Nonequilibrium Steady States and MacLennan-Zubarev Ensembles in a Quantum Junction System

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Based on a recent progress in nonequilibrium statistical mechanics of infinitely extended quantum systems, a nonequilibrium steady state (NESS) is constructed for a single-level quantum dot interacting with two free reservoirs under less general but more practically useful conditions than the previous works. As an example, a model of an Ahoronov-Bohm ring with a quantum dot is studied in detail. Then, NESS is shown to be regarded as a MacLennan-Zubarev ensemble. A formal relation between response and correlation at NESS is derived as well.

§1. Introduction

Nonequilibrium statistical ensembles have been studied for many years, but no consensus has been made. As an illustration, let us consider a MacLennan-Zubarev ensemble for a system consisting of identical particles. The system is assumed to be divided into $M$ independent parts, each of which has the energy $H_j$ and the particle number $N_j$ ($j = 1, \cdots, M$) and which are interacting by an interaction $W$. According to the MacLennan-Zubarev approach,\(^1,2\), a steady state close to a local equilibrium state is described by:

\[
\rho_+ = \frac{e^{-\sum_{j=1}^{M} \beta_j (\tilde{H}_j - \mu_j \tilde{N}_j)}}{Z} = \frac{1}{Z} \exp \left\{ -\sum_{j=1}^{M} \beta_j (H_j - \mu_j N_j) + \int_{-\infty}^{0} dse^{s} J_S(s) \right\},
\]

where $Z$ is the normalization constant, $1/\beta_j$ and $\mu_j$ are, respectively, the temperature and chemical potential of the $j$th subsystem, $\tilde{H}_j \equiv H_j + \int_{-\infty}^{0} dse^{s} \frac{dH_j(s)}{ds}$, and $\tilde{N}_j \equiv N_j + \int_{-\infty}^{0} dse^{s} \frac{dN_j(s)}{ds}$ are Zubarev’s local integrals of motion,\(^2\) and $H_j(s) = e^{iHs/\hbar} H_j e^{-iHs/\hbar}$, $N_j(s) = e^{iHs/\hbar} N_j e^{-iHs/\hbar}$ with $H \equiv \sum_j H_j + W$ the total Hamiltonian. The integrand in the left-hand side is given by $J_S(s) = \sum_{j=1}^{M} \beta_j J_j^q(s)$ where $J_j^q(s) \equiv \frac{dH_j(s)}{ds} - \mu_j \frac{dN_j(s)}{ds}$ stands for non-systematic energy flow, or heat flow, to the $j$th subsystem. A convergence factor $e^{\epsilon s}$ ($\epsilon > 0$) is introduced in the time integral, where the limit $\epsilon \to 0$ is taken after all the calculations. As discussed in Ref. 2), this ensemble well describes nonequilibrium phenomena, but it has a fundamental difficulty. Indeed, because $J_S(s)$ is the sum of heat flows divided by subsystem temperatures, it is the entropy production rate of the whole system. Hence, if the ensemble (1.1) would describe a state consistent with the second law of thermodynamics, the average of $J_S(s)$ over $\rho_+$ should be a positive constant and, as a consequence, the integral in (1.1) would diverge in the limit of $\epsilon \to 0$. 

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On the other hand, rigorous researches have been carried out on nonequilibrium steady states (NESS) of infinitely extended systems and are developed further in recent years. Those include studies on NESSs of harmonic crystals, unharmonic chains, a one-dimensional gas, unharmonic chains, an isotropic XY-chain, systems with asymptotic abelianness, a one-dimensional quantum conductor, an interacting fermion-spin system, fermionic junction systems, a quasi-spin model of superconductors, a Bose-Einstein condensate in a junction system, a Bose-Einstein condensate in a small system coupled with a large reservoir, a quantum dot coupled with several reservoirs, on nonequilibrium entropy productions and on linear responses. Moreover, we have shown that NESS constructed by this method well explains experiments on transports of some mesoscopic systems.

In this article, we illustrate the above-mentioned features in terms of a spinless-electron model of a single-level quantum dot interacting with two two-dimensional reservoirs and show that NESS can be regarded as a MacLennan-Zubarev ensemble in an appropriate sense. In the next section, the basic features of the C*-algebraic method are summarized in a less technical way. In Sec. 3, a nonequilibrium steady state (NESS) is constructed starting from a local equilibrium state with the aid of the scattering theory. Since general results were proved by Ruelle and Fröhlich, Merkli, Ueltschi, here we describe the construction under restricted but practically useful conditions and apply it to a model of an Aharonov-Bohm ring with a quantum dot. In Sec. 4, we show that NESS is an analog to the Zubarev-MacLennan ensemble under slightly different conditions from Ref. 23). As an application of this observation, we study a formal relation between response and fluctuation at NESS. The last section is devoted to concluding remarks.

Before closing this section, we describe the spinless-electron model of a single-level quantum dot interacting with two reservoirs. The system is described by creation (annihilation) operators of the reservoir electron with wave number $k \in \mathbb{R}^2$: $a_{kr}^\dagger(a_{kr})$ ($r = L$: for the left reservoir, $r = R$: for the right reservoir) and the dot electron: $c^\dagger(c)$, which satisfy the canonical anticommutation relations:

$$[a_{kr}, a_{k'r'}^\dagger]_+ = \delta_{rr'} \delta(k - k') \mathbf{1}, \quad [c, c^\dagger]_+ = \mathbf{1},$$

where $[A, B]_+ \equiv AB + BA$ is the anticommutator, $\delta_{rr'}$ the Kronecker delta, $\delta(k - k')$ the Dirac delta function, $\mathbf{1}$ the unit operator and the other anticommutators vanish. The total Hamiltonian is $H = H_L + H_R + H_D + W$ where

$$H_r \equiv \int dk \omega_{kr} a_{kr}^\dagger a_{kr} \quad (r = L \text{ or } R) \quad (1.2)$$

are the reservoir Hamiltonians, $H_D = \epsilon_0 c^\dagger c$ the dot energy and $W$ stands for the interaction among the reservoirs and the dot. In the above, $\omega_{kr} (r = L, R)$ stands for the single-electron energy of reservoir electrons: $\omega_{kL} = \omega_{kR} - eV = \hbar^2 k^2/(2m) - eV/2$ where $V$ is the bias voltage, $e$ the elementary charge, $\hbar$ the Planck constant and $m$ the effective mass, and $\epsilon_0$ is the energy of the dot level. The numbers of particles in the reservoirs and the dot are given, respectively, by $N_{L/R} = \int dk a_{kL/R}^\dagger a_{kL/R}$ and $N_D = c^\dagger c$. 
\section*{2. C*-algebraic approach}

\subsection*{2.1. C*-algebra and Time Evolution\cite{27,28}}

An essential feature of the C*-algebraic method is to discuss the properties of infinitely extended systems through the investigation of finite observables. We start from a set \( \mathcal{F} \) of operators \( A \) such that the maximum eigenvalue (more precisely, the maximum spectrum) of \( A^\dagger A \) is finite and its square root, denoted as \( \|A\| \), is used for measuring the size of \( A \) (or \( \|\cdot\| \) is a norm). The set \( \mathcal{F} \) is a complex linear space where the product and the ‘conjugation’ \( A \rightarrow A^\dagger \) are defined\(^1\), and the norm \( \|\cdot\| \) satisfies (i) \( \|A\| \geq 0 \) and \( \|A\| = 0 \) implies \( A = 0 \), (ii) \( \|A+B\| \leq \|A\| + \|B\| \) (\( \alpha \in \mathbb{C}, A, B \in \mathcal{F} \)), (iii) \( \|AB\| \leq \|A\|\|B\| \) and (iv) the C*-property: \( \|A^\dagger A\| = \|A\|^2 \). Also \( \mathcal{F} \) is complete with respect to this norm\(^*\). Such \( \mathcal{F} \) is called a C*-algebra\(,27,28\).

For the spinless electron model of a quantum dot, \( \mathcal{F} \) is a set of operators which can be approximated, with arbitrary precision, by a finite sum\(^**\):

\[
\alpha 1 + \sum_{\zeta} C_\zeta b_1(\zeta)^\dagger \cdots b_s(\zeta)^\dagger b_{s+1}(\zeta) \cdots b_{N_\zeta}(\zeta), \tag{2.1}
\]

where \( \alpha, C_\zeta \) are complex numbers, \( 1 \in \mathcal{F} \) is the unit and \( b_j(\zeta) (j = 1, \cdots N_\zeta) \) is either \( c \) or \( a_r(f) \equiv \int dkf(k)^*a_{kr} (r = L, R) \) with \( f(k) \) a square integrable function over \( \mathbb{R}^2 \), i.e., \( f \in L^2(\mathbb{R}^2) \). Namely, the algebra \( \mathcal{F} \) is generated by \( 1, c, a_L(f) \) and \( a_R(f) \). Because of the canonical anticommutation relations, one has \([a_r(f), a_r(g)]^\dagger = 0, [a_r(f), a_r(g)]^\dagger = (f, g)\delta_{rr}1 \) where \( (f, g) = \int dkf(k)g(k) \). The definition of \( \mathcal{F} \) is meaningful since \( a_r(f) \) is bounded. Indeed, the C*-property leads to

\[
\|a_r(f)\|^4 = \|a_r(f)^\dagger a_r(f)\|^2 = \|a_r(f)^\dagger a_r(f)^\dagger a_r(f)\| = \|a_r(f)^\dagger (f, f) - a_r(f)^\dagger a_r(f)^\dagger a_r(f)\| = \|a_r(f)^\dagger a_r(f)\|^2
\]

or \( \|a_r(f)\| = \sqrt{(f, f)} < +\infty \). For later use, we introduce a subset \( \mathcal{F}_{\text{res}}(\subset \mathcal{F}) \) of reservoir operators, each element of which is approximated, with arbitrary precision, by a finite sum: \( \alpha 1 + \sum_{\zeta} C_\zeta a_{l_1}(f_{\zeta,1})^\dagger \cdots a_{l_s}(f_{\zeta,s})^\dagger a_{r_{s+1}}(f_{\zeta,s+1}) \cdots a_{r_{N_\zeta}}(f_{\zeta,N_\zeta}) \) (\( r_j = L \) or \( R, f_{\zeta,j} \in L^2(\mathbb{R}^2) \), and \( \alpha, C_\zeta \) are complex numbers).

Now we turn to the description of the time evolution. Because of their unboundedness, the Hamiltonians \( H_L, H_R \) are not included in \( \mathcal{F} \) and, thus, are not observables. But, the time evolution can be defined within the framework of \( \mathcal{F} \). As an example, let us consider the free evolution.

