Cumulants of heat transfer across nonlinear quantum systems

Huanan Li$^1$, Bijay Kumar Agarwalla$^1$, Baowen Li$^{1,2,3}$, and Jian-Sheng Wang$^1$

$^1$ Department of Physics and Center for Computational Science and Engineering, National University of Singapore, Singapore 117542, Republic of Singapore
$^2$ NUS Graduate School for Integrative Sciences and Engineering, Singapore 117456, Republic of Singapore
$^3$ NUS-Tongji Center for Phononics and Thermal Energy Science, School of Physical Science and Engineering, Tongji University, 200092 Shanghai, China

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We consider thermal conduction across a general nonlinear phononic junction. Based on two-time observation protocol and the field theoretical/algebraic method, the cumulants of the heat transferred in both transient and steady-state regimes are studied on an equal footing, and practical formulae for the calculation of the cumulant generating function of heat transfer are obtained. As an application, the developed general formalism is used to study anharmonic effects on fluctuation of steady-state heat transfer across a single-site junction with a quartic nonlinear on-site pinning potential. An explicit nonlinear modification to cumulant generating function exact up to the first order is given, in which Gallavotti-Cohen fluctuation symmetry is verified. Numerically a self-consistent procedure is introduced, which works well for strong nonlinearity.

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I. INTRODUCTION

The physics of nonequilibrium many-body systems is one of the most rapidly expanding areas which attract much attentions recently. With the development of the modern nanoscale technology, a full understanding of the general features of thermal conduction is needed. And it is well-known that the noise generated by nanodevices contains valuable information on microscopic transport processes not available from current, which is simply related to the lowest order moment of the full distribution function for heat transfer. To this end, the full counting statistics (FCS) regarding the distribution of transferred quantity, such as heat in phononic case, has to be determined.

The extensive study of the FCS started from the field of electronic transport pioneered by Levitov and Lesovik, while much less attention is given to heat transfer. Saito and Dhar are the first ones to borrow this concept to thermal transport. However, both of them, including many subsequent works, are mainly restricted to noninteracting systems although some works have already been devoted to the analysis of fluctuation considering the effect of nonlinearity in the classical limit through Langevin simulations, or approximately in a restricted electronic transport case, such as the FCS in molecular junctions with electron-phonon interaction.

In recent years, phononics, i.e., the counterpart technology of electronics, has great interest to both theorists and experimentalists, and presents an unforeseen wealth of applications. And the nonlinearity, such as the phonon-phonon interaction, has been found of special importance in the construction of phononic devices. In addition, recently it has been noted that the nonlinearity of interaction is crucial to the manifestation of geometric heat flux. Therefore, it is desirable to establish a systematic and practical formalism to properly deal with cumulants of heat transfer in the presence of nonlinearity.

In this work, we shall study the FCS for heat transfer flowing across a quantum junction in the presence of general phonon-phonon interactions. Then, based on two-time observation protocol, we construct a concise and rigorous cumulant generating function (CGF) expression for the heat transfer in this general situation, in which both the transient and steady-state case are dealt with on equal footing. Furthermore, as an illustration of this general formalism, a single-site junction with a quartic nonlinear on-site pinning potential is introduced and the corresponding CGF exact up to first order of the nonlinear interaction strength is given. Finally, a self-consistent scheme is employed to numerically illustrate the nonlinear effects on first three cumulants of heat transfer. In short, the paper is organized as follows. We introduce the model and elaborate the general formalism in Sec. II which is taken as the main part of the work. And in Sec. III an application is introduced to verify the general formalism. Finally we summarize in Sec. V.

II. MODEL AND THE GENERAL FORMALISM

We consider the lead-junction-lead model initially prepared in a product state $\rho_{ini} = \Pi_{\alpha=L,C,R} \prod_{i} e^{-\beta_\alpha u \hat{c}^\dagger_i \hat{a}_{\alpha i}}$. It can be imagined that left lead ($L$), center junction ($C$), and right lead ($R$) in this model were in contact with three different heat baths at the inverse temperatures $\beta_L = (k_B T_L)^{-1}$, $\beta_C = (k_B T_C)^{-1}$ and $\beta_R = (k_B T_R)^{-1}$, respectively, for time $t < t_0$. At time $t = t_0$, all the heat baths are removed, and couplings of the center junction with the leads $H_{LC} = u_L^T V^{LC} u_C$ and $H_{CR} = u_R^T V^{CR} u_R$ and the interested nonlinear term $H_n$ appearing only in the center junction are switched on abruptly. Now the
total Hamiltonian is given by

\[ H_{\text{tot}} = H_L + H_C + H_R + H_{\text{LC}} + H_{\text{CR}} + H_n, \]

where \( H_a = \frac{1}{2}p_a^T p_a + \frac{1}{2}m_a \dot{x}_a, \) \( \alpha = L, C, R, \) represents coupled harmonic oscillators, \( u_a = \sqrt{m_a} x_a \) and \( p_a \) are column vectors of transformed coordinates and corresponding conjugate momenta in region \( \alpha \). \( K_a \) is force constant matrix; the superscript \( T \) stands for matrix transpose.

