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Nonequilibrium density matrix for quantum transport: Hershfield approach as a McLennan-Zubarev form of the statistical operator

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In this paper, we formally demonstrate that the nonequilibrium density matrix developed by Hershfield for the steady state has the form of a McLennan-Zubarev nonequilibrium ensemble. The correction term in this pseudoequilibrium Gibbs-like ensemble is directly related to the entropy production in the quantum open system. The fact that both methods state that a nonequilibrium steady state can be mapped onto a pseudoequilibrium, permits us to develop nonequilibrium quantities from formal expressions equivalent to the equilibrium case. We provide an example: the derivation of a nonequilibrium distribution function for the electron population in a scattering region in the context of quantum transport.

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I. INTRODUCTION

The understanding of irreversible phenomena including nonequilibrium (NE) steady state is a long-standing problem of statistical mechanics. The task of NE statistical mechanics is to understand and describe how a system, initially at thermodynamical equilibrium, will try to respond and adjust to an external stimulus by evolving towards a new macroscopic state that is compatible with this external constraint. This involves the understanding of the transient and steady-state regimes, as well as the derivation of the corresponding kinetic and balance equations of NE thermodynamics.

Since Gibbs formulation of the method of statistical ensembles for equilibrium many-body systems, it has been expected that some formal advantages may be given by an approach to NE processes in which the Gibbs ensembles play a prominent role [1]. The construction of such Gibbs-like ensembles for the NE steady state has been explored by many authors.

On one hand, early attempts have been performed by McLennan [1] for classical systems and by Zubarev [2–6] for both classic and quantum systems. In simple terms, it is found that the steady-state ensembles can be expressed in terms of the external forces which maintain the deviation from equilibrium. In Zubarev's formulation of NE steady state, the Gibbsian statistical mechanics method is extended to include steady-state boundary conditions in the density matrix leading to his so-called NE statistical operator (SO) method (NESOM). Such method consists in constructing a time-independent density matrix (statistical operator) by solving an equation of motion with the proper NE boundary conditions.

A rigorous analysis of the existence and stability of such NE steady state, i.e., its independence of the way the division into subsystems and reservoirs is performed and its stability against local perturbations, have been performed using C^* algebraic methods in Refs. [7–10]. Furthermore, rigorous definition of MacLennan-Zubarev ensembles have been given in Refs. [8,11].

There is also extensive literature which shows that the NESOM turns out to be very convenient for concrete application (for example, see the review, Ref. [6], and the references therein). More recently, applications of the McLennan-Zubarev form of the NE density matrix have been done in the context of quantum electron transport. For example, the problem of quantum transport for noninteracting electrons in effective one-dimensional systems can be found in Refs. [12,13], where the authors rederive Zubarev's NESOM from a maximum entropy principle, since in essence a Gibbs state is characterized by the principle of maximum entropy at fixed energy (see also Ref. [3]). Applications for interacting electron-nuclei systems is provided in Ref. [14], in which the authors derive the kinetic equations governing time evolution of positions and momenta of atoms (in the classic limit) interacting with a quantum electron gas using the NESOM.

On the other hand, in the early 1990s, Hershfield reformulated the problem of NE steady-state quantum statistical mechanics (QSM) in Ref. [15]. This was done by rewriting the conventional perturbation theory of NE QSM for the steady-state regime in a form similar to that of an equilibrium QSM (called below a pseudoequilibrium). In this reformulation, an explicit expression for the NE density matrix was provided as well as a scheme upon which one can build nonperturbative calculations in NE quantum systems. This approach has permitted us to understand more clearly the nonequilibrium ensembles, and how NE boundary conditions can be imposed as a statistical operator. It has also been successfully applied in numerical applications for the problem of quantum transport, in the presence or absence of interaction between electrons [16,17]. Other applications have been performed by Han and co-workers in the context of quantum transport for electron-phonon interaction in quantum dots [18], for strongly correlated electron systems within a slave boson approach [19]. Han and co-workers also developed an equivalent formulation within the framework of the imaginary time formalism [20–24].

