Bound on the exponential growth rate of out-of-time-ordered correlators

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(Received 28 August 2017; revised manuscript received 27 May 2018; published 30 July 2018)

It has been conjectured by Maldacena, Shenker, and Stanford [J. Maldacena, S. H. Shenker, and D. Stanford, J. High Energy Phys. 08 (2016) 106] that the exponential growth rate of the out-of-time-ordered correlator (OTOC) $F(t)$ has a universal upper bound $2\pi k_B T/\hbar$. Here we introduce a one-parameter family of out-of-time-ordered correlators $F_\gamma(t)$ $(0 \leqslant \gamma \leqslant 1)$, which has as good properties as $F(t)$ as a regularization of the out-of-time-ordered part of the squared commutator $\langle[\hat{A}(t), \hat{B}(0)]^2\rangle$ that diagnoses quantum many-body chaos, and coincides with $F(t)$ at $\gamma = 1/2$. We rigorously prove that if $F_\gamma(t)$ shows a transient exponential growth for all γ in $0 \leqslant \gamma \leqslant 1$, that is, if the OTOC shows an exponential growth regardless of the choice of the regularization, then the growth rate λ does not depend on the regularization parameter γ and satisfies the inequality $\lambda \leqslant 2\pi k_B T/\hbar$.

DOI: 10.1103/PhysRevE.98.012216

I. INTRODUCTION

Chaos in classical systems is characterized by the Lyapunov exponent, which represents the exponential growth rate of the distance between different classical orbits that initially lie in the immediate vicinity of each other in phase space. The phenomenon in which a tiny change in the initial condition blows up exponentially in time is known as the butterfly effect. A quantum analog of the Lyapunov exponent has attracted much interest recently, and is given by an out-of-time-ordered correlator (OTOC) [1], a four-point correlation function such as $\langle\hat{A}(t)\hat{B}(0)\hat{A}(t)\hat{B}(0)\rangle$ that does not obey the usual time-ordering rule. Such a correlator arises from the squared commutator $-\langle[\hat{A}(t), \hat{B}(0)]^2\rangle$, which is a second moment of the variation of the operator $\hat{A}$ at time t against a perturbation of a force $\hat{B}$ at time 0, and represents the sensitivity of the time-evolving observable to the initial perturbation. If the OTOC grows exponentially in time, the growth rate of the OTOC is expected to play a role similar to that of the Lyapunov exponent in quantum many-body systems [2,3].

Recently, a remarkable conjecture has been made by Maldacena, Shenker, and Stanford (MSS) [3] to the effect that in thermal equilibrium there exists a universal upper bound on the exponential growth rate λ of the OTOCs

$$\lambda \leqslant \frac{2\pi k_B T}{\hbar}, \tag{1}$$

where k_B is the Boltzmann constant, T is the temperature of the system, and $\hbar$ is the Planck constant. Precisely speaking, they introduce an OTOC of the form

$$F(t) \equiv \mathrm{Tr}[\hat{\rho}^{\frac{1}{4}}\hat{A}(t)\hat{\rho}^{\frac{1}{4}}\hat{B}(0)\hat{\rho}^{\frac{1}{4}}\hat{A}(t)\hat{\rho}^{\frac{1}{4}}\hat{B}(0)], \tag{2}$$

where $\hat{\rho} = e^{-\beta\hat{H}}/Z$ is the thermal density-matrix operator, $\beta = 1/k_B T$ is the inverse temperature, $\hat{H}$ is the Hamiltonian, $Z = \mathrm{Tr}(e^{-\beta\hat{H}})$ is the partition function, and $\hat{A}$ and $\hat{B}$ are arbitrary Hermitian operators. They focus on a situation where there is a clear separation between the dissipation time at which a usual time-ordered correlator decays to a constant and the scrambling time (or the Ehrenfest time) until which an OTOC grows exponentially. Let us suppose that the OTOC (2) shows an exponential growth

$$F(t) = c_0 - \epsilon c_1 e^{\lambda t} + O(\epsilon^2), \quad (c_1, \lambda > 0), \tag{3}$$

with time t well after the dissipation time but before the scrambling time. Here ϵ is a certain small positive expansion parameter such as $\hbar^2$ in the semiclassical approximation or $1/N^2$ in large-N theories. Then the MSS conjecture states that λ always satisfies the inequality (1) regardless of the choices of $\hat{A}$ and $\hat{B}$ and the details of $\hat{H}$. In this sense, the bound is completely universal, and is thought to be a fundamental property of quantum systems. It may be viewed as a refinement of the fast scrambling conjecture [4]. Several examples are known to saturate the bound (1), including black holes in Einstein gravity [3,5–7] and the Sachdev-Ye-Kitaev model [2,8–10]. Various analytical as well as numerical calculations have been performed for the growth rate of OTOCs in many different systems [11–22]. No clear counterexample that violates the bound (1) has been presented so far.

The motivation to consider $F(t)$ in Eq. (2) rather than the squared commutator is that in quantum field theory $\langle[\hat{A}(t), \hat{B}(0)]^2\rangle = \mathrm{Tr}(\hat{\rho}[\hat{A}(t), \hat{B}(0)]^2)$ is not necessarily well-defined since two operators can approach in time arbitrarily close to each other. A convenient prescription is to regularize it as $\mathrm{Tr}(\hat{\rho}^{\frac{1}{2}}[\hat{A}(t), \hat{B}(0)]\hat{\rho}^{\frac{1}{2}}[\hat{A}(t), \hat{B}(0)])$ [3], which is called the bipartite OTOC [23]. The difference between the squared commutator and the bipartite OTOC, $\mathrm{Tr}(\hat{\rho}[\hat{A}(t), \hat{B}(0)]^2) - \mathrm{Tr}(\hat{\rho}^{\frac{1}{2}}[\hat{A}(t), \hat{B}(0)]\hat{\rho}^{\frac{1}{2}}[\hat{A}(t), \hat{B}(0)])$, can be expressed in terms of the Wigner-Yanase (WY) skew information defined by $I_{\frac{1}{2}}(\hat{\rho}, \hat{O}) \equiv \mathrm{Tr}(\hat{\rho}\hat{O}^2) - \mathrm{Tr}(\hat{\rho}^{\frac{1}{2}}\hat{O}\hat{\rho}^{\frac{1}{2}}\hat{O})$ for a Hermitian operator $\hat{O}$ [23,24]. The WY skew information is known as an information-theoretic measure of quantum fluctuations. In the semiclassical regime of our interest (i.e., before the scrambling time), we expect that the difference of the skew information is expected to be suppressed. The out-of-time-ordered ($ABAB$

and $BABA$) part of the bipartite OTOC is defined by

$$F_0(t) \equiv \frac{1}{2}\mathrm{Tr}[\hat{\rho}^{\frac{1}{2}}\hat{A}(t)\hat{B}(0)\hat{\rho}^{\frac{1}{2}}\hat{A}(t)\hat{B}(0)] + \frac{1}{2}\mathrm{Tr}[\hat{\rho}^{\frac{1}{2}}\hat{B}(0)\hat{A}(t)\hat{\rho}^{\frac{1}{2}}\hat{B}(0)\hat{A}(t)]. \quad (4)$$

$F(t)$ in Eq. (2) may be viewed as a variant of the regularization of the out-of-time-ordered part of the squared commutator. As we will see below, $F(t)$ and $F_0(t)$ are related to each other through the analytic continuation into the complex time domain [see Eq. (15)].

