

The Entropy Production of a Nonequilibrium Open System

Ming Bao Yu*

407 Oak Tree Square, Athens, Georgia 30606, USA

Abstract

A nonequilibrium open system is studied in the projection operator formalism. The environment may linearly deviate from its initial state under the reaction from the open system. If the relevant statistical operator of the system is a generalized canonical one, the transport equation, the second kind of fluctuation-dissipation theorem and the entropy production rate of the open system can be derived and expressed in terms of correlation functions of fluctuations of random forces and interaction random forces.

Keywords: Non equilibrium open system; Projection operator; Entropy production rate

Introduction

In the study of nonequilibrium systems different projection operators are introduced to present a macroscopic description of the system in order to simplify the problem [1-6]. In this approach the macroscopic state of the system is determined by expectation values of a set of basis macro variables, and equations of motions for these expectation values, the transport equations, are derived in the projection operator formalism.

When studying a nonequilibrium open system, the influence of the environment upon the open system is one of the important topics in such studies. It has been shown [7] that the influence from the environment comes from two parts: one is the time-rate of the averaged macro variables resulting from the interaction Hamiltonian H_{SR} and the other from an additional influence term, therefore, the influence of the environment can be completely separated from the corresponding closed system.

When the relevant statistical operator of the system is of a generalized canonical statistical operator (GCSO) by which the entropy of the open system is defined, if the environment is a reservoir, then the memory and influence terms in the transport equation can be given in terms of correlation functions of fluctuations of random forces and interacting random forces, and they can be cast into the Volterra equation formalism.

The purpose of the present paper is to generalize the results to the case that the environment is not a reservoir which may linearly deviate from its initial state under the reaction from the open system. We will show that the memory and influence terms can still be expressed in terms of correlation functions of fluctuations of random forces and interaction random forces, but no longer be able to cast into the Volterra equation formalism, so is the entropy production rate of the open system.

The results obtained in this paper are compared with approaches in linear thermodynamics and statistical mechanics, focusing on the entropy production of a nonequilibrium open system, which is local in both space and time. In contract, the entropy generation [8] is also important in the study of nonequilibrium systems, which is global in space and time, being especially useful in cases involving effects of irreversibility. In addition, another important development in physics today is the so-called quantum thermodynamics [9-14] which has extended the thermodynamics study from the macroscopic scale to the nanometer scale, and even down to the single atom and single

photon scale. In Section 2, transport equations of the system are briefly reviewed. In Section 3, a GCSO is introduced. The entropy production rate is derived in Section 4. The influence term and its contribution to the entropy production is studied in Section 5. Comparison of the results with well-known approaches is presented in Section 6 and conclusions are drawn in Section 7.

Transport equations

Consider an open system S under the influence of its environment R. The total system $S \oplus R$ is characterized by Hamiltonian $H=H_S+H_R+\lambda H_{SR}$ and statistical operator (so) $W(t)$. The open system s is described by a reduced statistical operator $\rho(t)=tr_R W(t)$ satisfying $\partial \rho(t)/\partial t=-iL_S \rho(t)+\eta(t)$ with

$$\eta(t)=-i\lambda tr_R [L_{SR} W(t)] \tag{2.1}$$

describing the influence of R upon S, where $L_S X=i [H_S, X]$, $h=1$.

Suppose we are satisfied with the description of system S at the macroscopic level by expectation values (EVs) of a set of basis macrovariables $\{A_j, j=1, \dots, m\}$ of S, such macroscopic description can be realized by a relevant so $\rho_r(t)$ which is picked up by a time-dependent projection operator $\rho(t)$ from $\rho(t): \rho_r(t)=\rho(t)\rho(t)$. We may choose the following projection operator as $\rho(t)$ [3]:

$$\rho(t)X = \left[\rho_r(t) - \sum_k \frac{\partial \rho_r(t)}{\partial \langle A_k(t) \rangle} \langle A_k(t) \rangle \right] tr_r X + \sum_k \frac{\partial \rho_r(t)}{\partial \langle A_k(t) \rangle} tr_r (A_k X) \tag{2.2}$$

Introduce $q(t)=1-\rho(t)$, $p(t)q(t)=0$, we have [6]

$$\rho(t) = \rho_r(t) + g(t,0)q(0)\rho(0) - \int_0^t du g(t,u)q(u)iL_S \rho_r(u) + \int_0^t du g(t,u)q(u)\eta(u) \tag{2.3}$$

with $\dot{p}(t)\rho(t)=0$; $g(t,u)=T_+ \exp\{-i \int_u^t du_1 q(u_1)L_S\}$ ($t > u$) is a time-ordered evolution operator satisfying

$$\partial g(t,u)/\partial u = ig(t,u)q(u)L_S \text{ and } g(t,t)=1.$$

*Corresponding author: Ming Bao Yu, 407 Oak Tree Square, Athens, Georgia 30606, USA, Tel: 706-410-2137; E-mail: mingbyu@gmail.com

