Out-of-time-order fluctuation-dissipation theorem

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We prove a generalized fluctuation-dissipation theorem for a certain class of out-of-time-ordered correlators (OTOCs) with a modified statistical average, which we call bipartite OTOCs, for general quantum systems in thermal equilibrium. The difference between the bipartite and physical OTOCs defined by the usual statistical average is quantified by a measure of quantum fluctuations known as the Wigner-Yanase skew information. Within this difference, the theorem describes a universal relation between chaotic behavior in quantum systems and a nonlinear-response function that involves a time-reversed process. We show that the theorem can be generalized to higher-order n-partite OTOCs as well as in the form of generalized covariance.

I. INTRODUCTION

The fluctuation-dissipation theorem (FDT) relates nonequilibrium transport coefficients to equilibrium fluctuations and plays a pivotal role in statistical mechanics. It dates back to Einstein's theory of Brownian motion [1] and the Nyquist relation between resistance and a thermal noise in voltage [2], culminating in linear response theory [3] (for a review, see, e.g., Ref. [4]).

The FDT establishes the relationship between the expectation values of the commutator and the anticommutator,

$$C_{[A,B]}(t,t') \equiv \langle [\hat{A}(t),\hat{B}(t')] \rangle, \qquad (1)$$

$$C_{\{A,B\}}(t,t') \equiv \langle \{\hat{A}(t),\hat{B}(t')\} \rangle, \qquad (2)$$

of arbitrary (bosonic or fermionic[1]) Heisenberg operators $\hat{A}(t) = e^{\frac{i}{\hbar}\hat{H}t} \hat{A} e^{-\frac{i}{\hbar}\hat{H}t}$ and $\hat{B}(t) = e^{\frac{i}{\hbar}\hat{H}t} \hat{B} e^{-\frac{i}{\hbar}\hat{H}t}$. Here $\hat{H}$ is the Hamiltonian of the system, $\hbar$ is the Planck constant, $\langle \cdot \rangle \equiv \text{Tr}(\hat{\rho} \cdot)$, and $\hat{\rho} = e^{-\beta\hat{H}}/Z$ ($Z = \text{Tr}e^{-\beta\hat{H}}$) with $\beta = (k_B T)^{-1}$ being the inverse temperature (k_B is the Boltzmann constant). In the Fourier representation [i.e., $C_{\{A,B\}}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} C_{\{A,B\}}(t,0)$, etc.], the FDT is expressed as

$$C_{\{A,B\}}(\omega) = \coth\left(\frac{\beta\hbar\omega}{2}\right) C_{[A,B]}(\omega). \qquad (3)$$

If either $\hat{A}$ or $\hat{B}$ is bosonic, then $C_{\{A,B\}}(\omega)$ represents thermal fluctuations and $C_{[A,B]}(\omega)$ represents dissipation (and vice versa if both $\hat{A}$ and $\hat{B}$ are fermionic) [3,5,6].

What is the law that governs higher-order fluctuations beyond the FDT (3) and beyond the linear response regime? The generalization of the FDT has led to deeper understanding of nonequilibrium statistical mechanics. The prime examples are the fluctuation theorem [7,8] and the Jarzynski equality

[9], which are valid in arbitrary far off-equilibrium situations, reproduce the FDT (3) at zero frequency if applied to near thermal equilibrium, and place constraints on higher-order fluctuations [10–14].

Here we pursue a different direction of generalization of the FDT by considering the second moments of fluctuation and dissipation such as $\langle \{\hat{A}(t),\hat{B}(t')\}^2 \rangle$ and $\langle [\hat{A}(t),\hat{B}(t')]^2 \rangle$. They involve the operator sequences $\hat{A}(t)\hat{B}(t')\hat{A}(t)\hat{B}(t')$ and $\hat{B}(t')\hat{A}(t)\hat{B}(t')\hat{A}(t)$ that constitute out-of-time-ordered correlators (OTOCs) [15].

The OTOC has attracted growing attention as a measure to characterize chaotic behavior in quantum systems [16]. The relation to chaos can be seen in the semiclassical approximation: If $\hat{A}$ and $\hat{B}$ form a canonically conjugate pair, then $\langle [\hat{A}(t),\hat{B}(0)]^2 \rangle \sim -\hbar^2 \langle\langle \{A(t),B(0)\}_P^2 \rangle\rangle = -\hbar^2 \langle\langle (\frac{\partial A(t)}{\partial A(0)})^2 \rangle\rangle$, where $\langle\langle \cdot \rangle\rangle$ is the classical phase-space average with respect to the Gibbs ensemble, and $\{,\}_P$ is the Poisson bracket. This quantity indicates the sensitivity of the time-evolving quantity $A(t)$ to its initial value $A(0)$ and is expected to grow exponentially in time for chaotic systems ("butterfly effect") as $\sim e^{\lambda t}$, where λ is an analog of the Lyapunov exponent in classical chaotic systems (see also Ref. [17]). The interest in OTOCs has recently surged in various contexts, including the Sachdev-Ye-Kitaev model [16,18,19], black holes and the holography principle [20–22], quantum information [23–25], many-body localization [26–29], and strongly correlated systems [30–34]. The OTOC has recently been observed in experiments [35–38].

In this paper, we show that a generalized fluctuation-dissipation theorem holds for a certain class of OTOCs with an arbitrary frequency. The theorem describes a universal relation between chaotic properties in quantum systems and a nonlinear response function for a perturbation involving a time-reversed process. To be more precise, there is a difference in operator ordering between OTOCs defined by the usual statistical average $[\langle \hat{A}(t)\hat{B}(t')\hat{A}(t)\hat{B}(t') \rangle = \text{Tr}(\hat{\rho}\hat{A}(t)\hat{B}(t')\hat{A}(t)\hat{B}(t'))]$ and those that do obey the out-of-time-order FDT. This difference can be expressed in terms of the Wigner-Yanase skew information [39], which is known in the context of quantum information theory and serves as a measure of information

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[1]We call an operator $\hat{A}$ bosonic (fermionic) if $\hat{A}$ is a linear combination of operators, each of which contains an even (odd) number of fermion creation and/or annihilation operators.

contents contained in quantum fluctuations of observables. Within the difference of the skew information, the out-of-time-order FDT relates the chaotic behavior and the nonlinear response function.

The rest of this paper is organized as follows. In Sec. II, we present the statement of one of the main results in the paper, the out-of-time-order FDT. In Sec. III, we discuss the physical meaning of the out-of-time-order FDT. We prove the out-of-time-order FDT in Sec. IV. In Sec. V, we generalize the theorem to higher-order OTOCs as well as other operator ordering of OTOCs. In Sec. VI, we conclude the paper. In Appendix, we present the proofs of some relations among OTOCs used in the main text.

II. MAIN RESULTS

The FDT is generalized for OTOCs not in a straightforward manner but in a twisted form. Namely, we should split $\hat{\rho}$ into two $\hat{\rho}^{\frac{1}{2}}$'s, one of which is inserted in between commutators and/or anticommutators of $\hat{A}(t)$ and $\hat{B}(t')$ and the other is placed in front of them. To be specific, we define a *bipartite OTOC* (also called a regularized OTOC) [22,40–42] as

$$
\begin{aligned}
C_{AB}^{\alpha_1\alpha_2}(t,t') &\equiv C_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}}(t,t') \\
&\equiv \mathrm{Tr}\big(\hat{\rho}^{\frac{1}{2}}[\hat{A}(t),\hat{B}(t')]_{\alpha_1}\hat{\rho}^{\frac{1}{2}}[\hat{A}(t),\hat{B}(t')]_{\alpha_2}\big), \quad (4)
\end{aligned}
$$

where $\alpha_1,\alpha_2 = \pm$, and $[,]_{-(+)}$ represents the (anti)commutator. Note that (4) is different from an ordinary OTOC which takes the form of the expectation value $[\mathrm{Tr}(\hat{\rho}\cdots)]$ of products of (anti)commutators for a given state $\hat{\rho}$,

$$
\begin{aligned}
C_{AB}^{\mathrm{phys},\alpha_1\alpha_2}(t,t') &\equiv C_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}}^{\mathrm{phys}}(t,t') \\
&\equiv \mathrm{Tr}\big(\hat{\rho}[\hat{A}(t),\hat{B}(t')]_{\alpha_1}[\hat{A}(t),\hat{B}(t')]_{\alpha_2}\big). \quad (5)
\end{aligned}
$$

Since this quantity is written in the form of the expectation value that allows for a direct physical interpretation, we shall refer to (5) as a *physical* OTOC. Depending on $\alpha_1,\alpha_2 = \pm$, Eq. (4) introduces four types of bipartite OTOCs, of which $C_{\{A,B\}[A,B]}$ and $C_{[A,B]\{A,B\}}$ are equal due to the cyclic invariance of the trace. Hence there are three independent bipartite OTOCs for a given pair of $\hat{A}$ and $\hat{B}$.

