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Possibility of the total thermodynamic entropy production rate of a finite-sized isolated quantum system to be negative for the Gorini-Kossakowski-Sudarshan-Lindblad-type Markovian dynamics of its subsystem

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We investigate a total thermodynamic entropy production rate of an isolated quantum system. In particular, we consider a quantum model of coupled harmonic oscillators in a star configuration, where a central harmonic oscillator (system) is coupled to a finite number of surrounding harmonic oscillators (bath). In this model, when the initial state of the total system is given by the tensor product of the Gibbs states of the system and the bath, every harmonic oscillator is always in a Gibbs state with a time-dependent temperature. This enables us to define time-dependent thermodynamic entropy for each harmonic oscillator and total nonequilibrium thermodynamic entropy as the summation of them. We analytically confirm that the total thermodynamic entropy satisfies the third law of thermodynamics. Our numerical solutions show that, even when the dynamics of the system is well approximated by the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL)-type Markovian master equation, the total thermodynamic entropy production rate can be negative, while the total thermodynamic entropy satisfies the second law of thermodynamics. This result is a counterexample to the common belief that the total entropy production rate is non-negative when the system is under the GKSL-type Markovian dynamics.

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I. INTRODUCTION

Thermodynamics of macroscopic systems explains their macroscopic thermodynamic changes, where microscopic fluctuations can be neglected [1–3]. On the other hand, because of the development of nanotechnology, researchers in recent years have tried to extend the conventional thermodynamics to the microscopic world, where not only thermal but also quantum fluctuations cannot be neglected. This research field is called quantum thermodynamics [4–6], which explains microscopic thermodynamic changes of microscopic systems and macroscopic ones.

One of the most fundamental problems in quantum thermodynamics is how to define thermodynamic quantities such as thermodynamic entropy, temperature, heat, and work. Of particular importance is the thermodynamic entropy, because it characterizes the irreversibility of thermodynamics. This is why researchers have suggested several definitions of thermodynamic entropy [7–9] and various definitions of entropy production and of its rate; see Ref. [10] and references therein. However, there is no consensus for now. The connection between the entropy production and quantum information [11, Sec. 5.4], such as quantum cryptography [12], is also currently being investigated.

One of the typical setups in quantum thermodynamics is a quantum system coupled with a bath. The system is open [13,14], and the total system, which is a compound of the system and the bath, is isolated (closed) when the total Hamiltonian is time independent (time dependent) [14, Sec. 3.1.1]. There is active research [15–20] into the relation between non-Markovianity [21] of the dynamics of an open quantum system and a negative entropy production rate of the total system. However, there is no agreement about this relation mainly because there is no unified definition of the entropy production rate or of non-Markovianity. On the other hand, when an open quantum system is under the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL)-type Markovian dynamics [13,14,22–24], it is widely believed that the entropy production rate of the total system is non-negative [15–20], and researchers often use the von Neumann entropy production rate [25], which is the minus time-derivative of the von Neumann relative entropy [26, Sec. 11.8] between the reduced state of the system and the reference stationary state of the GKSL master equation. As we will see later, there is an implicit assumption in the form of the von Neumann entropy production rate that the size of a bath is so macroscopically large that its temperature does not change during the dynamics. However, when the size of the bath is finite, the temperature of the bath varies with time in general [7]. Then, we cannot use the von Neumann entropy production rate.

In this paper, we define and investigate a total thermodynamic entropy production rate of an isolated quantum system which consists of a system and a finite-sized bath. In particular, we consider a quantum model of coupled harmonic

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oscillators in a star configuration. We show that, contrary to the common belief, the entropy production rate of the total system can be negative even when the dynamics of the central harmonic oscillator (system) is well approximated by the GKSL master equation. This comes from the temperature changes of the surrounding harmonic oscillators (bath).

This paper is organized as follows. In Sec. II we review thermodynamic entropy of macroscopic systems and the von Neumann entropy production rate. In Sec. III we introduce our model, the initial state, and the dynamics. In Sec. IV we show that every harmonic oscillator is in a Gibbs state with a time-dependent temperature in our settings. We thus define the time-dependent thermodynamic entropy of each harmonic oscillator in a similar way to the definition in equilibrium thermodynamics and statistical mechanics. Then we define the nonequilibrium thermodynamic entropy of the total system as the summation of them. This total thermodynamic entropy satisfies the third law of thermodynamics. In Sec. V, considering the GKSL-type Markovian dynamics of the system, we show numerically that our total thermodynamic entropy production rate can take negative values, while our total thermodynamic entropy satisfies the second law of thermodynamics. In Sec. VI we draw a conclusion.

II. REVIEW OF THERMODYNAMIC ENTROPY AND OF ENTROPY PRODUCTION RATE

A. Thermodynamic entropy of macroscopic systems

Equilibrium thermodynamics of macroscopic systems is an established theory [1,2]. The irreversibility of thermodynamics is expressed by its second law, which can be cast into the form of the principle of increasing total thermodynamic entropy [1, Sec. 14.2] [27]. Let us prepare an adiabatic system in an equilibrium state with some constraints (for example, a system consisting of the two subsystems with different temperatures separated by an adiabatic wall). If we get rid of the constraints (e.g., remove the wall) at time $t_{\rm ini}$, the system would change to a new equilibrium state at time $t_{\rm fin}$. The final total thermodynamic entropy $S^{\rm th}_{\rm tot}(t_{\rm fin})$ must be greater than or equal to the initial one $S^{\rm th}_{\rm tot}(t_{\rm ini})$:

$$\Delta S^{\rm th}_{\rm tot}(t_{\rm fin}) = S^{\rm th}_{\rm tot}(t_{\rm fin}) - S^{\rm th}_{\rm tot}(t_{\rm ini}) \geqslant 0, \tag{1}$$

where $\Delta S^{\rm th}_{\rm tot}(t) := S^{\rm th}_{\rm tot}(t) - S^{\rm th}_{\rm tot}(t_{\rm ini})$ denotes the total thermodynamic entropy production from $t_{\rm ini}$ to t. This is the principle of increasing total thermodynamic entropy. Here, the word "total" refers to the adiabatic system itself, excluding its environment, and is used to distinguish $\Delta S^{\rm th}_{\rm tot}(t)$ from the internal thermodynamic entropy production, which we will explain later. Note that the principle deals with the thermodynamic-entropy difference only between the initial and final equilibrium states. This does not forbid the total thermodynamic entropy from decreasing during the intermediate nonequilibrium process [1, Sec. 14.2]. In other words, the total thermodynamic entropy production rate $\Pi^{\rm th}_{\rm tot}(t) := dS^{\rm th}_{\rm tot}(t)/dt$ can be negative for some time t.

Actually, the theory of nonequilibrium thermodynamics of macroscopic systems, including a proper definition of nonequilibrium thermodynamic entropy $S^{\rm th}(t)$, has not been established yet [3]. However, the entropy balance [3, Sec. 2.3], which we will explain below, is considered to hold universally. Let us consider a system A and its environment B, whose thermodynamic entropies are defined as $S^{\rm th}_A(t)$ and $S^{\rm th}_B(t)$, respectively. The time derivative of $S^{\rm th}_A(t)$ is written as the sum of the internal thermodynamic entropy production rate of the system $d^{\rm int}S^{\rm th}_A(t)/dt$ and the thermodynamic entropy flux into the system $d^{\rm ext}S^{\rm th}_A(t)/dt$ as follows:

$$\frac{d}{dt}S^{\rm th}_A(t) = \frac{d^{\rm int}}{dt}S^{\rm th}_A(t) + \frac{d^{\rm ext}}{dt}S^{\rm th}_A(t). \tag{2}$$

This is the entropy balance. We must distinguish the internal thermodynamic entropy production, which is the time integral of its rate, from the total one. When the temperature $T_A(t)$ of the system A is defined, the entropy flux into the system A is defined as [3, Sec. 1.3.3.2]

$$\frac{d^{\rm ext}}{dt}S^{\rm th}_A(t) := \frac{1}{T_A(t)}\frac{đQ_A(t)}{dt}, \tag{3}$$

where $đQ_A(t)/dt$ is the heat flux into the system A and the bar in $đQ_A(t)$ means that it is an inexact differential [3, Sec. 1.3.2]. Then, the internal entropy production rate of the system A is determined from Eqs. (2) and (3). On the other hand, when the temperature $T_A(t)$ of the system A is not defined, it is a subject of research how to define $d^{\rm int}S^{\rm th}_A(t)/dt$ and $d^{\rm ext}S^{\rm th}_A(t)/dt$. A similar relation to Eq. (2) holds for the environment:

$$\frac{d}{dt}S^{\rm th}_B(t) = \frac{d^{\rm int}}{dt}S^{\rm th}_B(t) + \frac{d^{\rm ext}}{dt}S^{\rm th}_B(t). \tag{4}$$

The point is that the entropy flux into the system does not equal that out of the environment in general:

$$\frac{d^{\rm ext}}{dt}S^{\rm th}_A(t) \neq -\frac{d^{\rm ext}}{dt}S^{\rm th}_B(t). \tag{5}$$

In order to recognize this point, let us consider the following example [2, Sec. 4.3] [3, Sec. 7.1.1]. Prepare an isolated system composed of the two subsystems A and B. There are two fixed walls between A and B: an adiabatic wall and a diathermal wall. The subsystem A (B) is in an equilibrium state with temperature T^0_A ($T^0_B(> T^0_A)$). The total system is also at equilibrium. Then remove the adiabatic wall at time $t_{\rm ini}$, and heat begins to flow from B to A through the diathermal wall and continues flowing until the two subsystems are of equal temperature at time $t_{\rm fin}$. Let us assume that the thermal conductivity of the diathermal wall is so small that each of the two subsystems should be always in an equilibrium state and that their temperatures $T_A(t)$ and $T_B(t)$ change very slowly during the process. We call this process quasistatic [2, Sec. 4.3] for both A and B, meaning that they are always in an equilibrium state. We note that there are other definitions of quasistatic processes; see, for example, Sec. 12.6 in Ref. [1].

Let us describe the internal energy of the subsystem A as $E_A(t)$. From the first law of thermodynamics, the change of $E_A(t)$ equals to the sum of the heat Q_A into A and the work W_A done on A: $\Delta E_A(t) = Q_A + W_A$. In the present example, W_A is always zero because of the fixed diathermal wall. Hence the heat flux into the subsystem A is given by $dE_A(t)/dt$. From the law of energy conservation, the heat flux into the subsystem B

is given by $-dE_A(t)/dt$. Then the entropy fluxes into the two subsystems are defined as

$$\frac{d^{\rm ext}}{dt}S_A^{\rm th}(t)=\frac{1}{T_A(t)}\frac{dE_A(t)}{dt}, \tag{6}$$

$$\frac{d^{\rm ext}}{dt}S_B^{\rm th}(t)=-\frac{1}{T_B(t)}\frac{dE_A(t)}{dt}. \tag{7}$$

These equations show that the entropy flux into A does not equal that out of B at $t\neq t_{\rm fin}$ because $T_A(t)\neq T_B(t)$. As the process is quasistatic for both A and B, the time derivatives of the thermodynamic entropies of the two subsystems are given by [2, Sec. 4.3]

$$\frac{d}{dt}S_A^{\rm th}(t)=\frac{1}{T_A(t)}\frac{dE_A(t)}{dt}, \tag{8}$$

$$\frac{d}{dt}S_B^{\rm th}(t)=-\frac{1}{T_B(t)}\frac{dE_A(t)}{dt}. \tag{9}$$

Combining Eqs. (2), (4), and (6)–(9), we find that the internal thermodynamic entropy production rates of the two subsystems are both zero:

$$\frac{d^{\rm int}}{dt}S_A^{\rm th}(t)=\frac{d^{\rm int}}{dt}S_B^{\rm th}(t)=0. \tag{10}$$

We regard this as the sign that the process is quasistatic for both A and B.

