Stationary solution of master equations in the large-system-size limit

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To study the stationary probability distribution of master equations in the large-system-size limit, we introduce a kind of master Hamiltonian which is similar to the Fokker-Planck Hamiltonian suggested by Graham *et al.* in the study of Fokker-Planck equations in the weak-noise limit. The general procedure to associate the potential of the master equation with a certain separatrix of the master Hamiltonian system is described. With some solvable models we show how the smoothness of the potential of the master equation is related to the integrability of the corresponding master Hamiltonian system.

The study of stationary probability distributions of Fokker-Planck equations which do not manifest detailed balance turns out to be of great interest, and has received much attention.[1-5] In many physically interesting cases the noise, represented by the diffusion term of the Fokker-Planck equation, is very small, and then the limit of weak noise is desirable. In this limit the stationary probability distribution—or, more precisely, the logarithm of the distribution—appears to be a good candidate of a nonequilibrium potential.[6,7] Recently, Graham and his co-workers have shown that in the weak-noise limit the Fokker-Planck equation becomes equivalent to the Hamilton-Jacobi equation of a certain Hamiltonian system in which the potential

$$\phi_0(x) = -\lim_{\epsilon \to 0} \{\epsilon \ln[p(x,\epsilon)]\}$$

plays the role of the action on a separatrix at energy zero.[8-11] This approach sheds new light on the study of the Fokker-Planck process.

In practice, many important physical and chemical systems cannot be modeled by Fokker-Planck equations, although they can often be successfully modeled by master equations in which variables may take discrete values.[12] Therefore, in order to construct a complete stochastical theory of nonequilibrium systems we should study the master equation as well as the Fokker-Planck equation thoroughly. However, the master equation, lacking detailed balance, is much less known than the Fokker-Planck equation. In Ref. 13 I succeeded in solving the potential of the one-dimensional master equation without detailed balance, in the leading order of system size. In Ref. 14 the system-size expansion of the stationary probability distribution has been obtained systematically. The Lyapunov property of the potential was shown in Ref. 15, and a comparison between the master equation and the Fokker-Planck equation in the one-dimensional case was presented in Ref. 16.

The main purpose of the present work is to extend Graham's theory to the master equation. First, we reduce the stationary master equation to a Hamilton-Jacobi equation, in the large-size limit, and define a master Hamiltonian. The relationship between the stationary probability distribution of the master equation and a particular separatrix of the master Hamiltonian system will be formulated. Then, all the approaches dealing with the Fokker-Planck equation based on the Hamiltonian formalism,[8-11] including calculation of the stationary probability distribution by specifying the separatrix of the Fokker-Planck Hamiltonian system and discussion of the smoothness of the potential according to the smoothness of the separatrix in cases for which the explicit form of the potential is not available, can be applied to the master equation. The presentation is organized as follows.

In Sec. I I present briefly the basic equation of the stationary probability distribution of the multidimensional master equation, in the leading order of the system size. In Sec. II the master Hamiltonian approach is formulated. Section III investigates several solvable examples with which I show how the new approach works. The general relationship between integrability of the master Hamiltonian and the smoothness of the potential will be briefly discussed at the end of the presentation.

I. BASIC EQUATION

It is well known that detailed balance, which provides a strict constraint on the master equation, exists in equilibrium. In the following we treat the master equation lacking detailed balance. Then we are dealing with nonequilibrium systems, taking equilibrium systems as special cases.

A nonequilibrium system may undergo a stochastical process described by a master equation

$$\frac{\partial}{\partial t} P(\mathbf{X},t) = \sum_{\mathbf{r}} P(\mathbf{X}-\mathbf{r},t) M(\mathbf{X}-\mathbf{r},\mathbf{r}) - \sum_{\mathbf{r}} P(\mathbf{X},t) M(\mathbf{X},\mathbf{r}) , \tag{1.1}$$

where $\mathbf{X}$ and $\mathbf{r}$ are q-dimensional vectors,

$$\mathbf{X}=(X_1,X_2,\ldots,X_q), \quad \mathbf{r}=(r_1,r_2,\ldots,r_q) ,$$

and the notation $\sum_{\mathbf{r}}$ indicates the summations over all the components r_i, $i=1,2,\ldots,q$,

$$\sum_{\mathbf{r}}=\sum_{r_q}\cdots\sum_{r_2}\sum_{r_1}.$$

By means of the Kramer-Moyal expansion, Eq. (1.1) can be transformed to a partial differential equation[17,18]

$$\epsilon\left[\frac{\partial}{\partial t}\right]p(\mathbf{x},t)=\sum_{\mathbf{n}}(1/\mathbf{n}!)\left[-\epsilon\frac{\partial}{\partial\mathbf{x}}\right]^{\mathbf{n}}\times[A_{\mathbf{n}}(\mathbf{x})p(\mathbf{x},t)], \tag{1.2}$$

where

$$\epsilon=1/\Omega,\quad p(\mathbf{x},t)=\Omega P(\mathbf{x},t),$$
$$A_{\mathbf{n}}(\mathbf{x})=\sum_{\mathbf{r}}\left[\prod_i r_i^{n_i}\right]m(\mathbf{x},\mathbf{r}),\quad m(\mathbf{x},\mathbf{r})=M(\mathbf{X},\mathbf{r})/\Omega, \tag{1.3}$$

with Ω being the size of the system and x_i, $i=1,2,\ldots,q$ being the concentrations of the variables. The notations $\mathbf{n}$, $\mathbf{n}!$, and $\Omega^{\mathbf{n}}$ are defined, respectively, as

$$\mathbf{n}=(n_1,n_2,\ldots,n_q),\quad \mathbf{n}!=\prod_i(n_i!),\quad \Omega^{\mathbf{n}}=\Omega^{\sum n_i}. \tag{1.4}$$