One of the main results in this paper is that for *any* quantum system in thermal equilibrium the three bipartite OTOCs are related via

$$
C_{\{A,B\}^2}(\omega) + C_{[A,B]^2}(\omega) = 2\coth\left(\frac{\beta\hbar\omega}{4}\right)C_{\{A,B\}[A,B]}(\omega), \tag{6}
$$

which we call the out-of-time-order FDT. If we ignore the difference in operator ordering between (4) and (5) (the physical meaning of this is explained in Sec. III), then the equality (6) implies a universal relation among the second moments of fluctuation and dissipation, and their cross-correlation. In this sense, the equality (6) can be viewed as a second-order extension of the FDT (3).

III. PHYSICAL MEANING OF THE OUT-OF-TIME-ORDER FLUCTUATION-DISSIPATION THEOREM

To see the physical meaning of the equality (6), let us first note that the difference between $C_{AB}^{\alpha_1\alpha_2}(t,t')$ (4) and $C_{AB}^{\mathrm{phys},\alpha_1\alpha_2}(t,t')$ (5) takes a form reminiscent of the Wigner-Yanase (WY) skew information[2] [39] defined by

$$
\begin{aligned}
I_{\frac{1}{2}}(\hat{\rho},\hat{O}) &\equiv -\frac{1}{2}\mathrm{Tr}\big([\hat{\rho}^{\frac{1}{2}},\hat{O}]^2\big) \\
&= \mathrm{Tr}(\hat{\rho}\hat{O}^2) - \mathrm{Tr}\big(\hat{\rho}^{\frac{1}{2}}\hat{O}\hat{\rho}^{\frac{1}{2}}\hat{O}\big) \quad (7)
\end{aligned}
$$

for a Hermitian operator $\hat{O}$. It serves as a measure of information contents concerning quantum fluctuations. Here by quantum fluctuations we mean the following [43]. Let us consider the variance of $\hat{O}$, $\langle(\Delta\hat{O})^2\rangle$, where $\Delta\hat{O} \equiv \hat{O} - \langle\hat{O}\rangle$. The variance $\langle(\Delta\hat{O})^2\rangle$ generally contains classical mixing and quantum uncertainty, so that we are tempted to decompose the variance as

$$
\langle(\Delta\hat{O})^2\rangle = C(\hat{\rho},\hat{O}) + Q(\hat{\rho},\hat{O}). \tag{8}
$$

If $C(\hat{\rho},\hat{O})$ and $Q(\hat{\rho},\hat{O})$ satisfy the following conditions, we call them the classical and quantum fluctuations of $\hat{O}$:

(a) $C(\hat{\rho},\hat{O}),Q(\hat{\rho},\hat{O}) \geqslant 0$.

(b) If $\hat{\rho}$ is pure, then $C(\hat{\rho},\hat{O}) = 0$ and $Q(\hat{\rho},O) = \langle(\Delta\hat{O})^2\rangle$.

(c) If $\hat{\rho}$ and $\hat{O}$ commute, then $C(\hat{\rho},O) = \langle(\Delta\hat{O})^2\rangle$ and $Q(\hat{\rho},\hat{O}) = 0$.

(d) $C(\hat{\rho},\hat{O})$ is concave and $Q(\hat{\rho},O)$ is convex as functions of $\hat{\rho}$, i.e.,

$$
C(\lambda\hat{\rho}_1 + (1-\lambda)\hat{\rho}_2,\hat{O}) \geqslant \lambda C(\hat{\rho}_1,\hat{O}) + (1-\lambda)C(\hat{\rho}_2,\hat{O}),
$$

$$
Q(\lambda\hat{\rho}_1 + (1-\lambda)\hat{\rho}_2,\hat{O}) \leqslant \lambda Q(\hat{\rho}_1,\hat{O}) + (1-\lambda)Q(\hat{\rho}_2,\hat{O}),
$$

for $0 \leqslant \lambda \leqslant 1$.

The condition (d) means that classical fluctuations should increase and quantum fluctuations should decrease by a classical mixing of states. These conditions are in accordance with our intuition of quantum fluctuations.

Although such a decomposition is not unique [44], the WY skew information provides one realization of the measure of quantum fluctuations $[Q(\hat{\rho},\hat{O}) = I_{\frac{1}{2}}(\hat{\rho},\hat{O})]$. In fact, it satisfies the inequalities

$$
0 \leqslant I_{\frac{1}{2}}(\hat{\rho},\hat{O}) \leqslant \langle(\Delta\hat{O})^2\rangle. \tag{9}
$$

The equality on the left-hand side of (9) is satisfied when $[\hat{\rho},\hat{O}] = 0$, and the one on the right-hand side is met when $\hat{\rho}$ is a pure state. Furthermore, the WY skew information is convex as a function of a quantum state [45],

$$
I_{\frac{1}{2}}(\lambda\hat{\rho}_1 + (1-\lambda)\hat{\rho}_2,\hat{O}) \leqslant \lambda I_{\frac{1}{2}}(\hat{\rho}_1,\hat{O}) + (1-\lambda)I_{\frac{1}{2}}(\hat{\rho}_2,\hat{O}),
$$
$$ \tag{10}$$

for $0 \leqslant \lambda \leqslant 1$. That is, it decreases under a classical mixing of quantum states, justifying [with (9)] the use of $I_{\frac{1}{2}}(\hat{\rho},\hat{O})$ as an information-theoretic measure of quantum fluctuations.

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[2]There is a one-parameter generalization of the WY skew information due to Dyson, i.e., $I_\alpha(\hat{\rho},\hat{O}) = \mathrm{Tr}(\hat{\rho}\hat{O}^2) - \mathrm{Tr}(\hat{\rho}^\alpha\hat{O}\rho^{1-\alpha}\hat{O})$ $(0 \leqslant \alpha \leqslant 1)$.

If $\hat{A}$ and $\hat{B}$ are Hermitian, then $C_{AB}^{\alpha_1\alpha_2}(t,t')$ and $C_{AB}^{\mathrm{phys},\alpha_1\alpha_2}(t,t')$ are related to the WY skew information via

$$C_{\{A,B\}^2}(t,t') = C_{\{A,B\}^2}^{\mathrm{phys}}(t,t') - I_{\frac{1}{2}}(\hat{\rho},\{\hat{A}(t),\hat{B}(t')\}), \quad (11)$$

$$C_{[A,B]^2}(t,t') = C_{[A,B]^2}^{\mathrm{phys}}(t,t') + I_{\frac{1}{2}}(\hat{\rho},i[\hat{A}(t),\hat{B}(t')]), \quad (12)$$

$$\begin{aligned}
C_{\{A,B\}[A,B]}(t,t') &= \frac{1}{2}\big[C_{\{A,B\}[A,B]}^{\mathrm{phys}}(t,t') + C_{[A,B]\{A,B\}}^{\mathrm{phys}}(t,t')\big] \\
&+ \frac{i}{4}I_{\frac{1}{2}}(\hat{\rho},\{\hat{A}(t),\hat{B}(t')\} + i[\hat{A}(t),\hat{B}(t')]) \\
&- \frac{i}{4}I_{\frac{1}{2}}(\hat{\rho},\{\hat{A}(t),\hat{B}(t')\} - i[\hat{A}(t),\hat{B}(t')]).
\end{aligned} \quad (13)$$

