Full-counting statistics of heat transport in harmonic junctions: Transient, steady states, and fluctuation theorems

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We study the statistics of heat transferred in a given time interval t_M, through a finite harmonic chain, called the center, which is connected to two heat baths, the left (L) and the right (R), that are maintained at two temperatures. The center atoms are driven by external time-dependent forces. We calculate the cumulant generating function (CGF) for the heat transferred out of the left lead, Q_L, based on the two-time quantum measurement concept and using the nonequilibrium Green's function method. The CGF can be concisely expressed in terms of Green's functions of the center and an argument-shifted self-energy of the lead. The expression of the CGF is valid in both transient and steady-state regimes. We consider three initial conditions for the density operator and show numerically, for a one-atom junction, how their transient behaviors differ from each other but, finally, approach the same steady state, independent of the initial distributions. We also derive the CGF for the joint probability distribution $P(Q_L, Q_R)$, and discuss the correlations between Q_L and Q_R. We calculate the CGF for total entropy production in the reservoirs. In the steady state we explicitly show that the CGFs obey steady-state fluctuation theorems. We obtain classical results by taking $\hbar \to 0$. We also apply our method to the counting of the electron number and electron energy, for which the associated self-energy is obtained from the usual lead self-energy by multiplying a phase and shifting the contour time, respectively.

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I. INTRODUCTION

Nonequilibrium systems are common in nature because they are, in general, subject to thermal gradients or chemical potential gradients or may be triggered by nonconservative forces. Heat transport is one such example of nonequilibrium systems where the heat carriers could be electrons, phonons, magnons, etc. To study heat transport in phononic systems, one considers a finite junction part, which can be an insulator, connected to two heat baths that are maintained at different temperatures. In the past decade, the main focus was on the calculation of the steady-state heat current or heat flux flowing through the junction part from the leads [1–10]. For diffusive systems, the answer is given by Fourier's law [11–13], which is true only in the linear response regime, i.e., when the temperature difference between the baths is small. However, for harmonic or ballistic systems, the heat current is given by a Landauer-like formula [3,7,10] which was first derived for electronic transport. The Landauer formula, contrary to Fourier's law, is true for arbitrary temperature differences between the leads. No such explicit expression for current is known for transient states. Recently, several works [14,15] have tried to answer what happens to current in the transient regime. This is an important question from both the theoretical and the experimental points of view.

Another aspect in phonon transport is on thermal devices and on controlling heat flow [16]. With the advent of new technology, it is now possible to study transport problems and observe a single mode of vibration in small systems with few degrees of freedom [17]. These systems show strong thermal fluctuations which can lead to instantaneous heat transfer from colder to hotter lead and hence could be a violation of the second law of thermodynamics. It is therefore necessary to talk about the statistical distribution of heat flux for these systems. In the electronic literature the distribution $P(Q_L)$ of the charge Q_L, flowing from the left lead to the junction part, was answered by calculating the corresponding generating function (GF), $\mathcal{Z}(\xi) = \langle e^{i\xi Q_L} \rangle$, and is given by the celebrated Levitov-Lesovik formula [18–20]. This methodology is also known as the *full counting statistics* [21–30] in the field of electronic transport. Experimentally the electron counting statistics has been measured in quantum-dot systems [31,32]. However, few experiments have been done on phonons [33]. In the phononic case Saito and Dhar [34] gave an explicit expression of the cumulant GF (CGF). Ren *et al.* gave results for two-level systems [35,36]. Full counting statistics of energy fluctuations in a driven quantum resonator was studied by Clerk [37]. The main focus in these papers was on the long-time limit and steady-state fluctuation theorem (SSFT) [38–43]. Using the nonequilibrium Green's function (NEGF) method [44,45] and two-time measurement [41,42,46,47] concept, Wang *et al.* [40] gave an explicit expression for the CGF which is valid for both transient and steady-state regimes.

In this paper, we extend our previous work in Ref. [40] and derive the CGF in a more general scenario, i.e., in the presence of both a temperature difference and time-dependent driving forces, for three different initial conditions of the density operator [Eqs. (45) and (61)]. We analyze the cumulants of heat Q_L by doing numerical simulations and study the effects on both transient and steady-state regimes for these initial conditions. We also derive the CGF for the joint probability

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distribution of left- and right-lead heat $P(Q_L,Q_R)$, which helps us to obtain the correlations between Q_L and Q_R. By calculating CGF for $P(Q_L,Q_R)$ we can immediately obtain the CGF for the total entropy production in the reservoirs. We present analytical expressions for the CGFs in the steady state and discuss the SSFT. Our method can be easily generalized for multiple heat baths and also in higher dimensions. Our derivation is also formally valid for a finite size of the heat baths and hence it is possible to study its effects on the cumulants and also on the fluctuation theorem, which has recently received much attention [48,49]. We do not, however, discuss this effect here and consider the semi-infinite limit of the heat baths, which is important for achieving irreversibility. We also discuss another definition of CGF due to Nazarov [Eq. (10)] and derive the corresponding long-time limit [Eq. (116)]. We find that, using this definition, the GF does not obey the Gallavotti-Cohen (GC) fluctuation symmetry, however, the first two cumulants of heat are the same.

The plan of the paper is as follows. We start in Sec. II by introducing our model. Then in Sec. III we define current and corresponding quantum heat operator, followed by the CGF for Q_L using the two-time measurement concept in Sec. IV. In Sec. V we derive the CGF for a projected initial condition [defined in Eq. (15)] using Feynman's path integral method, and in Sec. VI we use Feynman's diagrammatic technique to derive the CGF for the product initial state. The expressions for the CGFs are true for any transient time and also for any finite size of the leads. We show analytically that in the long-time limit the CGFs are the same independent of the initial distributions and also discuss the fluctuation theorems in Sec. VII. In Sec. VIII we present numerical results for the one-dimensional (1D) linear chain model, connected by Rubin heat baths, for three different initial conditions. Then in Sec. IX we obtain the CGF for the joint probability distribution of heat transferred $P(Q_L,Q_R)$ and discuss correlations and total entropy production in the leads. In Sec. X we give the long-time limit expression for the driven part of the full CGF. In Sec. XI we obtain the classical limit for the GFs. In Sec. XII we discuss Nazarov's CGF. Finally, we conclude with a short discussion in Sec. XIII. The appendixes give some details of a technical nature. In particular, the electron system of a tight-binding model is treated using our method.

II. THE MODEL

Our model consists of a finite harmonic junction of arbitrary dimension, which we denote C, coupled to two heat baths, the left (L) and the right (R), kept at two different temperatures, T_L and T_R, respectively. To model the heat baths, we consider an infinite collection of coupled harmonic oscillators. We take the three systems to be decoupled initially and to be described by the Hamiltonians,

$$\mathcal{H}_\alpha = \tfrac{1}{2}p_\alpha^T p_\alpha + \tfrac{1}{2}u_\alpha^T K^\alpha u_\alpha, \quad \alpha = L,C,R, \tag{1}$$

for the left, right, and finite central region. Masses are absorbed by defining $u = \sqrt{m}\,x$; u_α and p_α are column vectors of coordinates and momenta. K^α is the spring constant matrix of region α. Couplings of the center region with the leads are turned on either adiabatically from time $t = -\infty$, or switched on abruptly at $t = 0$. The interaction Hamiltonian takes the form

$$\mathcal{H}_{\rm int} = u_L^T\, V^{LC}\, u_C + u_R^T\, V^{RC}\, u_C. \tag{2}$$

For $t > 0$, an external time-dependent force is applied to the center atoms, which is of the form

$$\mathcal{V}_C(t) = -f^T(t)\, u_C, \tag{3}$$

where $f(t)$ is the time-dependent force vector. The driving force couples only with the position operators of the center. The force can be in the form of an electromagnetic field. Coupling of this form helps us to obtain an analytical solution for the CGF of heat flux. The full Hamiltonian for $t > 0$ (in the Schrödinger picture) is

$$\mathcal{H}(t) = \mathcal{H}(0^-) + \mathcal{V}_C(t) = \mathcal{H}_C + \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_{\rm int} + \mathcal{V}_C(t). \tag{4}$$

In the next section we define the current operator and the corresponding heat operator based on this Hamiltonian.

III. DEFINITION OF CURRENT AND HEAT OPERATORS

The current operator $\mathcal{I}$ depends on where we want to measure the current. Here we consider the current flowing from the left lead to the center system and $\mathcal{I}_L$ is defined (in the Heisenberg picture) as

$$\mathcal{I}_L(t) = -\frac{d\mathcal{H}_L^H(t)}{dt} = \frac{i}{\hbar}\big[\mathcal{H}_L^H(t),\mathcal{H}^H(t)\big] = p_L^T(t)\, V^{LC}\, u_C(t), \tag{5}$$

where $\mathcal{H}^H(t)$ is the (time-dependent) Hamiltonian in the Heisenberg picture at time t. The corresponding heat operator can be written as

$$\mathcal{Q}_L(t) = \int_0^t \mathcal{I}_L(t')\,dt' = \mathcal{H}_L(0) - \mathcal{H}_L^H(t), \tag{6}$$

where $\mathcal{H}_L[=\mathcal{H}_L(0)]$ is the Schrödinger operator of the free left lead and

$$\mathcal{H}_L^H(t) = \mathcal{U}(0,t)\,\mathcal{H}_L\,\mathcal{U}(t,0), \tag{7}$$

and $\mathcal{U}(t,t')$ is the evolution operator corresponding to the full Hamiltonian $\mathcal{H}(t)$ with the formal solution (assuming $t \geqslant t'$)

$$\mathcal{U}(t,t') = T\exp\left\{-\frac{i}{\hbar}\int_{t'}^t \mathcal{H}(\bar{t})\,d\bar{t}\right\}, \tag{8}$$

where T is the time-ordering operator and time increases from right to left. Also, $\mathcal{U}^\dagger(t,t') = \mathcal{U}(t',t)$. Note that $\mathcal{Q}$ of noncalligraphic font is a classical variable.

In the following section we derive the CGF based on this definition of heat operator and using a two-time measurement scheme.

IV. DEFINITION OF THE GENERATING FUNCTION FOR THE HEAT OPERATOR

Our primary interest here is to calculate the moments or cumulants of the heat energy transferred in a given time interval t_M. Hence, it is advantageous to calculate the GF instead of calculating moments directly. Correspondingly, the probability distribution can be obtained by doing an inverse Fourier transform of the GF. Since $\mathcal{Q}_L$ is a quantum operator,

there are subtleties as to how exactly the GF should be defined. Naively, we may use $\langle e^{i\xi \mathcal{Q}_L}\rangle$. But this definition fails the fundamental requirement of positive definiteness of the probability distribution.

Here we give two different definitions that are used to calculate the GF for such problem. The first definition comes from the idea of two-time measurements, and based on this concept the GF can be written down as

$$\mathcal{Z}(\xi) = \left\langle e^{i\xi \mathcal{H}_L}\, e^{-i\xi \mathcal{H}_L^H(t)}\right\rangle', \tag{9}$$

where the meaning of $\langle\cdots\rangle'$ is discussed just after Eq. (15).

The second definition of the GF is

$$\mathcal{Z}_1(\xi) = \langle \bar{T} e^{i\xi \mathcal{Q}_L/2} T e^{i\xi \mathcal{Q}_L/2}\rangle, \tag{10}$$

where $\bar{T}$ is the anti-time order operator. The time (or antitime) order is meant to apply to the integrand when the exponential is expanded and $\mathcal{Q}_L$ is expressed as an integral over $\mathcal{I}_L$ as in Eq. (6). This definition is used by Nazarov *et al.* [21,22] mostly for electronic transport. In the last section we show how this GF can be derived starting from $\mathcal{Z}(\xi)$ given in Eq. (9) under a particular approximation and also present the long-time limit expression for $\mathcal{Z}_1(\xi)$ for the harmonic model.

In the following we derive Eq. (9) based on a two-time measurement concept. Our derivation is similar to Ref. [41] except that the measured operator in this case is $\mathcal{H}_L$. Readers who are familiar with two-time measurement may skip this section and start from Sec. IV B.

A. Two-time quantum measurement

The heat operator in Eq. (6) depends on the left-lead Hamiltonian $\mathcal{H}_L$ at time 0 and t. The concept of two-time measurement implies the measurement of a certain operator (in this case $\mathcal{H}_L$) at two different times. Here the measurement is in the sense of quantum measurement of von Neumann [50].

Let us first assume that the full system is in a pure state $|\Psi_0\rangle$ at $t = 0$. We want to do measurement of the energy associated with the operator $\mathcal{H}_L$. According to quantum mechanics, the result of a measurement can only be an eigenvalue of the (Schrödinger) operator $\mathcal{H}_L$ and the wave function collapses into an eigenstate of $\mathcal{H}_L$. Let

$$\mathcal{H}_L|\phi_a\rangle = a|\phi_a\rangle, \quad \Pi_a = |\phi_a\rangle\langle\phi_a|, \tag{11}$$

where Π_a is the projector into the state $|\phi_a\rangle$ satisfying $\Pi_a^2 = \Pi_a$, and $\sum_a \Pi_a = 1$. We assume that the eigenvalues are discrete (this is always so if the lattice system is finite). After the measurement at time $t = 0$, the wave function is proportional to $\Pi_a|\Psi_0\rangle$ if the result of the measurement is the energy a and the probability of such an event happening is $\langle\Psi_0|\Pi_a^2|\Psi_0\rangle$. Let us propagate this state to time t and do a second measurement of the lead energy, finding that the result is b. The wave function now becomes proportional to $\Pi_b\,\mathcal{U}(t,0)\,\Pi_a\,|\Psi_0\rangle$. The joint probability of getting a at time 0 and b at time t is the square norm (inner product) of the above (unnormalized) state.

If the initial state is in a mixed state, we add up the initial probability classically, i.e., if

$$\rho(0) = \sum_k w_k \left|\Psi_0^k\right\rangle\left\langle\Psi_0^k\right|, \quad w_k > 0, \quad \sum_k w_k = 1, \tag{12}$$

the joint probability distribution of two-time measurement output is

$$\begin{aligned} P(b,a) &= \sum_k w_k \left\langle\Psi_0^k\right|\Pi_a\,\mathcal{U}(0,t)\,\Pi_b\,\mathcal{U}(t,0)\,\Pi_a\left|\Psi_0^k\right\rangle \\ &= \mathrm{Tr}[\Pi_a\,\rho(0)\,\Pi_a\,\mathcal{U}(0,t)\,\Pi_b\,\mathcal{U}(t,0)]. \end{aligned} \tag{13}$$

By definition, we see that $P(b,a)$ is a proper probability in the sense that $P(b,a) \geqslant 0$ and $\sum_{a,b} P(b,a) = 1$. Then the GF for $\mathcal{Q}_L = a - b$ is defined as

$$\begin{aligned} \mathcal{Z}(\xi) &= \langle e^{i\xi(a-b)}\rangle = \sum_{a,b} e^{i\xi(a-b)} P(b,a) \\ &= \sum_{a,b} e^{i\xi(a-b)} \mathrm{Tr}[\Pi_a\,\rho(0)\,\Pi_a\,\mathcal{U}(0,t)\,\Pi_b\,\mathcal{U}(t,0)] \\ &= \left\langle e^{i\xi\mathcal{H}_L}\, e^{-i\xi\mathcal{H}_L^H(t)}\right\rangle' \\ &= \left\langle e^{i\xi\mathcal{H}_L/2}\, e^{-i\xi\mathcal{H}_L^H(t)}\, e^{i\xi\mathcal{H}_L/2}\right\rangle', \end{aligned} \tag{14}$$

where the prime indicates that the average is with respect to

$$\rho'(0) = \sum_a \Pi_a\,\rho(0)\Pi_a, \tag{15}$$

which we call the *projected* density matrix [50].

If the initial state at $t = 0$ is a product state, i.e., $\rho(0) = \rho(-\infty) = \rho_L \otimes \rho_C \otimes \rho_R$, where the left, center, and right density matrices are in equilibrium distributions corresponding to the respective temperatures—$\rho_\alpha = e^{-\beta_\alpha \mathcal{H}_\alpha}/\mathrm{Tr}[e^{-\beta_\alpha\mathcal{H}_\alpha}]$ for $\alpha = L,C,R$ and $\beta_\alpha = 1/(k_B T_\alpha)$—then the initial projection operators Π_a do not play any role and $\langle\ldots\rangle' = \mathrm{Tr}[\rho(-\infty)\cdots] = \langle\ldots\rangle$.

B. Initial conditions

Here we derive the CGF for three initial conditions.

(1) The product initial state $\rho(-\infty)$; the coupling between the leads and the center is suddenly switched on at $t = 0$ and the system is let to evolve for a finite time t_M by the dynamics determined by $\mathcal{H}$.

(2) The steady state as the initial state, i.e., $\rho(0)$, which we can obtain, starting with the decoupled Hamiltonians at $t = -\infty$; the couplings between the center region and the leads are switched on adiabatically up to time $t = 0$.

(3) The *projected* density matrix $\rho'(0)$ considering $\rho(0)$ as the steady state, i.e., taking the effects of measurements into account.

