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Master Equations with a Unique Stationary State

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An effective method which allows one to verify whether a master equation on the Gibbs space has a unique stationary state is proposed. For a unique stationary state the formula establishing its dependence on matrix elements of the generator of the master equation is obtained. Examples of one-step processes with a unique stationary state are studied.

1 Introduction

In the last two decades a considerable progress has been made in the theory of nonequilibrium processes as well as in the theory of classical open systems. Much of this progress has resulted from systematic use of the so-called mesoscopic description of physical systems [1] or, in other words, from the use of classical dynamical semigroups.

The starting point of the mesoscopic description of a system $\mathcal{S}$ is the introduction of coarse-grained phase space obtained from the phase space of $\mathcal{S}$ by its proper fragmentation into a finite number of phase space cells. By definition, the (statistical) state of the system at a given instant t is known provided that the probability vector $p(t) = \big(p_1(t), p_2(t), \ldots, p_n(t)\big)$ is given. Here p_i's stand for probabilities of finding the system $\mathcal{S}$ in phase cells numbered $1, \ldots, n$. The time evolution of a state is described by the master equation

$$\frac{dp_i(t)}{dt} = \sum_{j=1}^{n} \left\{ \pi(i|j)p_j(t) - \pi(j|i)p_i(t) \right\}. \tag{1.1}$$

The nonnegative quantity $\pi(i|j)$ appearing in (1.1) is a transition rate from the state j to the state i. It depends on internal rate constants as well as on external conditions imposed by the coupling of the system $\mathcal{S}$ to reservoir systems.

Equations of this type play a very important rôle in the description of kinetics of physical, chemical and biological systems [1 - 4].

In every particular case an essential difficulty with the derivation of the master equation lies in establishing an explicit form of $\pi(i|j)$'s. Usually the problem of finding the particular form of (1.1) can be solved by assuming the definite model of phenomena which occur in the system in question, and practically the only criterion for the correctness of (1.1) is based on an experiment.

Within the problems described by a linear stochastic dynamics we are mostly interested in such a time evolution which leads to exactly one stationary state. In the case of an isolated system one obtains $\{\frac{1}{n}\}$ as a counterpart of a microcanonical distribution, while for a system interacting with a heat-bath — the corresponding Gibbs state [5]. In a more complicated situation when the system is coupled to reservoir systems which are not in mutual equilibrium, it cannot achieve an equilibrium state either, but at most tends to some nonequilibrium steady state [4].

As it was mentioned above, master equations are usually modelled. Therefore, it seems useful to give an effective criterion which would allow one to verify whether the postulated dynamics would lead to a unique stationary state. The aim of this paper is to formulate such a criterion possibly with a wide range of applications; therefore, we do not make any particular assumptions about transition rates. For the master equation with a unique stationary state we obtain the formula expressing components of a stationary state via matrix elements of the generator of the master equation.

Let us, for convenience, rewrite master equation (1.1) in a more compact form

$$\frac{dp(t)}{dt} = \boldsymbol{L}p(t), \qquad t \geq 0 \tag{1.2}$$

with $\boldsymbol{L} = [L_{ij}]$ given by the formula

$$L_{ij} := \pi(i|j) - \delta_{ij} \sum_k \pi(k|i). \tag{1.3}$$

It follows from the definition of $\pi(i|j)$'s that

$$L_{ii} \leq 0 \quad (i = 1, \ldots, n), \qquad L_{ij} \geq 0 \quad (i \neq j = 1, \ldots, n) \tag{1.4}$$

and

$$\sum_{i=1}^{n} L_{ij} = 0 \qquad (j = 1, \ldots, n). \tag{1.5}$$

The solution to the master equation (1.2) is given by the formula

$$p(t) = \boldsymbol{\Phi}(t)p(0), \qquad t \geq 0 \tag{1.6}$$

with the flow

$$\boldsymbol{\Phi}(t) := \exp(t\boldsymbol{L}). \tag{1.7}$$

If the operator L is time-dependent, then the above expression is not valid. However, in this case one can always rewrite (1.2) in the form

$$\frac{dp(t)}{dt} = \sum_{i=1}^{m} a_i(t) L_i p(t), \qquad t \geq 0, \tag{1.8}$$

where $m \leq n^2$ and L_{ij} are time-independent. Now, using the so-called Wei-Norman method [6] we can represent locally the general solution to the master equation (1.8) as a finite product of the exponential operators

$$p(t) = \left[\prod_{k=1}^{r} \exp\left(g_k(t) T_k\right)\right] p(t_0), \tag{1.9}$$