Note that $\{\hat{A}(t),\hat{B}(t')\}$, $i[\hat{A}(t),\hat{B}(t')]$, and $\{\hat{A}(t),\hat{B}(t')\} \pm i[\hat{A}(t),\hat{B}(t')]$ are Hermitian. We thus find that the difference between the bipartite (4) and physical OTOCs (5) can be expressed in terms of the skew information. Within this difference, which is negligible when quantum fluctuations are small, Eq. (6) shows the relation among the second moments of fluctuation and dissipation and their cross-correlation. We can explicitly express this by rewriting Eq. (6) in terms of the physical OTOCs,

$$\begin{aligned}
&C_{\{A,B\}^2}^{\mathrm{phys}}(\omega) + C_{[A,B]^2}^{\mathrm{phys}}(\omega) \\
&= \coth\left(\frac{\beta\hbar\omega}{4}\right)\big[C_{\{A,B\}[A,B]}^{\mathrm{phys}}(\omega) + C_{[A,B]\{A,B\}}^{\mathrm{phys}}(\omega)\big] \\
&+ I_{AB}(\omega),
\end{aligned} \quad (14)$$

where

$$\begin{aligned}
&I_{AB}(\omega) \\
&= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\bigg\{I_{\frac{1}{2}}(\hat{\rho},\{\hat{A}(t),\hat{B}(0)\}) - I_{\frac{1}{2}}(\hat{\rho},i[\hat{A}(t),\hat{B}(0)]) \\
&+ \frac{i}{2}\coth\left(\frac{\beta\hbar\omega}{4}\right)I_{\frac{1}{2}}(\hat{\rho},\{\hat{A}(t),\hat{B}(0)\} + i[\hat{A}(t),\hat{B}(0)]) \\
&- \frac{i}{2}\coth\left(\frac{\beta\hbar\omega}{4}\right)I_{\frac{1}{2}}(\hat{\rho},\{\hat{A}(t),\hat{B}(0)\} - i[\hat{A}(t),\hat{B}(0)])\bigg\}
\end{aligned} \quad (15)$$

is a linear combination of the skew information.

The physical meaning of Eq. (6) [or Eq. (14)] is as follows. The right-hand side of (6) is related to a certain type of a nonlinear-response function (Fig. 1). To see this, let us consider the following experimental protocol. The initial state is set to be in thermal equilibrium with $\hat{\rho}$. At time $t = 0$, we perturb the system with a variation of the Hamiltonian $\delta\hat{H}(t) = \hbar\varepsilon_B\delta(t)\hat{B}$ ($\varepsilon_B \in \mathbb{R}$). Then we let the system evolve from $t = 0$ to t_0 with the Hamiltonian $+\hat{H}$. At $t = t_0$ (>0), we perturb the system with $\delta\hat{H}(t) = \hbar\varepsilon_A\delta(t - t_0)\hat{A}$ ($\varepsilon_A \in \mathbb{R}$). Then we let the system evolve from $t = t_0$ to $2t_0$ with the inverted Hamiltonian $-\hat{H}$ (as in spin echo, Loschmidt echo, or ultracold atom [32] experiments), i.e., the time propagation is effectively reversed. Finally, we measure $\hat{B}$ at $t = 2t_0$. Let us suppose that ε_A and ε_B are sufficiently small, which allows us to expand $\langle\hat{B}(2t_0)\rangle$
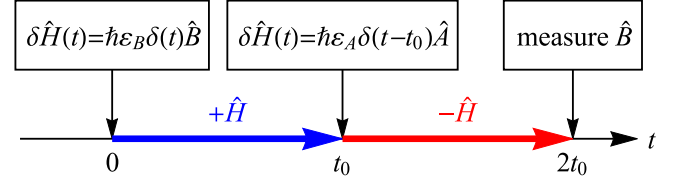

FIG. 1. Measurement protocol for the nonlinear response function $L_{(AB)^2}^{(3)}(t_0,0)$. The system is perturbed by the pulsed fields at $t = 0$ and $t = t_0$. The system evolves with the Hamiltonian $+\hat{H}$ from $t = 0$ to $t = t_0$ and then with $-\hat{H}$ from $t = t_0$ to $t = 2t_0$. The measurement of $\hat{B}$ is performed at $t = 2t_0$.

with respect to ε_A and ε_B,

$$\langle\hat{B}(2t_0)\rangle = \sum_{m,n=0}^{\infty} \varepsilon_A^m \varepsilon_B^n\big[\delta_{A^m B^n}^{m+n}\langle\hat{B}(2t_0)\rangle\big]. \quad (16)$$

Here $\delta_{A^m B^n}^{m+n}\langle\hat{B}(2t_0)\rangle$ represents the expansion coefficient at the mth and nth orders with respect to the perturbation strength ε_A and ε_B. The lowest order at which OTOCs appear is the third order ($m + n = 3$). We define a nonlinear response function $L_{(AB)^2}^{(3)}(t_0,0)$ as a coefficient of the third-order variation of $\langle\hat{B}(2t_0)\rangle$ that is proportional to $\varepsilon_A^2\varepsilon_B$, i.e.,

$$\delta_{A^2 B}^3\langle\hat{B}(2t_0)\rangle =: \frac{1}{2}L_{(AB)^2}^{(3)}(t_0,0). \quad (17)$$

The density matrix at $t = 2t_0$ is given by

$$\hat{\rho}(2t_0) = e^{\frac{i}{\hbar}\hat{H}t_0}e^{-i\varepsilon_A\hat{A}}e^{-\frac{i}{\hbar}\hat{H}t_0}e^{-i\varepsilon_B\hat{B}}\hat{\rho}\,e^{i\varepsilon_B\hat{B}}e^{\frac{i}{\hbar}\hat{H}t_0}e^{i\varepsilon_A\hat{A}}e^{-\frac{i}{\hbar}\hat{H}t_0}. \quad (18)$$

By expanding $\langle\hat{B}(2t_0)\rangle = \mathrm{Tr}[\hat{\rho}(2t_0)\hat{B}]$ with respect to ε_A and ε_B, and collecting terms proportional to $\varepsilon_A^2\varepsilon_B$, we obtain

$$\begin{aligned}
L_{(AB)^2}^{(3)}(t_0,0) &= -i\big[C_{\{A,B\}[A,B]}^{\mathrm{phys}}(t_0,0) + C_{[A,B]\{A,B\}}^{\mathrm{phys}}(t_0,0)\big] \\
&+ iC_{[A^2,B^2]}(t_0,0).
\end{aligned} \quad (19)$$

The two terms in the square bracket in Eq. (19) coincide with those in the square bracket in Eq. (13) (with $t = t_0$ and $t' = 0$),[3] while the last term in Eq. (19), $L_{A^2 B^2}^{(1)}(t_0,0) \equiv -iC_{[A^2,B^2]}(t_0,0)$, is a linear-response function with respect to $\hat{A}^2$ and $\hat{B}^2$ (i.e., a linear response of $\langle\hat{A}(t_0)^2\rangle$ against a perturbation $\delta\hat{H}(t) = \hbar\varepsilon_B\delta(t)\hat{B}^2$), which can be measured independently. One can see that the right-hand side of (6), $2C_{\{A,B\}[A,B]}(t,t')$, is related to the response function $i[L_{(AB)^2}^{(3)}(t,t') + L_{A^2 B^2}^{(1)}(t,t')]$ within the difference of the WY skew information,

$$\begin{aligned}
2C_{\{A,B\}[A,B]}(t,t') &= i\big[L_{(AB)^2}^{(3)}(t,t') + L_{A^2 B^2}^{(1)}(t,t')\big] \\
&+ \frac{i}{4}I_{\frac{1}{2}}(\hat{\rho},\{\hat{A}(t),\hat{B}(t')\} + i[\hat{A}(t),\hat{B}(t')]) \\
&- \frac{i}{4}I_{\frac{1}{2}}(\hat{\rho},\{\hat{A}(t),\hat{B}(t')\} - i[\hat{A}(t),\hat{B}(t')]).
\end{aligned} \quad (20)$$

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[3]The present protocol measures $L_{(AB)^2}^{(3)}(t_0,0)$ for $t_0 > 0$. The remaining part ($t_0 < 0$) can be obtained by changing the protocol such that the system evolves with $-H$ from $t = 0$ to t_0 and with $+H$ from $t = t_0$ to $2t_0$.