In the following sections we show analytically that the CGFs corresponding to different initial conditions reach the unique steady state in the long-time limit, hence are independent of the initial distributions. However, the transient behavior depends significantly on the initial conditions and also on the measurements.

V. CALCULATION FOR $\mathcal{Z}(\xi)$ USING THE FEYNMAN PATH INTEGRAL FORMALISM FOR INITIAL STATES $\rho(0)$ AND $\rho'(0)$

A. Removing the projection Π_a at $t = 0$

The projection by Π_a at $t = 0$ in Eq. (15) creates a problem for formulation in path integrals. We can remove this by putting it into part of an evolution of $\mathcal{H}_L$, just like the

factor associated with the GF variable ξ, but we must pay a price—the introduction of another integration variable, λ. The key observation is that we can represent the projector by the Dirac δ function

$$\Pi_a \propto \delta(a-\mathcal{H}_L) = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi}\, e^{-i\lambda(a-\mathcal{H}_L)}. \tag{16}$$

For this to make sense, we assume that the spectrum of the energy of $\mathcal{H}_L$ is continuous, which is valid if we take the large size limit first. Identifying Π_a as $\delta(a-\mathcal{H}_L)$ with a continuous variable a introduces a constant proportional to the Dirac $\delta(0)$ to $\rho'(0)$, since Π_a is now normalized as $\Pi_a\Pi_b = \delta(a-b)\Pi_a$. However, this constant can be easily fixed by the condition $\mathcal{Z}(0)=1$. So using $\Pi_a = \delta(a-\mathcal{H}_L)$ will not cause difficulty.

Substituting the Fourier integral representation into the expression for ρ', we obtain

$$\rho'(0) \propto \int da\, \Pi_a\, \rho(0)\Pi_a \tag{17}$$

$$= \int \frac{d\lambda}{2\pi} e^{i\lambda\mathcal{H}_L}\rho(0)e^{-i\lambda\mathcal{H}_L}. \tag{18}$$

Using the symmetric form of $\mathcal{Z}$, Eq. (14), we have

$$\mathcal{Z}(\xi) \propto \int \frac{d\lambda}{2\pi}\mathrm{Tr}\{\rho(0)\mathcal{U}_{\xi/2-\lambda}(0,t)\mathcal{U}_{-\xi/2-\lambda}(t,0)\}$$
$$= \int \frac{d\lambda}{2\pi}\, \mathcal{Z}(\xi,\lambda), \tag{19}$$

where $\mathcal{U}_x(t,t')$ is the modified evolution operator of an effective Hamiltonian given by

$$\mathcal{H}_x(t) = e^{ix\mathcal{H}_L}\mathcal{H}(t)e^{-ix\mathcal{H}_L}, \tag{20}$$

where x is a real parameter which, in this case, is $\xi/2-\lambda$ or $-\xi/2-\lambda$. Finally, $\mathcal{U}_x(t,t')$ is given by ($t \geqslant t'$)

$$\mathcal{U}_x(t,t') = e^{ix\mathcal{H}_L}\mathcal{U}(t,t')e^{-ix\mathcal{H}_L}$$
$$= \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 \cdots \int_{t'}^{t_{n-1}} dt_n$$
$$\times e^{ix\mathcal{H}_L}\mathcal{H}(t_1)\mathcal{H}(t_2)\cdots\mathcal{H}(t_n)e^{-ix\mathcal{H}_L}$$
$$= T\exp\left\{-\frac{i}{\hbar}\int_{t'}^{t}\mathcal{H}_x(t')dt'\right\}. \tag{21}$$

It is important to note that substituting $\lambda=0$ in $\mathcal{Z}(\xi,\lambda)$ gives us the result for the initial density matrix $\rho(0)$.

Now we give an explicit expression of the modified Hamiltonian $\mathcal{H}_x$ which helps us to calculate the CGF using the path integral.

B. Expression for the effective Hamiltonian $\mathcal{H}_x$

The modified Hamiltonian is the central quantity for calculating the CGF. It is the Heisenberg evolution of the full Hamiltonian $\mathcal{H}(t)$ (in the Schrödinger picture) with respect to $\mathcal{H}_L$. Since $\mathcal{H}_L$ commutes with every term $\tilde{\mathcal{H}}$ where $\mathcal{H}(t) = \tilde{\mathcal{H}} + u_L^T V^{LC} u_C$, except the coupling term $u_L^T V^{LC} u_C$, we can write

$$\mathcal{H}_x(t) = e^{ix\mathcal{H}_L}\mathcal{H}(t)e^{-ix\mathcal{H}_L}$$
$$= e^{ix\mathcal{H}_L}\left(\tilde{\mathcal{H}} + u_L^T V^{LC} u_C\right)e^{-ix\mathcal{H}_L}$$
$$= \mathcal{H}(t) + (u_L(\hbar x) - u_L)^T V^{LC} u_C, \tag{22}$$

where $u_L(\hbar x) = e^{ix\mathcal{H}_L}u_L e^{-ix\mathcal{H}_L}$ is the free left-lead Heisenberg evolution to time $t=\hbar x$. $u_L(\hbar x)$ can be obtained explicitly as

$$u_L(\hbar x) = \cos(\sqrt{K_L}\hbar x)u_L + \frac{1}{\sqrt{K_L}}\sin(\sqrt{K_L}\hbar x)p_L. \tag{23}$$

The matrix $\sqrt{K_L}$ is well defined, as the matrix K_L is positive definite. u_L and p_L are the initial values at $t=0$. The final expression for $\mathcal{H}_x(t)$ is

$$\mathcal{H}_x(t) = \mathcal{H}(t) + \left[u_L^T\mathcal{C}(x) + p_L^T\mathcal{S}(x)\right]u_C, \tag{24}$$

where

$$\mathcal{C}(x) = (\cos(\hbar x\sqrt{K_L}) - I)V^{LC}, \tag{25}$$

$$\mathcal{S}(x) = (1/\sqrt{K_L})\sin(\hbar x\sqrt{K_L})V^{LC}. \tag{26}$$

The effective Hamiltonian now has two additional terms with respect to the full $\mathcal{H}(t)$. The term $u_L^T\mathcal{C}(x)u_C$ is like the harmonic coupling term which modifies the coupling matrix V^{LC}.

In the following we calculate the two-parameter GF $\mathcal{Z}(\xi,\lambda)$ given in Eq. (19).

C. Expression for $\mathcal{Z}(\xi,\lambda)$

The expression for $\mathcal{Z}(\xi,\lambda)$ can be written down on the contour as (see Fig. 1)

$$\mathcal{Z}(\xi,\lambda) = \mathrm{Tr}[\rho(0)T_c e^{-\frac{i}{\hbar}\int_C \mathcal{H}_x(\tau)d\tau}], \tag{27}$$

where T_c is the contour-ordered operator, which orders operators according to their contour time argument; an earlier contour time places an operator to the right. The contour function $x(\tau)$ is defined as 0 whenever $t<0$ or $t>t_M$, and when $0<t<t_M$, i.e., within the measurement time interval, for the upper branch of the contour $x^+(t) = -\xi/2-\lambda$, and for the lower branch $x^-(t) = \xi/2-\lambda$.

For the moment, let us forget about the other lead and concentrate only on the left lead and center. The effect of the other lead simply modifies the self-energy of the leads additively, according to Feynman and Vernon [51]. Using the

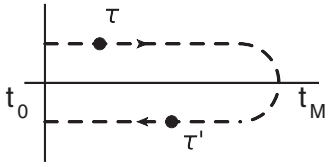

FIG. 1. Complex-time contour in the Keldysh formalism. The path of the contour begins at time t_0, goes to time t_M, and then goes back to time $t=t_0$. τ and τ' are complex-time variables along the contour. $t_0=-\infty$ and 0 correspond to Keldysh contours K and C, respectively.

Feynman path integral technique we can write

$$\mathcal{Z}(\xi,\lambda) = \int \mathcal{D}[u_C]\mathcal{D}[u_L]\rho(-\infty)e^{(i/\hbar)\int_K d\tau(\mathcal{L}_C+\mathcal{L}_L+\mathcal{L}_{LC})}. \tag{28}$$

Note that in Eq. (27), the contour C is from 0 to t_M and back, while that in Eq. (28) is on the Keldysh contour K, that is, from $-\infty$ to t_M and back, to take into account adiabatic switch-on, replacing $\rho(0)$ with $\rho(-\infty)$. Their relation is

$$\rho(0) = \mathcal{U}(0,-\infty)\rho(-\infty)\mathcal{U}(-\infty,0). \tag{29}$$

We can identify the Lagrangians as

$$\begin{aligned}\mathcal{L}_L &= \tfrac{1}{2}\dot{u}_L^2 - \tfrac{1}{2}u_L^T K^L u_L,\\ \mathcal{L}_C &= \tfrac{1}{2}\dot{u}_C^2 + f^T u_C - \tfrac{1}{2}u_C^T(K^C - \mathcal{S}^T\mathcal{S})u_C,\\ \mathcal{L}_{LC} &= -\dot{u}_L^T\mathcal{S}u_C - u_L^T(V^{LC}+\mathcal{C})u_C.\end{aligned} \tag{30}$$

For notational simplicity, we have dropped the argument τ. The vector f or matrices $\mathcal{C}$ and $\mathcal{S}$ are parametrically dependent on the contour time τ. They are 0 except on the interval $0 < t < t_M$. f is the same on the upper and lower branches, while $\mathcal{C}$ and $\mathcal{S}$ take different values depending on $x(\tau)$.

Now the lead part can be integrated out by performing the Gaussian integral [51]. To find exactly what it is, we convert the path integral back to the interaction picture (with respect to $\mathcal{H}_L$) operator form and evaluate the expression by the standard perturbative expansion. The only difference is that now the coupling with the center involves both u_L and $\dot{u}_L$. The result for the influence functional is given by [52]

$$\begin{aligned}I_L[u^C(\tau)] &\equiv \int \mathcal{D}[u_L]\rho_L(-\infty)e^{\frac{i}{\hbar}\int d\tau(\mathcal{L}_L+\mathcal{L}_{LC})}\\ &= \mathrm{Tr}\left[\frac{e^{-\beta_L H_L}}{Z_L}T_c e^{-\frac{i}{\hbar}\int d\tau\mathcal{V}_I^x(\tau)}\right]\\ &= e^{-\frac{i}{2\hbar}\int d\tau\int d\tau' u_C^T(\tau)\Pi^x(\tau,\tau')u_C(\tau')}.\end{aligned} \tag{31}$$

In the influence functional, the contour function $u_C(\tau)$ is not a dynamical variable but a parametric function. $\mathcal{V}_I^x(\tau)$ is the interaction picture operator with respect to the Hamiltonian $\mathcal{H}_L$ and is given by

$$\begin{aligned}\mathcal{V}_I^x(\tau) &= p_L^T\mathcal{S}u_C + u_L^T(V^{LC}+\mathcal{C})u_C + \tfrac{1}{2}u_C^T\mathcal{S}^T\mathcal{S}u_C\\ &= u_L^T(\tau+\hbar x(\tau))V^{LC}u_C + \tfrac{1}{2}u_C^T\mathcal{S}^T\mathcal{S}u_C.\end{aligned} \tag{32}$$

The important influence functional self-energy on the contour is given by

$$\Pi^x(\tau,\tau') = \Sigma_L^A(\tau,\tau') + \Sigma_L(\tau,\tau') + \mathcal{S}^T\mathcal{S}\,\delta(\tau,\tau'), \tag{33}$$

$$\begin{aligned}\Sigma_L^A(\tau,\tau') + \Sigma_L(\tau,\tau') &= V^{CL}g_L(\tau+\hbar x(\tau),\tau'+\hbar x(\tau'))V^{LC}\\ &= \Sigma_L(\tau+\hbar x(\tau),\tau'+\hbar x(\tau')),\end{aligned} \tag{34}$$

where we obtain a shifted self-energy $\Sigma_L(\tau+\hbar x(\tau),\tau'+\hbar x(\tau'))$, which is the usual self-energy of the lead in contour time with arguments shifted by $\hbar x(\tau)$ and $\hbar x(\tau')$. We define the self-energy Σ_L^A as the difference between the shifted self-energy and the usual one $\Sigma_L(\tau,\tau')$. Σ_L^A turns out to be a central quantity for this problem, as we show that $\mathcal{Z}(\xi)$ can be concisely expressed in terms of the center Green's function G_0 and Σ_L^A.

Substituting the explicit expression for the influence functionals of both the left and the right leads to the path integral expression given in Eq. (28), we have

$$\begin{aligned}\mathcal{Z}(\xi,\lambda) &= \int \mathcal{D}[u_C]\rho_C(-\infty)e^{(i/\hbar)\int d\tau\mathcal{L}_C}I_L[u_C]I_R[u_C]\\ &= \int \mathcal{D}[u_C]\rho_C(-\infty)e^{\frac{i}{\hbar}S_{\mathrm{eff}}},\end{aligned} \tag{35}$$

where the effective action is given by

$$\begin{aligned}S_{\mathrm{eff}} &= \int d\tau\left[\frac{1}{2}\dot{u}_C^2 - \frac{1}{2}u_C^T K^C u_C + f^T u_C\right]\\ &\quad - \frac{1}{2}\int d\tau\int d\tau' u_C^T(\tau)(\Sigma(\tau,\tau') + \Sigma_L^A(\tau,\tau'))u_C(\tau'),\end{aligned} \tag{36}$$

where $\Sigma = \Sigma_L + \Sigma_R$, taking into account the effect of both leads. The $\mathcal{S}^T\mathcal{S}$ term in $I_L[u_C]$ cancels exactly with the one in $\mathcal{L}_C$. We can perform an integration by part on the $\dot{u}^2$ term, assuming that the surface term does not matter (since it is at $t = -\infty$), we can write the expression in a standard quadratic form,

$$\begin{aligned}S_{\mathrm{eff}} &= \frac{1}{2}\int d\tau\int d\tau' u_C^T(\tau)D(\tau,\tau')u_C(\tau')\\ &\quad + \int f^T(\tau)u_C(\tau)d\tau.\end{aligned} \tag{37}$$

$D(\tau,\tau')$ is a differential operator and is given by

$$\begin{aligned}D(\tau,\tau') &= -I\frac{\partial^2}{\partial\tau^2}\delta(\tau,\tau') - K^C\delta(\tau,\tau')\\ &\quad - \Sigma(\tau,\tau') - \Sigma_L^A(\tau,\tau')\\ &= D_0(\tau,\tau') - \Sigma_L^A(\tau,\tau').\end{aligned} \tag{38}$$

The above equation defines the Dyson equation on Keldysh contour. The GF is obtained by doing another Gaussian integration and is of the following form:

$$\mathcal{Z} \propto \det(D)^{-1/2}e^{-\frac{i}{2\hbar}f^T D^{-1}f}. \tag{39}$$

(The meaning of the determinant is explained in Appendix C.) We define the Green's function G and G_0 by $DG = 1$ and $D_0G_0 = 1$, or more precisely,

$$\int D(\tau,\tau'')G(\tau'',\tau')d\tau'' = I\delta(\tau,\tau'), \tag{40}$$

and similarly for G_0. G can be written in terms of G_0 in the following Dyson equation form:

$$\begin{aligned}G(\tau,\tau') &= G_0(\tau,\tau')\\ &\quad + \int\int d\tau_1 d\tau_2 G_0(\tau,\tau_1)\Sigma_L^A(\tau_1,\tau_2)G(\tau_2,\tau').\end{aligned} \tag{41}$$

We view the differential operator (integral operator) D and D^{-1} as matrices that are indexed by space j and contour time τ. f is a column vector. The exponential factor term can also be written as a trace, $f^T D^{-1} f = \mathrm{Tr}_{(j,\tau)}(Gff^T)$. We can fix the proportionality constant by noting that $\mathcal{Z}(\xi = 0,\lambda = 0) = 1$. Since when $\xi = 0$, $\lambda = 0$, we have $x = 0$ and thus $\Sigma_L^A(\tau,\tau') = \Sigma_L(\tau+\hbar x,\tau'+\hbar x') - \Sigma_L(\tau,\tau') = 0$,

so $D = D_0$. The properly normalized GF is

$$\mathcal{Z}(\xi,\lambda) = \det\left(D_0^{-1}D\right)^{-1/2} e^{-\frac{i}{2\hbar}f^T D^{-1} f}. \tag{42}$$

We do not need to do anything for the exponential factor for the following reason. We note that

$$\begin{aligned} f^T G_0 f &= \int\int d\tau d\tau' f(\tau)^T G_0(\tau,\tau') f(\tau') \\ &= \sum_{\sigma,\sigma'} \int\int \sigma dt\, \sigma' dt' f(t)^T G_0^{\sigma\sigma'}(t,t') f(t'). \end{aligned} \tag{43}$$

Since the driven force f does not depend on the branch indices, i.e., $f^+(t) = f^-(t)$, we can take the summation inside and obtain

$$\sum_{\sigma\sigma'} \sigma\sigma' G_0^{\sigma\sigma'} = G_0^t + G_0^{\bar{t}} - G_0^> - G_0^< = 0. \tag{44}$$

Finally, making use of the formulas for operators or matrices $\det(M) = e^{\mathrm{Tr}\ln M}$ and $\ln(1-y) = -\sum_{k=1}^{\infty}\frac{y^k}{k}$, we can write the CGF in terms of Σ_L^A for the *projected* initial condition case as

$$\begin{aligned} \ln \mathcal{Z}(\xi) &= \lim_{\lambda\to\infty} \ln \mathcal{Z}(\xi,\lambda) \\ &= \lim_{\lambda\to\infty} \left\{ -\frac{1}{2}\mathrm{Tr}_{j,\tau} \ln\left(1 - G_0\Sigma_L^A\right) - \frac{i}{2\hbar}\mathrm{Tr}_{j,\tau}(Gff^T) \right\} \\ &= \lim_{\lambda\to\infty} \sum_{n=1}^{\infty} \frac{1}{2n}\mathrm{Tr}_{(j,\tau)}\left[\left(G_0\Sigma_L^A\right)^n\right] - \frac{i}{2\hbar} f^T G f \\ &= \frac{1}{2}\mathrm{Tr}_{(j,\tau)}\left(G_0\Sigma_L^A\right) + \frac{1}{4}\mathrm{Tr}_{(j,\tau)}\left(G_0\Sigma_L^A G_0\Sigma_L^A\right) + \cdots \\ &\quad - \frac{i}{2\hbar} f^T G_0\Sigma^A G_0 f + \cdots. \end{aligned} \tag{45}$$

This expression for CGF is valid for any transient time t_M present in the self-energy Σ_L^A and is the starting point for the calculation in transient regime. The notation $\mathrm{Tr}_{(j,\tau)}$ means trace both in space index j and contour time τ (see Appendix C). In order to obtain $\mathcal{Z}(\xi)$ from $\mathcal{Z}(\xi,\lambda)$ we have to take the limit $\lambda\to\infty$ because $\mathcal{Z}(\xi,\lambda)$ approaches a constant as $|\lambda|\to\infty$, and hence the value of the integral is dominated by the value at infinity. Since $\Sigma_L^A(\tau,\tau') = 0$ for $\xi = 0$ we have the correct normalization $\mathcal{Z}(0) = 1$.