The growth of the commutator is bounded by the Lieb-Robinson bound [25–28], which gives a fundamental limit on the spread of information: $\|[\hat{A}_{\boldsymbol{x}}(t), \hat{B}_{\boldsymbol{y}}(0)]\| \leqslant c\|\hat{A}\|\,\|\hat{B}\|e^{-(|\boldsymbol{x}-\boldsymbol{y}|-vt)/\xi}$. Here $\hat{A}$ and $\hat{B}$ are local operators inserted at positions $\boldsymbol{x}$ and $\boldsymbol{y}$, respectively; $\|\cdot\|$ represents the operator norm; and c, v, and ξ are some constants that depend on the Hamiltonian, $\hat{A}$, and $\hat{B}$. In contrast to the growth rate v/ξ in the Lieb-Robinson bound, the conjectured bound for λ in Eq. (1) depends on the state of the quantum system, and the state dependence of the bound appears only through the thermodynamic temperature (the relation between the Lieb-Robinson bound and the quantum butterfly effect was discussed in Refs. [13,29,30]). Thus the bound (1) constitutes a novel fundamental limit on information spreading in general quantum systems.

A compelling argument was given in Ref. [3] to establish the conjecture (1). The original derivation uses analytic properties of $F(z)$ [analytic continuation of $F(t)$ to complex time z], and assumes a factorization of a time-ordered correlation functions

$$\mathrm{Tr}[\hat{\rho}^{\frac{1}{2}}\hat{A}(t)\hat{B}(0)\hat{\rho}^{\frac{1}{2}}\hat{B}(0)\hat{A}(t)] \leqslant \mathrm{Tr}[\hat{\rho}^{\frac{1}{2}}\hat{A}(t)\hat{\rho}^{\frac{1}{2}}\hat{A}(t)] \times \mathrm{Tr}[\hat{\rho}^{\frac{1}{2}}\hat{B}(0)\hat{\rho}^{\frac{1}{2}}\hat{B}(0)] + \varepsilon, \quad (\forall t \geqslant t_0), \quad (5)$$

with a small constant ε and time t_0. Note that ε is different from the expansion parameter ϵ for $F(t)$. The factorization (5) has not been proved but used as a physical input [3]. We remark that the assumption (5) is a bit too strong for the present purpose since (5) requires the factorization for *all the time after* t_0 whereas the exponential growth of our interest occurs only up to a finite scrambling time. There is also a subtle issue concerning the Poincaré recurrence that may invalidate the factorization (5) at very long time [3]. It is desirable that one avoid assuming the factorization and make the argument restricted to within a finite time.

The purpose of the present work is to rigorously prove without assuming the factorization (5) that the inequality (1) holds true if the OTOC shows a transient exponential growth over a certain range of time *irrespective of the way to regularize the squared commutator*. There are not only $F(t)$ in Eq. (2) and $F_0(t)$ in Eq. (4), but in fact, infinitely many other possible ways to regularize $\langle[\hat{A}(t), \hat{B}(0)]^2\rangle$. Here we introduce a one-parameter family of OTOCs $F_\gamma(t)$ $(0 \leqslant \gamma \leqslant 1)$ [see Eq. (6)] that interpolates between $F_0(t) = F_{\gamma=0}(t) = F_{\gamma=1}(t)$ and $F(t) = F_{\gamma=\frac{1}{2}}(t)$. We show that $F_\gamma(t)$ has as good properties as $F(t)$ in Eq. (2) and $F_0(t)$ in Eq. (4) as a regularization of the out-of-time-ordered part of $\langle[\hat{A}(t), \hat{B}(0)]^2\rangle$. If the exponential growth of the OTOC is physically meaningful (or universal), it should not depend on the choice of the regularization. Hence it is reasonable to require that all the members in the one-parameter family of the OTOCs $F_\gamma(t)$ $(0 \leqslant \gamma \leqslant 1)$ grow exponentially in time. Under this requirement, we rigorously prove the existence of the bound (1) on the exponential growth rate of the OTOCs.

The rest of the paper is organized as follows. In Sec. II, we introduce a one-parameter family of OTOCs that make as much sense as $F(t)$ in Eq. (2) and $F_0(t)$ in Eq. (4) as a regularization of the out-of-time-ordered part of the squared commutator. In Sec. III, we describe the statement of the main theorem in this paper that claims the existence of the bound on the exponential growth rate of OTOCs, and prove it. In Sec. IV, we generalize the theorem for the bound on the exponential growth rate to higher-order OTOCs. In Sec. V, we discuss various issues related to the theorem and its proof. In Sec. VI, we summarize the paper.

II. ONE-PARAMETER FAMILY OF OTOCS

We introduce a one-parameter family of OTOCs

$$F_\gamma(t) \equiv \frac{1}{2}\mathrm{Tr}[\hat{\rho}^{\frac{1-\gamma}{2}}\hat{A}(t)\hat{\rho}^{\frac{\gamma}{2}}\hat{B}(0)\hat{\rho}^{\frac{1-\gamma}{2}}\hat{A}(t)\hat{\rho}^{\frac{\gamma}{2}}\hat{B}(0)] + \frac{1}{2}\mathrm{Tr}[\hat{\rho}^{\frac{1-\gamma}{2}}\hat{B}(0)\hat{\rho}^{\frac{\gamma}{2}}\hat{A}(t)\hat{\rho}^{\frac{1-\gamma}{2}}\hat{B}(0)\hat{\rho}^{\frac{\gamma}{2}}\hat{A}(t)] \quad (6)$$