In this paper, we show and prove that the Hershfield approach for the NE density matrix is actually a specific form of the McLennan-Zubarev NESOM. By specific, we mean that the Hershfield approach can be seen as a particular case of the NESOM applied to the problem of quantum transport,

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where a central scattering region (with interaction or not) is connected to two (or more) leads and the whole system is at the same temperature T. Our work provides a clear and formal connection between these two approaches which are widely used for applications in quantum transport.

Both McLennan-Zubarev and Hershfield show that the properties of a NE steady state can be obtained in a formally equivalent manner as in an equilibrium state but using a NE density matrix in a Gibbs form instead of the equilibrium Gibbs statistical ensembles. Hence it is also possible to derive NE quantities, such as distribution functions, from formal expressions used in the equilibrium case. We consider the development of such distribution functions for the population of electrons in the context of quantum transport in the last part of the paper.

The paper is organized as follows. In Secs. II and III, we briefly recall the main ingredients of the McLennan-Zubarev NESOM and of the Hershfield approach, respectively. Section IV is the main part of the paper where we formally establish the connection between the two methods. In Sec. V we derived the expression for the NE steady-state distribution of the electron population of a central region (in the presence of interaction) connected to two (noninteracting) electron reservoirs. Finally, we discuss further developments and present our conclusion in Sec. VI.

II. MCLENNAN-ZUBAREV NONEQUILIBRIUM STATISTICAL OPERATOR METHOD

Classic and quantum statistical mechanics should provide microscopic foundations for the thermodynamics description of many-body systems. For the equilibrium case, the method of statistical ensembles developed by Gibbs gives a rigorous formulation of the thermodynamic quantities and relations. Within the same line of reasoning, an extension of Gibbs method to the nonquilibrium cases would permit one to formulate the basic postulates of irreversible thermodynamics. Such a formulation of nonequilibrium statistical mechanics has been provided by McLennan [1] and Zubarev [2–6].

For a system composed of N independent parts (with $j = 1,\dots,N$ Hamiltonian H_j, at temperature β_j, and with $\lambda = 1,\dots,L$ species of particle λ with number $N_j^{(\lambda)}$ and chemical potential $\mu_j^{(\lambda)}$) which are interacting by an interaction W, the McLennan-Zubarev form of the NE statistical operator is given by

$$\rho = \frac{1}{Z}\exp\left\{-\sum_{j=1}^{N}\beta_j\left[H_j - \sum_{\lambda=1}^{L}\mu_j^{(\lambda)}N_j^{(\lambda)}\right] - \int_{-\infty}^{0} ds\, e^{\eta s} J_S(s)\right\}, \tag{1}$$

where Z is the normalization factor $Z = \mathrm{Tr}[\rho]$ and the quantity $J_S(s)$ is obtained from $J_S(s) = \sum_j \beta_j J_j^q(s)$ with $J_j^q(s)$ being the so-called nonsystematic energy flow [9], or heat flow, to the jth subsystem defined as

$$J_j^q(s) = \frac{d}{ds}\left(H_j(s) - \sum_{\lambda}\mu_j^{(\lambda)}N_j^{(\lambda)}(s)\right). \tag{2}$$

The operators are given in the Heisenberg representation, with the total Hamiltonian $H = \sum_j H_j + W$ and $H_j(s) = e^{iHs}H_j e^{-iHs}$, $N_j(s) = e^{iHs}N_j e^{-iHs}$. A convergence factor $e^{\eta s}$ ($\eta > 0$) is introduced in the time integral, where the limit $\eta \to 0$ is taken in the end, after all the calculations are done.

The quantity $J_S(s)$ being the sum of heat flows divided by subsystem temperatures, is therefore the entropy production rate of the whole system [3,9].

III. HERSHFIELD APPROACH FOR NONEQUILIBRIUM DENSITY MATRIX

Hershfield reformulated the problem of NE steady state in quantum statistical mechanics [15] by developing an iterative scheme for the NE density matrix expressed in terms of a series of power of $(W)^n$ where W is the perturbative part of the total Hamiltonian $H = H_0 + We^{\eta t}$ that drives the system out of equilibrium (and eventually also contains the interaction between the particles).