Let us confirm that the above example satisfies the principle of increasing total thermodynamic entropy (1). The total thermodynamic entropy production rate is the sum of the variation rates of the thermodynamic entropies of the two subsystems:

$$\begin{aligned}\Pi_{\rm tot}^{\rm th}(t)&=\frac{d}{dt}S_{\rm tot}^{\rm th}(t)=\frac{d}{dt}S_A^{\rm th}(t)+\frac{d}{dt}S_B^{\rm th}(t)\\&=\frac{T_B(t)-T_A(t)}{T_A(t)T_B(t)}\frac{dE_A(t)}{dt}\geqslant 0,\end{aligned} \tag{11}$$

where the last inequality follows from $T_B(t)\geqslant T_A(t)$ and $dE_A(t)/dt\geqslant 0$. This leads to the satisfaction of the principle of increasing total thermodynamic entropy:

$$\Delta S_{\rm tot}^{\rm th}(t_{\rm fin})=\int_{t_{\rm ini}}^{t_{\rm fin}}dt\,\Pi_{\rm tot}^{\rm th}(t)\geqslant 0. \tag{12}$$

Note that the total thermodynamic entropy production rate is not the sum of the internal thermodynamic entropy production rates:

$$\Pi_{\rm tot}^{\rm th}(t)\neq\frac{d^{\rm int}}{dt}S_A^{\rm th}(t)+\frac{d^{\rm int}}{dt}S_B^{\rm th}(t). \tag{13}$$

B. The von Neumann entropy production rate

Let us consider an undriven open quantum system A (different from A in the previous section) which is coupled to a thermal bath B with initial temperature T_B^0. If the coupling is sufficiently weak, the dynamics of the system is well approximated by the GKSL-type Markovian master equation. Then the following von Neumann entropy production rate [25] is typically used:

$$\Pi^{\rm vN}(t):=-\frac{d}{dt}K^{\rm vN}\big(\hat\rho_A(t)||\hat\rho_A^{\rm th}\big), \tag{14}$$

where $\hat\rho_A(t)$ is the density operator of the system, $\hat\rho_A^{\rm th}:=\mathrm{e}^{-\beta_B^0\hat H_A}/\mathrm{Tr}[\mathrm{e}^{-\beta_B^0\hat H_A}]$ with $\beta_B^0=1/(k_BT_B^0)$ and with $\hat H_A$ being the Hamiltonian of the system is the steady state of the GKSL master equation, and

$$\begin{aligned}K^{\rm vN}(\hat\rho_1||\hat\rho_2)&:=k_B\mathrm{Tr}[\hat\rho_1(\ln\hat\rho_1-\ln\hat\rho_2)]\\&=-S^{\rm vN}(\hat\rho_1)-k_B\mathrm{Tr}[\hat\rho_1\ln\hat\rho_2]\end{aligned} \tag{15}$$

is the von Neumann relative entropy [26, Sec. 11.8] with $S^{\rm vN}(\hat\rho):=-k_B\mathrm{Tr}[\hat\rho\ln\hat\rho]$ being the von Neumann entropy.

We can transform Eq. (14) as follows [14, Sec. 3.2.5]:

$$\begin{aligned}\Pi^{\rm vN}(t)&=-\frac{d}{dt}K^{\rm vN}\big(\hat\rho_A(t)||\hat\rho_A^{\rm th}\big)\\&=\frac{d}{dt}S_A^{\rm vN}(t)+k_B\frac{d}{dt}\mathrm{Tr}\left[\hat\rho_A(t)\ln\frac{\mathrm{e}^{-\beta_B^0\hat H_A}}{\mathrm{Tr}[\mathrm{e}^{-\beta_B^0\hat H_A}]}\right]\\&=\frac{d}{dt}S_A^{\rm vN}(t)-\frac{1}{T_B^0}\frac{d}{dt}\mathrm{Tr}[\hat\rho_A(t)\hat H_A]\\&\quad-k_B\ln\mathrm{Tr}[\mathrm{e}^{-\beta_B^0\hat H_A}]\frac{d}{dt}\mathrm{Tr}[\hat\rho_A(t)]\\&=\frac{d}{dt}S_A^{\rm vN}(t)-\frac{1}{T_B^0}\frac{d}{dt}E_A(t)\\&=\frac{d}{dt}S_A^{\rm vN}(t)+\frac{1}{T_B^0}\frac{d}{dt}E_B(t),\end{aligned} \tag{16}$$

where $E_A(t)$ ($E_B(t)$) is the mean energy of the system (bath). The last term in the third line of Eq. (16) becomes zero because $\mathrm{Tr}[\hat\rho_A(t)]=1$ all the time. From the conservation of the total energy, we have derived the last line in Eq. (16), ignoring the interaction energy due to weak coupling. The first term in the last line of Eq. (16) is the time derivative of the von Neumann entropy of the system and the second term is the time derivative of the thermodynamic entropy of the bath under the quasistatic process. Note that there appears an implicit assumption that the temperature of the bath does not change from the initial temperature T_B^0 in this second term. However, when the size of the bath is finite, the temperature of a part of the bath changes, as we will show in Sec. V B. Then we cannot use the von Neumann entropy production rate.

If we regarded the von Neumann entropy of the system as its nonequilibrium thermodynamic entropy, the von Neumann entropy production rate (16) would be regarded as the total thermodynamic entropy production rate. However, this is a delicate matter, because the von Neumann entropy does not equal the thermodynamic entropy in general. For example, let us decouple the system from the bath in the middle of the dynamics. Then the system is isolated, in general out of equilibrium, and undergoes the unitary dynamics. If the system shows thermalization [28], its nonequilibrium thermodynamic entropy should change. However, its von Neumann entropy does not change under the unitary dynamics [26, Sec. 11.1.1]. Hence we do not regard the von Neumann entropy of the system as its thermodynamic entropy in general. However, when the system is in a Gibbs state, its von Neumann entropy coincides with its thermodynamic entropy. Actually, we will consider such a case by adopting special settings in the next section.

It is shown that the von Neumann entropy production rate is always non-negative during the dynamics [25]:

$$\Pi^{\mathrm{vN}}(t) \geqslant 0 \quad {}^{\forall}t. \tag{17}$$

This leads to the non-negative von Neumann entropy production:

$$\Delta S^{\mathrm{vN}}(t) := \int_{t_{\mathrm{ini}}}^{t} ds\, \Pi^{\mathrm{vN}}(s) \geqslant 0 \quad {}^{\forall}t \geqslant t_{\mathrm{ini}}. \tag{18}$$

The above two inequalities are often regarded as signs of irreversibility. Here the total system is not necessarily at equilibrium at t_{ini} or t. Hence, inequality (18) with $t = t_{\mathrm{fin}}$ is different from the principle of increasing total thermodynamic entropy (1) unless each of the total system and the system A is in an equilibrium state at both t_{ini} and t_{fin}.

III. SETTINGS

A. Hamiltonian

We consider a quantum model of coupled harmonic oscillators in a star configuration. It consists of a central harmonic oscillator $j = 1$, which we refer to as system A, and N surrounding harmonic oscillators $j = 2, \ldots, N+1$, which we refer to as bath B. The system A and each harmonic oscillator j in B interact with each other with the coupling constant g_j. The total system is isolated, and hence its Hamiltonian is time independent as in

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_I, \tag{19}$$

where

$$\hat{H}_A = \hbar\omega_1\big(\hat{a}_1^{\dagger}\hat{a}_1 + \tfrac{1}{2}\big), \tag{20}$$

$$\hat{H}_B = \sum_{j=2}^{N+1} \hbar\omega_j\left(\hat{a}_j^{\dagger}\hat{a}_j + \frac{1}{2}\right), \tag{21}$$

$$\hat{H}_I = \sum_{j=2}^{N+1} \hbar g_j(\hat{a}_1^{\dagger}\hat{a}_j + \hat{a}_1\hat{a}_j^{\dagger}), \tag{22}$$

with $\hat{a}_j$ ($\hat{a}_j^{\dagger}$) denoting the annihilation (creation) operator of the jth harmonic oscillator, which satisfies the following commutation relations:

$$[\hat{a}_j, \hat{a}_k^{\dagger}] = \delta_{j,k}, \tag{23}$$

$$[\hat{a}_j, \hat{a}_k] = \big[\hat{a}_j^{\dagger}, \hat{a}_k^{\dagger}\big] = 0 \quad \text{for} \quad j, k = 1, \ldots, N+1. \tag{24}$$

This total Hamiltonian is a type of Fano-Anderson Hamiltonian in condensed-matter physics and of Lee-Friedrichs Hamiltonian in atomic physics [29–34]. If the counter-rotating terms $\sum_{j=2}^{N+1} \hbar g_j(\hat{a}_1^{\dagger}\hat{a}_j^{\dagger} + \hat{a}_1\hat{a}_j)$ are added to the interaction Hamiltonian in Eq. (22), the total Hamiltonian will become the Caldeira-Leggett Hamiltonian [34,35]. When N is large enough, the system is damped by the bath and is called a damped harmonic oscillator [13,22].

