PERTURBATIVE ANALYSIS OF NONEQUILIBRIUM STEADY STATES IN QUANTUM SYSTEMS

Ayumu Sugita

Department of Applied Physics, Osaka City University,
3-3-138 Sugimoto, Sumiyoshi-ku, Osaka, 558-8585, Japan

Abstract

We study the nonequilibrium steady state (NESS) in a quantum system in contact with two heat baths at different temperatures. We use a time-independent perturbative expansion with respect to the coupling with the two heat baths to obtain the density matrix for the NESS. In particular, we show an explicit representation of the density matrix for the reflection symmetric and weakly nonequilibrium case. We also calculate the expectation value of the energy current and show that the Kubo formula holds in this case.

1 Introduction

Construction of nonequilibrium statistical mechanics is a challenging open problem in physics. Since nonequilibrium phenomena are so diverse, probably it is impossible to make a theory which explains all nonequilibrium phenomena. Then a natural first step would be statistical mechanics for nonequilibrium steady states (NESSs). The most ambitious goal in this direction is to find a simple theoretical expression for the density matrix of the NESSs.

Although there are many theoretical frameworks to treat NESSs, it is quite difficult to write down the density matrix explicitly. For example, in the linear response theory [1] the density matrix for the NESS is obtained in the long-time limit of the dynamics under an external field

\[ \hat{\rho}_{\text{NESS}} = \hat{\rho}_{\text{eq}} + \lim_{t \to \infty} \int_0^t dt' e^{-i(t-t')\hat{H}/\hbar} \frac{1}{i\hbar} [\hat{H}_{\text{ext}}, \hat{\rho}_{\text{eq}}] e^{i(t-t')\hat{H}/\hbar}, \]

and the system has to be infinitely large. (Otherwise we obtain another equilibrium state.) Although this equation is useful to calculate some nonequilibrium properties like transport coefficients, \( \hat{\rho}_{\text{NESS}} \) itself is very hard to calculate in this formalism. Most of formalisms to treat NESS contain this kind of long time evolution, which makes it difficult to calculate \( \hat{\rho}_{\text{NESS}} \).

In this paper, we consider a system with two heat baths. We consider the stationary solution of a quantum master equation, and calculate it explicitly using a perturbative expansion with respect to the coupling parameter between the system and the heat baths. In particular, in the reflection symmetric case we show an explicit form of density matrix for the NESS in the weakly nonequilibrium regime.
2 Equation of Motion

We start with the equation of motion for the total system:

\[ \frac{d}{dt} \hat{\rho}_{\text{tot}}(t) = \frac{1}{i\hbar} [\hat{H}_{\text{tot}}, \hat{\rho}_{\text{tot}}(t)], \]

(2)

where

\[ \hat{H}_{\text{tot}} = \hat{H}_S + \hat{H}_B + u \hat{H}_{BS}. \]

(3)

Here \( \hat{H}_S, \hat{H}_B \) and \( \hat{H}_{BS} \) are the Hamiltonians of the system, the heat baths and the interactions, respectively. We use \( u \) as the perturbation parameter. In this paper, we consider a system with two heat baths:

\[ \hat{H}_B = \hat{H}_L + \hat{H}_R, \]

(4)

\[ \hat{H}_{BS} = \hat{H}_{LS} + \hat{H}_{RS}. \]

(5)

Here, \( \hat{H}_L \) and \( \hat{H}_R \) are the Hamiltonians for the left and right reservoirs, respectively. We assume that the heat bath \( \alpha (\alpha = L, R) \) is in equilibrium with the inverse temperature \( \beta_\alpha \) (See Fig. [1]). The interaction Hamiltonians \( \hat{H}_{LS} \) and \( \hat{H}_{RS} \) can be written in the form

\[ \hat{H}_{LS} = \sum_j \hat{X}_j^L \hat{Y}_j^L, \quad \hat{H}_{RS} = \sum_j \hat{X}_j^R \hat{Y}_j^R \]

(6)

where \( \hat{X}_j^\alpha \) acts on the system, and \( \hat{Y}_j^\alpha \) (\( \hat{Y}_j^\alpha \)) acts on the left (right) heat bath. In the following we assume \( \hat{X}_j^\alpha \) and \( \hat{Y}_j^\alpha \) are Hermitian for simplicity. However, our main results in this paper hold without this assumption.

