

## Asymptotic nonequilibrium steady-state operators

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We present a method for the calculation of asymptotic operators for nonequilibrium steady-state quantum systems. The asymptotic steady-state operator is obtained by averaging the corresponding operator in Heisenberg representation over infinitely long time. Several examples are considered to demonstrate the utility of our method. The results obtained within our approach are compared to those obtained within the Schwinger-Keldysh nonequilibrium Green's functions.

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### I. INTRODUCTION

If we place a finite quantum or classical system into the contact with several different macroscopic thermal baths or particle reservoirs and wait for some time, which is much longer than typical relaxation time of the system, the system will reach a nonequilibrium time-independent steady state. Like an equilibrium represents stationary state of a closed system, nonequilibrium steady state is the time-invariant state of an open system. The steady state is established by the delicate balance between irreversible processes and the driving forces produced by the reservoirs. Nonequilibrium steady-state systems are ubiquitous and their theoretical description has been a challenging fundamental problem for many years [1]. They are also of significant practical interest for various nanotechnological and biological applications. Examples of steady-state nonequilibrium systems include quantum contacts [2], molecular motors [3–5], molecular junctions and nanowires [6], low-dimensional heat conducting quantum and classical systems [7–9]. Recent experiments on these systems have revealed a wealth of interesting new nonequilibrium phenomena such as nondiffusive heat transfer, negative differential resistance, stochastic switching and hysteresis of electric current, and direct harnessing of thermal fluctuations [10–12].

The understanding of the fundamental mechanisms as well as the interpretation of these experimental observations require the development of new theoretical methods for the description of nonequilibrium quantum systems. Many theoretical approaches have been developed to deal with nonequilibrium steady-state systems, such as Keldysh-Schwinger Green's functions [13–19], scattering theory based approaches [20,21], different variations of Zubarev method of nonequilibrium statistical operator [22–26], and constrained current methods [27–34]. Most of the methods are based on the calculations of nonequilibrium averages of the operators of interest. Although average values, such as correlation functions, densities, and currents, are very important and directly related to the measurable quantities, it is very useful to have explicit expressions for asymptotic operators. Here we propose a general theoretical approach which directly defines and computes asymptotic nonequilibrium steady-state operators.

### II. ASYMPTOTIC OPERATORS

Let us consider a quantum mechanical observable which corresponds to a Hermitian operator  $A$ . We assume the existence of a unique steady state for our system. It implies the existence of the limit  $t \rightarrow +\infty$  for observable quantities. It means that the asymptotic value of the operator  $A$  in Heisenberg representation is uniquely defined and can be computed as

$$\bar{A} = \lim_{t \rightarrow +\infty} e^{iHt} A e^{-iHt}, \quad (1)$$

where the Hamiltonian  $H$  includes the system Hamiltonian  $H_S$ , the bath Hamiltonian  $H_B$ , and the system-bath interaction  $H_{SB}$ ,

$$H = H_S + H_B + H_{SB}. \quad (2)$$

We denote all thermal baths and particle reservoirs collectively by  $B$ . The Hamiltonian  $H$  is assumed to be time independent. We begin calculation of limit (1) by the use of the following self-evident identity, which is valid for any time-dependent operator  $O(t)$ :

$$O(t) = O(0) + \int_0^t dt' \frac{dO(t')}{dt'}. \quad (3)$$

Applying this identity to Eq. (1), we get

$$\bar{A} = A + \int_0^{+\infty} dt \frac{d}{dt} e^{iHt} A e^{-iHt}. \quad (4)$$

The existence of the unique steady state implies the convergence of the integral in Eq. (4), therefore we can introduce the infinitesimal factor  $\eta$ ,

$$\bar{A} = A + \lim_{\eta \rightarrow +0} \int_0^{+\infty} dt e^{-\eta t} \frac{d}{dt} e^{iHt} A e^{-iHt}. \quad (5)$$

This regularization of the integral is equivalent to the assumption that there exist some dissipation mechanisms in our system which we do not specify explicitly but which are efficient enough to lead to the unique steady state. The integration by parts of Eq. (5) yields

$$\bar{A} = \lim_{\eta \rightarrow +0} \eta \int_0^{+\infty} dt e^{-\eta t} e^{iHt} A e^{-iHt}. \quad (6)$$

This expression for the nonequilibrium asymptotic operator is interesting physically since the integral is multiplied by the infinitesimal number  $\eta$ . Therefore, only singular terms proportional to  $1/\eta$  give nonvanishing contribution from the integral to  $\bar{A}$ . Using Abel's theorem [22]