\footnote{\( ^1 \) In the mathematical literatures such as Ref. \cite{27}, \( A^* \) is used instead of \( A^\dagger \).}

\footnote{\( ^* \) Namely, if \( \{A_n\}_{n=1}^\infty \subset \mathcal{F} \) is a sequence such that \( \|A_n - A_m\| \rightarrow 0 \) for \( n, m \rightarrow \infty \), then there is \( A \in \mathcal{F} \) such that \( \|A_n - A\| \rightarrow 0 \) as \( n \rightarrow \infty \), or \( \{A_n\}_{n=1}^\infty \) has a limit in \( \mathcal{F} \).}

\footnote{\( ^** \) Let \( A \in \mathcal{F} \), then, for arbitrary \( \epsilon > 0 \), there exist \( \alpha, C_\zeta \) and \( b_j(\zeta) (j = 1, \cdots N_\zeta) \) such that \( \|A - \{\alpha 1 + \sum_{\zeta} C_\zeta b_1(\zeta)^\dagger \cdots b_s(\zeta)^\dagger b_{s+1}(\zeta)^\dagger \cdots b_{N_\zeta}(\zeta)\}\| < \epsilon \) holds.}
evolution is denoted as $\tau_t^{(0)}(A) \equiv e^{iHt/\hbar}Ae^{-iHt/\hbar}$, then the map $A \rightarrow \tau_t^{(0)}(A)$ is linear and preserves the product, conjugation and norm: $\tau_t^{(0)}(AB) = \tau_t^{(0)}(A)\tau_t^{(0)}(B)$, $\tau_t^{(0)}(A)^\dagger = \tau_t^{(0)}(A^\dagger)$ and $\|\tau_t^{(0)}(A)\| = \|A\|$. Its infinitesimal generator is given by $\dot{\delta}(A) \equiv \left. \frac{d}{dt} \tau_t^{(0)}(A) \right|_{t=0}$ on some dense subset $D(\delta) \subset \mathcal{F}$, called the domain of $\delta^\ast$. For instance, $\dot{\delta}(a_r(f)) = -i/\hbar \int dk \omega kr \{ f(k)^\ast akr \}$ ($r = L, R$) is meaningful only when $\omega kr f(k) \in L^2(\mathbb{R}^2)$, and a set of finite sums generated by such $a_r(f)$ ($r = L, R$) together with $1$ and $c$ provide the domain $D(\delta)$ of $\delta$. The evolution $\tau_t$ generated by the total Hamiltonian $H = H_0 + W$ is defined as a solution of
\[
\frac{d}{dt} \tau_t(A) = \tau_t \left( \hat{\delta}(A) + \frac{i}{\hbar}[W, A] \right), \quad (\forall A \in D(\delta))
\]
under the initial condition $\tau_t(A)\bigr|_{t=0} = A$. The map $\tau_t$ has similar properties as $\tau_t^{(0)}$.

2.2. States\textsuperscript{(27), (28)}

Usually, a statistical state is given by a density matrix. However, within the algebraic approach, it is specified by listing the average value $\langle A \rangle$ of an arbitrary element $A \in \mathcal{F}$, i.e., by a complex-valued linear map, called a normalized positive linear functional: $A \rightarrow \langle A \rangle$, which satisfies $\langle A^\dagger A \rangle \geq 0$, $\langle 1 \rangle = 1$ and $\|A\|$. Within the algebraic approach, canonical states are formulated without explicit reference to the Hamiltonian. Remind that the grand canonical state with temperature $\beta^{-1}$ and chemical potential $\mu$ of a finite degree-of-freedom system is given by $\langle A \rangle_{gc} = \text{Tr}(Ae^{-\beta(H-\mu N)})/Z_{gc}$ with $H$ the Hamiltonian, $N$ the total number of particles and $Z_{gc}$ the normalization constant. Then, it is easy to see that the Kubo-Martin-Schwinger (KMS) boundary condition\textsuperscript{(30), (31)} $\langle A\sigma^g_{i\beta}(B)\rangle_{gc} = \langle BA \rangle_{gc}$ is satisfied with respect to $\sigma^g_{i\beta}(A) = e^{i(H-\mu N)s}Ae^{-i(H-\mu N)s}$. For infinite systems, the KMS condition defines canonical ensembles\textsuperscript{(27), (28)}. As an example, let us consider the grand canonical state with temperature $\beta^{-1}$ and chemical potential $\mu$ of the reservoir system described by $\mathcal{F}_{res}$. Let $\sigma^g_{i\beta}(a_r(f)) \equiv \int dk f(k)^\ast e^{-i(\omega kr - \mu)s}akr$ ($r = L, R$) and $\mathcal{F}^{a,g}_{res}$ be a dense set such that, for any $A \in \mathcal{F}^{a,g}_{res}$, $\sigma^g_{i\beta}(A)$ is analytic in $|\text{Im}s| \leq \beta^\ast$, then the grand canonical state is defined as a state satisfying
\[
\langle A\sigma^g_{i\beta}(B)\rangle_{gc} = \langle BA \rangle_{gc}, \quad (A, B \in \mathcal{F}^{a,g}_{res})
\]
This equation and the canonical anticommutation relation lead to
\[
\langle a_r^\dagger(f)\{\sigma^g_{i\beta}(a_{r'}(g))+a_{r'}(g)\}\rangle_{gc} = \langle [a_{r'}(g), a_r^\dagger(f)]_+ \rangle_{gc} = \delta_{rr'} \langle g, f \rangle = \delta_{rr'} \int dk g(k)^\ast f(k).
\]
Since $\sigma^g_{i\beta}(a_r(g)) + a_{r'}(g) = \int dk g(k)^\ast (e^{i(\omega kr - \mu)} + 1)akr$, by replacing $g(k)$ by $g(k)F(\omega kr)$ with $F(x) \equiv 1/\{e^{\beta(x-\mu)} + 1\}$ the Fermi distribution function, one obtains
\[
\langle a_r^\dagger(f)a_{r'}(g)\rangle_{gc} = \delta_{rr'} \int dk g(k)^\ast f(k)F(\omega kr).
\]
\textsuperscript{(*)} Namely, any $A \in \mathcal{F}$ can be approximated by an element of $D(\delta)$ with arbitrary precision.
\textsuperscript{(**)} $\mathcal{F}^{a,g}_{res}$ can be a set of finite sums generated by $a_r(f)$ with $f(k)e^{i(\omega kr - \mu)s} \in L^2(\mathbb{R}^2) \ (|\text{Im}s| \leq \beta)$. 
In the same way, one can show that the state \( \langle \cdots \rangle_{gc} \) satisfies Wick’s theorem. In short, the KMS condition fully determines the state \( \langle \cdots \rangle_{gc} \). In general, if no phase transition takes place, the KMS state is unique and, if a phase transition occurs, several KMS states exist as a result of spontaneous symmetry breaking.

A local equilibrium state can also be defined as a KMS state. As an example, we consider a local equilibrium state where the left (right) reservoir is in the equilibrium state with temperature \( 1/\beta_L \) and chemical potential \( \mu_L \) (\( \mu_R \)). Consider a map \( \sigma_s \) formally expressed as \( \sigma_s(A) = e^{i\sum r \beta_r (H_r - \mu_r N_r)} A e^{i\sum r \beta_r (H_r - \mu_r N_r)} \) and defined by \( \sigma_s(a_r(f)) = \int dk f(k)^* e^{i\beta_r (\omega_{kr} - \mu_r)} a_{kr} \) (\( r = L, R \)) and \( \sigma_s(c) = c \), then a local equilibrium state \( \langle \cdots \rangle_{loc} \) is given by a KMS condition \( \langle A \sigma_s(B) \rangle_{loc} = \langle BA \rangle_{loc} \) (\( A \in F, B \in F_{\text{res}} \)), where \( B \in F_{\text{res}} \) implies that \( \sigma_s(B) \) is analytic in \( |\text{Im}s| \leq 1 \). It again satisfies Wick’s theorem and its nonvanishing two-point functions are

\[
\langle a_r^\dagger(f) a_r(g) \rangle_{loc} = \int dk g(k)^* f(k) F_r(\omega_{kr}) \quad (r = L, R), \quad \langle c^\dagger c \rangle_{loc} = \frac{1}{2}
\]

where \( F_r(x) = 1/\{e^{\beta_r (x - \mu_r)} + 1 \} \) (\( r = L, R \)) are the Fermi distribution functions.

### 2.3. Ergodicity \( ^{27, 28} \)

If the decay of dynamical correlations is sufficiently fast, certain states have ergodicity. One of such dynamical conditions is the asymptotic abelian property: \( ^{27} \)

\[
\lim_{|t| \to \infty} \| [A, \tau_t(B)] \| = 0, \quad (A \text{ or } B \in F_{\text{even}}) \tag{2.3}
\]

\[
\lim_{|t| \to \infty} \| [A, \tau_t(B)]_+ \| = 0, \quad (A \text{ and } B \in F_{\text{odd}}) \tag{2.4}
\]

where \( F_{\text{even/odd}} \equiv \{A \in F : A \text{ consists of even/odd numbers of Fermion operators.} \} \) and \( [A, B] \) stands for the commutator: \( [A, B] = AB - BA \). Then, as stated below (Example 4.3.24 of Ref. 27), a clustering property is satisfied by a class of states called \( \text{‘factor’ states} \), which include unique KMS states. Roughly speaking, a state \( \langle \cdots \rangle \) is called \( \text{‘factor’} \) if any \( D \in F \) satisfying \( \langle [A, D] \rangle = 0 \) (\( \forall A \in F \)) behaves as some complex number \( \gamma \) in the sense of \( \langle ADB \rangle = \gamma \langle AB \rangle \) (\( \forall A, B \in F \)).

**Clustering Property:** \( ^{27} \) For an asymptotic abelian evolution \( \tau_t \) and a factor state \( \langle \cdots \rangle \), one has

\[
\lim_{|t| \to \infty} \{|\langle A \tau_t(B) C \rangle - \langle AC \rangle \langle \tau_t(B) \rangle|\} = 0.
\]

If \( \langle \tau_t(A) \rangle = \langle A \rangle \) (\( \forall A \in F \)), it is mixing: \( \lim_{|t| \to \infty} \langle A \tau_t(B) C \rangle = \langle AC \rangle \langle B \rangle \).