The protocol has advantages that it can be applied to arbitrary thermal initial states and avoids multiple measurements that cause measurement back action. This is in contrast to the protocols described in Refs. [32,35], where the initial state is set to be an eigenstate of the operator $\hat{A}$ or $\hat{B}$ to readout the OTOC. This is equivalent to making a projection measurement at the initial time, which causes measurement back actions. A Loschmidt-echo-type protocol similar to the one shown in Fig. 1 has been proposed in Ref. [24]. The difference is that in the former one measures the nonlinear response function $L_{(AB)^2}(t,0)$ to reconstruct $\mathrm{Re}\langle\hat{A}(t)\hat{B}(0)\hat{A}(t)\hat{B}(0)\rangle = \frac{1}{4}[C^{\mathrm{phys}}_{\{A,B\}^2}(t,0) + C^{\mathrm{phys}}_{[A,B]^2}(t,0)]$ for Hermitian operators $\hat{A}$ and $\hat{B}$ via the out-of-time-order FDT (6), while in the latter one measures $|\langle\psi|\hat{W}^\dagger(t)\hat{V}^\dagger(0)\hat{W}(t)\hat{V}(0)|\psi\rangle|^2$ for unitary operators $\hat{V}$ and $\hat{W}$. The latter also requires the projection onto the initial state $|\psi\rangle$. We note that there are various other types of protocols which have been proposed to measure OTOCs [24,34,41,46–48].

The left-hand side of (6), on the other hand, is related to chaotic behavior in quantum many-body systems [16,22]. As we have mentioned, if $\hat{A}$ and $\hat{B}$ constitute a canonically conjugate pair, then $C^{\mathrm{phys}}_{[A,B]^2}(t,0) \sim -\hbar^2\langle\langle(\frac{\partial A(t)}{\partial A(0)})^2\rangle\rangle$ in the semiclassical regime, indicating an initial-value sensitivity of $A(t)$. In chaotic systems, $-\hbar^2\langle\langle(\frac{\partial A(t)}{\partial A(0)})^2\rangle\rangle$ is expected to grow exponentially in time ($\sim e^{\lambda t}$), where λ is an analog of the Lyapunov exponent. The exponential growth in $C^{\mathrm{phys}}_{[A,B]^2}(t,0)$ arises from its out-of-time-ordered part $\langle(\hat{A}(t)\hat{B}(0))^2\rangle + \langle(\hat{B}(0)\hat{A}(t))^2\rangle$ [22], which is equal to $\frac{1}{2}[C^{\mathrm{phys}}_{\{A,B\}^2}(t,0) + C^{\mathrm{phys}}_{[A,B]^2}(t,0)]$. Therefore, the left-hand side of Eq. (6) represents an initial-value sensitivity of a time-evolving observable (within the difference of the WY skew information). Based on these observations, we are led to a general principle that the nonlinear response defined in Eq. (17) is related to chaotic behavior in quantum systems through the out-of-time-order FDT (6). This allows one to access the exponentially growing part of the OTOC $\langle[\hat{A}(t),\hat{B}(0)]^2\rangle$ in chaotic systems by the nonlinear-response experiment. As far as the exponential growth of $\langle[\hat{A}(t),\hat{B}(0)]^2\rangle$ is concerned, the difference of the WY skew information, a measure of quantum fluctuations, is suppressed in the semiclassical regime of our interest.

In the strictly classical limit with $\hbar \to 0$, the out-of-time-order FDT (6) can be expressed as

$$\partial_t\langle\langle A(t)^2 B(t')^2\rangle\rangle = k_B T\langle\langle\{A(t)^2, B(t')^2\}_P\rangle\rangle. \quad (21)$$

We can see that the classical limit of (6) reduces to that of the conventional FDT (3) with $A(t)$ and $B(t)$ replaced by $A(t)^2$ and $B(t)^2$, respectively.

IV. PROOF OF THE OUT-OF-TIME-ORDER FLUCTUATION-DISSIPATION THEOREM

We now prove the equality (6). To this end, we introduce a representation of the bipartite OTOCs different from (4):

$$C^{\mu_1\mu_2}_{AB}(t,t') \equiv \mathrm{Tr}\big(\hat{\rho}^{\frac{1}{2}}(\hat{A}(t)\hat{B}(t'))^{\mu_1}\hat{\rho}^{\frac{1}{2}}(\hat{A}(t)\hat{B}(t'))^{\mu_2}\big), \quad (22)$$

where $\mu_1,\mu_2 = >, <$, and

$$(\hat{A}(t)\hat{B}(t'))^{\mu_i} \equiv \begin{cases} \hat{A}(t)\hat{B}(t') & \text{for } \mu_i = >, \\ \hat{B}(t')\hat{A}(t) & \text{for } \mu_i = <. \end{cases} \quad (23)$$

In the above definition, we do not include the minus sign for $\mu_i = <$ when both $\hat{A}$ and $\hat{B}$ are fermionic. However, all the arguments below can equally be applied to this case without any change. Again we have $C^{>>}_{AB} = C^{<>}_{AB}$ due to the cyclic invariance of the trace. The two representations (4) and (22) are connected by a linear transformation

$$L\begin{pmatrix} C^{>>}_{AB} & C^{><}_{AB} \\ C^{<>}_{AB} & C^{<<}_{AB} \end{pmatrix}L^T = \frac{1}{2}\begin{pmatrix} C_{[A,B]^2} & C_{[A,B]\{A,B\}} \\ C_{\{A,B\}[A,B]} & C_{\{A,B\}^2} \end{pmatrix}, \quad (24)$$

where

$$L \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad (25)$$

is an orthogonal matrix and L^T is the transpose of L. For convenience, we use notations $C_{(AB)^2}(t,t') \equiv C^{>>}_{AB}(t,t')$ and $C_{(BA)^2}(t',t) \equiv C^{<<}_{AB}(t,t')$. We note the parallelism of the formulation with that for Keldysh Green's functions [49–52].

We first show that $C_{(AB)^2}$ and $C_{(BA)^2}$ are related to each other by

$$C_{(BA)^2}(\omega) = e^{\frac{\beta\hbar\omega}{2}}C_{(AB)^2}(-\omega). \quad (26)$$

This relation is analogous to the Kubo-Martin-Schwinger condition $C_{BA}(\omega) = e^{\beta\hbar\omega}C_{AB}(-\omega)$ [3,53] for conventional correlation functions $C_{AB}(t,t') \equiv \mathrm{Tr}(\hat{\rho}\hat{A}(t)\hat{B}(t'))$. The equality (26) can be proven as follows. We insert four complete sets of the eigenstates $\sum_k|k\rangle\langle k|$ of the Hamiltonian $\hat{H}$ (with the eigenenergies E_k) in the definitions of $C_{(AB)^2}(t,t')$ and $C_{(BA)^2}(t,t')$, obtaining

$$C_{(AB)^2}(t,t') = \frac{1}{Z}\sum_{k,l,m,n} e^{-\frac{\beta}{2}(E_k+E_m)}e^{\frac{i}{\hbar}(E_k-E_l+E_m-E_n)(t-t')}$$
$$\times \langle k|\hat{A}|l\rangle\langle l|\hat{B}|m\rangle\langle m|\hat{A}|n\rangle\langle n|\hat{B}|k\rangle, \quad (27)$$

$$C_{(BA)^2}(t,t') = \frac{1}{Z}\sum_{k,l,m,n} e^{-\frac{\beta}{2}(E_k+E_m)}e^{\frac{i}{\hbar}(E_k-E_l+E_m-E_n)(t-t')}$$
$$\times \langle k|\hat{B}|l\rangle\langle l|\hat{A}|m\rangle\langle m|\hat{B}|n\rangle\langle n|\hat{A}|k\rangle. \quad (28)$$

