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 non-equilibrium density matrix developed by Hershfield for the steady state has the form of a McLennan-Zubarev non-equilibrium ensemble. The correction term in this pseudo equilibrium Gibbs-like ensemble is directly related to the entropy production in the quantum open system. The fact the both methods state that a non-equilibrium steady state can be mapped onto a pseudo-equilibrium, permits us to develop non-equilibrium quantities from formal expressions equivalent to the equilibrium case. We provide an example: the derivation of a non-equilibrium 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 non-equilibrium (NE) steady state is a longstanding 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. 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 for classical systems and by Zubarev 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 on 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. [3,10]. Furthermore, rigorous definition of McLennan-Zubarev ensembles have been given in Refs. [3,11].

There is also an 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 non-interacting electrons in effective one-dimensional systems can be found in Ref. [12,13], where the authors derive Zubarev’s NESOM from a maximum entropy principle, since by essence a Gibbs state is characterized by the principle of maximum entropy at fixed energy (see also Ref. [4]). 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 nineties, 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 pseudo-equilibrium). In this reformulation, an explicit expression for the NE density matrix was provided as well as a scheme upon which one can build non-perturbative calculations in NE quantum systems. This approach has permitted us to understand more clearly the non-equilibrium 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. Most of such applications have been performed by Han and co-workers in the context of quantum transport for electron-phonon interaction in quantum dots, for strongly correlated electrons within a slave boson approach. Han and co-workers also developed an equivalent formulation within the framework of the imaginary time formalism.

In this paper, we show and prove that Hershfield approach for the NE density matrix is actually a specific form of the McLennan-Zubarev NESOM. By specific, we mean that Hershfield approach can be seen as a particular
case of the NESOM applied to the problem of quantum transport, 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 organised as follows. In Sec. II and Sec. III we briefly recall the main ingredients of the McLennan-Zubarev NESOM and of Hershfield approach respectively. Sec. 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 (non-interacting) electron reservoirs. Finally, we discuss further developments and present our conclusion in Sec. VI.

II. MCLENNAN-ZUBAREV NON-EQUILIBRIUM 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 non-equilibrium cases would permit to formulate the basic postulates of irreversible thermodynamics. Such a formulation of non-equilibrium statistical mechanics has been provided by McLennan and Zubarev.

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

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

where $Z$ is the normalisation factor $Z = \text{Tr}[\rho]$ and the quantity $J_S(s)$ is obtained from $J_S(s) = \sum_j \beta_j J_j(s)$ with $J_j(s)$ being the so-called non-systematic energy flow, or heat flow, to the $j$th subsystem defined as

$$J_j(s) = \frac{d}{ds} \left( H_j(s) - \sum_{\lambda} \mu^{(\lambda)}_j N^{(\lambda)}_j(s) \right) .$$

The operators are given in the Heisenberg representation, with the total Hamiltonian $H = \sum_j H_j + W$ and $H_j(s) = e^{iH_j s} H_j e^{-iH_j s}$, $N_j(s) = e^{iH_j s} N_j e^{-iH_j s}$. 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.

III. HERSHFIELD APPROACH FOR NON-EQUILIBRIUM DENSITY MATRIX

Hershfield reformulated the problem of NE steady state in quantum statistical mechanics, 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 $H = H_0 + W e^{st}$ 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 pseudo equilibrium as follows:

$$\langle A \rangle = \frac{1}{Z_{\text{NE}}} \text{Tr}[\rho_{\text{NE}} A] ,$$

with the NE density matrix

$$\rho_{\text{NE}} = e^{-\beta(H-Y)} ,$$

and the partition function $Z_{\text{NE}} = \text{Tr}[\rho_{\text{NE}}]$. 

In the interaction representation (where the operators \( X \) are given by \( X_I(t) = e^{iH_0 t} X e^{-iH_0 t} \)), the density matrix follows the usual equation of motion

\[
\frac{\partial \rho(t)}{\partial t} = i[\rho(t), W_I(t)] .
\]

(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 \( Y_n \) follows the same differential equation as the density matrix but in a recursive way:

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

(6)

The index of the operators \( Y_n \) differs in each side of Eq. (8) in order to have the same power of the perturbation \( W \) on both sides.

The differential equation Eq. (8) can also be rewritten in terms of commutators as

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

(7)

where the positive infinitesimal \( \eta \) is included to make the equation well defined.