We can cast the total Hamiltonian into the form

$$\begin{aligned}\hat{H} &= \sum_{j=1}^{N+1} \frac{\hbar\omega_j}{2}\big(\hat{r}_{2j-1}^2 + \hat{r}_{2j}^2\big) + \sum_{j=2}^{N+1} \hbar g_j(\hat{r}_1\hat{r}_{2j-1} + \hat{r}_2\hat{r}_{2j}) \\ &=: \frac{\hbar}{2}\hat{\mathbf{r}}^{\mathrm{T}} H \hat{\mathbf{r}},\end{aligned} \tag{25}$$

where we have introduced the modified position operator $\hat{r}_{2j-1}$ and the modified momentum operator $\hat{r}_{2j}$,

$$\hat{r}_{2j-1} := \frac{\hat{a}_j + \hat{a}_j^{\dagger}}{\sqrt{2}}, \quad \hat{r}_{2j} := \frac{\hat{a}_j - \hat{a}_j^{\dagger}}{\sqrt{2}\,\mathrm{i}}, \tag{26}$$

and their vector representation

$$\hat{\mathbf{r}} = (\hat{r}_1, \hat{r}_2, \ldots, \hat{r}_{2N+1}, \hat{r}_{2N+2})^{\mathrm{T}} \tag{27}$$

as well as a $2(N+1)$-dimensional symmetric matrix H, whose nonzero elements are

$$\begin{aligned} &H_{2j-1,2j-1} = H_{2j,2j} = \omega_j \quad \text{for} \quad j = 1, \ldots, N+1, \\ &H_{1,2j-1} = H_{2j-1,1} = H_{2,2j} = H_{2j,2} = g_j \\ &\text{for} \quad j = 2, \ldots, N+1. \end{aligned} \tag{28}$$

B. Initial state and unitary dynamics

Let us impose the constraint $\hat{H}_I = 0$ for $t < 0$ and prepare the following initial state:

$$\begin{aligned}\hat{\rho}(t \leqslant 0) &= \frac{\mathrm{e}^{-\beta_A^0\hat{H}_A}}{Z_A} \otimes \frac{\mathrm{e}^{-\beta_B^0\hat{H}_B}}{Z_B} \\ &= \frac{\mathrm{e}^{-\beta_A^0\hat{H}_A}}{Z_A} \otimes \left(\bigotimes_{j=2}^{N+1} \frac{\mathrm{e}^{-\beta_B^0\hat{H}_j}}{Z_j}\right),\end{aligned} \tag{29}$$

where

$$Z_A = \mathrm{Tr}[\mathrm{e}^{-\beta_A^0\hat{H}_A}], \quad Z_B = \mathrm{Tr}[\mathrm{e}^{-\beta_B^0\hat{H}_B}], \tag{30}$$

$$\hat{H}_j = \hbar\omega_j\big(\hat{a}_j^{\dagger}\hat{a}_j + \tfrac{1}{2}\big), \quad Z_j = \mathrm{Tr}[\mathrm{e}^{-\beta_B^0\hat{H}_j}]. \tag{31}$$

That is, the system and the bath are both in the Gibbs states with inverse temperatures β_A^0 and β_B^0, respectively, and they are uncorrelated. Because of the constraint $\hat{H}_I = 0$, the initial state (29) is an equilibrium state:

$$\begin{aligned}\hat{\rho}(t_2) &= e^{-\mathrm{i}\frac{\hat{H}_A+\hat{H}_B}{\hbar}(t_2-t_1)}\hat{\rho}(t_1)e^{\mathrm{i}\frac{\hat{H}_A+\hat{H}_B}{\hbar}(t_2-t_1)} \\ &= \hat{\rho}(t_1) \quad \text{for} \quad t_1 \leqslant t_2 \leqslant 0.\end{aligned} \tag{32}$$

At time $t = 0$, we remove the constraint $\hat{H}_I = 0$ and let the state of the total system evolve under the total Hamiltonian (25). The interaction sets in between the system and the bath, which creates correlations.

As $\hat{H}_A$ and $\hat{H}_B$ are purely quadratic, the initial state (29) is a Gaussian state [36–40] with vanishing first moments: $\mathrm{Tr}[\hat{\mathbf{r}}\hat{\rho}(0)] = \mathbf{0}$. Moreover, as the total Hamiltonian is purely quadratic, the total density operator

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^{\dagger}(t) \quad \text{with} \quad \hat{U}(t) = \exp\left(-\mathrm{i}\frac{\hat{H}}{\hbar}t\right) \tag{33}$$

is always a Gaussian state with vanishing first moments: $\mathrm{Tr}[\hat{\mathbf{r}}\hat{\rho}(t)] = \mathbf{0}$. Therefore, $\hat{\rho}(t)$ is completely characterized by the $2(N+1)\times 2(N+1)$ covariance matrix $\sigma(t)$ whose (j,k)-element is given by

$$\sigma_{j,k}(t) = \mathrm{Tr}[\hat{\rho}(t)\{\hat{r}_j, \hat{r}_k\}], \tag{34}$$

where the curly parentheses $\{\bullet, \bullet\}$ denote the anticommutator. Note that the covariance matrix is a symmetric matrix. Because of Eq. (33), the following relation holds [36, Sec. 5.1.2]:

$$\sigma(t) = V(t)\sigma(0)V(t)^{\mathrm{T}} \quad \text{with} \quad V(t) = \mathrm{e}^{\Omega H t}, \tag{35}$$

where

$$\Omega = \bigoplus_{j=1}^{N+1}\Omega_1 = \begin{pmatrix} \Omega_1 & & \\ & \ddots & \\ & & \Omega_1 \end{pmatrix}, \quad \Omega_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{36}$$

and H is the $2(N+1)$-dimensional symmetric matrix introduced in Eq. (25).

If the total system is in a Gaussian state, its subsystems are also in Gaussian states. Thus, each of the states of the system and the bath is Gaussian and is completely characterized by the covariance matrices $\sigma_A(t)$ and $\sigma_B(t)$, respectively, which are the submatrices of $\sigma(t)$ [36, Sec. 5.2]:

$$\sigma(t) = \begin{pmatrix} \sigma_A(t) & \sigma_{AB}(t) \\ \sigma_{AB}(t)^{\mathrm{T}} & \sigma_B(t) \end{pmatrix}, \tag{37}$$

where $\sigma_A(t)$ is a two-dimensional symmetric matrix, $\sigma_B(t)$ is a $2N$-dimensional symmetric matrix, and $\sigma_{AB}(t)$ is a $2\times 2(N+1)$ matrix. Each harmonic oscillator in the total system is also in a Gaussian state which is totally determined by the following covariance matrix:

$$\sigma_j(t) := \begin{pmatrix} \sigma_{2j-1,2j-1}(t) & \sigma_{2j-1,2j}(t) \\ \sigma_{2j-1,2j}(t) & \sigma_{2j,2j}(t) \end{pmatrix} \tag{38}$$

for $j = 1, \dots, N+1$. The initial covariance matrix for the state (29) is [36, Sec. 3.3]

$$\begin{aligned} \sigma(0) &= \begin{pmatrix} \sigma_A(0) & 0 \\ 0 & \sigma_B(0) \end{pmatrix}, \\ \sigma_A(0) &= \sigma_1(0) = \coth\left(\frac{\hbar\omega_1}{2k_BT_A^0}\right)I_2, \\ \sigma_B(0) &= \bigoplus_{j=2}^{N+1}\sigma_j(0), \quad \sigma_j(0) = \coth\left(\frac{\hbar\omega_j}{2k_BT_B^0}\right)I_2, \end{aligned} \tag{39}$$

where $T_A^0 = 1/(k_B\beta_A^0)$, $T_B^0 = 1/(k_B\beta_B^0)$, and I_2 is the two-dimensional identity matrix.

C. The GKSL master equation

If the couplings $\{g_j\}$ of the harmonic oscillators are sufficiently weak, the dynamics of the system is well approximated by the GKSL master equation [13,14,22–24]:

$$\begin{aligned} \frac{d}{dt}\hat{\rho}_A(t) = &-\frac{\mathrm{i}}{\hbar}[\hat{H}_A, \hat{\rho}_A(t)] \\ &+ \Gamma(\bar{n}+1)(2\hat{a}_1\hat{\rho}_A(t)\hat{a}_1^\dagger - \{\hat{a}_1^\dagger\hat{a}_1, \hat{\rho}_A(t)\}) \\ &+ \Gamma\bar{n}(2\hat{a}_1^\dagger\hat{\rho}_A(t)\hat{a}_1 - \{\hat{a}_1\hat{a}_1^\dagger, \hat{\rho}_A(t)\}), \end{aligned} \tag{40}$$

where

$$\bar{n} = \frac{1}{\mathrm{e}^{\beta_B^0\hbar\omega_1} - 1} \tag{41}$$

is the mean excitation number of a harmonic oscillator at thermal equilibrium with frequency ω_1 at inverse temperature β_B^0, and

$$\Gamma = \pi J(\omega_1) \tag{42}$$

is the relaxation rate of the system, with

$$J(\omega) = \sum_{j=2}^{N+1} g_j^2\,\delta(\omega - \omega_j) \tag{43}$$

being the spectral density of the bath. Note that when we calculate Γ in Eq. (42), we need to specify the form of $J(\omega)$ in the continuous limit. For example, if we consider an Ohmic bath [21,22], the spectral density is written as $J(\omega) = \eta\omega\mathrm{e}^{-\omega/\omega_c}$, where η is the coupling strength between the system and the bath, and ω_c is the cutoff frequency. Under this GKSL master equation, the system is equilibrated with the bath in the limit $t\to\infty$:

$$\hat{\rho}_A(\infty) = \hat{\rho}_A^{\mathrm{th}} = \frac{\mathrm{e}^{-\beta_B^0\hat{H}_A}}{\mathrm{Tr}[\mathrm{e}^{-\beta_B^0\hat{H}_A}]}. \tag{44}$$

As we will show in the next section, $[\hat{H}_A, \hat{\rho}_A(t)] = 0$ always holds in our settings. Then the GKSL master equation (40) becomes

$$\begin{aligned} \frac{d}{dt}\hat{\rho}_A(t) = &\ \Gamma(\bar{n}+1)(2\hat{a}_1\hat{\rho}_A(t)\hat{a}_1^\dagger - \{\hat{a}_1^\dagger\hat{a}_1, \hat{\rho}_A(t)\}) \\ &+ \Gamma\bar{n}(2\hat{a}_1^\dagger\hat{\rho}_A(t)\hat{a}_1 - \{\hat{a}_1\hat{a}_1^\dagger, \hat{\rho}_A(t)\}). \end{aligned} \tag{45}$$

Under this GKSL master equation and the initial covariance matrix in Eq. (39), the covariance matrix of the system at time t is written as [40, Sec. 4.1.1]

$$\begin{aligned} \sigma_A(t) = \bigg[&\coth\left(\frac{\hbar\omega_1}{2k_BT_A^0}\right)\mathrm{e}^{-2\Gamma t} \\ &+ \coth\left(\frac{\hbar\omega_1}{2k_BT_B^0}\right)(1-\mathrm{e}^{-2\Gamma t})\bigg]I_2. \end{aligned} \tag{46}$$

IV. ANALYTICAL RESULTS

A. Gibbs states

We show that each harmonic oscillator is always in a Gibbs state with a time-dependent temperature under the unitary dynamics (33) of the total system. Note that there is a one-to-one correspondence between the density operator and the covariance matrix of each harmonic oscillator. As the covariance matrix is easier to calculate than the density matrix, we first calculate the covariance matrix. By substituting Eq. (39) into Eq. (35), we find (see Appendix A)

$$\sigma_j(t) = \sigma_{2j-1,2j-1}(t)I_2 \quad \text{for} \quad j = 1, \dots, N+1. \tag{47}$$

According to the calculation in Appendix A, the density operator is expressed with the covariance matrix (47) in the following form:

$$\hat{\rho}_j(t) = \frac{\mathrm{e}^{-\beta_j(t)\hat{H}_j}}{Z_j(t)}, \tag{48}$$

$$Z_j(t) = \mathrm{Tr}[\mathrm{e}^{-\beta_j(t)\hat{H}_j}] = \frac{1}{2}\sqrt{\sigma_{2j-1,2j-1}(t)^2 - 1}, \tag{49}$$

$$\begin{aligned}\beta_j(t) &= \frac{1}{k_B T_j(t)} = \frac{2}{\hbar\omega_j}\coth^{-1}[\sigma_{2j-1,2j-1}(t)]\\ &= \frac{1}{\hbar\omega_j}\ln\left(\frac{\sigma_{2j-1,2j-1}(t)+1}{\sigma_{2j-1,2j-1}(t)-1}\right)\\ &= \frac{1}{\hbar\omega_j}\ln\left(\frac{2E_j(t)+\hbar\omega_j}{2E_j(t)-\hbar\omega_j}\right),\end{aligned} \tag{50}$$

where $E_j(t)$ is the mean energy of the jth harmonic oscillator:

$$E_j(t) = \mathrm{Tr}[\hat{H}_j\hat{\rho}_j(t)] = \frac{\hbar\omega_j}{2}\sigma_{2j-1,2j-1}(t). \tag{51}$$

We find that each harmonic oscillator is always in a Gibbs (thermal equilibrium) state with a time-dependent temperature $T_j(t)$. In this meaning, the dynamics is quasistatic for every harmonic oscillator.