For the spinless electron model of a quantum dot, we show that the local equilibrium state \( \langle \cdots \rangle_{loc} \) restricted to the subalgebra \( F_{\text{res}} \) generated by \( 1, a_L(f) \) and \( a_R(f) \) is

\( ^{27} \) Given a state \( \langle \cdots \rangle \) over a \( C^* \)-algebra \( F \), it can be represented as a subalgebra \( \pi(F) \) of the algebra \( B \) of all bounded operators on some Hilbert space \( \mathcal{H} \) as \( \langle A \rangle = \langle \Omega, \pi(A) \Omega \rangle \) with a cyclic vector \( \Omega \in \mathcal{H} \) (GNS representation). Let \( \pi(F)' \equiv \{a \in B : [a, b] = 0, \forall b \in \pi(F)\} \) and \( \pi(F)'' \equiv \{c \in B : [c, a] = 0, \forall a \in \pi(F)\} \), then \( \langle \cdots \rangle \) is called a factor state iff \( \pi(F)' \cap \pi(F)'' = \mathbb{C}1 \), where \( \mathbb{C} \) is the set of complex numbers and \( 1 \) is the unit of \( \pi(F) \).
mixing with respect to the evolution \( \tau_t^{(0)} \). The state \( \langle \cdots \rangle_{loc} \) is a factor state as a unique KMS state and is easily shown to be \( \tau_t^{(0)} \)-invariant. On the other hand, for \( A, B \in \mathcal{F}_{res} \), their commutator \([A, \tau_t^{(0)}(B)]\) can be approximated with arbitrary precision by a finite sum of the terms like \( C_t[a_r(f), \tau_t^{(0)}(a_r(g)^\dagger)]_+ D_t \) \( (C_t, D_t \in \mathcal{F}_{res}) \) and its conjugate. Then, the Riemann-Lebesgue theorem\(^{32} \) gives

\[
\| C_t[a_r(f), \tau_t^{(0)}(a_r(g)^\dagger)]_+ D_t \| \leq \sup_t \| C_t \| \| D_t \| \int dk f(k)^* g(k)e^{i\omega_k t/h} \rightarrow 0 \quad (|t| \rightarrow \infty). 
\]

Thus, one has \( \lim_{|t| \rightarrow \infty} \| [A, \tau_t^{(0)}(B)] \| = 0 \), or \( \tau_t^{(0)} \) is asymptotic abelian. Therefore, as a result of Clustering Property, local equilibrium state \( \langle \cdots \rangle_{loc} \) restricted to \( \mathcal{F}_{res} \) is mixing with respect to \( \tau_t^{(0)} \):

\[
\lim_{|t| \rightarrow \infty} \langle A \tau_t^{(0)}(B)C \rangle_{loc} = \langle AC \rangle_{loc} \langle B \rangle_{loc} \quad (A, B, C \in \mathcal{F}_{res})
\]

(2.5)

Note that the state \( \langle \cdots \rangle_{loc} \) is not ergodic on the whole algebra \( \mathcal{F} \) with respect to \( \tau_t^{(0)} \) because \( \langle c^\dagger \tau_t^{(0)}(c) \rangle_{loc} = e^{-i\omega t/h} \langle c^\dagger c \rangle_{loc} \) does not converge for \( |t| \rightarrow \infty \).

§3. Nonequilibrium Steady States

3.1. Scattering Problem and Nonequilibrium Steady States

As discussed in Refs. 3, 6, 7, 9–14, 18, 19, 22–24, a nonequilibrium steady state (NESS) \( \langle \cdots \rangle_{+/-} \) is constructed dynamically as an asymptotic state starting from the local equilibrium state \( \langle \cdots \rangle_{loc} \) introduced in Sec. 2.2 \( \langle A \rangle_{+/-} \equiv \lim_{t \rightarrow \pm \infty} \langle \tau_t(A) \rangle_{loc} \) as discussed by Ruelle\(^7 \) for systems with \( L^1 \)-asymptotic abelian property and by Fröhlich, Merkli and Ueltschi\(^{12} \) for quantum junction systems, the construction of NESS is closely related to the scattering problem. Here we give a restrictive but practically useful characterization used in Refs. 25, 26).

For the spinless model of a quantum dot, the interaction \( W \) induces scattering of the left/right-reservoir electrons and the process is described by asymptotic fields:\(^{28} \)

\[
a_r^{(in/out)}(f) = \lim_{t \rightarrow -\infty/+\infty} \tau_t^{-1}(\tau_t^{(0)}(a_r(f))), \quad (r = L, R)
\]

(3.1)

where \( a_r^{(in/out)}(f) \) are incoming/outgoing fields and the limit is taken in an appropriate sense. Here we consider a case where the limit exists in norm:

\[
\lim_{t \rightarrow -\infty/+\infty} \| \tau_t^{-1}(\tau_t^{(0)}(a_r(f))) - a_r^{(in/out)}(f) \| = 0, \quad (r = L, R)
\]

(3.2)

and the initial state \( \langle \cdots \rangle_{loc} \) is \( \tau_t^{(0)} \)-invariant. Then, one has\(^{25, 26} \)

**Proposition 1:** If, for some subset \( D_0 \subset L^2(\mathbb{R}^2) \), (i) the limits exist for any \( f \in D_0 \), (ii) the fields \( a_r^{(in/out)}(f) \) \( (r = L, R, f \in D_0 \subset L^2(\mathbb{R}^2)) \) generate the whole algebra \( \mathcal{F} \) and (iii) \( \langle \cdots \rangle_{loc} \) is \( \tau_t^{(0)} \)-invariant, then, the limit

\[
\langle A \rangle_{+/-} \equiv \lim_{t \rightarrow +\infty/-\infty} \langle \tau_t(A) \rangle_{loc}, \quad (\forall A \in \mathcal{F})
\]

(3.3)
exists and defines a (nonequilibrium) $\tau$-invariant state $\langle \cdots \rangle_{+/\mp}$. Moreover,

$$
\langle a_{r_1}^{\text{out}}(f_1)^\dagger \cdots a_{r_N}^{\text{out}}(f_N)^\dagger a_{r_{s+1}}^{\text{out}}(f_{s+1}) \cdots a_{r_N}^{\text{out}}(f_N) \rangle_{\text{loc}} = \langle a_{r_1}^{\text{in}}(f_1)^\dagger \cdots a_{r_N}^{\text{in}}(f_N)^\dagger a_{r_{s+1}}^{\text{in}}(f_{s+1}) \cdots a_{r_N}^{\text{in}}(f_N) \rangle_{\text{loc}}.
$$

(3.4)

**N.B.** For a model of a single-level quantum dot coupled with free reservoirs (SEBB model) where the interaction is bilinear with respect to field operators, Aschbacher, Jakšić, Pautrat and Pillet derive an equivalent characterization to Proposition 1, but the present form is applicable, in principle, even to the case where the interaction is not bilinear.

In the previous section, we have seen that the unperturbed evolution restricted to the reservoir algebra $F_{\text{res}}$ is mixing. As a consequence, as first shown by Ruelle (see also Ref. 24), the steady states $\langle \cdots \rangle_{\pm}$ are mixing with respect to the full evolution $\tau_t$ in both directions of time:

**Proposition 2:** Under the same conditions as Proposition 1, the steady state $\langle \cdots \rangle_{+/\mp}$ satisfies

$$
\lim_{|t| \to \infty} \langle A \tau_t(B)C \rangle_{+/\mp} = \langle AC \rangle_{+/\mp} \langle B \rangle_{+/\mp}, (A, B, C \in F).
$$

(3.5)

**Proof of Proposition 1:** It can be shown immediately from the following lemma:

**Lemma 3:** If the limits $\lim_{r=L,R} a_r^{\text{in/out}}(f)$ exist and the fields $a_r^{\text{in/out}}(f)$ ($r = L, R$) generate the whole algebra $F$, there exists $\gamma_{+/\mp}(A) \in F$ for any $A \in F$ such that $\lim_{t \to \pm \infty} \| A - \tau_t(\gamma_{+/\mp}(A)) \| = 0$. The map $\gamma_{+/\mp}$ is a *-isomorphism between $F$ and the reservoir algebra $F_{\text{res}}$ generated by $a_r(f)$ ($r = L, R$), namely, (i) $\gamma_{+/\mp}(A) \in F_{\text{res}}$, (ii) $\gamma_{+/\mp}(\alpha A) = \alpha \gamma_{+/\mp}(A)$, (iii) $\gamma_{+/\mp}(AB) = \gamma_{+/\mp}(A)\gamma_{+/\mp}(B)$, (iv) $\gamma_{+/\mp}(A^\dagger) = \gamma_{+/\mp}(A)^\dagger$, and (v) $\gamma_{+/\mp}$ is one-to-one and onto. Moreover, (vi) $\| A \| = \| \gamma_{+/\mp}(A) \|$ and

$$
\gamma_+ \left( a_{r_1}^{\text{out}}(f_1)^\dagger \cdots a_{r_N}^{\text{out}}(f_N)^\dagger a_{r_{s+1}}^{\text{out}}(f_{s+1}) \cdots a_{r_N}^{\text{out}}(f_N) \right) = a_{r_1}^{\text{in}}(f_1)^\dagger \cdots a_{r_N}^{\text{in}}(f_N)^\dagger a_{r_{s+1}}^{\text{in}}(f_{s+1}) \cdots a_{r_N}^{\text{in}}(f_N),
$$

\(3.6\)

The maps $\gamma_{+/\mp}$ are nothing but the Møller morphisms $\gamma_{+/\mp}$. Therefore, the $\tau(0)$-invariance of $\langle \cdots \rangle_{\text{loc}}$ gives

$$
\lim_{t \to \pm \infty} \frac{\| \tau_t^{(0)}(A) \|}{\| A \|} = 0.
$$

(3.7)

Indeed, this lemma and $\tau_t^{(0)}$-invariance of $\langle \cdots \rangle_{\text{loc}}$ give

$$
\left| \langle \tau_t(A) \rangle_{\text{loc}} - \langle \gamma_{+/\mp}(A) \rangle_{\text{loc}} \right| = \left| \langle \tau_t^{(0)}(A) - \tau_t^{(0)}(\gamma_{+/\mp}(A)) \rangle_{\text{loc}} \right|.
$$
\begin{align*}
\leq &\|\tau_t\left(A - \tau_{-t}(\tau_{-t}^{-1}(\gamma_\pm(A)))\right)\| = \|A - \tau_{-t}(\tau_{-t}^{-1}(\gamma_\pm(A)))\| \to 0 \quad (t \to \pm \infty),
\end{align*}

or \((A)_\pm \equiv \lim_{t \to \pm \infty} \langle \tau_t(A) \rangle_{\text{loc}} = \langle \gamma_\pm(A) \rangle_{\text{loc}}\) exists. Clearly, the map \(A \to \langle A \rangle_\pm\) is linear and, as \(\langle A^1A \rangle_\pm = \lim_{t \to \pm \infty} \langle \tau_t(A)^1\tau_t(A) \rangle_{\text{loc}} \geq 0\) and \((1)_\pm = \lim_{t \to +\infty} \langle \tau_t(1) \rangle_{\text{loc}} = 1,\)
\(\langle \cdot \cdot \cdot \rangle_\pm\) defines a state. And it is invariant: \(\langle \tau_t(A) \rangle_\pm \equiv \lim_{t' \to \pm \infty} \langle \tau_{t+t'}(A) \rangle_{\text{loc}} = \langle A \rangle_\pm\).
By substituting \(A = a_{r_1}^{(\text{in/out})}(f_1)^{±} \cdots a_{r_s}^{(\text{in/out})}(f_s)^{±} a_{r_{s+1}}^{(\text{in/out})}(f_{s+1}) \cdots a_{r_N}^{(\text{in/out})}(f_N)\) into \(\langle A \rangle_\pm = \langle \gamma_\pm(A) \rangle_{\text{loc}},\)
\(\text{(3.3)}\) immediately follows from \(\text{(3.1)}\). \(\text{(Q.E.D.)}\)