for $0 \leqslant \gamma \leqslant 1$. We note that $F_\gamma(t)$ is symmetric around $\gamma = \frac{1}{2}$ [i.e., $F_\gamma(t) = F_{1-\gamma}(t)$], and agrees with $F_0(t)$ (4) at $\gamma = 0, 1$ and $F(t)$ (2) at $\gamma = \frac{1}{2}$. This form of the OTOC appears in the study of the out-of-time-order fluctuation-dissipation theorem [23]. If one defines

$$C^{\gamma}_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}}(t,0) \equiv \mathrm{Tr}[\hat{\rho}^{\frac{1-\gamma}{2}}(\hat{A}(t)\hat{\rho}^{\frac{\gamma}{2}}\hat{B}(0) + \alpha_1\hat{B}(0)\hat{\rho}^{\frac{\gamma}{2}}\hat{A}(t)) \times \hat{\rho}^{\frac{1-\gamma}{2}}(\hat{A}(t)\hat{\rho}^{\frac{\gamma}{2}}\hat{B}(0) + \alpha_2\hat{B}(0)\hat{\rho}^{\frac{\gamma}{2}}\hat{A}(t))], \quad (7)$$

where $\alpha_1, \alpha_2 = \pm$ and $[,]_{-(+)} = [,]$ $(\{,\})$ is the (anti)commutator, then $4F_\gamma(t) = C^{\gamma}_{\{A,B\}^2}(t,0) + C^{\gamma}_{[A,B]^2}(t,0)$ coincides with the inverse Fourier transform of the left-hand side of the out-of-time-order fluctuation-dissipation theorem [23]

$$C^{\gamma}_{\{A,B\}^2}(\omega) + C^{\gamma}_{[A,B]^2}(\omega) = 2\coth\left((1-2\gamma)\frac{\beta\hbar\omega}{4}\right)C^{\gamma}_{\{A,B\}[A,B]}(\omega). \quad (8)$$

Here $C^{\gamma}_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}}(\omega) \equiv \int_{-\infty}^{\infty} dt\, e^{i\omega t} C^{\gamma}_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}}(t,0)$ is the Fourier transform of Eq. (7). In other words, $F_\gamma(t)$ corresponds to the "fluctuation" part of the fluctuation-dissipation relation.

Each term in the OTOCs can be represented as a contour-ordered function

$$\frac{1}{Z}\mathrm{Tr}[\mathcal{T}_{\mathcal{C}} e^{-\frac{i}{\hbar}\int_{\mathcal{C}} dz \hat{H}(z)}\hat{A}(z_1)\hat{B}(z_2)\hat{A}(z_3)\hat{B}(z_4)], \quad (z_i \in \mathbb{C}), \quad (9)$$

where the contour $\mathcal{C}$ has double-folded branches [3,31–33] in the complex time domain as depicted in Fig. 1, and $\mathcal{T}_{\mathcal{C}}$ is the contour-ordering operator defined along $\mathcal{C}$. The positions

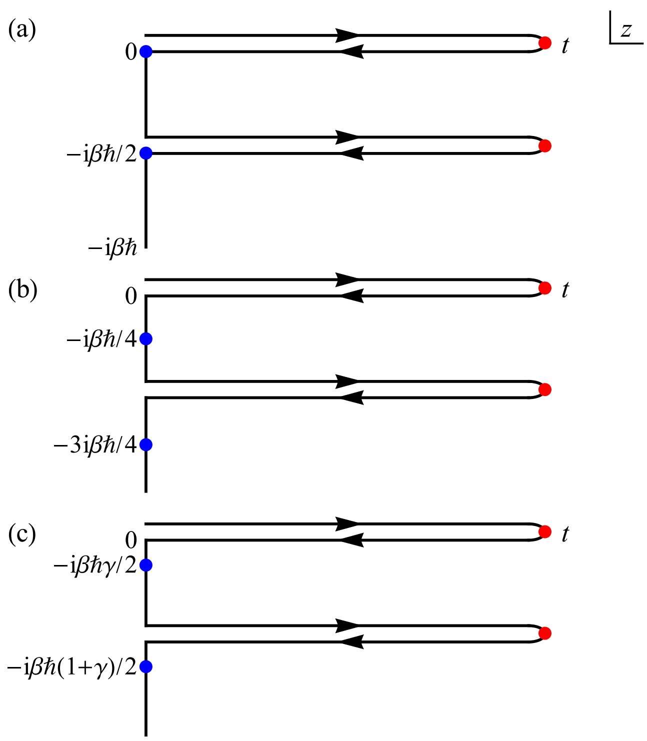

FIG. 1. Positions of the operators $\hat{A}(z)$ $[\hat{B}(z)]$ inserted along the contour $\mathcal{C}$ in the complex time domain represented by red dots on $\mathrm{Re}(z) = t$ [blue dots on $\mathrm{Re}(z) = 0$] for (a) the bipartite OTOC $F_0(t)$, (b) the symmetric OTOC $F(t) = F_{\frac{1}{2}}(t)$, and (c) the generalized OTOC $F_\gamma(t)$ $(0 \leqslant \gamma \leqslant 1)$.

of the operators inserted along the contour $\mathcal{C}$ are shown for $F_0(t)$, $F(t) = F_{\frac{1}{2}}(t)$, and $F_\gamma(t)$ in Figs. 1(a), 1(b), and 1(c), respectively.

The one-parameter family of the OTOC $F_\gamma(t)$ $(0 \leqslant \gamma \leqslant 1)$ (6) has as good properties as $F(t)$ as a regularization of the out-of-time-ordered part of $\langle[\hat{A}(t), \hat{B}(0)]^2\rangle$. First, $F_\gamma(t)$ is real if $\hat{A}$ and $\hat{B}$ are Hermitian. Hence it makes sense to discuss the sign of the variation of $F_\gamma(t)$, which plays an important role below. Second, $F_\gamma(t)$ smoothly interpolates between $F_0(t)$ in Eq. (4) and $F(t) = F_{\frac{1}{2}}(t)$ in Eq. (2), corresponding to the continuous shift of the positions of the operators inserted on the imaginary-time axis from Figs. 1(a) to 1(b) through 1(c). Third, $F_\gamma(t)$ is the out-of-time-ordered ($ABAB$ and $BABA$) part of $\frac{1}{2}C^\gamma_{[A,B]^2}(t,0)$, which is a generalization of the squared commutator. If one defines a generalized commutator as

$$[\hat{A}, \hat{B}]_\gamma \equiv \hat{A}\hat{\rho}^{\frac{\gamma}{2}}\hat{B} - \hat{B}\hat{\rho}^{\frac{\gamma}{2}}\hat{A}, \quad (0 \leqslant \gamma \leqslant 1), \tag{10}$$