As the system is always in a Gibbs state, the relation $[\hat{H}_A, \hat{\rho}_A(t)] = [\hat{H}_A, \mathrm{e}^{-\beta_A(t)\hat{H}_A}/Z_A(t)] = 0$ holds all the time. Therefore the GKSL master equation (40) transforms into Eq. (45). Using Eq. (46) for the time-dependent temperature $T_j(t)$ in Eq. (50), we find that the system under the GKSL master equation is equilibrated with the bath in the limit $t \to \infty$:

$$T_A(\infty) = T_1(\infty) = T_B^0; \tag{52}$$

we will plot this in Fig. 4 below.

B. Thermodynamic entropy

We define the time-dependent free energy and the time-dependent thermodynamic entropy of the jth harmonic oscillator simply following the analog of equilibrium statistical mechanics and thermodynamics:

$$F_j(t) := -k_B T_j(t)\ln Z_j(t), \tag{53}$$

$$S_j^{\mathrm{th}}(t) := \frac{E_j(t) - F_j(t)}{T_j(t)}. \tag{54}$$

In fact, the von Neumann entropy of the jth harmonic oscillator coincides with its thermodynamic entropy because it is in a Gibbs state [1, Sec. 21.1]:

$$\begin{aligned}S_j^{\mathrm{vN}}(t) &:= -k_B\mathrm{Tr}[\hat{\rho}_j(t)\ln\hat{\rho}_j(t)]\\ &= -k_B\mathrm{Tr}\left[\hat{\rho}_j(t)\ln\left(\frac{\mathrm{e}^{-\beta_j(t)\hat{H}_j}}{Z_j(t)}\right)\right]\\ &= \frac{1}{T_j(t)}\mathrm{Tr}[\hat{\rho}_j(t)\hat{H}_j] + k_B\ln Z_j(t)\\ &= \frac{E_j(t)-F_j(t)}{T_j(t)} = S_j^{\mathrm{th}}(t).\end{aligned} \tag{55}$$

We can rewrite $S_j^{\mathrm{th}}(t)$ in Eq. (54) as a strictly monotonically increasing function of $E_j(t)$:

$$\begin{aligned}\frac{S_j^{\mathrm{th}}(t)}{k_B} &= \frac{2E_j(t)+\hbar\omega_j}{2\hbar\omega_j}\ln\left(\frac{2E_j(t)+\hbar\omega_j}{2\hbar\omega_j}\right)\\ &\quad - \frac{2E_j(t)-\hbar\omega_j}{2\hbar\omega_j}\ln\left(\frac{2E_j(t)-\hbar\omega_j}{2\hbar\omega_j}\right).\end{aligned} \tag{56}$$

This is followed by

$$\frac{\partial S_j^{\mathrm{th}}(t)}{\partial E_j(t)} = \frac{k_B}{\hbar\omega_j}\ln\left(\frac{2E_j(t)+\hbar\omega_j}{2E_j(t)-\hbar\omega_j}\right) = \frac{1}{T_j(t)} \tag{57}$$

and

$$\frac{d}{dt}S_j^{\mathrm{th}}(t) = \frac{1}{T_j(t)}\frac{d}{dt}E_j(t). \tag{58}$$

We regard $dE_j(t)/dt$ as the heat flux into the jth harmonic oscillator because its Hamiltonian $\hat{H}_j$ is time independent [5, Sec. 2.1]. Then, Eq. (58) is a manifestation of the quasistatic process; see Eq. (8). We define the thermodynamic entropy flux into the jth harmonic oscillator as

$$\frac{d^{\mathrm{ext}}}{dt}S_j^{\mathrm{th}}(t) = \frac{1}{T_j(t)}\frac{d}{dt}E_j(t), \tag{59}$$

just as Eq. (6). Then we find that the internal thermodynamic entropy production rate of the jth harmonic oscillator is zero:

$$\frac{d^{\mathrm{int}}}{dt}S_j^{\mathrm{th}}(t) = \frac{d}{dt}S_j^{\mathrm{th}}(t) - \frac{d^{\mathrm{ext}}}{dt}S_j^{\mathrm{th}}(t) = 0, \tag{60}$$

which is also a manifestation of the quasistatic process.

In order to define the nonequilibrium thermodynamic entropy of the total system, we impose the additivity of the thermodynamic entropy, which is satisfied in equilibrium thermodynamics of macroscopic systems (see Secs. 11.5 and 13.11 in Ref. [1]). We thereby arrive at

$$\begin{aligned}S_{\mathrm{tot}}^{\mathrm{th}}(t) &:= \sum_{j=1}^{N+1} S_j^{\mathrm{th}}(t)\\ &= k_B\sum_{j=1}^{N+1}\left[\frac{2E_j(t)+\hbar\omega_j}{2\hbar\omega_j}\ln\left(\frac{2E_j(t)+\hbar\omega_j}{2\hbar\omega_j}\right)\right.\\ &\quad \left. - \frac{2E_j(t)-\hbar\omega_j}{2\hbar\omega_j}\ln\left(\frac{2E_j(t)-\hbar\omega_j}{2\hbar\omega_j}\right)\right].\end{aligned} \tag{61}$$

We analytically confirm that our thermodynamic entropy (61) satisfies the third law of thermodynamics [1, Sec. 23.7] as follows. The temperature $T_j(t)$ in Eq. (50) and the thermodynamic entropy $S_j^{\mathrm{th}}(t)$ in Eq. (56) become zero for the vacuum state:

$$T_j(t) \to +0, \quad S_j^{\mathrm{th}}(t) \to +0 \quad \text{as} \quad E_j(t) \to \frac{\hbar\omega_j}{2} + 0. \tag{62}$$

As $T_j(t)$ and $S_j^{\mathrm{th}}(t)$ are both strictly monotonically increasing functions of $E_j(t)$, the thermodynamic entropy $S_j^{\mathrm{th}}(t)$ becomes zero if and only if $T_j(t)$ becomes zero:

$$S_j^{\mathrm{th}}(t) \to +0 \quad \text{as} \quad T_j(t) \to +0. \tag{63}$$

This and Eq. (61) lead to the third law of thermodynamics:

$$S^{\rm th}_{\rm tot}(t) \to +0 \quad \text{as} \quad T_j(t) \to +0 \quad {}^{\forall} j, \tag{64}$$

which supports the validity of our definition of the total thermodynamic entropy in Eq. (61).

C. Total thermodynamic entropy production and its rate

We define the total thermodynamic entropy production as

$$\begin{aligned}\Delta S^{\rm th}_{\rm tot}(t) &:= S^{\rm th}_{\rm tot}(t) - S^{\rm th}_{\rm tot}(0)\\ &= S^{\rm th}_{A}(t) - S^{\rm th}_{A}(0) + \sum_{j=2}^{N+1}\left[S^{\rm th}_{j}(t) - S^{\rm th}_{j}(0)\right] \end{aligned}\tag{65}$$

and its rate as

$$\begin{aligned}\Pi^{\rm th}_{\rm tot}(t) &:= \frac{d}{dt}S^{\rm th}_{\rm tot}(t) = \sum_{j=1}^{N+1}\frac{1}{T_j(t)}\frac{d}{dt}E_j(t)\\ &= \frac{1}{T_A(t)}\frac{d}{dt}E_A(t) + \sum_{j=2}^{N+1}\frac{1}{T_j(t)}\frac{d}{dt}E_j(t).\end{aligned}\tag{66}$$

Let us transform this into the form which we can easily calculate in terms of the covariance matrix. Using Eqs. (B7) and (B8) in Appendix B, we obtain

$$\begin{aligned}\Pi^{\rm th}_{\rm tot}(t) &= \frac{\hbar\omega_1}{T_A(t)}\sum_{j=2}^{N+1} g_j\sigma_{1,2j}(t) - \sum_{j=2}^{N+1}\frac{\hbar\omega_j}{T_j(t)}g_j\sigma_{1,2j}(t)\\ &= k_B\sum_{j=2}^{N+1} g_j\sigma_{1,2j}(t)\left[\ln\left(\frac{\sigma_{1,1}(t)+1}{\sigma_{1,1}(t)-1}\right)\right.\\ &\quad \left. - \ln\left(\frac{\sigma_{2j-1,2j-1}(t)+1}{\sigma_{2j-1,2j-1}(t)-1}\right)\right].\end{aligned}\tag{67}$$

This total thermodynamic entropy production rate can be negative as we will see later.

D. The difference between our total thermodynamic entropy production rate and the conventional one

Let us consider the weak-coupling regime so that the dynamics of the system is well approximated by the GKSL master equation in Eq. (45). In our settings, the von Neumann entropy of the system coincides with its thermodynamic entropy as in Eq. (55), and hence the conventional entropy production rate $\Pi^{\rm vN}(t)$ in Eq. (16) has the following form:

$$\begin{aligned}\Pi^{\rm vN}(t) &= \frac{1}{T_A(t)}\frac{d}{dt}E_A(t) + \frac{1}{T_B^0}\frac{d}{dt}E_B(t)\\ &= \frac{1}{T_A(t)}\frac{d}{dt}E_A(t) + \sum_{j=2}^{N+1}\frac{1}{T_B^0}\frac{d}{dt}E_j(t).\end{aligned}\tag{68}$$

Let us transform Eq. (68) into the form which we can easily calculate. As we consider the weak-coupling regime, we neglect the interaction energy: $dE_B(t)/dt = -dE_A(t)/dt$. From the first line in Eq. (68), we obtain

$$\begin{aligned}\Pi^{\rm vN}(t) &= \left(\frac{1}{T_A(t)} - \frac{1}{T_B^0}\right)\frac{d}{dt}E_A(t)\\ &= \hbar\omega_1\Gamma\left(\frac{1}{T_B^0} - \frac{1}{T_A(t)}\right)\left[\frac{2E_A(t)}{\hbar\omega_1} - \coth\left(\frac{\hbar\omega_1}{2k_BT_B^0}\right)\right]\\ &= \hbar\omega_1\Gamma\left(\frac{1}{T_B^0} - \frac{1}{T_A(t)}\right)\\ &\quad\times\left[\coth\left(\frac{\hbar\omega_1}{2k_BT_A(t)}\right) - \coth\left(\frac{\hbar\omega_1}{2k_BT_B^0}\right)\right],\end{aligned}\tag{69}$$

where the second line follows from Eqs. (51) and (46), and the last line follows from Eq. (50).