We can construct a consistent framework consisting of two-time quantum histories to study the heat transfer across arbitrary nonlinear systems in a given time duration. A realization of the quantum history \( P_{t_0}^a \otimes P_{t_M}^b \) means that the result of the measurement at time \( t_0 \) of energy of the left lead associated with the operator \( H_L \) is the eigenvalue \( a \) of \( H_L \), then the measurement at time \( t_M \) yields the eigenvalue \( b \) of \( H_L \). Using this consistent quantum framework, we can define the generating function (GF) for heat transfer in the time duration \( t_M - t_0 \) to be

\[ Z(\xi) \equiv \sum_{a,b} e^{i(a-b)\xi} \text{Pr} \left( P_{t_0}^a \otimes P_{t_M}^b \right) \]
\[ = \langle U_{\xi/2}(t_0,t_M) U_{-\xi/2}(t_2,t_0) \rangle, \tag{2} \]

where \( \text{Pr} \left( P_{t_0}^a \otimes P_{t_M}^b \right) \) stands for the joint probability for the quantum history \( P_{t_0}^a \otimes P_{t_M}^b \); \( U_{\xi/2}(t_0,t_M) \) means evolution operator associated with the counting-field dependent total Hamiltonian

\[ H^{\xi/2}_{\text{tot}} = e^{i(-\xi/2)H_L} H_{\text{tot}} e^{-i(-\xi/2)H_L} \]

similarly for \( U_{\xi/2}(t_0,t_M) \) and \( \langle . \rangle \) denotes the ensemble average over the initial state \( \rho_{ini} \).

\[ \text{FIG. 1. An illustration of the contour C. The upper branch is called + and lower one } - \text{ so that a particular time point } \tau_1 \text{ on the upper branch is denoted by } t_1^+ \text{ while } \tau_2 \text{ on the lower one by } t_2^-. \text{ The time order follows the direction of the arrows.} \]

The first step for the study of the GF is to relate it to the Green’s function, by which the closed equation satisfied can be found out. To this end, we generalize the GF to be

\[ Z(\lambda_2 - \lambda_1) \equiv \langle U_{\lambda_2}(t_0,t_M) U_{\lambda_1}(t_M,t_0) \rangle \]
\[ = \langle e^{i(\lambda_2 - \lambda_1)H_L} U(t_0,t_M) e^{-i(\lambda_2 - \lambda_1)H_L} U(t_M,t_0) \rangle \]
\[ = \langle T^{+} e^{-i\int_{t}^{t} d\tau T_{\lambda}(\tau)} \rangle, \tag{3} \]

\[ = \int_{t_0}^{t_M} dt \langle \tilde{G}_{\text{LC}}(t, t') V^{\text{CL}} \rangle \bigg|_{t' = t}, \tag{12} \]

Notice that the tilde on the Green’s functions emphasizes the fact that they are counting field \( \xi \)-dependent, and real-time Green’s functions can be obtained by specifying the variation range of the time arguments in contour-ordered Green’s functions such as

\[ \tilde{G}_{\text{LC}}(\tau_1, \tau_2) \rightarrow \tilde{G}_{\text{LC}}(t_1^+, t_2) \]
\[ \tilde{G}_{\text{LC}}(t_1, t_2^+) \]

where, \( T \) is a \( \tau \)-ordering super-operator arranging operators with earlier \( \tau \) on the contour \( C \) (from \( t_0 \) to \( t_M \) and back to \( t_0 \)) to the right, see Fig. 11. In the second equality we have used the cyclic property of the trace and the commutator relation \([H_L, \rho_{ini}] = 0\); in the third equality we go to the interaction picture with respect to the free Hamiltonian \( h = H_L + H_C + H_R \) so that \( T_{\lambda}(\tau) = u_{\lambda}^{T}(\tau) V^{\text{LC}} \bar{u}_{\lambda}(\tau) + \bar{u}_{\lambda}(\tau) V^{\text{CR}} u_{\lambda}(\tau) + H_n(\tau) \) with caret put above operators to denote the interaction-picture \( \tau \) dependence such as \( \bar{u}_{\lambda}(\tau) = e^{-i\lambda h_{\tau}} \bar{u}_{\lambda}(\tau) e^{-i\lambda h_{\tau}} \), where \( u_{\lambda}(\tau) = u_{\lambda}(h_{\tau} + \tau) \) with \( x_{\tau} = \lambda_1(\lambda_2) \) with \( \tau = t^+ (t^-) \) on the upper (lower) branch of the contour \( C \).

Furthermore, we define the adiabatic potential \( U(t, \lambda_2, \lambda_1) \) according to

\[ Z(\lambda_2 - \lambda_1) = e^{-\int_{t_0}^{t_M} dt U(t, \lambda_2, \lambda_1)}. \]

Thus we could apply the nonequilibrium version of the Feynman-Hellman theorem to get

\[ \frac{\partial}{\partial \lambda_1} U(t, \lambda_2, \lambda_1) = \frac{1}{Z(\lambda_2 - \lambda_1)} \left\langle T^{+} \frac{\partial T_{\lambda}(t)}{\partial \lambda_1} e^{-\int_{t}^{t} d\tau T_{\lambda}(\tau)} \right\rangle, \tag{7} \]

\[ \equiv \left\langle T^{+} \frac{\partial T_{\lambda}(t)}{\partial \lambda_1} \right\rangle_{\lambda}. \tag{8} \]

Since

\[ \frac{\partial T_{\lambda}(t)}{\partial \lambda_1} = \hbar \frac{\partial \tilde{u}_{\lambda}^{T}(t)}{\partial t^+} V^{\text{LC}} \bar{u}_{\lambda}(t^+) \tag{9} \]

and introducing contour-ordered Green’s functions \( \tilde{G}_{\text{LC}} \) and \( \tilde{G}_{\text{CL}} \) defined as

\[ \tilde{G}_{\text{LC}}(\tau_1, \tau_2) = -\frac{i}{\hbar} \left\langle T_{\lambda} \tilde{u}_{\lambda}(\tau_1) \tilde{u}_{\lambda}^{T}(\tau_2) \right\rangle_{\lambda}, \tag{10} \]

\[ \tilde{G}_{\text{CL}}(\tau_1, \tau_2) = -\frac{i}{\hbar} \left\langle T_{\lambda} \tilde{u}_{\lambda}(\tau_1) \tilde{u}_{\lambda}^{T}(\tau_2) \right\rangle_{\lambda}, \tag{11} \]

we can get

\[ \frac{\partial \ln Z(\lambda_2 - \lambda_1)}{\partial \lambda_1} \]
\[ = \int_{t_0}^{t_M} dt \hbar \frac{\partial}{\partial t^+} \left[ \tilde{G}_{\text{LC}}(t^+, t) V^{\text{CL}} \right] \bigg|_{t' = t}, \tag{12} \]
According to the basic analysis of Feynman diagrams, the contour-ordered Green’s functions $\hat{G}_{LC}$ and $\hat{G}_{CL}$ are given as