We expand the density matrix up to \( O(u^2) \), trace out the heat bath variables, and apply the Markov approximation. Then we obtain the equation of motion for the system [2]

\[ \frac{d}{dt} \hat{\rho}(t) = \frac{1}{i\hbar} [\hat{H}'_S, \hat{\rho}(t)] + u^2 \sum_{\alpha=L,R} \Gamma_\alpha \hat{\rho}(t). \]

(7)
Here,
\[ \hat{H}'_S \equiv \hat{H}_S + u \sum_{\alpha=L,R} \sum_j \hat{X}_j^\alpha \langle \hat{Y}_j^\alpha \rangle \]  
(8)
is the system Hamiltonian with the averaged interaction terms, where \( \langle \hat{A}^\alpha \rangle \) represents the average of \( \hat{A}^\alpha \) with respect to the heat bath \( \alpha \). Hereafter \( \hat{H}'_S \) is denoted as \( \hat{H}_S \) for simplicity. \( \Gamma^\alpha \) is the heat bath superoperator, whose explicit form is
\[ \Gamma^\alpha \hat{\rho}(t) = -\frac{1}{\hbar^2} \sum_{j,l} \int_0^\infty dt' \left\{ \hat{X}_j^\alpha \hat{X}_l^\alpha (-t') \hat{\rho}(t') \hat{X}_j^\alpha (t' - t) \hat{X}_l^\alpha (t') \hat{\rho}(t') \hat{X}_j^\alpha (-t') \hat{\rho}(t) \hat{X}_j^\alpha (t') \hat{\rho}(t) \hat{X}_j^\alpha (-t') \right\} \]  
(9)
Here, \( \hat{X}(t) \equiv e^{-i\hat{H}_S t/\hbar} \hat{X} e^{i\hat{H}_S t/\hbar} \) represents the operator in the interaction picture.
\[ \Phi^\alpha_{jl}(t) \equiv \langle \Delta \hat{Y}_j^\alpha(t) \Delta \hat{Y}_l^\alpha \rangle \]  
(10)
is a correlation function in the heat bath \( \alpha \), where
\[ \Delta \hat{Y}_j^\alpha \equiv \hat{Y}_j^\alpha - \langle \hat{Y}_j^\alpha \rangle. \]  
(11)
Note that we used
\[ \langle \Delta \hat{Y}_j^\alpha(t) \Delta \hat{Y}_l^\beta \rangle = \delta_{\alpha\beta} \langle \Delta \hat{Y}_j^\alpha(t) \Delta \hat{Y}_l^\alpha \rangle \]  
(12)
to derive Eq. (7). Since we assumed \( \hat{Y}_j^\alpha \)'s are Hermitian,
\[ \Phi_{jl}(t)^* = \Phi_{lj}(-t). \]  
(13)
The heat bath superoperator (9) can be rewritten as
\[ \Gamma^\alpha = \Gamma^\alpha_1 + \Gamma^\alpha_2, \]  
(14)
where
\[ \Gamma^\alpha_1 \hat{\rho} = -\frac{1}{2\hbar^2} \sum_{j,l} \left( \hat{X}_j^\alpha \hat{R}_{jl}^\alpha \hat{\rho} \right) + \left[ \hat{X}_j^\alpha, \hat{R}_{jl}^\alpha \hat{\rho} \right]^\dagger, \]  
(15)
\[ \Gamma^\alpha_2 \hat{\rho} = -\frac{i}{2\hbar^2} \sum_{j,l} \left( \hat{X}_j^\alpha \hat{W}_{jl}^\alpha \hat{\rho} - \left[ \hat{X}_j^\alpha, \hat{W}_{jl}^\alpha \hat{\rho} \right]^\dagger \right). \]  
(16)
The operators \( \hat{R}_{jl}^\alpha \) and \( \hat{W}_{jl}^\alpha \) are defined as
\[ \langle E_p | \hat{R}_{jl}^\alpha | E_q \rangle = \langle E_p | \hat{X}_j^\alpha | E_q \rangle \Phi_{jl}(\omega_{pq}), \]  
(17)
\[ \langle E_p | \hat{W}_{jl}^\alpha | E_q \rangle = \langle E_p | \hat{X}_j^\alpha | E_q \rangle \Psi_{jl}(\omega_{pq}), \]  
(18)
where \( |E_i\rangle \) is an energy eigenvector of the system with eigenenergy \( E_i \), \( \omega_{pq} \equiv (E_p - E_q)/\hbar \) and
\[ \Phi_{jl}(\omega) = \int_{-\infty}^{\infty} dt e^{-\imath \omega t} \Phi_{jl}(t) \]  
(19)
\[ \Psi_{jl}(\omega) = \mathcal{P} \int_{-\infty}^{\infty} d\omega' \frac{\Phi_{jl}(\omega')}{\pi} \frac{1}{\omega' - \omega}. \]  
(20)
Here $\mathcal{P}$ denotes the Cauchy principal value. Note that
\begin{align}
\tilde{\Phi}^{\alpha}_{jl}(\omega)^* &= \tilde{\Phi}^{\alpha}_{lj}(\omega), \\
\tilde{\Psi}^{\alpha}_{jl}(\omega)^* &= \tilde{\Psi}^{\alpha}_{lj}(\omega).
\end{align}

The correlation functions satisfy the Kubo-Martin-Schwinger (KMS) condition
\begin{equation}
\tilde{\Phi}^{\alpha}_{jl}(-\omega) = e^{\beta_{\alpha}\hbar\omega} \tilde{\Phi}^{\alpha}_{lj}(\omega),
\end{equation}
which is equivalent to the following operator identity:
\begin{equation}
\hat{R}^{\alpha}_{jl} = e^{\beta_{\alpha}\hbar\Omega} \hat{R}^{\alpha}_{lj} e^{-\beta_{\alpha}\hbar\Omega}.
\end{equation}
Using this identity it is easy to show that
\begin{equation}
\Gamma^{\alpha}_{1} e^{-\beta_{\alpha}\hbar\Omega} = 0,
\end{equation}
which guarantees the existence of the equilibrium solution for Eq. (7) when $\beta_{L} = \beta_{R}$.