The difference between our total thermodynamic entropy production rate $\Pi^{\rm th}_{\rm tot}(t)$ in Eq. (66) and the conventional entropy production rate $\Pi^{\rm vN}(t)$ in Eq. (68) arises from the gaps between $\{T_j(t)\}$ and T_B^0:

$$\Pi^{\rm vN}(t) - \Pi^{\rm th}_{\rm tot}(t) = \sum_{j=2}^{N+1}\left(\frac{1}{T_B^0} - \frac{1}{T_j(t)}\right)\frac{d}{dt}E_j(t). \tag{70}$$

V. NUMERICAL RESULTS

A. Parameters

For a numerical example, we use an Ohmic bath [21,22], whose spectral density is

$$J(\omega) = \sum_{j=2}^{N+1} g_j^2\delta(\omega-\omega_j) = \eta\omega \mathrm{e}^{-\omega/\omega_c}, \tag{71}$$

where η is the coupling strength between the system and the bath, and ω_c is the cutoff frequency. For numerical demonstration, we fix the parameters as follows [22, Appendix A]:

$$\begin{gathered}\omega_1 = 4\ \text{MHz},\ \omega_c = 3\ \text{MHz},\ \omega_{\rm min} = 0.026\ \text{MHz},\\ \omega_{\rm max} = 20\ \text{MHz},\ \Delta\omega = \frac{\omega_{\rm max}-\omega_{\rm min}}{N-1},\\ \omega_j = \omega_{\rm min} + (j-2)\Delta\omega \quad \text{for} \quad j = 2,\dots,N+1,\\ \eta = 10^{-3},\ T_A^0 = 10\ \mu\text{K},\ T_B^0 = 50\ \mu\text{K}.\end{gathered}\tag{72}$$

We set the coupling constant g_j by integrating Eq. (71) over ω as in

$$\sum_{j=2}^{N+1} g_j^2 = \int_{\omega_{\rm min}-\epsilon}^{\omega_{\rm max}+\epsilon} d\omega\, \eta\omega \mathrm{e}^{-\omega/\omega_c} \simeq \sum_{j=2}^{N+1}\eta\Delta\omega\omega_j \mathrm{e}^{-\omega_j/\omega_c}, \tag{73}$$

which gives

$$g_j = \sqrt{\eta\Delta\omega\omega_j \mathrm{e}^{-\omega_j/\omega_c}}. \tag{74}$$

Let us check whether the dynamics of the system obeys the GKSL master equation when $N = 4000$, 6000, and 8000. Note that the quantum state of the system is totally determined only by $\sigma_{1,1}(t)$. Thus, in Fig. 1 we compare $\sigma_{1,1}(t)$ which we calculate from the unitary dynamics of the total system (35) and that we calculate from the GKSL master equation (46). We find that the two curves coincide with each other for $t \lesssim 2\pi/\Delta\omega$, and hence we conclude that the dynamics of the

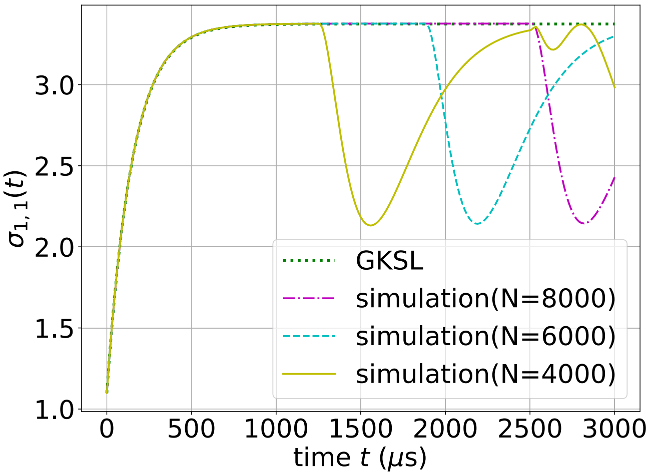

FIG. 1. The time evolution of $\sigma_{1,1}(t)$. We set $\omega_1 = 4$ MHz, $\omega_c = 3$ MHz, $\omega_{\min} = 0.026$ MHz, $\omega_{\max} = 20$ MHz, $\eta = 10^{-3}$, $T_A^0 = 10\ \mu$K, and $T_B^0 = 50\ \mu$K. The green dotted line is obtained from the solution of the GKSL master equation (46). The other lines are obtained from the unitary dynamics of the total system (35).

system is well approximated by the GKSL master equation in that time range. However, the dynamics of the system no longer obeys the GKSL master equation for $t \gtrsim 2\pi/\Delta\omega$ because at $t = t_1 := 2\pi/\Delta\omega$, we have $e^{i\omega_j t_1} = e^{2\pi i\omega_{\min}/\Delta\omega}$ for $j = 2, \ldots, N+1$, and hence all harmonic oscillators in the bath have almost the same phase and recurrencelike behavior happens; see Fig. 1. Hence we restrict ourselves to $t_{\max} < t_1 = 2\pi/\Delta\omega$ in the following calculations. Note that t_1 is almost proportional to N for large N because $\Delta\omega = (\omega_{\max} - \omega_{\min})/(N-1)$; we thus need not worry about the recurrencelike behavior for sufficiently large N. We also remark that the interaction energy $E_I(t) := \mathrm{Tr}[\hat{\rho}(t)\hat{H}_I]$ is negligibly small under the parameters in Eq. (72) for large N; see Fig. 2. This justifies the transformation from the first line of Eq. (68) to that of Eq. (69).

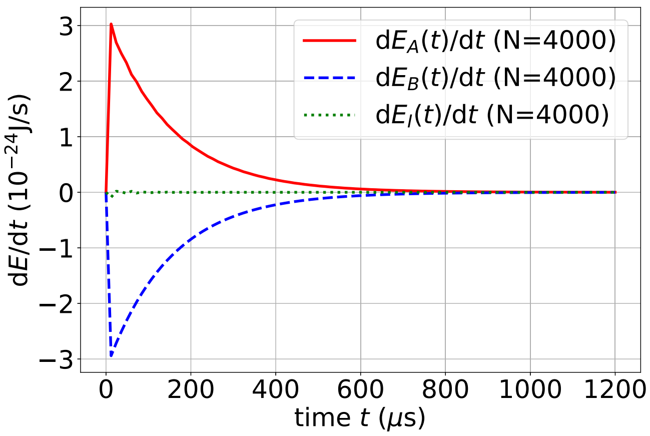

FIG. 2. The time evolution of $dE_A(t)/dt$ in Eq. (B7), $dE_B(t)/dt$ in Eq. (B11), and $dE_I(t)/dt$ in Eq. (B12) when $N = 4000$ under the unitary dynamics of the total system (35). All the parameters except N are the same as those in Fig. 1.

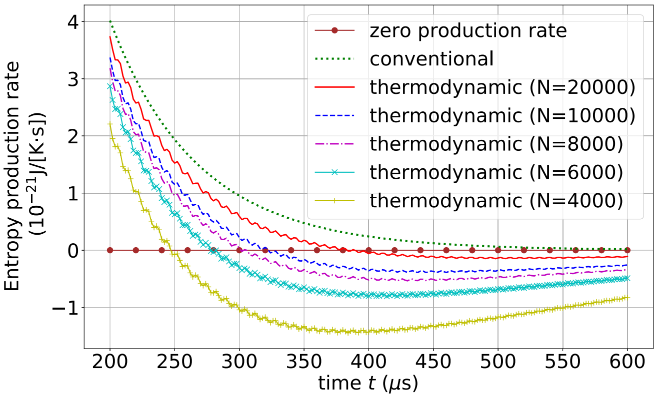

FIG. 3. The total thermodynamic entropy production rate $\Pi_{\mathrm{tot}}^{\mathrm{th}}(t)$ in Eq. (67) and the conventional entropy production rate $\Pi^{\mathrm{vN}}(t)$ in Eq. (69). All the parameters except N are the same as those in Fig. 1.

B. Negative total thermodynamic entropy production rate

We compare in Fig. 3 our total thermodynamic entropy production rate $\Pi_{\mathrm{tot}}^{\mathrm{th}}(t)$ in Eq. (67) with the conventional entropy production rate $\Pi^{\mathrm{vN}}(t)$ in Eq. (69). We find that our total thermodynamic entropy production rate $\Pi_{\mathrm{tot}}^{\mathrm{th}}(t)$ is negative in a certain time range, in contrast to the conventional entropy production rate $\Pi^{\mathrm{vN}}(t)$, which is always non-negative. As we said in Sec. IV D, $\Pi_{\mathrm{tot}}^{\mathrm{th}}(t)$ differs from $\Pi^{\mathrm{vN}}(t)$ because some of $\{T_j(t)\}$ differ from T_B^0; see Eq. (70). Let us see the behaviors of $\{T_j(t)\}$ below. We find in Fig. 4 that the temperature of the system $T_A(t)$ relaxes to the initial temperature of the bath T_B^0, while some of the temperatures $\{T_j(t)\}$ of the harmonic oscillators in the bath decrease. The harmonic oscillators which show temperature decreasing have almost the same

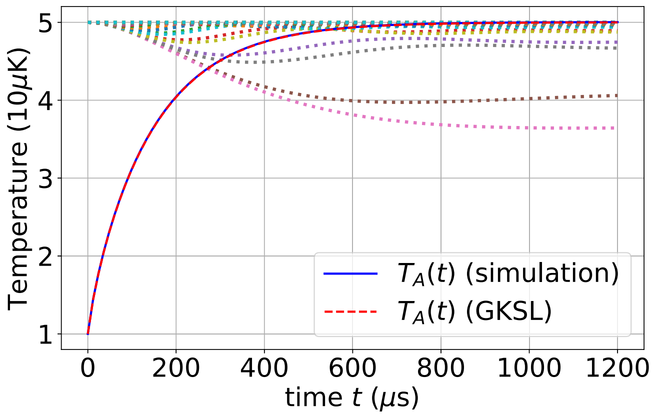

FIG. 4. Time-dependent temperature $T_j(t)$ in Eq. (50) of each harmonic oscillator. We set $N = 4000$. All the parameters except N are the same as those in Fig. 1. The blue solid line is the time-dependent temperature of the system obtained from the unitary dynamics of the total system (35). The red dashed line, which is almost identical to the blue solid line, is the time-dependent temperature of the system obtained from the solution of the GKSL master equation (46). The dotted lines are the time-dependent temperatures of all the harmonic oscillators in the bath obtained from the unitary dynamics of the total system.