$$\hat{G}_{LC}(\tau_1, \tau_2) = \int_C \hat{g}^L(\tau_1, \tau) V^{LC} \hat{G}_{CC}(\tau, \tau_2) d\tau, \quad (13)$$

$$\hat{G}_{CL}(\tau_1, \tau_2) = \int_C \hat{G}_{CC}(\tau, \tau) V^{CL} \hat{g}^L(\tau, \tau_2) d\tau, \quad (14)$$

with the shifted bare Green’s function for the left lead being

$$\hat{g}^L(\tau_1, \tau_2) = -\frac{i}{\hbar} \langle T_\tau \hat{u}_L^\tau(\tau_1) \hat{u}^\tau_L(\tau_2) \rangle, \quad (15)$$

where

$$\hat{G}_{CC}(\tau_1, \tau_2) = -\frac{i}{\hbar} \langle T_\tau \hat{u}_C(\tau_1) \hat{u}^\tau_C(\tau_2) \rangle \quad (16)$$

is the central quantity for the study of the GF of the heat transfer, which we will discuss later. Before that we use the treatment of symmetrization to simplify $\frac{\partial}{\partial \lambda_l} \hat{Z}$ in Eq. (12) further according to the time-order version of Eq. (13) and Eq. (14), i.e.,

$$\hat{G}_{CL}^t(t', t) = \int_{t_0}^{t_{LM}} \hat{g}_{\tau}^L(t', t_1) V^{LC} \hat{G}_{CC}^t(t_1, t) d\tau_1$$

$$- \int_{t_0}^{t_{LM}} \hat{g}_{\tau}^L(t_1, t') V^{LC} \hat{G}_{CC}^t(t_1, t) d\tau_1, \quad (17)$$

$$\hat{G}_{CL}^t(t, t') = \int_{t_0}^{t_{LM}} \hat{G}_{CC}^t(t, t_1) V^{CL} \hat{g}_{\tau}^L(t, t_1') d\tau_1$$

$$- \int_{t_0}^{t_{LM}} \hat{G}_{CC}^t(t, t_1) V^{CL} \hat{g}_{\tau}^L(t, t_1') d\tau_1, \quad (18)$$

which explicitly means that

$$\frac{\partial}{\partial \lambda_l} \hat{Z}(\lambda_2 - \lambda_1)$$

$$= \frac{h}{2} \int_{t_0}^{t_{LM}} dt' \frac{d}{dt'} Tr \left[ \hat{G}_{CL}^t(t, t') V^{LC} + \hat{G}_{CL}^t(t', t) V^{CL} \right] \bigg|_{t'=t} \quad (19)$$

$$= -\frac{h}{2} \int_{t_0}^{t_{LM}} dt dt' Tr \left[ \hat{G}_{CC}^t(t, t') \frac{\partial \hat{\Sigma}^t_{\tau} (t', t)}{\partial t'} \right]$$

$$+ \hat{G}_{CC}^t(t, t') \frac{\partial \hat{\Sigma}^t_{\tau} (t', t)}{\partial t} \quad (20)$$

with the self-energy defined to be $\hat{\Sigma}_{\tau}(\tau_1, \tau_2) = V^{CL} \hat{g}_{\tau}(\tau_1, \tau_2) V^{LC}$, Eq. (20) is a generalized Meir-Wingreen formula. In obtaining the second equality we have used the relation $\frac{\partial \hat{\Sigma}^t_{\tau} (t', t)}{\partial t'} = -\frac{\partial \hat{\Sigma}^t_{\tau} (t', t)}{\partial t}$, since $\hat{\Sigma}_{\tau}^t(t', t_1) = \hat{\Sigma}_{\tau}^t(t' - t)$. Essentially we employ the procedure of symmetrization to get rid of the time-ordered version of $\hat{G}_{CC}(\tau_1, \tau_2)$, i.e., $\hat{G}_{CC}^t(t_1, t_2)$.

Setting $\lambda_1 = -\xi/2$ and $\lambda_2 = \xi/2$, and noticing that $\frac{\partial \hat{\Sigma}^t_{\tau} (t', t_1)}{\partial t'} = -\frac{1}{h} \frac{\partial \hat{\Sigma}^t_{\tau} (t', t_1)}{\partial \xi}$ and $\frac{\partial \hat{\Sigma}^t_{\tau} (t', t_1)}{\partial \xi} = 0$, we can obtain a compact expression for $\frac{\partial}{\partial \lambda_l} \hat{Z}$ from the generalized Meir-Wingreen formula Eq. (21).

$$\frac{\partial}{\partial \lambda_l} \int \frac{d\tau}{d\xi} = \frac{1}{2} \int_{t_0}^{t_{LM}} dt \int_{t_0}^{t_{LM}} dt' Tr \left\{ \left( \frac{\partial \hat{G}^t_{CC}(t, t')}{\partial \xi} \right) \right\} = \frac{1}{2} \int_C d\tau \int d\tau' Tr \left[ \hat{G}_{CC}(\tau, \tau') \frac{\partial \hat{\Sigma}_{\tau}(\tau', \tau)}{\partial \xi} \right]. \quad (21)$$

It is worth mentioning that, Eq. (21) could be also obtained based on the field theoretical/diagrammatic method. If needed, the proper normalization for the CGF, i.e., $ln Z(\xi)$, can be determined by the constraint $ln Z(0) = 0$.

