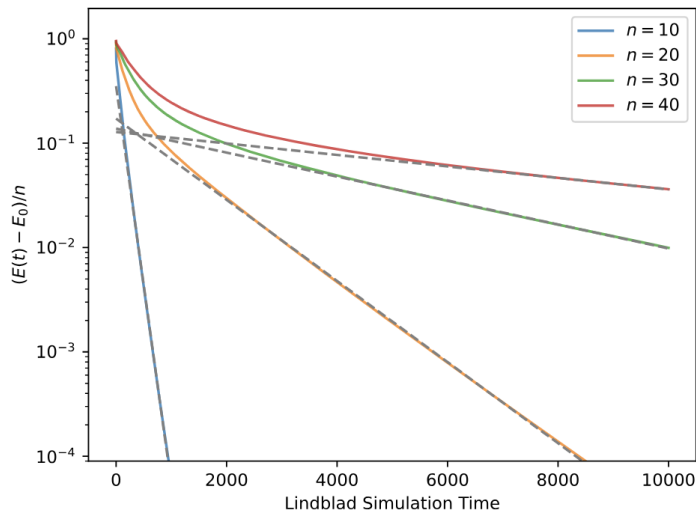
$$\hat{H} = -J \sum_{i=1}^{n-2} X_i Z_{i+1} X_{i+2} - h_1 \sum_{i=1}^n Z_i.$$

The coupling operators are  $\mathbf{A} = X_1, X_n, Y_1, Y_n$ .

We choose  $h_1/J = 0.1$ , where the Hamiltonian is in the SPT phase and has a fourfold degenerate ground state.

# Mixing time of cluster Hamiltonian (boundary dissipation)

Energy decay of Lindbladian dynamics and the loglog plot of mixing time, showing mixing time scales polynomially with system size.  $T_{mix} = O(n^3)$



# Mixing time of non-quasi free systems: Tensor network methods

We represent all operators as MPOs and evaluating the mixing time by directly propagating the Lindbladian.

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k K_k \rho K_k^\dagger - \frac{1}{2} \{K_k^\dagger K_k, \rho\}.$$

$$K_k = \int_{-\infty}^{\infty} f(s) e^{iHs} A e^{-iHs} ds$$

The mixing time is defined as

$$\tau_{\text{mix}}(\epsilon) = \min \{t \mid \langle \psi | \rho_t | \psi \rangle \geq 1/2 \text{ for input state } \rho_0 = \mathbb{I}/2^n\}$$

# Mixing time of non-quasi free systems: Tensor network methods

Assumption: All the jump operators and states during time evolution have low bond dimension structure.

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k K_k \rho K_k^\dagger - \frac{1}{2} \{K_k^\dagger K_k, \rho\}.$$
$$K_k = \int_{-\infty}^{\infty} f(s) e^{iHt} A e^{-iHt} ds$$

After each time step, we compress the bond dimension of  $\rho$ .

Main difficulty:

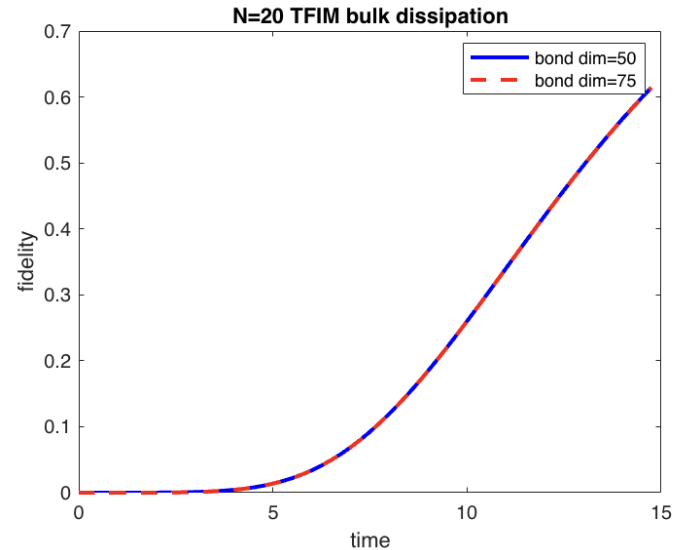
Fast compression method.

Direct tensor network compression is very slow, so we use an approximate fitting method that is 100 times faster

# Tensor network methods are reliable

We verify the low bond dimension assumption by showing that the TN results with different bond dimensions match very well.

For the Lindbladian dynamics of  $N=20$  TFIM, the relative error of TN results with different bond dimension is less than 0.1%.