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The transport equation for EV $\langle A_j(t) \rangle = \text{tr}_S[\rho(t)A_j] = \text{tr}_S[\rho(t)A_j]$ takes the form [6]

$$\frac{\partial}{\partial t} \langle A_j(t) \rangle = \frac{\partial}{\partial t} \langle A_j(t) \rangle^{(0)} + Y_j(t) \quad (j=1,2,\dots,m).$$

In Heisenberg picture,

$$\frac{\partial}{\partial t} \langle A_j(t) \rangle^{(0)} = \text{tr}_S[\rho(0)\dot{A}_j] + \text{tr}_S[\rho(0)Q(0)G(0,t)\dot{A}_j] + \int_0^t \text{d}u \text{tr}_S[\rho(u)iL_S Q(u)G(u,t)\dot{A}_j], \quad (2.5)$$

here the first term gives the organized motion, the second term the initial condition and the third term the disorganized motion or the memory term [4] and

$$Y_j(t) = \int_0^t \text{d}u \text{tr}_S \left[\eta(u)Q(u)G(u,t)\dot{A}_j \right] \quad (2.6)$$

is an additional term describing the external influence from the environment upon the open system; $G(u,t) = T_{-} \exp \left[i \int_u^t \text{d}u' L Q(u') \right]$ ($t > u$) is an anti-time-ordered evolution operator defined by $\partial G(u,t) / \partial u = -iL_S Q(u)G(u,t)$ and $G(t,t) = 1$; $Q(t) = 1 - P(t)$, $P(t)$ is the transposed projection operator of $P(t)$ [4],

$$P(t)X = \text{tr}_S[\rho_r(t)X] + \sum_k [A_k - \langle A_k(t) \rangle] \text{tr}_S \left[\frac{\partial \rho_r(t)}{\partial \langle A_k(t) \rangle} X \right]; \quad (2.7)$$

Satisfying

$$\text{tr}_S[X(t)g(t,u)q(u)Y(u)] = \text{tr}_S[Y(u)Q(u)G(u,t)X(t)] \quad (2.8)$$

Since $\dot{A}_j = i(L_S + \lambda L_{SR})A_j$, (2.4) may be written as [7]

$$\frac{\partial}{\partial t} \langle A_j(t) \rangle^{(0)} = \text{tr}_S[\rho_r(t)(iL_S A_j)] + \text{tr}_S[\rho(0)Q(0)G(0,t)(iL_S A_j)] + \int_0^t \text{d}u \text{tr}_S[\rho(u)iL_S Q(u)G(u,t)(iL_S A_j)] \quad (j = 1, 2, \dots, m), \quad (2.9)$$

Where

$$\frac{\partial}{\partial t} \langle A_j(t) \rangle^{(0)} = \text{tr}_S[\rho_r(t)(iL_S A_j)] + \text{tr}_S[\rho(0)Q(0)G(0,t)(iL_S A_j)] + \int_0^t \text{d}u \text{tr}_S[\rho(u)iL_S Q(u)G(u,t)(iL_S A_j)]$$

(2.10a) is the transport equation of the corresponding closed system, i.e. the time rate of EV resulting from H_S , the Hamiltonian of the system S itself; and

$$\frac{\partial}{\partial t} \langle A_j(t) \rangle^{(0)} = \text{tr}_S[\rho_r(t)(iL_{SR} A_j)] + \text{tr}_S[\rho(0)Q(0)G(0,t)(iL_{SR} A_j)] + \int_0^t \text{d}u \text{tr}_S[\rho(u)iL_{SR} Q(u)G(u,t)(iL_{SR} A_j)] \quad (2.10b)$$

is the time rate resulting from the interaction H_{SR} .

The meaning of (2.9) is clear and simple: The transport equation of an open system is the sum of transport equation of the corresponding closed system, the time-rate of the EV due to the interaction Hamiltonian H_{SR} and the additional influence term $Y_j(t)$.