then the bracket $[\cdot,\cdot]_\gamma$ satisfies the bilinearity $[a\hat{A} + b\hat{B}, \hat{C}]_\gamma = a[\hat{A}, \hat{C}]_\gamma + b[\hat{B}, \hat{C}]_\gamma$ and $[\hat{C}, a\hat{A} + b\hat{B}]_\gamma = a[\hat{C}, \hat{A}]_\gamma + b[\hat{C}, \hat{B}]_\gamma$ $(a, b \in \mathbb{C})$, the alternativity $[\hat{A}, \hat{A}]_\gamma = 0$, and the Jacobi identity $[\hat{A}, [\hat{B}, \hat{C}]_\gamma]_\gamma + [\hat{B}, [\hat{C}, \hat{A}]_\gamma]_\gamma + [\hat{C}, [\hat{A}, \hat{B}]_\gamma]_\gamma = 0$. Hence the bracket $[\cdot,\cdot]_\gamma$ satisfies the axiom of the commutator (or the Lie algebra). If $\hat{A}$ and $\hat{B}$ are Hermitian, then the generalized commutator $[\hat{A}, \hat{B}]_\gamma$ is skew-Hermitian, i.e., $([\hat{A}, \hat{B}]_\gamma)^\dagger = -[\hat{A}, \hat{B}]_\gamma$. We note that $C^\gamma_{[A,B]^2}(t,0)$ can be expressed as $C^\gamma_{[A,B]^2}(t,0) = \mathrm{Tr}(\hat{\rho}^{\frac{1-\gamma}{2}}[\hat{A}(t), \hat{B}(0)]_\gamma \hat{\rho}^{\frac{1-\gamma}{2}}[\hat{A}(t), \hat{B}(0)]_\gamma)$, which contains two generalized commutators. Since $C^\gamma_{[A,B]^2}(t,0)$ can be viewed as the trace of the square of the skew-Hermitian operator, it is negative semidefinite, $C^\gamma_{[A,B]^2}(t,0) \leqslant 0$, as is the case for the squared commutator $\langle[\hat{A}(t), \hat{B}(0)]^2\rangle$. Therefore, if $C^\gamma_{[A,B]^2}(t,0)$ grows exponentially in such a manner that the initial-perturbation sensitivity increases, it should grow to the negative direction. Since the exponential growth of our interest arises from the out-of-time-ordered ($ABAB$ and $BABA$) part [3], $F_\gamma(t)$ in Eq. (6) should also grow to the negative direction. This is why we require that $F_\gamma(t) = c_0(\gamma) - \epsilon c_1(\gamma) e^{\lambda(\gamma)t} + O(\epsilon^2)$ with $c_1(\gamma) \geqslant 0$ for $0 \leqslant \gamma \leqslant 1$.

There is a heuristic argument that supports the bound (1) from the out-of-time-order fluctuation-dissipation theorem (8). If $F_0(t)$ in Eq. (4) grows exponentially as $F_0(t) = c_0 - \epsilon c_1 e^{\lambda t}$, then it follows from the relation (8) that $C^\gamma_{\{A,B\}[A,B]}(t,0) = 2i \tan(\frac{\beta\hbar}{4}\partial_t) F_0(t) = -2i\epsilon c_1 \tan(\frac{\beta\hbar\lambda}{4}) e^{\lambda t}$. In Ref. [23], we showed that $C^\gamma_{\{A,B\}[A,B]}(t,0)$ corresponds to a certain nonlinear response function, $C^\gamma_{\{A,B\}[A,B]}(t,0) \sim \frac{i}{2} L^{(3)}_{(AB)^2}(t)$ (up to the difference of the skew information). This implies that $L^{(3)}_{(AB)^2}(t) \sim -4\epsilon c_1 \tan(\frac{\beta\hbar\lambda}{4}) e^{\lambda t}$. Here we notice that should λ exceed the bound $\frac{2\pi}{\beta\hbar}$, something strange would happen: The sign of the response function $L^{(3)}_{(AB)^2}(t)$ changes. Usually, we expect that response functions have definite signs (e.g., spins align under a magnetic field in a definite direction, or current flows under a dc electric field in a definite direction). Here the direction of the exponential sensitivity against perturbations would be reversed, which is unlikely to happen. Although this argument is not rigorous, it serves as a hint to focus on the sign of the exponential growth of OTOCs, which turns out to be a key to our proof.

III. BOUND ON THE EXPONENTIAL GROWTH RATE OF OTOCS

Now we describe the statement of the main theorem that gives a rigorous bound on the exponential growth rate for the OTOCs, and prove it in two ways: One is to use a differential equation, and the other is to use analytic continuation.

Theorem. If the one-parameter family of the OTOC $F_\gamma(t)$ $(0 \leqslant \gamma \leqslant 1)$ in Eq. (6) for Hermitian operators $\hat{A}$ and $\hat{B}$ has a uniform asymptotic expansion of

$$F_\gamma(t) = c_0(\gamma) - \epsilon c_1(\gamma) e^{\lambda(\gamma)t} + O(\epsilon^2) \tag{11}$$

in the region $D = \{(t,\gamma)\,|\,0 < t_1 \leqslant t \leqslant t_2\ (t_1 \neq t_2), 0 \leqslant \gamma \leqslant 1\}$ with $c_1(\gamma) \geqslant 0$ and $\lambda(\gamma) > 0$ $(0 \leqslant \gamma \leqslant 1)$, and if $c_1(\gamma)$ is nonzero at least at one γ in $0 \leqslant \gamma \leqslant 1$, then the following properties hold.

(i) The exponent $\lambda(\gamma)$ is independent of γ [hence we write $\lambda(\gamma) = \lambda$].

(ii) The coefficient $c_1(\gamma)$ is fully determined as

$$c_1(\gamma) = \tilde{c}_1 \cos\left((1 - 2\gamma)\frac{\beta\hbar\lambda}{4}\right), \quad (0 \leqslant \gamma \leqslant 1), \tag{12}$$

with $\tilde{c}_1 > 0$.