**Proof of Proposition 2.** We only show it in case of \((\cdot \cdot \cdot)_+\). Eq.\((3.1)\) gives
\(\|\tau_t^{(0)}(\gamma_+(A)) - \gamma_+(\tau_t(A))\| \leq \|\tau_t^{(0)}(\gamma_+(A)) - \tau_t^{(0)}(\tau_s^{(0)}(\gamma_+(A)))\| \to 0 \quad (s \to +\infty),\)
i.e., \(\tau_t^{(0)}(\gamma_+(A)) = \gamma_+(\tau_t(A)) (\forall t \in \mathbb{R})\). On the other hand, as shown in the proof of Proposition 1, we have \(\langle A \rangle_+ = \langle \gamma_+(A) \rangle_{\text{loc}}\) and \(\gamma_+(A) \in \mathcal{F}_{\text{res}}\), thus, \(\text{(2.3)}\) gives
\begin{align*}
\lim_{|t| \to \infty} \langle A \tau_t(B)C \rangle_+ &= \lim_{|t| \to \infty} \langle \gamma_+(A)\gamma_+(\tau_t(B))\gamma_+(C) \rangle_{\text{loc}} \\
&= \lim_{|t| \to \infty} \langle \gamma_+(A)\tau_t^{(0)}(\gamma_+(B))\gamma_+(C) \rangle_{\text{loc}} = \langle \gamma_+(A)\gamma_+(C) \rangle_{\text{loc}} \langle \gamma_+(B) \rangle_{\text{loc}} \\
&= \langle AC \rangle_+ \langle B \rangle_+. \quad (\text{Q.E.D.})
\end{align*}

**Proof of Lemma 3:** Let us consider the case of incoming fields. Because of \(\text{(3.3)}\) and \(\|\tau_t^{(0)}(a_r(f)^{±})\| = \|a_r(f)^{±}\|\), one has
\begin{align*}
\|\tau_t^{(0)}(a_r(f)^{±})a_r^{(\text{in})}(g)\| &\leq \|a_r^{(\text{in})}(f)^{±}\| \|\tau_t^{(0)}(a_r^{(\text{in})}(g))\| - a_r^{(\text{in})}(g)\| + \|\tau_t^{(0)}(a_r(f)^{±}) - a_r^{(\text{in})}(f)^{±}\| \|a_r^{(\text{in})}(g)\| \to 0 \quad (t \to -\infty).
\end{align*}
Repeating the same arguments, one finds
\begin{align*}
\lim_{t \to -\infty} \|\tau_t^{(0)}(a_{r_1}(f_1)^{±_1} \cdots a_{r_N}(f_N)^{±_N}) - a_{r_1}^{(\text{in})}(f_1)^{±_1} \cdots a_{r_N}^{(\text{in})}(f_N)^{±_N}\| &= 0, \quad (3.8)
\end{align*}
where \(\zeta_j \ (j = 1, \cdots N)\) stands for \(\dagger\) or no symbol. Therefore, for any finite sum:
\begin{align*}
A_f \equiv \alpha 1 + \sum_{\zeta} C_{\zeta} a_{r_1}^{(\text{in})}(f_{\zeta,1})^{±_1} \cdots a_{r_s}^{(\text{in})}(f_{\zeta,s})^{±_s} a_{r_{s+1}}^{(\text{in})}(f_{\zeta,s+1})^{±_{s+1}} \cdots a_{r_N}^{(\text{in})}(f_{\zeta,N})^{±_N}, \quad (3.9)
\end{align*}
where \(\alpha, C_{\zeta} \in \mathbb{C}\), there exists
\begin{align*}
B_f \equiv \alpha 1 + \sum_{\zeta} C_{\zeta} a_{r_1}(f_{\zeta,1})^{±_1} \cdots a_{r_s}(f_{\zeta,s})^{±_s} a_{r_{s+1}}(f_{\zeta,s+1})^{±_{s+1}} \cdots a_{r_N}(f_{\zeta,N})^{±_N} \in \mathcal{F}_{\text{res}} \quad (3.10)
\end{align*}
such that \(\lim_{t \to -\infty} \|A_f - \tau_t^{(0)}(B_f)\| = 0\). On the other hand, as the fields \(a_r^{(\text{in})}(f)\) \((r = L, R)\) generate \(\mathcal{F}\), any \(A \in \mathcal{F}\) can be approximated by a finite sum \(\text{(3.9)}\) with arbitrary precision. Thus, for any \(A \in \mathcal{F}\), there exists \(B \in \mathcal{F}_{\text{res}}\) such that
\begin{align*}
\lim_{t \to -\infty} \|A - \tau_t^{(0)}(B)\| = 0. \quad \text{As such B is unique, we define B \equiv \gamma_+(A),}
\end{align*}
Then, the properties (ii), (iii), (iv) and (vi) can be shown immediately. For example, (vi) follows from $\|\gamma_+(A)\| - \|A\| \leq \|\tau_t^{(0)}(\gamma_+(A)) - A\| \to 0$ $(t \to -\infty)$. The property (vi) implies that $\gamma_+$ is one-to-one. Moreover, since any $B \in \mathcal{F}_{\text{res}}$ can be approximated by a finite sum $\sum_k$, one can find $A \in \mathcal{F}$ such that $\gamma_+(A) = B$ or $\gamma_+$ is onto. The second equality of (3.12) follows from the definition of $\gamma_+$ and (3.8). The properties of $\gamma_-$ can be proved in the same way. (Q.E.D.)

3.2. Nonequilibrium Steady States for Aharonov-Bohm Ring with Quantum Dot

In this subsection, we further investigate the properties of NESS $\langle \cdots \rangle_+$ when the reservoir-dot interaction is described by a sum of two tunneling interactions:

$$W = \int dk \left\{ u_{kL} a_{kL}^\dagger c + u_{kR} a_{kR}^\dagger c \right\} + we^{i\varphi} \int dk dq u_{kL} u_{qR} a_{kL}^\dagger a_{qR} + (\text{h.c.}) ,$$

(3.11)

where the first term corresponds to a tunneling via a quantum dot and the second to a direct tunneling between the two reservoirs. Real parameters $w$ and $\varphi$ are, respectively, the relative strength and phase between the two processes. This model describes an Aharonov-Bohm (AB) ring with a quantum dot and, when $w = 0$, it reduces to a model of a single-level quantum dot embedded between two reservoirs studied in Ref. 24. The tunneling matrix elements are assumed to satisfy:

(a) The real-valued functions $u_{kr}$ ($r = L, R$) are infinitely differentiable with respect to $k \in \mathbb{R}^2$ and $u_{kr} = 0$ when $|k| \leq k_0$ or $|k| \geq k_1$ (for some $0 < k_0 < k_1$). Then, the functions $\Gamma_r(\omega) \equiv 2\pi \int dk |u_{kr}|^2 \delta(\omega - \omega_{kr})$ ($r = L, R$) are integrable and infinitely differentiable on the whole real axis.

(b) Let $M_r(z) \equiv \int dk |u_{kr}|^2/(z - \omega_{kr})$, then the function

$$A(z) = (1 - w^2 M_L(z) M_R(z))(z - \epsilon_0) - \sum_{r=L,R} M_r(z) - 2w \cos \varphi M_L(z) M_R(z)$$

has no real zeros and, hence, $1/A_\pm(\omega) \equiv \lim_{\epsilon \to 0, \epsilon > 0} 1/A(\omega \pm i\epsilon)$ is bounded.

3.2.1. Construction of NESS

To derive incoming fields, it is enough to study the evolution $\tau_{-t} \tau_t^{(0)}(a_{r_0}(f))$ where $f(k)$ is in a set $C_0^\infty(\mathbb{R}^2)$ of infinitely differentiable localized functions as $C_0^\infty(\mathbb{R}^2)$ is dense in $L^2(\mathbb{R}^2)$. Then, thanks to the bilinearity of $W$, $\tau_{-t}(a_{r_0}(f))$ is written as

$$\tau_{-t}(a_{r_0}(f)) = \sum_{r'=L,R} a_{r'}(\psi_{r'}(t)) + \psi_0(t)^*c .$$

From the equation of motion $\frac{d}{dt} \tau_{-t}(a_{r_0}(f)) = -\frac{i}{\hbar} [W, \tau_{-t}(a_{r_0}(f))]$, the functions $\psi_{r'}(k; t)$ and $\psi_0(t)$ are found to satisfy

$$ih \frac{\partial}{\partial t} \psi_{r'}(k; t) = \omega_{kr} \psi_{r'}(k; t) + u_{r'}(k) \left\{ \psi_0(t) + we^{i\varphi_{r'}} \int dk' u_{r'}^*(k') \psi_{r'}(k'; t) \right\} ,$$

$$ih \frac{\partial}{\partial t} \psi_0(t) = \epsilon_0 \psi_0(t) + \sum_{r'=L,R} \int dk' u_{r'}(k') \psi_{r'}(k'; t) ,$$

(3.12)