The influence term (2.6) can be written as ($j=1,2,\dots,m$) ($j=1,2,\dots,m$), (2.11)

Where $f_j(u,t) = Q(u)G(u,t)\dot{A}_j$ denotes the random force, which may be split into two:

$$f_j(u,t) = f_j^s(u,t) + \lambda f_j^{SR}(u,t), \quad (2.12a)$$

$$f_j^s(u,t) = Q(u)G(u,t)(iL_S A_j),$$

$$f_j^{SR}(u,t) = Q(u)G(u,t)(iL_{SR} A_j) \quad (2.12b)$$

being respectively the random force and interaction random force associated with the time rate of the basis variable A_j due to H_S and H_{SR} respectively. Since the average of the random force over given ensembles vanishes, so $f_j(u,t) = \delta f_j(u,t)$ In the rest of the paper we will no longer distinguish $f_j(u,t)$ from its fluctuation $\delta f_j(u,t)$.

Generalized canonical statistical operator In order to go steps further

let us assume $\rho_r(t)$ to be a GCSO:

$$\rho_r(t) = e^{-\sum_l \lambda_l(t)A_l} / z_r(t) = \text{tr}_S \left[e^{-\sum_l \lambda_l(t)A_l} \right] \quad (3.1)$$

where $\lambda_l(t)$ ($l=1,\dots,m$) are conjugate parameters of the basis macrovariables $\{A_l\}$

Making use of the Kubo identity $[X, e^Y] = \int_0^1 d\alpha e^{\alpha Y} [X, Y] e^{(1-\alpha)Y}$ we have

$$iL_S \rho_r(t) = -\sum_l \int_0^1 d\alpha e^{-\alpha \sum_l \lambda_l(t)A_l} (iL_S A_l) e^{\alpha \sum_l \lambda_l(t)A_l} \rho_r(t) \lambda_l(t) \quad (3.2a)$$

$$iL_{SR} \rho_r(t) = -\sum_l \int_0^1 d\alpha e^{-\alpha \sum_l \lambda_l(t)A_l} (iL_{SR} A_l) e^{\alpha \sum_l \lambda_l(t)A_l} \rho_r(t) \lambda_l(t) \quad (3.2b)$$

Introducing the generalized quantum correlation function

$$(X(t), Y(u))_r = \int_0^1 d\alpha \text{tr}_S \left[X(t) e^{-\alpha \sum_l \lambda_l(t)A_l} Y(u) e^{\alpha \sum_l \lambda_l(t)A_l} \rho_r(u) \right] \quad (3.3)$$

and making use of (3.2), the integrand in (2.5) may be written as

$$\text{tr}_S[\rho_r(u) iL_S f_j(u,t)] = \sum_l (f_j(u,t), iL_S A_l)_r \lambda_l(u) \quad (3.4)$$

Since $f_j(u,t)$ is in the irregular space because of $Q(u)$ while is in the regular space, their correlation is zero, thus

$$\text{tr}_S[\rho_r(u) iL_S f_j(u,t)] = \sum_l (f_j(u,t), f_l^s(u,u))_r \lambda_l(u) \quad (3.5)$$

Where $f_l^s(u,u)$ is given by (2.12b). Same argument will apply to similar cases later.

Therefore Eq.(2.5) takes the form

$$\frac{\partial}{\partial t} \langle A_j(t) \rangle^{(0)} = \text{tr}_S[\rho_r(t)\dot{A}_j] + \text{tr}_S[\rho(0)Q(0)G(0,t)\dot{A}_j] + \int_0^t \text{d}u \text{tr}_S[\rho(u)Q(u)G(u,t)f_j^s(u,u)] \lambda_j(u) \quad (3.6)$$

here the memory term is expressed in terms of quantum correlation function of fluctuations of random forces. The influence term $Y_j(t)$ will be further analysed in Section 5.

Entropy production rate

Now define the entropy of the nonequilibrium open system through its relevant statistical operator [1,15,16]

$$S(t) = -k_B \text{tr}_S[\rho_r(t) \ln \rho_r(t)] \quad (4.1)$$

where k_B is the Boltzmann constant. The entropy production rate reads [7]

$$\frac{\partial S(t)}{\partial t} = k_B \sum_j \frac{\partial \langle A_j(t) \rangle}{\partial t} j(t) \quad (4.2)$$

which is the sum of products of transport equations and the conjugate parameters. If assume that the initial state of the system is a GCSO: $\rho(0) = \rho_r(0)$ then the initial term in (3.6) vanishes. Combining (4.2) with (2.4) given by (3.6) and (2.11), we obtain

$$\frac{\partial S_1(t)}{\partial t} = \frac{\partial S_1(t)}{\partial t} + \frac{\partial S_2(t)}{\partial t} + \frac{\partial S_3(t)}{\partial t}, \quad (4.3)$$

the first term resulting from the organized motion in (3.6) reads [7]