where $T_1, \ldots, T_r$ represent an arbitrary basis for the finite-dimensional Lie-algebra $\mathcal{L}$ generated by the operators $L_1, \ldots, L_m$ $(r := \dim \mathcal{L})$ and the time-dependent functions $g_k(t)$, $k = 1, \ldots, r$ are defined by a set of differential equations (Wei-Norman equations)

$$a_k(t) = \sum_{j=1}^{r} \Omega_{kj} \dot{g}_j(t), \qquad g_i(0) = 0, \tag{1.10}$$

for i, $k = 1, \ldots, r$. In the above Ω's denote some analytic functions of the g_i's. The representation (1.9) is valid globally provided the algebra $\mathcal{L}$ is solvable [7].

2 Remarks about the flow $\Phi(t)$

We would like to emphasize that the solution of the master equation given by (1.6) and (1.7) should not be treated only as a formal expression. On the contrary, by virtue of an expansion of the flow (1.7) in terms of a finite number of powers of L it has a practical meaning. Throughout this paragraph we want to discuss this problem. To this end we will utilize the resolvent technique, cf. for instance [8]. Let $R(\lambda) = (\lambda I - L)^{-1}$ be the resolvent of L and let $\sigma(L)$ stand for the spectrum of L. One can check that for any polynomial

$$\nu(\lambda) = \sum_{k=0}^{p} a_k \lambda^k \quad \text{with} \quad \lambda \notin \sigma(L),$$

the following equality holds

$$\big(\nu(\lambda) I - \nu(L)\big) R(\lambda) = \sum_{k=0}^{p-1} \nu_k(\lambda) L^k, \tag{2.1}$$

where

$$\nu_k(\lambda) = \sum_{i=0}^{p-k-1} a_{i+k+1} \lambda^i. \tag{2.2}$$

In particular, substituting for $\nu(\lambda)$ the minimal polynomial of a generator L, $\mu(\lambda, L) = \sum_{k=0}^{m} a_k \lambda^k$ $(m = \deg(\mu(\lambda, L)))$, (2.1) takes the form

$$R(\lambda) = \frac{1}{\mu(\lambda, L)} \sum_{k=0}^{m-1} \mu_k(\lambda) L^k , \tag{2.3}$$

where

$$\mu_k(\lambda) = \sum_{i=0}^{m-k-1} a_{i+k+1} \lambda^i . \tag{2.4}$$

According to the definition of the function of an operator we have

$$\Phi(t) = \exp(tL) = \frac{1}{2\pi i} \oint_{\partial D} (zI - L)^{-1} \exp(tz)\, dz, \tag{2.5}$$

where D is an arbitrary region of the complex plane C such that $\sigma(L) \subset D$. Substituting (2.3) into (2.5) we obtain

$$\Phi(t) = \sum_{k=0}^{m-1} c_k(t) L^k \tag{2.6}$$

with the coefficients $c_k(t)$ given by

$$c_k(t) = \frac{1}{2\pi i} \oint_{\partial D} \frac{\mu_k(z)}{\mu(z, L)} \exp(tz)\, dz . \tag{2.7}$$

The use of the minimal polynomial of the generator L to obtain the expansion (2.6) assures the simplest mathematical representation of the flow $\Phi(t)$ in terms of L. (The flow is expressed as a polynomial in L of a possibly lowest order with the expansion coefficients calculated from the coefficients of the lowest order polynomial annihilating L.) An analogous expansion can be obtained with the help of an arbitrary annihilator of L, which follows from the fact that (2.3) is true for an arbitrary annihilator of L. If in a particular case finding the minimal polynomial is difficult, one can get the expansion with the help of the characteristic polynomial of L.

3 Asymptotic behavior of a stochastic system

The number of linearly independent stationary states and, consequently, the asymptotic behavior of the system described by a limiting probability distribution

$$p(\infty) = \lim_{t \to \infty} \Phi(t) p(0) \tag{3.1}$$

depend on the geometric multiplicity of zero as a characteristic value of L. It is easy to see that zero is always contained in the spectrum of L. The coefficients χ_k appearing in the characteristic equation for L

$$\chi(\lambda, L) = \det(\lambda I - L) = \lambda^n + \chi_1 \lambda^{n-1} + \ldots + \chi_k \lambda^{n-k} + \ldots + \chi_n = 0 \tag{3.2}$$

are connected with matrix elements of L by the formula

$$\chi_k = (-1)^k S_k \,, \tag{3.3}$$

where S_k denotes the sum of all kth order principal minors of L. In particular, $\chi_n = (-1)^n \det L$ which is equal to zero due to (1.5).