The derivative $(\partial/\partial\mathbf{x})^{\mathbf{n}}$ represents

$$\frac{\partial^{\mathbf{n}}}{\partial\mathbf{x}^{\mathbf{n}}}f(\mathbf{x},t)=\frac{\partial^{n_1+n_2+\cdots+n_q}f(\mathbf{x},t)}{\partial x_1^{n_1}\partial x_2^{n_2}\cdots\partial x_q^{n_q}}. \tag{1.5}$$

A common approach is to truncate the infinite terms of Eq. (1.2) to the second order of ϵ, and then to reduce the master equation (or the Kramers-Moyal expansion) to a Fokker-Planck equation. Unfortunately, this approach does not work.[16,19,20] Provided the system size is very large, the local properties of the stationary probability peaks, such as the positions of the peaks and the widths of the peaks, of both equations are identical. However, the global properties, such as the relative heights of the peaks, for both equations are completely different, even if the limit of large size is taken. Hence, all the infinite terms in the Kramers-Moyal expansion have to be taken as a whole, and the approach used for the Fokker-Planck equation cannot be directly applied to the master equation. How can one treat the infinite coupled equations in (1.1) or, equivalently, the partial differential equation (1.2) which contains infinite terms and defies any truncation?

Fortunately, the difficulty may be largely reduced by taking the large-size limit. In physically and chemically interesting cases and in most practical systems, the size of the systems Ω is found to be very large

$$\Omega\gg 1,\quad X_i\gg 1, \tag{1.6}$$

while the concentrations of the variables are finite,

$$x_i=X_i/\Omega\quad\text{finite}.$$

The large-size limit for the master equation is analogous to the weak-noise limit for the Fokker-Planck equation.

In the large-size limit we may expand the stationary probability distribution as

$$P(\mathbf{x})=N\exp[-u(\mathbf{x})],$$
$$u(\mathbf{x})=u_0(\mathbf{x})/\epsilon+u_1(\mathbf{x})+\cdots, \tag{1.7}$$

with N being the normalization constant and $\lim_{\epsilon\to 0}(\epsilon N)=0$. We assume that the master equation has a unique time-independent solution which is approached from any given initial state. It is well known that $p(\mathbf{x})$ has an essential singularity for $\epsilon\to 0$. In many cases the logarithm $\epsilon\ln[p(\mathbf{x})/N]$ may be regular at $\epsilon=0$. However, it is not always so. In certain cases, $\ln[p(\mathbf{x})/N]$ may include terms like $\ln(\epsilon)f(\mathbf{x})$ because of which $u_1(\mathbf{x})$ and some other terms in (1.7) may be divergent. We do not intend to consider this matter in detail in the present work, but simply rewrite $u_0(\mathbf{x})$, the so-called potential, as

$$u_0(\mathbf{x})=\lim_{\epsilon\to 0}\{-\epsilon\ln[p(\mathbf{x})]\}. \tag{1.8}$$

Equation (1.8) rules out terms such as $\ln(\epsilon)$. Consequently, the divergence problem due to $\ln(\epsilon)$ no longer exists. Nevertheless, both Eqs. (1.7) and (1.8) give no difference to $u_0(\mathbf{x})$.

Inserting Eq. (1.7) into Eq. (1.2), keeping the leading terms of the system size, exchanging the summations over $\mathbf{n}$ and $\mathbf{r}$, and summing $\mathbf{n}$, a rather compact equation for $u_0(\mathbf{x})$ then follows:

$$\sum_{\mathbf{r}}m(\mathbf{x},\mathbf{r})\{\exp[\mathbf{r}\cdot\nabla u_0(\mathbf{x})]-1\}=0, \tag{1.9}$$

where the vector $\nabla u_0(\mathbf{x})$ reads

$$\nabla u_0(\mathbf{x})=(u_0^1(\mathbf{x}),u_0^2(\mathbf{x}),\ldots,u_0^q(\mathbf{x})),$$

with

$$u_0^i(\mathbf{x})=\frac{\partial u_0(\mathbf{x})}{\partial x_i}.$$

In Ref. 15, we have proved that the potential defined by Eq. (1.9), if it exists, must be a Lyapunov function of the corresponding kinetic equation,

$$\frac{d\mathbf{x}}{dt}=A_1(\mathbf{x})=(A_{(1)}(\mathbf{x}),A_{(2)}(\mathbf{x}),\ldots,A_{(q)}(\mathbf{x})),$$
$$A_{(i)}(\mathbf{x})=\sum_{\mathbf{r}}r_i m(\mathbf{x},\mathbf{r}), \tag{1.10}$$

i.e.,

$$\frac{du_0(\mathbf{x})}{dt}=\nabla u_0(\mathbf{x})\cdot A_1(\mathbf{x})\le 0, \tag{1.11}$$

where the equality holds only for

$$\frac{\partial u_0(\mathbf{x})}{\partial x_i}=0,\quad i=1,2,\ldots,q. \tag{1.12}$$