(iii) The exponent λ satisfies the inequality

$$\lambda \leqslant \frac{2\pi}{\beta\hbar} = \frac{2\pi k_B T}{\hbar}. \tag{13}$$

Some technical remarks are in order here. In the theorem, we assume not only that $F_\gamma(t)$ has an asymptotic expansion of the form of Eq. (11), but also that the asymptotic expansion is *uniform*, that is, the speed of the convergence of the expansion depends on neither t nor γ in D. More precisely, $F_\gamma(t)$ converges to $c_0(\gamma)$ uniformly in D in the limit of $\epsilon \to 0$, and $[F_\gamma(t) - c_0(\gamma)]/\epsilon$ converges to $-c_1(\gamma)e^{\lambda(\gamma)t}$ uniformly in D in the limit of $\epsilon \to 0$. The assumption of uniform convergence is physically natural since there is no *a priori* reason that the convergence slows down at certain t and γ in the finite region D. When $c_1(\gamma)$ vanishes for all γ in $0 \leqslant \gamma \leqslant 1$, $F_\gamma(t)$ does not show an exponential growth at all. In this case, the MSS bound is obviously satisfied ($\lambda = 0$). Therefore, we only consider the case in which $c_1(\gamma)$ is nonzero at least at one γ in $0 \leqslant \gamma \leqslant 1$ in the theorem.

Another remark is that in the theorem we assume that the expansion parameter ϵ and $\hbar$ are independent of each other. In the context of large N theories, this is indeed the case. However, it is not the case for semiclassical approximations where ϵ is taken to be $\hbar^2$. In order for the theorem to make sense in this case, one should understand Eq. (11) as an asymptotic expansion with respect to ϵ with $\beta\hbar$ being fixed. Note that $\hbar$ always appears together with β in the theorem.

Proof. Let us write

$$\begin{aligned}
F_\gamma(t) = {} & \frac{1}{2}\mathrm{Tr}\big[\hat\rho^{\frac14}\hat A\big(t - i\big(\gamma - \tfrac12\big)\tfrac{\beta\hbar}{2}\big)\hat\rho^{\frac14}\hat B(0) \\
& \times \hat\rho^{\frac14}\hat A\big(t - i\big(\gamma - \tfrac12\big)\tfrac{\beta\hbar}{2}\big)\hat\rho^{\frac14}\hat B(0)\big] \\
& + \frac{1}{2}\mathrm{Tr}\big[\hat\rho^{\frac14}\hat A\big(t + i\big(\gamma - \tfrac12\big)\tfrac{\beta\hbar}{2}\big)\hat\rho^{\frac14}\hat B(0) \\
& \times \hat\rho^{\frac14}\hat A\big(t + i\big(\gamma - \tfrac12\big)\tfrac{\beta\hbar}{2}\big)\hat\rho^{\frac14}\hat B(0)\big] \\
= {} & \frac{1}{2}F\big(t - i\big(\gamma - \tfrac12\big)\tfrac{\beta\hbar}{2}\big) + \frac{1}{2}F\big(t + i\big(\gamma - \tfrac12\big)\tfrac{\beta\hbar}{2}\big).
\end{aligned} \tag{14}$$

If we denote $z = t + i(\gamma - \frac12)\frac{\beta\hbar}{2}$, then $F_\gamma(t)$ can be expressed as

$$F_\gamma(t) = \frac{1}{2}F(z) + \frac{1}{2}F(\bar z). \tag{15}$$

Since $F(\bar z)$ is the complex conjugate of $F(z)$ [i.e., $F(\bar z) = \overline{F(z)}$], $F_\gamma(t)$ is the real part of the complex function $F(z)$. Let us define $c_0 \equiv c_0(\frac12)$, $\tilde c_1 \equiv c_1(\frac12) \geqslant 0$, and $\lambda \equiv \lambda(\frac12) > 0$ [later it turns out that $c_0(\gamma)$ and $\lambda(\gamma)$ do not depend on γ, so that we use the same notations for c_0 and λ at $\gamma = \frac12$]. At $\gamma = \frac12$, we have

$$F_{\frac12}(t) = F(t) = c_0 - \epsilon\tilde c_1 e^{\lambda t} + O(\epsilon^2), \quad (t_1 \leqslant t \leqslant t_2). \tag{16}$$

It has been shown in Ref. [3] that $F(z)$ is analytic in the strip region $-\frac{\beta\hbar}{4} \leqslant \mathrm{Im}\, z \leqslant \frac{\beta\hbar}{4}$ (except at $z = \pm i\frac{\beta\hbar}{4}$) [34], and especially in the region of $\Omega \equiv \{z \in \mathbb{C} \,|\, 0 < t_1 \leqslant \mathrm{Re}\, z \leqslant t_2, -\frac{\beta\hbar}{4} \leqslant \mathrm{Im}\, z \leqslant \frac{\beta\hbar}{4}\}$. Hence $F(t)$ is infinitely differentiable, and can be Taylor expanded around t with the convergence radius of $\frac{\beta\hbar}{4}$. This allows us to rewrite Eq. (14) in the form of the following differential equation:

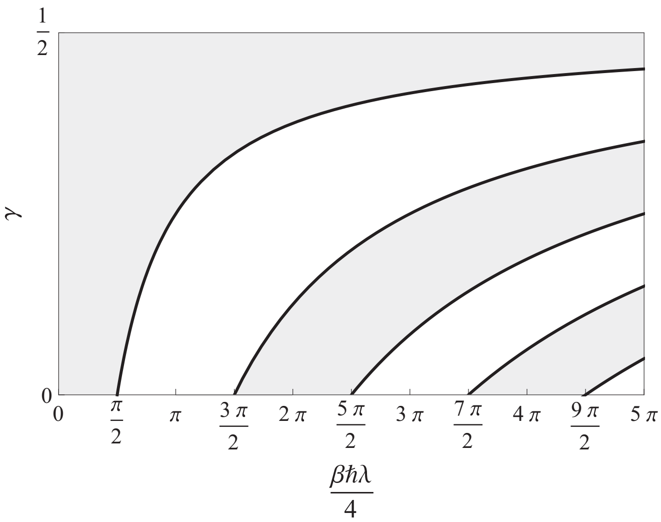

FIG. 2. Regions (shaded in gray) of $c_1(\gamma) \geqslant 0$.

$$\begin{aligned}
F_\gamma(t) &= \frac{1}{2}e^{-\frac{\beta\hbar}{2}(\gamma-\frac12)i\partial_t}F(t) + \frac{1}{2}e^{\frac{\beta\hbar}{2}(\gamma-\frac12)i\partial_t}F(t) \\
&= \cos\left((1-2\gamma)\frac{\beta\hbar}{4}\partial_t\right)F(t).
\end{aligned} \tag{17}$$

If $F(t)$ has the uniform asymptotic expansion (16) in $t_1 \leqslant t \leqslant t_2$, arbitrary-order derivatives of $F(t)$ also have uniform asymptotic expansions in $t_1 \leqslant t \leqslant t_2$ since $F(z)$ is holomorphic in Ω. Therefore, we can exchange the order of the derivative ∂_t and the limit $\epsilon \to 0$ in Eq. (17), obtaining

$$F_\gamma(t) = c_0 - \epsilon\tilde c_1 \cos\left((1-2\gamma)\frac{\beta\hbar\lambda}{4}\right)e^{\lambda t} + O(\epsilon^2). \tag{18}$$

This completely determines the γ dependencies of $c_0(\gamma)$, $c_1(\gamma)$, and $\lambda(\gamma)$. Especially, $\lambda(\gamma) = \lambda$ (independent of γ) and $c_1(\gamma) = \tilde c_1 \cos[(1-2\gamma)\frac{\beta\hbar\lambda}{4}]$. If $\tilde c_1 = 0$, $c_1(\gamma)$ vanishes for all γ in $0 \leqslant \gamma \leqslant 1$, which contradicts the assumption of the theorem. Hence $\tilde c_1 > 0$, and the statements (i) and (ii) of the theorem follow.