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt f(t) = \lim_{\eta \rightarrow +0} \eta \int_0^{+\infty} dt e^{-\eta t} f(t), \quad (7)$$

we see that Eq. (6) yields the part of the operator which is conserved after averaging over the infinitely long time. Equation (6) is the definition of the asymptotic nonequilibrium steady-state operator. It will be the starting point for our calculations. Definition (6) has been initially introduced by Kubo in his work on irreversible thermodynamics (so-called time invariant part of the operator) [35] and Zubarev during his development of nonequilibrium statistical operator method [22]. It was used by Grandy [36] and Hershfield [23] in their formulations of steady-state nonequilibrium statistical mechanics. Recently, Tasaki and Takahashi also employed asymptotic operators (6) to continue the advances of Zubarev method in application to transport in quantum junctions [24]. The time invariant current defined via Eq. (7) was used by Bokes *et al.* as a term constrained by the Lagrange multiplier in their development of variational transport theory [31]. In this paper, we develop a general practical method for computing asymptotic nonequilibrium operators.

To carry out our program it is convenient to represent the Hamiltonian and operator  $A$  in the second quantization form. We assume that the Hamiltonian and the operator  $A$  are quadratic in creation and annihilation operators,

$$H = \sum_{ij} H_{ij} a_i^\dagger a_j, \quad (8)$$

$$A = \sum_{ij} A_{ij} a_i^\dagger a_j. \quad (9)$$

The creation  $a^\dagger$  and annihilation  $a$  operators obey the standard commutation (for bosons) and anticommutation (for fermions) relations. The methods developed in this paper are applicable to both, Fermi and Bose, systems. With the use of the following operator identity

$$e^{iHt} A e^{-iHt} = \sum_{ij} (e^{i\mathbf{H}t} \mathbf{A} e^{-i\mathbf{H}t})_{ij} a_i^\dagger a_j, \quad (10)$$

where  $\mathbf{H}$  and  $\mathbf{A}$  are matrices with matrix elements  $H_{ij}$  [Eq. (8)] and  $A_{ij}$  [Eq. (9)], the expression for asymptotic operator (6) becomes

$$\bar{A} = \lim_{\eta \rightarrow +0} 2\eta \int_0^{+\infty} dt \sum_{ij} [e^{-i(\omega - \mathbf{H} - i\eta)t} \mathbf{A} e^{i(\omega - \mathbf{H} + i\eta)t}]_{ij} a_i^\dagger a_j. \quad (11)$$

This integral can further be transformed by inserting the delta function  $\delta(t-t') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{i\omega(t-t')}$  and integrating over  $t$  and  $t'$ ,

$$\bar{A} = \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{ij} [\mathbf{G}^*(\omega) \mathbf{A} \mathbf{G}(\omega)]_{ij} a_i^\dagger a_j, \quad (12)$$

where  $\mathbf{G}(\omega) = [\omega - \mathbf{H} + i\eta]^{-1}$  is the total Green's function. This is the general formula for the asymptotic steady-state nonequilibrium operator, which is applicable to any systems with quadratic Hamiltonians.

The indexes  $i$  and  $j$  run over the system  $s$  and bath  $b$  single-particle states in Eqs. (8) and (9). Therefore the total Hamiltonian matrix can be written in the following form:

$$\mathbf{H} = \begin{bmatrix} \mathbf{H}_B & \mathbf{H}_{SB} \\ \mathbf{H}_{BS} & \mathbf{H}_S \end{bmatrix}, \quad (13)$$

where  $\mathbf{H}_S$  is the matrix of the system Hamiltonian,  $\mathbf{H}_B$  is the matrix of the bath Hamiltonians, and  $\mathbf{H}_{SB}$  is the matrix of the system-bath interaction. Likewise, we can partition the matrix  $\mathbf{A}$

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_B & \mathbf{A}_{SB} \\ \mathbf{A}_{BS} & \mathbf{A}_S \end{bmatrix}, \quad (14)$$

and the Green's function

$$\mathbf{G}(\omega) = [\omega - \mathbf{H} + i\eta]^{-1} = \begin{bmatrix} \mathbf{G}_B(\omega) & \mathbf{G}_{SB}(\omega) \\ \mathbf{G}_{BS}(\omega) & \mathbf{G}_S(\omega) \end{bmatrix}. \quad (15)$$

The block matrix elements of the Green's function, which can be computed by the Frobenius formula [37], have the following form:

$$\mathbf{G}_S(\omega) = [(\omega + i\eta)\mathbf{I}_S - \mathbf{H}_S - \Sigma_B(\omega)]^{-1}, \quad (16)$$

$$\mathbf{G}_{SB}(\omega) = -\mathbf{G}_S(\omega) \mathbf{H}_{SB} \mathbf{g}_B(\omega), \quad (17)$$

$$\mathbf{G}_B(\omega) = \mathbf{g}_B(\omega) + \mathbf{g}_B(\omega) \mathbf{H}_{BS} \mathbf{G}_S(\omega) \mathbf{H}_{SB} \mathbf{g}_B(\omega). \quad (18)$$