At the first glimpse, Eq. (1.9), which governs the potential of the master equation in the large-system-size limit, is completely different from the equation

$$\sum_{\mu}\sum_{\nu} Q_{\mu\nu}(\mathbf{x})\frac{\partial\phi}{\partial x_{\mu}}\frac{\partial\phi}{\partial x_{\nu}}+\sum_{\mu} K_{(\mu)}(\mathbf{x})\frac{\partial\phi}{\partial x_{\mu}}=0 , \tag{1.13}$$

which governs the potential of the Fokker-Planck equation in the weak-noise limit. In the study of the Fokker-Planck equation of nonequilibrium systems, an important ideal is to separate the drift into two orthogonal parts, the circulation and the gradient of the potential,[6,10] which are analogous to the reversible and the dissipative currents in thermodynamical systems, respectively. The orthonormality between the circulation and the gradient is an important fact in describing the relationship between the potential of the Fokker-Planck equation and the drift force. For the master equation [cf. Eq. (1.9)] no circulation can be properly defined and then no simple relationship between the potential and the transition probabilities can be found.

Nevertheless, an important similarity between Eqs. (1.9) and (1.13) is implied. Due to Eqs. (1.9) and (1.11), the potential, evolved by the deterministic equation (1.10), decreases as time increases. As $t\to\infty$, $u_0(\mathbf{x})$ will approach one of its minimal values while the trajectory of Eq. (1.10) approaches one of its attractors. In the limit sets (they may be attractors, repellors, and saddles; from another point of view, they may be fixed points, limit cycles, and so on; the limit sets which have fractional dimensions will be excluded from our consideration in this presentation), we have

$$\left.\frac{\partial u_0(\mathbf{x})}{\partial x_i}\right|_{\mathbf{x}(\Gamma)}=0 , \tag{1.14}$$

where Γ denotes the limit sets. (In somewhat weakened form, Γ may be replaced by A, which denotes the attracting points.) The same boundary condition has been found for the Fokker-Planck equation and plays a key role in the Fokker-Planck Hamiltonian description.[8-11] According to Eqs. (1.13) and (1.14), Graham *et al.*, suggested a mechanical analogy to relate the potential of the Fokker-Planck equation to a separatrix of a certain Hamiltonian system. It is obvious that Eqs. (1.9) and (1.14) fit the essential condition of the analogy.

II. MASTER HAMILTONIAN

Equation (1.9) can be regarded as a Hamilton-Jacobi equation. The Hamiltonian reads

$$H=\sum_{\mathbf{r}} m(\mathbf{x},\mathbf{r})[\exp(\mathbf{r}\cdot\mathbf{p})-1] , \tag{2.1}$$

with

$$\mathbf{p}=(p_1,p_2,\ldots,p_q) ,$$

$$P_i=\partial u_0(\mathbf{x})/\partial x_i .$$

Here and henceforward we write the action of the system directly by $u_0(\mathbf{x})$. Actually, only the special action of the Hamiltonian system at zero energy and constrained by the boundary condition (1.14) is really related to the stationary probability distribution of the original master equation. Since the Hamiltonian is derived from the master equation, we shall henceforth refer to it as the master Hamiltonian. For an actual stable system, the stationary probability distribution should be normalizable. In the present paper we assume that the normalization condition is automatically valid. Whenever an unnormalizable probability distribution appears it is always implied that we consider only a local problem.

The Hamiltonian (2.1) has a very strange form. It has no obvious analogy to any real mechanical system, and it is rather different from the Fokker-Planck Hamiltonian. Thus, we cannot regard (2.1) as a meaningful energy; it is only a formal representation of the master equation. On the other hand, Eq. (2.1) shows how useful the Hamiltonian formalism initiated by mechanics is.

The canonical equations of the master Hamiltonian system are given as

$$\frac{dx_i}{dt}=\sum_{\mathbf{r}} r_i m(\mathbf{x},\mathbf{r})\exp(\mathbf{r}\cdot\mathbf{p}) , \tag{2.2a}$$

$$\frac{dp_i}{dt}=\sum_{\mathbf{r}} m^i(x,r)[\exp(\mathbf{r}\cdot\mathbf{p})-1] , \tag{2.2b}$$

$$m^i(\mathbf{x},\mathbf{r})=\frac{\partial m(\mathbf{x},\mathbf{r})}{\partial x_i} .$$

Now we are in the position from whence the relationship between the trajectory of the deterministic equation in the $2q$-dimensional Hamiltonian phase space and the potential of the master equation (1.9) can be described.

It is apparent that the q-dimensional sheet Q_1,

$$p_i=0, \quad i=1,2,\ldots,q ,$$

is an invariant subspace of Eq. (2.2). In this subspace the trajectory of the master Hamiltonian is exactly the deterministic path of the kinetic equation (1.10), $\dot{\mathbf{x}}_i=\sum_{\mathbf{r}} r_i m(\mathbf{x},\mathbf{r})$. For the stationary probability distribution, Eq. (1.9) corresponds to the Hamilton-Jacobi equation at zero energy,