It is straightforward to prove the statement (iii) from the condition $c_1(\gamma) \geqslant 0$, which is equivalent to

$$\cos\left((1-2\gamma)\frac{\beta\hbar\lambda}{4}\right) \geqslant 0 \tag{19}$$

for $0 \leqslant \gamma \leqslant 1$. Since the condition (19) is symmetric around $\gamma = \frac12$, it is sufficient to restrict ourselves to $0 \leqslant \gamma \leqslant \frac12$. The allowed region of (λ, γ) is depicted in Fig. 2. The condition (19) means that $\cos\theta \geqslant 0$ for $-\frac{\beta\hbar\lambda}{4} \leqslant \theta \leqslant \frac{\beta\hbar\lambda}{4}$. Therefore the interval $[-\frac{\beta\hbar\lambda}{4}, \frac{\beta\hbar\lambda}{4}]$ must be included in the interval $[-\frac{\pi}{2}, \frac{\pi}{2}]$, which is satisfied if and only if $\frac{\beta\hbar\lambda}{4} \leqslant \frac{\pi}{2}$. This proves the inequality (13). ∎

Alternative proof. There is another way to show the statements (i) and (ii) of the theorem by using analytic continuation. As we have seen above, $F(z)$ is analytic in the region of Ω, and on the real axis ($z = t \in \Omega \cap \mathbb{R}$) $F(z)$ is given by Eq. (16). If (a) there exists an asymptotic expansion of $F(z)$ with respect to ϵ up to $O(\epsilon^2)$, and if (b) each term in the expansion is also analytic in the region of Ω, then due to the uniqueness of analytic continuation we obtain

$$F(z) = c_0 - \epsilon\tilde{c}_1 e^{\lambda z} + O(\epsilon^2) \tag{20}$$

for $\forall z \in \Omega$. Substituting Eq. (20) in Eq. (15) gives

$$\begin{aligned} F_\gamma(t) &= c_0 - \epsilon\tilde{c}_1 \mathrm{Re}\big[e^{\lambda(t+i(\gamma-\frac{1}{2})\frac{\beta\hbar}{2})}\big] + O(\epsilon^2) \\ &= c_0 - \epsilon\tilde{c}_1 \cos\left((1-2\gamma)\frac{\beta\hbar\lambda}{4}\right)e^{\lambda t} + O(\epsilon^2), \end{aligned} \tag{21}$$

which is equivalent to (i) and (ii).

The remaining task is to show that the assumptions (a) and (b) made in the above argument are true. To this end, we first need to show that $\lim_{\epsilon\to 0} F(z)$ exists and that $\lim_{\epsilon\to 0} F(z)$ is holomorphic [note that $F(z)$ itself is holomorphic in Ω for each fixed ϵ]. Let us recall that the real part of $F(z)$ is $F_\gamma(t)$, which converges uniformly in the region Ω in the limit of $\epsilon \to 0$. Since $F(z) = F_\gamma(t)$ for $\mathrm{Im}\, z = 0$, $F(z)$ converges in the limit of $\epsilon \to 0$ for $z \in \Omega \cap \mathbb{R}$. Now we invoke the following mathematical fact in complex analysis [35]: Suppose that $f_n(z)$ ($n = 1,2,3,\ldots$) is holomorphic in the region Ω, $u_n(z)$ is the real part of $f_n(z)$, $\{u_n(z)\}$ converges uniformly on any compact subset of Ω, and $\{f_n(z)\}$ converges for at least one $z \in \Omega$. Then $\{f_n(z)\}$ converges uniformly on any compact subset of Ω. From this fact, it follows that $F(z)$ converges uniformly in the region Ω in the limit of $\epsilon \to 0$. Uniform convergence guarantees that $\lim_{\epsilon\to 0} F(z)$ is holomorphic in Ω. By analytic continuation, we obtain $\lim_{\epsilon\to 0} F(z) = c_0$ for $z \in \Omega$. We repeat the same argument with $F(z)$ replaced by $[F(z) - c_0]/\epsilon$, showing that $[F(z) - c_0]/\epsilon$ converges uniformly in Ω in the limit of $\epsilon \to 0$ and that $\lim_{\epsilon\to 0}[F(z) - c_0]/\epsilon$ is holomorphic in Ω. Thus the assumptions (a) and (b) are shown to be true, and the proof of the theorem is completed. ∎

IV. GENERALIZATION OF THE MSS BOUND TO HIGHER-ORDER OTOCS

The theorem derived in the previous section can be generalized to higher even-order OTOCs. We define the higher-order generalization of the one-parameter family of the OTOCs $F_\gamma(t)$ (6) as

$$\begin{aligned} F_\gamma^n(t) \equiv{}& \frac{1}{2}\mathrm{Tr}([\hat\rho^{\frac{1-\gamma}{2n}}\hat A(t)\hat\rho^{\frac{\gamma}{2n}}\hat B(0)]^{2n}) \\ &+ \frac{1}{2}\mathrm{Tr}([\hat\rho^{\frac{1-\gamma}{2n}}\hat B(0)\hat\rho^{\frac{\gamma}{2n}}\hat A(t)]^{2n}), \end{aligned} \tag{22}$$

with $0 \leqslant \gamma \leqslant 1$ and $n = 1,2,3,\ldots$. We note that $F_\gamma^n(t) = F_\gamma(t)$ for $n = 1$, $F_\gamma^n(t)$ is real for arbitrary n and γ, and $F_\gamma^n(t)$ is the $(AB)^{2n} + (BA)^{2n}$ part of the regularized $\langle[\hat A(t), \hat B(0)]^{2n}\rangle$. Again $F_\gamma^n(t)$ has appeared in the left-hand side ("fluctuation" part) of the $2n$th-order out-of-time-order fluctuation-dissipation theorem [23]