Similarly, for the steady-state initial condition $\rho(0)$, the CGF is given by

$$\ln \mathcal{Z}(\xi) = \lim_{\lambda\to 0} \ln \mathcal{Z}(\xi,\lambda). \tag{46}$$

The difference in this two cases is in the matrix Σ_L^A.

Similar relations also exist if we want to calculate the CGF for the right-lead heat operator $\mathcal{Q}_R$. In this case one has to do two-time measurement on the right lead corresponding to the Hamiltonian $\mathcal{H}_R$. The final formula for the CGF remains the same except Σ_L^A should be replaced with Σ_R^A.

Now in order to calculate the cumulants $\langle\langle Q_\alpha^n\rangle\rangle$ with $\alpha = L,R$, we need to go to the real time using Langreth's rule [45]. In this case, it is more convenient to work with a Keldysh rotation (see Appendix C) for the contour functions while keeping $\mathrm{Tr}(ABC\ldots D)$ invariant. The effect of the Keldysh rotation is to change any given matrix $\mathcal{D}^{\sigma\sigma'}(t,t')$, with $\sigma,\sigma' = \pm$ for branch indices, to

$$\begin{aligned} \breve{\mathcal{D}} &= \begin{pmatrix} \mathcal{D}^r & \mathcal{D}^K \\ \mathcal{D}^{\bar{K}} & \mathcal{D}^a \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} \mathcal{D}^t - \mathcal{D}^< + \mathcal{D}^> - \mathcal{D}^{\bar{t}}, & \mathcal{D}^t + \mathcal{D}^{\bar{t}} + \mathcal{D}^< + \mathcal{D}^> \\ \mathcal{D}^t + \mathcal{D}^{\bar{t}} - \mathcal{D}^< - \mathcal{D}^>, & \mathcal{D}^< - \mathcal{D}^{\bar{t}} + \mathcal{D}^t - \mathcal{D}^> \end{pmatrix}. \end{aligned} \tag{47}$$

In this case we define the quantities $\mathcal{D}^r$, $\mathcal{D}^a$, $\mathcal{D}^K$, and $\mathcal{D}^{\bar{K}}$ as above. In particular, $\mathcal{D}^K \neq \mathcal{D}^< + \mathcal{D}^>$, as one would usually think it is.

Using the above definition for the center Green's function G_0, we get

$$\breve{G}_0 = \begin{pmatrix} G_0^r & G_0^K \\ 0 & G_0^a \end{pmatrix}. \tag{48}$$

The $G_0^{\bar{K}}$ component is 0 due to the standard relation among Green's functions. But the $\bar{K}$ components are not 0 for Σ_L^A and G, as we compute later.

It is useful computationally to work in Fourier space even if there is no time-translational invariance. We define the two-frequency Fourier transform by

$$\breve{A}[\omega,\omega'] = \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' \breve{A}(t,t') e^{i(\omega t + \omega' t')}. \tag{49}$$

Since $\breve{G}_0$ is time translationally invariant, it is "diagonal':

$$\breve{G}_0[\omega,\omega'] = 2\pi\delta(\omega+\omega')\breve{G}_0[\omega]. \tag{50}$$

(The expressions for different components of $\breve{G}_0[\omega]$ and $\breve{\Sigma}[\omega]$ are given in Appendix A.) Using $\breve{G}_0[\omega]$, we can save one integration due to the δ function and, finally, have

$$\begin{aligned} \ln \mathcal{Z}(\xi) = &-\tfrac{1}{2}\mathrm{Tr}_{j,\sigma,\omega} \ln[1 - \breve{G}_0[\omega]\breve{\Sigma}_L^A[\omega,\omega']] \\ &- \frac{i}{2\hbar}\mathrm{Tr}_{j,\sigma,\omega}[\breve{G}[\omega,\omega']\breve{\mathcal{F}}[\omega',\omega]], \end{aligned} \tag{51}$$

where $\breve{G}_0[\omega]\breve{\Sigma}_L^A[\omega,\omega']$ is viewed as a matrix indexed by ω and ω'. The trace is performed on the frequency as well as the usual space and branch components. (The meaning of the trace in the frequency domain is defined in Appendix C.) $\breve{\mathcal{F}}$ is given by

$$\breve{\mathcal{F}}[\omega,\omega'] = \begin{pmatrix} 0 & 2f[\omega]f[\omega']^T \\ 0 & 0 \end{pmatrix}. \tag{52}$$

In the next section we derive the CGF for the product initial condition using the Feynman diagrammatic technique.

VI. CALCULATION FOR $\mathcal{Z}(\xi)$ FOR THE PRODUCT INITIAL STATE $\rho(-\infty)$ USING THE FEYNMAN DIAGRAMMATIC TECHNIQUE

In this section, we derive the CGF for the product initial state; i.e., the density matrix at time $t = 0$ is given by $\rho(-\infty) = \rho_C \otimes \rho_L \otimes \rho_R$. Since this density matrix commutes with the projection operator Π_a, the initial projection does not play any role and hence the projection parameter λ is absent. Working in the interaction picture with respect to the decoupled Hamiltonian $\mathcal{H}(-\infty) = \sum_{\alpha=L,C,R}\mathcal{H}_\alpha$, the interaction part of

the Hamiltonian on the contour $C = [0,t_M]$ is

$$\mathcal{V}_I^x(\tau) = -f^T(\tau)u_C(\tau) + u_R(\tau)V^{RC}u_C(\tau) + u_L(\tau+\hbar x(\tau))V^{LC}u_C(\tau). \quad (53)$$

In the last term for u_L, the argument is shifted by $\hbar x$, where $x^+(t) = -\xi/2$, $x^-(t) = \xi/2$ for $0 < t < t_M$, which is similar to the result with $\lambda = 0$.

The density matrix remains unaffected by the transformation to the interaction picture, because it commutes with $\mathcal{H}(-\infty)$. The GF can now be written as

$$\mathcal{Z}(\xi) = \mathrm{Tr}\big[\rho(-\infty)T_c\, e^{-\frac{i}{\hbar}\int_C \mathcal{V}_I^x(\tau)\,d\tau}\big]. \quad (54)$$

Expanding the exponential, we generate various terms of the product of u_α. These terms can be decomposed in pairs according to Wick's theorem [45]. Since the system is decoupled, each type of u comes in an even number of times for a nonvanishing contribution because $\langle u_C\rangle = 0$, $\langle u_C u_L\rangle = 0$, and we know that

$$-\frac{i}{\hbar}\langle T_C u_\alpha(\tau)u_{\alpha'}(\tau')^T\rangle_{\rho(-\infty)} = \delta_{\alpha,\alpha'}g_\alpha(\tau,\tau'). \quad (55)$$

We collect the diagrams of all orders to sum the series. Since $\mathcal{V}_I$ contains only two-point couplings, the graphs are all ring type. The combinatorial factors can be worked out as $1/(2n)$ for a ring containing n vertices. We now make use of the linked-cluster theorem [53], which says that $\ln\mathcal{Z}$ contains only connected graphs, and the disconnected graphs cancel exactly when we take the logarithm. The final result can be expressed as

$$\ln\mathcal{Z}(\xi) = -\frac{1}{2}\mathrm{Tr}_{j,\tau}\ln[1 - g_C\Sigma^{\mathrm{tot}}] - \frac{i}{2\hbar}f^T G f, \quad (56)$$

where

$$\Sigma^{\mathrm{tot}} = \Sigma_L(\tau+\hbar x,\tau'+\hbar x') + \Sigma_R(\tau,\tau') = \Sigma + \Sigma_L^A \quad (57)$$

and Σ is the total self-energy due to both leads. $G(\tau,\tau')$ obeys the following Dyson's equation:

$$G(\tau,\tau') = g_C(\tau,\tau') + \int\int d\tau_1 d\tau_2 g_C(\tau,\tau_1)\Sigma^{\mathrm{tot}}(\tau_1,\tau_2)G(\tau_2,\tau'). \quad (58)$$

The above expression for CGF can be written down more explicitly, by getting rid of the vacuum diagrams. Let us define a new type of Dyson's equation,

$$G_0(\tau,\tau') = g_C(\tau,\tau') + \int_C\int_C d\tau_1 d\tau_2\, g_C(\tau,\tau_1)\Sigma(\tau_1,\tau_2)G_0(\tau_2,\tau'), \quad (59)$$

where g_C is the contour ordered Green's function of the isolated center. (The Green's functions for an isolated single harmonic oscillator is given in Appendix A.) Using this definition we can write

$$1 - g_C\Sigma^{\mathrm{tot}} = 1 - g_C\big(\Sigma + \Sigma_L^A\big) = (1 - g_C\Sigma)\big(1 - G_0\Sigma_L^A\big). \quad (60)$$

The two factors above are in matrix (and contour time) multiplication. Using the relation between trace and determinant, $\ln\det(M) = \mathrm{Tr}\ln M$, and the fact, $\det(AB) = \det(A)\det(B)$, we find that the two terms give two factors for $\mathcal{Z}$, and the factor due to $1 - g_C\Sigma$ is exactly 1. We then have

$$\ln\mathcal{Z}(\xi) = -\frac{1}{2}\mathrm{Tr}_{j,\tau}\ln\big[1 - G_0\Sigma_L^A\big] - \frac{i}{2\hbar}f^T G f, \quad (61)$$

where the $G(\tau,\tau')$ can now be expressed in terms of $G_0(\tau,\tau')$ as

$$G^{-1} = G_0^{-1} - \Sigma_L^A. \quad (62)$$

which is similar in form to Eq. (41), except that the current one is on contour C.

Equations (45) and (61) are the central results of our paper, which have the following importance for this particular model.

(1) The expressions for the CGFs are true for any arbitrary measurement time t_M, which need not be large.

(2) The effect of the measurement of $\mathcal{H}_L$ is to shift the time argument of the corresponding self-energy Σ_L by $\hbar x$. The information about the measurement time is contained in Σ_L^A.

(3) The expressions are true for systems of any dimensions, and it is also easy to generalize to a system connected to multiple heat baths; see Eq. (79).

(4) The expressions are also correct for a finite size of the heat baths and it is an interesting problem to study the corresponding effects.

(5) In the long-time limit the CGFs are the same independent of the initial distributions, which confirms that the steady state is unique for this model.

To compute the cumulants $\langle\langle Q^n\rangle\rangle$, we need to take derivatives of $\ln\mathcal{Z}$ with respect to $i\xi$ n times and setting $\xi = 0$; i.e.,

$$\langle\langle Q^n\rangle\rangle = \frac{\partial\ln\mathcal{Z}(\xi)}{\partial(i\xi)}|_{\xi=0}. \quad (63)$$

Note that the shifted self-energy for $0 < t < t_M$ is (for all three initial conditions)

$$\begin{aligned}\Sigma_A^t(t,t') &= 0, \quad \Sigma_A^{\bar{t}}(t,t') = 0,\\ \Sigma_A^<(t,t') &= \Sigma_L^<(t-t'-\hbar\xi) - \Sigma_L^<(t-t'),\\ \Sigma_A^>(t,t') &= \Sigma_L^>(t-t'+\hbar\xi) - \Sigma_L^>(t-t').\end{aligned} \quad (64)$$

We note $\Sigma_L^A(\xi = 0) = 0$. The derivatives at $\xi = 0$ can be obtained as

$$\begin{aligned}\frac{\partial^n\Sigma_A^<}{\partial\xi^n}\Big|_{\xi=0} &= (-\hbar)^n\Sigma_L^{<,(n)}(t-t'),\\ \frac{\partial^n\Sigma_A^>}{\partial\xi^n}\Big|_{\xi=0} &= \hbar^n\Sigma_L^{>,(n)}(t-t'),\end{aligned} \quad (65)$$

where the superscript (n) means derivatives with respect to the argument of the function n times. In the following sections we first show the explicit expression of the CGF in the long-time limit and then discuss the SSFT.

VII. LONG-TIME LIMIT AND STEADY-STATE FLUCTUATION THEOREM

For the long-time limit calculation we can use either Eq. (51) or Eq. (61). For the convenience of taking the long-time limit, i.e., t_M large, we prefer to set the interval

to $(-t_M/2,t_M/2)$. In this way, when $t_M \to \infty$, the interval becomes the full domain, and Fourier transforms of all the Green's functions and self-energy can be performed (where translational invariance is restored). Applying the convolution theorem to the trace formula in Eq. (61), we find that there is one more time integral left with an integrand independent of t. This last one can be set from $-t_M/2$ to $t_M/2$, obtaining an overall factor of t_M, and we have

$$\mathrm{Tr}_{(j,\tau)}(AB\cdots D) = t_M \int \frac{d\omega}{2\pi}\mathrm{Tr}[\breve{A}(\omega)\breve{B}(\omega)\cdots\breve{D}(\omega)]. \quad (66)$$

In the long-time limit, Σ_L^A is given by Eq. (64), which becomes the function of time difference $t - t'$. So by performing Fourier transformation we obtain

$$\Sigma_A^>[\omega] = \Sigma_L^>[\omega](e^{-i\hbar\omega\xi} - 1) = a, \quad (67)$$

$$\Sigma_A^<[\omega] = \Sigma_L^<[\omega](e^{i\hbar\omega\xi} - 1) = b. \quad (68)$$

We note that Σ_L^A is supposed to depend on both ξ and λ. However in the long-time limit, the λ dependence drops out, which makes the steady-state result independent of the initial distribution.

Finally, we can express the CGF as

$$\ln \mathcal{Z}(\xi) = -t_M \int \frac{d\omega}{4\pi}\mathrm{Tr}\ln\left[1 - \breve{G}_0[\omega]\breve{\Sigma}_L^A[\omega]\right] - \frac{i}{\hbar}\int \frac{d\omega}{4\pi}\mathrm{Tr}[\breve{G}[\omega]\breve{\mathcal{F}}[\omega,-\omega]], \quad (69)$$

where $\breve{G}[\omega]$ is obtained by solving the Dyson equation in the frequency domain and, in the long-time limit, obeys time-translational invariance. So the full CGF can be written as the sum of contributions due to the driving force and due to the temperature difference between the leads, i.e.,

$$\ln \mathcal{Z}(\xi) = \ln \mathcal{Z}^s(\xi) + \ln \mathcal{Z}^d(\xi). \quad (70)$$

In the following and subsequent sections we discuss $\mathcal{Z}^s(\xi)$ and we return to $\mathcal{Z}^d(\xi)$ in Sec. XI.