$$H=0 . \tag{2.3}$$

Equation (1.14), the boundary condition, may be used to fix the $q-1$ invariants other than the Hamiltonian. Then Eqs. (1.9) and (1.14), from which the potential may be solved, determine a q-dimensional hypersurface Q_2. According to Eqs. (2.2a) and (1.14), in all the limit sets of the deterministic equation the momenta associated with the potential must vanish. Consequently, a clear mechanical picture is the following: In the $2q$-dimensional phase space, the deterministic motion takes place on the q-dimensional plane $p_i=0$, while the stationary master equation (in the large-size limit) characterizes motion on other q-dimensional subspace Q_2 which intersects the sheet of the deterministic dynamics in all the limit sets $[\mathbf{x}(\Gamma),\mathbf{p}=0]$. All the limit set points

are the stationary solutions of the Hamiltonian canonical equation (2.2). Moreover, they are hyperbolic points in $2q$-dimensional phase space. Therefore, the surface Q_2 is a separatrix of the Hamiltonian system which connects all the limit sets of the deterministic dynamics. This mechanical picture is just what one has obtained for the Fokker-Planck Hamiltonian system.

It is difficult to treat Eq. (2.2) due to the fact that the momenta p_i appear in the exponents. The canonical equations can be considerably simplified by making use of the generating function

$$f=\sum_{i=1}^{q} x_i \ln s_i \tag{2.4}$$

to transform the original coordinates and the momenta x_i and p_i to new coordinates and the momenta s_i and w_i as

$$p_i=\ln s_i \ ,$$
$$w_i=-x_i/s_i \quad \text{or} \quad x_i=-s_i w_i \ . \tag{2.5}$$

The master Hamiltonian can be rewritten as

$$H=\sum_{\mathbf{r}} m(-s_i w_i,\mathbf{r})\left[\prod_j s_j^{r_j}-1\right] . \tag{2.6}$$

An important advantage of Eq. (2.6) is that the master Hamiltonian is polynomial whenever the transition probabilities are polynomial. [Suppose the master equation (1.1) represents chemical reactions $\sum_{i=1}^{q} R_i(j)X_i \xrightarrow{k_j} \sum_{i=1}^{q} \bar{R}_i(j)X_i$, $j=1,2,\ldots,n$, where k_j are constant and $r_i(j)=\bar{R}_i(j)-R_i(j)$. The arguments s_i can never appear in denominators though some of r_i may be negative.] The new momenta are associated with a new action as

$$w_i=\frac{\partial \eta(\mathbf{s})}{\partial s_i}, \quad i=1,2,\ldots,q \tag{2.7}$$

since the transformation (2.5) is canonical. The problem of solving $u_0(\mathbf{x})$ is equivalent to that of solving $\eta(\mathbf{s})$ from

$$H(\mathbf{s},\mathbf{w})=0 \ . \tag{2.8}$$

The canonical equations of the master Hamiltonian (2.6) read

$$\frac{ds_i}{dt}=-\sum_{\mathbf{r}} s_i m^{i}(-s_i w_i,\mathbf{r})\left[\prod_j s_j^{r_j}-1\right] , \tag{2.9a}$$

$$\frac{dw_i}{dt}=-\sum_{\mathbf{r}} r_i m(-s_i w_i,\mathbf{r}) \prod_{j\ (j\neq i)} \cdot s_i^{r_i-1} + \sum_{\mathbf{r}} w_i m^{i}(-s_i w_i,\mathbf{r})\left[\prod_j s_j^{r_j}-1\right] . \tag{2.9b}$$

From Eq. (2.9) it is easily verified that the q-dimensional plane

$$s_i=1, \quad i=1,2,\ldots,q$$

becomes the invariant plane in $(\mathbf{s},\mathbf{w})$ phase space, replacing the plane $p_i=0$ in the old representation. The deterministic motion takes place right in this plane. [Replacing s_i, w_i by 1 and $-w_i$, respectively, Eq. (2.9b) may reduce to Eq. (1.10).] Equation (2.5) transforms the $2q$-dimensional limit set points $[\mathbf{x}(\Gamma),\mathbf{p}=0]$ to $s_i=1$ and

$$w_i=-x_i(\Gamma) \ , \tag{2.10}$$

which are the stationary solutions of Eq. (2.9). Equation (2.10) is the boundary condition under which the special action associated with the potential can be identified. Again, Eqs. (2.8) and (2.10) define a q-dimensional separatrix in $(\mathbf{s},\mathbf{w})$ representation.

In the preceding discussion, we approached Eqs. (2.6) and (2.8) by a type of transformation that seems to be merely a mathematical trick. In fact, the transformation is physically meaningful. Defining a generating function of the probability distribution as

$$F(\mathbf{s},t)=\sum_{\mathbf{n}} \prod_i s_i^{n_i} P(\mathbf{X},t)$$

and then an accumulating generating function as

$$\Psi(\mathbf{s},t)=\epsilon \ln[F(\mathbf{s},t)] \ ,$$

we find the stationary $\Psi(\mathbf{s})$ as (readers may check it directly)

$$\lim_{\epsilon\to 0} \Psi(\mathbf{s})=-\eta(\mathbf{s}) \ ,$$

if the limit exists. Thus, in $(\mathbf{s},\mathbf{w})$ representation the master Hamiltonian (2.6) is related to the behaviors of the spectrum of the stationary probability distribution of the master equation. In the subsequent sections we will not proceed further with this affair, but use both representations alternatively for the sake of mathematical convenience.

