arXiv:1705.07597v1 [quant-ph] 22 May 2017

Finite-size scaling of out-of-time-ordered correlators at late times

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May 23, 2017

Abstract

Chaotic dynamics in quantum many-body systems scrambles local information so that at late times it can no longer be accessed locally. This is reflected quantitatively in the out-of-time-ordered correlator of local operators which is expected to decay to zero with time. However, for systems of finite size, out-of-time-ordered correlators do not decay exactly to zero and we show in this paper that the residue value can provide useful insights into the chaotic dynamics. In particular, we show that when energy is conserved, the late-time saturation value of out-of-time-ordered correlators for generic traceless local operators scales inverse polynomially with the system size. This is in contrast to the inverse exponential scaling expected for chaotic dynamics without energy conservation. We provide both analytical arguments and numerical simulations to support this conclusion.

1 Introduction

Non-integrable quantum many-body systems are expected to exhibit 'chaotic' dynamics, which implies not only thermalization but also scrambling of local information into a nonlocal form. In the Heisenberg picture, the support of a local operator A is expected to grow with time under the chaotic dynamics. Such a growth can be reflected in the non-commutativity of $A(t) = e^{iHt}Ae^{-iHt}$ with another local operator B at a different site, which leads to the decay of the out-of-time-ordered correlator (OTOC) $\mathrm{Re}\langle A^\dagger(t)B^\dagger A(t)B\rangle$ [15, 21, 22, 19, 13, 14]. Without loss of generality, here we take A and B to be unitary and get

$$\mathrm{Re}\langle A^\dagger(t)B^\dagger A(t)B\rangle = 1 - \langle [A(t), B][A(t), B]^\dagger\rangle/2 \tag{1}$$

so that when the commutator [...] grows, the OTOC decays. The chaotic nature of the dynamics is reflected in two ways: 1. the fast decay of OTOC away from 1 at relatively short time scales; 2. the approaching of OTOC to 0 at late times. If the dynamics is not chaotic, OTOC may approach a finite value at late times; see, e.g., Refs. [9, 7, 5, 25, 8, 4].

Why does chaotic dynamics result in such decaying behavior of OTOC? While it is not possible to exactly solve the dynamics of non-integrable systems in general, we might be able to extract some universal features, at least in certain limits. For simplicity, let us consider a system of n qubits at infinite temperature so that $\langle ...\rangle = \mathrm{tr}(...)/2^n$. In the limit of $t \to \infty$, a naive way to understand why the OTOC approaches 0 is to assume that after undergoing the chaotic evolution for a sufficiently long time, a local operator A would have support in the whole system and if we expand it in terms of, for example, the Pauli operator basis (σ_0, σ_x, σ_y, σ_z), we would find

$$A(t) = \sum_{k_1,k_2...} a_{k_1,k_2...}\sigma_{k_1}\sigma_{k_2}..., \quad k_i = 0, x, y, z. \tag{2}$$

and we expect that $a_{k_1,k_2,k_3...}$'s behave as uncorrelated random variables for different $k_1, k_2, k_3...$ due to the chaotic nature of the dynamics. As $A(t)$ is unitary, we have

$$\sum_{k_1,k_2...} |a_{k_1,k_2...}|^2 = 1. \tag{3}$$

If we choose B to be a local Pauli operator σ_x on the first spin, then half of the terms in the expansion of $A(t)$ commute with B and half of them do not. We can then estimate the term involving the commutator in Eq. (1) to be

$$\begin{aligned}\langle [A(t), B][A(t), B]^\dagger\rangle &= \Bigg\langle \Bigg(- \sum_{y,k_2...} 2ia_{y,k_2...}\sigma_z\sigma_{k_2}... + \sum_{z,k_2...} 2ia_{z,k_2...}\sigma_y\sigma_{k_2}...\Bigg) \\ &\quad \times \Bigg(- \sum_{y,k_2...} 2ia_{y,k_2...}\sigma_z\sigma_{k_2}... + \sum_{z,k_2...} 2ia_{z,k_2...}\sigma_y\sigma_{k_2}...\Bigg)^\dagger \Bigg\rangle \\ &= 4\sum_{k_2,...} |a_{y,k_2...}|^2 + |a_{z,k_2...}|^2 \approx 4 \times (1/2) = 2. \end{aligned} \tag{4}$$

The approximation step comes from the fact that we are summing over half of the random variables. Plugging this into Eq. (1), we see that the OTOC decays to zero at late times.

Equation (2) is a very simple way to approximate operator evolution at late times in chaotic systems and it may be oversimplified in certain aspects. For example, one major difference between Eq. (2) and $A(t) = e^{iHt}Ae^{-iHt}$ is that the latter preserves the spectrum of A while the former does not. An immediate question that needs to be answered is: how does this discrepancy affect our understanding of OTOC behavior at late times? Is it necessary to use better and more sophisticated approximation method in order to fully capture the essence of chaotic dynamics at late times?

One question we can ask is the scaling of late-time OTOC with the system size. In finite-size systems, it is possible for a generic OTOC to decay to a small yet nonzero value which goes to zero when the system size goes to infinity. Using the approximation in Eq. (2), we might estimate this residue value to be exponentially small in the system size as we are summing over an exponential number of uncorrelated random variables. However, as we are going to show below, this scaling should be inverse polynomial if we use a more careful approximation. In particular, we show that this power law scaling is closely related to the conservation of energy by the time evolution which is not captured by the approximation in Eq. (2).