*) More precisely, functions with compact support.
with an initial condition: \( \psi^{\nu'}(k; 0) = \delta^{\nu'}_{\varphi} f(k) \), \( \psi_c(0) = 0 \), where \( \bar{L} = R, \bar{R} = L \), \( \varphi_L = -\varphi_R = \varphi \). The linear equations (3.12) can be solved easily and one has

\[
\psi^{\nu'}(k; t) = \sum_{r' = L, R} \int \frac{d k}{2} \frac{u_{r'}(k) \chi_{r'}^+(\omega_{kr'})}{A_+(\omega_{kr'})} F_{kr'}(t) + \sum_{r' = L, R} \int \frac{d k}{2} \frac{u_{r'}(k) \chi_{r'}^+(\omega_{kr'})}{A_+(\omega_{kr'})} F_{kr'}(t)
\]

where \( A_\pm(\omega) \) is introduced in (b), \( \xi^\pm(x) \equiv 1 + M_\pm(x)(2w \cos \varphi + w^2(x - \epsilon_0)), \)
\( \kappa_r(x) \equiv 1 + re^{i\varphi_r}(x-\epsilon_0), \chi^\pm(x) \equiv 1 + re^{i\varphi}, M^\pm_L(x) \) with \( M_r^\pm(x) = \lim_{\epsilon \to 0} M_r(x \pm i\epsilon) \),

\[
F_{kr}(t) = e^{-i\omega_{kr} t} \left[ \psi_r(k) + \frac{u_r(k)}{A_-(\omega_{kr})} \int \frac{d k'}{2} \frac{\xi^+(\omega_{kr}) u_r(k') \psi_r(k')}{\omega_{kr} - \omega_{kr'} - i0} \right],
\]

with \( \psi_r(k) = \delta_{r \varphi}^L f(k) \). When \( f(k) \in C^\infty_0(\mathbb{R}^2) \) and the conditions (a), (b) are satisfied, the limits like \( \int dk h(k)/(x - \omega_{kr} \pm i0) \equiv \lim_{\epsilon \to 0} \int dk h(k)/(x - \omega_{kr} \pm i\epsilon) \)

converge pointwise and uniformly with respect to \( x \). As a consequence, \( \tau_{-t} \tau_t^{(0)}(a_{r_0}(f)) \) is again a linear combination

\[
\tau_{-t} \tau_t^{(0)}(a_{r_0}(f)) = \sum_{r' = L, R} a_{r'}(\psi^{(in)}_{r_0r'}(f)) + \psi^{(in)}_{r_0c}(f) c + \sum_{r' = L, R} a_{r'}(\Delta \bar{\psi}_r(t)) + \Delta \bar{\psi}_c(t) c
\]

where \( \psi^{(in)}_{r_0r'}(k; f), \psi^{(in)}_{r_0c}(f) \) are derived from (3.13) by replacing \( F_{kr}(t) \) to \( \delta_{r \varphi}^L f(k) \):

\[
\psi^{(in)}_{r_0r'}(k; f) \equiv f(k) + \int \frac{d k'}{2} \frac{u_{r_0}(k) u_{r_0}(k') \xi^+(\omega_{kr'_0})}{A_+(\omega_{kr'_0})} f(k'),
\]

\[
\psi^{(in)}_{r_0r}(k; f) \equiv \int \frac{d k'}{2} \frac{u_{r_0}(k) u_{r_0}(k') \xi^+(\omega_{kr'_0})}{A_+(\omega_{kr'_0})} f(k'),
\]

\[
\psi^{(in)}_{r_0c}(f) \equiv \int \frac{d k'}{2} \frac{u_{r_0}(k') \chi_{r_0}^+(\omega_{kr'_0})}{A_+(\omega_{kr'_0})} f(k'),
\]

and \( \Delta \bar{\psi}_r(t), \Delta \bar{\psi}_c(t) \) are obtained from (3.13) by replacing \( F_{kr}(t) \) to

\[
\Delta \bar{F}_{kr}(t) = \frac{u_r(k)}{A_-(\omega_{kr})} \eta_{r_0}(\omega_{kr}) \int \frac{d k'}{2} \frac{u_{r_0}(k') f(k')}{\omega_{kr} - \omega_{kr'} - i0} e^{i(\omega_{kr} - \omega_{kr'}) t/h},
\]

with \( \eta_{r_0}(x) = \xi^+_r(x), \eta_{r_0}(x) = \kappa_r(x) \). Reminding \( \lim_{t \to +\infty} e^{-i\omega t}/(x + i0) = -2\pi \delta(x) \)

in the sense of distribution, one expects \( \Delta \bar{F}_{kr}(t) \to 0 \) \( (t \to +\infty) \) and thus,

\[
\tau_{-t} \tau_t^{(0)}(a_{r_0}(f)) \to \sum_{r' = L, R} a_{r'}(\psi^{(in)}_{r_0r'}(f)) + \psi^{(in)}_{r_0c}(f) c \equiv a_{r_0}^{(in)}(f), \quad (t \to +\infty).
\]

Indeed, if the conditions (a) and (b) are satisfied and \( f \in C^\infty_0(\mathbb{R}^2) \), an argument similar to those of Refs. 14, 29 gives

\[
\|\tau_{-t} \tau_t^{(0)}(a_{r_0}(f)) - a_{r_0}^{(in)}(f)\| \leq \sum_{r' = L, R} \|a_{r'}(\Delta \bar{\psi}_r(t))\| + |\Delta \bar{\psi}_c(t)|
\]
Moreover, under the condition (a), the original operators are expressed as
\[
    a_r(f) = \sum_{r'=L,R} a_{r'}^{(in)} (\varphi_{r'r}(f)) , \quad c = \sum_{r'=L,R} a_{r'}^{(in)} (\varphi_{r'r}) ,
\]
where the functions \(\varphi_{r'r}(k; f)\) and \(\varphi_{r'r}(k)\) are given by
\[
    \varphi_{r'r}(k; f) = \delta_{r'r} f(k) + \frac{u_{r'}(k) \gamma_{r'r}(\omega_{kr'})}{\Lambda_{-}(\omega_{kr'})} \int dk' \frac{u_{r'}(k') f(k')}{\omega_{kr'} - \omega_{kr'} - i0} ,
\]
\[
    \varphi_{r'r}(k) = \frac{u_{r'}(k) \gamma_{r'r}(\omega_{kr'})*}{\Lambda_{-}(\omega_{kr'})} .
\]
This implies that the incoming fields generate the whole algebra \(\mathcal{F}\). Then, because of Proposition 1 and the fact that Wick’s theorem holds for the expectation value of a product of \(a_r(f)\) and \(a_{r'}(f')^\dagger\) with respect to \(\langle \cdot \cdot \cdot \rangle_{loc}\), we find:

**Proposition 4:** For the model where the interaction is given by Eq. (3.11), if the tunneling matrix elements satisfy the conditions (a) and (b), then the limit: \(\lim_{t \to +\infty} \langle \tau(t) (A) \rangle_{loc} \equiv \langle A \rangle_+\) exists for any \(A \in \mathcal{F}\) and defines a steady state. Moreover, the steady state \(\langle \cdot \cdot \cdot \rangle_+\) satisfies Wick’s theorem with respect to the incoming fields \(a_r^{(in)}(f)\) introduced in Eqs. (3.14) and (3.15), and the nonvanishing two-point functions are given by
\[
    \langle a_{r_1}^{(in)}(f_1)^\dagger a_{r_2}^{(in)}(f_2) \rangle_+ = \langle a_{r_1}^{(in)}(f_1) a_{r_2}^{(in)}(f_2) \rangle_{loc} = \int dk f_2(k)^* f_1(k) F_r(\omega_{kr_1}) ,
\]
where \(F_r(x) = 1/\{e^{\beta_r(x-\mu_r)} + 1\}\) \((r = L, R)\) is the Fermi distribution function of inverse temperature \(\beta_r\) and chemical potential \(\mu_r\).

A simple interpretation could be given to this result. Suppose that there exists an invariant vacuum state \(|\text{vac.}\rangle\), then, due to the difference between the Schrödinger and Heisenberg pictures, the vector \(\tau_{-t}(a_r^{(in)}(f)^\dagger)|\text{vac.}\rangle\) describes a one-particle state at time \(t\) starting from an initial state: \(a_r^{(in)}(f)^\dagger|\text{vac.}\rangle\). When \(t \ll 0\), one may regard \(\tau_{-t}(a_r^{(in)}(f)^\dagger)|\text{vac.}\rangle \simeq \tau_{-t}^{(0)}(a_r(f)^\dagger)|\text{vac.}\rangle\) as a consequence of a relation: \(\lim_{t \to -\infty} \|\tau_{-t}^{(0)}(a_r(f)^\dagger) - \tau_{-t}(a_r^{(in)}(f)^\dagger)\| = 0\) (cf. Eq. (3.2)). In this sense, \(a_r^{(in)}(f)^\dagger\) describes a particle which was an unperturbed particle of the \(r\)th reservoir in the far past. Thus, \(\langle \cdot \cdot \cdot \rangle_+\) is a steady state such that particles carry the temperature and chemical potential of the reservoir from which they come.

### 3.2.2. Transports

As an application of Proposition 4, transports in the steady state \(\langle \cdot \cdot \cdot \rangle_+\) will be studied. Formally the energy and the particle number of the reservoir are expressed, respectively, by \(H_r = \int dk \omega_{kr} a_{kr}^\dagger a_{kr}\) and \(N_r = \int dk a_{kr}^\dagger a_{kr}\) \((r = L, R)\), and a formal calculation leads to
\[
    \frac{d}{dt} e^{iHt/\hbar} N_r e^{-iHt/\hbar} \bigg|_{t=0} = -\frac{i}{\hbar} \left( a_r(u_r)^\dagger \{ c + we^{i\varphi_r} a_r(u_r) \} - (\text{h.c.}) \right) \equiv J_r ,
\]
where \( u_r(k) \) is the tunneling matrix elements, \( u^E_r(k) = \omega_k u_r(k) \), and \( J_r, J_r^E \in \mathcal{F} \) are defined by the middle expressions. Therefore, \( J_r \) and \( J_r^E \) \((r = L, R)\) can be regarded as the particle and energy flows to the reservoirs. Then, \( \text{Ref. 16} \), \( \text{Ref. 17} \) and Proposition 4 give

**Proposition 5:** The steady state considered in Proposition 4 carries the particle and energy flows:

\[
\langle J_L \rangle_+ = -\langle J_R \rangle_+ = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} d\omega T(\omega) \{ F_R(\omega) - F_L(\omega) \} , \tag{3.20}
\]

\[
\langle J_L^E \rangle_+ = -\langle J_R^E \rangle_+ = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} d\omega T(\omega) \{ F_R(\omega) - F_L(\omega) \} . \tag{3.21}
\]

where

\[
T(\omega) = \left| \frac{1 + we^{i\omega}(\omega - \epsilon_0)}{\Lambda_+^{(\omega)}} \right|^2 \Gamma_L(\omega) \Gamma_R(\omega) .
\]

The entropy production rate \( J_S \equiv \sum_\beta \beta_r J^0_\beta \), where \( J^0_r = J^E_r - \mu_r J_r \) are heat flows to the reservoirs, has the following NESS average

\[
\langle J_S \rangle_+ = \int_{-\infty}^{\infty} d\omega \frac{T(\omega)}{2\pi\hbar} \{ F_R(\omega) - F_L(\omega) \} \{ \beta_L(\omega - \mu_L) - \beta_R(\omega - \mu_R) \} ,
\]

which is nonnegative and vanishes if and only if \( \beta_L = \beta_R \) and \( \mu_L = \mu_R \).