# Mixing time of Heisenberg model in a magnetic field (boundary dissipation)

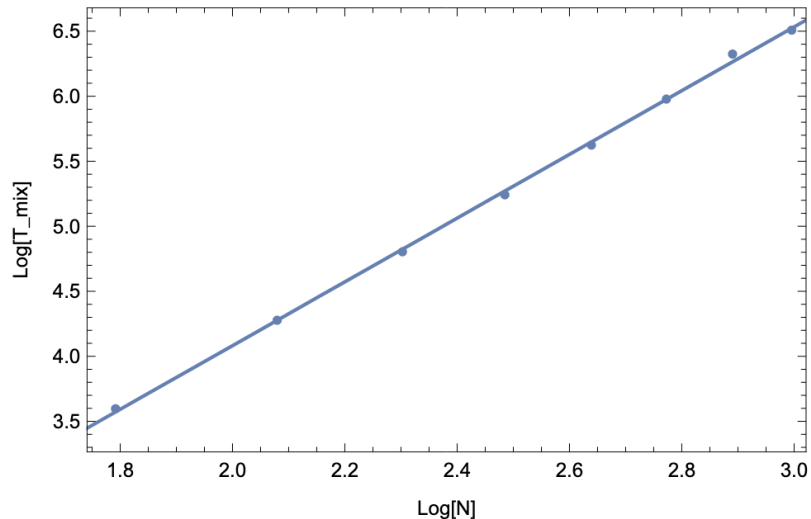
Consider the Hamiltonian:

$$H = -J \sum_{i=1}^{n-1} X_i X_{i+1} - \Delta \sum_{i=1}^{n-1} (Y_i Y_{i+1} + Z_i Z_{i+1}) - \sum_{i=1}^n g_i Z_i,$$

with  $A = X_1, Y_1, Z_1, X_n, Y_n, Z_n$

The numerical result shows

$$T_{mix} = O(n^{2.5})$$



Boundary dissipation  $\rightarrow$  *poly*  $N$  mixing time



# Rapid mixing of 1D gapped local Hamiltonians

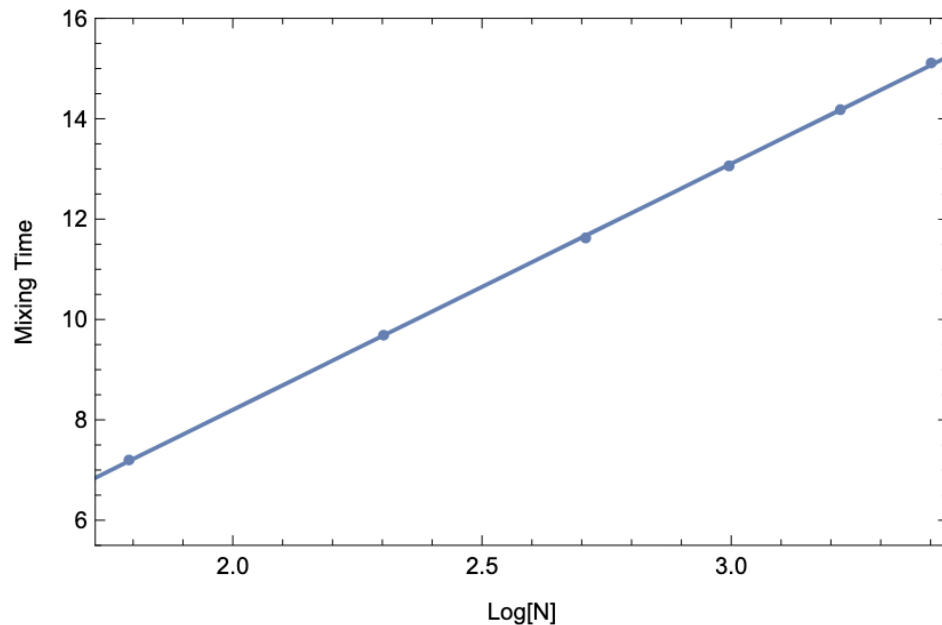
For the TFIM Hamiltonian,

$$H = - \sum_{i=1}^n g_i Z_i - J \sum_{i=1}^{n-1} X_i X_{i+1}$$

we use all  $3N$  Pauli operators as coupling operators.