From the general theorem of Gerschgorin it follows, in particular, that the real part of the non-zero characteristic value of L must be negative [9]. Hence, if zero is a simple characteristic value of L, the evaluation of the limit (3.1) presents no difficulties. In this case the most interesting feature of the distribution $p(\infty)$ is its independence of the initial probability distribution $p(0)$.

However, if zero is an r-fold characteristic value, the existence of the limit (3.1) is possible only if L is of rank $n - r$. It is a remarkable property of generators that the last condition is always fulfilled [10]. For L with zero as an r-fold characteristic value, the last r coefficients in (3.2) must vanish

$$\chi_n = \chi_{n-1} = \ldots = \chi_{n-r+1} = 0$$

while $\chi_{n-r} \neq 0$ and $\dim\ker L = r$. The limiting probability distribution (3.1) has the form

$$p(\infty) = f_1(p(0))\, q_1 + \ldots + f_r(p(0))\, q_r \,, \tag{3.4}$$

where $q_1, \ldots, q_r$ are linearly independent vectors which span the kernel of L and $f_1(p(0)), \ldots, f_r(p(0))$ are scalars depending on the initial probability distribution.

4 The criterion for a unique stationary state

It follows from the preceding remarks about limiting states of a master equation that the necessary and sufficient condition for a master equation to have a unique limiting state reads $\chi_{n-1} \neq 0$ or by (3.3)

$$S_{n-1} \neq 0. \tag{4.1}$$

Condition (4.1) is an effective one but still the computation of determinants of a large matrix is a cumbersome problem. The effectiveness of our criterion (4.1) can be considerably improved by expressing (4.1) in terms of traces of powers of L. In that way the numerically difficult problem can be reduced to a rather simple problem of matrix products. To this end let us first remind that symmetric polynomials of the form

$$a_k = x_1^k + x_2^k + \ldots + x_n^k \qquad (k = 1, \ldots n) \tag{4.2}$$

are connected with elementary symmetric polynomials

$$
\begin{aligned}
s_1 &= x_1 + x_2 + \ldots + x_n \\
s_2 &= x_1x_2 + x_1x_3 + \ldots + x_{n-1}x_n \\
&\ldots \\
s_n &= x_1x_2\ldots x_n
\end{aligned}
\tag{4.3}
$$

by Newton formulas

$$
a_k - a_{k-1}s_1 + a_{k-2}s_2 + \ldots + (-1)^{k-1}a_1s_{k-1} + (-1)^k k s_k = 0 \quad (k \leq n)\,. \tag{4.4}
$$

Let us denote by $\lambda_1, \ldots, \lambda_n$ the characteristic values of L and let

$$
\sigma_k = s_k(\lambda_1, \ldots, \lambda_n) \qquad (k = 1, \ldots, n)\,. \tag{4.5}
$$

Then by Viete formulas the coefficients of characteristic equation (3.2) are connected with σ_k in the following manner

$$
\sigma_k = (-1)^k \chi_k \qquad (k = 1, \ldots, n) \tag{4.6}
$$

and because of (3.3)

$$
\sigma_k = S_k\,. \tag{4.7}
$$

Let

$$
\alpha_k = a_k(\lambda_1, \ldots, \lambda_n) \qquad (k = 1, \ldots, n)\,, \tag{4.8}
$$

then

$$
\alpha_k = \sum_{i=1}^{n} (\lambda_i)^k = \mathrm{Tr}(L^k)\,. \tag{4.9}
$$

Because of (4.5) — (4.9), (4.4) yields

$$
(-1)^{k+1} k S_k = \alpha_k - \alpha_{k-1}S_1 + \alpha_{k-2}S_2 + \ldots + (-1)^{k-1}\alpha_1 S_{k-1} \tag{4.10}
$$

with $k = 1, \ldots, n$ and $\alpha_1 = S_1 = \mathrm{Tr}\, L$. By a successive application of (4.10) one can express sums of kth order principal minors of L in terms of traces of powers of L. The explicit expression (Waring formula) reads

$$
S_k = \sum \frac{(-1)^{l_1 + l_2 + \ldots + l_k + k}}{1^{l_1} 2^{l_2} \ldots k^{l_k} l_1! l_2! \ldots l_k!} \alpha_1^{l_1} \alpha_2^{l_2} \ldots \alpha_k^{l_k} \qquad (k \leq n)\,, \tag{4.11}
$$

where the sum is taken over all non-negative integers $l_1, \ldots, l_k$ which fulfil the condition $l_1 + 2l_2 + \ldots + kl_k = k$.