2 Results

In this section, we introduce basic definitions and then provide a summary of results. All technical details are deferred to the following sections.

Throughout this paper, we make extensive use of asymptotic notations. Let $f, g : \mathbf{R}^+ \to \mathbf{R}^+$ be two positive functions. One writes $f(x) = O(g(x))$ if and only if there exist positive real numbers M, x_0 such that $f(x) \le Mg(x)$ for all $x > x_0$; $f(x) = \Omega(g(x))$ if and only if there exist positive real numbers M, x_0 such that $f(x) \ge Mg(x)$ for all $x > x_0$; $f(x) = \Theta(g(x))$ if and only if there exist positive real numbers M_1, M_2, x_0 such that $M_1 g(x) \le f(x) \le M_2 g(x)$ for all $x > x_0$. For notational simplicity, let $\tilde{O}(f(x)) := O(f(x) \operatorname{poly}\log f(x))$ hide a polylogarithmic factor.

For concreteness, consider a chain of n spin-1/2's with total Hilbert space dimension $d = 2^n$ governed by a translationally invariant local Hamiltonian $H = \sum_{i=1}^n H_i$, where H_i acts on the spin i and its neighbors (short-range interaction). While our discussion is based on a one-dimensional spin system, our results do not rely on the dimensionality of the system or the degrees of freedom being spins. A minor modification of our method leads to similar results in other settings, e.g., fermionic systems in higher spatial dimensions. Without loss of generality, we assume $\operatorname{tr} H_i = 0$ (traceless) and $\|H_i\| \le 1$ (bounded operator norm).

Let A, B, C, D be local (not necessarily unitary) operators with $\|A\| = \|B\| = \|C\| = \|D\| = 1$. The late-time value of OTOC is given by

$$\mathrm{OTOC}(\infty) := \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau \mathrm{d}t \langle AB(t)CD(t)\rangle, \tag{5}$$

where $X(t) = e^{iHt} X e^{-iHt}$ is the time-evolved operator in the Heisenberg picture, and $\langle X\rangle = \frac{1}{d} \operatorname{tr} X$ denotes the expectation value of an operator at infinite temperature.

Let $|1\rangle, |2\rangle, \ldots, |d\rangle$ be a complete set of eigenstates of H with the corresponding energies $E_1 \le E_2 \le \cdots \le E_d$ in non-descending order. Let $X_{jk} = \langle j|X|k\rangle$ be the matrix element of an operator in the energy basis. We propose the following formula for calculating late-time OTOC in strongly chaotic systems:

$$\mathrm{OTOC}(\infty) = \frac{1}{d} \sum_j \langle A, B, C, D\rangle_j + \text{error terms}, \tag{6}$$

where

$$\langle A, B, C, D\rangle_j := (AC)_{jj} B_{jj} D_{jj} + A_{jj} C_{jj} (BD)_{jj} - A_{jj} B_{jj} C_{jj} D_{jj}. \tag{7}$$

Based on this, we are going to argue that

- OTOC $\langle AB(t)A^\dagger B^\dagger(t)\rangle$ for traceless operators A, B vanishes (on average) at late times in the thermodynamic limit $n \to \infty$, where n is the system size;
- for systems of finite size, its saturation value is $\Theta(1/n)$ if either A or B (or both) has a finite overlap with the Hamiltonian H. In particular,

$$\lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau \mathrm{d}t \langle AB(t)A^\dagger B^\dagger(t)\rangle = \frac{\langle BB^\dagger\rangle |\langle HA\rangle|^2 + \langle AA^\dagger\rangle |\langle HB\rangle|^2}{\langle HH_i\rangle n} + \tilde{O}(n^{-1.5}). \tag{8}$$

This is our main result. The remainder of this paper is organized as follows. In Section 3, we provide a heuristic (non-rigorous) derivation of Eq. (6) using techniques from the theory of random unitaries. We begin by reviewing a previous approach, which takes into consideration the unitarity of the Hamiltonian dynamics by approximating e^{-iHt} with a random unitary. Similar to Eq. (2), this approach suggests that the residue value of the late-time OTOC is exponentially small in the system size. Unfortunately, this approximation is still too crude. In particular, we show that once energy conservation is also taken into consideration by requiring the random unitary to act within a small energy window, the scaling of late-time OTOC becomes inverse polynomial in the system size. In Section 4, we take a different approach by assuming a 'generic' spectrum and the eigenstate thermalization hypothesis [6, 23, 18] (both of which are mild assumptions in chaotic systems). Then, we give a fully rigorous proof of Eq. (6) and the two statements itemized above. As shown in Eq. (8), we provide upper bounds (which are not necessarily tight) on the error terms and even work out the prefactor hided in the notation $\Theta(1/n)$ for late-time OTOC. In Section 5, we support our analytical arguments with numerical simulations of a non-integrable spin chain model. The numerical results suggest that the last term in Eq. (8) can be improved to $O(n^{-2})$.

3 Dynamics as random unitary

In this section, we derive Eq. (6) using techniques from random unitary theory. The derivation is not rigorous, but provides a heuristic picture showing the extent to which chaotic dynamics can be approximated by a random unitary.

To improve the approximation in Eq. (2), the first thing one can do is to take into consideration the unitarity of the dynamics. In strongly chaotic systems, it is tempting to expect

Assumption 1. The time evolution operator e^{-iHt} for large t behaves like a random unitary.