3 Perturbative expansion

We put $\rho = \text{const.}$ in the equation of motion (7). Then we have the equation for the steady state
\begin{equation}
L_{0}\hat{\rho} + v L_{1}\hat{\rho} = 0,
\end{equation}
where
\begin{align}
L_{0}\hat{\rho} &= \frac{1}{i\hbar} [\hat{H}_{S}, \hat{\rho}], \\
L_{1}\hat{\rho} &= \Gamma^{L}\hat{\rho} + \Gamma^{R}\hat{\rho},
\end{align}
and $v \equiv u^2$. We expand $\hat{\rho}$ with respect to $v$:
\begin{equation}
\hat{\rho} = \hat{\rho}_0 + v\hat{\rho}_1 + v^2\hat{\rho}_2 + \ldots
\end{equation}

Then we obtain a series of equations
\begin{align}
L_{0}\hat{\rho}_0 &= 0, \\
L_{0}\hat{\rho}_1 + L_{1}\hat{\rho}_0 &= 0, \\
L_{0}\hat{\rho}_2 + L_{1}\hat{\rho}_1 &= 0,
\end{align}
3.1 Separation of diagonal and off-diagonal parts

In a normal perturbation theory, we can determine \( \hat{\rho} \) step by step starting from the 0th order solution \( \hat{\rho}_0 \). In this case, however, the 0th order equation (29) is degenerate, and any diagonal density matrices in the energy representation satisfy it. Therefore we cannot fix the 0th order term \( \hat{\rho}_0 \) from the 0th order equation (29).

To handle this problem, we introduce a projection superoperator \( P \), which is defined by

\[
P|E_i\rangle\langle E_j| = \begin{cases} |E_i\rangle\langle E_i| & (i = j) \\ 0 & (i \neq j) \end{cases}.
\]

Namely, \( P \) is the projection to the diagonal part. We also define \( Q \equiv 1 - P \), which is the projection to the off-diagonal part.

Hereafter we assume that \( \hat{H}_S \) is non-degenerate. Then the 0th order equation (29) means that \( \hat{\rho}_0 \) is diagonal. Since \( L_0 \) satisfies \( P L_0 = L_0 P = 0 \), we obtain

\[
P \hat{L}_1 \hat{\rho}_0 = P \hat{L}_1 \hat{\rho}_0 = 0
\]

from the 1st order equation (30). Eq. (35) means \( PL_1 P \) has a zero eigenvalue, and we assume that it is non-degenerate. Then Eq. (35) determines the 0th order term \( \hat{\rho}_0 \) uniquely.

The unperturbed Liouvillian \( L_0 \) acts on the density matrix as

\[
(L_0 \hat{\rho})_{jk} = \frac{1}{i\hbar} \left( [\hat{H}_S, \hat{\rho}] \right)_{jk} = \frac{E_j - E_k}{i\hbar} \rho_{jk},
\]

where \( A_{jk} \equiv \langle E_i| \hat{A} | E_k \rangle \) denotes a matrix element in the energy representation. \( L_0 \) does not have its inverse because it has zero eigenvalues. Nevertheless we can define its inverse in the off-diagonal subspace:

\[
\left( (Q L_0 Q)^{-1} \hat{\rho} \right)_{jk} = \frac{i\hbar}{E_j - E_k} \rho_{jk},
\]

Then from (30) we obtain the off-diagonal part of the first order term

\[
Q \hat{\rho}_1 = - (Q L_0 Q)^{-1} \hat{L}_1 \hat{\rho}_0.
\]

The diagonal part of the second order equation (31) can be rewritten as

\[
P \hat{L}_1 (P + Q) \hat{\rho}_1 = 0.
\]

\( P \hat{L}_1 P \) has a zero eigenvalue, and the corresponding eigenvector is \( \hat{\rho}_0 \). Therefore the general solution of (40) is

\[
P \hat{\rho}_1 = - (P \hat{L}_1 P)^{-1} P \hat{L}_1 Q \hat{\rho}_1 + \gamma \hat{\rho}_0,
\]

where \( (P \hat{L}_1 P)^{-1} \) is the inverse of \( P \hat{L}_1 P \) in the subspace spanned by non-zero eigenvectors of \( P \hat{L}_1 P \), and \( \gamma \) is a number determined by the normalization condition \( \text{Tr} \hat{\rho}_1 = 0 \).

In the same procedure we can determine \( Q \hat{\rho}_2, P \hat{\rho}_2, Q \hat{\rho}_3 \) and so on. These higher order terms, however, may be physically irrelevant because Eq. (25) was derived from the approximation up to the first order of \( v \).
3.2 Perturbative expansion with respect to $\Delta \beta$

The perturbative solution we have obtained in the previous subsection is still very formal because we do not know the explicit form of the 0th order term $\rho_0$. In this and following subsections we try to find a more explicit solution by expanding $\hat{\rho}$ with respect to $\Delta \beta$, the inverse temperature difference between the two heat bath.