$$\frac{\partial S_1(t)}{\partial t} = \lambda k_B \sum_{j=1}^m \lambda_j(t) tr_S \left[\rho_r(t) tr_S (iL_{SR} A_j) \right] \quad (4.4)$$

the second term resulting from the disorganized motion in (3.6) takes the form

$$\frac{\partial S_2(t)}{\partial t} = k_B \sum_{j,1} \int_0^t du (f_j(u,t), f_1^S(u,u))_r \lambda_l(u) \lambda_j(t) \quad (4.5)$$

because of (3.5); and the third term resulting from the influence term (2.11) is

$$\frac{\partial S_3(t)}{\partial t} = k_B \sum_j \int_0^t du tr_S \left[\eta(u) f_j(u,t) \right] \lambda_j(t) \quad (4.6)$$

These expressions represent the contributions of each term in the transport equation to the entropy production, respectively. Besides, Eq.(4.4) does not involve $iL_S A_j$, indicating that in the organized motion term H_S contributes nothing to the rate.

Non-reservoir environment

Now we further analyze the contribution of the influence term $Y_j(t)$. Suppose that the environment R is not a reservoir and may linearly deviate from its initial state under the reaction from S. For simplicity, we assume $H_{SR} = \sum_k \gamma_k A_k B_k$, A_k and B_k respectively pertain to S and R, and they are initially independent:

$$W(0) = \rho(0) R(0) \text{ where } R(t) = tr_S W(t).$$

By $W(0) = \rho(0) R(0)$, we have $W(u) = \rho(u) R(u)$, here $\rho(u) = e^{-i(L_S + \lambda L_{SR})u} \rho(0)$ and $R(u) = e^{-i(L_R + \lambda L_{SR})u} R(0)$. By (2.1), $\eta(u)$ may be written as

$$\eta(u) = -i\lambda \langle L_{SR}(u) \rangle_{R0} \rho(u) = -i\lambda \left[\langle H_{SR}(u) \rangle_{R0}, \rho_r(t) \right]_- \quad (5.1)$$

$$\langle H_{SR}(u) \rangle_{R0} = \sum_k \gamma_k A_k \langle B_k(u) \rangle_{R0},$$

$$\langle B_k(u) \rangle_{R0} = tr_R \left[B_k(u) R(0) \right] \quad (5.2)$$

$\langle B_k(u) \rangle_{R0}$ determines the evolution of the EV of macrovariable B_k .

Since $\partial B_k(t) / \partial t = iL_R B_k(t) + i\lambda L_{SR} B_k(t)$ thus $B_k(t) = e^{iL_R t} B_k(0) + i\lambda \int_0^t du e^{iL_R(t-u)} L_{SR} B_k(u)$

For weak interaction, keeping only the linear term in λ , we obtain

$$B_k(t) = e^{iL_R t} \left[1 + i\lambda \int_0^t du L_{SR}(u) \right] B_k(0) + o(\lambda^2), L_{SR}(u) = e^{iL_R u} L_{SR} e^{iL_R u}$$

$$\langle B_k(u) \rangle_{R0} = \langle B_k(u) \rangle_{R0}^{(0)} + B_k(u) \rangle_{R0}^{(1)} \quad (5.3a)$$

$$\langle B_k(u) \rangle_{R0}^{(1)} = tr_R \left[R(0) e^{iL_R u} B_k(0) \right], \quad (5.3b)$$

$$\langle B_k(u) \rangle_{R0}^{(1)} = i\lambda tr_R \left[R(0) e^{iL_R u} \int_0^u du_1 L_{SR}(u_1) B_k(0) \right] \quad (5.3c)$$

being the zeroth and first order terms of the EV of B_k when R linearly deviates from its initial state under the weak reaction from S. By (5.1) and (5.2), the integrand in (2.11) takes the form

$$tr_S \{ \eta(u) f_j(u,t) \} = -i\lambda \sum_k \gamma_k tr_S \{ f_j(u,t) [A_k, \rho(u)]_- \} \langle B_k(u) \rangle_{R0} \quad (5.4a)$$

$$= -i\lambda \sum_k \gamma_k tr_S \left\{ F_j(u,t) [A_k(u), \rho(0)]_- \right\} \langle B_k(u) \rangle_{R0} \quad (5.4b)$$

in Schrodinger and Heisenberg pictures, respectively; where

$$F_j(u,t) = e^{i(L_S + L_{SR})u} f_j(u,t) \text{ and } A_k(u) = e^{i(L_S + L_{SR})u} A_k.$$