Our numerical result shows

$$T_{mix} = O(\log N)$$



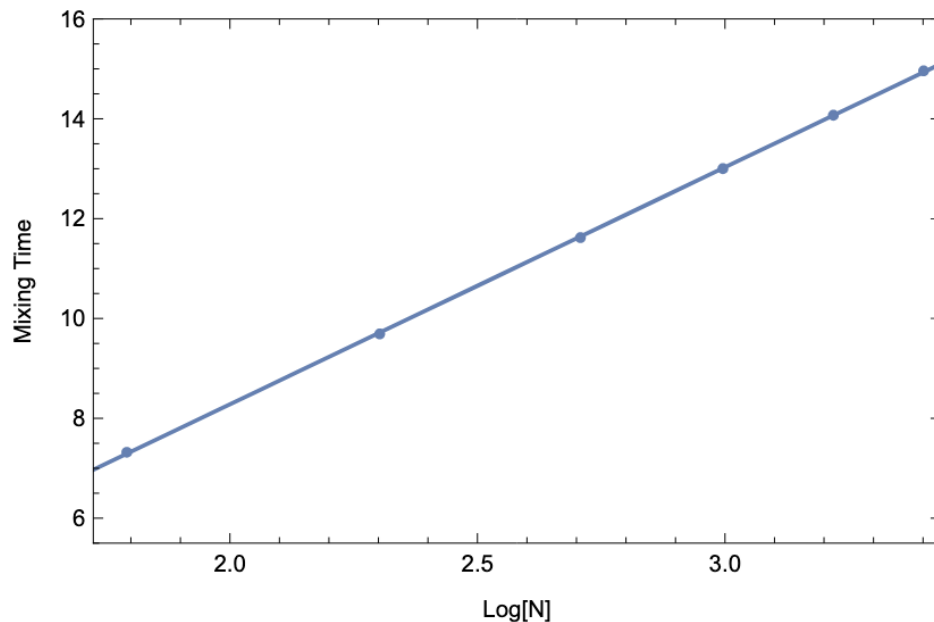
# Rapid mixing of 1D gapped local Hamiltonians

For the Heisenberg model  
in a magnetic field,

$$H = -J \sum_{i=1}^{n-1} X_i X_{i+1} - \Delta \sum_{i=1}^{n-1} (Y_i Y_{i+1} + Z_i Z_{i+1}) - \sum_{i=1}^n g_i Z_i,$$

Our numerical result shows

$$T_{mix} = O(\log N)$$



# Current challenges in proving mixing time



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- It is difficult to improve  $O(\text{poly } N)$  mixing time to  $O(\log N)$ .

Theoretical analysis of mixing time faces many serious difficulties.

# Current challenges in proving mixing time

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- ~~• It is difficult to improve  $O(\text{poly } N)$  mixing time to  $O(\log N)$ .~~

Theoretical analysis of mixing time faces many serious difficulties.

However, our numerical method directly shows strong evidence of rapid mixing in non-commuting Hamiltonians for ground state preparation.

# Mixing time of quantum systems: Existing results

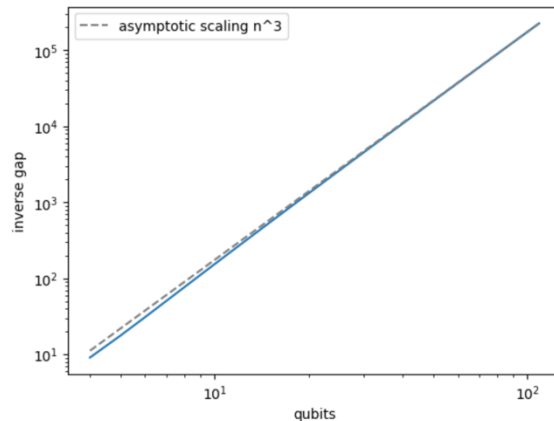
	Commuting	Non-Commuting	
Gibbs state	1D commuting Local Hamiltonian: $O(N) \rightarrow O(\log N)$ 2D toric code: $O(N)$	?	High temperature: $O(N)$
Ground state	1D gapped local Hamiltonian Boundary: $O(\text{poly } N)$ Bulk: $O(\log N)$		

# An interesting observation

- We find that the mixing time of Lindbladian can often be characterized by the non-Hermitian part.

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k \cancel{K_k \rho K_k^\dagger} - \frac{1}{2} \{K_k^\dagger K_k, \rho\}.$$

For boundary dissipative TFIM, the non-Hermitian part also has an  $O(n^{-3})$  gap

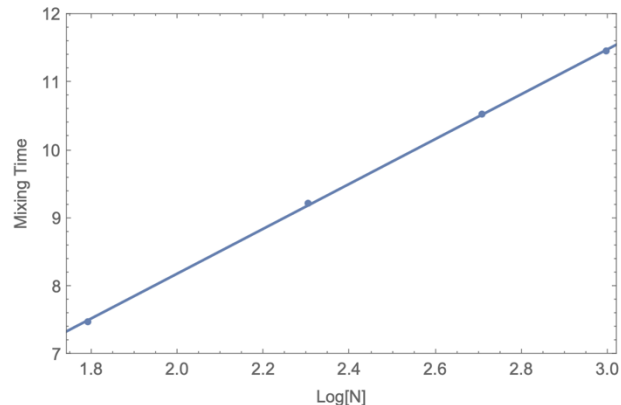


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$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k \cancel{K_k \rho K_k^\dagger} - \frac{1}{2} \{K_k^\dagger K_k, \rho\}.$$

For bulk dissipative TFIM, direct propagation of the non-Hermitian part also shows  $O(\log N)$  mixing time



# Outlook

- Generalize previous results about fast mixing of commuting Hamiltonians to non-commuting ones.
- Numerical simulation of Lindbladian dynamics of 2D local Hamiltonians.
- Quantum advantage in 2D, or even 1D?