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The steady state distribution of the master equation

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Abstract

The steady states of the master equation are investigated. We give two expressions for the steady state distribution of the master equation *à la* the Zubarev–McLennan steady state distribution, i.e., the exact expression and the expression near equilibrium. The latter expression obtained looks similar to that of recent attempts to construct steady state thermodynamics.

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1. Introduction

In daily life, nonequilibrium steady states (NESS) are observed in various situations, such as electric current, heat conduction, and so on. Usually the linear response theory (Kubo formula [1]) and Onsager's reciprocal relation [2] are used to describe the NESS, i.e., the NESS near equilibrium. Recent advances in experimental aspects need the study of the NESS far from equilibrium. Thus, the understanding of the NESS is one of the challenges in nonequilibrium statistical mechanics. However, our knowledge on the NESS has been limited until the discovery of the fluctuation theorem [3–10]. The fluctuation theorem is not restricted to near equilibrium. Thus, the fluctuation theorem provides us with some clues to investigate the NESS for general settings.

In this paper, the NESS of the master equation is investigated. The master equation describes the number of physical, chemical, biological and even social phenomena. Usually, the master equation was investigated by the Ω -expansion [11–14]. Without the use of the Ω -expansion, we develop a theory for the NESS of the master equation using the recent development of the fluctuation theorem. Here, we note that an exact expression for the NESS has already been obtained by Schnakenberg using the graph theory [15] or by other authors [16, 17]. However, its expression is not a useful form. We derive an alternative expression for the NESS. The key relation is the detailed imbalance relation, which is used to show the fluctuation theorem. Thanks to the detailed imbalance relation; the master equation is exactly solved, and we obtain the steady state distribution in a similar form to the Zubarev–McLennan steady state distribution [18, 19]. However, this expression is not convenient to handle. Therefore, we consider an easier case, i.e., near equilibrium. In [24], for the case near

equilibrium, a different attempt was given, but its explicit evaluation has not been obtained. In our treatment, in a linear approximation near equilibrium, a very familiar expression is obtained, which is, indeed, in the form of the Zubarev–McLennan steady state distribution. This is done by evaluating the time evolution of the statistical entropy and the distribution function. Here, it should also be mentioned that the linear approximation used is not the linear approximation in terms of the degree of nonequilibrium property, such as temperature difference in the thermal conduction problem, chemical potential difference in the diffusion problem, and so on. This point will be stressed in the latter section. Compared with the result on the NESS of the master equation [15, 20], we examine the expression obtained for the steady state distribution, and compare it with the recent results [21–23].

2. Master equation

The master equation is given by

$$\frac{\partial}{\partial t} P(\omega; t) = - \sum_{\omega'} w_{\omega\omega'} P(\omega; t) + \sum_{\omega'} w_{\omega'\omega} P(\omega'; t), \quad (1)$$

where $\omega = (\omega_1, \omega_2, \dots, \omega_N)^t$ is the discrete variable of the state. $P(\omega; t)$ is the probability distribution that the system is in the state ω at time t . $w_{\omega\omega'}$ is the transition rate that the system performs a transition from the state ω to the state ω' in a unit time. By definition, the transition rates, $w_{\omega\omega'}$, are non-negative. Equation (1) can be rewritten into the following form [15]:

$$\frac{\partial}{\partial t} P(\omega; t) = \sum_{\omega'} W_{\omega'\omega} P(\omega'; t), \quad (2)$$

where

$$W_{\omega'\omega} = w_{\omega'\omega} - \delta_{\omega\omega'} \sum_{\omega''} w_{\omega\omega''}. \quad (3)$$

Since the master equation conserves the total probability, the transition rates $W_{\omega\omega'}$ satisfy the following condition:

$$\sum_{\omega'} W_{\omega\omega'} = 0. \quad (4)$$

This relation can be confirmed directly. Therefore, an alternative form of the master equation is obtained:

$$\frac{\partial}{\partial t} P(\omega; t) = - \sum_{\omega'} W_{\omega\omega'} P(\omega; t) + \sum_{\omega'} W_{\omega'\omega} P(\omega'; t). \quad (5)$$

Note that the transition rates $W_{\omega\omega'}$ are no longer non-negative, and the diagonal elements $W_{\omega\omega}$ are non-positive.

As a first attempt, the exact expression for the NESS of the master equation was given by Schnakenberg [15]. He used the graph theory to obtain the expression for the NESS. However, its derivation contains counting complicated trees associated with a given graph. Its derivation is lengthy. Schnakenberg's result is practically not convenient.