Based on this assumption, late-time OTOC can be estimated as

$$\mathrm{OTOC}(\infty) = \int \mathrm{d}U \langle A(U^\dagger BU)C(U^\dagger DU)\rangle, \tag{9}$$

where the unitary U is taken from the unitary group with respect to the Haar measure.

Lemma 1 ([12, 20])**.** *We have*

$$\int \mathrm{d}U \langle A(U^\dagger BU)C(U^\dagger DU)\rangle = \langle A, B, C, D\rangle - \langle AC\rangle_c \langle BD\rangle_c/(d^2-1), \tag{10}$$

where $\langle XY\rangle_c = \langle XY\rangle - \langle X\rangle\langle Y\rangle$ *is the connected correlator and*

$$\langle A, B, C, D\rangle := \langle AC\rangle\langle B\rangle\langle D\rangle + \langle A\rangle\langle C\rangle\langle BD\rangle - \langle A\rangle\langle B\rangle\langle C\rangle\langle D\rangle. \tag{11}$$

Note that the right-hand side of Eq. (7) resembles that of Eq. (11) in the sense of replacing each $\langle\cdots\rangle$ (infinite-temperature average) by $\langle j|\cdots|j\rangle$ (expectation value with respect to eigenstates).

Corollary 1 ([12, 20])**.** *Combining Lemma 1 and Assumption 1, we obtain*

$$\mathrm{OTOC}(\infty) = \langle A, B, C, D\rangle - \langle AC\rangle_c \langle BD\rangle_c/(d^2-1), \tag{12}$$

from which we can immediately see that

- *OTOC* $\langle AB(t)A^\dagger B^\dagger(t)\rangle$ *for traceless operators* A, B *vanish (on average) at late times in the thermodynamic limit* ($d\to\infty$)*;*
- *for systems of finite size, the saturation value of OTOC is exponentially small in the system size (as* d *is exponential in* n*).*

However, we are going to show that the approximation stated in Assumption 1 is still too crude. In particular, we propose a refined version of Assumption 1 by incorporating energy conservation and argue (non-rigorously) that Eq. (6) is an implication of this refinement.

The key idea of the refined assumption is that time evolution does not change the energy while local operators can only change the energy of a state by an order 1 amount. This idea is quantified using the following lemma. Let

$$P(\epsilon, \epsilon') = \sum_{j:\epsilon\le E_j<\epsilon'} |j\rangle\langle j|. \tag{13}$$

be the projector onto the energy window $[\epsilon, \epsilon')$.

Lemma 2 ([1])**.** *Let* $\epsilon < \epsilon'$*. For any local operator* X*,*

$$\|P(-\infty, \epsilon)XP(\epsilon', +\infty)\| \le c\|X\|e^{-(\epsilon'-\epsilon)/\epsilon_0}, \tag{14}$$

where c *and* ϵ_0 *are constants.*

The action of the operator $AB(t)CD(t)$ is then (approximately) restricted to each microcanonical emsemble defined as:

Definition 1 (microcanonical ensemble)**.** A microcanonical ensemble of energy E and bandwidth 2Δ is the set

$$\{|\psi\rangle : |\psi\rangle = P(E-\Delta, E+\Delta)|\psi\rangle\}. \tag{15}$$

This observation motivates the following refinement of Assumption 1 in strongly chaotic systems:

Assumption 2. The time evolution operator e^{-iHt} for large t behaves like a random unitary in each microcanonical ensemble (of constant bandwidth).

Conceptually, this assumption is related to the notion of random diagonal unitaries [17, 16].

Based on Assumption 2, we now argue for Eq. (6). As the bandwidth of H is $\Theta(n)$, we divide the energy spectrum into the disjoint union of $\Theta\left(\frac{n}{2\Delta}\right)$ microcanonical ensembles

$$I = \sum_k P_k, \quad P_k := P((2k-1)\Delta, (2k+1)\Delta), \tag{16}$$

where I is the identity operator, and the bandwidth 2Δ of each microcanonical ensemble is some constant. (Note that it might more precise to take $\Delta = \Theta(\log n)$; see Eq. (18) below. Here we neglect this technical subtlety in order to simplify the physical picture.) Define $[A, B, C, D]_k$ as the right-hand side of Eq. (11) with each $\langle\cdots\rangle$ replaced by the expectation value $\mathrm{tr}(P_k \cdots)/\,\mathrm{tr}\, P_k$ of the maximally mixed state in the microcanonical ensemble. We expect

$$\lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau \mathrm{d}t \frac{\mathrm{tr}(P_k AB(t)CD(t))}{\mathrm{tr}\, P_k} \approx [A, B, C, D]_k \approx \frac{1}{\mathrm{tr}\, P_k} \sum_{j:(2k-1)\Delta\le E_j<(2k+1)\Delta} \langle A, B, C, D\rangle_j. \tag{17}$$

The first step of Eq. (17) is a consequence of Lemma 1 and Assumption 2. Indeed, it is just Eq. (12) restricted to the microcanonical ensemble P_k. The second step of Eq. (17) is a weak variant of the eigenstate thermalization hypothesis which says that eigenstates with similar energies have similar local expectation values. Equation (6) then follows immediately from Eq. (17).