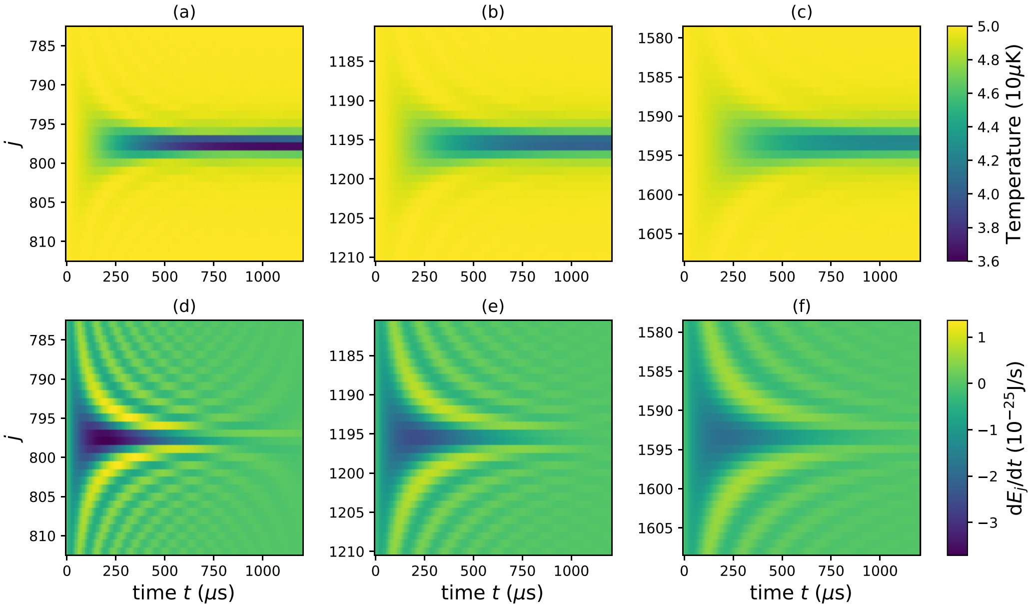

FIG. 5. The time-dependent temperatures $\{T_j(t)\}$ (upper panels) and the time derivatives of the mean energies $\{dE_j(t)/dt\}$ (lower panels) of the harmonic oscillators in the bath which have almost the same frequency as that of the system. The color expresses the value of $T_j(t)$ ($dE_j(t)/dt$) in the upper (lower) panels. The vertical axis corresponds to the number j of each harmonic oscillator. The horizontal axis corresponds to time. We set $N = 4000$ in (a) and (d), $N = 6000$ in (b) and (e), and $N = 8000$ in (c) and (f). The other parameters are the same as those in Fig. 1.

frequency as the system (Fig. 5). This can be explained as follows. The mean energy of the system $E_A(t)$ is a strictly monotonically increasing function of the temperature of the system $T_A(t)$, and hence $E_A(t)$ increases as $T_A(t)$ relaxes to T_B^0, which is higher than the initial temperature of the system T_A^0. In order for $E_A(t)$ to increase, the system must receive particles with energy $\hbar\omega_1$. Note that the total particle number operator $\sum_{j=1}^{N+1} \hat{a}_j^\dagger \hat{a}_j$ commutes with the total Hamiltonian (25), so that the total particle number is conserved. Thus, in order for the system to receive a particle with energy $\hbar\omega_1$, the bath must provide the particle, and only the harmonic oscillators whose frequencies are almost the same as that of the system can do so. When the harmonic oscillators provide the particle, their mean energies $\{E_j(t)\}$ decrease. Hence, the time-dependent temperature $T_j(t)$, which is a strictly monotonically increasing function of $E_j(t)$, also decreases. We see from Fig. 5 that as $|\omega_j - \omega_1|$ becomes smaller, $[T_B^0 - T_j(t)]$ and $|dE_j(t)/dt|$ become larger, and so does $[1/T_B^0 - 1/T_j(t)]dE_j(t)/dt$. As N becomes larger, more harmonic oscillators in the bath take part in the energy exchange with the system, and hence $[T_B^0 - T_j(t)]$ and $|dE_j(t)/dt|$ for each harmonic oscillator become smaller; see Fig. 5. In addition, $\sum_{j=2}^{N+1} dE_j(t)/dt = dE_B(t)/dt = -dE_A(t)/dt$ does not depend on N as long as the dynamics of the system obeys the GKSL master equation. Therefore as N becomes larger, $\Pi^{\rm vN}(t) - \Pi_{\rm tot}^{\rm th}(t)$ in Eq. (70) becomes smaller as in Fig. 3.

C. The second law of thermodynamics

We compare in Fig. 6 our total thermodynamic entropy production $\Delta S_{\rm tot}^{\rm th}(t)$ in Eq. (65) with the conventional entropy production, which in our settings is given by

$$\Delta S^{\rm vN}(t) := \int_0^t dt\, \Pi^{\rm vN}(t)$$
$$= S_A^{\rm th}(t) - S_A^{\rm th}(0) - \frac{E_A(t) - E_A(0)}{T_B^0}. \qquad (75)$$

As the entropy production is the time integral of the entropy production rate, our total thermodynamic entropy production approaches the conventional entropy production as N becomes larger, which is similar to the case of the total entropy

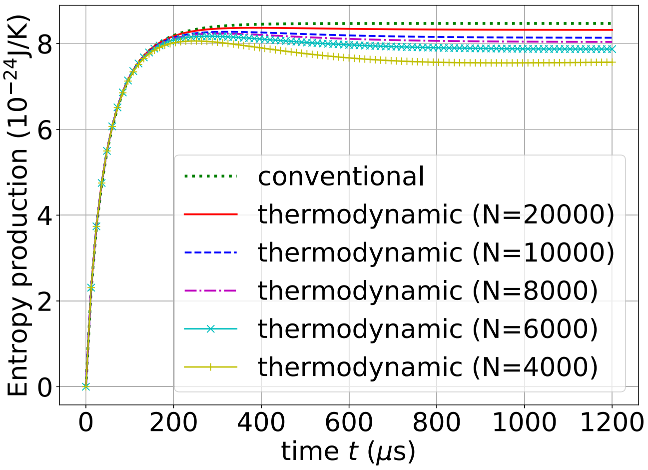

FIG. 6. The thermodynamic entropy production $\Delta S_{\rm tot}^{\rm th}(t)$ in Eq. (65) and the conventional entropy production $\Delta S^{\rm vN}(t)$ in Eq. (75). All the parameters except N are the same those in Fig. 1.

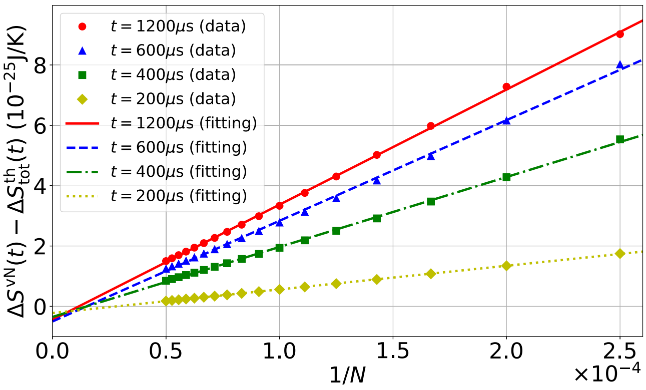

FIG. 7. The difference $\Delta S^{\mathrm{vN}}(t) - \Delta S^{\mathrm{th}}_{\mathrm{tot}}(t)$ in Eq. (76) against N^{-1} for four different times. All the parameters except N are the same as those in Fig. 1.

production rate. In fact, the difference

$$\Delta S^{\mathrm{vN}}(t) - \Delta S^{\mathrm{th}}_{\mathrm{tot}}(t) = \frac{E_A(0) - E_A(t)}{T_B^0} + \sum_{j=2}^{N+1}\left[S_j^{\mathrm{th}}(0) - S_j^{\mathrm{th}}(t)\right] \tag{76}$$

is almost proportional to N^{-1} for large N; see Fig. 7. This suggests that $\Delta S^{\mathrm{th}}_{\mathrm{tot}}(t)$ may converge to $\Delta S^{\mathrm{vN}}(t)$ in the limit $N \to \infty$.

Our total thermodynamic entropy production changes little for 800 μs $\lesssim t \leqslant$ 1200 μs, as shown in Fig. 6. We therefore regard the quantum state of the total system $\hat{\rho}(t)$ in this time range as an equilibrium state. Since $\Delta S^{\mathrm{th}}_{\mathrm{tot}}(t) > 0$ for 800 μs $\lesssim t \leqslant$ 1200 μs, we judge that our total thermodynamic entropy $S^{\mathrm{th}}_{\mathrm{tot}}(t)$ satisfies the principle of increasing total thermodynamic entropy (1).

VI. CONCLUSION

In conclusion, we have defined the nonequilibrium thermodynamic entropy for the quantum model of coupled harmonic oscillators in a star configuration. We analytically confirmed that our total thermodynamic entropy satisfies the third law of thermodynamics. We have found numerically that our total thermodynamic entropy production rate can be negative even when the dynamics of the central harmonic oscillator (system) is well approximated by the GKSL-type Markovian master equation, while our total thermodynamic entropy satisfies the second law of thermodynamics.

Because of the specific Hamiltonian and the special initial state in our settings, all harmonic oscillators are in Gibbs states for all the time. This allows us to define the thermodynamic entropy of each harmonic oscillator in the present work. If we instead prepare a different initial state, each harmonic oscillator will be no longer in a Gibbs state. Defining the nonequilibrium thermodynamic entropy of each harmonic oscillator and of the total system in this case can be an interesting future work.

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APPENDIX A: EVERY HARMONIC OSCILLATOR IS IN A GIBBS STATE WITH A TIME-DEPENDENT TEMPERATURE

In this Appendix, we show that every harmonic oscillator is in a Gibbs state all the time. As each harmonic oscillator is in a single-mode Gaussian state with vanishing first moments, its density operator is totally determined by its covariance matrix (38). Since the time evolution of the covariance matrix is easier to calculate than that of the density operator, we first calculate the covariance matrix of each harmonic oscillator at time t in the next two paragraphs. Then, in the last paragraph, using the relation between the density operator and the covariance matrix in Eq. (A14), we show that each harmonic oscillator is in a Gibbs state with a time-dependent temperature $T_j(t)$.

The matrix H in Eq. (25) with the elements (28) has a form of the following symmetric block matrix:

$$H = \begin{pmatrix} \omega_1 I_2 & g_2 I_2 & g_3 I_2 & \cdots & g_{N+1} I_2 \\ g_2 I_2 & \omega_2 I_2 & 0 & \cdots & 0 \\ g_3 I_2 & 0 & \omega_3 I_2 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ g_{N+1} I_2 & 0 & \cdots & 0 & \omega_{N+1} I_2 \end{pmatrix}. \tag{A1}$$

Therefore, the nth power of H has a form of the following symmetric block matrix:

$$H^n = \begin{pmatrix} h_{1,1}(n) I_2 & \cdots & h_{1,N+1}(n) I_2 \\ \vdots & \ddots & \vdots \\ h_{1,N+1}(n) I_2 & \cdots & h_{N+1,N+1}(n) I_2 \end{pmatrix}, \tag{A2}$$

whose elements satisfy

$$(H^n)_{2j-1,2k-1} = (H^n)_{2j,2k}, \quad (H^n)_{2j-1,2k} = (H^n)_{2j,2k-1} = 0$$
$$\text{for} \quad n \in \mathbb{N}, \quad j,k = 1,\ldots,N+1. \tag{A3}$$