III. PICTURE ON THE CONTOUR

The nonlinear effects on the GF are completely included in the $\hat{G}_{CC}$, for which we try to obtain the closed Dyson equations now. To this end, we need to introduce the picture on the contour. A key concept appearing in the picture on the contour is an evolution operator $U^S(\tau_2, \tau_1)$ defined on the contour $C$. Assuming that $\tau_2 \succ \tau_1$, namely $\tau_2$ succeeds $\tau_1$ on the contour, we will encounter three different situations depending on the relative position of the arguments $\tau_2$ and $\tau_1$:

$$U^S(\tau_2, \tau_1) = \begin{cases} U^S_{\tau_2, \tau_1} & (\tau_2 = t_2^+), \\ U^-_{\tau_2, \tau_1} U^S_{\tau_2, \tau_1} & (\tau_2 = t_2^+, \tau_1 = t_1^+), \\ U^-_{\tau_2, \tau_1} & (\tau_2 = t_2^-) \end{cases} \quad (22)$$

Where in the second situation we need not specify the relative magnitude of $t_2^+$ and $t_1^+$, since the time on the lower branch always succeeds the time on the upper branch along the contour. Also we should notice that the superscript $+$ or $-$ for the evolution operator simply tell us that the ordinary Schrödinger evolution operator is for the upper branch or the lower branch, respectively. Compactely, the evolution operator defined on the contour $U^S(\tau_2, \tau_1)$ when $\tau_2 \succ \tau_1$ could be written as

$$U^S(\tau_2, \tau_1) = T, \exp \left( -\frac{i}{\hbar} \int_{C[\tau_2, \tau_1]} H_{tot}(\tau) d\tau \right), \quad (23)$$

where $C[\tau_2, \tau_1]$ denotes the path along the contour $C$ from $\tau_2$ to $\tau_1$. In order to keep group properties of the evolution operator, the evolution operator $U^S(\tau_1, \tau_2)$ when $\tau_2 \succ \tau_1$ is defined to be

$$U^S(\tau_1, \tau_2) = U^S(\tau_2, \tau_1)^{-1} = U^S(\tau_2, \tau_1)^\dagger. \quad (24)$$
After this general discussion, we will use the same notation $U^S(\tau_2, \tau_1)$ to denote the Schrödinger-picture evolution operator on the contour without causing confusion, which is determined by the effective total Hamiltonian $H_{tot}^\tau(\tau) \equiv e^{ix_s H_L} H_{tot} e^{-ix_s H_L}$. Then the Heisenberg-picture operator on the contour such as $u_C^H(\tau_1)$ is defined as

$$u_C^H(\tau_1) = U^S(t_0^+, \tau_1) u_C U^S(\tau_1, t_0^+) .$$  (25)


By virtue of the Heisenberg-picture on the contour, we can rewrite the $\tilde{G}_{CC}$ from Eq. \ref{eq:30} as

$$\tilde{G}_{CC}(\tau_1, \tau_2) =$$

$$= -i \hbar \left\langle U^S(t_0^+, \tau_1) U^S(\tau_1, \tau_2) U^S(\tau_2, t_0^+) \right\rangle$$

$$\times e^{-\frac{1}{\hbar} \int_C \tau^d C \cdot dr' H_n'(\tau')} \left\langle U^S(t_0^+, \tau_2) U^S(\tau_2, \tau_1) U^S(\tau_1, \tau_1) \right\rangle$$

$$+ e^{-\frac{1}{\hbar} \int_C \tau^d C \cdot dr' H_n'(\tau')}.$$  (26)


Now we define the interaction picture on the contour. The modified total Hamiltonian can be split into two parts, i.e.,

$$H_{tot}^\tau(\tau) = H_0^\tau(\tau) + H_n.$$  (27)


The interaction-picture evolution operator is defined as

$$U_I(\tau_1, \tau_2) = U^S(t_0^+, \tau_1) U^S(\tau_1, \tau_2) U^S(\tau_2, t_0^+),$$  (28)


where $U^S_0$ is similar to $U^S$ but determined by $H_0^\tau(\tau)$. According to the interaction-picture evolution operator, we can define the interaction-picture operator such as $u_C(\tau_1)$ as

$$u_C^I(\tau_1) = U^S(t_0^+, \tau_1) u_C U^S_0(\tau_1, t_0^+).$$  (29)


The relation between the Heisenberg-picture operator and the interaction-picture one turns out to be

$$u_C^H(\tau_1) = U_I(\tau_1, \tau_1) u_C^I(\tau_1) U_I(\tau_1, t_0^+).$$  (30)


Further, the interaction-picture evolution operator can be expressed as

$$U_I(\tau_1, \tau_2) = T_\tau e^{-\frac{i}{\hbar} \int_C C_{[\tau_1, \tau_2]} H_n'(\tau) d\tau}$$  (31)


for $\tau_1$ succeeds $\tau_2$. Using the interaction picture on the contour, we can rewrite the $\tilde{G}_{CC}$ from Eq. \ref{eq:30} as

$$\tilde{G}_{CC}(\tau_1, \tau_2) =$$

$$= -i \hbar \left\langle U^S(t_0^+, \tau_1) T_\tau u_C^I(\tau_1) u_C^{\dagger I}(\tau_2) e^{-\frac{i}{\hbar} \int_C \tau^d C \cdot dr' H_n'(\tau')} \right\rangle$$

$$\times \frac{1}{Z_0},$$  (32)


which is shown below assuming that $\tau_1$ succeeds $\tau_2$ without loss of generality:

$$\tilde{G}_{CC}(\tau_1, \tau_2) =$$

$$= -i \hbar \left\langle U^S(t_0^+, \tau_1) U^S(\tau_1, \tau_2) U^S(\tau_2, t_0^+) \right\rangle$$

$$\times e^{-\frac{1}{\hbar} \int_C \tau^d C \cdot dr' H_n'(\tau')} \left\langle U^S(t_0^+, \tau_2) U^S(\tau_2, \tau_1) U^S(\tau_1, \tau_1) \right\rangle$$

$$+ e^{-\frac{1}{\hbar} \int_C \tau^d C \cdot dr' H_n'(\tau')}.$$  (33)