An important subtlety here, which does not appear in Eq. (12), requires further explanation. For an eigenstate $|j\rangle$ in a microcanonical ensemble P_k, $AB(t)CD(t)|j\rangle$ may not be completely in the microcanonical ensemble. However, as long as A, B, C, D are local operators, Lemma 2 implies

$$\|P_k AB(t)CD(t)|j\rangle\| \ge 1 - e^{-\Omega(\min\{E_j-(2k-1)\Delta,(2k+1)\Delta-E_j\})}, \tag{18}$$

i.e., the "leakage" outside the microcanonical ensemble is exponentially small. This is why Eq. (6) requires the locality of A, B, C, D, although Corollary 1 does not.

The argument for the other claim in Section 2 that Eq. (6) implies the $\Theta(1/n)$ scaling of the late-time OTOC $\langle AB(t)A^\dagger B^\dagger(t)\rangle$ with system size is deferred to the next section.

4 Implications of eigenstate thermalization

In this section, we provide an alternative argument for the claims made in Section 2. This argument is fully rigorous assuming a generic spectrum and the eigenstate thermalization hypothesis. In the special case where the local operators in OTOC are the terms in the Hamiltonian, the eigenstate thermalization hypothesis trivially holds and thus we obtain a rigorous proof of the $\Theta(1/n)$ scaling for late-time OTOC assuming only a generic spectrum.

In strongly chaotic systems, we expect that the spectrum satisfies a 'generic' condition that

Assumption 3 (generic spectrum; see, e.g., Ref. [24])**.**

$$E_p + E_r = E_q + E_s \qquad \text{implies} \qquad ((p = q) \text{ and } (r = s)) \quad \text{or} \quad ((p = s) \text{ and } (r = q)). \tag{19}$$

Writing out the matrix elements, it is easy to see

$$\begin{aligned} \langle AB(t)CD(t)\rangle &= \frac{1}{d}\sum_{p,q,r,s} A_{pq}B_{qr}C_{rs}D_{sp}e^{i(E_q-E_r+E_s-E_p)t} \\ \implies \quad \mathrm{OTOC}(\infty) &= \frac{1}{d}\sum_{p,q,r,s} A_{pq}B_{qr}C_{rs}D_{sp}\delta_{E_p+E_r,E_q+E_s}, \end{aligned} \tag{20}$$

where δ is the Kronecker delta function. Assumption 3 implies

$$\mathrm{OTOC}(\infty) = \frac{1}{d}\sum_{j,k} A_{jj}B_{jk}C_{kk}D_{kj} + \frac{1}{d}\sum_{j,k} A_{jk}B_{kk}C_{kj}D_{jj} - \frac{1}{d}\sum_{j} A_{jj}B_{jj}C_{jj}D_{jj}. \tag{21}$$

Consider the following estimate for the first term on the right-hand side of Eq. (21):

$$\begin{aligned} &\frac{1}{d}\sum_{j,k} A_{jj}B_{jk}C_{kk}D_{kj} \approx \frac{1}{d}\sum_{j}\sum_{k:|E_j-E_k|<3\epsilon_0\ln n} A_{jj}B_{jk}C_{kk}D_{kj} \\ \approx\; &\frac{1}{d}\sum_{j}\sum_{k:|E_j-E_k|<3\epsilon_0\ln n} A_{jj}B_{jk}C_{jj}D_{kj} \approx \frac{1}{d}\sum_{j,k} A_{jj}C_{jj}B_{jk}D_{kj} = \frac{1}{d}\sum_{j} A_{jj}C_{jj}(BD)_{jj}. \end{aligned} \tag{22}$$

We now bound the error in each step of this equation chain. Let

$$Q = \sum_{k:|E_j-E_k|\geq 3\epsilon_0\ln n} |k\rangle\langle k|, \quad \tilde{C} = \sum_k C_{kk}|k\rangle\langle k|. \tag{23}$$

As $\tilde{C}$ is the "diagonal part" of C (in the energy basis), it is easy to see $\|\tilde{C}\| \leq \|C\|$. In the first step of Eq. (22), the approximation error can be upper bounded by

$$\begin{aligned} &\frac{1}{d}\left|\sum_{j}\sum_{k:|E_j-E_k|\geq 3\epsilon_0\ln n} A_{jj}B_{jk}C_{kk}D_{kj}\right| \leq \frac{1}{d}\sum_j |A_{jj}|\left|\sum_{k:|E_j-E_k|\geq 3\epsilon_0\ln n} B_{jk}C_{kk}D_{kj}\right| \\ \leq\; &\frac{\|A\|}{d}\sum_j \langle j|BQ\tilde{C}QD|j\rangle \leq \frac{\|A\|}{d}\sum_j \|QB^\dagger|j\rangle\|\|\tilde{C}\|\|QD|j\rangle\| \leq \|A\|\|B\|\|C\|\|D\|O(n^{-3}), \end{aligned} \tag{24}$$

where we used Lemma 2. Note that we considered microcanonical ensembles of bandwidth $\Theta(\log n)$ instead of $\Theta(1)$. This is because by doing so we can rigorously bound the approximation error, as given on the right-hand side of Eq. (14), to be inverse polynomial in n. The approximation error in the third step of Eq. (22) can be controlled similarly.