By a Legendre transformation we may formulate the Lagrangian associated to the Hamiltonian

$$L_0(\mathbf{x},\dot{\mathbf{x}})=\sum_i p_i x_i - H \ , \tag{2.11}$$

where $\mathbf{p}$ may be replaced by $\dot{\mathbf{x}}$ via the canonical equations,

$$\dot{\mathbf{x}}_i=\frac{\partial H(\mathbf{x},\mathbf{p})}{\partial p_i} \ . \tag{2.12}$$

The potential can be represented by the extremum principle

$$u_0(\mathbf{x},E_j)=\min_j \left\{ \int_{\mathbf{x}(E_j)(t=-\infty)}^{\mathbf{x}(t=0)} L_0(\mathbf{x},\dot{\mathbf{x}})+C(E_j) \right\} , \quad j=1,2,\ldots,n \tag{2.13a}$$

$$u_0(\mathbf{x})=\min_j \{u_0(\mathbf{x},E_j)\} \ , \tag{2.13b}$$

where the minimum in (2.13a) is taken over all paths starting in attractor E_j for $t\to-\infty$ and ending in the point $\mathbf{x}$ at $t=0$. The constant $C(E_j)$ is the value of the potential on the jth attractor. The solutions of Eq. (2.13a) [or Eq. (1.9)] may not be unique; then, the minimum in (2.13b) requires one to take the absolute

minimum among all $u_0(\mathbf{x},E_j)$ in any given $\mathbf{x}$. Finally, $u_0(\mathbf{x})$ is a single-valued function. At all points where the minimum is transferred from one branch to another, the first derivative of $u_0(\mathbf{x})$ may be discontinuous while the potential itself remains continuous. These arguments were originally postulated by Graham *et al.*, for the Fokker-Planck equation. We expect that it is true for the master equation.

In spite of the great difference between the master equation and the Fokker-Planck equation, both equations can be treated identically by Eqs. (2.3) and (1.14). The approach used for the Fokker-Planck equation can be applied to the master equation. The master equation differs from the Fokker-Planck equation only in the form of the Hamilton-Jacobi equations, namely, by Eqs. (1.9) and (1.13). The smoothness of the potential of the master equation is related to the smoothness of a separatrix of the master Hamiltonian. An integrable Hamiltonian may guarantee the smoothness of the separatrices, and hence the smoothness of the potential. However, in mechanics we know that smooth separatrices are structurally unstable and integrable Hamiltonian systems are really exceptional among all Hamiltonian systems. Arbitrary weak perturbations (not of exceptional form) may destroy the smoothness of separatrices. Thus, we may expect that master equations which represent nonequilibrium systems and have smooth potentials must be exceptional. Equations (2.1), (2.2), and (2.13) provide a useful method to calculate the potential of the master equation by studying the master Hamiltonian system. The dynamics of Hamiltonian systems have been studied much more extensively than that of the master equation lacking detailed balance. In recent years, there appear numerous works dealing with Hamiltonian dynamics, both numerically and analytically. Thus, the master Hamiltonian formalism may appear to be a remarkable new approach in the study of the stationary probability distribution of nonequilibrium master equations.

III. EXAMPLES

In this section we apply the general approach stated in Secs. I and II to certain solvable models and discuss the potentials of the master equations and the conserved phase-space functions of the corresponding master Hamiltonian systems.

A. One-dimensional master Hamiltonian

A simple solvable model is a one-dimensional master equation. The general form of the master Hamiltonian is

$$H=\sum_r m(x,r)[\exp(rp)-1] . \tag{3.1}$$

It is, of course, integrable at any value of energy. At zero energy $du_0(x)/dx$ can be worked out by solving the algebraic equation

$$\sum_r m(x,r)(T^r-1)=0 , \tag{3.2}$$

with

$$T=\exp\left[\frac{du_0(x)}{dx}\right] .$$

In Ref. 14 we have proved that Eq. (3.2) has one and only one positive solution which can be associated with the potential of the master equation.

It is well known that one-dimensional stationary birth-death master equations can be solved exactly without taking the large-size limit. However, in general, one cannot obtain an explicit form of the stationary probability distribution if the master equation does not manifest detailed balance. Here and in Ref. 14 we succeed in obtaining the explicit solution of the stationary distribution by taking the large-size limit.

B. Master equation with linear transition probabilities

First, let us consider a q-dimensional birth-death master equation which has linear transition probabilities. The master Hamiltonian is expressed in the form

$$H=\sum_i\sum_j A_{ij}x_i[\exp(-p_i+p_j)-1] + \sum_i B_i[\exp(p_i)-1]+\sum_i c_i x_i[\exp(-p_i)-1] . \tag{3.3}$$

The corresponding canonical equations,

$$\begin{aligned} dx_i/dt &= -\sum_{j\neq i} A_{ij}x_i\exp(-p_i+p_j) \\ &\quad +\sum_{j\neq i} A_{ji}x_j\exp(-p_j+p_i) \\ &\quad +B_i\exp(p_i)-C_i x_i\exp(-p_i) , \\ dp_i/dt &= -\sum_{j\neq i} A_{ij}[\exp(-p_i+p_j)-1] \\ &\quad -C_i[\exp(-p_i)-1] , \end{aligned} \tag{3.4}$$

look complex. By the transformation (2.5), the master Hamiltonian is considerably simplified. In $(\mathbf{s},\mathbf{w})$ representation the Hamiltonian becomes quadratic,

$$H=\sum_i\sum_j A_{ij}w_i(s_j-s_i)+\sum_i B_i(s_i-1) + \sum_i C_i w_i(1-s_i) . \tag{3.5}$$