In order to obtain an explicit expression for $\ln \mathcal{Z}^s(\xi)$, we need to compute the matrix product

$$\breve{G}_0[\omega]\breve{\Sigma}_L^A[\omega] = \frac{1}{2}\begin{pmatrix} G_0^r & G_0^K \\ 0 & G_0^a \end{pmatrix}\begin{pmatrix} a-b & a+b \\ -(a+b) & b-a \end{pmatrix}. \quad (71)$$

To simplify the expression, we rewrite the term $\mathrm{Tr}\ln(1-M)$ as a determinant and use the formula (assuming A to be an invertible matrix)

$$\det\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A)\det(D - CA^{-1}B) \quad (72)$$

to reduce the dimensions of the determinant matrix by half. The steady-state solution for $\mathcal{Z}^s(\xi)$ is given by

$$\ln \mathcal{Z}^s(\xi) = -t_M \int \frac{d\omega}{4\pi}\ln\det\left\{I - G_0^r\Gamma_L G_0^a\Gamma_R[(e^{i\xi\hbar\omega}-1)\times f_L(1+f_R) + (e^{-i\xi\hbar\omega}-1)f_R(1+f_L)]\right\}, \quad (73)$$

with $f_\alpha = 1/(e^{\beta_\alpha\hbar\omega}-1)$, $\alpha = L,R$, the Bose-Einstein distribution function, and $\Gamma_\alpha[\omega] = i(\Sigma_\alpha^r[\omega] - \Sigma_\alpha^a[\omega])$. If we consider the full system as a one-dimensional linear chain, then because of the special form of Γ_α matrices (only one entry in the Γ matrices is nonzero), it can easily be shown that

$$\det\left[I - \left(G_0^r\Gamma_L G_0^a\Gamma_R\right)\Xi(\xi)\right] = 1 - \mathcal{T}[\omega]\Xi(\xi), \quad (74)$$

where $\Xi(\xi)$ is any arbitrary function of ξ and $\mathcal{T}[\omega] = \mathrm{Tr}(G_0^r\Gamma_L G_0^a\Gamma_R)$ is known as the transmission function and is given by the Caroli formula [1,10]. The GF $\mathcal{Z}^s(\xi)$ in the steady state obeys the symmetry

$$\mathcal{Z}^s(\xi) = \mathcal{Z}^s(-\xi + i\,\mathcal{A}), \quad (75)$$

where $\mathcal{A} = \beta_R - \beta_L$ is known as the thermodynamic affinity. This relation is also known as GC symmetry [38]. The immediate consequence of this symmetry is that the probability distribution for heat transferred, Q_L, which is given by the Fourier transform of the GF, i.e., $P(Q_L) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\xi\, \mathcal{Z}(\xi)\, e^{-i\xi Q_L}$ obeys the following relation in the large t_M limit:

$$P_{t_M}(Q_L) = e^{\mathcal{A}Q_L}\, P_{t_M}(-Q_L). \quad (76)$$

This relation is known as the SSFT and was first derived by Saito and Dhar [34] in the phononic case. This theorem quantifies the ratio of positive and negative heat flux and second-law violation.

The first cumulant or heat flux is given by

$$\frac{\langle\langle Q\rangle\rangle}{t_M} = \int_{-\infty}^{\infty}\frac{d\omega}{4\pi}\hbar\,\omega\,\mathcal{T}(\omega)(f_L - f_R), \quad (77)$$

which is known as the Landauer-like formula in thermal transport. Similarly, the second cumulant $\langle\langle Q^2\rangle\rangle = \langle Q^2\rangle - \langle Q\rangle^2$, which describes the fluctuation of the heat transferred, can be written as [34,54,55]

$$\frac{\langle\langle Q^2\rangle\rangle}{t_M} = \int_{-\infty}^{\infty}\frac{d\omega}{4\pi}(\hbar\omega)^2\{\mathcal{T}^2(\omega)(f_L - f_R)^2 + \mathcal{T}(\omega)(f_L + f_R + 2\,f_L f_R)\}. \quad (78)$$

Our formalism can be easily generalized for multiple heat baths, and for N leads connected to the center C, the above formula for $\ln \mathcal{Z}(\xi)$ can be written as

$$\ln \mathcal{Z}^s(\xi) = -t_M \int \frac{d\omega}{4\pi}\ln\det\left\{I - \sum_{m\neq L}^{N} G_0^r\Gamma_L G_0^a\Gamma_m \times[(e^{i\xi\hbar\omega}-1)f_L(1+f_m) + (e^{-i\xi\hbar\omega}-1)f_m(1+f_L)]\right\}. \quad (79)$$

In the following section we present numerical results for one particle junction connected to Rubin heat baths, for different initial conditions. Details about how to obtain cumulants numerically are given in Appendixes D and E.

VIII. NUMERICAL RESULTS

The central quantity to calculate the CGF numerically is the shifted self-energy Σ_L^A, which is given by

$$\Sigma_L^A(\tau,\tau') = \Sigma_L(\tau + \hbar x(\tau), \tau' + \hbar x(\tau')) - \Sigma_L(\tau,\tau'). \quad (80)$$

Here τ is a contour variable which runs over the Keldysh contour $K = (-\infty,\infty)$ for the initial conditions $\rho(0)$ and $\rho'(0)$, whereas for $\rho(-\infty)$, τ runs over the contour $C = [0,t_M]$ (see Fig. 1). The contour function $x(\tau)$ is 0 whenever $t < 0$ or

$t > t_M$, and for $0 < t < t_M$, $x^+(t) = -\xi/2 - \lambda$, and $x^-(t) = \xi/2 - \lambda$. Depending on the values of t, t', and λ ($\lambda \to 0$ and $\lambda \to \infty$ correspond to the steady-state initial state and the *projected* initial state, respectively), Σ_L^A will have different functional forms. If $0 < t,t' < t_M$, then Σ_L^A's are given by Eq. (64). This is the region which dominates in the long-time limit and gives steady state GF. If both t and t' lie outside the measurement time, i.e., $t,t' < 0$ or $t,t' > t_M$, then Σ_L^A is 0.

The main computational task for a numerical evaluation of the cumulants is to compute the matrix series $-\ln(1 - M) = M + \frac{1}{2}M^2 + \cdots$. It can be seen that, due to the nature of Σ_L^A, for the product initial state, exact n terms up to M^n are required for the nth cumulants, as the infinite series terminates due to $\Sigma_L^A(\xi = 0) = 0$. Numerically, we also observed for the projected state $\rho'(0)$ that exact $3n$ terms are required (although we do not have a proof) if the calculation is performed in the time domain.

The computation can be performed in the time as well as in the frequency domain. However, for projected and steady-state initial conditions, since $G_0[\omega]$ is time translationally invariant, it is advantageous to work in the frequency domain. But for the product state there is no such preference and one has to solve Eq. (59) numerically. Details about obtaining Σ_L^A and solving the Dyson equation numerically are given in Appendixes D and E.

We now present some numerical results. In Figs. 2 and 3, we show the results for the first four cumulants for both $\mathcal{Q}_L$ and $\mathcal{Q}_R$ (measurement is on the right lead) for a 1D linear chain connected by Rubin baths, starting with the projected initial state $\rho'(0)$ and product state $\rho(-\infty)$, respectively. Rubin baths [57,58] mean, in our case, a uniform linear chain with a spring constant K and a small on-site K_0 for all the atoms. Only one atom is considered as the center. The atoms on the left and right sides of the center are considered baths. We use $K = 1\,\mathrm{eV}/(u\text{Å}^2)$ and the on-site potential $K_0 = 0.1\,\mathrm{eV}/(u\text{Å}^2)$ in all our calculations. First, cumulants greater than 2 are nonzero, which confirms that the distribution for $P(Q_L)$ or $P(Q_R)$ is not Gaussian. The generic features are almost the same in both cases. However, the fluctuations are larger for the product initial state $\rho(-\infty)$, as this state corresponds to the sudden switching-on of the couplings between the leads and the center, and hence the state is far away from the correct steady-state distribution. On the contrary, for the initial state $\rho'(0)$ the fluctuations are relatively small. For $\rho'(0)$, due to the effect of the measurement, at the starting time, energy goes into the leads, which is quite surprising. But for $\rho(-\infty)$, although the initial measurement does not play any role, energy still goes into the leads. This can also be shown analytically (see Appendix B). At the starting time the behavior of both $\mathcal{Q}_L$ and $\mathcal{Q}_R$ are very similar and can be understood since both the left and the right leads are identical and the effect of a temperature difference is not present. However, at longer times the odd cumulants start differing and, finally, grow linearly with time t_M and agree with the corresponding long-time predictions.

In Fig. 4 we show the results for the steady-state initial condition, i.e., $\rho(0)$, which can be obtained by mapping the projection operators as identity operators, i.e., taking the limit $\lambda \to 0$. So in this case the measurement effect is ignored and the dynamics starts with the actual steady state for the full system. The first cumulant increases linearly from the start, $\langle Q \rangle = tI$, and the slope gives the correct prediction with the Landauer-like formula. However, high-order cumulants still show transient behavior. In this case the whole system achieves steady state much more rapidly compared with the other two cases.

IX. CORRELATION BETWEEN LEFT- AND RIGHT-LEAD HEAT

A. Product initial state

In this section, we derive the CGF for the joint probability distribution $P(Q_L,Q_R)$ for the product initial state $\rho(-\infty)$. In order to calculate the CGF we need to measure both $\mathcal{H}_L$ and $\mathcal{H}_R$ at time 0 and at time t_M. Since the Hamiltonians for the left and the right lead commute at the same instant in time, i.e., $[\mathcal{H}_L,\mathcal{H}_R] = 0$, this type of measurement is allowed in quantum mechanics, and also Nelson's theorem [59] guarantees that $P(Q_L,Q_R)$ is a well-defined probability distribution. The immediate consequence of deriving such a CGF is that the correlations between the left- and the right-lead heat can be obtained, and it is also possible to calculate the CGF for total entropy flow (defined below) to the reservoirs. To calculate the GF we need two counting fields ξ_L and ξ_R and the GF in this case can be written as [41]

$$\mathcal{Z}(\xi_L,\xi_R) = \left\langle e^{i\,\xi_L\,\mathcal{H}_L + i\,\xi_R\,\mathcal{H}_R}\; e^{-i\,\xi_L\,\mathcal{H}_L^H(t) - i\,\xi_R\,\mathcal{H}_R^H(t)} \right\rangle', \quad (81)$$

where the average is defined as

$$\langle \cdots \rangle' = \sum_{a,c} \Pi_a^L\,\Pi_c^R\,\rho(0)\,\Pi_a^L\,\Pi_c^R. \quad (82)$$

Π_a^L and Π_c^R are the projectors onto the eigenstates of $\mathcal{H}_L$ and $\mathcal{H}_R$, with eigenvalues a and c, respectively, corresponding to the measurements at $t = 0$. Here we consider only the product state $\rho(-\infty)$; thus initial projections Π_a^L and π_c^R do not play any role. We can proceed as before, and finally, the CGF can be written down as

$$\ln \mathcal{Z}(\xi_L,\xi_R) = \sum_{k=1}^{\infty} \frac{1}{2k} \mathrm{Tr}_{(j,\tau)}\left[\left(G_0\left(\Sigma_L^A + \Sigma_R^A\right)\right)^k\right]; \quad (83)$$

i.e., in this case we need to shift the contour-time arguments for both left- and right-lead self-energies. In the long-time limit $\mathcal{Z}(\xi_L,\xi_R)$ becomes a function of the difference in counting fields ξ_L and ξ_R, i.e., $\xi_L - \xi_R$. The explicit expression for the CGF in the long-time limit is

$$\begin{aligned}\ln \mathcal{Z}(\xi_L - \xi_R) = -t_M \int \frac{d\omega}{4\pi} \ln\det\big\{ & I - G_0^r \Gamma_L G_0^a \Gamma_R \\ & \times [(e^{i(\xi_L-\xi_R)\hbar\omega} - 1) f_L (1 + f_R) \\ & + (e^{-i(\xi_L-\xi_R)\hbar\omega} - 1) f_R (1 + f_L)]\big\}, \end{aligned} \quad (84)$$

where G_0 obeys the same type of Dyson equation as Eq. (59). This CGF in the steady state obeys the same type of GC fluctuation symmetry, which in this case is given by

$$\mathcal{Z}(\xi_L - \xi_R) = \mathcal{Z}(-\xi_L + \xi_R + i\mathcal{A}). \quad (85)$$

Now performing Fourier transform of the CGF, the joint probability distribution is given by $P(Q_L,Q_R) = P(Q_L)\,\delta(Q_L +$

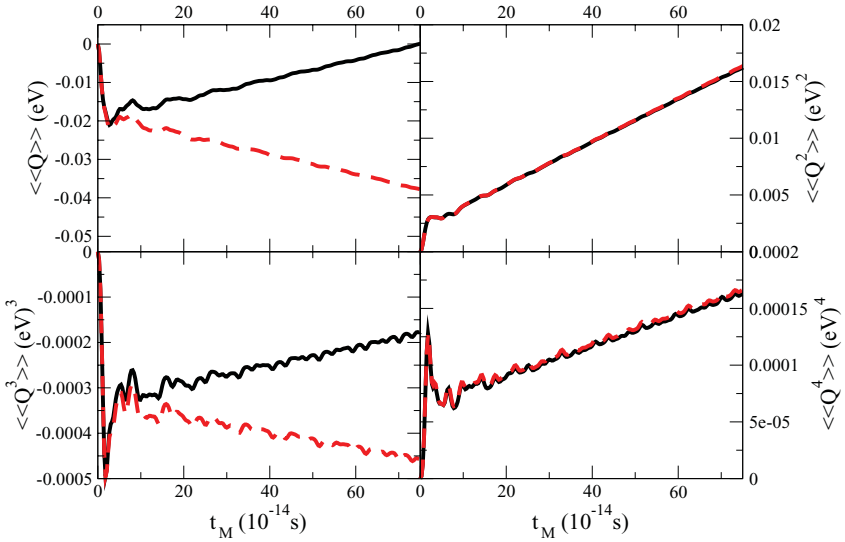

FIG. 2. (Color online) Cumulants $\langle\langle Q_L^n\rangle\rangle$ and $\langle\langle Q_R^n\rangle\rangle$ for $n = 1$, 2, 3, and 4 for a one-dimensional linear chain connected by Rubin baths, for the projected initial state $\rho'(0)$. Black (solid) and red (dotted) curves correspond to $\langle\langle Q_L^n\rangle\rangle$ and $\langle\langle Q_R^n\rangle\rangle$, respectively. The temperatures of the left and right leads are 310 and 290 K, respectively. The center (C) consists of one particle.

Q_R). The appearance of the δ function is a consequence of the energy conservation in the steady state, i.e., $I_L = -I_R$. In the steady state, knowing the probability distribution for either $\mathcal{Q}_L$ or $\mathcal{Q}_R$ is sufficient to know the joint probability distribution.

The cumulants can be obtained from the CGF by taking derivatives with respect to both ξ_L and ξ_R; i.e.,$\langle\langle Q_L^n Q_R^m\rangle\rangle = \partial^{n+m} \ln \mathcal{Z}/\partial(i\xi_L)^n \partial(i\xi_R)^m$, substituting $\xi_L = \xi_R = 0$. In the steady state the cumulants obey $\langle\langle Q_L^n Q_R^m\rangle\rangle = (-1)^m\langle\langle Q_L^{m+n}\rangle\rangle = (-1)^n\langle\langle Q_R^{m+n}\rangle\rangle$. The first cumulant gives us the left- and right-lead correlation $\langle\langle Q_L Q_R\rangle\rangle = \langle Q_L Q_R\rangle - \langle Q_L\rangle\langle Q_R\rangle$ and, in the steady state, is equal to $-\langle\langle Q_L^2\rangle\rangle$.

In Fig. 5 we plot the first three cumulants for a 1D linear chain connected by Rubin baths where the center consists of only one atom. Initially the cumulant $\langle\langle Q_L Q_R\rangle\rangle$ is positively correlated, as both Q_L and Q_R are negative, however, at a longer time, since $Q_L = -Q_R$ the correlation becomes negative. We also give plots for $\langle\langle Q_L^2 Q_R\rangle\rangle$ (black) and $\langle\langle Q_R^2 Q_L\rangle\rangle$ (red), which, in the long-time limit, are negative and positively correlated, respectively, and match the long-time predictions.

B. Entropy flow to the reservoir

From the two-parameter (ξ_L,ξ_R) CGF, one can also obtain the total entropy that flows into the leads. The total entropy flow to the reservoirs can be defined as [60,61]

$$\sigma = -\beta_L \mathcal{Q}_L - \beta_R \mathcal{Q}_R. \tag{86}$$

In order to calculate this CGF, we just make the substitutions $\xi_L \to -\beta_L\mu$ and $\xi_R \to -\beta_R\mu$ in Eq. (83). In the long-time limit the expression for entropy production is similar to $\ln \mathcal{Z}(\xi_L,\xi_R)$, with $\xi_L - \xi_R$ replaced by $\mathcal{A}$, and becomes an explicit function of thermodynamic affinity, $\beta_R - \beta_L$ [26]. The CGF in this case satisfies the following symmetry:

$$\mathcal{Z}(\mu) = \mathcal{Z}(-\mu + i). \tag{87}$$

In Fig. 6 we give the results for the first four cumulants of the entropy flow. All cumulants are positive and, in the long-time limit, give correct predictions.