By cyclically permuting the labels, $k \to l \to m \to n \to k$, we have

$$C_{(BA)^2}(t,t') = \frac{1}{Z}\sum_{k,l,m,n} e^{-\frac{\beta}{2}(E_l+E_n)}e^{-\frac{i}{\hbar}(E_k-E_l+E_m-E_n)(t-t')}$$
$$\times \langle k|\hat{A}|l\rangle\langle l|\hat{B}|m\rangle\langle m|\hat{A}|n\rangle\langle n|\hat{B}|k\rangle. \quad (29)$$

After the Fourier transformation, we obtain

$$C_{(AB)^2}(\omega) = \frac{1}{Z}\sum_{k,l,m,n} e^{-\frac{\beta}{2}(E_k+E_m)}$$
$$\times 2\pi\delta\left(\omega + \frac{1}{\hbar}(E_k - E_l + E_m - E_n)\right)$$
$$\times \langle k|\hat{A}|l\rangle\langle l|\hat{B}|m\rangle\langle m|\hat{A}|n\rangle\langle n|\hat{B}|k\rangle, \quad (30)$$

$$C_{(BA)^2}(\omega) = \frac{1}{Z}\sum_{k,l,m,n} e^{-\frac{\beta}{2}(E_l+E_n)}$$
$$\times 2\pi\delta\left(\omega - \frac{1}{\hbar}(E_k - E_l + E_m - E_n)\right)$$
$$\times \langle k|\hat{A}|l\rangle\langle l|\hat{B}|m\rangle\langle m|\hat{A}|n\rangle\langle n|\hat{B}|k\rangle. \quad (31)$$

Due to the presence of the δ function, we can replace $E_l + E_n$ in the exponential in Eq. (31) with $E_k + E_m - \hbar\omega$. By comparing it with Eq. (30), we obtain Eq. (26).

With the relation (26), the left-hand side of (6) is transformed as

$$C_{\{A,B\}^2}(\omega) + C_{[A,B]^2}(\omega) = 2C_{(AB)^2}(\omega) + 2C_{(BA)^2}(-\omega)$$
$$= 2\left(1 + e^{-\frac{\beta\hbar\omega}{2}}\right)C_{(AB)^2}(\omega), \quad (32)$$

while the right-hand side is

$$C_{\{A,B\}[A,B]}(\omega) = C_{(AB)^2}(\omega) - C_{(BA)^2}(-\omega)$$
$$= \left(1 - e^{-\frac{\beta\hbar\omega}{2}}\right)C_{(AB)^2}(\omega). \quad (33)$$

Combining Eqs. (32) and (33), we arrive at the out-of-time-order FDT (6). ∎

Let us recall that the FDT (3) can also be expressed as [3]

$$\beta\hbar\omega\,\Phi_{AB}(\omega) = C_{[A,B]}(\omega), \quad (34)$$

where Φ_{AB} is a canonical correlation (a quantum generalization of a classical correlator $\langle\langle A(t)B(t')\rangle\rangle$),

$$\Phi_{AB}(t,t') \equiv \int_0^1 d\lambda \,\text{Tr}(\hat{\rho}^{1-\lambda}\hat{A}(t)\hat{\rho}^{\lambda}\hat{B}(t')). \quad (35)$$

Analogously to this, the right-hand side of (6) can be rewritten in a form of a canonical bipartite OTOC defined as

$$\Phi_{(AB)^2}(t,t') \equiv \int_0^1 d\lambda \,\text{Tr}\left[\left(\hat{\rho}^{\frac{1-\lambda}{2}}\hat{A}(t)\hat{\rho}^{\frac{\lambda}{2}}\hat{B}(t')\right)^2\right]. \quad (36)$$

The second-order extension of (34) is written as

$$\beta\hbar\omega\,\Phi_{(AB)^2}(\omega) = 2C_{\{A,B\}[A,B]}(\omega). \quad (37)$$

The proof of (37) is given as a special case of (53) in Appendix A.

To clarify the meaning of Eq. (37), we note that $\Phi_{(AB)^2}(t,t')$ can be written as

$$\Phi_{(AB)^2}(t,t') = \int_0^1 d\lambda\, C_{(AB)^2}\left(t - i\lambda\frac{\beta\hbar}{2},t'\right). \quad (38)$$

That is, the time argument of the operator $\hat{A}$ is shifted to the direction of imaginary time. This type of deformation has been employed to regularize OTOCs in the context of quantum field theory [22]. Each λ represents a different choice of regularization. If the regularized OTOC $C_{(AB)^2}(t - i\lambda\frac{\beta\hbar}{2},0)$ shows an exponential growth for every choice of regularization (in order for the growth to be physical, it should not depend on the choice of the regularization), then its average (38) over the regularization parameter λ also shows an exponential growth. Then Eq. (37) says that the averaged exponential growth of the OTOCs on the left-hand side is related to the nonlinear response function on the right-hand side within the difference of the skew information [see Eq. (20)].

V. GENERALIZATION OF THE OUT-OF-TIME-ORDER FLUCTUATION-DISSIPATION THEOREM

The FDT (6) for OTOCs can be generalized in two ways. One is to extend the relation to higher-order OTOCs [52,54].

Let us define an n-partite OTOC,

$$C_{AB}^{\mu_1\mu_2\cdots\mu_n}(t,t') \equiv \text{Tr}\left[\prod_{i=1}^n \hat{\rho}^{\frac{1}{n}}(\hat{A}(t)\hat{B}(t'))^{\mu_i}\right], \quad (39)$$

with $\mu_1,\mu_2,\ldots,\mu_n = >,<$. In particular, we use abbreviations, $C_{(AB)^n}(t,t') \equiv C_{AB}^{>>\cdots>}(t,t')$ and $C_{(BA)^n}(t',t) \equiv C_{AB}^{<<\cdots<}(t,t')$. We perform a tensor transformation

$$C_{AB}^{\alpha_1\alpha_2\cdots\alpha_n}(t,t') \equiv 2^{\frac{n}{2}}\sum_{\mu_1,\ldots,\mu_n} L^{\alpha_1}{}_{\mu_1}L^{\alpha_2}{}_{\mu_2}\cdots L^{\alpha_n}{}_{\mu_n}$$
$$\times C_{AB}^{\mu_1\mu_2\cdots\mu_n}(t,t') \quad (40)$$

to switch to the commutator-anticommutator representation,

$$C_{AB}^{\alpha_1\alpha_2\cdots\alpha_n}(t,t') = C_{[A,B]_{\alpha_1}[A,B]_{\alpha_2}\cdots[A,B]_{\alpha_n}}(t,t')$$
$$= \text{Tr}\left(\prod_{i=1}^n \hat{\rho}^{\frac{1}{n}}[\hat{A}(t),\hat{B}(t')]_{\alpha_i}\right), \quad (41)$$

with $\alpha_1,\alpha_2,\ldots,\alpha_n = \pm$. The transformation (40) is a higher-order generalization of Eq. (24). There are redundancies in the definitions (39) and (41), $C_{AB}^{\mu_1\mu_2\cdots\mu_n}(t,t') = C_{AB}^{\mu_n\mu_1\cdots\mu_{n-1}}(t,t')$ and $C_{AB}^{\alpha_1\alpha_2\cdots\alpha_n}(t,t') = C_{AB}^{\alpha_n\alpha_1\cdots\alpha_{n-1}}(t,t')$, due to the cyclic invariance of the trace.