By introducing

$$Z_0 = \left\langle T_\tau e^{-\frac{i}{\hbar} \int_C \tau^d C \cdot dr'(\hat{u}_C^{\dagger I}(\tau) v^{LC}_C \hat{u}_C + v^{RC}_C \hat{u}_C)} \right\rangle,$$

which is the GF when $H_n = 0$, and defining $Z_n = Z/Z_0$, $G_{CC}$ in Eq. \ref{eq:32} is written as

$$G_{CC}(\tau_1, \tau_2) =$$

$$= -i \hbar \text{Tr} \left[ \rho_{ini} T_\tau u_C^I(\tau_1) u_C^{\dagger I}(\tau_2) e^{-\frac{i}{\hbar} \int_C \tau^d C \cdot dr' H_n'(\tau')} \right]$$

$$\times \frac{1}{Z_n},$$  (34)


where $\rho_{ini} = \rho_{ini} U^S(t_0^+, \tau_1) / Z_0$, $\text{Tr}(\rho_{ini}) = 1$. Notice that $\rho_{ini}$ and the interaction-picture operator on the contour, such as $u_C(\tau_1)$, after second quantization satisfy the sufficient conditions for the Wick theorem to be valid presented in the appendix A.


Observing the structure of Eq. \ref{eq:31} and realizing that the denominator $Z_n$ cancels the disconnected diagrams, we can obtain the Dyson equation for $G_{CC}$ as $G_{CC} = G_{CC}^0 + G_{CC}^0 \Sigma_n G_{CC}$, a symbolic notation of

$$\tilde{G}_{CC}(\tau_1, \tau_2) =$$

$$= G_{CC}^0(\tau_1, \tau_2) +$$

$$+ \int_C d\tau d\tau' \tilde{G}_{CC}^0(\tau_1, \tau) \Sigma_n(\tau, \tau') \tilde{G}_{CC}(\tau', \tau_2)$$  (35)


in terms of

$$G_{CC}^0(\tau_1, \tau_2) = -i \hbar \text{Tr} \left[ \rho_{ini} T_\tau u_C^I(\tau_1) u_C^{\dagger I}(\tau_2) \right]$$  (36)


and the nonlinear self-energy $\Sigma_n$ constructed by the bare propagator $G_{CC}^0$, whose vertices are solely due to the nonlinear Hamiltonian $H_n$.

Going to the interaction picture with respect to the free Hamiltonian $h = H_L + H_C + H_R$, $G_{CC}^0$ can be written as

$$\tilde{G}_{CC}(\tau_1, \tau_2) =$$

$$= -i \hbar \left\langle T_\tau \hat{u}_C(\tau_1) \hat{u}_C^T(\tau_2) \right\rangle$$

$$+ e^{-\frac{1}{\hbar} \int_C \tau^d C \cdot dr' H_n'(\tau')} V^{LC}_C \hat{u}_C(\tau) + V^{RC}_C \hat{u}_C(\tau) \right\rangle$$

$$\times \frac{1}{Z_0}$$  (37)
so that
\[ \tilde{G}^0_{CC} = g_C + g_C \left( \Sigma_L + \Sigma_R \right) \tilde{G}^0_{CC}, \]  
\hspace{1cm} (38)

where \( \Sigma_R (\tau_1, \tau_2) \) is the right-lead version of the ordinary contour-order self energy \( \Sigma_\nu = V^{\nu \mu} g_\nu V^{\mu \nu}, \nu = L, R, \) in which \( g_\alpha (\tau_1, \tau_2) \) is
\[ \langle T_a \bar{u}_{\alpha,j} (\tau_1) u_{\alpha,k} (\tau_2) \rangle \) for \( \alpha = L, C, \) \( R \) are the uncoupled contour-order Green’s functions.

Though Eq. (35) and Eq. (36) are enough for the calculation of \( G_{CC} \), for convenience one can introduce a counting-field independent auxiliary equation \( G_{CC}^0 = g_C + g_C (\Sigma_L + \Sigma_R) G_{CC}^0 \), and combine it with Eqs. (35) and (38) to obtain a closed Dyson equation for \( G_{CC} (\tau_1, \tau_2) \):
\[ \tilde{G}_{CC} = G^0_{CC} + G^0_{CC} \left( \Sigma + \Sigma_n \right) \tilde{G}_{CC}, \]  
\hspace{1cm} (39)

where the shifted self energy \( \Sigma_A \equiv \Sigma_s - \Sigma_L \), which first appears in Ref. 5, accounts for the distribution of heat in ballistic systems.

From now on, for notational simplicity, all the subscripts \( CC \) of the Green’s functions will be suppressed and the superscript 0 in both \( G_{CC}^0 \) and \( G_{CC}^0 \) will be re-expressed as a subscript.

Until now, the formalism for studying the distribution of heat transport across general nonlinear junctions has been completely established. In the case of steady state, one simply set \( t_0 \to -\infty \) and \( t_M \to +\infty \) simultaneously, and technically assume that real-time versions of \( \tilde{G} (\tau_1, \tau_2) \) are time-translationally invariant. Then going to the Fourier space, Eq. (21) for \( \partial \ln Z / \partial (i\xi) \) in steady state could be rewritten as
\[ \frac{\partial \ln Z}{\partial (i\xi)} (t_M - t_0) \int_{-\infty}^{\infty} d\omega \frac{\hbar \omega}{2\pi} \text{Tr} \left( \tilde{G}_{CC}^0 \Sigma_L^r e^{-i\hbar \omega \xi} \right) \]  
\hspace{1cm} (40)

after taking into account \( \tilde{G}^r [-\omega] = \tilde{G}^< [\omega]^T \) and \( \Sigma_L^r [-\omega] = \Sigma_L^> [\omega]^T \). In the Fourier space, due to Eq. (39) exact result for \( G [\omega] \) could be yielded as
\[ \tilde{G} [\omega] = \left( G_0 [\omega]^{-1} - \Sigma_A [\omega] - \Sigma_n [\omega] \right)^{-1} \]  
\hspace{1cm} (41)

when keeping in mind the convention that the contour-order Green’s function such as \( \tilde{G} (\tau_1, \tau_2) \) in frequency space is written as
\[ \tilde{G} [\omega] = \begin{bmatrix} \tilde{G}^t [\omega] & \tilde{G}^> [\omega] \\ -\tilde{G}^> [\omega] & -\tilde{G}^t [\omega] \end{bmatrix}. \]  
\hspace{1cm} (42)