The expectation value of any operator A in a NE steady state is then obtained from a pseudoequilibrium as follows:

$$\langle A\rangle = \frac{1}{Z^{\mathrm{NE}}}\mathrm{Tr}[\rho^{\mathrm{NE}}A], \tag{3}$$

with the NE density matrix

$$\rho^{\mathrm{NE}} = e^{-\beta(H-Y)}, \tag{4}$$

and the partition function $Z^{\mathrm{NE}} = \mathrm{Tr}[\rho^{\mathrm{NE}}]$.

In the interaction representation (where the operators X are given by $X_I(t) = e^{iH_0t}Xe^{-iH_0t}$), the density matrix follows the usual equation of motion

$$\frac{\partial\rho_I(t)}{\partial t} = i[\rho_I(t),W_I(t)]. \tag{5}$$

Hershfield introduced a new set of operators Y_n which are of the order $O(W^n)$ and from which the density matrix can be constructed by an iterative scheme.

The individual operators Y_n follow the same differential equation as the density matrix but in a recursive way:

$$\frac{\partial Y_{n+1,I}(t)}{\partial t} = i[Y_{n,I}(t),W_I(t)]. \tag{6}$$

The index of the operators Y_n differs in each side of Eq. (6) in order to have the same power of the perturbation W on both sides.

The differential equation (6) can also be rewritten in terms of commutators as

$$[H_0,Y_n] - i\eta Y_n = [Y_{n-1},W], \tag{7}$$

where the positive infinitesimal η is included to make the equation well defined [15].

The operator Y is then obtained from the sum $Y = \sum_{n=0}^{\infty} Y_n$. The initial expression of the Y_n operators is given by $Y_0 = \sum_i \mu_i N_i$. The important difference between the equilibrium and NE cases is that the operator Y_0 does not commute with the perturbation W. Furthermore, Hershfield showed that the full operator Y and the total Hamiltonian H commute in the limit of adiabatic switching of the perturbation ($\eta \to 0^+$). Because Y and H commute, Hershfield interpreted the Y operator as the operator into which Y_0 "evolves" under the action of the perturbation W.

We show in the next section that the NE density matrix $\rho^{\rm NE}$ with the presence of the Y operator is actually a McLennan-Zubarev form of a NE statistical operator (for a system at the same temperature $kT = 1/\beta$).

IV. HERSHFIELD DENSITY MATRIX AS A MCLENNAN-ZUBAREV FORM OF THE STATISTICAL OPERATOR

We now rewrite the McLennan-Zubarev NE statistical operator for the conditions considered by Hershfield, i.e., one specie of particle (electrons) $L = 1$ and a unique temperature $\beta_j = \beta$. Hence Eq. (1) becomes

$$\rho = \frac{1}{Z}\exp\left\{-\beta\sum_{j=1}^{N}\left(H_j - \mu_j N_j - \int_{-\infty}^{0} ds\, e^{\eta s} J_j^q(s)\right)\right\}$$
$$= \frac{1}{Z} e^{-\beta(H-\Upsilon)}. \tag{8}$$

In the second equality of Eq. (8), we have rewritten the NE statistical operator in the form of a NE density matrix with

$$\Upsilon = Y_0 + W + \int_{-\infty}^{0} dx\, e^{\eta x} e^{iHx} i[W,H_0 - Y_0]e^{-iHx}, \tag{9}$$

with the total Hamiltonian $H = \sum_j H_j + W = H_0 + W$, $Y_0 = \sum_j \mu_j N_j$, and

$$\begin{aligned}\sum_j \frac{1}{\beta} J_j^q(x) &= \sum_j \frac{d}{dx}\left(H_j - \mu_j N_j\right)(x)\\ &= \frac{d}{dx}\left[H_0(x) - Y_0(x)\right]\\ &= i[H,H_0(x) - Y_0(x)]\\ &= e^{iHx} i[W,H_0 - Y_0]e^{-iHx}\\ &= i[W(x),H_0(x) - Y_0(x)]\,.\end{aligned} \tag{10}$$

We use the fact that the operator Y_0 commutes with the unperturbed noninteracting Hamiltonian H_0.