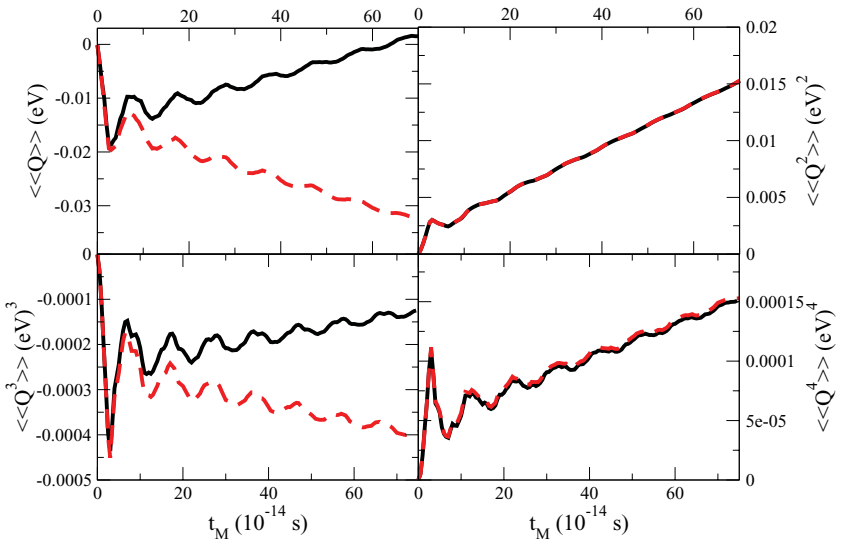

FIG. 3. (Color online) Same as Fig. 2 except for the product initial state $\rho(-\infty)$. Temperatures of the left, center, and right leads are 310, 300, and 290 K, respectively.

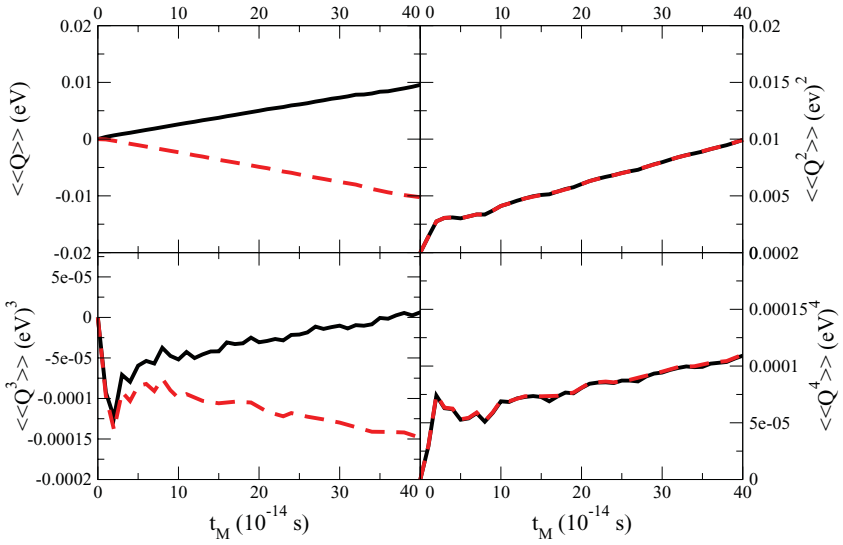

FIG. 4. (Color online) Same as Fig. 2 except for the steady-state initial state $\rho(0)$.

X. LONG-TIME RESULT FOR ln $\mathcal{Z}^d(\xi)$

In this section we derive the explicit expression for the long-time limit of ln $\mathcal{Z}^d(\xi)$, which is given by [Eq. (69)],

$$\ln \mathcal{Z}^d(\xi) = -\frac{i}{\hbar}\int \frac{d\omega}{4\pi}\mathrm{Tr}[\check{G}[\omega]\check{\mathcal{F}}[\omega,-\omega]], \tag{88}$$

where $G[\omega]$ obeys the Dyson equation given in Eq. (41). It is possible to write down $\check{G}[\omega]$ in terms of $\check{G}_0$ and $\check{\Sigma}_L^A$ as $\check{G}[\omega] = (I - \check{G}_0\check{\Sigma}_L^A)^{-1}\check{G}_0[\omega]$. This equation can be solved analytically. Next we assume that the product of $f(t)$ and $f(t')$ is a time translationally invariant function, i.e., $f(t)f^T(t') = F(t-t')$, in order to get rid of the $t+t'$ dependence term. In the Fourier domain this means $f[\omega]f^T[\omega'] = 2\pi F[\omega]\delta(\omega+\omega')$. So from Eq. (52) the matrix element $\mathcal{F}_{12}$ is given by $\check{\mathcal{F}}[\omega,-\omega]_{12} \propto \delta(0)F[\omega]$. We write $\delta(0) = t_M/2\pi$. Using these results the CGF can be expressed as

$$\ln \mathcal{Z}^d(\xi) = it_M\int \frac{d\omega}{4\pi\hbar}\frac{1}{\mathcal{N}(\xi)}\mathrm{Tr}\big[G_0^r[\omega](a+b)G_0^a[\omega]F[\omega]\big], \tag{89}$$

where a and b are defined in Eqs. (67) and (68). Using the expressions for the self-energy, the CGF reduces to

$$\ln \mathcal{Z}^d(\xi) = \int \frac{d\omega}{4\pi\hbar}\frac{\mathcal{K}(\xi)}{\mathcal{N}(\xi)}\mathrm{Tr}\big[G_0^r[\omega]\Gamma_L[\omega]G_0^a[\omega]F[\omega]\big], \tag{90}$$

with

$$\mathcal{K}(\xi) = (e^{-i\xi\hbar\omega}-1) + f_L(e^{i\xi\hbar\omega}+e^{-i\xi\hbar\omega}-2), \tag{91}$$

and

$$\mathcal{N}(\xi) = \det\big[I - \big(G_0^r\Gamma_L G_0^a\Gamma_R\big)\{(e^{i\xi\hbar\omega}-1)f_L(1+f_R) \times (e^{-i\xi\hbar\omega}-1)f_R(1+f_L)\}\big]. \tag{92}$$

It is important to note that $\mathcal{K}(\xi)$ depends only on the left-lead temperature and satisfies the symmetry $\mathcal{K}(\xi) = \mathcal{K}(-\xi - i\beta_L)$. So we can immediately write $\mathcal{Z}^d(-i\beta_L) = 1$, and this relation is completely independent of the right lead. If we consider the two leads at the same temperature ($\beta_L = \beta_R = \beta$), this form of symmetry is then closely related to the Jarzynski equality (JE) [62,63], and $\mathcal{Z}^d(-i\beta) = 1$ is one special form of the JE. However, since $\mathcal{N}(\xi)$ does not satisfy this particular symmetry of ξ at thermal equilibrium (it obeys the GC summary when the leads are at different temperatures), and the GF $\mathcal{Z}^d(\xi) \neq \mathcal{Z}^d(-\xi - i\beta)$, the JE is not satisfied. This, however, does not violate the JE, as the GF $\mathcal{Z}^d(\xi)$ is defined for the quantity heat, not for the work done by the external force. Let us now come back to the general scenario with leads at different temperatures and give the explicit expression of the first and second cumulants by taking the derivative of ln $\mathcal{Z}^d(\xi)$ with respect to $i\xi$.

The first cumulant or moment is given by [64]

$$\frac{\langle\langle Q_d\rangle\rangle}{t_M} = -\int \frac{d\omega}{4\pi}\,\omega\,\mathcal{S}[\omega], \tag{93}$$

where we define $\mathcal{S}[\omega]$ as the transmission function for the driven case and is given by

$$\mathcal{S}[\omega] = \mathrm{Tr}\big[G_0^r\Gamma_L G_0^a F\big]. \tag{94}$$

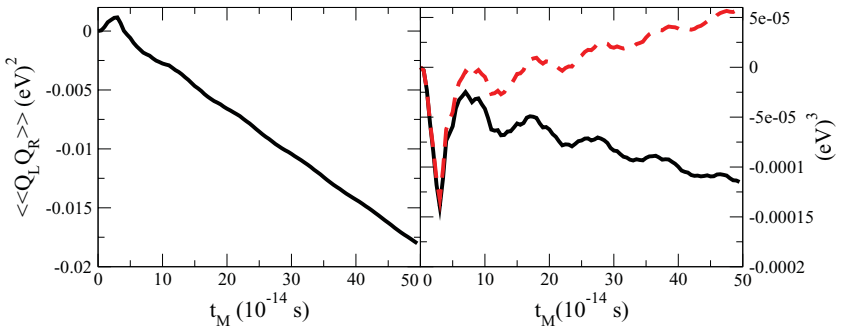

FIG. 5. (Color online) First three cumulants of the correlations between left- and right-lead heat flux for a one dimensional linear chain connected by Rubin baths, starting with the product initial state $\rho(-\infty)$. Left, $\langle\langle Q_L Q_R\rangle\rangle$; right, cumulants $\langle\langle Q_L^2 Q_R\rangle\rangle$ (black (solid) curve) and $\langle\langle Q_R^2 Q_L\rangle\rangle$ (red (dotted) curve). Left-, center-, and right-lead temperatures are 310, 290, and 300 K, respectively. The center consists of one particle.

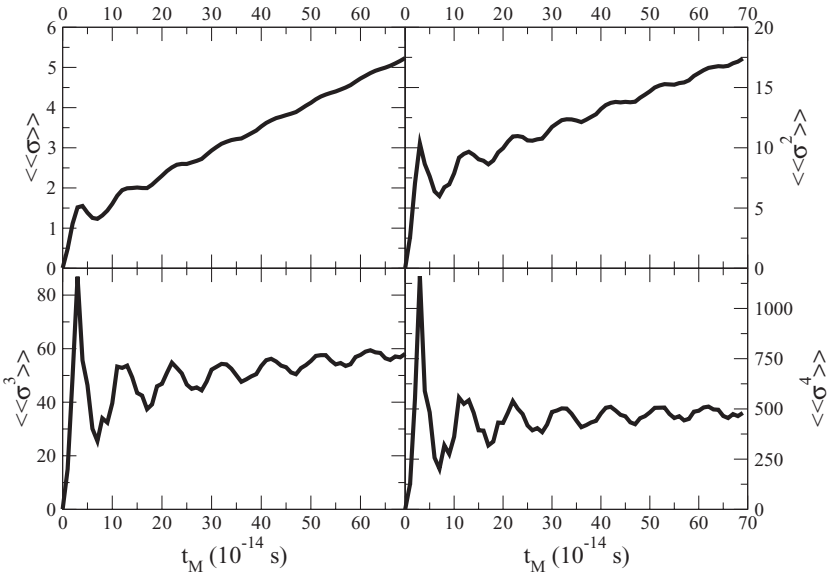

FIG. 6. Cumulants of entropy production $\langle\langle\sigma^n\rangle\rangle$ for $n = 1, 2, 3, 4$ for a one-dimensional linear chain connected by Rubin baths, for product initial state $\rho(-\infty)$. Left-, center-, and right-lead temperatures are 510, 400, and 290 K, respectively. The center consists of one particle.

From the expression of $\mathcal{S}[\omega]$ it is clear that the average energy current due to the driven force is independent of $\hbar$, and since it contains $G_0^{r,a}$ and Γ_L, which are independent of the temperature, we can conclude that the energy current is independent of the temperature of the heat baths in the ballistic transport case. However, the second cumulant and, similarly, the higher ones do depend on the temperature of the baths. The second cumulant can be written as

$$\frac{\langle\langle Q_d^2\rangle\rangle}{t_M} = \int \frac{d\omega}{4\pi\hbar}(\hbar\omega)^2\,\mathcal{S}[\omega][(1+2\,f_L) - 2\,\mathcal{T}(\omega)(f_L - f_R)]. \tag{95}$$

Similarly, all the higher cumulants can be obtained from the CGF and we can conclude that the distribution $P(Q_d)$ is not Gaussian.

XI. CLASSICAL LIMIT FOR GENERATING FUNCTIONS

In this section we give the classical limit of the steady-state expression for the CGFs $\ln\mathcal{Z}^s(\xi)$ and $\ln\mathcal{Z}^d(\xi)$ given in Eqs. (73) and (90). First, we note that the retarded and advanced Green's functions, i.e., G_0^r and G_0^a, are the same for the quantum and classical cases. We know that in the classical limit $f_\alpha \to k_B T_\alpha/\hbar\omega$ and also $e^{ix} = 1 + ix + (ix)^2/2 + \cdots$, where $x = \xi\hbar\omega$. Using this, we obtain from Eq. (73) the classical limit of $\mathcal{Z}^s(\xi)$:

$$\ln\mathcal{Z}^s_{\rm cls}(\xi) = \frac{t_M}{4\pi}\int d\omega\,\ln\det\left[I - \left(G_0^r\Gamma_L G_0^a\Gamma_R\right) \times k_B T_L\,k_B T_R\,i\xi(i\xi+\mathcal{A})\right]. \tag{96}$$

This result reproduces that in Ref. [43], which was obtained from Langevin dynamics with white-noise reservoirs. In the classical case also, the CGF obeys the GC symmetry, i.e., it remains invariant under the transformation $i\xi \to -i\xi - \mathcal{A}$.

Let us now get the classical limit for $\ln\mathcal{Z}^d(\xi)$ using Eq. (90). Following the above relations, the function $\mathcal{K}(\xi)$ in the limit $\hbar \to 0$ reduces to

$$\mathcal{K}_{\rm cls}(\xi) = -\hbar\omega\left(i\xi + \frac{\xi^2}{\beta_L}\right). \tag{97}$$

The transmission function $\mathcal{S}[\omega]$ stays the same, as it is independent of the temperature and $\hbar$. So in the classical limit, $\ln\mathcal{Z}^d(\xi)$ reduces to

$$\ln\mathcal{Z}^d_{\rm cls}(\xi) = t_M\int\frac{d\omega}{4\pi}\,\omega\,\mathcal{S}[\omega]\,\frac{\left(i\xi + \frac{\xi^2}{\beta_L}\right)}{\mathcal{N}_{\rm cls}(\xi)}, \tag{98}$$

where

$$\mathcal{N}(\xi)_{\rm cls} = \det\left[I - \left(G_0^r\Gamma_L G_0^a\Gamma_R\right)k_B T_L\,k_B T_R\,i\xi(i\xi+\mathcal{A})\right]. \tag{99}$$

Here we can easily see that $\mathcal{Z}^d(-i\beta_L) = 1$.

We can also derive the fluctuation dissipation theorem from Eq. (95) if we assume that the leads are at the same temperature, i.e., $\beta_L = \beta_R = \beta$; then we can write the second cumulant $\langle\langle Q_d^2\rangle\rangle$ as

$$\frac{\langle\langle Q_d^2\rangle\rangle}{t_M} = \int\frac{d\omega}{4\pi\hbar}(\hbar\omega)^2\,\mathcal{S}[\omega](1+2\,f_L). \tag{100}$$

In the high-temperature limit using $f_L \to \frac{k_B T_L}{\hbar\omega}$, we obtain

$$\langle\langle Q_d^2\rangle\rangle = \frac{2}{\beta_L}\langle Q_d\rangle, \tag{101}$$

which is always true if the distribution $P(Q_d)$ is Gaussian. However, the reverse statement is not true, which is the case here.

In the next section we present Nazarov's GF and give the long-time limit expression.

XII. NAZAROV'S DEFINITION OF THE GENERATING FUNCTION

In this section we derive another definition of the CGF given by Eq. (10), starting from the CGF, derived using the two-time measurement concept, i.e., Eq. (9). Equation (10) can be obtained from Eq. (9) in the small ξ approximation as follows. In the small ξ approximation the modified Hamiltonian given in Eq. (24) takes the form

$$\mathcal{H}_x(t) = \mathcal{H}(t) + \hbar x\mathcal{I}_L(0) + O(x^2), \tag{102}$$

because $\mathcal{C}(x) = O(x^2)$ and $\mathcal{S}(x) = \hbar x V^{LC} + O(x^2)$. $\mathcal{I}_L$ is defined by Eq. (5). So the modified unitary operator becomes

$$\mathcal{U}_x(t,0) = T e^{-\frac{i}{\hbar}\int_0^t [\mathcal{H}(\bar{t}) + \hbar x \mathcal{I}_L(0)] d\bar{t}}. \tag{103}$$

We can consider $\hbar x \mathcal{I}_L(0)$ as the interaction Hamiltonian and write the full unitary operator $\mathcal{U}_x$ as a product of two unitary operators as

$$\mathcal{U}_x(t,0) = \mathcal{U}(t,0)\mathcal{U}_x^I(t,0), \tag{104}$$

where

$$\begin{aligned} \mathcal{U}(t,0) &= T e^{-\frac{i}{\hbar}\int_0^t \mathcal{H}(t')dt'}, \\ \mathcal{U}_x^I(t,0) &= T e^{-\frac{i}{\hbar}\int_0^t \hbar x \mathcal{I}_L(t')dt'}, \end{aligned} \tag{105}$$

with $\mathcal{I}_L(t') = \mathcal{U}^\dagger(t',0)\mathcal{I}_L(0)\mathcal{U}(t',0)$ the current operator in the Heisenberg picture. Note that $\mathcal{U}$ is the usual unitary operator which evolves with the full Hamiltonian $\mathcal{H}(t)$ in Eq. (8) and has no ξ dependence.