The nonnegativity of \( \langle J_S \rangle_+ \) immediately follows from an inequality:

\[
\left( \frac{1}{e^y + 1} - \frac{1}{e^x + 1} \right) (x - y) \geq 0 ,
\]

where the equality holds if and only if \( x = y \). As shown in Refs. 16)–19), positivity of the entropy production can be proved for more general cases since it is related to the relative entropy between the initial state and the state at time \( t \): If the two states were described by density matrices, respectively, \( \rho_{\text{loc}} \) and \( \rho_t \), the relative entropy \( S(\rho_{\text{loc}}|\rho_t) \equiv \text{Tr}\{\rho_t(\log \rho_t - \log \rho_{\text{loc}})\} \) is related to the entropy production via

\[
\langle J_S \rangle_t = \frac{d}{dt} S(\rho_{\text{loc}}|\rho_t) , \tag{3.22}
\]

where \( \langle \cdots \rangle_t \) stands for the average with respect to \( \rho_t \). The same relation holds for a C*-generalization of the relative entropy given by Araki.\(27,33)\) Then, because of \( S(\rho_{\text{loc}}|\rho_t) \geq 0 \), l’Hospital’s rule gives the positivity of \( \langle J_S \rangle_+ \).\(^{18}\)

For states described by density matrices, \( \text{Ref. 16} \) can be easily shown.\(^{16}\) Then, we have \( \rho_{\text{loc}} = e^{-\sum_j \beta_j(H_j - \mu_j N_j)}/Z_0, \rho_t = e^{-iHt/\hbar}\rho_{\text{loc}}e^{iHt/\hbar} \) with \( Z_0 \) a constant, and

\[
S(\rho_{\text{loc}}|\rho_t) = \text{Tr}\{\rho_{\text{loc}} \left( -\sum_j \beta_j(H_j - \mu_j N_j) + \sum_j \beta_j(H_j(t) - \mu_j N_j(t)) \right) \} ,
\]
where \( H_j(t) = e^{iHt/\hbar} H_j e^{-iHt/\hbar} \) and \( N_j(t) = e^{iHt/\hbar} H_j e^{-iHt/\hbar} \), and which gives \(3.22\):

\[
\frac{d}{dt} S(\rho_{\text{loc}}|\rho_t) = \text{Tr}\left\{\rho_{\text{loc}} \sum_j \beta_j \left( \frac{dH_j(t)}{dt} - \mu_j \frac{dN_j(t)}{dt} \right) \right\} = \langle J_S(t) \rangle_{\text{loc}} = \langle J_S \rangle_t.
\]

This observation indicates that the features consistent with thermodynamics come from the second term of the relative entropy: \(-\text{Tr}(\rho_t \log \rho_{\text{loc}})\), which is similar to the nonequilibrium entropy of Zubarev:\(2\) 
\(S_Z = -\text{Tr}(\rho_t \log \rho_t)\) (cf. eq.(22.31) of Ref. 2) with \(\rho_t\) a reference local equilibrium state. An entropy of Zubarev type (more precisely, the relative entropy between the state \(\rho_t\) and a reference local equilibrium state \(\rho_t\): \(S(\rho_t|\rho_t)\)) was studied by Fröhlich, Merkli, Schwarz and Ueltschi\(20\) in a slightly different context.

The identification of \(J^T_r \equiv J^T_r - \mu_r J_r\) with the heat flow could be justified since \(\int_0^T dt J^T_r(t)\) behaves as a thermodynamic heat in the weak coupling limit for a small system coupled with a single reservoir.\(^{30,37}\)

Note that the expressions of the particle and energy flows agree with those of the Landauer formula.\(^{38,39}\) As discussed e.g., by Sivan and Imry,\(^{40}\) when the temperature difference \(\beta^{-1}_L - \beta^{-1}_R\) and chemical potential difference \(\mu_L - \mu_R\) are small, \(3.20\) and \(3.21\) reduce to linear relations between thermodynamic forces and flows, where Onsager’s reciprocal relations hold. The general proofs of linear response relations for nonlocal perturbations such as the temperature difference and/or chemical potential difference are discussed by Jakšić, Ogata and Pillet.\(^{21}\)

**§4. KMS Characterization of Nonequilibrium Steady States**

As discussed in Sec. 2.2 canonical and grand canonical states are characterized as KMS states. As shown for \(L^1\)-asymptotic abelian systems in Ref. 23), the nonequilibrium steady states discussed in the previous section can be characterized in a similar way:

**Proposition 6:** If the limits \(3.20\) exist, the fields \(a_r^{(\text{in/out})}(f)\) \((r = L, R)\) generate the whole algebra \(\mathcal{F}\) and \(\langle \cdots \rangle_{\text{loc}}\) is \(\tau^{(0)}\)-invariant, the nonequilibrium steady states \(\langle \cdots \rangle_{\pm}\) are KMS states with respect to the maps

\[
\sigma^{(\pm)}_s \equiv \gamma^{-1}_s \sigma_s \gamma^\pm , \tag{4.1}
\]

namely, \(\langle A \sigma^{(\pm)}_s(A) \rangle_{\pm} = \langle BA \rangle_{\pm}\) for \(A, B \in \mathcal{F}_s^\pm\) where \(i = \sqrt{-1}\), \(\sigma_x\) is a map defining \(\langle \cdots \rangle_{\text{loc}}\) as a KMS state, \(\gamma_{\pm}\) are maps introduced in Lemma 3 and \(\mathcal{F}_s^\pm \subset \mathcal{F}\) are (dense) subsets such that \(\sigma^{(\pm)}_s(A)\) is analytic in \(|\text{Im } z| \leq 1\) for any \(A \in \mathcal{F}_s^\pm\). Note that \(1.1\) is well-defined as \(\sigma_s \gamma_{\pm}(A) \in \mathcal{F}_{\text{res}}\ (\forall A \in \mathcal{F})\).

Let \(\hat{\omega}(A) \equiv \frac{d}{ds} \sigma_s(A)\) \((s = 0\) \((A \in D(\hat{\omega}))\) and \(\hat{\omega}^+ (A) \equiv \frac{d}{ds} \sigma_s^{(\pm)}(A)\) \((s = 0\) \((A \in D(\hat{\omega}^+))\)), where \(D(\hat{\omega})\) and \(D(\hat{\omega}^+)\) are (dense) subsets where the corresponding derivatives exist. Suppose that \(W \in D(\hat{\omega})\) and there exists a
On the other hand, if the state is described by a density matrix of the Zubarev ensemble:

\[ \langle \sigma \rangle \]

were applicable to finite-degree-of-freedom systems, one would have

\[ \langle \sigma \rangle \]

Before going to the proof of Proposition 6, we discuss its implications. Remind that

\[ \sigma_s(A) = e^i \sum_{r=L,R} \beta_r (H_r - \mu_r N_r) s A e^{-i \beta_r (H_r - \mu_r N_r) s} \]

for finite-degree-of-freedom systems, where \( H_r \) and \( N_r \) (\( r = L, R \)) are, respectively, the energy and the number of particles in each reservoir. Hence, \( \sigma_s(A) = i \sum_{r=L,R} \beta_r ([H_r - \mu_r N_r], A) \) and

\[ \sigma_s(W) = -i \sum_{r=L,R} \beta_r [H_r, H_r - \mu_r N_r] = - \sum_{r=L,R} \beta_r \frac{d \tau_r (H_r - \mu_r N_r)}{dt} \bigg|_{t=0} = -J_S , \]

where \( J_S \) is the entropy production operator discussed in Sec. 1. Therefore, if Proposition 6 were applicable to finite-degree-of-freedom systems, one would have

\[ \delta_s^+ (A) = \sum_{r=L,R} \beta_r ([H_r - \mu_r N_r], A) + i \int_{-\infty}^{0} dt \left[ \tau_r (J_S), A \right] . \]

On the other hand, if the state is described by a density matrix \( \rho \propto e^{-\Gamma} \), it satisfies a KMS condition: \( \langle A \sigma_s^\dagger (B) \rangle_\rho = \langle BA \rangle_\rho \), where \( \sigma_s^\dagger (B) = e^{i T s} B e^{-i T s} \). Hence, the density matrix of the steady state \( \langle \cdot \cdot \cdot \rangle_+ \), if it exists, is given by a MacLennan-Zubarev ensemble:

\[ \rho_+ = \frac{1}{Z} \exp \left\{ - \sum_{j=1}^{N} \beta_j (H_j - \mu_j N_j) + \int_{-\infty}^{0} ds J_S(s) \right\} . \]

As pointed out in Sec. 1, the original proposal (4.3) by MacLennan and Zubarev cannot be justified. Rather, KMS states with respect to \( \sigma_s^\dagger (\pm) \) which is generated by (4.4) should be regarded as a precise definition of the MacLennan-Zubarev ensembles.

**Proof of Proposition 6:** When the dynamics is L^1-asymptotic abelian and Möller morphisms are invertible, we have shown the same conclusion.23,37 Since the present conditions are different from the previous ones, we give the outline of the proof in case of \( \langle \cdot \cdot \cdot \rangle_+ \).

Remind that \( \langle A \sigma_s^\dagger (B) \rangle_{loc} = \langle BA \rangle_{loc} \) holds for some (dense) subset \( F^\alpha_{res} \subset F_{res} \). On the other hand, the map \( \gamma_+ \) defined in Lemma 3 has the inverse \( \gamma_+^{-1} \) on \( F_{res} \) and the steady state is given by \( \langle A \rangle_+ = \langle \gamma_+ (A) \rangle_{loc} \). Hence, one has

\[ \langle A \gamma_+^{-1} (\sigma_i (\gamma_+ (B))) \rangle_+ = \langle \gamma_+ (A) \sigma_i (\gamma_+ (B)) \rangle_{loc} = \langle \gamma_+ (B) \gamma_+ (A) \rangle_{loc} = \langle BA \rangle_+ , \]
for any two elements of the dense set \( \{ A\gamma_+(A) \in F_{\text{res}}^a \} \subset F \). Namely, the steady state is a KMS state with respect to \( \sigma_+^{(s)} = \gamma^{-1}_+ \sigma_+ \). This proves the first half.