$$\begin{aligned} &\sum_{\alpha_1,\alpha_2,\ldots,\alpha_{2n}=\pm}^{\alpha_1\alpha_2\cdots\alpha_{2n}=+} C^\gamma_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}\cdots[A,B]_{\alpha_{2n}}}(\omega) \\ &= \coth\left((1-2\gamma)\frac{\beta\hbar\omega}{4n}\right)\sum_{\alpha_1,\alpha_2,\ldots,\alpha_{2n}=\pm}^{\alpha_1\alpha_2\cdots\alpha_{2n}=-} \\ &\quad\times C^\gamma_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}\cdots[A,B]_{\alpha_{2n}}}(\omega), \end{aligned} \tag{23}$$

where $C^\gamma_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}\cdots[A,B]_{\alpha_{2n}}}(\omega)$ is the Fourier transform of

$$\begin{aligned} &C^\gamma_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}\cdots[A,B]_{\alpha_{2n}}}(t,0) \\ &\equiv \mathrm{Tr}\left(\prod_{i=1}^{2n}[\hat\rho^{\frac{1-\gamma}{2n}}\hat A(t)\hat\rho^{\frac{\gamma}{2n}}\hat B(0) + \alpha_i\hat\rho^{\frac{1-\gamma}{2n}}\hat B(0)\hat\rho^{\frac{\gamma}{2n}}\hat A(t)]\right) \end{aligned} \tag{24}$$

with $\alpha_i = \pm$. $F_\gamma^n(t)$ is related to the left-hand side of Eq. (23) via

$$F_\gamma^n(t) = \frac{1}{2^{2n}}\sum_{\alpha_1,\alpha_2,\ldots,\alpha_{2n}=\pm}^{\alpha_1\alpha_2\cdots\alpha_{2n}=+} C^\gamma_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}\cdots[A,B]_{\alpha_{2n}}}(t,0). \tag{25}$$

Since $(-1)^n\langle[\hat A(t), \hat B(0)]^{2n}\rangle$ is positive semidefinite, it is reasonable to expect that $F_\gamma^n(t)$ grows exponentially (if it does) to the positive (negative) direction for even (odd) n. Thus we assume that $F_\gamma^n(t)$ has a uniform asymptotic expansion of

$$F_\gamma^n(t) = c_{0,n}(\gamma) + (-1)^n\epsilon c_{1,n}(\gamma)e^{\lambda_n(\gamma)t} + O(\epsilon^2) \tag{26}$$

in the region $D = \{(t,\gamma)|t_1 \leqslant t \leqslant t_2\ (t_1 \neq t_2), 0 \leqslant \gamma \leqslant 1\}$ with $c_{1,n}(\gamma) \geqslant 0$ and $\lambda_n(\gamma) > 0$ for $0 \leqslant \gamma \leqslant 1$. If $c_{1,n}(\gamma)$ is nonzero at least at one γ in $0 \leqslant \gamma \leqslant 1$, then, due to the same argument as in Sec. III, we can prove that $\lambda_n(\gamma)$ does not depend on γ (hence we write $\lambda_n(\gamma) = \lambda_n$) and the γ dependence of $c_{1,n}(\gamma)$ is determined as

$$c_{1,n}(\gamma) = \tilde c_{1,n}\cos\left((1-2\gamma)\frac{\beta\hbar\lambda_n}{4n}\right) \tag{27}$$

with a positive constant $\tilde c_{1,n}$. In order for the coefficient $c_{1,n}(\gamma)$ to be positive semidefinite for $0 \leqslant \gamma \leqslant 1$, λ_n must satisfy the inequality

$$\lambda_n \leqslant \frac{2n\pi}{\beta\hbar} = \frac{2n\pi k_B T}{\hbar}. \tag{28}$$

This is a generalization of the MSS bound to the higher-order OTOCs $F_\gamma^n(t)$. If the bound (28) is saturated, the dominant exponential growth of the regularized $\langle[\hat A(t), \hat B(0)]^{2n}\rangle$ is given by $\exp\left(\frac{2n\pi}{\beta\hbar}t\right) = [\exp\left(\frac{2\pi}{\beta\hbar}t\right)]^n$. This is natural since the fastest exponential growth of the regularized $\langle[\hat A(t), \hat B(0)]^2\rangle$ is given by $\exp\left(\frac{2\pi}{\beta\hbar}t\right)$.

V. DISCUSSIONS

In this section, we discuss various issues on the theorem and its proof given in Sec. III.

The assumption about the form of $F_\gamma(t)$ in Eq. (11) for all γ in $0 \leqslant \gamma \leqslant 1$ is too strong for the purpose of showing (i) and (ii). As we have seen above, $F_\gamma(t)$ is uniquely determined from $F_{\frac{1}{2}}(t)$. In fact, to prove (i) and (ii), it is sufficient to adopt a weaker assumption that Eq. (11) holds for $\gamma = \frac{1}{2}$ and that there exists a uniform asymptotic expansion of $F_\gamma(t)$ in D. If one further assumes $c_1(\gamma) \geqslant 0$ for $0 \leqslant \gamma \leqslant 1$, then (iii) follows. Also, the assumption of the uniformity of the asymptotic expansion seems to be rather technical. Instead of uniformity, it is sufficient to assume (a) and (b) from the beginning to prove the statements (i), (ii), and (iii) of the theorem in the alternative proof.

Let us emphasize that in proving the theorem we cannot use the mathematical result employed in Ref. [3]: If $f(t+i\tau)$ is analytic in the half strip $\{(t,\tau)|t>0,-\frac{\beta\hbar}{4}\leqslant\tau\leqslant\frac{\beta\hbar}{4}\}$, $f(t)$ is real for $\tau=0$, and $|f(t+i\tau)|\leqslant 1$ in the entire half strip, then it follows that

$$\frac{1}{1-f}\left|\frac{df}{dt}\right|\leqslant\frac{2\pi}{\beta\hbar}+O(e^{-4\pi t/\beta\hbar}). \tag{29}$$

It is argued in Ref. [3] that the appropriately normalized OTOC f satisfies the assumptions of the above statement if one assumes a factorization of certain time-ordered functions. From the inequality (29), one can see that the exponential growth rate of f is bounded by $2\pi/\beta\hbar$. Here we cannot use this mathematical result simply because the theorem does not assume anything about the behavior of $F_\gamma(t)$ out of the region $D=\{(t,\gamma)|t_1\leqslant t\leqslant t_2, 0\leqslant\gamma\leqslant 1\}$. Thus it is impossible to bound $|F_\gamma(t)|$ in an entire region of a certain half strip such as $\{(t,\gamma)|t\geqslant t_1, 0\leqslant\gamma\leqslant 1\}$ in our case. Since we restrict ourselves to the finite-time range ($t_1\leqslant t\leqslant t_2$), we do not suffer from Poincaré recurrences (if the time range is shorter than the recurrence time), which would invalidate the factorization [3].