Hence we have the influence term

$$Y_j(t) = -i\lambda \sum_k \gamma_k \int_0^t du tr_S \{ f_j(u,t) [A_k, \rho(u)]_- \} \langle B_k(u) \rangle_{R0} \quad (5.5a)$$

$$= -i\lambda \sum_k \gamma_k \int_0^t du tr_S \{ F_j(u,t) [A_k(u), \rho(0)]_- \} \langle B_k(u) \rangle_{R0} \quad (5.5b)$$

and its contribution to the entropy production in Shrodinger and Heisenberg pictures:

$$\frac{\partial S_3(t)}{\partial t} = -i\lambda k_B \sum_{j,k} \gamma_k \int_0^t du tr_S \{ f_j(u,t) [A_k, \rho(u)]_- \} \langle B_k(u) \rangle_{R0} \lambda_j(t) \quad (5.6a)$$

$$-i\lambda k_B \sum_{j,k} \gamma_k \int_0^t du tr_S \{ F_j(u,t) [A_k(u), \rho(0)]_- \} \langle B_k(u) \rangle_{R0} \lambda_j(t) \quad (5.6b)$$

Now consider the case that the initial state of S is given by a GCSO:

$$\rho_r(0) = e^{-\sum_l \lambda_l(0) A_l} / tr_S e^{-\sum_l \lambda_l(0) A_l}. \quad (5.7)$$

By the Kubo identity and the initial condition $\rho(0) = \rho_r(0)$ we have

$$[A_k(u), \rho(0)]_- = -\sum_l \lambda_l(0) \int_0^1 d\alpha e^{-\alpha \sum_l \lambda_l(0) A_l} \rho_r(0),$$

Thus (5.4) may be written as

$$tr_S \{ \eta(u) f_j(u,t) \} = \lambda \sum_l (F_j(u,t), i \langle L_{SR}(u) \rangle_{R0} A_l)_{r0} \lambda_l(0) = \lambda \sum_l (F_j(u,t), f_l^{SR}(u,u))_{r0} \lambda_l(0)$$

here we have conducted argument similar to that leads (3.4) to (3.5), and

$$f_l^{SR}(u,u) = Q(u) G(u,u) [i \langle L_{SR}(u) \rangle_{R0} A_l] \quad (5.8)$$

is the averaged interaction random force. Thus we obtain

$$Y_j(t) = \lambda \sum_l \int_0^t du \left(F_j(u,t), f_l^{SR}(u,u) \right)_{r0} \lambda_l(0) \quad (5.9)$$

$$\frac{\partial S_3(t)}{\partial t} = \lambda k_B \sum_{j,l} \int_0^t du \left(F_j(u,t), f_l^{SR}(u,u) \right)_{r0} \lambda_l(0) \lambda_j(t) \quad (5.10)$$

$$\text{With } (X(t), Y(u))_{r0} = \int_0^1 d\alpha tr_S \left\{ X(t) e^{-\alpha \sum_l \lambda_l(0) A_l} \rho_r(0) \right\}$$

If the open system is initially in an equilibrium state

$$\rho(0) = \rho_r(0) = \rho_{eq} = e^{-\beta_0 H_S} / tr_S (e^{-\beta_0 H_S}), \quad (5.11)$$

$\beta_0 = 1/k_B T_0$ is the initial inverse temperature of the system, then ρ_{eq} is a special case of (5.7) in which $A_1 = H_S, \lambda_1(0) = \beta_0$ and $A_l = 0 (l \geq 2)$. Since A_1 is the only basic variable, so $\rho_r(t) = e^{-\beta(t) H_S} / tr_S [e^{-\beta(t) H_S}]$ and $\beta(t) = 1/k_B T(t)$ is the inverse temperature of S. Because $iL_S H_S = 0$, thus $\dot{H}_S = i\lambda L_{SR} H_S$ and $f_1^S(u,t) = 0, f_1(u,t) = \lambda f_1^{SR}(u,t); \quad (5.12)$

the memory term in (3.6) becomes $\lambda \int_0^t du (f_1^{SR}(u,t), f_1^S(u,u))_r \beta(u)$ and vanishes, so

$$\frac{\partial \langle H_S(t) \rangle^{(0)}}{\partial t} = \lambda tr_S [\rho_r(t) (iL_{SR} H_S)] \quad (5.13)$$

Besides, as a special case of (5.9) and (5.10), we have

$$Y_1(t) = \lambda^2 \beta_0 \int_0^t du \left(F_1^{SR}(u, t), \bar{f}_1^{SR}(u, u) \right)_{eq} \quad (5.14)$$

$$\frac{\partial S_3(t)}{\partial t} = \frac{\lambda^2}{T_0} \int_0^t du \left(F_1^{SR}(u, t), \bar{f}_1^{SR}(u, u) \right)_{eq} \beta(t) \quad (5.15)$$

$$\text{Here } (X(t), Y(u))_{eq} = \int_0^1 d\alpha tr_S \{ X(t) e^{-\alpha \beta_0 H_S} Y(u) e^{-\alpha \beta_0 H_S} \rho_{eq} \} \quad (5.16)$$