If we use product state $\rho(-\infty)$ as the initial state, the GF is given by

$$\mathcal{Z}(\xi) = \mathrm{Tr}[\rho(-\infty)\mathcal{U}_{\xi/2}(0,t)\mathcal{U}_{-\xi/2}(t,0)]. \tag{106}$$

In the small-ξ approximation and using the expression for $\mathcal{U}_x$, we can write the GF as

$$\mathcal{Z}_1(\xi) = \mathrm{Tr}[\rho(-\infty)\mathcal{U}^I_{\xi/2}(0,t)\mathcal{U}^I_{-\xi/2}(t,0)], \tag{107}$$

where we use the property of the unitary operator, i.e., $\mathcal{U}^\dagger(t,0)\mathcal{U}(t,0) = 1$. Finally, using the definition of the heat operator $\mathcal{Q}_L$ given in Eq. (6), the GF can be written as

$$\mathcal{Z}_1(\xi) = \langle \bar{T} e^{i\xi \mathcal{Q}_L(t)/2}\, T e^{i\xi \mathcal{Q}_L(t)/2} \rangle, \tag{108}$$

which is the same as Eq. (10). In the following we give the long-time limit expression for this GF.

In order to calculate the GF, we go to the interaction picture with respect to the Hamiltonian $\mathcal{H}_0 = \mathcal{H}_L + \mathcal{H}_C + \mathcal{H}_R$, as we know how to calculate Green's functions for operators which evolve with $\mathcal{H}_0$ and treat the rest as the interaction $\mathcal{V}_x = \mathcal{H}_{\rm int} + \hbar x \mathcal{I}_L(0)$. So the GF on the contour $C = [0,t_M]$ can be written as

$$\mathcal{Z}_1(\xi) = \left\langle T_c e^{-\frac{i}{\hbar}\int \mathcal{V}_x^I(\tau)d\tau} \right\rangle, \tag{109}$$

where $\mathcal{V}_x^I(\tau)$ is now given by

$$\begin{aligned} \mathcal{V}_x^I(\tau) = {} & u_L^T(\tau) V^{LC} u_C(\tau) + u_R^T(\tau) V^{RC} u_C(\tau) \\ & + \hbar x(\tau) p_L(\tau) V^{LC} u_C(\tau), \end{aligned} \tag{110}$$

where $p_L = \dot{u}_L$. The time dependence τ comes from the free evolution with respect to $\mathcal{H}_0$. $x(\tau)$ has a similar meaning as before; i.e., on the upper branch of the contour, $x^+(t) = -\xi/2$, and on the lower branch $x^-(t) = \xi/2$. Now using the same idea as before, we expand the series, use Wick's theorem, and finally, the CGF can be expressed as

$$\ln \mathcal{Z}(\xi) = -\tfrac{1}{2}\mathrm{Tr}_{j,\tau} \ln\left[1 - G_0 \Sigma_L^A\right]. \tag{111}$$

Here G_0 is the same as before and is given by Eq. (59). However, the shifted self-energy Σ_L^A in this case is different and is given by (in the contour-time argument)

$$\begin{aligned} \Sigma_L^A(\tau,\tau') = {} & \hbar\, x(\tau)\, \Sigma_{p_L u_L}(\tau,\tau') + \hbar\, x(\tau')\, \Sigma_{u_L p_L}(\tau,\tau') \\ & + \hbar^2\, x(\tau)\, x(\tau')\, \Sigma_{p_L p_L}(\tau,\tau'). \end{aligned} \tag{112}$$

The notation $\Sigma_{AB}(\tau,\tau')$ means

$$\Sigma_{AB}(\tau,\tau') = \left(-\frac{i}{\hbar}\right) V^{CL} \langle\, T_c A(\tau) B^T(\tau') \,\rangle\, V^{LC}. \tag{113}$$

The average here is with respect to the equilibrium distribution of the left lead. It is possible to express correlation functions such as $\Sigma_{p_L u_L}(\tau,\tau')$ in terms of the $\Sigma_{u_L,u_L}(\tau,\tau') = \Sigma_L(\tau,\tau')$ correlations. $\Sigma_{p_L u_L}(\tau,\tau')$ and $\Sigma_{u_L p_L}(\tau,\tau')$ are simply related to $\Sigma_L(\tau,\tau')$ by the contour-time derivative, whereas for $\Sigma_{p_L p_L}(\tau,\tau')$ the expression is

$$\Sigma_{p_L p_L}(\tau,\tau') = \frac{\partial^2 \Sigma_{u_L u_L}(\tau,\tau')}{\partial\tau\partial\tau'} + \delta(\tau,\tau')\Sigma_L^I, \tag{114}$$

where $\Sigma_L^I = V^{CL}V^{LC}$. Now in the frequency domain, different components of Σ_L^A take the following form:

$$\begin{aligned} \Sigma_A^t[\omega] &= \frac{\hbar^2\xi^2\omega^2}{4}\Sigma_L^t[\omega] + \frac{\hbar^2\xi^2}{4}\Sigma_L^I, \\ \Sigma_A^{\bar{t}}[\omega] &= \frac{\hbar^2\xi^2\omega^2}{4}\Sigma_L^{\bar{t}}[\omega] - \frac{\hbar^2\xi^2}{4}\Sigma_L^I, \\ \Sigma_A^<[\omega] &= \left(i\hbar\xi\omega - \frac{\hbar^2\xi^2\omega^2}{4}\right)\Sigma_L^<[\omega], \\ \Sigma_A^>[\omega] &= \left(-i\hbar\xi\omega - \frac{\hbar^2\xi^2\omega^2}{4}\right)\Sigma_L^>[\omega]. \end{aligned} \tag{115}$$

Finally, using the relations between the self-energy (see Appendix A), in the long-time limit the CGF can be written as

$$\begin{aligned} \ln \mathcal{Z}_1(\xi) = -t_M \int \frac{d\omega}{4\pi} \ln\Big[& 1 - (i\xi\hbar\omega)\mathcal{T}[\omega]\,(f_L - f_R) \\ & - \frac{(i\xi\hbar\omega)^2}{4}\big(\mathcal{T}[\omega](1+2f_L)(1+2f_R) - G_0^a\Sigma_L^r \\ & + G_0^r\Sigma_L^a - G_0^r\Gamma_L G_0^a\Gamma_L\big) + \mathcal{J}(\xi^2,\xi^4)\Big], \end{aligned} \tag{116}$$

where $\mathcal{J}(\xi^2,\xi^4)$ is given by

$$\begin{aligned} \mathcal{J}(\xi^2,\xi^4) = {} & -\frac{\hbar^2\xi^2}{4}\big(G_0^a + G_0^r\big)\Sigma_L^I - \frac{1}{4}\frac{(i\xi\hbar\omega)^2}{2}\frac{\hbar^2\xi^2}{2} \\ & + \big(G_0^r\Sigma_L^a G_0^a\Sigma_L^I + G_0^r\Sigma_L^I G_0^a\Sigma_L^r\big) + \frac{1}{4}\frac{(i\xi\hbar\omega)^4}{4} \\ & \times G_0^r\Sigma_L^a G_0^a\Sigma_L^r + \frac{1}{4}\frac{(\hbar^4\xi^4)}{4} G_0^r\Sigma_L^I G_0^a\Sigma_L^I. \end{aligned} \tag{117}$$

This CGF does not obey the GC fluctuation symmetry. However, it gives the correct first and second cumulants, as it should because the definition of the first and second cumulants turns out to be the same for both the GFs, $\mathcal{Z}(\xi)$ and $\mathcal{Z}_1(\xi)$, and is given by

$$\begin{aligned} \langle\langle Q\rangle\rangle &= \langle Q\rangle = \frac{\partial \ln \mathcal{Z}(\xi)}{\partial(i\xi)} = \frac{\partial \ln \mathcal{Z}_1(\xi)}{\partial(i\xi)} = \int_0^t dt_1 \langle \mathcal{I}_L(t_1)\rangle, \\ \langle\langle Q^2\rangle\rangle &= \langle Q^2\rangle - \langle Q\rangle^2 = \frac{\partial^2 \ln \mathcal{Z}(\xi)}{\partial(i\xi)^2} = \frac{\partial^2 \ln \mathcal{Z}_1(\xi)}{\partial(i\xi)^2} \\ &= \int_0^t dt_1 \int_0^t dt_2 \langle \mathcal{I}_L(t_1)\mathcal{I}_L(t_2)\rangle - \left[\int_0^t dt_1 \langle \mathcal{I}_L(t_1)\rangle\right]^2. \end{aligned} \tag{118}$$

Expressions for higher cumulants are different for the two GFs, and hence the final expressions for the CGFs are completely different from each other.

XIII. CONCLUSION

In summary, we present an elegant way of deriving the CGF for heat $\mathcal{Q}_{L,R}$ transferred from the leads to the center for driven linear systems using the two-time measurement concept with the help of the NEGF technique. The CGF is written in terms of the Green's function of the center and the self-energy Σ_L^A of the leads. The counting of the energy is related to the shifting in time of the self-energy. The expressions are valid in both transient and steady-state regimes, where the information about the measurement time t_M is contained in Σ_L^A. The form of the expression, $-(1/2)\mathrm{Tr}\ln(1-G_0\Sigma_L^A)$, is the same whether we use a product initial state or a projected initial state, except that the meaning of the Green's function has to be adjusted accordingly. We consider three initial conditions and show numerically, for 1D linear chains connected by Rubin baths, that transient behaviors differ significantly from each other, but eventually the system reaches a unique steady-state distribution in the long-time limit. We give an explicit expression of the CGF in the steady state invoking the symmetry of translational invariance in time. The CGF obeys GC fluctuation symmetry. We also give the steady-state expression for the CGF in the presence of time-dependent driving forces. We obtain a two-parameter CGF which is useful for calculating the correlations between heat fluxes and also the total entropy production in the leads. We also generalize our result for multiple heat baths, and our derivation is also valid for finite-size heat baths. We show in the appendixes that our method can be extended for electronic systems where we derive the CGF for a tight-binding model. It will be interesting to derive the CGF by including the magnetic field contribution in the Hamiltonian and also to study the cumulants in the presence of nonlinear interactions such as phonon-phonon or electron phonon interactions.

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APPENDIX A: EXPRESSIONS FOR DIFFERENT TYPES OF GREEN'S FUNCTIONS

Here we give the explicit expressions for the center Green's function $G_0[\omega]$ in the steady state, for a harmonic system which is connected to the leads. These formulas are required to derive the analytical form of the CGF given in Eq. (73). For basic definitions of the different types of Green's functions, we refer to Ref. [10].

The retarded Green's function $G_0^r[\omega]$ is given by

$$G_0^r[\omega] = \left[(\omega+i\eta)^2 - K^C - \Sigma_L^r[\omega] - \Sigma_R^r[\omega]\right]^{-1}. \quad \text{(A1)}$$

Here η is an infinitesimal positive number which is required to satisfy the condition of causality, i.e., $G_0^r(t)=0$ for $t<0$. The advanced Green's function is $G_0^a[\omega]=[G_0^r[\omega]]^\dagger$. The Keldysh Green's function $G_0^K[\omega]$ can be obtained by solving the corresponding Dyson equation, Eq. (59), and is given by

$$G_0^K[\omega] = G_0^r[\omega]\Sigma^K[\omega]G_0^a[\omega], \quad \text{(A2)}$$

where $\Sigma^K=\Sigma_L^K+\Sigma_R^K$ and $\Sigma_\alpha^K=\Sigma_\alpha^<+\Sigma_\alpha^>$, with $\alpha=L,R$. Alternatively, $G_0^K=G_0^<+G_0^>$. Another important identity is

$$G_0^r[\omega]-G_0^a[\omega] = -i\,G_0^r[\omega](\Gamma_L[\omega]+\Gamma_R[\omega])G_0^a[\omega], \quad \text{(A3)}$$

where $\Gamma_\alpha[\omega]=i(\Sigma_\alpha^r[\omega]-\Sigma_\alpha^a[\omega])$, and $\alpha=L,R$. The self-energies for the leads are given by

$$\begin{aligned}\Sigma_\alpha^<[\omega] &= f_\alpha[\omega]\left(\Sigma_\alpha^r[\omega]-\Sigma_\alpha^a[\omega]\right),\\ \Sigma_\alpha^>[\omega] &= (1+f_\alpha[\omega])\left(\Sigma_\alpha^r[\omega]-\Sigma_\alpha^a[\omega]\right),\end{aligned} \quad \text{(A4)}$$

where $f_\alpha[\omega]=1/(e^{\beta_\alpha\hbar\omega_\alpha}-1)$ is the Bose distribution function.

Explicit expressions for $G_0^r[\omega]$ and $\Sigma_L^r[\omega]$ can be obtained for a 1D homogeneous linear chain, with interparticle force constant K and on-site spring constant K_0, which is divided into three parts: the center, the left, and the right. The classical equation of motion for the atoms in all three regions is

$$\ddot{u}_j = Ku_{j-1}+(-2K-K_0)u_j+Ku_{j-1}, \quad \text{(A5)}$$

where the index j runs over all the atoms in the whole system.

The retarded Green's function $G_0^r[\omega]$ can be obtained [9] by solving $[(\omega+i\eta)^2-\tilde{K}]G_0^r=I$, where matrix $\tilde{K}$ is infinite in both directions and is $2K+K_0$ on the diagonals and $-K$ on the first off-diagonals. The solution is translationally invariant in space index and is given by

$$G_{0,jk}^r[\omega] = \frac{\lambda^{|j-k|}}{K\left(\lambda-\frac{1}{\lambda}\right)}, \quad \text{(A6)}$$

with $\lambda=-\frac{\Omega}{2K}\pm\frac{1}{2K}\sqrt{\Omega^2-4K^2}$ and $\Omega=(\omega+i\eta)^2-2K-K_0$, choosing between plus and minus sign such that $|\lambda|\leqslant 1$.

The surface Green's function $g_L^r[\omega]$ can be similarly obtained in the frequency domain, and this gives the self-energy $\Sigma_L^r[\omega]=-K\lambda$. Since in equilibrium only one Green's function is independent, knowing $\Sigma_L^r[\omega]$ is sufficient to obtain all other Green's functions.

Here we also give the expressions for Green's functions g_C in the time and frequency domain for an isolated single harmonic oscillator with frequency ω_0 (we have omitted the subscript C in g_C) [65,66]:

$$\begin{aligned} g^r(t) &= -\theta(t)\frac{\sin\omega_0 t}{\omega_0}, \quad g^r[\omega]=\frac{1}{(\omega+i\eta)^2-\omega_0^2},\\ g^<(t) &= \frac{-i}{2\omega_0}[(1+f)e^{i\omega_0 t}+fe^{-i\omega_0 t}],\\ g^>[\omega] &= \frac{-i\pi}{\omega_0}\left[\delta(\omega+\omega_0)(1+f)+\delta(\omega-\omega_0)f\right], \end{aligned} \quad \text{(A7)}$$

where $f=f(\omega_0)=\frac{1}{e^{\beta\hbar\omega_0}-1}$. Other components can be obtained by exploiting the symmetry between the Green's functions such as $g^a(-t)=g^r(t)$ for $t>0$, hence $g^r[\omega]=g^a[-\omega]$. The greater component is related to the lesser

component via $g^>(t) = g^<(-t)$, which, in the frequency domain, satisfies $g^>[\omega] = g^<[-\omega]$.

APPENDIX B: CURRENT AT A SHORT TIME FOR THE PRODUCT INITIAL STATE

Using the definition of current operator given in Eq. (5), the energy current flowing from the left lead to the center is [here we assume that there is no driving force $f(t)$]

$$\langle \mathcal{I}_L(t)\rangle = -\left\langle \frac{d\mathcal{H}_L(t)}{dt}\right\rangle = \frac{i}{\hbar}\langle[\mathcal{H}_L(t),\mathcal{H}]\rangle, \tag{B1}$$

where the average is with respect to $\rho(-\infty)$. If t is small, we can expand $\mathcal{H}_L(t)$ in a Taylor series, and it is given by $\mathcal{H}_L(t) = \mathcal{H}_L(0) + t\dot{\mathcal{H}}_L(0) + \cdots$.

Now since $[\rho(-\infty),\mathcal{H}_L(0)] = 0$, then it immediately follows that $\langle[\mathcal{H}_L(0),\mathcal{H}]\rangle = 0$ by using the cyclic property of trace. So in linear order of t the current is given by

$$\langle \mathcal{I}_L(t)\rangle = t\frac{i}{\hbar}\langle[\dot{\mathcal{H}}_L(0),\mathcal{H}]\rangle = -t\frac{i}{\hbar}\langle\left[p_L^T V^{LC} u_C,\mathcal{H}\right]\rangle. \tag{B2}$$

The only term of the full $\mathcal{H}$ that will contribute to this is $\mathcal{H}_{LC} = u_L^T V^{LC} u_C$.