To prove that the Hershfield approach is actually a McLennan-Zubarev form of the NE statistical operator, we have to prove that the operator Υ is just the operator Y in the Hershfield method.

For that, we expand the time dependence of the commutator $A = i[W,H_0 - Y_0]$ in a series expansion

$$\begin{aligned}A(x) &= e^{iHx} A e^{-iHx}\\ &= A + [iHx,A] + \tfrac{1}{2}[iHx,[iHx,A]]\\ &\quad + \tfrac{1}{3}[iHx,[iHx,[iHx,A]]] + \cdots\end{aligned} \tag{11}$$

of powers of $(W)^n$, knowing that $H = H_0 + W = O(W^1)$ and $A = O(W^1)$.

It is then natural to expand, as in the Hershfield approach, the operator Υ in a series $\Upsilon = \sum_n \Upsilon_n$ where each term Υ_n corresponds to a power W^n. The aim of the derivation is to identify the terms of each order of the perturbation W in the interaction representation scheme of Hershfield for $Y_{n,I}(t)$ and in the Heisenberg representation used for the expression of Υ in the NESOM. This is easily done for the lowest order terms.

At the zeroth order of the perturbation, it is clear from Eq. (9) that $\Upsilon_0 = Y_0$. For the higher order, it is convenient to generalize Eq. (9) as

$$\Upsilon(\tau) = Y_0 + W + \int_{-\infty}^{\tau} dx\, e^{\eta s} e^{iHx} i[W,H_0 - Y_0]e^{-iHx}, \tag{12}$$

and take the limit $\tau = 0$ in the end to make the connection between the NESOM and Hershfield approach. Hence we have

$$\frac{\partial\Upsilon(\tau)}{\partial\tau} = e^{iH\tau} i[We^{\eta\tau},H_0 - Y_0]e^{-iH\tau} + \frac{\partial Y_0}{\partial\tau} + \frac{\partial W}{\partial\tau}, \tag{13}$$

with $\partial_\tau Y_0 = i[H,Y_0(\tau)]$ and $\partial_\tau W = i[H,W(\tau)]$.

To get the term linear in W, we have to consider the lowest order expansion in Eq. (11) for the time evolution operator in terms of the noninteracting Hamiltonian H_0 only, i.e., $H \to H_0$ and $X(\tau) \to X_I(\tau)$. Hence the right-hand side of Eq. (12) becomes $i[W_I(\tau),H_0 - Y_{0,I}(\tau)] + i[H_0,W_I(\tau)]$, where the term $e^{\eta\tau}$ is included in $W_I(\tau)$. For the left-hand side of Eq. (12), we assume that the Heisenberg representation of Υ can rearrange as $e^{iH_0\tau}$[sum of terms in $O(W^n)$]$e^{-iH_0\tau}$, i.e., $e^{iH_0\tau}[\sum_n \Upsilon_n]e^{-iH_0\tau}$. Hence at the lowest order in W, we get the interaction representation of $\Upsilon_{n=1}$, and therefore we find the lowest order version of Eq. (6) for Υ_n:

$$\partial_\tau \Upsilon_{1,I}(t) = -i[W_I(t),Y_{0,I}(\tau)]. \tag{14}$$

The same result can also be obtained more directly from Eq. (9) by considering the lowest order expansion of the time evolution operator:

$$\Upsilon_1 = W + \int_{-\infty}^{0} dx\, e^{\eta s} e^{iH_0x} i[W,H_0 - Y_0]e^{-iH_0x}, \tag{15}$$

and integrating by part the term in $e^{iH_0x} i[W,H_0]e^{-iH_0x} = -\partial_x W_I(x)$ to find

$$\Upsilon_1 = i\int dx\, e^{iH_0x}[Y_0,W]e^{-iH_0x}, \tag{16}$$

which is just the integrated version of Eq. (14) or Eq. (6).