Defining

$$s_i'=s_i-1 ,$$

one may rewrite the Hamiltonian and the Hamilton-Jacobi equation as

$$H=\mathbf{w}\cdot\underline{M}\cdot\mathbf{s}'+\mathbf{B}\cdot\mathbf{s}' \tag{3.6}$$

and

$$\nabla\eta\cdot\underline{M}\cdot\mathbf{s}'+\mathbf{B}\cdot\mathbf{s}'=0 , \tag{3.7}$$

respectively, where

$$\mathbf{s}'=(s_1',s_2',\ldots,s_q')\ ,$$

$$\mathbf{w}=(w_1,w_2,\ldots,w_q)\ ,$$

$$\nabla\eta=\left(\frac{\partial\eta}{\partial s_1},\frac{\partial\eta}{\partial s_2},\ldots,\frac{\partial\eta}{\partial s_q}\right)\ ,$$

$$\mathbf{B}=(B_1,B_2,\ldots,B_q)\ ,$$

and

$$M_{ij}=A_{ij},\quad i\neq j;\quad M_{ii}=-\left[\prod_{j(\neq i)}A_{ij}\right]-C_i\ . \tag{3.8}$$

$\underline{M}$ can be easily diagonalized by a similarity transformation with $\underline{D}$ as

$$\underline{\bar{M}}=\underline{D}^{-1}\underline{M}\underline{D}\ ,$$

$$\underline{\bar{M}}=\begin{pmatrix} m_i & \cdots & 0 & \cdots & 0\\ 0 & \cdots & m_i & \cdots & 0\\ 0 & \cdots & 0 & \cdots & m_q\end{pmatrix}\ . \tag{3.9}$$

(The transformation may be nonunitary since $A_{ij}\neq A_{ji}$, in general.) Here we assume that the eigenvalues $m_1,m_2,\ldots,m_q$, are different from each other. If some of them are degenerate, one has to work a little more with the transformation. Nevertheless, there is no essential difficulty. The Hamiltonian is diagonalized by $\underline{D}$

$$\begin{aligned}H&=\mathbf{w}\cdot\underline{D}\underline{\bar{M}}\underline{D}^{-1}\cdot\mathbf{s}'+\mathbf{B}\cdot\underline{D}\underline{D}^{-1}\cdot\mathbf{s}'\\&=\sum_i(m_ih_il_i+B_i'h_i)\ ,\end{aligned} \tag{3.10}$$

with

$$\mathbf{h}=\underline{D}^{-1}\mathbf{s}',\quad l=\mathbf{w}\underline{D}\ ,$$

and

$$\mathbf{B}'=\mathbf{B}\underline{D}\ .$$

The q-dimensional transformation (3.9) has very special properties. On the one hand, it induces a canonical transformation in the $2q$-dimensional Hamiltonian phase space; on the other hand, it does not change the action. [Remember that the transformation (2.5) does change the action.] The first point preserves the Poisson bracket. Given any phase-space function $N(\mathbf{s},\mathbf{w})=N(\mathbf{h},l)$, we have

$$\begin{aligned}\frac{dN(\mathbf{s},\mathbf{w})}{dt}&=\sum_i\left[\frac{\partial N}{\partial s_i}\frac{\partial H}{\partial w_i}\right]-\sum_i\left[\frac{\partial N}{\partial w_i}\frac{\partial H}{\partial s_i}\right]\\&=\sum_i\left[\left[\sum_\mu\underline{D}^{-1}{}_{i\mu}\frac{\partial N}{\partial h_\mu}\right]\left[\sum_\nu\underline{D}'{}_{i\nu}\frac{\partial H}{\partial l_\nu}\right]\right.\\&\qquad\left.-\left[\sum_\nu\underline{D}'{}_{i\nu}\frac{\partial N}{\partial l_\nu}\right]\left[\sum_\mu\underline{D}^{-1}{}_{i\mu}\frac{\partial H}{\partial h_\mu}\right]\right]\\&=\left[\sum_\mu\sum_\nu\sum_i\underline{D}^{-1}{}_{i\mu}\underline{D}'{}_{i\nu}\left[\frac{\partial N}{\partial h_\mu}\frac{\partial H}{\partial l_\nu}\right]\right]\\&\quad-\left[\sum_\mu\sum_\nu\sum_i\underline{D}^{-1}{}_{i\mu}\underline{D}'{}_{i\nu}\left[\frac{\partial N}{\partial l_\nu}\frac{\partial H}{\partial h_\mu}\right]\right]\\&=\sum_\mu\left[\frac{\partial N}{\partial h_\mu}\frac{\partial H}{\partial l_\mu}-\frac{\partial N}{\partial l_\mu}\frac{\partial H}{\partial h_\mu}\right]\ ,\end{aligned} \tag{3.11}$$

where $\underline{D}'$ is the transpose of $\underline{D}$. The coordinate transformation (3.9) transforms Eq. (3.7) to

$$H=\sum_\mu\left[m_\mu h_\mu\frac{\partial\eta}{\partial h_\mu}+B_\mu'h_\mu\right]=0\ , \tag{3.12}$$

which is just the Hamilton-Jacobi equation in (h,l) representation. Thus, the second point is proven $(\partial\eta/\partial h_\mu=l_\mu)$.