Finally we obtain the transport equation for the only basis variable H_S :

$$\frac{\partial S(t)}{\partial t} = \frac{\lambda}{T(t)} tr_S [\rho_r(t) (iL_{SR} H_S)] + \frac{\lambda^2}{T_0} \int_0^t du \left(F_1^{SR}(u, t), \bar{f}_1^{SR}(u, u) \right)_{eq} \beta(t) \quad (5.17)$$

Eqs.(5.9), (5.10) and (5.14), (5.15) involve the averaged interaction random force (5.8) which has incorporated the linear deviation of the environment from its initial state.

Now consider the case without a given initial condition. By (3.1) and the Kubo identity, we have

$$i \langle L_{SR}(u) \rangle_{r_0} \rho_r(u) = -\sum_i \lambda_i(u) \int_0^1 d\alpha e^{-\alpha \sum_i \lambda_i(u) A_i} [i \langle L_{SR}(u) \rangle_{r_0} A_i] e^{-\alpha \sum_i \lambda_i(u) A_i} \rho_r(u) \quad (5.18)$$

With (5.1) and (2.3),

$$tr_S \{ \eta(u) f_j(u, t) \} = -\lambda tr_S [f_j(u, t) i \langle L_{SR}(u) \rangle_{r_0} \rho(u)] = J_1 + J_2 + J_3 \quad (5.19)$$

Eq.(5.19) is similar to Eq.(22) in [17] where the environment is a reservoir and $\langle L_{SR} \rangle_{r_0}$ is time-independent. In the following, we will follow the argument in [17], however, take into consideration that $\langle L_{SR}(u) \rangle_{r_0}$ is time-dependent. Making use of (5.18) and (3.3), leads to

$$J_1 = -\lambda tr_S \{ f_j(u, t) i \langle L_{SR}(u) \rangle_{r_0} \rho_r(u) \} = \lambda \sum_i \lambda_i(u) \langle f_j(u, t), i \langle L_{SR}(u) \rangle_{r_0} A_i \rangle_r \quad (5.20)$$

$$J_2 = \lambda \int_0^u du_1 tr_S \{ f_j(u, t) i \langle L_{SR}(u) \rangle_{r_0} \tilde{K}_1(u, u_1) \rho_r(u_1) \} \\ = \lambda \sum_i \int_0^u du_1 \lambda_i(u_1) \langle K_1(u_1, u) f_j(u, t), i \langle L_{SR}(u) \rangle_{r_0} A_i \rangle_r \quad (5.21)$$

$$\tilde{K}_1(u, u_1) = g(u, u_1) q(u_1) iL_S, \\ K_1(u_1, u) = iL_S Q(u_1) G(u_1, u) \quad (5.22)$$

$$J_3 = -\lambda \int_0^u du_1 tr_S [f_j(u, t) i \langle L_{SR}(u) \rangle_{r_0} g(u, u_1) q(u_1) \eta(u_1)] \\ = \lambda^2 \int_0^u du_1 tr_S \{ \rho(u_1) \tilde{K}(u_1, u) \tilde{K}(u, t) \dot{A}_j \} \quad (5.23)$$

$$\tilde{K}(u, t) = i \langle L_{SR}(u) \rangle_{r_0} Q(u) G(u, t). \quad (5.24)$$

Substituting (2.3) into (5.23) and repeating the above arguments, we have

$$tr_S [\eta(u) f_j(u, t)] = \lambda \sum_i \{ \lambda_i(u) \langle f_j(u, t), i \langle L_{SR}(u) \rangle_{r_0} A_i \rangle_r + \\ \int_0^u du_1 \lambda_i(u_1) \langle K_1(u_1, u) f_j(u, t), i \langle L_{SR}(u) \rangle_{r_0} A_i \rangle_{r_1} + \dots \}$$

$$+ \lambda^2 \sum_i \int_0^u du_1 \lambda_i(u_1) \langle K(u_1, u) f_j(u, t), i \langle L_{SR}(u) \rangle_{r_0} A_i \rangle_r \\ + \int_0^u du_2 \lambda_i(u_2) \langle K_1(u_2, u_1) f_j(u, t), i \langle L_{SR}(u_1) \rangle_{r_0} A_i \rangle_{r_1} + \dots \} \\ K(u_1, u) = Q(u_1) G(u_1, u) i \langle L_{SR}(u) \rangle_{r_0}, \quad (5.25)$$