The second step of Eq. (22) is due to a weak variant of the eigenstate thermalization hypothesis which says that eigenstates with similar energies have similar local expectation values:

Assumption 4 (Eigenstate thermalization in the middle of the spectrum)**.** Let δ be an arbitrarily small positive constant and $1/\operatorname{poly} n$ represent an inverse polynomial of sufficiently high order. For any local operator X with $\|X\| \leq 1$, there is a function $f_X : [-\delta, \delta] \to [-1, 1]$ such that

$$|X_{jj} - f_X(E_j/n)| \leq 1/\operatorname{poly} n \tag{25}$$

for all $|j\rangle$ with $|E_j| \leq \delta n$. Furthermore, we assume that f_X is smooth in the sense of allowing the Taylor expansion to some low order.

It was proposed analytically [24] and supported by numerical simulations [11] that the right-hand side of Eq. (25) can be improved to $e^{-\Omega(n)}$. For our purposes, however, it suffices to assume a (much weaker) inverse polynomial upper bound as in Eq. (25).

The eigenvalues of H are highly concentrated in the sense that

Lemma 3. *Almost all eigenstates have zero energy density:*

$$|\{j : |E_j| \geq n^{0.51}\}|/d \leq O(n^{-0.01m}), \quad \forall m = O(1). \tag{26}$$

Proof. Expanding each term H_i in the Pauli basis, we obtain

$$\frac{1}{d}\sum_j E_j^m = \langle H^m \rangle = \Theta(n^{m/2}) \tag{27}$$

for any even positive integer m. Then, Eq. (26) follows from Markov's inequality. (Note that Eq. (27) is related to the fact that E_j's approach a normal distribution in the thermodynamic limit [10, 3].) □

This lemma allows us to bound the contributions from eigenstates away from the middle of the spectrum, e.g.,

$$\frac{1}{d}\sum_{j:|E_j|\geq n^{0.51}} E_j^2 \leq O(n^{2-0.01m}). \tag{28}$$

For any local operator X,

$$\frac{1}{d}\operatorname{tr} X = \frac{1}{d}\sum_j X_{jj} \approx \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} X_{jj} \approx \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} f_X(0) \approx \frac{1}{d}\sum_j f_X(0) = f_X(0), \tag{29}$$

where we used Eq. (26) in the second and fourth steps. The third step is due to the continuity of $f_X(x)$ at $x = 0$. Taking the limit $n \to \infty$, all errors vanish and thus Eq. (29) is exact. In particular, $f_A(0) = 0$ for any traceless local operator A. Furthermore,

$$\begin{aligned} \frac{1}{d}\operatorname{tr}(HA) &= \frac{1}{d}\sum_j E_j A_{jj} \approx \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} E_j A_{jj} \approx \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} \frac{E_j^2}{n} f'_A(0) \approx \frac{1}{d}\sum_j \frac{E_j^2}{n} f'_A(0) \\ &= \operatorname{tr}(HH_i) f'_A(0)/d, \end{aligned} \tag{30}$$

where we used Eqs. (26) (28) in the second and fourth steps, respectively. In the third step, we used Eq. (25) and the Taylor expansion

$$f_A(E_j/n) = f_A(0) + f'_A(0)E_j/n + f''_A(0)E_j^2/(2n^2) + O(|E_j|^3/n^3) \tag{31}$$

with the approximation error upper bounded by

$$\frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}} \frac{|E_j|^3}{n^2} \leq O(n^{-0.47}). \tag{32}$$

Taking the limit $n \to \infty$, all errors vanish and thus

$$f'_A(0) = \operatorname{tr}(HA)/\operatorname{tr}(HH_i), \tag{33}$$

As the (normalized) overlap between A and the Hamiltonian, $f'_A(0)$ is finite for a generic traceless operator A.

Consider the following estimate:

$$\frac{1}{d}\sum_j |A_{jj}|^2 \approx \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} |A_{jj}|^2 \approx \frac{|f'_A(0)|^2}{d}\sum_{j:|E_j|<n^{0.51}} \frac{E_j^2}{n^2} \approx \frac{|f'_A(0)|^2}{d}\sum_j \frac{E_j^2}{n^2} = \frac{|\operatorname{tr}(HA)|^2}{dn\operatorname{tr}(HH_i)}, \quad (34)$$

where we used Eqs. (26) (28) (33) in the first, third, and fourth steps, respectively. In the second step, we used Eqs. (25) (31) with the approximation error upper bounded by

$$\begin{aligned} &\frac{O(1)}{d}\left|\sum_{j:|E_j|<n^{0.51}} \frac{E_j^3}{n^3}\right| + \frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}} \frac{E_j^4}{n^4} + \frac{1}{\operatorname{poly} n} \approx \frac{O(1)}{d}\left|\sum_j \frac{E_j^3}{n^3}\right| + \frac{O(1)}{d}\sum_j \frac{E_j^4}{n^4} \\ = &\; O(n^{-2}) + O(n^{-2}) = O(n^{-2}), \end{aligned} \quad (35)$$

where we used Eq. (27) and

$$\left|\frac{1}{d}\sum_j E_j^3\right| = |\langle H^3\rangle| = O(n). \quad (36)$$

This is the error of leading order in Eq. (34). Similarly, we have

$$\frac{1}{d}\sum_j |A_{jj}|^4 \approx \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} |A_{jj}|^4 \approx \frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}} \frac{E_j^4}{n^4} \approx \frac{O(1)}{d}\sum_j \frac{E_j^4}{n^4} = O(n^{-2}). \quad (37)$$