We put

$$
\beta_L = \beta - \frac{\Delta \beta}{2},
$$

$$
\beta_R = \beta + \frac{\Delta \beta}{2}.
$$

Then we expand the heat bath superoperators and the density matrix as

$$
\Gamma^L(\beta_L) = \Gamma^L(\beta) - \frac{\Delta \beta}{2} \partial_\beta \Gamma^L(\beta) + O(\Delta \beta^2),
$$

$$
\Gamma^R(\beta_R) = \Gamma^R(\beta) + \frac{\Delta \beta}{2} \partial_\beta \Gamma^L(\beta) + O(\Delta \beta^2),
$$

$$
\hat{\rho} = \hat{\rho}_{00} + \Delta \beta \hat{\rho}_{01} + \nu(\hat{\rho}_{10} + \Delta \beta \hat{\rho}_{11}) + O(\nu^2) + O(\Delta \beta^2).
$$

We obtain an equation for each order $O(\nu^n \Delta \beta^m)$:

$$
O(1) : \quad \mathcal{L}_0 \hat{\rho}_{00} = 0,
$$

$$
O(\Delta \beta) : \quad \mathcal{L}_0 \hat{\rho}_{01} = 0,
$$

$$
O(\nu) : \quad \mathcal{L}_0 \hat{\rho}_{10} + (\Gamma^L + \Gamma^R) \hat{\rho}_{00} = 0,
$$

$$
O(\nu \Delta \beta) : \quad \mathcal{L}_0 \hat{\rho}_{11} + (\Gamma^L + \Gamma^R) \hat{\rho}_{01} + \frac{1}{2}(\partial_\beta \Gamma^L + \partial_\beta \Gamma^R) \hat{\rho}_{00} = 0.
$$

Note that $\Gamma^\alpha$ and $\partial_\beta \Gamma^\alpha$ in the above equations are evaluated at the inverse temperature $\beta$.

Eqs. (48) and (49) mean that $\hat{\rho}_{00}$ and $\hat{\rho}_{01}$ are diagonal. Since $\Gamma^\alpha_2$ satisfies

$$
P \Gamma^\alpha_2 P = 0,
$$

we obtain

$$
P(\Gamma^L_1 + \Gamma^R_1) \hat{\rho}_{00} = 0
$$

by applying $P$ to (50). It has the equilibrium solution

$$
\hat{\rho}_{00} = \frac{1}{Z} e^{-\beta H_S},
$$

where $Z$ is the partition function. Then from (50) we obtain

$$
Q \hat{\rho}_{10} = -\frac{1}{Z}(Q \mathcal{L}_0 Q)^{-1}(\Gamma^L_2 + \Gamma^R_2)e^{-\beta H_S}.
$$
3.3 Symmetric case

By applying $P$ to (51) we obtain
\[
P(\Gamma^L_1 + \Gamma^R_1)\hat{\rho}_{01} + \frac{1}{2}P(-\partial_\beta \Gamma^L_1 + \partial_\beta \Gamma^R_1)\hat{\rho}_{00} = 0.
\] (56)

In principle, $\hat{\rho}_{01}$ is determined by solving this equation. However, the inverse of $P(\Gamma^L_1 + \Gamma^R_1)P$ is hard to calculate analytically.

Here we assume that the system and the heat baths are reflection symmetric. More precisely, we assume that $\hat{\Pi} \hat{H}_{\text{tot}} \hat{\Pi} = \hat{H}_{\text{tot}}$, where $\hat{\Pi}$ is the parity operator which satisfies $\hat{\Pi}^2 = 1$. Then we have
\[
\hat{\Pi} \hat{H}_S \hat{\Pi} = \hat{H}_S, \tag{57}
\]
\[
\hat{\Pi} \hat{X}_j^L \hat{\Pi} = \hat{X}_j^R, \tag{58}
\]
\[
\hat{\Pi} \hat{R}_j^L \hat{\Pi} = \hat{R}_j^R, \tag{59}
\]
\[
\hat{\Pi} \hat{W}_j^L \hat{\Pi} = \hat{W}_j^R. \tag{60}
\]

Note that the operators are evaluated at the same inverse temperature $\beta$ in Eqs. (59) and (60).