### IV. APPLICATION TO SINGLE-SITE JUNCTION

Now we apply the general formalism developed above to study a single-site junction with a quartic nonlinear on-site pinning potential, that is, \( H_n = \frac{1}{4} \lambda u_{\xi,0} \) in Eq. (1). In this case, nonlinear contour-order self energy exact up to first order in nonlinear strength is
\[ \Sigma_n (\tau, \tau') = 3i\hbar \lambda G_0 (\tau, \tau') \delta (\tau, \tau'), \]  
where the generalized \( \delta \)-function \( \delta (\tau, \tau') \) is the counterpart of the ordinary Dirac delta function on the contour \( C \), see, for example, Ref. 13. Thus the corresponding frequency-space nonlinear self energy is
\[ \tilde{\Sigma}_n [\omega] = 3i\hbar \lambda \begin{bmatrix} \tilde{G}_0^t (0) & 0 \\ 0 & \tilde{G}_0^r (0) \end{bmatrix}. \]  
\hspace{1cm} (43)

Consequently, exact up to first order in nonlinear strength the CGF for the molecular junction could be given as
\[ \frac{1}{(t_M - t_0)} \frac{\partial \ln Z (\xi)}{\partial (i\xi)} = -\int_{-\infty}^{\infty} d\omega \frac{\partial \ln D [\omega]}{\partial (i\xi)} - 3i\hbar \lambda \times \begin{bmatrix} \tilde{G}_0^t (0) G_0^r [\omega] - \tilde{G}_0^r (0) G_0^t [\omega] \end{bmatrix} \frac{\partial}{\partial (i\xi)} \frac{1}{D [\omega]} \]  
\hspace{1cm} (44)

with
\[ D [\omega] \equiv \det \left[ I - G_0 [\omega] \Sigma_A [\omega] \right] = 1 - T [\omega] \left[ (e^{i\hbar \omega} - 1) f_L (1 + f_R) + (e^{-i\hbar \omega} - 1) f_R (1 + f_L) \right] \]  
\hspace{1cm} (45)

and \( \tilde{G}_0^t (0) = \int_{-\infty}^{\infty} d\omega \frac{\partial \Sigma_\xi}{\partial (i\xi)} ) D [\omega] \right), \) where \( T [\omega] = \text{Tr} (G_0^t \Gamma_R G_0^r \Gamma_L) \) is the transmission coefficient in the ballistic system, and \( f_{(L,R)} = \left\{ \exp (\beta_{(L,R)} \hbar \omega) - 1 \right\}^{-1} \) is the Bose-Einstein distribution function for phonons. Here \( G_0^t = G_0 - G_0^< \) and \( G_0^r = G_0^< - G_0^t \) are retarded and advanced Green’s functions, respectively. Also \( \Gamma_{(L,R)} = i (\Sigma_{(L,R)}^r - \Sigma_{(L,R)}^s ) \), related to the spectral density of the baths, are expressed by retarded and advanced self energies similarly defined as Green’s functions. Eq. (44) satisfies Gallavotti-Cohen symmetry for the derivatives, since \( D [\omega] \) remains invariant under the transformation \( \xi \to -\xi + i (\beta_R - \beta_L) \) while \( \partial D [\omega] / \partial (i\xi) \) changes sign.

One could easily use this CGF in Eq. (44) to evaluate cumulants. The steady current out of the left lead is closely related to the first cumulant so that
\[ I^{ss}_L = \frac{d}{dt_M} \left( \frac{\partial \ln Z (\xi)}{\partial (i\xi)} \right) \bigg|_{\xi = 0} \]  
\hspace{1cm} (46)

where \( \Lambda [\omega] \equiv 3i\hbar \lambda G_0^t (0) (G_0^r [\omega] + G_0^r [\omega]) \) is the first-order nonlinear correction to the transmission coefficient. The fluctuation for steady-state heat transfer in the molecular junction is obtained by taking the second derivative with respect to \( i\xi \), and then setting \( \xi = 0 \):
\[ \langle (Q^2) \rangle / (t_M - t_0) = \int_{-\infty}^{\infty} d\omega \left\{ (\hbar \omega)^2 T^2 [\omega] (1 + 2 \Lambda [\omega]) (f_L - f_R)^2 + 3i\hbar \lambda^2 \left[ G_0^t [\omega] \delta \tilde{G}_0^r - G_0^r [\omega] \delta \tilde{G}_0^t \right] T [\omega] (f_L - f_R) \right\} + \left( \hbar \omega \right)^2 T [\omega] (1 + \Lambda [\omega]) (f_L + f_R + 2f_L f_R), \]  
\hspace{1cm} (47)
are considered and the two off-diagonals. And only the nearest interaction using a self-consistent procedure though the expressions are messy.

As the nonlinear contour-order self energy is taken that the nonlinear contour-order self energy is not Gaussian. In this numerical illustration, the nonzero implies that the distribution for transferred energy is not Gaussian. As shown, the effect of nonlinearity is to reduce the current as well as higher order fluctuations, and the fact predictions for the FCS.

As shown, the effect of nonlinearity is to reduce the current in the case of a extremely accurate results for the current in the case of a nonlinear quantum junctions. The CGF for the heat transfer in both transient and steady-state regimes is studied on an equal footing and useful formulas for the CGF are obtained. A new feature of this formalism is that counting-field dependent full Green’s function $G_{CC}$ can be expressed solely through the nonlinear term $H^L_n(\tau)$ with the help of an interaction-picture transformation defined on a contour. Although we focus on the distribution of heat transfer in pure nonlinear phononic systems, there is no doubt that this general formalism can be readily employed to handle any other nonlinear systems, such as electron-phonon interaction and Joule heating problems. Up to the first order in the nonlinear strength for the single-site quartic model, the CGF for steady-state heat transfer is obtained and explicit results for the steady current and fluctuation of steady-state heat transfer are given. A self-consistent procedure, which works well for strong nonlinearity, is also introduced to numerically check our general formalism.