After Schnakenberg, a more direct form of the NESS was given in [16, 17]. Its expression involves the determinant of a submatrix of the matrix $W_{\omega\omega'}$:

$$P^{st}(\omega) = \frac{\text{adj}(-W)_{\omega\omega}}{\sum_{\omega'} \text{adj}(-W)_{\omega'\omega'}}, \quad (6)$$

where $\text{adj}(A)_{ij}$ is the cofactor of the matrix A for the matrix element A_{ij} . Note that this expression is for the case that the size of the matrix $W_{\omega\omega'}$ is finite. But it is still hard to extract its physical meaning of the NESS.

We will give another procedure for the case near equilibrium in the following section.

3. An expression for the NESS near equilibrium

In this section, the master equation (5) is considered. Now, we assume the detailed imbalance relation (sometimes it is called the nonequilibrium detailed balance relation):

$$\frac{P(\omega; t-0)W_{\omega\omega'}}{P(\omega'; t+0)W_{\omega'\omega}} = \exp[\sigma_{\omega\omega'}(t)], \quad (7)$$

where $\sigma_{\omega\omega'}(t)$ is the entropy production for one jump $\omega \rightarrow \omega'$. Equation (7) is the starting point to derive various fluctuation theorems. For instance, Hatano and Sasa derived steady state thermodynamics of the Langevin system, and showed the fluctuation theorem and Jarzynski (in)equality starting from equation (7) [25]. Using the Onsager–Machlup path integral and equation (7), a work fluctuation theorem was derived for a Langevin system in [26]. In [14], the entropy production for the master equation was examined, and equation (7) was a key relation there. Moreover, in [27], equation (7) has been shown both at the single trajectories and at the average level, and was confirmed in experiments.

Using equation (7), equation (5) is rewritten as

$$\frac{\partial}{\partial t} P(\omega; t) = P(\omega; t) \sum_{\omega'} (\exp[-\sigma_{\omega\omega'}(t)] - 1) W_{\omega\omega'}. \quad (8)$$

Equation (8) is easily solved:

$$P(\omega; t) = C(\omega; 0) \exp \left[\int_0^t dt' \sum_{\omega'} (\exp[-\sigma_{\omega\omega'}(t')] - 1) W_{\omega\omega'} \right], \quad (9)$$

where $C(\omega; 0)$ will be determined later. As in the standard definition, here we set

$$P(\omega; t) = \exp[-S(\omega; t)]. \quad (10)$$

Thus, the statistical entropy of the probability distribution is given as a Shannon entropy:

$$S(t) = - \sum_{\omega} P(\omega; t) \ln P(\omega; t) = \sum_{\omega} P(\omega; t) S(\omega; t). \quad (11)$$

For comparison with thermodynamical entropy, equation (11) should be modified. For its definition, see [28, 29]. In this paper, we use the definition of equation (11). Equation (9) is rewritten as

$$\begin{aligned} P(\omega; t) &= C(\omega; 0) \exp \left[\int_0^t dt' \frac{\partial P(\omega; t') / \partial t'}{P(\omega; t')} \right] \\ &= C(\omega; 0) \exp \left[- \int_0^t dt' \dot{S}(\omega; t') \right] \\ &= C(\omega; 0) \exp[S(\omega; 0) - S(\omega; t)]. \end{aligned} \quad (12)$$

To be consistent with equation (10), it should be $C(\omega; 0) = \exp[-S(\omega; 0)]$. Thus, equation (9) is a formal (exact) solution.

For the NESS, the steady state distribution is given by

$$\begin{aligned} P^{st}(\omega) &= \exp \left[-S(\omega; 0) + \int_0^{\infty} dt' \sum_{\omega'} (\exp[-\sigma_{\omega\omega'}(t')] - 1) W_{\omega\omega'} \right] \\ &= \exp \left[-S(\omega; 0) + \int_0^{\infty} dt' \sum_{\omega'} W_{\omega\omega'} \sum_{n=1}^{\infty} \frac{1}{n!} (-\sigma_{\omega\omega'}(t'))^n \right]. \end{aligned} \quad (13)$$