Now using the relation that $[p_L,u_L] = -i\hbar$, for a 1D linear chain we can write

$$\langle \mathcal{I}_L(t)\rangle = -t\,K^2\langle\left(u_1^C\right)^2\rangle = -t\,K^2\frac{\hbar}{\omega_0}\left(f_C(\omega_0)+\frac{1}{2}\right), \tag{B3}$$

where u_1^C is the first particle in the center, which is connected to the first particle of the left lead with force constant K. Now since the average is with respect to $\rho(-\infty)$, $\langle(u_1^C)^2\rangle$ can be easily computed. Here $f_C(\omega_0)$ is the Bose distribution function of the particle with characteristic frequency ω_0. So we can see that for a short time the current is negative, i.e., it goes into the lead. It is now easy to see that a similar expression should also hold for $\langle \mathcal{I}_R(t)\rangle$. The negative sign in currents means that the energy flows into the leads initially irrespective of the temperatures of the leads. This is consistent with the numerical results obtained by Cuansing *et al.* [14,15].

APPENDIX C: CONVOLUTION, TRACE, AND DETERMINANT ON THE KELDYSH COUNTOUR

Here we discuss the meaning of convolution, trace, and determinant on the Keldysh contour, which we used to derive the CGFs for heat flux. We define the convolution on the contour in the following way:

$$AB\cdots D \to \sum_{j_2,j_3,\cdots,j_n}\int d\tau_2\cdots\int d\tau_n A_{j_1,j_2}(\tau_1,\tau_2) \times B_{j_2,j_3}(\tau_2,\tau_3)\cdots D_{j_n,j_{n+1}}(\tau_n,\tau_{n+1}). \tag{C1}$$

From the convolution we define the trace by substituting $\tau_{n+1} = \tau_1$, $j_{n+1} = j_1$, integrating also over τ_1, and summing over j_1, i.e.,

$$\mathrm{Tr}_{j,\tau}(AB\cdots D) = \int d\tau_1\int d\tau_2\cdots\int d\tau_n \times \mathrm{Tr}_j[A(\tau_1,\tau_2)B(\tau_2,\tau_3)\cdots D(\tau_n,\tau_1)]. \tag{C2}$$

Changing from contour to real-time integration from $-\infty$ to $+\infty$, i.e., using $\int d\tau = \sum_\sigma \int \sigma dt$, we have

$$\begin{aligned}&\mathrm{Tr}_{j,\tau}(AB\cdots D)\\ &= \sum_{\sigma_1,\sigma_2,\cdots,\sigma_n}\int dt_1\int dt_2\cdots\int dt_n\\ &\times \mathrm{Tr}_j[\sigma_1 A^{\sigma_1\sigma_2}(t_1,t_2)\sigma_2 B^{\sigma_2\sigma_3}(t_2,t_3)\cdots\\ &\times \sigma_n D^{\sigma_n\sigma_1}(t_n,t_1)].\end{aligned} \tag{C3}$$

Let us absorb the extra σ into the definition of branch components, i.e., define

$$\bar{A}_{\sigma\sigma'} = \sigma A^{\sigma\sigma'} \quad \text{or} \quad \bar{A} = \sigma_z A, \tag{C4}$$

where A is viewed as a 2×2 block matrix with the usual $+$, $-$ component,

$$A = \begin{pmatrix} A^{++} & A^{+-}\\ A^{-+} & A^{--}\end{pmatrix} = \begin{pmatrix} A^t & A^<\\ A^> & A^{\bar{t}}\end{pmatrix}, \tag{C5}$$

and σ_z is defined as

$$\sigma_z = \begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix}; \tag{C6}$$

then it can easily be seen that

$$\begin{aligned}\mathrm{Tr}_{j,\tau}(AB\cdots D) &= \int dt_1\int dt_2\cdots\int dt_n \mathrm{Tr}_j[\bar{A}(t_1,t_2)\\ &\times \bar{B}(t_2,t_3)\cdots\bar{D}(t_n,t_1)]\\ &= \mathrm{Tr}_{t,j,\sigma}(\bar{A}\bar{B}\cdots\bar{D}).\end{aligned} \tag{C7}$$

Then we can do a rotation, where the rotation matrix is given by

$$O = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1\\ -1 & 1\end{pmatrix}, \quad OO^T = I, \tag{C8}$$

and we define, for any matrix A, the rotated matrix as

$$\breve{A} = O^T\sigma_z A O = O^T\bar{A}O. \tag{C9}$$

This is known as the Keldysh rotation. The effect of the Keldysh rotation is given in Eq. (47). Since this is an orthogonal transformation, the trace remains invariant, and hence we can write

$$\mathrm{Tr}_{t,j,\sigma}(\bar{A}\bar{B}\cdots\bar{D}) = \mathrm{Tr}_{t,j,\sigma}(\breve{A}\breve{B}\cdots\breve{D}). \tag{C10}$$

If we now go to the frequency domain, using the definition of two-time Fourier transform given in Eq. (49), then we can compute the trace in the frequency domain as

$$\begin{aligned}&\mathrm{Tr}_{(j,\tau)}(AB\cdots D)\\ &= \int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\cdots\int\frac{d\omega_n}{2\pi}\\ &\times \mathrm{Tr}\{\breve{A}[\omega_1,-\omega_2]\breve{B}[\omega_2,-\omega_3]\cdots\breve{D}[\omega_n,-\omega_1]\}\\ &= \mathrm{Tr}_{j,\sigma,\omega}(\breve{A}\breve{B}\cdots\breve{D}).\end{aligned} \tag{C11}$$

The last line above defines what we mean by the trace over the frequency domain given in Eq. (51). Unlike the trace in the time domain, the second argument of each of the variables needs a minus sign.

Let us now define what we mean by 1 on the contour. In the sense of convolution we define 1 as

$$A1\,D = AD, \tag{C12}$$

which means

$$\int d\tau_1 \int d\tau_2\, A(\tau,\tau_1) I\delta(\tau_1,\tau_2) D(\tau_2,\tau') = \int d\tau_1 A(\tau,\tau_1) D(\tau_1,\tau'). \quad \text{(C13)}$$

Note that $\delta(\tau,\tau')$ in real time has the following form:

$$\delta^{\sigma,\sigma'}(t,t') = \sigma\delta_{\sigma,\sigma'}\delta(t-t'). \quad \text{(C14)}$$

The inverse on the contour is defined as

$$\int d\tau_1 A(\tau,\tau_1) B(\tau_1,\tau') = I\delta(\tau,\tau'), \quad \text{(C15)}$$

where the identity matrix I takes care about the space index. Similarly to above, we go to the real time and multiply the above equation by the branch index σ, and we can write

$$\int dt_1 \bar{A}(t,t_1)\bar{B}(t_1,t') = I\bar{\delta}(t-t'), \quad \text{(C16)}$$

where

$$\bar{\delta}(t-t') = \sigma\delta^{\sigma,\sigma'}(t,t') = \sigma^2\delta_{\sigma,\sigma'}\delta(t-t') = \delta_{\sigma,\sigma'}\delta(t-t'). \quad \text{(C17)}$$

If we now discretize the time and write $\delta(t_i,t_{i'}) = \delta_{i,i'}/\Delta t$ with $\Delta t = |t_i - t_{i'}|$, then we have

$$\tilde{A}\tilde{B} = \tilde{I}, \quad \text{(C18)}$$

with $\tilde{A} = A\Delta t$, and similarly for other matrices.

With similar notation, we can now write different types of Dyson's equations given in Eqs. (41) and (59) as follows. In contour time we have

$$G_0(\tau,\tau') = g_C(\tau,\tau') + \int\int d\tau_1 d\tau_2\, g_C(\tau,\tau_1)\Sigma(\tau_1,\tau_2)G_0(\tau_2,\tau'). \quad \text{(C19)}$$

In real time, following the above arguments, we write

$$\bar{G}_0(t,t') = \bar{g}_C(t,t') + \int\int dt_1 dt_2\, \bar{g}_C(t,t_1)\bar{\Sigma}(t_1,t_2)\bar{G}_0(t_2,t'). \quad \text{(C20)}$$

After Keldysh rotation we can write

$$\breve{G}_0(t,t') = \breve{g}_C(t,t') + \int\int dt_1 dt_2\, \breve{g}_C(t,t_1)\breve{\Sigma}(t_1,t_2)\breve{G}_0(t_2,t'). \quad \text{(C21)}$$

Finally, in discretized time t we write

$$\tilde{G}_0 = \tilde{g}_C + \tilde{g}_C\tilde{\Sigma}\tilde{G}_0, \quad \text{(C22)}$$

which is a matrix equation. Similar equations can also be written for Eq. (41).

Now we define the determinant via the relation $\det(A) = \exp(\mathrm{Tr}\ln A)$; i.e., the determinant is defined in terms of the trace. In order for $\ln A$ to be defined, we have to assume a Taylor expansion. For example, we can define $\ln(1+M) = M - M^2/2 + M^3/3 + \cdots$, where 1 means $\delta_{jj'}\delta(\tau,\tau')$ in contour space.

APPENDIX D: CALCULATION OF $\Sigma_L^A(\omega,\omega')$ FOR THE PROJECTED INITIAL STATE

Here we discuss the calculation for $\Sigma_L^A(\omega,\omega')$ for $\rho'(0)$, which is the starting point for doing the numerical calculation. To calculate $\Sigma_L^A(\omega,\omega')$ for the projected initial state $\rho'(0)$ we define two types of θ functions, $\theta_1(t,t')$ and $\theta_2(t,t')$. $\theta_1(t,t')$ is nonzero and has the value 1 when

$$0 \leqslant t \leqslant t_M, \quad \text{and} \quad t' \leqslant 0 \quad \text{or} \quad t' \geqslant t_M, \quad \text{(D1)}$$

or

$$0 \leqslant t' \leqslant t_M, \quad \text{and} \quad t \leqslant 0 \quad \text{or} \quad t \geqslant t_M, \quad \text{(D2)}$$

and $\theta_2(t,t')$ is nonzero only in the regime where $0 \leqslant t,t' \leqslant t_M$. For regions where $\theta_1(t,t')$ is nonzero, the expression for Σ_L^A after taking the limit $\lambda \to \infty$ is (assuming that all correlation functions decay to 0 as $t \to \pm\infty$)

$$\Sigma_A^{t,\bar{t},\langle,\rangle}(t,t') = -\Sigma_L^{t,\bar{t},\langle,\rangle}(t-t'). \quad \text{(D3)}$$

So using θ functions we may write $\Sigma_L^A(t,t')$ in the full t,t' domain as

$$\begin{aligned}
\Sigma_A^{t,\bar{t}}(t,t') &= -\theta_1(t,t')\Sigma_L^{t,\bar{t}}(t-t'),\\
\Sigma_A^{<}(t,t') &= -\theta_1(t,t')\Sigma_L^{<}(t-t') + \theta_2(t,t')\\
&\quad\times[\Sigma_L^{<}(t-t'-\hbar\xi) - \Sigma_L^{<}(t-t')],\\
\Sigma_A^{>}(t,t') &= -\theta_1(t,t')\Sigma_L^{>}(t-t') + \theta_2(t,t')\\
&\quad\times[\Sigma_L^{>}(t-t'+\hbar\xi) - \Sigma_L^{>}(t-t')]. \quad \text{(D4)}
\end{aligned}$$

By doing a Fourier transform, it can easily be shown that

$$\Sigma_A^{t,\bar{t}}[\omega,\omega'] = -\int_{-\infty}^{\infty}\frac{d\omega_c}{2\pi}\,\theta_1[\omega-\omega_c,\omega'+\omega_c]\Sigma_L^{t,\bar{t}}(\omega_c) \quad \text{(D5)}$$

and

$$\begin{aligned}
&\Sigma_A^{>,<}[\omega,\omega']\\
&= -\int_{-\infty}^{\infty}\frac{d\omega_c}{2\pi}\theta_1[\omega-\omega_c,\omega'+\omega_c]\Sigma_L^{>,<}(\omega_c)\\
&\quad+\int_{-\infty}^{\infty}\frac{d\omega_c}{2\pi}\theta_2[\omega-\omega_c,\omega'+\omega_c]\Sigma_L^{>,<}(\omega_c)(e^{i\omega_c\eta\xi}-1), \quad \text{(D6)}
\end{aligned}$$

where $\eta = \pm 1$. The positive sign is for $\Sigma_A^{<}$ and the negative sign for $\Sigma_A^{>}$.

The θ functions are now given by

$$\begin{aligned}
\theta_1(\omega_a,\omega_b) &= f(\omega_a)g(\omega_b) + f(\omega_b)g(\omega_a),\\
\theta_2(\omega_a,\omega_b) &= f(\omega_a)f(\omega_b), \quad \text{(D7)}
\end{aligned}$$

where

$$f(\omega) = \frac{e^{i\omega t_M}-1}{i\omega}, \quad g(\omega) = \frac{1}{i\omega+\epsilon} - \frac{e^{i\omega t_M-\eta t_M}}{i\omega-\epsilon}, \quad \text{(D8)}$$

with $\epsilon \to 0^+$. The θ functions are of immense importance, as they carry all information on the measurement time t_M.

In the limit $t_M \to \infty$, the region $0 \leqslant t, t' \leqslant t_M$ dominates and the corresponding θ function, i.e., $\theta_2(\omega,\omega')$, reduces to

$$\theta_2(\omega-\omega_c,\omega'+\omega_c) \approx \delta(\omega-\omega_c)\delta(\omega'+\omega_c) \quad \text{(D9)}$$

and is responsible for obtaining the steady state result.

To calculate all the cumulants we only need to take the derivative of $\Sigma_A(\omega,\omega')$ with respect to $i\xi$ since G_0 does not have any ξ dependence. Also, Σ^A has ξ dependence only for $0 \leqslant t, t' \leqslant t_M$, and hence the derivatives are given by

$$\frac{\partial^n \Sigma_A^{>,<}}{\partial (i\xi)^n}[\omega,\omega'] = \int_{-\infty}^{\infty} \frac{d\omega_c}{2\pi} (\eta\hbar\omega_c)^n \theta_2[\omega-\omega_c,\omega'+\omega_c] \times \Sigma_L^{>,<}(\omega_c) e^{i\omega_c\eta\xi}. \tag{D10}$$

Here n refers to the order of the derivative.

APPENDIX E: SOLVING THE DYSON EQUATION NUMERICALLY FOR THE PRODUCT INITIAL STATE

Here we discuss solving the Dyson equation for G_0 given in Eq. (59) for product initial state $\rho(-\infty)$. In order to compute the matrix $\check{G}_0(t,t')$, we have to calculate two components, G_0^r and G_0^K, which are written in the integral form by applying Langreth's rule [45,54]:

$$G_0^r(t,t') = g_C^r(t-t') + \int_0^{t_M} dt_1 \int_0^{t_M} dt_2 g_C^r(t-t_1)\Sigma^r(t_1-t_2)G_0^r(t_2,t'), \tag{E1}$$

and

$$\begin{aligned} G_0^K(t,t') = {} & g_C^K(t-t') \\ & + \int_0^{t_M} dt_1 \int_0^{t_M} dt_2\, g_C^r(t-t_1)\,\Sigma^r(t_1-t_2)G_0^K(t_2,t') \\ & + \int_0^{t_M} dt_1 \int_0^{t_M} dt_2\, g_C^r(t-t_1)\Sigma^K(t_1-t_2)G_0^a(t_2,t') \\ & + \int_0^{t_M} dt_1 \int_0^{t_M} dt_2\, g_C^K(t-t_1)\Sigma^a(t_1-t_2)G_0^a(t_2,t'). \end{aligned} \tag{E2}$$

Note that the argument for the center Green's function g_C and lead self-energy Σ are written as the time difference $t-t'$ because they are Green's functions for the isolated center part and leads, respectively, and hence are calculated at equilibrium. The analytical expressions for Σ and g_C are known in the frequency domain and are given in Appendix A. To determine their time dependence we numerically calculate their inverse Fourier transforms using the trapezoidal rule [56]. Then in order to solve the above equations for any t_M, we discretize the time variable into N total intervals of incremental length $\Delta t = t_M/N$, thus converting the integral into a sum. After discretization, the above equations can be written in matrix form, indexed by space j and discrete time t, as

$$\begin{aligned} \tilde{G}_0^r &= \tilde{g}_C^r + \tilde{g}_C^r \tilde{\Sigma}^r \tilde{G}_0^r, \\ \tilde{G}_0^K &= \tilde{G}_0^r \tilde{\Sigma}^K \tilde{G}_0^a + \left(I + \tilde{G}_0^r \tilde{\Sigma}^r\right)\tilde{g}_C^K \left(I + \tilde{\Sigma}^a \tilde{G}_0^a\right). \end{aligned} \tag{E3}$$

So $\tilde{G}_0^r$ can be obtained by doing an inverse of the matrix $(I - \tilde{g}_C^r \tilde{\Sigma}^r)$ and then multiplying by $\tilde{g}_C^r$. $\tilde{G}_0^r$ in this case also obeys time-translational invariance, so it can also be obtained by direct inverse Fourier transform. $\tilde{G}_0^a$ can be obtained by taking the transpose of $\tilde{G}_0^r$. Once $\tilde{G}_0^r$ and $\tilde{G}_0^a$ are obtained, we use the second equation to calculate $\tilde{G}_0^K$, which is simply multiplying matrices.