The higher order terms $\Upsilon_{n\geqslant 2}$ can be found from

$$\Upsilon_{n\geqslant 2} = i\int_{-\infty}^{0} dx\, e^{iHx}[We^{\eta s},H_0 - Y_0]e^{-iHx}, \tag{17}$$

however, the derivation is much more cumbersome than for the lowest order terms.

Instead, one can use Eq. (9) and perform an analysis and decomposition order by order of the powers in $O(W^n)$. For that we first rewrite Eq. (9) as

$$\begin{aligned}\Upsilon = Y_0 + W &- \int_{-\infty}^{0} dx\, \partial_x W(x)\\ &- i\int_{-\infty}^{0} dx\, e^{iHx}[We^{\eta x},Y_0]e^{-iHx},\end{aligned} \tag{18}$$

using the fact that $e^{iHx} i[W,H_0]e^{-iHx} = e^{iHx} i[W,H]e^{-iHx} = i[W(x),H] = -\partial_x W(x)$. Note that when not explicitly written, the term $e^{\eta x}$ is included in the perturbation W. Finally, using the fact that, in leading order, the operator Y in the Hershfield approach is the time evolution of Y_0, $Y = e^{iHx} Y_0 e^{-iHx}$, we get in leading order

$$\Upsilon = Y_0 - i \int_{-\infty}^{0} dx [W(x), Y(x)]. \tag{19}$$

Hence again, in leading order, we find that by expanding Eq. (19) in powers of $O(W^n)$, we keep only the time dependence in terms of H_0 in the series expansion, and we find $\Upsilon_0 = Y_0$, $\Upsilon_1 = -i \int_{-\infty}^{0} dx [W_I(x), Y_{0,I}(x)]$, and $\Upsilon_{n+1} = -i \int_{-\infty}^{0} dx [W_I(x), Y_{n,I}(x)]$ which is the integrated expression of the right-hand side of Eq. (6).

Finally to conclude this section, we consider Eq. (13) and rewrite it in terms of commutators to find that

$$\begin{aligned} \partial_\tau \Upsilon(\tau) &= i[W(\tau), H_0(\tau) - Y_0(\tau)] + i[H, Y_0(\tau)] + i[H, W(\tau)] \\ &= i[W(\tau), -Y_0(\tau)] + i[H, Y_0(\tau)] \\ &= i[H_0(\tau), Y_0(\tau)] = e^{iH\tau} i[H_0, Y_0] e^{-iH\tau} = 0. \end{aligned} \tag{20}$$

Hence $\Upsilon(\tau) = \Upsilon$ is constant of motion, and $\partial_\tau \Upsilon(\tau) = i[H, \Upsilon(\tau)] = 0$ implies that the operator Υ commutes with the total Hamiltonian H, as the Hershfield operator Y commutes with H.

Therefore we have shown that the NE density matrix $e^{-\beta(H-Y)}$ of the Hershfield approach is indeed a McLennan-Zubarev form of the NE statistical operator. Finally, we can note that the NE density matrix/statistical operator depends, via the operator Y/Υ, on the NE conditions as expected, i.e., on the different chemical potentials μ_i in Y_0, but also on the interaction W and on how the initial Y_0 evolves under the perturbation W.

V. AN APPLICATION FOR NONEQUILIBRIUM DISTRIBUTION

The fact that the NE steady state can be described as a pseudoequilibrium state, with a modified Gibbs-like statistics, permit us to determine NE quantities from formal expressions used in the equilibrium case [compare Eqs. (23) Eq. (24) below]. In this section, we derive an expression for the NE distribution function of the electron population in a central region connected to two reservoirs. The study of other NE thermodynamical quantities for noninteracting quantum transport (current-induced forces and thermodynamical potentials) has been addressed in [25–28].

As an example, we consider in the following the NE distribution function of a central region consisting of a single level (with interaction) connected to two (left and right) reservoirs at their own equilibrium. The statistics in each reservoir is given by the Fermi-Dirac distribution with chemical potentials μ_L and μ_R and temperature T_L and T_R. In the NE conditions $\mu_L \neq \mu_R$ and/or $T_R \neq T_R$.