This is the first main result, and is nothing but the exact expression of the NESS, which is similar to the Zubarev–McLennan steady state distribution. However, equation (13) is not in

a useful form. Thus, we consider a NESS near equilibrium. Near equilibrium, the entropy production is small. So we can approximate as $\exp(-\sigma) \approx 1 - \sigma$, i.e., the linear approximation near equilibrium. Note that this linear approximation does not mean the linear approximation in terms of the degree of nonequilibrium property, such as temperature difference in the thermal conduction problem, chemical potential difference in the diffusion problem, and so on. This point will be discussed later again. Then, we obtain the probability distribution,

$$P(\omega; t) \simeq \exp \left[-S(\omega; 0) - \int_0^t dt' \sum_{\omega'} \sigma_{\omega\omega'}(t') W_{\omega\omega'} \right]. \quad (14)$$

Near equilibrium, the steady state distribution is approximated as

$$\begin{aligned} P^{st}(\omega) &\simeq \exp \left[-S(\omega; 0) - \int_0^\infty dt' \sum_{\omega'} \sigma_{\omega\omega'}(t') W_{\omega\omega'} \right] \\ &= \exp \left[-S(\omega; 0) - \int_0^\infty dt' \{ \Sigma(\omega; t') - \langle J(\omega) \rangle \} \right], \end{aligned} \quad (15)$$

where

$$\Sigma(\omega; t) = \sum_{\omega'} \{ S(\omega'; t) - S(\omega; t) \} W_{\omega\omega'}, \quad (16)$$

and

$$\langle J(\omega) \rangle = - \sum_{\omega'} W_{\omega\omega'} \ln \frac{W_{\omega\omega'}}{W_{\omega'\omega}}. \quad (17)$$

This is the second main result. $\Sigma(\omega; t)$ is the total entropy production including the incoming entropy production flow, i.e., $\frac{1}{\tau} \Delta S(\omega)$. $\langle J(\omega) \rangle$ is the entropy production flow, i.e., $\frac{1}{\tau} \Delta_e S(\omega)$. Thus, $\Sigma(\omega; t) - \langle J(\omega) \rangle$ is the (internal) entropy production, i.e., $\frac{1}{\tau} \Delta_i S(\omega) = \frac{1}{\tau} (\Delta S(\omega) - \Delta_e S(\omega))$. Thus, the argument of the exponential function in the second line of equation (15) expresses the time integration of the minus of the excess entropy production or the internal entropy production.

The averaged entropy production in the NESS is given by [15, 20]

$$\langle \sigma \rangle = \sum_{\omega, \omega'} P^{st}(\omega) W_{\omega\omega'} \ln \frac{P^{st}(\omega) W_{\omega\omega'}}{P^{st}(\omega') W_{\omega'\omega}}. \quad (18)$$

This expression can be written in terms of Kolmogorov–Sinai (KS) entropy [20]:

$$\langle \sigma \rangle = h^R - h, \quad (19)$$

where h is the KS entropy, and h^R is the KS entropy for the reversed process. Since

$$\sum_{\omega'} \sigma_{\omega\omega'}(t) W_{\omega\omega'} = \sum_{\omega'} W_{\omega\omega'} \ln \frac{P(\omega; t) W_{\omega\omega'}}{P(\omega'; t) W_{\omega'\omega}}, \quad (20)$$

thus, this quantity resembles the content inside of the sum in the right-hand side of equation (18). This quantity can be identified with the excess entropy production in the state ω .

Consider $S(\omega; t)$. From equation (14), we obtain

$$\begin{aligned} S(\omega; t) &= -\ln P(\omega; t) \\ &= S(\omega; 0) + \sum_{\omega'} \int_0^t dt' \left\{ W_{\omega\omega'} (S(\omega'; t') - S(\omega; t')) + W_{\omega\omega'} \ln \frac{W_{\omega\omega'}}{W_{\omega'\omega}} \right\}. \end{aligned} \quad (21)$$

This equation expresses the time evolution of $S(\omega; t)$. Taking time derivative of equation (21) and noting equation (4), we have

$$\frac{d}{dt}S(\omega; t) = \sum_{\omega'} W_{\omega\omega'} S(\omega'; t) - \langle J(\omega) \rangle. \quad (22)$$