which many be written as

$$tr_S [\eta(u) f_j(u, t)] = \lambda \sum_i \left\{ \lambda_i(u) \langle f_j(u, t), \bar{f}_i^{SR}(u, u) \rangle_r + M_i(u, t) \right\} \quad (5.26)$$

$$M_i(u, t) = \sum_{n=1}^{\infty} \lambda^{n-1} \int_0^u du_1 \dots \int_0^{u_{n-1}} du_n \lambda_i(u_n) \langle (K_1(u_{n-1}, u_{n-2}) \dots K(u_1, u) f_j(u, t), \bar{f}_i^{SR}(u_{n-1}, u_{n-1}))_r, \\ + \lambda K(u_n, u_{n-1}) K(u_{n-1}, u_{n-2}) \dots K(u_1, u) f_j(u, t), \bar{f}_i^{SR}(u_n, u_n) \rangle_r \quad (5.27)$$

here we have had argument similar to that leads (3.4) to (3.5). Thus we obtain the influence term and its contribution to the entropy production:

$$Y_j(t) = \lambda \sum_i \int_0^t du \left\{ \lambda_i(u) \langle f_j(u, t), \bar{f}_i^{SR}(u, u) \rangle_r + M_i(u, t) \right\} \quad (5.28)$$

$$\frac{\partial S_3(t)}{\partial t} = \lambda k_B \sum_{j,l} \int_0^t du \left\{ \lambda_j(u) \langle f_j(u, t), \bar{f}_j^{SR}(u, u) \rangle_r + M_l(u, t) \right\} \lambda_l(t) \quad (5.29)$$

If we are satisfied with keeping the linear term of λ in $M_i(u, t)$, then

$$M_i(u, t) = \int_0^u du_1 \lambda_i(u_1) \langle K_1(u_1, u) f_j(u, t), \bar{f}_i^{SR}(u, u) \rangle_r + o(\lambda^2) \quad (5.30)$$

$$tr_S [\eta(u) f_j(u, t)] = \lambda \sum_i \left(\phi_i(u) f_j(u, t), \bar{f}_i^{SR}(u, u) \right)_r + o(\lambda^3) \quad (5.31)$$

$$\phi_i(u) = \lambda_i(u) + \int_0^u du_1 \lambda_i(u_1) K_1(u_1, u) \quad (5.32)$$

Therefore we have the approximate expressions

$$Y_j(t) = \lambda \sum_i \int_0^t du \left(\phi_i(u) f_j(u, t), \bar{f}_i^{SR}(u, u) \right)_r \quad (5.33)$$

$$\frac{\partial S_3(t)}{\partial t} = \lambda k_B \sum_{j,l} \int_0^t du \left(\phi_l(u) f_j(u, t), \bar{f}_l^{SR}(u, u) \right)_r \lambda_j(t) \quad (5.34)$$

they are up to λ^2 by (2.12a). Comparing (5.34) with (4.5), we see clearly that $\phi_i(u)$ plays the role of $\lambda_i(u)$ in the case of corresponding isolate system.

Now we rewrite the results obtained above in the form of special dependent. For simplicity, we focus on the simpler expression (5.34). The entropy production of the open system reads

$$\frac{\partial S(x, t)}{\partial t} = \frac{\partial S_1(x, t)}{\partial t} + \frac{\partial S_2(x, t)}{\partial t} + \frac{\partial S_3(x, t)}{\partial t} \quad (5.35)$$

Where

$$\frac{\partial S_1(x, t)}{\partial t} = \lambda k_B \sum_{j=1}^m \lambda_j(x, t) tr_S [\rho_r(x, t) (iL_{SR} A_j)] \quad (5.36a)$$

results from the organized motion in the transport equation due to H_{SR}^2

$$\frac{\partial s_2(x,t)}{\partial t} = k_B \sum_{j,l} \int_0^t du (f_j(u,t), f_l^S(u,u))_r \lambda_l(x,u) \lambda_j(x,t) \quad (5.36b)$$

from the disorganized motion and

$$\frac{\partial s_3(x,t)}{\partial t} = \lambda k_B \sum_{j,l} \int_0^t du (\phi_l(x,u), f_j(u,t))_r \overset{-SR}{f_l}(u,u)_r \lambda_j(x,t) \quad (5.36c)$$

from the influence term, respectively.