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 \( Y_0 = \sum_j \mu_j N_j \). 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 \( (\eta \rightarrow 0^+) \). 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 \( \rho_{\text{NE}} \) 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. (10) becomes

\[
\rho = \frac{1}{Z} \exp \left\{ -\beta \sum_{j=1}^{N} \left( H_j - \mu_j N_j - \int_{-\infty}^{0} ds e^{\eta s} J^q_j(s) \right) \right\} = \frac{1}{Z} e^{-\beta(H-Y)} .
\]

(8)

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

\[
Y = Y_0 + W + \int_{-\infty}^{0} dx e^{\eta x} e^{iHx} \left[ W, H_0 - Y_0 \right] e^{-iHx} ,
\]

(9)

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

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

(10)

We use the fact that the perturbation \( W \) in the unperturbed non-interacting 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 \( Y \) is just the operator \( Y \) in Hershfield method.

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

\[
A(x) = e^{iHx} A e^{-iHx} = A + [iHx, A] + \frac{1}{2} [iHx, [iHx, A]] + \ldots
\]

(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 Hershfield approach, the operator \( Y \) in a series \( Y = \sum_n Y_n \) where each term \( Y_n \) 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 \( Y \) in the NESOM. This is easily done for the lowest order terms.

At the zero-th order of the perturbation, it is clear from Eq. (9) that \( Y_0 = Y_0 \). For the higher order, it is
convenient to generalise Eq. (9) as
\[
\Upsilon(\tau) = Y_0 + W + \int_{-\infty}^{\tau} dx e^{\eta x} e^{-iHx} i[W, H_0 - Y_0] e^{-iHx},
\]
and take the limit \( \tau = 0 \) in the end to make the connection between the NESOM and Hershfield approach. Hence we have
\[
\frac{\partial \Upsilon(\tau)}{\partial \tau} = e^{iH\tau} i[W e^{\eta \tau}, H_0 - Y_0] e^{-iH\tau} + \frac{\partial Y_0}{\partial \tau} + \frac{\partial W}{\partial \tau},
\]
(13)
with \( \partial_x \Upsilon = i[H, Y_0(\tau)] \) and \( \partial_x W = i[H, W(\tau)] \).

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 non-interacting Hamiltonian \( H_0 \) only, i.e. \( H \rightarrow H_0 \) and \( X(\tau) \rightarrow X_1(\tau) \). Hence the right hand side of Eq. (12) becomes \( i[W_I(\tau), H_0 - Y_0(\tau)] + i[H_0, W_I(\tau)] \), 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 \( \Upsilon \) can rearrange as \( e^{iH_0 \tau} \) sum of terms in \( O(W^n) e^{-iH_0 \tau} \) i.e. \( e^{iH_0 \tau} \sum_n Y_n e^{-iH_0 \tau} \). Hence at the lowest order in \( W \), we get the interaction representation of \( Y_{n=1} \) and therefore we find the lowest order version of Eq. (13) for \( Y_n \):\[
\partial_x Y_{1,1}(t) = -i[W_I(t), Y_0(\tau)].
\]
(14)
The same result can also be obtained more directly from Eq. (9) by considering the lowest order expansion of the time evolution operator:
\[
Y_1 = W + \int_{-\infty}^{0} dx e^{\eta x} e^{iH_0 x} i[W, H_0 - Y_0] e^{-iH_0 x},
\]
(15)
and integrating by part the term in \( e^{iH_0 x} i[W, H_0] e^{-iH_0 x} = -\partial_x W_I(x) \) to find
\[
Y_1 = i \int_{-\infty}^{0} dx e^{iH_0 x} [Y_0, W] e^{-iH_0 x},
\]
(16)
which is just the integrated version of Eq. (14) or Eq. (9).

The higher order terms \( Y_{n \geq 2} \) can be found from
\[
Y_{n \geq 2} = i \int_{-\infty}^{0} dx e^{iH_0 x} [W e^{\eta x}, Y_0] e^{-iH_0 x},
\]
(17)
however the derivation is much more cumbersome that for the lowest order terms.

Instead, one can use Eq. (9) and perform an analysis and decomposition by order of the powers in \( O(W^n) \). For that we first rewrite Eq. (9) as
\[
Y = Y_0 + W - \int_{-\infty}^{0} dx \partial_x W(x) + i \int_{-\infty}^{0} dx e^{iH_0 x} [W e^{\eta x}, Y_0] e^{-iH_0 x},
\]
(18)
using the fact that \( e^{iH_0 x} i[W, H_0] e^{-iH_0 x} = e^{iH_0 x} i[W, H] e^{-iH_0 x} = i=W(x), H = -\partial_x W(x) \). 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 Hershfield approach is the time evolution of \( Y_0 \), \( Y = e^{iH_0 \tau} Y_0 e^{-iH_0 \tau} \), we get in leading order
\[
Y = Y_0 - i \int_{-\infty}^{0} dx [W(x), Y(\tau)].
\]
(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 \( Y_0 = Y_0, Y_1 = -i \int_{-\infty}^{0} dx [W_I(x), Y_0(\tau)] \), and \( Y_{n+1} = -i \int_{-\infty}^{0} dx [W_I(x), Y_n(\tau)] \) which is the integrated expression of the right hand side of Eq. (16).