Then let us consider the second term of Eq. (56). Since $\rho_{00}$ is symmetric, we have
\[
\hat{\Pi} \partial_\beta \Gamma^L_1 \rho_{00} \hat{\Pi} = \partial_\beta \Gamma^R_1 \rho_{00}, \tag{61}
\]
\[
\hat{\Pi} \partial_\beta \Gamma^R_1 \rho_{00} \hat{\Pi} = \partial_\beta \Gamma^L_1 \rho_{00}. \tag{62}
\]

A diagonal element in the second term of (56) is
\[
\langle E_p | (-\partial_\beta \Gamma^L_1 + \partial_\beta \Gamma^R_1)\hat{\rho}_{00} | E_p \rangle = \langle E_p | \hat{\Pi}(-\partial_\beta \Gamma^L_1 + \partial_\beta \Gamma^R_1)\hat{\rho}_{00} \hat{\Pi} | E_p \rangle \tag{63}
\]
\[
= \langle E_p | (-\partial_\beta \Gamma^R_1 + \partial_\beta \Gamma^L_1)\hat{\rho}_{00} | E_p \rangle \tag{64}
\]
\[
= \langle E_p | (-\partial_\beta \Gamma^L_1 + \partial_\beta \Gamma^L_1)\hat{\rho}_{00} | E_p \rangle \tag{65}
\]

Hence
\[
\langle E_p | (-\partial_\beta \Gamma^L_1 + \partial_\beta \Gamma^L_1)\hat{\rho}_{00} | E_p \rangle = 0 \tag{66}
\]

and the second term of (56) vanishes. Then we have
\[
P(\Gamma^L_1 + \Gamma^R_1)\hat{\rho}_{01} = 0, \tag{68}
\]

whose solution is
\[
\hat{\rho}_{01} \propto \hat{\rho}_{00} = \frac{1}{Z} e^{-\beta \hat{H}_S}. \tag{69}
\]

To keep the normalization condition $\text{Tr} \hat{\rho} = 1$, we should put
\[
\hat{\rho}_{01} = 0. \tag{70}
\]

Then we obtain the lowest order nonequilibrium term
\[
Q \hat{\rho}_{11} = -\frac{1}{2Z}(Q \mathcal{L}_0 Q)^{-1}Q(-\partial_\beta \Gamma^L_1 + \partial_\beta \Gamma^R_1)e^{-\beta \hat{H}_S}. \tag{71}
\]

from (51). This is our main result. Note that diagonal elements do not contribute to nonequilibrium properties like the energy current and the temperature gradient.
4 Energy current

4.1 Energy current operator

Let us consider the energy current going through the system. We divide the system into two parts. Then the system Hamiltonian is

\[ \hat{H}_S = \hat{H}_l + \hat{H}_r, \]  

(72)

where \( \hat{H}_l \) and \( \hat{H}_r \) are the Hamiltonians for the left and right parts of the system, respectively, and \( \hat{H}_i \) is the interaction between them. Note that \([\hat{H}_l, \hat{H}_r] = 0\). The energy current which goes from the left part to the right part can be defined as the energy loss of the left part:

\[ \hat{J}_l \equiv -\dot{\hat{H}}_l = -\frac{1}{i\hbar}[\hat{H}_l, \hat{H}_S] = -\frac{1}{i\hbar}[\hat{H}_l, \hat{H}_i]. \]  

(73)

It is also possible to define another current operator by the energy gain of the right part:

\[ \hat{J}_r \equiv \dot{\hat{H}}_r = \frac{1}{i\hbar}[\hat{H}_r, \hat{H}_S] = \frac{1}{i\hbar}[\hat{H}_r, \hat{H}_i]. \]  

(74)

We can also define the energy current at a boundary between the system and a heat bath. The total energy of the system changes as

\[ \frac{d}{dt} \langle \hat{H}_S \rangle = \text{Tr} \left( \hat{H}_S \frac{d}{dt} \hat{\rho} \right) \]  

(75)

\[ = \text{Tr} \left\{ \hat{H}_S \left( [\hat{H}_S, \hat{\rho}] + v\Gamma^L \hat{\rho} + v\Gamma^R \hat{\rho} \right) \right\} \]  

(76)

\[ = v \text{Tr} \left( \hat{H}_S \Gamma^L \hat{\rho} \right) + v \text{Tr} \left( \hat{H}_S \Gamma^R \hat{\rho} \right). \]  

(77)

The left (right) term can be interpreted as the energy current at the left (right) boundary. Therefore we define two current operators \( \hat{J}_L \) and \( \hat{J}_R \) so that the following relations hold.

\[ \langle \hat{J}_L \rangle = v \text{Tr} \left( \hat{H}_S \Gamma^L \hat{\rho} \right), \]  

(78)

\[ \langle \hat{J}_R \rangle = -v \text{Tr} \left( \hat{H}_S \Gamma^R \hat{\rho} \right). \]  

(79)

Then

\[ \text{Tr}(\hat{J}_L \hat{\rho}) = -\frac{v}{2\hbar^2} \sum_{ji} \text{Tr} \left\{ \hat{H}_S \left( [\hat{X}_j^L, \hat{R}_{ji}^L \hat{\rho}] + [\hat{X}_j^L, \hat{R}_{ji}^L \hat{\rho}]^\dagger \right) + i \left( [\hat{X}_j^L, \hat{W}_{ji}^L \hat{\rho}] - [\hat{X}_j^L, \hat{W}_{ji}^L \hat{\rho}]^\dagger \right) \right\} \]  