Let n be sufficiently large such that $3\epsilon_0 \ln n < \delta n/2$, and define

$$\tilde{C}^{(j)} := \sum_{k:|E_j-E_k|<3\epsilon_0\ln n} (C_{jj} - C_{kk})|k\rangle\langle k|. \quad (38)$$

For j,k such that $|E_j| < \delta n/2$ and $|E_j - E_k| \le 3\epsilon_0 \ln n$, Assumption 4 implies

$$|C_{jj} - C_{kk}| \le |f_C(E_j/n) - f_C(E_k/n)| + 1/\operatorname{poly} n = O(|E_j - E_k|)/n + 1/\operatorname{poly} n. \quad (39)$$

Thus, we have $\|\tilde{C}^{(j)}\| = \tilde{O}(1/n)$ for any j such that $|E_j| < \delta n/2$. The approximation error in the second step of Eq. (22) is upper bounded by

$$\begin{aligned} &\frac{1}{d}\left|\sum_j \sum_{k:|E_j-E_k|<3\epsilon_0\ln n} A_{jj}B_{jk}(C_{jj}-C_{kk})D_{kj}\right| \le \frac{1}{d}\sum_j |A_{jj}|\left|\sum_{k:|E_j-E_k|<3\epsilon_0\ln n} B_{jk}\tilde{C}^{(j)}_{kk}D_{kj}\right| \\ = &\; \frac{1}{d}\sum_j |A_{jj}||\langle j|B\tilde{C}^{(j)}D|j\rangle| \le \frac{1}{d}\sum_j |A_{jj}|\|\tilde{C}^{(j)}\| = \frac{1}{d}\sum_{j:|E_j|<\delta n/2} |A_{jj}|\|\tilde{C}^{(j)}\| \\ &+ \frac{1}{d}\sum_{j:|E_j|\ge\delta n/2} |A_{jj}|\|\tilde{C}^{(j)}\| \le \frac{1}{d}\sum_{j:|E_j|<\delta n/2} |A_{jj}|\tilde{O}(1/n) + \frac{1}{d}\sum_{j:|E_j|\ge\delta n/2} |A_{jj}|O(1) \\ \le &\; \frac{\tilde{O}(1/n)}{d}\sum_j |A_{jj}| + \frac{1}{d}\sum_{j:|E_j|\ge\delta n/2} O(1) \le \tilde{O}(1/n)\sqrt{\frac{1}{d}\sum_j |A_{jj}|^2} + 1/\operatorname{poly} n \le \tilde{O}(n^{-1.5}). \end{aligned} \quad (40)$$

This is the error of leading order in Eq. (22).

Equation (22) shows that the first term on the right-hand side of Eq. (21) corresponds to the second term on the right-hand side of Eq. (7). Similarly, the second term on the right-hand side of Eq. (21) can be approximated by the first term on the right-hand side of Eq. (7). Obviously, the third terms on the right-hand sides of Eqs. (7), (21) are the same. Thus, we obtain Eq. (6) with an error that scales as $\tilde{O}(n^{-1.5})$.

We now show that Eq. (6) implies the $\Theta(1/n)$ scaling of the late-time OTOC $\langle AB(t)A^\dagger B^\dagger(t)\rangle$ with the system size for generic traceless local operators A, B. Specialized to this OTOC, Eq. (6) becomes

$$\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \mathrm{d}t\langle AB(t)A^\dagger B^\dagger(t)\rangle = \frac{1}{d}\sum_j (AA^\dagger)_{jj}|B_{jj}|^2 + |A_{jj}|^2(BB^\dagger)_{jj} - |A_{jj}B_{jj}|^2 + \tilde{O}(n^{-1.5}). \quad (41)$$

Consider the following estimate for the first term on the right-hand side of Eq. (41):

$$\begin{aligned}\frac{1}{d}\sum_j (AA^\dagger)_{jj}|B_{jj}|^2 &\approx \frac{1}{d}\sum_{j:|E_j|<n^{0.51}}(AA^\dagger)_{jj}|B_{jj}|^2 \approx \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} f_{AA^\dagger}(0)|B_{jj}|^2\\ &\approx \frac{f_{AA^\dagger}(0)}{d}\sum_j |B_{jj}|^2 \approx \frac{\mathrm{tr}(AA^\dagger)|\,\mathrm{tr}(HB)|^2}{dn\,\mathrm{tr}(HH_i)},\end{aligned} \quad (42)$$

where we used Eq. (26) in the first and third steps; the continuity of $f_{AA^\dagger}(x)$ at $x=0$ in the second step; Eqs. (29) (34) in the fourth step. The approximation error in the fourth step is upper bounded by $O(n^{-1.96})$ as in Eq. (35). The Taylor expansion for $f_{AA^\dagger}(x)$ at $x=0$ allows us to estimate the approximation error in the second step as

$$\begin{aligned}&\frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}}\frac{|B_{jj}|^2E_j}{n} + \frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}}\frac{|B_{jj}|^2E_j^2}{n^2} + \frac{1}{\mathrm{poly}\,n} \approx \frac{O(1)}{d}\left|\sum_{j:|E_j|<n^{0.51}}\frac{E_j^3}{n^3}\right|\\ &+\frac{1}{d}\sum_{j:|E_j|<n^{0.51}}\frac{E_j^4}{n^4} + \frac{O(n^{-0.98})}{d}\sum_{j:|E_j|<n^{0.51}}|B_{jj}|^2 \approx \frac{O(1)}{d}\left|\sum_j\frac{E_j^3}{n^3}\right| + \frac{1}{d}\sum_j\frac{E_j^4}{n^4} + O(n^{-1.98})\\ &\approx O(n^{-2}) + O(n^{-2}) + O(n^{-1.98}) = O(n^{-1.98}),\end{aligned} \quad (43)$$