The complete set of integrals is, obviously,

$$L_\mu=m_\mu h_\mu l_\mu+B_\mu'h_\mu,\quad \mu=1,2,\ldots,q\ . \tag{3.13}$$

The separatrix represented by Eq. (2.8) and the boundary condition (2.10) is determined by

$$L_\mu=0\ ,$$

which gives rise to

$$\frac{\partial\eta}{\partial h_\mu}=-B_\mu'/m_\mu$$

and

$$\eta(\mathbf{s})=-\sum_i g_i(s_i-1)\ , \tag{3.14}$$

with

$$g_i=\left[\sum_\mu D^{-1}{}_{i\mu}B_\mu'/m_\mu\right]\ .$$

Transforming $(\mathbf{s},\mathbf{w})$ back to $(\mathbf{x},\mathbf{p})$ we obtain

$$p_i=\ln(x_i/g_i)$$

that produces the stationary probability distribution

$$\begin{aligned}p(\mathbf{x})&=\prod_i p(x_i)\\&=\prod_i(\sqrt{\Omega/(2\pi g_i)}\\&\qquad\times\exp\{[x_i-g_i-x_i\ln(x_i/g_i)]\Omega\})\ ,\end{aligned} \tag{3.15}$$

or, equivalently,

$$P(\mathbf{X})=\prod_i[\exp(-g_i\Omega)(g_i\Omega)^{X_i}/X_i!]\ , \tag{3.16}$$

which is a production of q-Poisson distributions of which each argument has its average

$$\bar{X}_i=g_i\Omega=\Omega\sum_\mu\underline{D}^{-1}{}_{i\mu}B_\mu^1/m_\mu\ .$$

In fact, Eq. (3.16) is the exact stationary solution of the master equation, though we started from the equation of the large-system-size limit. Usually to solve a master equation is much more difficult than to solve a Fokker-Planck equation corresponding to the same kinetic equation. However, for the present model, the result of the master equation is even much simpler than that of the Fokker-Planck equation, of which the stationary probability distribution cannot be factorized if the arguments in the drift force are coupled to each other. In the stationary solution (3.16) various arguments

are decoupled and the probability distribution is factorized, though the arguments are coupled to each other in transition probabilities.

The model is exactly solvable. Here, by studying the model in detail we manifest clearly the way by which the master Hamiltonian approach works. Moreover, the method for solving the stationary probability distribution of the master equation by diagonalizing the Hamiltonian is completely new, and obviously much easier than that of directly solving Eq. (1.9).

A multidimensional equation with linear transition probabilities can be very complex if it is not of the birth-death type. Let us study a set of chemical reactions

$$X \underset{k_2}{\overset{k_1}{\rightleftarrows}} Y, \quad Y \xrightarrow{k_3} X+Z ,$$

$$A \xrightarrow{k_4} Y, \quad Z \xrightarrow{k_5} X+Y, \quad Z \xrightarrow{k_6} B .$$

Given

$$k_1=\sigma, \quad k_3=k_5=1, \quad k_2=k_4=\gamma ,$$

$$k_6=(b-1), \quad A/\Omega=1 ,$$

we may specify the master Hamiltonian and the corresponding canonical equation by the standard procedures. Owing to the linearity of the transition probabilities, the equations in the three-dimensional coordinate space (s_x,s_y,s_z) are independent of the momenta [cf. Eq. (2.9)]. They read

$$\begin{aligned} \frac{ds_x}{dt} &= -\sigma(s_x-s_y) , \\ \frac{ds_y}{dt} &= \beta s_x s_z+\gamma s_x-s_y , \\ \frac{ds_z}{dt} &= s_x s_y-b s_z , \end{aligned} \tag{3.17}$$

where $\beta=1$. Replacing $\beta=1$ by $\beta=-1$, Eq. (3.17) is just the well-known Lorenz equation,[21] which is a typical model for showing chaotic behaviors. We have not yet investigated Eq. (3.17). In this paper we are only restricted to solvable systems. However, it is obvious that with (3.17) no explicit constant of motion other than energy can be found. It is not surprising if one finds the potential of the master equation nonsmooth for such a seemingly simple model.

C. Multidimensional master equations with nonlinear transition probabilities

To date there is no general way to discuss the master equation of this kind, even in the large-size limit. We can only cite some especially simple models as our solvable examples.

The first apparently solvable model of this kind is the decoupled master equation. The master Hamiltonian is given by

$$H=\sum_i \sum_{r_i} m(x_i,r_i)[\exp(r_i p_i)-1] . \tag{3.18}$$

The following q first integrals

$$L_i=\sum_{r_i} m(x_i,r_i)[\exp(r_i p_i)-1], \quad i=1,2,\ldots,q$$

are manifest. The potential is the sum of $u_{0i}(x_i)$,

$$u_0(\mathbf{x})=\sum_i u_{0i}(x_i) ,$$

where $u_{0i}(x_i)$ is the solution of the Hamilton-Jacobi equation $L_i=0$. Hence, the problem is substantially one dimensional.