5 The unique stationary state expressed in terms of the matrix elements of L

Now we would like to express a unique limiting state (3.1) of the master equation in terms of the matrix elements of the generator $\boldsymbol{L}$.

Let us first observe that $\boldsymbol{p}(\infty)$ is a unique limiting state if and only if

$$\boldsymbol{\Phi}(\infty) := \lim_{t\to\infty} \boldsymbol{\Phi}(t) \tag{5.1}$$

has the form

$$\boldsymbol{\Phi}(\infty) = \begin{bmatrix} q_1 & q_1 & \cdots & q_1 \\ q_2 & q_2 & \cdots & q_2 \\ \vdots & \vdots & \ddots & \vdots \\ q_n & q_n & \cdots & q_n \end{bmatrix}, \tag{5.2}$$

where $q_i \equiv p_i(\infty) \quad (i = 1, \dots, n)$. Obviously, if (5.2) holds then (3.1) is fulfilled for every $\boldsymbol{p}(0)$. On the other hand, because $\boldsymbol{q}$ is independent of the initial state, $\boldsymbol{\Phi}(\infty)$ can depend on $\boldsymbol{q}$ only. Suppose that

$$\boldsymbol{\Phi}(\infty) = \begin{bmatrix} f_{11}(\boldsymbol{q}) & f_{12}(\boldsymbol{q}) & \cdots & f_{1n}(\boldsymbol{q}) \\ f_{21}(\boldsymbol{q}) & f_{22}(\boldsymbol{q}) & \cdots & f_{2n}(\boldsymbol{q}) \\ \vdots & \vdots & \ddots & \vdots \\ f_{n1}(\boldsymbol{q}) & f_{n2}(\boldsymbol{q}) & \cdots & f_{nn}(\boldsymbol{q}) \end{bmatrix}. \tag{5.3}$$

Because $\boldsymbol{q} = \boldsymbol{\Phi}(\infty)\boldsymbol{p}(0)$ for any $\boldsymbol{p}(0)$, let us take as $\boldsymbol{p}(0)$ all pure states, i.e. states of the form $(0, \dots, 1_i, \dots, 0)\,, \quad (i = 1, \dots, n)$, then (5.2) follows easily.

We have

$$\boldsymbol{L}\,\boldsymbol{\Phi}(\infty) = 0 \tag{5.4}$$

and simultaneously

$$\boldsymbol{L}\,\mathrm{adj}(-\boldsymbol{L}) = 0\,. \tag{5.5}$$

(We take adj$(-\boldsymbol{L})$ instead of adj$(\boldsymbol{L})$ because all cofactors of matrix elements of $-\boldsymbol{L}$ are positive [10].) In order to find the dependence of $\boldsymbol{\Phi}(\infty)$ on $\boldsymbol{L}$ let us first observe that $\boldsymbol{\Phi}(t)$ admits the following expansion [11]

$$\boldsymbol{\Phi}(t) = \exp(t\boldsymbol{L}) = \sum_{k=1}^{s} \frac{1}{(n_k - 1)!}[\mathrm{adj}(\lambda_k \boldsymbol{I} - \boldsymbol{L}) \exp(\lambda_k t)/\Delta_k(\lambda)]\,, \tag{5.6}$$

where

$$\Delta_k(\lambda) = \chi(\lambda, \boldsymbol{L})/(\lambda - \lambda_k)^{n_k}\,, \tag{5.7}$$

n_k denotes the algebraic multiplicity of λ_k and $s < n$ is the number of different roots of $\chi(\lambda, \boldsymbol{L})$. Because the real part of the non-zero characteristic value of $\boldsymbol{L}$ must be negative, in the limit $\lim_{t\to\infty} \boldsymbol{\Phi}(t)$ all constituents of (5.6) corresponding to non-zero eigenvalues of $\boldsymbol{L}$ do not contribute. Taking into account that zero is a simple characteristic value of $\boldsymbol{L}$ we get

$$\boldsymbol{\Phi}(\infty) = \mathrm{adj}(-\boldsymbol{L})/\chi'(0,\boldsymbol{L}). \tag{5.8}$$

By comparison of (5.2) and (5.8) we obtain that

$$\mathrm{adj}(-\boldsymbol{L})_{ij} = \mathrm{adj}(-\boldsymbol{L})_{ii}, \qquad (i,j = 1,\ldots,n). \tag{5.9}$$

In other words

$$A_{1i} = A_{2i} = \ldots = A_{ni} \qquad (i = 1,\ldots,n), \tag{5.10}$$

i.e. all cofactors of matrix elements from any column of $-\boldsymbol{L}$ are equal.