where we used the Taylor expansion for $f_B(x)$ at $x=0$ in the first step; Eqs. (26) (34) in the second step; Eqs. (27) (36) in the third step. The second term on the right-hand side of Eq. (41) can be estimated similarly as we did in Eq. (42). The third term on the right-hand side of Eq. (41) is upper bounded by

$$\frac{1}{d}\sum_j |A_{jj}B_{jj}|^2 \le \frac{1}{2d}\sum_j |A_{jj}|^4 + |B_{jj}|^4 \le O(n^{-2}), \quad (44)$$

where we used Eq. (37). Thus, we have proved Eq. (8) based on Assumptions 3, 4. This completes the argument for all the claims made in Section 2.
□

In the special case where the local operators in OTOC are the terms in the Hamiltonian, the eigenstate thermalization hypothesis (Assumption 4) trivially holds and thus we obtain a rigorous proof of the $\Theta(1/n)$ scaling assuming only a generic spectrum.

Note that given H, there are multiple ways of writing it as the sum of local terms: $H=\sum_i H_i$. For simplicity, we fix this ambiguity by expanding H in the Pauli basis and assigning all Pauli string operators stating at the site i to H_i (see Eq. (52) as an example). This convention implies $\mathrm{tr}(H_jH_k)=0$ for $j\neq k$ and hence $\langle H_i^2\rangle = \langle HH_i\rangle = \langle H^2\rangle/n$. Using this convention,

Theorem 1. *Assumption 3 implies*

$$\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \mathrm{d}t\langle H_1H_i(t)H_1H_i(t)\rangle = 2\langle H_i^2\rangle^2/n + O(n^{-2}). \tag{45}$$

Proof. We provide two slightly different proofs of this theorem. Both proofs make use of the fact that $(H_i)_{jj} = E_j/n$ for any i due to translational invariance.

In the first proof, we follow the argument given above, and observe that the analog of Eq. (41)

$$\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \mathrm{d}t\langle H_1H_i(t)H_1H_i(t)\rangle = \frac{1}{d}\sum_j 2(H_i^2)_{jj}(E_j/n)^2 - (E_j/n)^4 + \tilde{O}(n^{-1.5}) \tag{46}$$

can be established rigorously. In Eq. (22), the first and third steps are already rigorous with errors inverse polynomial in n. In the second step of Eq. (22), we use the eigenstate thermalization hypothesis (Assumption 4), which trivially holds for the terms in the Hamiltonian. In particular, we take

$$f_{H_i}(x) = x. \tag{47}$$

The first term on the right-hand side of Eq. (46) is equal to

$$\frac{2}{dn^2}\sum_j (H_i^2)_{jj}E_j^2 = \frac{2}{dn^2}\sum_j (H_i^2H^2)_{jj} = \frac{2}{dn^2}\operatorname{tr}(H_i^2H^2). \tag{48}$$

The remainder of the first proof is essentially the same as the "second half" of the second proof given below. It should be noted that the error term in the first proof is $\tilde{O}(n^{-1.5})$, which is slightly worse than $O(n^{-2})$ as in Eq. (45).

The second proof is more direct. For the present choice of local operators in OTOC, the first term on the right-hand side of Eq. (21) reads

$$\begin{aligned}
&\frac{1}{d}\sum_{j,k=1}^{d}(H_1)_{jj}(H_i)_{jk}(H_1)_{kk}(H_i)_{kj} = \frac{1}{dn^2}\sum_{j,k=1}^{d}E_j\langle j|H_i|k\rangle E_k\langle k|H_i|j\rangle \\
&= \frac{1}{dn^2}\operatorname{tr}\left(\sum_{j=1}^{d}|j\rangle E_j\langle j|H_i\sum_{k=1}^{d}|k\rangle E_k\langle k|H_i\right) = \frac{\operatorname{tr}(HH_iHH_i)}{dn^2} = \frac{1}{n^2}\sum_{j,k=1}^{n}\langle H_jH_iH_kH_i\rangle.
\end{aligned} \tag{49}$$

There are n^2 terms in the last summation. However, most of them are zero because $\operatorname{tr}H_j = \operatorname{tr}H_k = 0$. Furthermore, the convention specified above implies $\operatorname{tr}(H_jH_k) = 0$ for $j \neq k$. Thus, we see that the number of non-vanishing terms in the last summation of Eq. (49) is $n + \Theta(1)$ (n comes from the terms with $j = k$ and $\Theta(1)$ accounts for the remainder). Equation (49) is equal to

$$\frac{1}{n^2}\sum_{j=1}^{n}\langle H_jH_iH_jH_i\rangle + O(1/n^2) = \langle H_i^2\rangle^2/n + O(1/n^2) + O(1/n^2) = \langle H_i^2\rangle^2/n + O(1/n^2). \tag{50}$$