The $(2n-1)$th and the $(2n)$th powers of the matrix Ω in Eq. (36) are given by

$$\Omega^{2n-1} = (-1)^{n-1}\Omega, \quad \Omega^{2n} = (-1)^n I_{2N+2} \quad \text{for} \quad n \in \mathbb{N}, \tag{A4}$$

where I_{2N+2} is the $(2N+2)$-dimensional identity matrix. The matrices H and Ω commute with each other:

$$H\Omega = \Omega H. \tag{A5}$$

Using Eqs. (A4) and (A5), we can rewrite $V(t) = \mathrm{e}^{\Omega H t}$ in Eq. (35) as

$$V(t) = \mathrm{e}^{\Omega H t}$$
$$= \sum_{n=0}^{\infty} \frac{\Omega^{2n}(Ht)^{2n}}{(2n)!} + \sum_{n=1}^{\infty} \frac{\Omega^{2n-1}(Ht)^{2n-1}}{(2n-1)!}$$

$$
\begin{aligned}
&= \sum_{n=0}^{\infty} \frac{(-1)^n (Ht)^{2n}}{(2n)!} + \Omega \sum_{n=1}^{\infty} \frac{(-1)^{n-1} (Ht)^{2n-1}}{(2n-1)!} \\
&= \cos Ht + \Omega \sin Ht, \qquad \text{(A6)}
\end{aligned}
$$

whose transpose is

$$V(t)^{\mathrm{T}} = \cos Ht - [\sin Ht]\Omega \qquad \text{(A7)}$$

because $\Omega^{\mathrm{T}} = -\Omega$. From Eq. (A3), we find

$$
\begin{aligned}
&(\cos Ht)_{2j-1,2k-1} = (\cos Ht)_{2j,2k}, \quad (\cos Ht)_{2j-1,2k} = (\cos Ht)_{2j,2k-1} = 0, \\
&(\sin Ht)_{2j-1,2k-1} = (\sin Ht)_{2j,2k}, \quad (\sin Ht)_{2j-1,2k} = (\sin Ht)_{2j,2k-1} = 0 \\
&\text{for} \quad j, k = 1, \dots, N+1.
\end{aligned}
\qquad \text{(A8)}
$$

As the initial covariance matrix (39) is diagonal, each element of $\sigma(t) = V(t)\sigma(0)V(t)^{\mathrm{T}}$ is written as

$$
\begin{aligned}
&\sigma_{j,k}(t) = \sum_{l=1}^{2N+2} (\cos Ht + \Omega \sin Ht)_{j,l} \sigma_{l,l}(0) (\cos Ht - [\sin Ht]\Omega)_{l,k} \\
&\text{for} \quad j, k = 1, \dots, 2N+2.
\end{aligned}
\qquad \text{(A9)}
$$

Let us calculate the elements of the covariance matrix of the jth harmonic oscillator (38). We first obtain

$$
\begin{aligned}
\sigma_{2j-1,2j-1}(t) &= \sum_{l=1}^{2N+2} (\cos Ht + \Omega \sin Ht)_{2j-1,l} \sigma_{l,l}(0) (\cos Ht - [\sin Ht]\Omega)_{l,2j-1} \\
&= \sum_{l=1}^{2N+2} [(\cos Ht)_{2j-1,l} + (\sin Ht)_{2j,l}] \sigma_{l,l}(0) [(\cos Ht)_{l,2j-1} + (\sin Ht)_{l,2j}] \\
&= \sum_{m=1}^{N+1} [(\cos Ht)_{2j-1,2m-1} \sigma_{2m-1,2m-1}(0) (\cos Ht)_{2m-1,2j-1} + (\sin Ht)_{2j,2m} \sigma_{2m,2m}(0) (\sin Ht)_{2m,2j}] \\
&= \sum_{m=1}^{N+1} [(\cos Ht)_{2j-1,2m-1} \sigma_{2m-1,2m-1}(0) (\cos Ht)_{2m-1,2j-1} + (\sin Ht)_{2j-1,2m-1} \sigma_{2m-1,2m-1}(0) (\sin Ht)_{2m-1,2j-1}],
\end{aligned}
\qquad \text{(A10)}
$$

where the second line follows from the form of Ω in Eq. (36), the third line follows from Eq. (A8), and the last line follows from Eq. (A8) and the form of $\sigma(0)$ in Eq. (39). Similarly, we have

$$
\begin{aligned}
\sigma_{2j,2j}(t) &= \sum_{l=1}^{2N+2} (\cos Ht + \Omega \sin Ht)_{2j,l} \sigma_{l,l}(0) (\cos Ht - [\sin Ht]\Omega)_{l,2j} \\
&= \sum_{l=1}^{2N+2} [(\cos Ht)_{2j,l} - (\sin Ht)_{2j-1,l}] \sigma_{l,l}(0) [(\cos Ht)_{l,2j} - (\sin Ht)_{l,2j-1}] \\
&= \sum_{m=1}^{N+1} [(\cos Ht)_{2j,2m} \sigma_{2m,2m}(0) (\cos Ht)_{2m,2j} + (\sin Ht)_{2j-1,2m-1} \sigma_{2m-1,2m-1}(0) (\sin Ht)_{2m-1,2j-1}] \\
&= \sum_{m=1}^{N+1} [(\cos Ht)_{2j-1,2m-1} \sigma_{2m-1,2m-1}(0) (\cos Ht)_{2m-1,2j-1} + (\sin Ht)_{2j-1,2m-1} \sigma_{2m-1,2m-1}(0) (\sin Ht)_{2m-1,2j-1}] \\
&= \sigma_{2j-1,2j-1}(t),
\end{aligned}
\qquad \text{(A11)}
$$

$$
\begin{aligned}
\sigma_{2j-1,2j}(t) &= \sum_{l=1}^{2N+2} (\cos Ht + \Omega \sin Ht)_{2j-1,l} \sigma_{l,l}(0) (\cos Ht - [\sin Ht]\Omega)_{l,2j} \\
&= \sum_{l=1}^{2N+2} [(\cos Ht)_{2j-1,l} + (\sin Ht)_{2j,l}] \sigma_{l,l}(0) [(\cos Ht)_{l,2j} - (\sin Ht)_{l,2j-1}] \\
&= \sum_{m=1}^{N+1} [-(\cos Ht)_{2j-1,2m-1} \sigma_{2m-1,2m-1}(0) (\sin Ht)_{2m-1,2j-1} + (\sin Ht)_{2j,2m} \sigma_{2m,2m}(0) (\cos Ht)_{2m,2j}]
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_{m=1}^{N+1}[-(\cos Ht)_{2j-1,2m-1}\sigma_{2m-1,2m-1}(0)(\sin Ht)_{2m-1,2j-1} + (\sin Ht)_{2j-1,2m-1}\sigma_{2m-1,2m-1}(0)(\cos Ht)_{2m-1,2j-1}]\\
&= \sum_{m=1}^{N+1}[-(\cos Ht)_{2j-1,2m-1}\sigma_{2m-1,2m-1}(0)(\sin Ht)_{2m-1,2j-1} + (\sin Ht)_{2m-1,2j-1}\sigma_{2m-1,2m-1}(0)(\cos Ht)_{2j-1,2m-1}]\\
&= 0,
\end{aligned}
\tag{A12}
$$

where the fifth line follows from the symmetry of $\cos Ht$ and $\sin Ht$. We thus arrive at

$$\sigma_j(t) = \sigma_{2j-1,2j-1}(t)I_2, \tag{A13}$$

which appears in Eq. (47) in the main text.

As the jth harmonic oscillator is in a single-mode Gaussian state with vanishing first moments, its density operator is completely characterized by the covariance matrix in Eq. (A13) and has the following form [41]:

$$\hat{\rho}_j(t) = \frac{\exp\left[-\frac{1}{2}\hat{\mathbf{r}}_j^{\mathrm{T}}G_j(t)\hat{\mathbf{r}}_j\right]}{Z_j(t)}, \tag{A14}$$

where

$$\hat{\mathbf{r}}_j = (\hat{r}_{2j-1}, \hat{r}_{2j})^{\mathrm{T}}, \tag{A15}$$

$$G_j(t) = 2\mathrm{i}\Omega_1 \coth^{-1}[\sigma_j(t)\mathrm{i}\Omega_1] = 2\coth^{-1}[\sigma_{2j-1,2j-1}(t)]I_2 \quad \text{with} \quad \Omega_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{A16}$$

$$Z_j(t) = \frac{1}{2}\sqrt{\det(\sigma_j(t) + \mathrm{i}\Omega_1)} = \frac{1}{2}\sqrt{\sigma_{2j-1,2j-1}(t)^2 - 1}. \tag{A17}$$

Let us show that $\hat{\rho}_j(t)$ in Eq. (A14) is a Gibbs state below. The numerator of Eq. (A14) is transformed using Eqs. (A15) and (A16) as

$$\exp\left[-\frac{1}{2}\hat{\mathbf{r}}_j^{\mathrm{T}}G_j(t)\hat{\mathbf{r}}_j\right] = \exp\left[-\frac{2}{\hbar\omega_j}\coth^{-1}[\sigma_{2j-1,2j-1}(t)]\frac{\hbar\omega_j}{2}\left(\hat{r}_{2j-1}^2 + \hat{r}_{2j}^2\right)\right] = \exp\left[-\beta_j(t)\hat{H}_j\right], \tag{A18}$$

where

$$\beta_j(t) = \frac{1}{k_B T_j(t)} = \frac{2}{\hbar\omega_j}\coth^{-1}[\sigma_{2j-1,2j-1}(t)] = \frac{1}{\hbar\omega_j}\ln\left(\frac{\sigma_{2j-1,2j-1}(t)+1}{\sigma_{2j-1,2j-1}(t)-1}\right). \tag{A19}$$

The trace of the numerator of Eq. (A14) is equal to the denominator:

$$
\begin{aligned}
&\mathrm{Tr}\left[\exp\left[-\frac{1}{2}\hat{\mathbf{r}}_j^{\mathrm{T}}G_j(t)\hat{\mathbf{r}}_j\right]\right]\\
&= \mathrm{Tr}[\exp[-\beta_j(t)\hat{H}_j]]\\
&= \mathrm{Tr}\left[\exp\left[-\beta_j(t)\hbar\omega_j\left(\hat{a}_j^\dagger\hat{a}_j + \frac{1}{2}\right)\right]\right]\\
&= \sum_{n=0}^{\infty}\exp\left[-\beta_j(t)\hbar\omega_j\left(n + \frac{1}{2}\right)\right]\\
&= \frac{\exp[-\beta_j(t)\hbar\omega_j/2]}{1 - \exp[-\beta_j(t)\hbar\omega_j]}\\
&= \frac{1}{\exp[\beta_j(t)\hbar\omega_j/2] - \exp[-\beta_j(t)\hbar\omega_j/2]}\\
&= \frac{1}{\sqrt{\frac{\sigma_{2j-1,2j-1}(t)+1}{\sigma_{2j-1,2j-1}(t)-1}} - \sqrt{\frac{\sigma_{2j-1,2j-1}(t)-1}{\sigma_{2j-1,2j-1}(t)+1}}}\\
&= \frac{1}{2}\sqrt{\sigma_{2j-1,2j-1}(t)^2 - 1} = Z_j(t),
\end{aligned}
\tag{A20}
$$

where in the sixth line, we have used Eq. (A19). Therefore, we have derived Eqs. (48) and (49):

$$
\begin{aligned}
\hat{\rho}_j(t) &= \frac{\mathrm{e}^{-\beta_j(t)\hat{H}_j}}{Z_j(t)},\\
Z_j(t) &= \mathrm{Tr}[\mathrm{e}^{-\beta_j(t)\hat{H}_j}]\\
&= \frac{1}{2}\sqrt{\sigma_{2j-1,2j-1}(t)^2 - 1},
\end{aligned}
\tag{A21}
$$

which shows that the jth harmonic oscillator is in the Gibbs state with the time-dependent inverse temperature $\beta_j(t)$.