In the same way as for $n = 2$ [Eq. (26)], we can prove (see Appendix A)

$$C_{(BA)^n}(\omega) = e^{\frac{\beta\hbar\omega}{n}}C_{(AB)^n}(-\omega) \quad (42)$$

for arbitrary $n = 1,2,3,\ldots$. To rewrite the equality (42) in the form of the FDT, we carry out (anti)symmetrization like Eqs. (32) and (33),

$$C_{(\{A,B\}+[A,B])^n}(\omega) \pm C_{(\{A,B\}-[A,B])^n}(\omega)$$
$$= 2^n[C_{(AB)^n}(\omega) \pm C_{(BA)^n}(-\omega)]$$
$$= 2^n\left(1 \pm e^{-\frac{\beta\hbar\omega}{n}}\right)C_{(AB)^n}(\omega). \quad (43)$$

By taking the ratio of both sides of Eq. (43) between the ones with $+$ and $-$ signs and explicitly expanding $(\{A,B\} \pm [A,B])^n$, we arrive at

$$\sum_{\alpha_1,\alpha_2,\ldots,\alpha_n=\pm}^{\alpha_1\alpha_2\cdots\alpha_n=+} C_{AB}^{\alpha_1\alpha_2\cdots\alpha_n}(\omega)$$
$$= \coth\left(\frac{\beta\hbar\omega}{2n}\right)\sum_{\alpha_1,\alpha_2,\ldots,\alpha_n=\pm}^{\alpha_1\alpha_2\cdots\alpha_n=-} C_{AB}^{\alpha_1\alpha_2\cdots\alpha_n}(\omega). \quad (44)$$

Equation (44) is the nth-order generalization of the out-of-time-order FDT.

The right-hand side of Eq. (44) can be expressed in the form of a canonical correlation, similarly to Eq. (37). We define an n-partite canonical OTOC as

$$\Phi_{(AB)^n}(t,t') \equiv \int_0^1 d\lambda\,\text{Tr}\left[\left(\hat{\rho}^{\frac{1-\lambda}{n}}\hat{A}(t)\hat{\rho}^{\frac{\lambda}{n}}\hat{B}(t')\right)^n\right]. \quad (45)$$

Following the same calculation as for $n = 2$, we can prove (see Appendix A)

$$\sum_{\alpha_1,\alpha_2,\ldots,\alpha_n=\pm}^{\alpha_1\alpha_2\cdots\alpha_n=+} C_{AB}^{\alpha_1\alpha_2\cdots\alpha_n}(\omega) = \frac{2^{n-1}}{n}\beta\hbar\omega\coth\left(\frac{\beta\hbar\omega}{2n}\right)\Phi_{(AB)^n}(\omega).$$
$$(46)$$

In this way, we have obtained infinitely many rigorous equalities [(44) and (46)] for OTOCs. The classical limit of Eq. (44) formally becomes

$$\partial_t \langle\langle A(t)^n B(t')^n \rangle\rangle = k_B T \langle\langle \{A(t)^n, B(t')^n\}_P \rangle\rangle, \qquad (47)$$

which corresponds to that of the conventional FDT (3) with $A(t)$ and $B(t)$ replaced by $A(t)^n$ and $B(t)^n$, respectively.

The other generalization is that the FDT holds not only for OTOCs in the form of $\mathrm{Tr}(\hat{\rho}^{\frac{1}{2}} \hat{A}(t) \hat{B}(t') \hat{\rho}^{\frac{1}{2}} \hat{A}(t) \hat{B}(t'))$ but also in the form of $\mathrm{Tr}(\hat{\rho}^{\frac{1-\gamma}{2}} \hat{A}(t) \hat{\rho}^{\frac{\gamma}{2}} \hat{B}(t') \hat{\rho}^{\frac{1-\gamma}{2}} \hat{A}(t) \hat{\rho}^{\frac{\gamma}{2}} \hat{B}(t'))$, i.e., the operator ordering is rearranged. For usual time-ordered correlators, this type of rearrangement of operator ordering shows up in the context of the generalized covariance [55,56] defined by

$$C_{AB}^f(t,t') \equiv \mathrm{Tr}\big(\hat{A}(t) \boldsymbol{K}_{\hat{\rho}}^f[\hat{B}(t')]\big), \qquad (48)$$

where $\boldsymbol{K}_{\hat{\rho}}^f \equiv f(\boldsymbol{L}_{\hat{\rho}} \boldsymbol{R}_{\hat{\rho}}^{-1}) \boldsymbol{R}_{\hat{\rho}}$ is a superoperator, $\boldsymbol{R}_{\hat{\rho}}$ ($\boldsymbol{L}_{\hat{\rho}}$) denotes an operation of multiplying $\hat{\rho}$ from the right-hand side (left-hand side), and $f(x)$ is an operator monotone function satisfying $0 \leqslant \hat{A} \leqslant \hat{B} \Rightarrow f(\hat{A}) \leqslant f(\hat{B})$. Equation (48) generalizes the classical covariance for two observables that do not necessarily commute with $\hat{\rho}$. The generalized covariance has played a key role in estimation theory involving the quantum Fisher information [57–59]. The conventional FDT (3) has recently been generalized to [60]

$$C_{AB}^f(\omega) = \beta\hbar\omega \frac{f(e^{-\beta\hbar\omega})}{1 - e^{-\beta\hbar\omega}} \Phi_{AB}(\omega), \qquad (49)$$

which provides a means to measure the generalized covariance through the response function. The relation (34) is a special case of Eq. (49) with $f(x) = \frac{1+x}{2}$.

With the generalized covariance, the n-partite OTOC is generalized in the form of

$$C_{(AB)^n}^f(t,t') \equiv \mathrm{Tr}\big(\big[\hat{A}(t) \boldsymbol{K}_{\hat{\rho}^{1/n}}^f[\hat{B}(t')]\big]^n\big). \qquad (50)$$

In particular, if we take $f(x) = x^\gamma$ with $0 \leqslant \gamma \leqslant 1$, then Eq. (50) reads

$$C_{(AB)^n}^f(t,t') = C_{(AB)^n}^\gamma(t,t') = \mathrm{Tr}\big(\big[\hat{A}(t) \hat{\rho}^{\frac{\gamma}{n}} \hat{B}(t') \hat{\rho}^{\frac{1-\gamma}{n}}\big]^n\big). \qquad (51)$$

Following similar calculations used in deriving Eqs. (42) and (44), we can prove (see Appendix A)

$$C_{(BA)^n}^\gamma(\omega) = e^{\frac{1-2\gamma}{n}\beta\hbar\omega} C_{(AB)^n}^\gamma(-\omega), \qquad (52)$$

which reduces to Eq. (42) for $\gamma = 0$ and leads to a generalized out-of-time-order FDT,

$$\sum_{\alpha_1,\alpha_2,\ldots,\alpha_n=\pm}^{\alpha_1\alpha_2\cdots\alpha_n=+} C_{AB}^{\gamma,\alpha_1\alpha_2\cdots\alpha_n}(\omega) = \coth\left((1-2\gamma)\frac{\beta\hbar\omega}{2n}\right) \sum_{\alpha_1,\alpha_2,\ldots,\alpha_n=\pm}^{\alpha_1\alpha_2\cdots\alpha_n=-} C_{AB}^{\gamma,\alpha_1\alpha_2\cdots\alpha_n}(\omega) \qquad (53)$$

$$= \frac{2^{n-1}}{n} \beta\hbar\omega \coth\left((1-2\gamma)\frac{\beta\hbar\omega}{2n}\right) \Phi_{(AB)^n}^\gamma(\omega). \qquad (54)$$

Here we define

$$C_{AB}^{\gamma,\alpha_1\alpha_2\cdots\alpha_n}(t,t')$$
$$\equiv \mathrm{Tr}\left(\prod_{i=1}^n \big[\hat{A}(t) \hat{\rho}^{\frac{\gamma}{n}} \hat{B}(t') \hat{\rho}^{\frac{1-\gamma}{n}} + \alpha_i \hat{B}(t') \hat{\rho}^{\frac{\gamma}{n}} \hat{A}(t) \hat{\rho}^{\frac{1-\gamma}{n}}\big]\right), \qquad (55)$$

$$\Phi_{(AB)^n}^\gamma(t,t') \equiv \int_\gamma^{1-\gamma} d\lambda \, \mathrm{Tr}\big[\big(\hat{\rho}^{\frac{1-\lambda}{n}} \hat{A}(t) \hat{\rho}^{\frac{\lambda}{n}} \hat{B}(t')\big)^n\big]. \qquad (56)$$

The equality (53) is the most general form of the out-of-time-order FDT derived in this paper, which includes Eqs. (6) and (44) as special cases. Let us remark that for $f(x) = x^\gamma$ to be operator monotone we need $0 \leqslant \gamma \leqslant 1$. However, the equalities (52), (53), and (54) hold for arbitrary $\gamma \in \mathbb{R}$.