APPENDIX F: A QUICK DERIVATION OF THE LEVITOV-LESOVIK FORMULA FOR ELECTRONS USING THE NEGF

The GF for noninteracting electrons was first derived by Levitov and Lesovik [18,19] using the Landauer type of wave scattering approach. Klich [24] and Schönhammer [23] rederived the formula using a trace and determinant relation to reduce the problem from a many-body to a single-particle Hilbert-space problem. Esposito *et al.* reported an approach using the superoperator nonequilibrium Green's function [41]. A more rigorous treatment is given in Ref. [67].

Our method for calculating the CGF can be easily extended to the electron case. Here we derive the CGF for the joint probability distribution for the particle number and energy without a time-dependent driving force. The Hamiltonian for the whole system can be written as (using the tight-binding model)

$$\mathcal{H}^e = \sum_{\alpha=L,C,R} c_\alpha^\dagger h^\alpha c_\alpha + \sum_{\alpha=L,R} \left(c_\alpha^\dagger V_e^{\alpha C} c_C + \text{H.c.}\right), \tag{F1}$$

where c_α is a column vector consisting of all the annihilation operators in region α. $c_\alpha^\dagger$ is a row vector of the corresponding creation operators. h^α is the single-particle Hamiltonian matrix. $V_e^{\alpha C}$ has a meaning similar to that of $V^{\alpha C}$ in the phonon Hamiltonian, and $V_e^{\alpha C} = (V_e^{C\alpha})^\dagger$.

We are interested in calculating the GF corresponding to the particle operator $\mathcal{N}_L$ and energy operator $\mathcal{H}_L$ of the left lead, where $\mathcal{H}_L = c_L^\dagger h^L c_L$ and $\mathcal{N}_L = c_L^\dagger c_L$ [68]. One can easily generalize the formula for the right lead also, as we did in the phonon case. For electrons, $\mathcal{N}_L$ and $\mathcal{H}_L$ can be measured simultaneously because they commute; i.e., $[\mathcal{H}_L,\mathcal{N}_L] = 0$. In order to calculate the CGF we introduce two counting fields, ξ_p and ξ_e, for particle and energy, respectively. Here we consider the product initial state (with fixed temperatures and chemical potentials for the leads) and derive the long-time result.

Similarly to the phonon case we can write the GF as

$$\mathcal{Z}(\xi_e,\xi_p) = \left\langle e^{i(\xi_e\mathcal{H}_L + \xi_p\mathcal{N}_L)}\, e^{-i(\xi_e\mathcal{H}_L^H + \xi_p\mathcal{N}_L^H)}\right\rangle, \tag{F2}$$

where superscript H means that the operators are in the Heisenberg picture at time t. In terms of the modified Hamiltonian the GF can be expressed as

$$\mathcal{Z}(\xi_e,\xi_p) = \left\langle \mathcal{U}_{\left(\frac{\xi_e}{2},\frac{\xi_p}{2}\right)}(0,t)\,\mathcal{U}_{\left(-\frac{\xi_e}{2},-\frac{\xi_p}{2}\right)}(t,0)\right\rangle, \tag{F3}$$

where

$$\begin{aligned} \mathcal{U}_{x,y}(t,0) &= e^{ix\mathcal{H}_L + iy\mathcal{N}_L}\,\mathcal{U}(t,0)\,e^{-ix\mathcal{H}_L - iy\mathcal{N}_L} \\ &= e^{-\frac{i}{\hbar}\mathcal{H}_{x,y}t}, \end{aligned} \tag{F4}$$

with $x = \xi_e/2$ and $y = \xi_p/2$, and $\mathcal{U}(t,0) = e^{-i\mathcal{H}t/\hbar}$. $\mathcal{H}_{x,y}$ is the modified Hamiltonian, which evolves with both $\mathcal{H}_L$ and $\mathcal{N}_L$ and is given by

$$\begin{aligned} \mathcal{H}_{x,y} &= e^{ix\mathcal{H}_L + iy\mathcal{N}_L}\,\mathcal{H}\,e^{-ix\mathcal{H}_L - iy\mathcal{N}_L} \\ &= \mathcal{H}_L + \mathcal{H}_C + \mathcal{H}_R + \left(e^{iy}c_L^\dagger(\hbar x)V_e^{LC}c_C + \text{H.c.}\right) \\ &\quad + \left(c_R^\dagger V_e^{RC} c_C + \text{H.c.}\right), \end{aligned} \tag{F5}$$

where we have used the fact that

$$e^{ix\mathcal{H}_L}c_L e^{-ix\mathcal{H}_L} = c_L(\hbar x),$$
$$e^{iy\mathcal{N}_L}c_L e^{-iy\mathcal{N}_L} = e^{-iy}c_L. \tag{F6}$$

So the evolution with $\mathcal{H}_L$ and $\mathcal{N}_L$ is to shift the time argument and produce a phase for c_L and $c_L^\dagger$, respectively. Next we go to the interaction picture of the modified Hamiltonian $\mathcal{H}_{x,y}$ with respect to $\mathcal{H}_0 = \sum_{\alpha=L,C,R}\mathcal{H}_\alpha$, and the GF can then be written on the contour running from 0 to t_M and back as

$$\mathcal{Z}(\xi_e,\xi_p) = \mathrm{Tr}\big[\rho(-\infty)T_c e^{-\frac{i}{\hbar}\int d\tau \mathcal{V}^I_{x,y}(\tau)}\big], \tag{F7}$$

where $\mathcal{V}^I_{x,y}(\tau)$ is written in contour time:

$$\mathcal{V}^I_{x,y}(\tau) = \big(e^{iy}c_L^\dagger(\tau+\hbar x)V_e^{LC}c_C(\tau) + \mathrm{H.c.}\big) + \big(c_R(\tau)^\dagger V_e^{RC}c_C(\tau) + \mathrm{H.c.}\big). \tag{F8}$$

Now we can expand the exponential in the GF and use Feynman diagrams to sum the series, and finally, the CGF can be shown to be

$$\ln\mathcal{Z}(\xi_e,\xi_p) = \mathrm{Tr}_{j,\tau}\ln\big[1 - G_0^e\Sigma^A_{L,e}\big], \tag{F9}$$

where we define the shifted self-energy for the electron as

$$\Sigma^A_{L,e}(\tau,\tau') = e^{i(y(\tau')-y(\tau))}\Sigma_{L,e}(\tau+\hbar x,\tau'+\hbar x') - \Sigma_{L,e}(\tau,\tau'). \tag{F10}$$

The counting of the electron number is associated with the factor of a phase, while the counting of the energy is related to the translation in time. Note that the CGF does not have the characteristic 1/2 prefactor, compared to the phonon case, because c and $c^\dagger$ are independent variables. In the long-time limit, following the same steps as we did for phonons, the CGF can be written as (after doing Keldysh rotation)

$$\ln\mathcal{Z}(\xi_e,\xi_p) = t_M\int\frac{dE}{2\pi\hbar}\mathrm{Tr}\ln\big(I - \check{G}_0^e(E)\check{\Sigma}^A_{L,e}(E)\big). \tag{F11}$$

In the energy E domain, different components of the shifted self-energy are

$$\Sigma_A^t(E) = \Sigma_A^{\bar{t}}(E) = 0,$$
$$\Sigma_A^<(E) = (e^{i(\xi_p+\xi_e E)} - 1)\Sigma_L^<(E), \tag{F12}$$
$$\Sigma_A^>(E) = (e^{-i(\xi_p+\xi_e E)} - 1)\Sigma_L^>(E).$$

Finally, the CGF can be simplified as

$$\ln\mathcal{Z} = t_M\int\frac{dE}{2\pi\hbar}\ln\det\big\{I + G_0^r\Gamma_L G_0^a\Gamma_R[(e^{i\alpha}-1) \times f_L(1-f_R) + (e^{-i\alpha}-1)f_R(1-f_L)]\big\}, \tag{F13}$$

where $\alpha = \xi_p + \xi_e E$, and f_L and f_R are the Fermi distribution functions for the left and right lead, respectively. Note the difference in the signs of the CGF compared to the phonons. If we replace α with $(E-\mu_L)\xi$, the resulting formula is for the counting of the heat $\mathcal{Q}_L = \mathcal{H}_L - \mu_L\mathcal{N}_L$ transferred, where μ_L is the chemical potential of the left lead. The CGF obeys the following fluctuation symmetry [39]:

$$\mathcal{Z}(\xi_e,\xi_p) = \mathcal{Z}(-\xi_e + i(\beta_R - \beta_L), -\xi_p - i(\beta_R\mu_R - \beta_L\mu_L)). \tag{F14}$$

[1] C. Caroli, R. Combescot, P. Nozieres, and D. Saint-James, J. Phys. C **4**, 916 (1971).
[2] Y. Meir and N. S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).
[3] L. G. C. Rego and G. Kirczenow, Phys. Rev. Lett. **81**, 232 (1998).
[4] D. Segal, A. Nitzan, and P. Hänggi, J. Chem. Phys. **119**, 6840 (2003).
[5] N. Mingo and L. Yang, Phys. Rev. B **68**, 245406 (2003).
[6] T. Yamamoto and K. Watanabe, Phys. Rev. Lett. **96**, 255503 (2006).
[7] A. Dhar and D. Roy, J. Stat. Phys. **125**, 805 (2006).
[8] J.-S. Wang, J. Wang, and N. Zeng, Phys. Rev. B **74**, 033408 (2006).
[9] J.-S. Wang, N. Zeng, J. Wang, and C. K. Gan, Phys. Rev. E **75**, 061128 (2007).
[10] J.-S. Wang, J. Wang, and J. T. Lü, Eur. Phys. J. B **62**, 381 (2008).
[11] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, *Fourier's Law: A Challenge to Theorists, Mathematical Physics 2000* (Imperial College Press, London, 2000).
[12] A. Dhar, Adv. Phys. **57**, 457 (2008).
[13] S. Lepri, R. Livi, and A. Politi, Phys. Rep. **377**, 1 (2003).
[14] E. C. Cuansing and J.-S. Wang, Phys. Rev. B **81**, 052302 (2010); **83**, 019902(E) (2011).
[15] E. C. Cuansing and J.-S. Wang, Phys. Rev. E **82**, 021116 (2010).
[16] N. Li, J. Ren, L. Wang, G. Zhang, P. Hänggi, and B. Li, e-print arXiv:1108.6120.
[17] A. D. O'Connell, M. Hofheinz, M. Ansmann, R. C. Bialczak, M. Lenander, E. Lucero, M. Neeley, D. Sank, H. Wang, M. Weides, J. Wenner, J. M. Martinis, and A. N. Cleland, Nature **464**, 697 (2010).
[18] L. S. Levitov and G. B. Lesovik, JETP Lett. **58**, 230 (1993).
[19] L. S. Levitov, H.-W. Lee, and G. B. Lesovik, J. Math. Phys. **37**, 4845 (1996).
[20] L. S. Levitov and M. Reznikov, Phys. Rev. B **70**, 115305 (2004).
[21] W. Belzig and Y. V. Nazarov, Phys. Rev. Lett. **87**, 197006 (2001).
[22] Y. V. Nazarov and M. Kindermann, Eur. Phys. J. B **35**, 413 (2003).
[23] K. Schönhammer, Phys. Rev. B **75**, 205329 (2007); J. Phys.: Condens. Matter **21**, 495306 (2009).
[24] I. Klich, in *Quantum Noise in Mesoscopic Physics, NATO Science Series II, Vol. 97*, edited by Yu. V. Nazarov (Kluwer, Dordrecht, 2003).
[25] S. Pilgram, A. N. Jordan, E. V. Sukhorukov, and M. Büttiker, Phys. Rev. Lett. **90**, 206801 (2003).
[26] K. Saito and Y. Utsumi, Phys. Rev. B **78**, 115429 (2008).
[27] D. A. Bagrets and Y. V. Nazarov, Phys. Rev. B **67**, 085316 (2003).
[28] A. O. Gogolin and A. Komnik, Phys. Rev. B **73**, 195301 (2006).
[29] D. F. Urban, R. Avriller, and A. Levy Yeyati, Phys. Rev. B **82**, 121414(R) (2010).

[30] D. B. Gutman, Y. Gefen, and A. D. Mirlin, Phys. Rev. Lett. **105**, 256802 (2010).
[31] S. Gustavsson, R. Leturcq, B. Simovič, R. Schleser, T. Ihn, P. Studerus, K. Ensslin, D. C. Driscoll, and A. C. Gossard, Phys. Rev. Lett. **96**, 076605 (2006).
[32] C. Flindt, C. Fricke, F. Hohls, T. Novotný, K. Netočný, T. Brandes, and R. J. Haug, Proc. Natl. Acad. Sci. USA **106**, 10116 (2009).
[33] A. A. Clerk, F. Marquardt, and J. G. E. Harris, Phys. Rev. Lett. **104**, 213603 (2010).
[34] K. Saito and A. Dhar, Phys. Rev. Lett. **99**, 180601 (2007); Phys. Rev. E **83**, 041121 (2011).
[35] J. Ren, P. Hänggi, and B. Li, Phys. Rev. Lett. **104**, 170601 (2010).
[36] L. Nicolin and D. Segal, J. Chem. Phys. **135**, 164106 (2011).
[37] A. A. Clerk, Phys. Rev. A **84**, 043824 (2011).
[38] G. Gallavotti and E. G. D. Cohen, Phys. Rev. Lett. **74**, 2694 (1995); C. Jarzynski, *ibid.* **78**, 2690 (1997).
[39] D. Andrieux, P. Gaspard, T. Monnai, and S. Tasaki, New J. Phys. **11**, 043014 (2009).
[40] J.-S. Wang, B. K. Agarwalla, and H. Li, Phys. Rev. B **84**, 153412 (2011).
[41] M. Esposito, U. Harbola, and S. Mukamel, Rev. Mod. Phys. **81**, 1665 (2009).
[42] M. Campisi, P. Hänggi, and P. Talkner, Rev. Mod. Phys. **83**, 771 (2011).
[43] A. Kundu, S. Sabhapandit, and A. Dhar, J. Stat. Mech (2011) P03007.
[44] J. Schwinger, J. Math. Phys. **2**, 407 (1961); L. V. Keldysh, Sov. Phys. JETP **20**, 1018 (1965).
[45] For a review, see J. Rammer and H. Smith, Rev. Mod. Phys. **58**, 323 (1986).
[46] M. Campisi, P. Talkner, and P. Hänggi, Phys. Rev. E **83**, 041114 (2011).
[47] M. Campisi, P. Talkner, and P. Hänggi, Phys. Rev. Lett. **105**, 140601 (2010).
[48] M. Campisi, P. Talkner, and P. Hänggi, Phys. Rev. E **80**, 031145 (2009).
[49] E. C. Cuansing, H. Li, and J.-S. Wang, e-print arXiv:1105.2233.
[50] J. von Neumann, *Mathematical Fundations of Quantum Mechanics* (Princeton University Press, Princeton, NJ, 1955).
[51] R. P. Feynman and F. L. Vernon, Ann. Phys. **24**, 118 (1963).
[52] J. T. Stockburger and H. Grabert, Phys. Rev. Lett. **88**, 170407 (2002).
[53] G. D. Mahan, *Many-Particle Physics*, 3rd ed. (Kluwer Academic, New York, 2000).
[54] H. Haug and A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors*, 2nd ed. (Springer, New York, 2008).
[55] Ya. M. Blanter and M. Büttiker, Phys. Rep. **336**, 2 (2000).
[56] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes: The Art of Scientific Computing*, 3rd ed. (Cambridge University Press, New York, 2007).
[57] R. J. Rubin and W. L. Greer, J. Math. Phys. **12**, 1686 (1971).
[58] U. Weiss, *Quantum Dissipative Systems*, 2nd ed. (World Scientific, Singapore, 1999).
[59] H.-P. Breuer and F. Peteruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
[60] M. Esposito, K. Lindenberg, and C. van den Broeck, New J. Phys. **12**, 013013 (2010).
[61] S. Deffner and E. Lutz, Phys. Rev. Lett. **107**, 140404 (2011).
[62] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997).
[63] P. Talkner, P. S. Burada, and P. Hänggi, Phys. Rev. E **78**, 011115 (2008).
[64] B. K. Agarwalla, J.-S. Wang, and B. Li, Phys. Rev. E **84**, 041115 (2011).
[65] N. Zeng, Ph.D. thesis, National University of Singapore (2008); available at: [http://staff.science.nus.edu.sg/~phywjs/NEGF/negf.html].
[66] P. Brouwer, *Theory of Many-Particle Systems* (Lecture Notes for P654, Spring) (Cornell University, Ithaca, NY, 2005).
[67] D. Bernard and B. Doyon, e-print arXiv:1105.1695.
[68] F. Zhan, S. Denisov, and P. Hänggi, Phys. Rev. B **84**, 195117 (2011).