Finally to conclude this section, we consider Eq. (13) and rewrite it in terms of commutators to find that:
\[
\partial_x \Upsilon(\tau) = i[W(\tau), H(\tau) - Y_0(\tau)] + i[H, Y_0(\tau)] + i[H, W(\tau)]
\]
\[
= i[W(\tau), Y_0(\tau)] + i[H, Y_0(\tau)]
\]
\[
= i[H_0(\tau), Y_0(\tau)] = e^{iH_0 \tau} [H_0, Y_0] e^{-iH_0 \tau} = 0.
\]
(20)
Hence \( \Upsilon(\tau) = Y \) is constant of motion, and \( \partial_x \Upsilon(\tau) = i[H, Y(\tau)] = 0 \) implies that the operator \( \Upsilon \) 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 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 \( Y/T \), on the NE conditions as expected, i.e. on the different chemical potentials \( \mu_i \) 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 NON-EQUILIBRIUM DISTRIBUTION

The fact that both methods clearly show that the NE steady state can be described as a pseudo equilibrium state, with a Gibbs-like statistics, permit us to determine NE quantities in a formally similar way as done for the equilibrium case (compare Eq. (23) and Eq. (24) below).

In this section, we derive an explicit expression for the NE distribution function of the electron population in a central region connected to two reservoirs, in the context of quantum transport. The study of other NE thermodynamical quantities for non-interacting quantum transport, such as the current-induced forces and thermodynamical potentials, can be found in Refs. [31] [34].

In the following, we considered on the NE distribution function of a central region consisting of a single level (with interaction) connected to two reservoirs at their own equilibrium (same temperature \( T \) and two different
chemical potentials $\mu_L$ and $\mu_R$). We use and calculate NE Green’s functions (GF), which are just specific objects (correlation functions) whose thermodynamical averages are formally identical to those calculated in Hershfield approach to the steady state regime.

There is a huge literature which deals with electron transport in quantum junctions using NEGF methods, see for example Refs. [35–37] and references therein. The different GF in the central region can be obtained from two correlation functions (i.e. the so-called lesser and greater GF):

$$G^<(t, t') = -i[d(t')d(t)] ,$$

$$G^>(t, t') = i[d(t)d(t')] ,$$

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

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

$$G^*/a(t, t') = \pm \theta(\pm(t-t'))G^>(t, t') - G^<(t, t') .$$  \hspace{1cm} (22)

The interaction in the central region is obtained from a perturbation expansion, via partial resummation of Feynman diagrams, and enters the definition of the GF via the self-energy $\Sigma(t, t')$ in the Dyson equations of $G^\tau/a$ and in the quantum kinetic equations of $G^S$.

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 $G^>(\omega) - G^<(\omega) = G^\tau(\omega) - G^\eta(\omega)$ and the KMS condition [35, 36] $G^\sigma(\omega) = -e^{(\omega - i\mu)^\gamma}G^\sigma(\omega)$, one recovers the conventional relation

$$G^\tau = -f^\eta(G^> - G^<) = -f^\eta(G^\tau - G^\eta) ,$$

with $f^\eta(\omega) = [1 - G^\tau / G^\eta]^{-1} = [1 + e^{(\omega - i\mu)^\gamma}]^{-1}$ being the equilibrium Fermi-Dirac distribution.

We can now extend this formal definition to the NE conditions by defining a NE distribution function $f^\text{NE}(\omega)$ for the electron population in the NE steady state as follows:

$$G^<(\omega) = -f^\text{NE}(\omega) (G^\tau(\omega) - G^\eta(\omega)) ,$$

where we are now considering full NE GF. This is entirely justified by the fact that a NE steady-state can be seen as a pseudo-equilibrium defined by a Gibbs-like ensemble provided by either Hershfield or McLennan-Zubarev methods. In this generalised Gibbs-like ensemble, we get a generalised KMS-like relation for the NE steady state of the type $G^\tau(\omega) = -e^{\pi\omega\mu^\gamma}G^\tau(\omega)$.