(80)

\[ = -\frac{v}{2\hbar^2} \sum_{ji} \text{Tr} \left\{ \left( [\hat{H}_S, \hat{X}_j^L] \left( \hat{R}_{ji}^L + i\hat{W}_{ji}^L \right) + \left( \hat{R}_{ji}^L + i\hat{W}_{ji}^L \right)^\dagger \right) \hat{\rho} \right\}. \]  

(81)

Hence

\[ \hat{J}_L = -\frac{v}{2\hbar^2} \sum_{ji} \left\{ \left( [\hat{H}_S, \hat{X}_j^L] \left( \hat{R}_{ji}^L + i\hat{W}_{ji}^L \right) + \left( \hat{R}_{ji}^L + i\hat{W}_{ji}^L \right)^\dagger \right) \left[ \hat{H}_S, \hat{X}_j^L \right]^\dagger \hat{\rho} \right\}. \]  

(82)

In the same way we obtain

\[ \hat{J}_R = \frac{v}{2\hbar^2} \sum_{ji} \left\{ \left( [\hat{H}_S, \hat{X}_j^R] \left( \hat{R}_{ji}^R + i\hat{W}_{ji}^R \right) + \left( \hat{R}_{ji}^R + i\hat{W}_{ji}^R \right)^\dagger \right) \left[ \hat{H}_S, \hat{X}_j^R \right]^\dagger \hat{\rho} \right\}. \]  

(83)

In the steady state all current operators should have the same expectation value.
4.2 Expectation value

Let us consider the expectation value of an energy current operator in the system. In our perturbation theory, \( Q\hat{\rho}_{11} \) is the leading nonequilibrium term. Therefore we evaluate

\[
\text{Tr}(\hat{J}_t Q\hat{\rho}_{11}) = \frac{1}{2i\hbar} \left\{ [\hat{H}_t, \hat{H}_S](Q\mathcal{L}_0 Q)^{-1}(-\partial_\beta \Gamma^L + \partial_\beta \Gamma^R)\hat{\rho}_{00} \right\} 
\]

\[
= -\frac{1}{2} \left\{ (\mathcal{L}_0 \hat{H}_t)(Q\mathcal{L}_0 Q)^{-1}Q(-\partial_\beta \Gamma^L + \partial_\beta \Gamma^R)\hat{\rho}_{00} \right\} .
\]

Note that

\[
\text{Tr} \left\{ (\mathcal{L}_0 \hat{A})(Q\mathcal{L}_0^{-1} Q)^{-1} Q\hat{B} \right\} = -\text{Tr}(\hat{A}\hat{Q}\hat{B})
\]

holds in general, because

\[
\text{Tr} \left\{ (\mathcal{L}_0 \hat{A})(Q\mathcal{L}_s^{-1} Q)^{-1} Q\hat{B} \right\} = \sum_{l,m} \langle E_l | \mathcal{L}_0 \hat{A} | E_m \rangle \langle E_m | (Q\mathcal{L}_0^{-1} Q)^{-1} Q\hat{B} | E_l \rangle
\]

\[
= \sum_{l \neq m} (E_l - E_m) \langle E_l | \hat{A} | E_m \rangle \frac{1}{E_m - E_l} \langle E_m | \hat{B} | E_l \rangle
\]

\[
= -\sum_{l \neq m} \langle E_l | \hat{A} | E_m \rangle \langle E_m | \hat{B} | E_l \rangle
\]

\[
= -\text{Tr}(\hat{A}\hat{Q}\hat{B}).
\]

Hence

\[
\text{Tr}(\hat{J}_t Q\hat{\rho}_{11}) = \frac{1}{2} \text{Tr} \left\{ \hat{H}_t Q(-\partial_\beta \Gamma^L + \partial_\beta \Gamma^R)\hat{\rho}_{00} \right\}
\]

\[
= \frac{1}{2} \text{Tr} \left\{ \hat{H}_t(-\partial_\beta \Gamma^L + \partial_\beta \Gamma^R)\hat{\rho}_{00} \right\} \quad (\because P(-\partial_\beta \Gamma^L + \partial_\beta \Gamma^R)\hat{\rho}_{00} = 0).
\]

Each term in \( \partial_\beta \Gamma^\alpha \hat{\rho}_{00} \) has the form \( \hat{X}_j^\alpha, \partial_\beta \hat{Z}_{ji}\hat{\rho}_{00} \) (\( Z = R, W \)). Then

\[
\text{Tr} \left( \hat{H}_t[X_j^\alpha, \partial_\beta \hat{Z}_{ji}\hat{\rho}_{00}] \right) = \text{Tr} \left( [\hat{H}_t, X_j^\alpha]\partial_\beta \hat{Z}_{ji}\hat{\rho}_{00} \right),
\]

which vanishes if \( \alpha = R \). Hence

\[
\text{Tr}(\hat{J}_t Q\hat{\rho}_{11}) = -\frac{1}{2} \text{Tr} \left( \hat{H}_t\partial_\beta \Gamma^L \hat{\rho}_{00} \right)
\]

\[
= -\frac{1}{2} \text{Tr} \left( \hat{H}_S \partial_\beta \Gamma^L \hat{\rho}_{00} \right)
\]

\[
= -\frac{1}{2} \text{Tr} \left\{ \hat{H}_S \left( \partial_\beta \Gamma^L_1 + \partial_\beta \Gamma^L_2 \right) \hat{\rho}_{00} \right\}.
\]