If the arguments in the master equation are coupled to each other the problem becomes nontrivial, and in particular, if the coupling is on one direction the problem may be solvable. Let us consider a master Hamiltonian with two degrees of freedom,

$$H=H_1+H_2+H_3 ,$$

in which

$$H_1=\sum_{r_1} m_1(x,r_1)[\exp(r_1 p_1)-1] ,$$

$$H_2=\sum_{r_2} m_2(y,r_2)[\exp(r_2 p_2)-1] ,$$

and

$$H_3=\sum_{r_1}\sum_{r_2} m_3(x,\bar{r}_1,\bar{r}_2)[\exp(\bar{r}_1 p_1+\bar{r}_2 p_2)-1] . \tag{3.19}$$

The coupling of the master equation which is represented in H_3 is only on the direction $x \rightarrow y$. The following three cases of Eq. (3.19) will be discussed, respectively.

1. H_1+H_3 is a birth-death master Hamiltonian and linear in x

The general forms of H_1,H_3 are specified by

$$H_1=a[\exp(p_1)-1]+x[\exp(-p_1)-1] ,$$

$$H_3=x[\exp(-p_1+p_2)-1] .$$

The second constant of motion besides the Hamiltonian can be easily found in $(\mathbf{s},\mathbf{w})$ representation [cf. Eq. (2.9)] in which the Hamiltonian is formulated as

$$\begin{aligned} H=&a(s_1-1)-w_1(s_2-s_1)-w_1(1-s_1) \\ &+\sum_{r_2} m_2(-s_2 w_2,r_2)(s_2^{r_2}-1) . \end{aligned} \tag{3.20}$$

The canonical equation for w_1 is independent of all the other arguments

$$\frac{dw_1}{dt}=-a-2w_1$$

that can be integrated as

$$L_A=(a+2w_1)\exp(2t) . \tag{3.21}$$

Apparently, the separatrix is defined as

$$2w_1+a=0 ,$$

or, more specificly, by

$$L_1 = a(s_1 - 1) - 2w_1(1 - s_1) = 0 , \tag{3.22a}$$

$$L_2 = \bar{x}(s_2 - 1) + \sum_{r_2} m_2(-s_2 w_2, r_2)(s_2^{r_2} - 1) = 0 . \tag{3.22b}$$

Equation (3.22a) yields

$$P(X) = \exp(-a\Omega/2)(a\Omega/2)^X / X! .$$

Equation (3.22b) is a one-dimensional Hamilton-Jacobi equation which has been generally solved in Sec. III A. The constant $\bar{x}$ in L_2 is nothing but the average concentration of x, $\bar{x} = a/2$. It should be noted that neither L_1 nor L_2 is the first integral. They remain constant only on the separatrix. The main nontrivial result is that the stationary probability distribution is still factorizable in this one-directionally coupled model and x enters the stationary probability distribution of y in such a way that it takes its average value.

To date, only a few examples of master equations without manifest detailed balance are known to be solvable. It is, of course, interesting to find new kinds of solvable models. Now, for the first time, the master equations of the type of Eq. (3.20) are solved in the large-system-size limit. The solution is obtained by finding a certain separatrix of the corresponding master Hamiltonian system [cf. Eqs. (3.22a) and (3.22b)].

2. $H_2 + H_3$ is a birth-death master Hamiltonian and linear in x

The Hamiltonian now becomes

$$H = \left[\sum_{r_1} m_1(-s_1 w_1, r_1)(s_1^{r_1} - 1 \right] - w_1(s_2 - s_1) + a(s_2 - 1) - w_2(1 - s_2) . \tag{3.23}$$

Now it is the equation of s_2 that is independent of the others,

$$\frac{ds_2}{dt} = -(1 - s_2) ,$$

which gives rise to a new time-dependent constant of motion,

$$L_B = (s_2 - 1)\exp(-t) . \tag{3.24}$$

Unlike Eq. (3.22), the stationary probability distribution in this case is no longer factorized. The potential is not associated with any value of the constant L_B. There is no general way to define the separatrices from time-dependent constants of motion, and we are not able to find the explicit form of the potential. However, due to the fact that the master Hamiltonian system is integrable, we may conclude the smoothness of the potential without really solving it. It is emphasized that this conclusion can not be obtained directly from Eq. (1.9).

3. General case

For the general one-directionally coupled master equation [cf. Eq. (3.19)], we can find neither the second constant of motion nor the explicit form of the potential. Provided the stationary solution of the master equation is $p(x,y)$, the distribution

$$p(x) = \int p(x,y)dy$$

can be evaluated by solving

$$L_1 = \sum_{r_1} m_1(x, r_1)\{\exp[r_1 du_0(x)/dx] - 1\} + \sum_{\bar{r}_1} \sum_{\bar{r}_2} m_3(x, \bar{r}_1, \bar{r}_2)\{\exp[\bar{r}_1 du_0(x)/dx] - 1\} = 0 ,$$

$$p(x) = N \exp\left[- \int [du_0(x)/dx]dx \right] ,$$

with N being the normalization constant.

To conclude our presentation, some remarks are necessary. In our solvable models, we always find that integrability of master Hamiltonians ensures the smoothness of potentials. However, complete integrability is a much stronger requirement than that of the existence of a smooth potential. For the Fokker-Planck equation, Graham *et al.* have shown that a system possessing a smooth potential (or, a smooth separatrix) is not necessarily integrable, even at $H = 0$. It may be the case for the master equation.

Most master equations of interest are not solvable. For practical purposes, one has to resort to various perturbation procedures. On this aspect, the understanding of the master equation is much less than that of the Fokker-Planck equation. Moreover, the numerical detection on the integrability of the master Hamiltonian has not yet been started. There is a wide field to be explored.

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