Now we consider the generator. Let \( \gamma_t(A) \equiv \tau_0^{(0)}(\tau_t(A)) \), then, for any \( A \in F \), \( \gamma_t(A) \) is differentiable and \( \frac{d}{dt}\gamma_t(A) = \frac{i}{\hbar}\gamma_t([\tau_t(W), A]) \), which leads to

\[
\frac{d}{dt}\gamma_t^{-1}\sigma_+ \gamma_t(A) = i\frac{\hbar}{\rho^2}[\tau_t^{-1}(\sigma_+(W) - W), \gamma_t^{-1}\sigma_+ \gamma_t(A)]
\]

or

\[
\gamma_t^{-1}\sigma_+ \gamma_t(A) = \sigma_+(A) + i\frac{\hbar}{\rho^2}\int_0^t dt' \left[ \tau_{t'}(\sigma_+(W) - W), \gamma_t^{-1}\sigma_+ \gamma_{t'}(A) \right]
\]

where we have used \( \gamma_t \tau_t^{-1} = \tau_0^{(0)} \), \( \tau_0^{(0)} \sigma_+ = \sigma_+ \tau_t^{-1} \), \( \gamma_t^{-1}\tau_t^{(0)} = \tau_t^{-1} \). Since \( W \in D(\delta_\omega) \) is assumed, for any \( A \in D(\delta_\omega) \), one has

\[
\delta_\omega^{(s)}(A) \equiv \frac{d}{ds}\gamma^{-1}_s \gamma_s(A) \bigg|_{s=0} = \delta_\omega(A) + i\frac{\hbar}{\rho^2}\int_0^1 dt' \left[ \tau_{t'}(\delta_\omega(W)), A \right].
\]

It can be shown that \( \delta_\omega^{(s)} \) is indeed the generator of \( \{ \gamma^{-1}_s \gamma_s \}_{s \in \mathbb{R}} \). On the other hand, since Lemma 3 implies

\[
\lim_{n \to \infty} \| \gamma_n^{-1}\gamma_n(A) - \sigma_+^+ (A) \| = 0,
\]

for any \( A \in F \), one has \( \delta_\omega^{(s)}(A) = \lim_{n \to \infty} \delta_\omega^{(n)}(A) \), if the limit exists\(^a\). Because of the assumption \( \{ \gamma_n \}_{n \geq 0} \), this is indeed the case for \( A \in D(\delta_\omega) \cap G_+ \) and we obtain the desired result \( 4.3 \). (Q.E.D.)

Originally, Kubo\(^b\) used the KMS condition to show the fluctuation-dissipation relations. Since we have a KMS characterization of NESS, it is interesting to explore a relation between response and fluctuation at NESS following Ref. 30.

Suppose that a spatially uniform electric field of strength \( E(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{i\omega t} \hat{E}(\omega) \) is applied to a finite domain, then, as shown e.g., by Gavish, Imry and Yurke,\(^c\) its effect is described by a perturbation Hamiltonian: \( \int_{-\infty}^{+\infty} dt'E(t')\hat{I} \) \( (I \in F): \) spatially averaged current) and we have

\[
\langle \hat{I} \rangle_{+,E(t)} = \langle \hat{I} \rangle + \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{i\omega t} G(\omega) \hat{E}(\omega) + O(E(t)^2),
\]

where \( \langle \cdots \rangle_{+,E(t)} \) is the state perturbed by \( E(t) \) and the frequency-dependent conductance \( G(\omega) \) is a distribution:

\[
G(\omega) = \frac{1}{\hbar(\omega - i0)} \int_{-\infty}^{0} dt e^{i\omega t} \langle [\tau_t(\hat{I}), \hat{I}] \rangle_+.
\]

\(^a\) One can show that the limit \( \delta_\omega^{(s)} \) is uniform on a finite closed \( s \)-interval. Then, the generator \( \delta_\omega^s \) of \( \sigma_+^+ \) is the graph limit of \( \{ \delta_\omega^{(n)} \}_{n \geq 0} \) (cf. Theorem 3.1.28 of Ref. 27)). Also \( \delta_\omega^{(n)} \) is proved to have the same domain: \( D(\delta_\omega^{(n)}) = D(\delta_\omega) \). Then, if \( \delta_\omega^{(n)}(A) \) converges, the limit is \( \delta_\omega^s(A) \).\(^{37}\)
When $\hat{E}(\omega)$ and the Fourier transform of $\langle \tau(\hat{I}, \hat{I}) \rangle_+$ have appropriate smoothness and integrability, the formal calculations can be justified as shown by Ruelle.\(^9\) Note that the zero-frequency limit $\text{Re} G(0+) = (\text{Re} 0)_{\text{formal}}$ corresponds to a dc-conductance, but is not necessarily agrees with the differential conductance $\frac{d}{dV}(\hat{I})_+$ as shown in Ref. 25) because the former comes from a local perturbation but the latter from a nonlocal perturbation.

Now we introduce a gauge transformation $g_\varphi : \mathcal{F} \to \mathcal{F}$, which is formally expressed as $g_\varphi(A) = e^{i(\sum_r N_r + c^+ c)} A e^{-i(\sum_r N_r + c^+ c)}$. Clearly, $g_\varphi$ is a linear map which preserves product and conjugation, and its action to the generators is $g_\varphi(c) = e^{-i\varphi} c$, $g_\varphi(a_r(f)) = e^{-i\varphi} a_r(f)$ ($r = L, R$). Then, we observe that, if the interaction $W$ is gauge-invariant: $g_\varphi(W) = W$, the maps $\tau_\lambda, \sigma_\lambda^+(\lambda)$ (cf. Proposition 6) and $g_\varphi$ commute with each other. And there exists a dense subset $\mathcal{F}_{g_\sigma\tau}$, where, for any $A \in \mathcal{F}_{g_\sigma\tau}$, $\tau_\lambda(A)$, $\sigma_\lambda^+(A)$ and $g_\varphi(A)$ are analytic on the whole complex plane of $z$ (cf. the arguments of Proposition 2.5.22 of Ref. 27)). Then, we have

**Corollary 7:** Let (i) $\hat{I} \in \mathcal{F}_{g_\sigma\tau} \cap D(\delta_N^\lambda) \cap D(\delta_E^\lambda)$ be gauge-invariant: $g_\varphi(\hat{I}) = \hat{I}$, (ii) $W \in D(\delta_N^\lambda) \cap D(\delta_E^\lambda)$ and

\[
\begin{align*}
&\int_{-\infty}^{+\infty} dt \langle \tau_\lambda(\delta\hat{I}) \delta\hat{I} \rangle_+ < +\infty, \quad (4.12) \\
&\int_{-\infty}^{+\infty} dt \| [\tau_\lambda(\delta^{(\lambda)}(W), \delta\hat{I})] \| < +\infty \quad (\lambda = N, E), \quad (4.13)
\end{align*}
\]

where $\delta\hat{I} \equiv \hat{I} - (\hat{I})_+$ stands for the fluctuation of $\hat{I}$ and $\delta^{(\lambda)}(\lambda = N, E)$ are the infinitesimal generators of $\xi^{(\lambda)}_s(\lambda = N, E)$ formally expressed as $\xi^{(N)}_s(A) = e^{i(N_L - N_R)_s} A e^{-i(N_L - N_R)_s}$ and $\xi^{(E)}_s(A) = e^{-i(H_L - H_R)_s} A e^{-i(H_L - H_R)_s}$ (i.e., $\delta^{(\lambda)}(A) = \frac{\partial}{\partial s}(\xi^{(\lambda)}_s(A))_{s=0}$). Consider the Fourier transform $S_I(\omega)$ of the symmetrized correlation function

\[
S_I(\omega) \equiv \frac{1}{2} \int_{-\infty}^{+\infty} dt e^{i\omega t} \langle \{ \tau_\lambda(\delta\hat{I}) \delta\hat{I} + \delta\hat{I} \tau_\lambda(\delta\hat{I}) \} \rangle_+, \quad (4.14)
\]

then

\[
(e^{\beta \omega} - 1) S_I(\omega) - (e^{\beta \omega} + 1) \text{Re}(\omega G(\omega)) = \frac{\Delta \beta}{2} \int_{-\infty}^{+\infty} dt e^{i\omega t} \int_0^1 d\nu \langle \tau_\lambda(\delta\hat{I}) \xi^{(+)}_s \rangle \left( i \delta^{(E)}_\xi(\delta\hat{I}) - \int_{-\infty}^{0} \frac{dt'}{\hbar} [\tau_\nu(\delta^{(E)}_\xi(W), \delta\hat{I})] \right)_+ \\
= \frac{\Delta N}{2} \int_{-\infty}^{+\infty} dt e^{i\omega t} \int_0^1 d\nu \langle \tau_\lambda(\delta\hat{I}) \xi^{(+)}_s \rangle \left( i \delta^{(N)}_\xi(\delta\hat{I}) - \int_{-\infty}^{0} \frac{dt'}{\hbar} [\tau_\nu(\delta^{(N)}_\xi(W), \delta\hat{I})] \right)_+, \quad (4.15)
\]

where $\xi^{(+)}_s$ is the map $\xi^{(+)}_s = \sigma^{(+)}_s - \beta h_s \xi^{(+)}_s$, $\bar{\beta} = (\beta_L + \beta_R)/2$ the average inverse temperature, $\Delta \beta = \beta_L - \beta_R$ the difference of inverse temperatures, $\Delta N = \beta_L \mu_L - \beta_R \mu_R$ the affinity difference and $\bar{\beta} = (\beta_L \mu_L + \beta_R \mu_R)/2$.
the average affinity. Note that the infinitesimal generator \( \delta^+ \) defined by 
\[
\delta^+ (A) \equiv \frac{d}{ds} \{ \xi_i^{(+)}(A) \}_{s=0} \text{ for } A \in D(\delta^+) \]
is of order of \( \Delta \beta \) and \( \Delta \delta \).