Higher-order cumulants can be also systematically given by corresponding higher-order derivatives, although the expressions are messy.

In Fig 2 we give a numerical illustration to the first three cumulants for heat transfer in this molecular junction using a self-consistent procedure, which means that the nonlinear contour-order self energy is taken as $\Sigma_n(\tau, \tau') = 3i\hbar\lambda G(\tau, \tau') \delta(\tau, \tau')$. Very recently, it is shown that such self-consistent calculation gives extremely accurate results for the current in the case of a single site model as compared with master equation approach, thus we believe that it should leads to excellent predictions for the FCS.

As shown, the effect of nonlinearity is to reduce the current as well as higher order fluctuations, and the fact that third and higher order cumulants are small but nonzero implies that the distribution for transferred energy is not Gaussian. In this numerical illustration, the Rubin baths are used, that is, $K_a, \alpha = L, R$ in Eq. 11 are both the semi-infinite tridiagonal spring constant matrix consisting of $2k + k_0$ along the diagonal and $-k$ along the two off-diagonals. And only the nearest interaction $V_{L,0}^L$ and $V_{0,R}^R$ between the molecular and the two baths are considered and $H_C = $\frac{1}{2}p^2_{C,0}+$\frac{1}{2}K_Cu_{C,0}^2. As expected, for weak nonlinearity the first-order perturbation results, presented as dotted lines, are consistent with the corresponding self-consistent ones.

\[ \delta G_0^{\tau,\bar{\tau}}(0) \equiv \frac{\partial G_0^{\tau,\bar{\tau}}(0)}{\partial \xi} \bigg|_{\xi=0} = -i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \hbar \omega T[\omega] (f_L - f_R) G_0^{\tau,\bar{\tau}}[\omega]. \]

(48)

V. SUMMARY

A formally rigorous formalism dealing with cumulants of heat transfer across nonlinear quantum junctions is established based on field theoretical and NEGF methods. The CGF for the heat transfer in both transient and steady-state regimes is studied on an equal footing and useful formulas for the CGF are obtained. A new feature of this formalism is that counting-field dependent full Green’s function $G_{CC}$ can be expressed solely through the nonlinear term $H^L_n(\tau)$ with the help of an interaction-picture transformation defined on a contour. Although we focus on the distribution of heat transfer in pure nonlinear phononic systems, there is no doubt that this general formalism can be readily employed to handle any other nonlinear systems, such as electron-phonon interaction and Joule heating problems. Up to the first order in the nonlinear strength for the single-site quartic model, the CGF for steady-state heat transfer is obtained and explicit results for the steady current and fluctuation of steady-state heat transfer are given. A self-consistent procedure, which works well for strong nonlinearity, is also introduced to numerically check our general formalism.

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Appendix A: The Wick Theorem (Phonons)

In this appendix, we give sufficient conditions for the Wick theorem to be valid which covers most of the situation we encounter. The discussion is limited to the case of bosonic operators which is the main interest in this paper. We mainly extend Gaudin’s approach. For an alternative proof, one can resort ro the Ref. 23.

First we explain what the Wick theorem is. The Wick theorem says that the average value of a product of creation and annihilation operators is equal to the sum of all complete systems of pairings, mathematically which can be stated as

\[
\begin{align*}
\text{Tr} \{ \rho^{i_1} \beta_1 \beta_2 \cdots \beta_s \} &= \text{Tr} \{ \rho^{i_1} \beta_1 \beta_2 \} \text{Tr} \{ \rho^{i_2} \beta_3 \cdots \beta_s \} \\
&+ \text{Tr} \{ \rho^{i_1} \beta_1 \beta_3 \} \text{Tr} \{ \rho^{i_2} \beta_4 \cdots \beta_s \} \\
&\quad \cdots \\
&+ \text{Tr} \{ \rho^{i_1} \beta_1 \beta_s \} \text{Tr} \{ \rho^{i_2} \beta_2 \cdots \beta_{s-1} \} \\
\end{align*}
\]
Now we explore the sufficient conditions for the Wick theorem to be justified, which simply means that Eq. (A1) is valid. Suppose the system’s degrees of freedom is $f$, and we define

$$\alpha = \left( \begin{array}{c} a \\ a^{\dagger} \end{array} \right), \quad \alpha_i = a_i, \quad \alpha_i^{\dagger} = a_i^{\dagger}, \quad i = 1, 2, \ldots, f,$$

where $a_i$ and $a_i^{\dagger}$ are annihilation and creation operators respectively.

Assume

$$\alpha_i \rho^{ini} = \sum_{k=1}^{2f} h_{ik} \rho^{ini} \alpha_k,$$  \hspace{1cm} (A3)

where $h_{ik}$ are c-numbers. We prove the Wick theorem for $\text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\}$, which is shown below:

$$\text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\} = \text{Tr} \left\{ \rho^{ini} [\alpha_i, \alpha_i] \cdots \alpha_i \right\} + \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\} + \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\} + \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\}$$

$$= \cdots$$

$$= \sum_{j=2}^{s} [\alpha_i, \alpha_j] \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\} + \text{Tr} \left\{ \alpha_i \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\}$$

$$= \sum_{j=2}^{s} [\alpha_i, \alpha_j] \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\} + \sum_{k=1}^{2f} h_{ik} \text{Tr} \left\{ \rho^{ini} \alpha_k \alpha_i \alpha_i \cdots \alpha_i \right\}$$

where the circle over the operator means that this operator is omitted. Then

$$= \sum_{k=1}^{2f} (1 - h)_{i,k} \text{Tr} \left\{ \rho^{ini} \alpha_k \alpha_i \alpha_i \cdots \alpha_i \right\}$$

$$= \sum_{j=2}^{s} [\alpha_i, \alpha_j] \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\} + \sum_{k=1}^{2f} h_{ik} \text{Tr} \left\{ \rho^{ini} \alpha_k \alpha_i \alpha_i \cdots \alpha_i \right\}$$

$$= \sum_{j=2}^{s} \left( \sum_{k=1}^{2f} (1 - h)_{i,k} \right) \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\} \quad \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\}$$