VI. CONCLUSION

In conclusion, we have found the generalized fluctuation-dissipation theorem [Eqs. (6) and (37)] for bipartite out-of-time-ordered correlation functions [Eq. (4)]. The theorem describes the general relationship between chaotic behavior in quantum systems and a nonlinear response. The difference between the bipartite and physical OTOCs is characterized by the Wigner-Yanase skew information [Eqs. (11)–(13)], which quantifies the information contents involved in the corresponding quantum fluctuations. We have further extended the theorem to n-partite OTOCs [Eqs. (44) and (46)] and in the form of the generalized covariance [Eqs. (53) and (54)]. Our results bring up various interesting open questions such as the physical meaning of the higher-order out-of-time-order FDTs ($n \geqslant 3$) that are expected to be related to higher-order response functions and the relation to the fluctuation theorem [7,8] (see also Ref. [47]), which merit further study.

APPENDIX: PROOF OF EQS. (37), (42), (46), (52), (53), AND (54)

In this appendix, we prove the equalities (52), (53), and (54) given in the main text, i.e.,

$$C_{(BA)^n}^{\gamma}(\omega) = e^{\frac{1-2\gamma}{n}\beta\hbar\omega} C_{(AB)^n}^{\gamma}(-\omega) \tag{A1}$$

and

$$\sum_{\alpha_1,\alpha_2,\ldots,\alpha_n=\pm}^{\alpha_1\alpha_2\cdots\alpha_n=+} C_{AB}^{\gamma,\alpha_1\alpha_2\cdots\alpha_n}(\omega) = \coth\left[(1-2\gamma)\frac{\beta\hbar\omega}{2n}\right] \sum_{\alpha_1,\alpha_2,\ldots,\alpha_n=\pm}^{\alpha_1\alpha_2\cdots\alpha_n=-} C_{AB}^{\gamma,\alpha_1\alpha_2\cdots\alpha_n}(\omega) \tag{A2}$$

$$= \frac{2^{n-1}}{n}\beta\hbar\omega \coth\left[(1-2\gamma)\frac{\beta\hbar\omega}{2n}\right]\Phi_{(AB)^n}^{\gamma}(\omega). \tag{A3}$$

with $n = 1,2,3,\ldots$. Here $C_{(AB)^n}^{\gamma}(\omega)$ and $C_{(BA)^n}^{\gamma}(\omega)$ in Eq. (A1) are the Fourier transforms of n-partite OTOCs

$$C_{(AB)^n}^{\gamma}(t,t') = \text{Tr}\left(\left[\hat{A}(t)\hat{\rho}^{\frac{\gamma}{n}}\hat{B}(t')\hat{\rho}^{\frac{1-\gamma}{n}}\right]^n\right), \tag{A4}$$

$$C_{(BA)^n}^{\gamma}(t,t') = \text{Tr}\left(\left[\hat{B}(t)\hat{\rho}^{\frac{\gamma}{n}}\hat{A}(t')\hat{\rho}^{\frac{1-\gamma}{n}}\right]^n\right). \tag{A5}$$

Equalities (42) and (46) in the main text are the special cases of Eqs. (A1) and (A3) with $\gamma = 0$, and the equality (37) in the main text is the special case of Eq. (A3) with $n = 2$ and $\gamma = 0$.

First, we expand $C_{(AB)^n}^{\gamma}(t,t')$ and $C_{(BA)^n}^{\gamma}(t,t')$ in the basis of the eigenstates of the Hamiltonian $\hat{H}$,

$$C_{(AB)^n}^{\gamma}(t,t') = \frac{1}{Z}\sum_{i_1\cdots i_{2n}} e^{-\frac{(1-\gamma)\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}})-\frac{\gamma\beta}{n}(E_{i_2}+E_{i_4}+\cdots+E_{i_{2n}})} e^{\frac{i}{\hbar}(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots+E_{i_{2n-1}}-E_{i_{2n}})(t-t')}$$
$$\times \langle i_1|\hat{A}|i_2\rangle\langle i_2|\hat{B}|i_3\rangle\langle i_3|\hat{A}|i_4\rangle\langle i_4|\hat{B}|i_5\rangle\cdots\langle i_{2n-1}|\hat{A}|i_{2n}\rangle\langle i_{2n}|\hat{B}|i_1\rangle, \tag{A6}$$

$$C_{(BA)^n}^{\gamma}(t,t') = \frac{1}{Z}\sum_{i_1\cdots i_{2n}} e^{-\frac{(1-\gamma)\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}})-\frac{\gamma\beta}{n}(E_{i_2}+E_{i_4}+\cdots+E_{i_{2n}})} e^{\frac{i}{\hbar}(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots+E_{i_{2n-1}}-E_{i_{2n}})(t-t')}$$
$$\times \langle i_1|\hat{B}|i_2\rangle\langle i_2|\hat{A}|i_3\rangle\langle i_3|\hat{B}|i_4\rangle\langle i_4|\hat{A}|i_5\rangle\cdots\langle i_{2n-1}|\hat{B}|i_{2n}\rangle\langle i_{2n}|\hat{A}|i_1\rangle. \tag{A7}$$

Then we permute the summation indices as $i_1 \to i_2 \to i_3 \to \cdots \to i_{2n-1} \to i_{2n} \to i_1$ in Eq. (A7), obtaining

$$C_{(BA)^n}^{\gamma}(t,t') = \frac{1}{Z}\sum_{i_1\cdots i_{2n}} e^{-\frac{(1-\gamma)\beta}{n}(E_{i_2}+E_{i_4}+\cdots+E_{i_{2n}})-\frac{\gamma\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}})} e^{-\frac{i}{\hbar}(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots+E_{i_{2n-1}}-E_{i_{2n}})(t-t')}$$
$$\times \langle i_1|\hat{A}|i_2\rangle\langle i_2|\hat{B}|i_3\rangle\langle i_3|\hat{A}|i_4\rangle\langle i_4|\hat{B}|i_5\rangle\cdots\langle i_{2n-1}|\hat{A}|i_{2n}\rangle\langle i_{2n}|\hat{B}|i_1\rangle. \tag{A8}$$

Fourier transforming Eqs. (A6) and (A8), we obtain

$$C_{(AB)^n}^{\gamma}(\omega) = \frac{1}{Z}\sum_{i_1\cdots i_{2n}} e^{-\frac{(1-\gamma)\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}})-\frac{\gamma\beta}{n}(E_{i_2}+E_{i_4}+\cdots+E_{i_{2n}})} 2\pi\delta\left(\omega + \frac{1}{\hbar}\left(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots+E_{i_{2n-1}}-E_{i_{2n}}\right)\right)$$
$$\times \langle i_1|\hat{A}|i_2\rangle\langle i_2|\hat{B}|i_3\rangle\langle i_3|\hat{A}|i_4\rangle\langle i_4|\hat{B}|i_5\rangle\cdots\langle i_{2n-1}|\hat{A}|i_{2n}\rangle\langle i_{2n}|\hat{B}|i_1\rangle, \tag{A9}$$

$$C_{(BA)^n}^{\gamma}(\omega) = \frac{1}{Z}\sum_{i_1\cdots i_{2n}} e^{-\frac{(1-\gamma)\beta}{n}(E_{i_2}+E_{i_4}+\cdots+E_{i_{2n}})-\frac{\gamma\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}})} 2\pi\delta\left(\omega - \frac{1}{\hbar}\left(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots+E_{i_{2n-1}}-E_{i_{2n}}\right)\right)$$
$$\times \langle i_1|\hat{A}|i_2\rangle\langle i_2|\hat{B}|i_3\rangle\langle i_3|\hat{A}|i_4\rangle\langle i_4|\hat{B}|i_5\rangle\cdots\langle i_{2n-1}|\hat{A}|i_{2n}\rangle\langle i_{2n}|\hat{B}|i_1\rangle. \tag{A10}$$