From the arguments of the previous section, we have \( \delta^+(N)(W) = h(J_R - J_L) \) and 
\( \delta^+(E)(W) = h(J_R^E - J_L^E) \), and, thus, the terms involving \( t' \)-integrals are correlation 
functions among three current operators. On the contrary, the terms \( i \delta^+(\delta \hat{I}) \) 
(\( \lambda = N, E \)) depend on the interaction \( W \) and, in general, do not have simple physical 
meaning. For the model of an AB ring with a dot, when \( w = 0, \beta_L = \beta_R = \beta \) and 
the left-hand side of \( 4.15 \) is absolutely integrable, the response and correlation 
functions with respect to the average current: \( \hat{I} = -e(J_R - J_L)/2 \) satisfy 

\[
\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \left\{ (e^{i\beta \omega} - 1) S_I(\omega) - (e^{i\beta \omega} + 1) \text{Re}(h\omega G(\omega)) \right\} 
= \frac{\beta \Delta \mu}{2i} \int_{0}^{1} dv \left( \tau_i(\delta \hat{I}) \xi_i^{(+)} \left( \frac{e}{2\hbar} W + \frac{2}{i\epsilon} \int_{-\infty}^{0} dt' \tau_i(\delta \hat{I}), \delta \hat{I} \right) \right) + 
= \frac{\beta \Delta \mu}{2i} \left\{ \frac{e}{2\hbar} \tau_i(\delta \hat{I}) W + \frac{2}{i\epsilon} \int_{-\infty}^{0} dt' \left( \tau_i(\delta \hat{I}) \tau_i(\delta \hat{I}) \right) + \right\} + O(\Delta \mu^2)
\]

where \( \Delta \mu = \mu_L - \mu_R \) is the chemical potential difference. Thus, the imperfection 
of the fluctuation dissipation relation is equal to a sum of two correlation functions, 
the one between the current and the interaction \( W \) and the other among three 
currents. We believe that this relation is a first step towards a quantum analog 
to the equality between the violation of fluctuation-dissipation relation and energy 
dissipation obtained for certain classical systems by Harada-Sasa \cite{42} and Teramoto- 
Sasa \cite{43} or to a nonequilibrium extension of fluctuation-dissipation relation derived 
for classical Langevin systems by Speck and Seifert. \cite{44}

**Proof of Corollary 7:** Integrability \( 4.12 \) guarantees the existence of \( S_I(\omega) \) 
and \( h\omega G(\omega) \). By integrating an analytic function \( e^{i\omega t}(\delta \hat{I})_i \) on a rectangle 
\( [-T_1, T_2] \cup [T_2, T_2 + i\hbar \beta] \cup [T_2 + i\hbar \beta, -T_1 + i\hbar \beta] \cup [-T_1 + i\hbar \beta, -T_1] \) in the 
complex \( t' \)-plane with \( [z_1, z_2] \) a segment starting from \( z_1 \) and terminating at \( z_2 \), and 
by taking the limit of \( T_1, T_2 \to +\infty \), we obtain 

\[
\int_{-\infty}^{+\infty} dte^{i\omega t} \langle \tau_i(\delta \hat{I}) \rangle = e^{-i\beta \omega} \int_{-\infty}^{+\infty} dte^{i\omega t} \langle \tau_i(\delta \hat{I}) \rangle + . \tag{4.16}
\]

Note that the intergals on the segments \( [T_2, T_2 + i\hbar \beta] \) and \( [-T_1 + i\hbar \beta, -T_1] \) vanish 
for \( T_1, T_2 \to +\infty \) because of the mixing property given by Proposition 2. On 
the other hand, Proposition 6 and the gauge invariance of \( \hat{I} \): \( g_i \bar{\hat{R}}(\hat{I}) = \hat{I} \) imply 

\[
\langle \tau_i(\delta \hat{I}) \rangle = \langle \tau_i(\delta \hat{I}) \rangle + = \langle \tau_i(\delta \hat{I}) \rangle + = \langle \tau_i(\delta \hat{I}) \rangle + \text{Re}(g_i \bar{\hat{R}}(\delta \hat{I})) + 
= \langle \tau_i(\delta \hat{I}) \rangle + i \int_{0}^{1} dv \langle \tau_i(\delta \hat{I}) \rangle + , \tag{4.17}
\]

where \( \delta \hat{I} \in D(\delta^+) \) is shown later. It is easy to see \( \xi_i^{(+)} = \gamma_{+}^{-1} \xi_i^{(0)} \gamma_{+} \) where 
\( \xi_i^{(0)} = \sigma_i \tau_{-h\beta s} g_{\bar{R} s} \), and \( \xi_i^{(0)}(A) = \xi_i^{(E)}(\xi_i^{(N)})(e^{i\beta \alpha - \bar{R}})^c \text{Re} A e^{i\beta \alpha - \bar{R}}^c \text{Re} A) \). Thus,
\[ \xi_s^{(+)}(\delta \hat{I}) = \gamma_+^{-1} \left( \xi_{s s_0}^{(E)}(\xi_{\Delta s_0/2}^{(N)}(\xi_{\Delta s_0/2}^{(N)}(\xi_{\Delta s_0/2}^{(N)}(\gamma_+^{(\delta \hat{I})))))) \right). \]

Since \( \xi_s^{(+)}(\delta \hat{I}) \) has the same structure as \( \sigma_s^{(+)}(A) \), one can show \( \delta \hat{I} \in D(\delta \hat{c}^+) \) and
\[
\begin{aligned}
\hat{c}^+_s(\delta \hat{I}) &= \frac{\Delta \beta}{2} \left\{ \xi_{\Delta s_0/2}^{(E)}(\delta \hat{I}) + i \int_{-\infty}^{0} d\tau [\tau(\xi_{\Delta s_0/2}^{(E)}(W)), \delta \hat{I}] \right\} \\
&- \frac{\Delta \Delta}{2} \left\{ \xi_{\Delta s_0/2}^{(N)}(\delta \hat{I}) + i \int_{-\infty}^{0} d\tau [\tau(\xi_{\Delta s_0/2}^{(N)}(W)), \delta \hat{I}] \right\},
\end{aligned}
\]

from the conditions (i)-(ii) and (iii) as in the proof of Proposition 6. Combining (4.16), (4.17), (4.18), and using \( S_1(\omega) - \text{Re}(\hbar \omega G(\omega)) = \int_{\mathbb{R}} d\tau e^{i\omega \tau} (\delta \hat{I} \tau_2(\delta \hat{I}))_+ \) and \( S_1(\omega) + \text{Re}(\hbar \omega G(\omega)) = \int_{\mathbb{R}} d\tau e^{i\omega \tau} (\tau(\delta \hat{I}) \hat{I})_+ \), we obtain the desired result. (Q.E.D)

§5. Conclusions

As pointed out by Ruelle\(^9\) and clearly seen from Proposition 1, nonequilibrium steady states investigated so far are constructed through the scattering approach. In this sense, the present approach can be regarded as an extension of Landauer-Büttiker’s approach\(^3\) to electronic transports in mesoscopic systems. And there exist a class of mesoscopic systems to which the present formalism is applicable, such as the Aharonov-Bohm ring with a quantum dot. Since we have a full characterization of NESS for non-interacting systems, one may develop approximations such as the mean-field approximation.\(^2\) These aspects will be discussed elsewhere.

Before closing this article, we look through a relation between the dynamical reversibility and irreversible evolution towards a steady state in the sense of Proposition 1.\(^2\) We assume that the dynamics is symmetric with respect to a time reversal operation, namely, there exists an antilinear operation \( A \rightarrow \iota(A) \) such that \( \iota(AB) = \iota(A)\iota(B) \), \( \iota(\alpha A + B) = \alpha^* \iota(A) + \iota(B) \), \( \iota^2(A) = A \) and \( \iota(\tau_2(\iota(A))) = \tau_{-2}(A) \) \( (A, B \in \mathcal{F}, \alpha \in \mathbb{C}) \). The time reversal operation on a state \( \langle \cdots \rangle \) is, then, defined by \( \langle A \rangle^{TR} = \langle \iota(A) \rangle \). For the present model, one can choose \( \iota(a_k(f)) = \int d\mathbf{k} f(-k)a_k \), \( \iota(c) = c \). Then, when \( \iota(W) = W \) (when \( \varphi = 0 \) for the model of an Aharonov-Bohm ring with a dot), the system has a time-reversal symmetry. Under the assumption that the initial state is time-reversal symmetric \( \langle A \rangle_{loc}^{TR} = \langle A \rangle_{loc} \), let us carry out the following thought experiment: (i) Let the system autonomously evolve up to \( t = t_0 \). (ii) The time reversal operation is performed at \( t = t_0 \). And (iii) let the system autonomously evolve once again. Just before the time reversal operation, the system is in the state \( \langle A \rangle_{t_0} = \langle \tau_{t_0}(A) \rangle_{loc} \) and, just after the time reversal operation, the state becomes
\[
\langle A \rangle_{t_0} = \langle A \rangle_{t_0}^{TR} = \langle \tau_{t_0}(\iota(A)) \rangle_{loc} = \langle \iota(\tau_{-t_0}(A)) \rangle_{loc} = \langle \tau_{-t_0}(A) \rangle_{loc},
\]
which evolves further as \( \langle A \rangle_t = \langle \tau_{-t_0}(A) \rangle_{loc} \). Then, the system comes back at \( t = 2t_0 \) to the state just before the time reversal operation, as expected. Note that, if \( t_0 > 0 \) is large enough, the state \( \langle A \rangle_{t_0} \) just before the time reversal operation is close to the steady state \( \langle A \rangle_+ \), while the state \( \langle A \rangle_{t_0} \) just after the time reversal operation is close to another steady state \( \langle A \rangle_- \). In other words, the time reversal operation
discontinuously derives the system from a state close to $\langle \cdots \rangle_+$ to the one close to $\langle \cdots \rangle_-$. On the other hand, by the ‘natural’ evolution $\tau$, the system changes towards the steady state $\langle \cdots \rangle_+$. Hence, the dynamical reversibility is fully consistent with irreversible state evolution in the sense of Proposition 1.\textsuperscript{23)}

It is interesting to revisit Loschmidt’s criticism to the work of Boltzmann.\textsuperscript{45)} Although the dynamical reversibility is consistent with the irreversible state evolution, Loschmidt’s criticism can be applied to the relative entropy $S(\rho_{\text{loc}}|\rho_t)$. Indeed, in the above thought experiment, let $\langle J_S \rangle_t$ be the entropy production at time $t$, then, when $t$ is slightly larger than $t_0$, $\langle J_S \rangle_t$ is close to $\langle J_S \rangle_- (< 0^*)$ and should itself be negative. Thus, because of (3.22), there is a period when the relative entropy $S(\rho_{\text{loc}}|\rho_t)$ decreases. Contrary to Boltzmann’s reply,\textsuperscript{45)} these states are typical in the sense that they evolve towards the steady state $\langle \cdots \rangle_+$ for $t \to \infty$. In other words, Loschmidt’s criticism does not deny the consistency of irreversible phenomena with dynamical reversibility and it just shows that the relative entropy is not an appropriate thermodynamic entropy for general cases. Another criticism to Boltzmann’s work by Zermelo\textsuperscript{45)} is not applicable to the present case since the recurrence time is infinitely long as a result of the infinite extension of the system.

From the point of view of the second law of thermodynamics, one may be satisfied with all these features, particularly the properties of the entropy production discussed in Sec. 3. However, one should remind that the ‘correct’ form of the entropy production is obtained because we start from a local equilibrium state where each subsystem is in a canonical state. As the canonical states are very outcome of the second law, the present results do not give a dynamical proof of the second law, but show that, once one starts from canonical ensembles or their combinations, the dynamics derives the system consistently with the second law of thermodynamics.

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\textsuperscript{*}) This follows from (3.22) and l’Hospital’s rule as the proof of $\langle J_S \rangle_+ \geq 0$. 
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