(A5)

After considering the special case

$$\text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \right\} = \sum_{k=1}^{2f} (1 - h)_{i,k} \alpha_k, \quad \alpha_i$$

we obtain from Eq. (A5)

$$\text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\}$$

$$= \sum_{j=2}^{s} \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \right\} \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\}$$

Assume

$$\beta_j = \sum_{i=1}^{2f} g_{ji} \alpha_i$$  \hspace{1cm} (A7)

where $g_{ji}$ are c-numbers. Then

$$\text{Tr} \left\{ \rho^{ini} \beta_1 \beta_2 \cdots \beta_s \right\}$$

$$= \sum_{i_1} \sum_{i_2} \cdots \sum_{i_s} g_{i_1} g_{i_2} g_{i_s} \alpha_i \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\}$$

$$= \sum_{i_1} \sum_{i_2} \cdots \sum_{i_s} g_{i_1} g_{i_2} g_{i_s} \sum_{j=2}^{s} \text{Tr} \left\{ \rho^{ini} \alpha_i \alpha_i \cdots \alpha_i \right\}$$

$$= \sum_{i_1} \sum_{i_2} \cdots \sum_{i_s} g_{i_1} g_{i_2} g_{i_s} \sum_{j=2}^{s} \text{Tr} \left\{ \rho^{ini} \beta_1 \beta_2 \cdots \beta_s \right\}$$

which is just the Eq. (A1).

In summary, the sufficient conditions for the Wick theorem Eq. (A1) to be valid are Eq. (A3) and Eq. (A7) and implicitly $\text{Tr} \left\{ \rho^{ini} \right\} = 1$.

In the following, we try to figure out the form of initial density matrix $\rho^{ini}$ satisfying Eq. (A3), which turns out to be

$$\rho^{ini} = e^{-\alpha^T A \alpha}$$  \hspace{1cm} (A8)

with $A$ to be a general square matrix. We neglect the normalization constant for $\text{Tr} \left\{ \rho^{ini} \right\} = 1$ here. To this end, we split the $A$ to be a symmetrical part and an anti-symmetrical part, that is

$$A = \frac{1}{2} (A + A^T) + \frac{1}{2} (A - A^T)$$

$$\equiv A^s + A^a.$$  \hspace{1cm} (A9)

Let us define

$$f_i(t) = e^{(\alpha^{T} A^{s}) \alpha \cdot A^{T} \alpha} e^{-\alpha^{T} A^{a} \alpha}$$

$$= e^{\frac{1}{2} \alpha^{T} A^{s} \alpha} e^{-\frac{1}{2} \alpha^{T} A^{a} \alpha}.$$  \hspace{1cm} (A10)

In obtaining the second equality, notice that $\alpha^{T} A^{a} \alpha$ is a c-number due to $[\alpha^{T}, \alpha] = \left( \begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right)$ and $A^{a \cdot T} = -A^{a}$. Thus

$$\frac{df_i(t)}{dt} = \frac{d}{dt} e^{\frac{1}{2} \alpha^{T} A^{s} \alpha} \left[ \begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right] e^{-\frac{1}{2} \alpha^{T} A^{a} \alpha}$$

$$= -\sum_{j} (\sigma A^{s})_{ij} f_j(t).$$
where $\sigma \equiv \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. So $f_i(t) = \sum_j (e^{-t\sigma A^*})_{ij} \alpha_j$ and 

$$f_i(1) = e^{\alpha^T A \alpha} e^{-\sigma A^*} = \sum_j (e^{-\sigma A^*})_{ij} \alpha_j \text{ or equivalently}$$

$$\alpha_i e^{-\sigma A^*} = \sum_j (e^{-\sigma A^*})_{ij} e^{-\sigma A^*} \alpha_j.$$  \hspace{1cm} (A11)

More generally, the multiplication of finite number of the form of Eq. (A8) still satisfies Eq. (A3), such as

$$\rho_{ini} = e^{-\sigma A^*} e^{-\sigma B^*},$$  \hspace{1cm} (A12)

which is shown below:

$$\begin{align*}
\alpha_i \rho_{ini} & = \alpha_i e^{-\sigma A^*} e^{-\sigma B^*} \\
& = \sum_j (e^{-\sigma A^*})_{ij} \alpha_j e^{-\sigma B^*} \\
& = \sum_j (e^{-\sigma A^*})_{ij} \sum_k (e^{-\sigma B^*})_{jk} \alpha_k \\
& = \sum_j \sum_k (e^{-\sigma A^*} e^{-\sigma B^*})_{jk} \rho_{ini} \alpha_k.
\end{align*}$$

Due to the sufficient conditions presented in this appendix, the Wick theorem used in this paper for the Feynman-diagrammatic analysis is justified. For example, for the case of the interaction picture on the contour, initial density matrix $\rho_{ini} = \rho_{ini} U_0 S(t_0, t_0^+) / Z_0 = \Pi_{i=C,R} e^{-\beta \alpha H_{\alpha}} e^{-\beta \alpha H_{\alpha}^*} e^{-\beta \alpha H_{\alpha}} e^{-\beta \alpha H_{\alpha}^*} / Z_0$ is the multiplication of finite number of the form of Eq. (A8) and $\text{Tr}(\rho_{ini}) = 1$. In addition, interaction-picture operator on the contour such as $u_C^{\tau_1}$ in the Eq. (29) can be expressed as the linear transformation of $\alpha$ defined in the Eq. (A2) according to the similar steps for the calculation of $f_i(t)$.

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