The Hamiltonian for the central scattering region C is simply given by $H_C = \varepsilon_0 d^\dagger d$, where $d^\dagger$ (d) creates (annihilates) an electron in the level ε_0. The specific model used for the leads connected to the central region does not need to be specified, as long as the leads can be described by an embedding self-energy Σ_α in the electron Green's function (GF) of the central region ($\alpha = L,R$).

At equilibrium, the average of the electron population of a single level coupled to a thermal bath $\langle d^\dagger d \rangle$ leads to the equilibrium Fermi-Dirac distribution $f^{\rm eq}$. For NE conditions, the average $\langle d^\dagger d \rangle$ as given by Eq. (3) is difficult to derive exactly, especially in the presence of interaction [16–18]. However, because of the pseudoequilibrium nature of the NE steady-state statistics, we can assume that such an average is well behaved and leads to a NE distribution $f^{\rm NE}$.

In order to obtain a compact form for $f^{\rm NE}$, we have found that, instead of calculating the series expansion of the operator Y, a more straightforward approach is obtained by using NE GFs in the steady-state regime [29]. The GFs are correlation functions whose thermodynamical averages are formally identical to those calculated in the Hershfield approach.

Both perturbation series used in the NE GF approach and in the derivations of the equations for the Y operator in the Hershfield approach start from the same nonequilibrium series expansion. They are just two different ways of summing that series. For a noninteracting problem for which the series can be resumed exactly, the NE GF and the Hershfield Y operator approach provide the same result [16,17]. For an interacting system, one must resort to approximations to partially resum the series, and therefore the two approaches are similar only when the same approximations are used.

The different GF in the central region can be obtained from two correlation functions (i.e., the so-called lesser and greater GF):

$$\begin{aligned} G^<(t,t') &= -i \langle d^\dagger(t') d(t) \rangle, \\ G^>(t,t') &= i \langle d(t) d^\dagger(t') \rangle, \end{aligned} \tag{21}$$

where $d^\dagger$ (d) creates (annihilates) an electron in the single level of the central region and $\langle \cdots \rangle$ is the average over the proper equilibrium or NE ensemble, as given in Eq. (3).

The other GFs, the advanced and retarded GFs, are obtained from the combination of the lesser and greater components as

$$G^{r/a}(t,t') = \pm\theta[\pm(t-t')][G^>(t,t') - G^<(t,t')]. \tag{22}$$

The interaction in the central region is obtained from a perturbation expansion, via partial resummation of Feynmann diagrams, and enters the definition of the GF via the self-energy $\Sigma_{\rm int}$ in the Dyson equations of $G^{r,a}$ and in the quantum kinetic equations of $G^{\lessgtr}$.

At equilibrium and in the steady state, all quantities depend only on the time difference $X(t,t') = X(t-t')$ and can be Fourier transformed in a single-energy representation $X(\omega)$.

At equilibrium, from the relation $G^> - G^< = G^r - G^a$ and the Kubo, Martin, and Schwinger (KMS) condition [30–34] $G^>(\omega) = -e^{\beta(\omega-\mu^{\rm eq})} G^<(\omega)$, one recovers the conventional relation

$$G^< = -f^{\rm eq}(G^> - G^<) = -f^{\rm eq}(G^r - G^a), \tag{23}$$

with $f^{\rm eq}(\omega) = [1 - G^>/G^<]^{-1} = [1 + e^{\beta(\omega-\mu^{\rm eq})}]^{-1}$ being the equilibrium Fermi-Dirac distribution. The equilibrium KMS condition arises from the fact that the statistical operator $e^{-\beta H}$ looks formally like the time evolution operator e^{-iHt} if one works with imaginary time $t \equiv -i\beta$. In general, for any two operators A and B, the KMS relation is given by $\langle A(t - i\beta) B(t') \rangle = \langle B(t') A(t) \rangle$ [30–34].