In the second line we used \( [\hat{H}_t, \hat{X}_j] = [\hat{H}_S, \hat{X}_j] \). With some algebra, one can easily show

\[
\text{Tr} \left( \hat{H}_S \partial_\beta \Gamma^L_2 \hat{\rho}_{00} \right) = 0.
\]

Since

\[
\Gamma^L_1(\beta) e^{-\beta R_S} = 0
\]
for any $\beta$,
\[
\partial_\beta \left( \Gamma_1^L(\beta) e^{-\beta H_S} \right) = \partial_\beta \Gamma_1^L(\beta) e^{-\beta H_S} + \Gamma_1^L(\beta) \partial_\beta e^{-\beta H_S} = 0.
\]
(101)
Therefore
\[
\partial_\beta \Gamma_1^L \hat{\rho}_{00} = -\Gamma_1^L \hat{H}_S \hat{\rho}_{00}
\]
(102)
and
\[
\text{Tr}(\hat{J}_l Q \hat{\rho}_{11}) = \frac{1}{2} \text{Tr}
\left( \hat{H}_S \Gamma_1^L \hat{H}_S \rho_{00} \right)
\]
(103)
\[
= -\frac{1}{2\hbar^2} \text{Re} \sum_{jl} \text{Tr}
\left( \hat{H}_S [\hat{X}_j^L, \hat{R}_{jl}^L \hat{H}_S \rho_{00}] \right)
\]
(104)
\[
= -\frac{1}{2\hbar^2} \text{Re} \sum_{jl} \text{Tr}
\left( [\hat{H}_S, \hat{X}_j^L] \hat{R}_{jl}^L \hat{H}_S \rho_{00} \right)
\]
(105)
\[
= -\frac{1}{4\hbar^2 Z} \sum_{jl} \sum_{pq} \left\{ E_p (E_p - E_q) \langle E_p | \hat{X}_j^L | E_q \rangle \langle E_p | \hat{X}_j^L | E_p \rangle \Phi_{jl}(\omega_{pq}) e^{-\beta E_p} + E_p (E_p - E_q) \langle E_q | \hat{X}_j^L | E_p \rangle \langle E_q | \hat{X}_j^L | E_p \rangle \Phi_{jl}(\omega_{pq}) e^{-\beta E_p} \right\}
\]
(106)
\[
= -\frac{1}{4\hbar^2 Z} \sum_{jl} \sum_{pq} \left\{ (E_p - E_q)^2 \langle E_p | \hat{X}_j^L | E_q \rangle \langle E_q | \hat{X}_j^L | E_p \rangle \Phi_{jl}(\omega_{pq}) e^{-\beta E_q} \right\}
\]
(107)
\[
= -\frac{1}{4\hbar^2} \sum_{jl} \left\langle [\hat{H}_S, \hat{X}_j^L][\hat{R}_{jl}^L, \hat{H}_S] \right\rangle_\beta.
\]
(108)
In the last line, the expectation value is evaluated for the system in equilibrium at the inverse temperature $\beta$.

In the same way we obtain
\[
\text{Tr}(\hat{J}_r Q \rho_{11}) = -\frac{1}{4\hbar^2} \sum_{jl} \left\langle [\hat{H}_S, \hat{X}_j^R][\hat{R}_{jl}^R, \hat{H}_S] \right\rangle_\beta.
\]
(110)
Since we have assumed the reflection symmetry, we obtain
\[
\langle \hat{J}_l \rangle = \langle \hat{J}_r \rangle = -\frac{1}{4\hbar^2} \sum_{jl} \left\langle [\hat{H}_S, \hat{X}_j^L][\hat{R}_{jl}^L, \hat{H}_S] \right\rangle_\beta \nu \Delta \nu + O(\nu^2) + O(\Delta \nu^2).
\]
(111)
We can also calculate the expectation values of the current operators at the boundaries. Let us consider $\hat{J}_L$. Since $\hat{J}_L$ is $O(\nu)$, the lowest order current comes from $O(\nu^0)$ terms of the density matrix. Because $\hat{\rho}_{01} = 0$ in the symmetric case, we have
\[
\langle \hat{J}_L \rangle = \text{Tr}(\hat{J}_L \hat{\rho}_{00}) + O(\nu^2) + O(\Delta \nu^2).
\]
(112)
Then, from Eq. (78)
\[
\text{Tr}(\hat{J}_L \hat{\rho}_{00}) = v \text{Tr}(\hat{H}_S \Gamma_L \hat{\rho}_{00}).
\] (113)