Here we introduced the Green's functions for the baths

$$\mathbf{g}_B(\omega) = [(\omega + i\eta)\mathbf{I}_B - \mathbf{H}_B]^{-1}, \quad (19)$$

and the corresponding self-energies

$$\Sigma_B(\omega) = \mathbf{H}_{SB} \mathbf{g}_B(\omega) \mathbf{H}_{BS}. \quad (20)$$

Note that the baths are assumed to be macroscopically large, so they have continuum energy levels. Therefore, when  $\eta$  tends to zero, the Green's function of the baths  $\mathbf{g}_B(\omega)$  has a pole on the real energy axis. The Green's function  $\mathbf{G}_S(\omega)$  is not singular in general, although special care should be taken to deal with the bound states [38].

We consider two practically important choices of the operator  $A$  at time  $t=0$ . First,  $A$  is defined in the system space only

$$\begin{aligned} \bar{A}_S &= \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{ij} [\mathbf{G}^*(\omega) \mathbf{A}_S \mathbf{G}(\omega)]_{ij} a_i^\dagger a_j \\ &= \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{bb'} [\mathbf{G}_{BS}^*(\omega) \mathbf{A}_S \mathbf{G}_{SB}(\omega)]_{bb'} a_b^\dagger a_{b'}. \end{aligned} \quad (21)$$

Second,  $A$  mixes the Fock spaces of the system and baths,

$$\begin{aligned}
\bar{A}_{SB} &= \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{ij} [\mathbf{G}^*(\omega) \mathbf{A}_{SB} \mathbf{G}(\omega)]_{ij} a_i^\dagger a_j \\
&= \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{bs'} [\mathbf{G}_{BS}^*(\omega) \mathbf{A}_{SB} \mathbf{G}_{BS}(\omega)]_{bs'} a_b^\dagger a_{s'} \\
&\quad + \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{bb'} [\mathbf{G}_S^*(\omega) \mathbf{A}_{SB} \mathbf{G}_B(\omega)]_{bb'} a_s^\dagger a_{b'} \\
&\quad + \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{bb'} [\mathbf{G}_{BS}^*(\omega) \mathbf{A}_{SB} \mathbf{G}_B(\omega)]_{bb'} a_b^\dagger a_{b'}.
\end{aligned} \tag{22}$$

Here the indexes  $b$  and  $s$  refer to the single-particle states of the baths and the system, respectively. We have retained only those terms under the integrals which are  $\sim 1/((\omega - \varepsilon_b)^2 + \eta^2)$ . Less singular terms give zero contributions upon the integration and multiplication by  $\eta$ . With an eye on the averaging of asymptotic operators over the initial equilibrium density matrix, which is the product of equilibrium system and bath density matrices, the expression for  $\bar{A}_{SB}$  can further be simplified,

$$\bar{A}_{SB} \approx \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{bb'} [\mathbf{G}_{BS}^*(\omega) \mathbf{A}_{SB} \mathbf{G}_B(\omega)]_{bb'} a_b^\dagger a_{b'}. \tag{23}$$

### III. COMPARISONS WITH NONEQUILIBRIUM GREEN'S FUNCTION METHOD

In order to compare our approach with existing theoretical methods, we consider a finite quantum system with discrete energy levels and noninteracting fermions (quantum dot, atom, atomic cluster, molecule, or atomic Fermi gas in a trap) which is attached to two macroscopic reservoirs. Such kind of systems can be described by the tunneling Hamiltonian [39], which has the form

$$H = H_0 + T. \tag{24}$$

Here  $H_0$  is the Hamiltonian of the isolated reservoirs and the system,

$$H_0 = \sum_{b=l,r} \varepsilon_b a_b^\dagger a_b + \sum_s \varepsilon_s a_s^\dagger a_s. \tag{25}$$

The indexes  $l$  and  $r$  refer to the continuum single-particle states in the left and right reservoirs, respectively, and  $s$  refers to the discrete single-particle states of the system. The tunneling interaction couples the reservoirs to the system,

$$T = \sum_{b=l,r} \sum_s t_{bs} (a_b^\dagger a_s + a_s^\dagger a_b). \tag{26}$$

We deal with fermions in this example; therefore the creation  $a^\dagger$  and annihilation  $a$  operators obey the standard anticommutation relations. We assume that the system is isolated from the reservoirs at  $t < 0$ . Therefore the system is in equilibrium at  $t < 0$  and it is described by the density matrix

$$\rho_0 = \frac{1}{\text{Tr}[e^{-\beta(H_0 - \mu_L N_L - \mu_R N_R)}]} e^{-\beta(H_0 - \mu_L N_L - \mu_R N_R)}. \tag{27}$$

Here  $N_L$  ( $N_R$ ) are the number of particles operators for the left (right) reservoirs and  $\mu_L$  ( $\mu_R$ ) are the corresponding chemical potentials. Then at  $t=0$  we turn on the reservoir-system coupling  $T$ .