APPENDIX B: THE TIME DERIVATIVE OF THE MEAN ENERGY OF EACH HARMONIC OSCILLATOR, THE BATH, AND THE INTERACTION

In this Appendix we calculate the time derivative of the mean energy of each harmonic oscillator so that we can transform the thermodynamic entropy production rate (66) to the more easily calculable form (67). We also calculate the time derivative of the mean energy of the bath and the interaction in order to show in Fig. 2 that the interaction energy is negligibly small.

The modified position and momentum operators introduced in Eq. (26) satisfy the canonical commutation relations:

$$[\hat{r}_j, \hat{r}_k] = \mathrm{i}\Omega_{j,k} \quad \text{for} \quad j, k = 1, \dots, 2(N+1). \tag{B1}$$

The total Hamiltonian in the Heisenberg picture is

$$\hat{H}^H(t) = \sum_{j=1}^{N+1} \frac{\hbar\omega_j}{2}\big(\hat{r}_{2j-1}^H(t)^2 + \hat{r}_{2j}^H(t)^2\big) + \sum_{j=2}^{N+1} \hbar g_j\big(\hat{r}_1^H(t)\hat{r}_{2j-1}^H(t) + \hat{r}_2^H(t)\hat{r}_{2j}^H(t)\big), \tag{B2}$$

where $\hat{r}_k^H(t) = \hat{U}^\dagger(t)\hat{r}_k\hat{U}(t)$ for $k = 1, \dots, N+1$. The Heisenberg equations of motions read

$$\frac{d}{dt}\hat{r}_1^H(t) = \frac{\mathrm{i}}{\hbar}\big[\hat{H}^H(t), \hat{r}_1^H(t)\big] = \omega_1\hat{r}_2^H(t) + \sum_{j=2}^{N+1} g_j\hat{r}_{2j}^H(t), \tag{B3}$$

$$\frac{d}{dt}\hat{r}_2^H(t) = \frac{\mathrm{i}}{\hbar}\big[\hat{H}^H(t), \hat{r}_2^H(t)\big] = -\omega_1\hat{r}_1^H(t) - \sum_{j=2}^{N+1} g_j\hat{r}_{2j-1}^H(t), \tag{B4}$$

$$\frac{d}{dt}\hat{r}_{2j-1}^H(t) = \frac{\mathrm{i}}{\hbar}\big[\hat{H}^H(t), \hat{r}_{2j-1}^H(t)\big] = \omega_j\hat{r}_{2j}^H(t) + g_j\hat{r}_2^H(t) \quad \text{for} \quad j = 2, \dots, N+1, \tag{B5}$$

$$\frac{d}{dt}\hat{r}_{2j}^H(t) = \frac{\mathrm{i}}{\hbar}\big[\hat{H}^H(t), \hat{r}_{2j}^H(t)\big] = -\omega_j\hat{r}_{2j-1}^H(t) - g_j\hat{r}_1^H(t) \quad \text{for} \quad j = 2, \dots, N+1. \tag{B6}$$

Then the time derivative of the mean energy of each harmonic oscillator is calculated as

$$\begin{aligned}
\frac{d}{dt}E_A(t) &= \frac{d}{dt}E_1(t)\\
&= \frac{\hbar\omega_1}{2}\frac{d}{dt}\sigma_{1,1}(t)\\
&= \frac{\hbar\omega_1}{2}\frac{d}{dt}\mathrm{Tr}\big[\hat{\rho}(0)\big\{\hat{r}_1^H(t), \hat{r}_1^H(t)\big\}\big]\\
&= \frac{\hbar\omega_1}{2}\mathrm{Tr}\left[\hat{\rho}(0)\left\{\frac{d}{dt}\hat{r}_1^H(t), \hat{r}_1^H(t)\right\}\right] + \frac{\hbar\omega_1}{2}\mathrm{Tr}\left[\hat{\rho}(0)\left\{\hat{r}_1^H(t), \frac{d}{dt}\hat{r}_1^H(t)\right\}\right]\\
&= \frac{\hbar\omega_1}{2}\mathrm{Tr}\left[\hat{\rho}(0)\left\{\left(\omega_1\hat{r}_2^H(t) + \sum_{j=2}^{N+1} g_j\hat{r}_{2j}^H(t)\right), \hat{r}_1^H(t)\right\}\right] + \frac{\hbar\omega_1}{2}\mathrm{Tr}\left[\hat{\rho}(0)\left\{\hat{r}_1^H(t), \left(\omega_1\hat{r}_2^H(t) + \sum_{j=2}^{N+1} g_j\hat{r}_{2j}^H(t)\right)\right\}\right]\\
&= \frac{\hbar\omega_1}{2}\left[\omega_1\sigma_{2,1}(t) + \sum_{j=2}^{N+1} g_j\sigma_{2j,1}(t)\right] + \frac{\hbar\omega_1}{2}\left[\omega_1\sigma_{1,2}(t) + \sum_{j=2}^{N+1} g_j\sigma_{1,2j}(t)\right]\\
&= \hbar\omega_1\left[\omega_1\sigma_{1,2}(t) + \sum_{j=2}^{N+1} g_j\sigma_{1,2j}(t)\right]\\
&= \hbar\omega_1\sum_{j=2}^{N+1} g_j\sigma_{1,2j}(t),
\end{aligned} \tag{B7}$$

$$\begin{aligned}
\frac{d}{dt}E_j(t) &= \frac{\hbar\omega_j}{2}\frac{d}{dt}\sigma_{2j-1,2j-1}(t)\\
&= \frac{\hbar\omega_j}{2}\frac{d}{dt}\mathrm{Tr}\big[\hat{\rho}(0)\big\{\hat{r}_{2j-1}^H(t), \hat{r}_{2j-1}^H(t)\big\}\big]\\
&= \frac{\hbar\omega_j}{2}\mathrm{Tr}\left[\hat{\rho}(0)\left\{\frac{d}{dt}\hat{r}_{2j-1}^H(t), \hat{r}_{2j-1}^H(t)\right\}\right] + \frac{\hbar\omega_j}{2}\mathrm{Tr}\left[\hat{\rho}(0)\left\{\hat{r}_{2j-1}^H(t), \frac{d}{dt}\hat{r}_{2j-1}^H(t)\right\}\right]\\
&= \frac{\hbar\omega_j}{2}\mathrm{Tr}\big[\hat{\rho}(0)\big\{\big(\omega_j\hat{r}_{2j}^H(t) + g_j\hat{r}_2^H(t)\big), \hat{r}_{2j-1}^H(t)\big\}\big] + \frac{\hbar\omega_j}{2}\mathrm{Tr}\big[\hat{\rho}(0)\big\{\hat{r}_{2j-1}^H(t), \big(\omega_j\hat{r}_{2j}^H(t) + g_j\hat{r}_2^H(t)\big)\big\}\big]\\
&= \frac{\hbar\omega_j}{2}[\omega_j\sigma_{2j,2j-1}(t) + g_j\sigma_{2,2j-1}(t)] + \frac{\hbar\omega_j}{2}[\omega_j\sigma_{2j-1,2j}(t) + g_j\sigma_{2j-1,2}(t)]\\
&= \hbar\omega_j[\omega_j\sigma_{2j-1,2j}(t) + g_j\sigma_{2,2j-1}(t)]\\
&= \hbar\omega_j g_j\sigma_{2,2j-1}(t)\\
&= -\hbar\omega_j g_j\sigma_{1,2j}(t) \quad \text{for} \quad j = 2, \dots, N+1,
\end{aligned} \tag{B8}$$

where the last line follows from

$$\begin{aligned}
\sigma_{1,2j}(t) &= \sum_{l=1}^{2N+2} (\cos Ht + \Omega \sin Ht)_{1,l}\sigma_{l,l}(0)(\cos Ht - [\sin Ht]\Omega)_{l,2j}\\
&= \sum_{l=1}^{2N+2} [(\cos Ht)_{1,l} + (\sin Ht)_{2,l}]\sigma_{l,l}(0)[(\cos Ht)_{l,2j} - (\sin Ht)_{l,2j-1}]\\
&= \sum_{m=1}^{N+1} [-(\cos Ht)_{1,2m-1}\sigma_{2m-1,2m-1}(0)(\sin Ht)_{2m-1,2j-1} + (\sin Ht)_{2,2m}\sigma_{2m,2m}(0)(\cos Ht)_{2m,2j}]\\
&= \sum_{m=1}^{N+1} [-(\cos Ht)_{1,2m-1}\sigma_{2m-1,2m-1}(0)(\sin Ht)_{2m-1,2j-1} + (\sin Ht)_{1,2m-1}\sigma_{2m-1,2m-1}(0)(\cos Ht)_{2m-1,2j-1}], \qquad \text{(B9)}
\end{aligned}$$

$$\begin{aligned}
\sigma_{2,2j-1}(t) &= \sum_{l=1}^{2N+2} (\cos Ht + \Omega \sin Ht)_{2,l}\sigma_{l,l}(0)(\cos Ht - [\sin Ht]\Omega)_{l,2j-1}\\
&= \sum_{l=1}^{2N+2} [(\cos Ht)_{2,l} - (\sin Ht)_{1,l}]\sigma_{l,l}(0)[(\cos Ht)_{l,2j-1} + (\sin Ht)_{l,2j}]\\
&= \sum_{m=1}^{N+1} [(\cos Ht)_{2,2m}\sigma_{2m,2m}(0)(\sin Ht)_{2m,2j} - (\sin Ht)_{1,2m-1}\sigma_{2m-1,2m-1}(0)(\cos Ht)_{2m-1,2j-1}]\\
&= \sum_{m=1}^{N+1} [(\cos Ht)_{1,2m-1}\sigma_{2m-1,2m-1}(0)(\sin Ht)_{2m-1,2j-1} - (\sin Ht)_{1,2m-1}\sigma_{2m-1,2m-1}(0)(\cos Ht)_{2m-1,2j-1}]\\
&= -\sigma_{1,2j}(t). \qquad \text{(B10)}
\end{aligned}$$

Inserting Eqs. (B7) and (B8) into Eq. (66), we obtain Eq. (67), which we can calculate from the covariance matrix $\sigma(t)$.

The time derivative of the mean energy of the bath is calculated as

$$\frac{d}{dt}E_B(t) = \sum_{j=2}^{N+1} \frac{d}{dt}E_j(t) = -\sum_{j=2}^{N+1} \hbar\omega_j g_j \sigma_{1,2j}(t). \qquad \text{(B11)}$$

From the conservation of the total energy, the time derivative of the interaction energy is calculated as

$$\frac{d}{dt}E_I(t) = -\frac{d}{dt}E_A(t) - \frac{d}{dt}E_B(t) = \sum_{j=2}^{N+1} \hbar(\omega_j - \omega_1)g_j\sigma_{1,2j}(t). \qquad \text{(B12)}$$

In Fig. 2, we compare $dE_A(t)/dt$ in Eq. (B7), $dE_B(t)/dt$ in Eq. (B11), and $dE_I(t)/dt$ in Eq. (B12).

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