Note that \(\Gamma_L\) is evaluated at \(\beta_L = \beta - \Delta \beta/2\) here. Substituting
\[
\Gamma_L(\beta_L) = \Gamma_L(\beta) - \frac{\Delta \beta}{2} \partial_\beta \Gamma_L(\beta)
\] (114)
we obtain
\[
\text{Tr}(\hat{J}_L \hat{\rho}_{00}) = -\frac{v \Delta \beta}{2} \text{Tr}(\hat{H}_S \partial_\beta \Gamma_L \hat{\rho}_{00}),
\] (115)
which is equivalent to (97). Then we obtain the same current expectation value again:
\[
\langle \hat{J}_L \rangle = \langle \hat{J}_R \rangle = -\frac{1}{4\hbar^2} \sum_{jl} \left[ \langle [\hat{H}_S, \hat{X}_j(t)] [\hat{X}_l(t), \hat{H}_S] \rangle_{\beta} v \Delta \beta + O(v^3) + O(\Delta \beta^2) \right]
\] (116)

### 4.3 Kubo formula

Let us consider the total system including the heat bath again. The current operator for the energy coming from the heat bath \(L\) to the system is defined as
\[
\hat{J}'_L = \frac{d}{dt}(\hat{H}_S + u \hat{H}_{RS} + \hat{H}_R)
\] (117)
\[
= \frac{1}{i\hbar} [\hat{H}_S + u \hat{H}_{RS} + \hat{H}_R, \hat{H}_{\text{tot}}]
\] (118)
\[
= \frac{1}{i\hbar} [\hat{H}_S, u \hat{H}_{LS}]
\] (119)
\[
= \frac{u}{i\hbar} \sum_{j} [\hat{H}_S, \hat{X}_j] \hat{Y}_j.
\] (120)

Then we define the correlation function
\[
C_L(t) \equiv \frac{1}{2} \langle \hat{J}'_L(t) \hat{J}'_L + \hat{J}'_L \hat{J}'_L(t) \rangle.
\] (121)

The expectation value is evaluated for the equilibrium of the total system with inverse temperature \(\beta\). Since \(\hat{J}'_L\) is \(O(v^3)\), we have
\[
C_L(t) = C^{(0)}(t) + O(v^3),
\] (122)
where
\[
C^{(0)}(t) = \frac{1}{2} \text{Tr} \left\{ \rho_S^{\text{eq}} \otimes \rho_B^{\text{eq}} \left( e^{i(\hat{H}_S + \hat{H}_B)t/\hbar} \hat{J}'_L e^{-i(\hat{H}_S + \hat{H}_B)t/\hbar} \hat{J}'_L + \hat{J}'_L e^{i(\hat{H}_S + \hat{H}_B)t/\hbar} \hat{J}'_L e^{-i(\hat{H}_S + \hat{H}_B)t/\hbar} \right) \right\}
\] (123)

Here, \(\rho_S^{\text{eq}}\) and \(\rho_B^{\text{eq}}\) represents the equilibrium state of the system and the heat baths, respectively. Then we have
\[
C^{(0)}_L(t) = -\frac{u^2}{2\hbar^2} \sum_{jl} \left\{ \langle [H_S, \hat{X}_j(t)] [H_S, \hat{X}_l] \rangle_{\beta} \Phi_{jl}(t) + \langle [H_S, \hat{X}_j][H_S, \hat{X}_l(t)] \rangle_{\beta} \Phi_{jl}(-t) \right\}
\] (124)
and

\[
\int_0^\infty dt \, C_L^{(0)}(t) = -\frac{u^2}{2\hbar} \sum_{jl} \sum_{p,q} e^{-\beta E_p} (E_p - E_q)^2 \langle E_p | \hat{X}_j | E_q \rangle \langle E_q | \hat{X}_l | E_r \rangle \\
\times \int_0^\infty dt \left\{ e^{-i\omega_{qp}t} \Phi_{jl}(t) + e^{i\omega_{qp}t} \Phi_{jl}(-t) \right\} 
\]

\[
= -\frac{u^2}{2\hbar} \sum_{jl} \sum_{p,q} e^{-\beta E_p} (E_p - E_q)^2 \langle E_p | \hat{X}_j | E_q \rangle \langle E_q | \hat{X}_l | E_r \rangle \Phi_{jl}(\omega_{qp}) 
\]

\[
= -\frac{v}{2\hbar} \sum_{jl} \left\langle [\hat{H}_S, \hat{X}_j] [\hat{R}_{jl}, \hat{H}_S] \right\rangle. 
\]

Therefore, in the lowest order, the current is written as

\[
\langle \hat{J}_L \rangle = \frac{\Delta \beta}{2} \int_0^t dt \, C_L(t), 
\]

which is the Kubo formula [3], or the fluctuation-dissipation theorem, in this case. Note that \(\Delta \beta/2\) is the inverse temperature difference at the boundary.

In spite of the formal similarity, physical content of Eq. (128) is quite different from the original Kubo formula [1]. For example, the transport coefficient contains the information of the heat baths, though the original one does not.

## 5 Summary

We have calculated the density matrix for the NESS using the time-independent perturbation theory. Our main result is Eq. (71), which is an explicit expression for the density matrix for the NESS in the reflection symmetric setting. We have also calculated the expectation value of the energy current and shown that the Kubo formula holds in this case.

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### References

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