From the definition $G^\tau = G^\tau\Sigma^\tau G^\tau$, where the total self-energy $\Sigma(\omega) = \Sigma_L(\omega) + \Sigma_R(\omega) + \Sigma_\text{int}(\omega)$ arises from the contributions of the leads self-energy $\Sigma_L, R$ and the self-energy $\Sigma_\text{int}$ of the interaction between particles, we can see that the total self-energy follows as well the same statistics, i.e. $\Sigma^\tau = -f^\text{NE}(\Sigma_L^\tau - \Sigma_R^\tau)$. However as we have clearly explained in Ref. [38], there is no reason for each contribution $\Sigma^\tau_L, R$ and $\Sigma_\text{int}$ 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 $f^\text{NE}(\omega)$:

$$f^\text{NE}(\omega) = \frac{f^\text{NE}_0(\omega) - i\Sigma^\tau(\omega)/\Gamma_{L+R}(\omega)}{1 + i(\Sigma^\tau_{\text{int}} - \Sigma^\tau)/\Gamma_{L+R}(\omega)} ,$$ \hspace{1cm} (25)

where $\Gamma_{L+R}(\omega)$ is the spectral function of the leads $\Gamma_{L+R} = \sum_{\alpha=L,R}(\Sigma^\alpha_{\text{int}} - \Sigma^\alpha)$, and $\Sigma^\tau_{\text{int}}$ are the lesser and greater components of the interaction self-energy.

The function $f^\text{NE}_0(\omega)$ is the NE distribution for the non-interacting case. It can be easily derived as the weighted average of the usual Fermi-Dirac distribution functions $f_{L/R}(\omega)$ of the left and right leads:

$$f^\text{NE}_0 = (\Gamma_L f_L(\omega) + \Gamma_R f_R(\omega))/\Gamma_{L+R}(\omega) .$$ \hspace{1cm} (26)

The distribution $f^\text{NE}_0(\omega)$ 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 $\mu_L - \mu_R = eV$ ($\mu_0$ 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.

The full NE distribution $f^\text{NE}(\omega)$ can be decomposed into two terms $f^\text{NE}(\omega) = f^\text{NE}_0(\omega) + \delta f^\text{NE}(\omega)$, one corresponds to the dynamically renormalized distribution $f^\text{NE}_0 = f^\text{NE}_0(\omega)/N(\omega)$ and the other is a “correction” term $\delta f^\text{NE}$ associated with the inelastic processes and given by $\Sigma_{\text{int}}$ renormalised by the same factor $N$. The renormalisation factor $N(\omega)$ is given by the sum $\sum_N^\text{NE}(\omega)$ of the spectral functions of the leads $\Gamma_{L+R}$ and of the interaction $\Gamma_{\text{int}} = i(\Sigma^\tau_{\text{int}} - \Sigma^\tau_{L} - \Sigma^\tau_{R})$, 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 $\Sigma^\text{int}(\omega) = \gamma_0(\alpha)(N_p G^S(\omega + \omega_0) + (N_p + 1)G^S(\omega + \omega_0))$. At low temperature $N_p = 0$, and we can expand Eq. (26) as a series expansion in terms of the electron-phonon coupling parameter $\gamma_0$. To lowest order, we find the following expression for the NE distribution function:

$$f^\text{NE}(\omega) \sim f^\text{NE}_0 + \frac{2\pi\gamma_0^2}{\Gamma} \times

[ A(\omega + \omega_0) (1 - f^\text{NE}_0(\omega)) f^\text{NE}_0(\omega + \omega_0) ]

- A(\omega - \omega_0) (1 - f^\text{NE}_0(\omega - \omega_0) f^\text{NE}_0(\omega)]$$ \hspace{1cm} (27)

where $A(\omega)$ is the spectral function of the central region, i.e. $A(\omega) = (G^\tau - G^\eta)/2\pi\tau$. The terms in $\gamma_0^2$ in Eq. (27) are correction terms to the non-interacting distribution $f^\text{NE}_0(\omega)$ and correspond to the lowest order contributions.
of the electron-phonon interacting (i.e. phonon emission by electron or hole in the presence of a finite bias). They are equivalent to the lowest order contributions of the interaction in the perturbation formulations of electron-phonon interaction given in Refs. [41–43].

VI. CONCLUSION

We have demonstrated that the NE density matrix developed by Hershfield for the steady state has the form of a McLennan-Zubarev non-equilibrium ensemble. According to McLennan-Zubarev NESOM and Hershfield methods, the stationary density of an open system can be written in the modified Gibbs form $\rho_{\text{NE}} = e^{-\beta(H-Y)} / Z$, with the non-equilibrium “correction term” $Y$. The operator $Y$ that was interpreted as the operator into which $Y_0 = \sum_{\mu} \mu N_{\mu}$ “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 nonequilibrium state, permits us to derive, in a rigorous way, NE quantities from the formal expressions given at equilibrium (compare Eq. (23) and Eq. (24)). We have derived an example of such quantities, i.e. the NE distribution function for the electron population in a scattering region in the context of quantum electronic transport.

Such NE distributions could be used to develop numerical schemes for quantum transport in the presence of interaction. They are also central to the understanding of other physical properties of NE quantum open systems and to the derivation of NE thermodynamical laws, such as NE fluctuation-dissipation relations and quantum entropy production.
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