Comparison

In this section, we compare the results obtained in the proceeding sections with the well known approaches in the linear nonequilibrium thermodynamics and statistical mechanics. The time rate of the entropy density $s(x, t)$ of a nonequilibrium system takes the form [8,18,19]:

$$\frac{\partial s(x,t)}{\partial t} = \sigma(x,t) - \nabla \cdot j_s(x,t) \quad (6.1)$$

$$\text{Where } \sigma(x,t) = \sum_i X_i(x,t) J_i(x,t) \quad (6.2)$$

is the entropy production density occurring inside the system which is given in terms of the sum of products of thermodynamic fluxes $J_i(x,t)$ and the conjugate thermodynamic forces $X_i(x,t)$; and $j_s(x,t)$ is the density of entropy flux through the border into the system.

Onsager proposed a linear relationship between the fluxes and forces

$$J_i(x,t) = \sum_k L_{ik} X_k(x,t) \quad (6.3)$$

with reciprocity relations

$$L_{ik} = L_{ki} \quad (6.4)$$

Thus we have

$$\frac{\partial s(x,t)}{\partial t} = \sum_{i,k} L_{ik} X_i(x,t) X_k(x,t) - \nabla \cdot j_s(x,t) \quad (6.5)$$

For the special case considered in Sect.5, the interaction between open system S and its environment R takes the form $H_{SR} = \sum_k \gamma_k A_k B_k$, for example, S and R are composed of different kinds of harmonic oscillator [7]. Such interaction implies no obvious border separating S and R, leading to absence of the divergence term on the right hand side of (6.5). Thus the variation of entropy density results from inner entropy production $\sigma(x,t)$ only:

$$\frac{\partial s(x,t)}{\partial t} = \sum_{i,k} L_{ik} X_i(x,t) X_k(x,t) \quad (6.6)$$

Besides, in the Green-Kubo formalism, the transport coefficients L_{ik} can be expressed in terms of time correlation functions of the time rate of corresponding variables [19,20].

$$L_{ik} \sim \int_0^\infty dt \langle \dot{A}_i(t) \dot{A}_k(0) \rangle_{eq} \quad (6.7)$$

where the average is taken over an equilibrium ensemble and the Markovian effect is taken into account.

In this paper, we study a nonequilibrium open system whose transport equations (2.9)-(2.11) are nonlinear differential-integral ones. Now let us compare (5.36b) with (6.6). We notice that (5.36b) share the same structure as (6.6) because of the facts : (1) parameters

$\{\lambda_j(x,t)\}$ ($j=1, \dots, m$) play the role Thermodynamic forces since they may involve spacial gradients of, e.g., temperature, velocity, chemical potential or electric, magnetic fields, etc.; (2) the random forces (2.12b) involve the time rates of variables because of using projection operator technique and (3) the average is taken over GCSO (3.1) instead of an equilibrium ensemble. As for (5.36c), the contribution of $Y_j(t)$ to the entropy production, in which the free term $\phi_l(x,u)$ in the Volterra equation is indeed a generalization of $\lambda_l(x,u)$ in (5.26b), hence (5.36c) possesses the same structure as (6.6) also. Accordingly, we see clearly that the entropy production rate (5.35) is a natural generalization of (6.6) where the non-linearity and the non-Markovian effect have been taken into consideration. In addition to the entropy production, the *entropy generation* is another useful tool in the study of nonequilibrium systems [8] and especially useful in the analysis of a process occurring in the system during a period of time τ . It is worth noticing the major differences between the two: the entropy production needs the hypothesis of local equilibrium but the entropy generation does not; the former does not consider the time but the latter introduces the lifetime τ of the process [8]. The two different approaches are closely related and complementary one to another.

Conclusion

In the present paper we have studied a nonequilibrium open system in interaction with its environment which may linearly deviate from its initial state under the reaction of the open system. We have shown that if the relevant statistical operator of the system is of the form of GCSO, then the transport equation is given by (3.6) and (5.28) or (5.33). The memory term in (3.6) and the influence term (5.28) or (5.33) can be expressed in terms of quantum correlation functions of fluctuations of random forces and interaction random forces, giving the second kind of fluctuation-dissipation theorem for this nonequilibrium open system. We have also shown that the entropy production rate is given by the sum of products of transport equations and the corresponding parameters. In the organized motion term, H_s contributes nothing to the rate, but H_{SR} does; the contributions of the memory and influence terms are expressed in terms of quantum correlation functions of fluctuations of random forces and interaction random forces. The total entropy production rate is given by the sum of contributions resulting from each term in the transport equation, given respectively by (4.4), (4.5) and (5.29) or (5.34). They are natural generalizations of those for a linear nonequilibrium closed system to a nonlinear open system.

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