First, we compute the asymptotic single-particle density matrix for the system

$$\bar{n}_{ss'} = \lim_{t \rightarrow +\infty} e^{iHt} a_s^\dagger a_s e^{-iHt}. \tag{28}$$

The use of formula (21) gives

$$\bar{n}_{ss'} = \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{bb'} [\mathbf{G}_{BS}^*(\omega)]_{bs'} [\mathbf{G}_{SB}(\omega)]_{sb'} a_b^\dagger a_{b'}, \tag{29}$$

where  $b$  and  $b'$  run over all single-particle states of the left and right reservoirs. Substituting the explicit expressions for Green's functions (17), we get

$$\begin{aligned}
\bar{n}_{ss'} &= \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{bb'} [\mathbf{g}_B^*(\omega) \mathbf{H}_{BS} \mathbf{G}_S^*(\omega)]_{bs'} \\
&\quad \times [\mathbf{G}_S(\omega) \mathbf{H}_{SB} \mathbf{g}_B(\omega)]_{sb'} a_b^\dagger a_{b'}.
\end{aligned} \tag{30}$$

Averaging asymptotic operator (30) over the equilibrium initial density matrix, we obtain the following expression for the steady-state single-particle density matrix:

$$\begin{aligned}
\text{Tr}\{\rho_0 \bar{n}_{ss'}\} &= \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega \sum_{B=L,R} f(\omega - \mu_B) \{ \mathbf{G}_S(\omega) [\Sigma_B^*(\omega) \\
&\quad - \Sigma_B(\omega)] \mathbf{G}_S^*(\omega) \}_{ss'},
\end{aligned} \tag{31}$$

$f(\omega)$  being the Fermi-Dirac occupation numbers. The same equation is obtained by the method of nonequilibrium Green's functions through the lesser Green's function  $G^<$  [40].

Now we calculate the asymptotic current operator. The current operator is defined by the continuity equation

$$J = \frac{d}{dt} N_L = i[H, N_L] = i \sum_{ls} t_{ls} (a_l^\dagger a_s - a_s^\dagger a_l), \tag{32}$$

$N_L$  being the particle number operator for the left reservoir [41].

We define the asymptotic value of the current operator as

$$\bar{J} = \lim_{t \rightarrow +\infty} e^{iHt} J e^{-iHt}. \tag{33}$$

The use of Eq. (23) leads to

$$\bar{J} = \lim_{\eta \rightarrow +0} \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\omega \sum_{bb'} [\mathbf{G}_{BS}^*(\omega) \mathbf{J} \mathbf{G}_B(\omega)]_{bb'} a_b^\dagger a_{b'}, \tag{34}$$

where the matrix, which represents the current, is

$$\mathbf{J} = \begin{bmatrix} 0 & \mathbf{T}_{LN} & 0 \\ -\mathbf{T}_{NL} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (35)$$

Substituting the expressions for  $G_B(\omega)$  and  $G_{SB}(\omega)$  into Eq. (34), and averaging over equilibrium initial density matrix (27) results into the following expression for the steady-state current:

$$\bar{J} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega [n(\omega - \mu_L) - n(\omega - \mu_R)] \text{Tr} \{ [\Sigma_L(\omega) - \Sigma_L^*(\omega)] \mathbf{G}_{NN}^*(\omega) [\Sigma_R(\omega) - \Sigma_R^*(\omega)] \mathbf{G}_{NN}(\omega) \}. \quad (36)$$

This is the so-called Landauer formula, which is typically obtained via the formalism of nonequilibrium Green's functions [14,16].

#### IV. CONCLUSIONS

We define a nonequilibrium steady state as an asymptotic state of a finite quantum system which is connected to sev-

eral different macroscopic thermal baths or particle reservoirs. We present a general method to compute asymptotic steady-state operators for such systems. The asymptotic operators can be computed exactly for the systems with quadratic Hamiltonians. For the tunneling Hamiltonian we recover the standard results obtained by the nonequilibrium Green's function method, thereby demonstrating equivalence of the two approaches. For example, we derive Landauer formula by a direct calculation of the asymptotic steady-state nonequilibrium current operator.

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