If we use the matrix notation for the transition rates $W_{\omega\omega'}$, and the vector notations for $S(\omega; t)$ and the steady entropy production current $\langle J(\omega) \rangle$, then we have

$$\dot{S}(t) = WS(t) - J. \quad (23)$$

This can be easily solved as

$$S(t) = e^{Wt} S(0) - \int_0^t ds e^{-W(s-t)} J. \quad (24)$$

In the NESS, the following condition is satisfied:

$$\sum_{\omega'} W_{\omega'\omega} P^{st}(\omega') = 0. \quad (25)$$

Here we have set the right-hand side of equation (2) to be zero. Equation (25) implies that there exist zero eigenvalues for the matrix W . Now we assume that at $t = \infty$, the state reaches the NESS. As a result, the steady state distribution is given by $P^{st}(\omega) = \exp[-S^{st}(\omega)] = \exp[-S(\omega; \infty)]$. Thus, we have

$$P^{st}(\omega) \simeq \exp \left[- \lim_{t \rightarrow \infty} \sum_{\omega'} \left\{ (e^{Wt})_{\omega\omega'} S(\omega'; 0) - \int_0^t ds (e^{-W(s-t)})_{\omega\omega'} \langle J(\omega') \rangle \right\} \right]. \quad (26)$$

This is the third main result. The rank of the matrix W is smaller than its matrix size. We assume that the matrix W has only one zero eigenvalue, and the others are negative eigenvalues, since the diagonal elements of the matrix W have negative values (see equation (3)). The first term in the argument of the right-hand side of equation (26) converges to the element of the eigenvector corresponding to the zero eigenvalue, i.e., the NESS.

4. Conclusions

We have demonstrated that near equilibrium, the solution of the master equation is solved analytically. The time evolution of the entropy and the distribution function was obtained, and the steady state distribution near equilibrium was evaluated. To include nonlinear effects far from equilibrium, i.e., beyond the linear approximation, one should include the nonlinear terms ($n = 2, 3, \dots$) in the argument of the exponential function in the second line of equation (13). But this task would be tedious. At present, there is no results in this direction.

We have derived the time evolution of the entropy (production) near equilibrium. We identify the (averaged) entropy production obtained with thermodynamical entropy production ($\sigma_{\text{th}} = \mathbf{J} \cdot \mathcal{A}$, where \mathbf{J} is the current, and \mathcal{A} is the affinity). Due to the property of the matrix W (i.e., zero eigenvalue and negative eigenvalues), the entropy production may decay exponentially. Near equilibrium the affinity \mathcal{A} is almost constant in time. Thus, the current \mathbf{J} should decay exponentially. This property may be observed in numerical simulation. Far from the equilibrium case, the above observation may break down. The time evolution of the entropy production may deviate from exponential decay by nonlinearity of the time evolution equation of the entropy production.

The expression of equation (15) is very similar to the result of a recent attempt of constructing steady state thermodynamics [21–23]. Now we rewrite equation (15) into the form

of the expression derived by Komatsu and Nakagawa [22]. Noting that $\sigma_{\omega\omega'}(t) = -\sigma_{\omega'\omega}(t)$, equation (15) can be rewritten as

$$P^{st}(\omega) \simeq \exp \left[-S(\omega; 0) + \frac{1}{2} \int_{-\infty}^0 dt' \sum_{\omega'} \sigma_{\omega'\omega}(t') W_{\omega\omega'} - \frac{1}{2} \int_0^{\infty} dt' \sum_{\omega'} \sigma_{\omega\omega'}(t') W_{\omega\omega'} \right]. \quad (27)$$

This equation is similar to equations (15a) and (15b) in [22]. But it should be noted that equation (27) has some differences compared with equations (15a) and (15b) in [22]. In [22], they derived the expression in the argument of the exponential function in terms of the degree of nonequilibrium property, say ϵ , such as the temperature difference in the thermal conduction problem or particle number difference in the diffusion problem, etc. Their expression is in the order of ϵ^2 in the argument of the exponential function. In equation (27), the expression is not in terms of ϵ . If one expands the argument of the exponential function, namely $\sigma_{\omega\omega'}$, in terms of ϵ , then we may get an infinite power series of ϵ , which starts from the order of ϵ^1 . This will be confirmed for the one-dimensional diffusion problem, which is treated in a different context in [14]. Therefore, the result of the master equation in this paper is somewhat different from that of the Hamiltonian system in [22]. But both expressions look similar. Thus, for master equations, a similar discussion as for Hamiltonian systems in [23] may be possible. Finally, we stress the following remark. To obtain equation (15) from equation (13), the condition that our expression is valid is that (1) the nonequilibrium property is small (i.e., the entropy production is small), and (2) the initial probability distribution is close to the NESS, because both equations (13) and (15) involve an integral over time.

Finally one (deep) question remains. ‘*Is the Zubarev–McLennan steady state distribution for the NESS near equilibrium?*’ At least, for the master equation, equation (15) (i.e., the expression near equilibrium) seems to correspond to the Zubarev–McLennan steady state distribution [18, 19].

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