If λ were to exceed the bound $2\pi/\beta\hbar$, something strange would happen. From the theorem, one can see that there exists some γ in $0\leqslant\gamma\leqslant 1$ such that $c_1(\gamma)<0$. This means that there exists an OTOC $F_\gamma(t)$ in the one-parameter family that grows exponentially in the direction *opposite* to the one in which the initial-perturbation sensitivity grows. That is, the direction of the exponential growth depends on the choice of the regularization of $\langle[\hat{A}(t),\hat{B}(0)]^2\rangle$. Although such a case is not excluded by the theorem, the exponential growth of the OTOC becomes regularization dependent, and it is no longer universal. As long as the exponential growth is universal, the growth rate must be bounded from the theorem.

The theorem can be extended to cases in which there is a subleading correction to the exponential growth in the $O(\epsilon)$ term in Eq. (11):

$$F_\gamma(t)=c_0(\gamma)-\epsilon[c_1(\gamma)e^{\lambda(\gamma)t}+f_\gamma(t)]+O(\epsilon^2). \tag{30}$$

Here $f_\gamma(t)$ represents a subleading correction such as $c_2(\gamma)e^{\lambda'(\gamma)t}$ with $\lambda'(\gamma)<\lambda(\gamma)$ for $0\leqslant\gamma\leqslant 1$. By applying the same argument as in the proof of the theorem, one obtains

$$F_\gamma(t)=c_0-\epsilon\left[\tilde{c}_1\cos\left((1-2\gamma)\frac{\beta\hbar\lambda}{4}\right)e^{\lambda t}+f_\gamma(t)\right]+O(\epsilon^2). \tag{31}$$

As long as one requires the positivity of the coefficient of the leading exponentially growing term [i.e., $c_1(\gamma)\geqslant 0$], the exponent λ in the leading term is bounded as in Eq. (13). Adding a subleading correction to the $O(\epsilon^0)$ term is also possible with the results unchanged.

The theorem does not exclude the growth of the OTOC faster than the exponential such as $e^{\lambda t^2}$. Originally, it has been conjectured [3] that

$$\frac{d}{dt}[F_d-F(t)]\leqslant\frac{2\pi}{\beta\hbar}[F_d-F(t)], \tag{32}$$

where F_d is a constant which $F(t)$ approaches after the dissipation time. This is stronger than our statement that assumes an exponential growth from the beginning. However, our argument in the proof of the theorem can be used to strongly constrain rapid growth of the OTOC. For example, if $F(t)$ takes the form of

$$F(t)=c_0-\epsilon\tilde{c}_1e^{\lambda t^2}+O(\epsilon^2) \tag{33}$$

for $t_1\leqslant t\leqslant t_2$, then a similar argument shows that

$$F_\gamma(t)=c_0-\epsilon c_1(\gamma,t)e^{\lambda t^2}+O(\epsilon^2) \tag{34}$$

with

$$c_1(\gamma,t)=\tilde{c}_1e^{-\lambda(1-2\gamma)^2(\frac{\beta\hbar}{4})^2}\cos\left((1-2\gamma)\frac{\beta\hbar\lambda}{2}t\right). \tag{35}$$

That is, $F_\gamma(t)$ not only grows as $e^{\lambda t^2}$ but also oscillates with t. If the duration of the growth t_2-t_1 is sufficiently large (i.e., $t_2-t_1>\frac{2\pi}{\beta\hbar\lambda}$), the $O(\epsilon^1)$ term of some of $F_\gamma(t)$ in $0\leqslant\gamma\leqslant 1$ must change its sign. Thus it is impossible that all the members of the OTOCs in the one-parameter family grows as $e^{\lambda t^2}$ to the "correct" direction (such that the initial perturbation-sensitivity grows) for a sufficiently long-time duration. The extension of the argument to other cases including $e^{\lambda t^n}$ ($n\geqslant 3$) is straightforward.

Finally, let us comment on the zero-temperature limit (i.e., $\beta\hbar\to\infty$) in the case of $\epsilon=\hbar^2$ (semiclassical approximations), where the theorem suggests that λ must be zero. Does this mean that there is no chaotic behavior at zero temperature? There is a subtle ambiguity which arises when we consider the two limits of $\hbar\to 0$ and $\beta\to\infty$ simultaneously. Depending on the precise definition of the limits, we have two possibilities: either (i) the semiclassical approximation itself breaks down, or (ii) the semiclassical approximation retains its validity as the temperature goes to zero. In the former case, the basis of the theorem [i.e., the presence of the asymptotic expansion (11)] does not hold, so that the theorem cannot be applied. In the latter case, the system approaches the lowest-energy state (i.e., the stable fixed point) of the classical Hamiltonian $H(q_i,p_i)$, around which the Hamiltonian can be approximated by quadratic terms in q_i and p_i (see, e.g., Ref. [36]). Thus the system becomes nearly integrable, and the chaotic behavior is suppressed at low temperature.

VI. SUMMARY

To summarize, we prove the inequality (1) for the growth rate of the OTOCs under the assumption that all the OTOCs in the one-parameter family [$F_\gamma(t)$ with $0\leqslant\gamma\leqslant 1$] show a transient exponential growth in the uniform asymptotic expansion by using only the analytic properties of the OTOCs. We do not exclude the possibility that some of the OTOCs in the one-parameter family might violate the MSS bound. However, in this case the sign of the exponentially growing part depends on the regularization parameter, which makes the exponential growth of the OTOC nonuniversal. Our argument places a strong constraint on the faster-than-exponential growth of the OTOC. The obtained results are independent of the choice of the operators $\hat{A}$ and $\hat{B}$ and any details of the system, and applicable to arbitrary quantum systems in thermal equilibrium, including quantum black holes and strongly interacting many-body systems. The theorem is further generalized to higher-order OTOCs (22), for which we derive a novel universal bound given by Eq. (28).

ACKNOWLEDGMENTS

N.T. is supported by JSPS KAKENHI Grant No. JP16K17729. T.S. acknowledges support from a Grant-in-Aid for JSPS Fellows (KAKENHI Grant No. JP16J06936) and the Advanced Leading Graduate Course for Photon Science (ALPS) of JSPS. M.U. acknowledges support by KAKENHI Grant No. JP18H01145 and KAKENHI Grant No. JP15H05855.

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