Due to the presence of the δ function, we can replace $E_{i_2} + E_{i_4} + \cdots + E_{i_{2n}}$ with $E_{i_1} + E_{i_3} + \cdots + E_{i_{2n-1}} - \hbar\omega$, and $E_{i_1} + E_{i_3} + \cdots + E_{i_{2n-1}}$ with $E_{i_2} + E_{i_4} + \cdots + E_{i_{2n}} + \hbar\omega$ in the exponential in Eq. (A10), which results in

$$C_{(BA)^n}^{\gamma}(\omega) = \frac{1}{Z}\sum_{i_1\cdots i_{2n}} e^{-\frac{(1-\gamma)\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}}-\hbar\omega)-\frac{\gamma\beta}{n}(E_{i_2}+E_{i_4}+\cdots+E_{i_{2n}}+\hbar\omega)}$$
$$\times 2\pi\delta\left(\omega - \frac{1}{\hbar}\left(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots+E_{i_{2n-1}}-E_{i_{2n}}\right)\right)$$
$$\times \langle i_1|\hat{A}|i_2\rangle\langle i_2|\hat{B}|i_3\rangle\langle i_3|\hat{A}|i_4\rangle\langle i_4|\hat{B}|i_5\rangle\cdots\langle i_{2n-1}|\hat{A}|i_{2n}\rangle\langle i_{2n}|\hat{B}|i_1\rangle. \tag{A11}$$

By comparing this with Eq. (A9), we prove the equality (52) [i.e., (A1)].

Next, we consider

$$
\sum_{\alpha_1,\alpha_2,\ldots,\alpha_n=\pm}^{\alpha_1\alpha_2\cdots\alpha_n=+(-)} C_{AB}^{\gamma,\alpha_1\alpha_2\cdots\alpha_n}(\omega)
$$

$$
= \int_{-\infty}^{\infty} dt\, e^{i\omega t} \frac{1}{2}\mathrm{Tr}\Big(\big[\big(\hat{A}(t)\hat{\rho}^{\frac{\gamma}{n}}\hat{B}(0)\hat{\rho}^{\frac{1-\gamma}{n}} + \hat{B}(0)\hat{\rho}^{\frac{\gamma}{n}}\hat{A}(t)\hat{\rho}^{\frac{1-\gamma}{n}}\big) + \big(\hat{A}(t)\hat{\rho}^{\frac{\gamma}{n}}\hat{B}(0)\hat{\rho}^{\frac{1-\gamma}{n}} - \hat{B}(0)\hat{\rho}^{\frac{\gamma}{n}}\hat{A}(t)\hat{\rho}^{\frac{1-\gamma}{n}}\big)\big]^n
$$

$$
+ (-)\big[\big(\hat{A}(t)\hat{\rho}^{\frac{\gamma}{n}}\hat{B}(0)\hat{\rho}^{\frac{1-\gamma}{n}} + \hat{B}(0)\hat{\rho}^{\frac{\gamma}{n}}\hat{A}(t)\hat{\rho}^{\frac{1-\gamma}{n}}\big) - \big(\hat{A}(t)\hat{\rho}^{\frac{\gamma}{n}}\hat{B}(0)\hat{\rho}^{\frac{1-\gamma}{n}} - \hat{B}(0)\hat{\rho}^{\frac{\gamma}{n}}\hat{A}(t)\hat{\rho}^{\frac{1-\gamma}{n}}\big)\big]^n\Big)
$$

$$
= \int_{-\infty}^{\infty} dt\, e^{i\omega t} 2^{n-1}\mathrm{Tr}\big(\big[\hat{A}(t)\hat{\rho}^{\frac{\gamma}{n}}\hat{B}(0)\hat{\rho}^{\frac{1-\gamma}{n}}\big]^n + (-)\big[\hat{B}(0)\hat{\rho}^{\frac{\gamma}{n}}\hat{A}(t)\hat{\rho}^{\frac{1-\gamma}{n}}\big]^n\big)
$$

$$
= 2^{n-1}\big[C_{(AB)^n}^{\gamma}(\omega) + (-)C_{(BA)^n}^{\gamma}(-\omega)\big] = 2^{n-1}\big[1 + (-)e^{-\frac{(1-2\gamma)}{n}\beta\hbar\omega}\big]C_{(AB)^n}^{\gamma}(\omega). \tag{A12}
$$

Here we have used the relation (52) in deriving the fourth equality. Taking the ratio of both sides of Eq. (A12) between the ones with $+$ and $-$ signs proves Eq. (53) [i.e., (A2)].

Finally, we expand the partial n-partite canonical OTOC $\Phi_{(AB)^n}^{\gamma}(t,t')$ defined by Eq. (56) in the basis of the eigenstates of the Hamiltonian $\hat{H}$,

$$
\Phi_{(AB)^n}^{\gamma}(t,t') = \frac{1}{Z}\int_{\gamma}^{1-\gamma} d\lambda \sum_{i_1\cdots i_{2n}} e^{-\frac{\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}})} e^{\frac{\lambda\beta}{n}(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots+E_{2n-1}-E_{2n})} e^{\frac{i}{\hbar}(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots+E_{2n-1}-E_{2n})(t-t')}
$$

$$
\times \langle i_1|\hat{A}|i_2\rangle\langle i_2|\hat{B}|i_3\rangle\langle i_3|\hat{A}|i_4\rangle\langle i_4|\hat{B}|i_5\rangle\cdots\langle i_{2n-1}|\hat{A}|i_{2n}\rangle\langle i_{2n}|\hat{B}|i_1\rangle, \tag{A13}
$$

which is Fourier transformed into

$$
\Phi_{(AB)^n}^{\gamma}(\omega) = \frac{1}{Z}\int_{\gamma}^{1-\gamma} d\lambda\, e^{-\frac{\lambda\beta}{n}\hbar\omega} \sum_{i_1\cdots i_{2n}} e^{-\frac{\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}})} 2\pi\delta\bigg(\omega + \frac{1}{\hbar}\big(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots-E_{2n}\big)\bigg)
$$

$$
\times \langle i_1|\hat{A}|i_2\rangle\langle i_2|\hat{B}|i_3\rangle\langle i_3|\hat{A}|i_4\rangle\langle i_4|\hat{B}|i_5\rangle\cdots\langle i_{2n-1}|\hat{A}|i_{2n}\rangle\langle i_{2n}|\hat{B}|i_1\rangle
$$

$$
= \frac{1}{Z}\frac{e^{-\frac{\gamma}{n}\beta\hbar\omega} - e^{-\frac{(1-\gamma)}{n}\beta\hbar\omega}}{\beta\hbar\omega/n} \sum_{i_1\cdots i_{2n}} e^{-\frac{\beta}{n}(E_{i_1}+E_{i_3}+\cdots+E_{i_{2n-1}})} 2\pi\delta\bigg(\omega + \frac{1}{\hbar}\big(E_{i_1}-E_{i_2}+E_{i_3}-E_{i_4}+\cdots-E_{2n}\big)\bigg)
$$

$$
\times \langle i_1|\hat{A}|i_2\rangle\langle i_2|\hat{B}|i_3\rangle\langle i_3|\hat{A}|i_4\rangle\langle i_4|\hat{B}|i_5\rangle\cdots\langle i_{2n-1}|\hat{A}|i_{2n}\rangle\langle i_{2n}|\hat{B}|i_1\rangle. \tag{A14}
$$

By comparing this with Eq. (A9), we obtain

$$
\Phi_{(AB)^n}^{\gamma}(\omega) = \frac{n}{\beta\hbar\omega}\big[1 - e^{-\frac{(1-2\gamma)}{n}\beta\hbar\omega}\big]C_{(AB)^n}^{\gamma}(\omega). \tag{A15}
$$

The combination of Eqs. (A12) and (A15) proves Eq. (54) [i.e., (A3)]. ∎

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