In the NE steady state the situation is different. Even if the steady state can be seen as a pseudoequilibrium state, with a statistical operator $e^{-\beta(H-Y)}$, the KMS relation is modified as follows: $\langle A(t-i\beta)B(t')\rangle = \langle e^{-\beta Y}B(t')e^{\beta Y}A(t)\rangle$. Depending on the nature of the operator B, additional contributions arise from the expansion $e^{-\beta Y}Be^{\beta Y} = B + [-\beta Y,B] + [-\beta Y,[-\beta Y,B]]/2! + \cdots$.

However, because of the intrinsic pseudoequilibrium nature of the NE steady state, it is entirely justified to use the Gibbs-like ensemble, provided by either the Hershfield or McLennan-Zubarev method, to define the NE distribution $f^{\rm NE}$ for the relationship between the GFs in a similar way as done for the equilibrium relation. That is, we can extend the formal definition of the equilibrium distribution to the NE conditions, i.e., the distribution $f^{\rm NE}$ of the electron population in the NE steady state [35–37]:

$$G^{<}(\omega) = -f^{\rm NE}(\omega)[G^{r}(\omega) - G^{a}(\omega)], \qquad (24)$$

where we are now considering full NE GFs [38]. This is a rigorous definition for the NE steady state, and not an ansatz.

With respect to Refs. [25,26,28], the NE distribution $f^{\rm NE}$ represents the statistics for the electron population of an open quantum system, i.e., the central region (in the presence of interaction) connected to the two reservoirs. It is not the "local" equilibrium statistics of states scattering in and out of the reservoirs which are themselves at their own equilibrium.

From the definition $G^{<} = G^{r}\Sigma^{<}G^{a}$, where the total self-energy $\Sigma(\omega) = \Sigma_L(\omega) + \Sigma_R(\omega) + \Sigma_{\rm int}(\omega)$ arises from the contributions of the leads self-energy $\Sigma_{L,R}$ and the self-energy $\Sigma_{\rm int}$ of the interaction between particles, we can see that the total self-energy follows as well the same statistics, i.e., $\Sigma^{<} = -f^{\rm NE}(\Sigma^{r} - \Sigma^{a})$. However, as we have clearly explained in Ref. [39], there is no reason for each contribution $\Sigma_{L,R}$ and $\Sigma_{\rm int}$ to follow individually the same statistics.

From this point of view, we find a compact and universal (with respect to the interaction) expression for the NE distribution function $f^{\rm NE}(\omega)$:

$$f^{\rm NE}(\omega) = \frac{f_0^{\rm NE}(\omega) - i\,\Sigma_{\rm int}^{<}(\omega)/\,\Gamma_{L+R}(\omega)}{1 + i\left(\Sigma_{\rm int}^{>} - \Sigma_{\rm int}^{<}\right)/\,\Gamma_{L+R}}, \qquad (25)$$

where $\Gamma_{L+R}(\omega)$ is the spectral function of the leads $\Gamma_{L+R} = \sum_{\alpha=L,R} i(\Sigma_\alpha^{r} - \Sigma_\alpha^{a})$, and $\Sigma_{\rm int}^{\lessgtr}$ are the lesser and greater components of the interaction self-energy.

The function $f_0^{\rm NE}(\omega)$ is the NE distribution for the noninteracting case. It can be easily derived [17,35–37,40] as the weighted average of the usual Fermi-Dirac distribution functions $f_{L,R}(\omega)$ of the left and right leads:

$$f_0^{\rm NE} = [\Gamma_L(\omega)f_L(\omega) + \Gamma_R(\omega)f_R(\omega)]\,/\,\Gamma_{L+R}(\omega). \qquad (26)$$

The distribution $f_0^{\rm NE}(\omega)$ is a double-step function, with more or less steep steps (depending on the temperature) located around $\omega = \mu_L$ and $\omega = \mu_R$, and separated by $\mu_L - \mu_R = eV$ (μ_α being the chemical potential of the lead $\alpha = L,R$ and V the applied bias). The use of such a distribution has already been implemented in realistic calculations based on single-particle elastic scattering [41].