The second term on the right-hand side of Eq. (21) gives the same result. The last term on the right-hand side of Eq. (21) is

$$\frac{1}{dn^4}\sum_j E_j^4 = \Theta(n^{-2}), \tag{51}$$

where we used Eq. (27) for $m = 4$. Therefore, we obtain Eq. (45). □

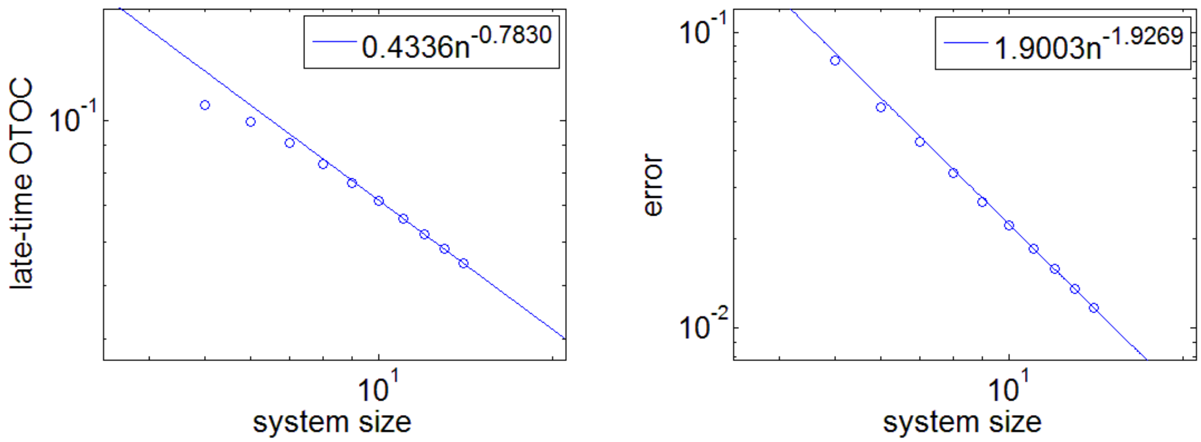

Figure 1: Left panel: Finite-size scaling of the late-time OTOC F_n for $n = 5, 6, \ldots, 14$. The line is a power-law fit $0.4336n^{-0.7830}$ for the last few data points. It noticeably deviates from the leading term $G_n := (14/15)n^{-1} \approx 0.9333n^{-1}$ of the theoretical calculation Eq. (8) due to finite-size effects. Right panel: Finite-size scaling of the error $G_n - F_n$ for $n = 5, 6, \ldots, 14$. The line is a power-law fit $1.9003n^{-1.9269}$ for the last few data points. We conjecture that the error should scale as $\Theta(n^{-2})$ in the thermodynamic limit $n \to \infty$.

5 Numerics

In this section, we support Eq. (8) with numerical simulations. Consider the spin-1/2 chain

$$H = \sum_{i=1}^{n} H_i, \quad H_i := \sigma_i^z \sigma_{i+1}^z - 1.05\sigma_i^x + 0.5\sigma_i^z + g\sigma_i^y \sigma_{i+1}^z \tag{52}$$

with periodic boundary conditions ($\sigma_{n+1}^z := \sigma_1^z$), where $\sigma_i^x, \sigma_i^y, \sigma_i^z$ are the Pauli matrices at the site i. For $g = 0$, this model is non-integrable in the sense of Wigner-Dyson level statistics [2]. Reference [19] calculated OTOC, but the focus there is the butterfly effect rather than the late-time behavior. It should be noted that for $g = 0$, most energy levels are two-fold degenerate so that Assumption 3 does not hold.

We take $g = 0.1$. Intuitively, the model is non-integrable for any value of g. We numerically confirmed the validity of Assumption 3 for $n = 5, 6, \ldots, 12$ (for larger n, it is necessary to perform high precision computations). Presumably, Assumption 3 holds for any integer $n \geq 5$. Let

$$F_n = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \mathrm{d}t \frac{1}{n} \sum_{i=1}^{n} \langle \sigma_1^x \sigma_i^x(t) \sigma_1^x \sigma_i^x(t) \rangle. \tag{53}$$

We use exact diagonalization and compute the integral in F by averaging over a sufficient number of randomly sampled t until convergence is clearly observed. The results are shown in Fig. 1.

6 Conclusion

In summary, we propose that in order to better approximate late-time behavior of chaotic dynamics generated by a time-independent Hamiltonian, one needs to take into account the conservation of energy. In particular, we show that approximation schemes with and without energy conservation make different predictions regarding OTOC at late times: without energy conservation, late-time OTOC scales inverse exponentially with system size; with energy conservation, the scaling becomes inverse polynomial. The latter prediction has been confirmed rigorously based on a few physically reasonable assumptions and is consistent with numerical simulation of a non-integrable spin chain model.

Of course, one open problem regarding the energy preserving approximation schemes discussed in this paper is that how good they are in terms of predicting, for example, the behavior of higher-order time-ordered or out-of-time-ordered correlators. Furthermore, it is not clear how to approximate the time evolution process of the chaotic dynamics and capture universal features like the early-time exponential decay of OTOC. These are interesting questions for future study.

Acknowledgments

We would like to thank Xie Chen, Yingfei Gu, Nick Hunter-Jones, Alexei Y. Kitaev, and Douglas Stanford for helpful discussions. We are especially grateful to X.C., who wrote a substantial portion of this paper. We acknowledge funding provided by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center (NSF Grant PHY-1125565) with support of the Gordon and Betty Moore Foundation (GBMF-2644). Additional funding support was provided by NSF DMR-1654340 (Y.H., Y.-L.Z.).

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