The full NE distribution $f^{\rm NE}$ can be decomposed into two terms $f^{\rm NE}(\omega) = \tilde{f}_0^{\rm NE}(\omega) + \delta f^{\rm NE}(\omega)$; one corresponds to the dynamically renormalized distribution $\tilde{f}_0^{\rm NE} = f_0^{\rm NE}(\omega)/\mathcal{N}(\omega)$ and the other is a "correction" term $\delta f^{\rm NE}$ associated with the inelastic processes and given by $\Sigma_{\rm int}^{<}$ renormalized by the same factor $\mathcal{N}$. The renormalization factor $\mathcal{N}(\omega)$ is given by the sum $\mathcal{N}(\omega) = \Gamma_{L+R} + i(\Sigma_{\rm int}^{>} - \Sigma_{\rm int}^{<})$ of the spectral functions of the leads Γ_{L+R} and of the interaction $\Gamma_{\rm int} = i(\Sigma_{\rm int}^{>} - \Sigma_{\rm int}^{<}) = i(\Sigma_{\rm int}^{r} - \Sigma_{\rm int}^{a})$, and does not contain direct information of the statistics of the system.

For local electron-phonon interaction in the central region, the interaction self-energy is given by $\Sigma_{\rm int}^{F,\lessgtr}(\omega) = \gamma_0^2[N_{\rm ph}G^{\lessgtr}(\omega \mp \omega_0) + (N_{\rm ph}+1)G^{\lessgtr}(\omega \pm \omega_0)]$ [42]. At low temperature $N_{\rm ph} = 0$, and we can expand Eq. (25) as a series expansion in terms of the electron-phonon coupling parameter γ_0. To lowest order, we find the following expression for the NE distribution function:

$$\begin{aligned} f^{\rm NE}(\omega) &\\ \sim f_0^{\rm NE} + \frac{2\pi\gamma_0^2}{\Gamma}&\big\{A(\omega+\omega_0)\big[1 - f_0^{\rm NE}(\omega)\big]f_0^{\rm NE}(\omega+\omega_0) \\ &- A(\omega-\omega_0)\big[1 - f_0^{\rm NE}(\omega-\omega_0)\big]\,f_0^{\rm NE}(\omega)\big\}, \end{aligned} \qquad (27)$$

where $A(\omega)$ is the spectral function of the central region, i.e., $A(\omega) = (G^{a} - G^{r})/i2\pi$. The terms in γ_0^2 in Eq. (27) are correction terms to the noninteracting distribution $f_0^{\rm NE}(\omega)$ and correspond to the lowest order contributions of the electron-phonon interaction (i.e., phonon emission by electron or hole in the presence of a finite bias). When they are included in the expression of the current [43] they generate an equivalent formulation of the lowest order treatment of the perturbation approaches to electron-phonon interaction provided in Refs. [44–46].

VI. CONCLUSION

We have demonstrated that the NE density matrix developed by Hershfield for the steady state has the form of a McLennan-Zubarev nonequilibrium ensemble. According to the McLennan-Zubarev NESOM and Hershfield methods, the stationary density of an open system can be written in the modified Gibbs form $\rho^{\rm NE} = e^{-\beta(H-Y)}/Z$, with the nonequilibrium "correction term" Y. The operator Y that was interpreted as the operator into which $Y_0 = \sum_i \mu_i N_i$ "evolves" under the action of the perturbation W, is actually the entropy production rate of the NE quantum system. It can be calculated in the absence and in the presence of interaction and gives information about the dissipation in the driven system.

The fact the both methods clearly show that a NE steady state can be mapped onto an effective pseudoequilibrium state, permits us to derive, in a rigorous way, NE quantities from the formal expressions given at equilibrium [compare Eqs. (23) and (24)]. We have derived an example of such quantities, i.e., the NE distribution function for the electron population in a scattering region connected to two reservoirs. Such a NE distribution function describes the statistics of an open quantum system in the NE steady-state regime. It is central to the understanding of the NE physical properties of open systems and to the derivation of NE thermodynamical laws, such as NE fluctuation-dissipation relations [39], NE charge susceptibility [37], or quantum entropy production.

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