Therefore, the unique normalized solution of (5.4) has the form

$$q_j = \frac{A_{jj}}{\sum_{j=1}^{n} A_{jj}} \qquad (j = 1,\ldots,n). \tag{5.11}$$

Formula (5.11) establishes the connection between the unique stationary solution of the master equation and matrix elements of its generator $\boldsymbol{L}$. For the computation of determinants see for instance [12].

6 An example: one-step processes

The method formulated in Sec. 4 can be applied in any case, i.e. regardless of the structure of the generator $\boldsymbol{L}$ of a dynamical evolution of a stochastic system. There are, however, processes for which the uniqueness of the stationary state can be deduced from the matrix structure of $\boldsymbol{L}$.

As an example of such a situation we will consider one-step processes (birth and death processes).

Let us remind that any one-step process can be represented in the form (1.2) if $\boldsymbol{L} = [L_{ij}]_{i,j=0,\ldots,n-1}$ is defined as follows

$$L_{ij} := \begin{cases} b_{i-1} & \text{for} \quad j = i-1 \\ -(b_i + c_i) & \text{for} \quad j = i \\ c_{i+1} & \text{for} \quad j = i+1 \\ 0 & \text{for} \quad |j-i| > 1 \end{cases} \tag{6.1}$$

with $b_{n-1} = c_0 = 0$ and all remaining b_i's and c_i's non-negative.

We will discuss several cases of such processes according to the values of parameters $b_i \quad (i = 0,\ldots,n-2)$ and $c_i \quad (i = 1,\ldots,n-1)$.

(a) Let us assume that

$$b_i c_{i+1} > 0 \qquad (i = 1,\ldots,n-2). \tag{6.2}$$

It is well-known that under assumption (6.2) the spectrum of the tri-diagonal (Jacobi) matrix is non-degenerate [13, 14]. In particular, zero is a simple eigenvalue of L; therefore $\dim\ker L = 1$ and the time-evolution generated by L has a unique stationary state.

Even if a single product from (6.2) was zero then the degeneration of any eigenvalue of L can occur. In particular, if both factors in such a product are equal to zero, then zero becomes the degenerated eigenvalue of L because in this case the system is decomposable [1]. Assumption (6.2), however, can be weakened in such a way that zero would remain a simple eigenvalue of L.

(b) Let us assume that all b_i's and all c_i's are positive apart from one, say c_k ($k \neq n-1$) which is equal to zero.
Then the characteristic polynomial of L can be written in the form

$$\chi(\lambda, L) \ = \ \chi(\lambda, \widetilde{L}_{(k)})\chi(\lambda, L^{(n-k)}), \tag{6.3}$$

where $\chi(\lambda, L^{(n-k)})$ denotes the characteristic polynomial of the generator $L^{(n-k)}$ which is obtained from L by the removal of its first k rows and columns and $\chi(\lambda, \widetilde{L}_{(k)})$ stands for the characteristic polynomial of the kth section of L. (By the kth section of L [13] we understand a $k \times k$ tri-diagonal matrix for which the sum of elements appearing in a column is equal to zero for each column apart from the last for which the corresponding sum is negative.) In this case all non-diagonal elements of $\widetilde{L}_{(k)}$ are positive and, according to [13], the spectrum of $\widetilde{L}_{(k)}$ does not contain zero. Due to positivity of all non-diagonal elements of $L^{(n-k)}$ its spectrum is non-degenerate, hence zero is the simple root of $\chi(\lambda, L^{(n-k)})$. Therefore, also in this case $\dim\ker L = 1$.

(c) The above observation can be easily generalized to the case of an arbitrary number of c_i's equal to zero while c_{n-1} and all b_i's remain positive.

Let $k_1 < k_2 < \ldots < k_r$ denote the values of an index i for which $c_{k_1} = c_{k_2} = \ldots = c_{k_r} = 0$. Then the characteristic polynomial of L can be written in the form

$$\chi(\lambda, L) \ = \ \chi(\lambda, \widetilde{L}_{(k_1)})\chi(\lambda, \widetilde{L}^{(n-k_1)}_{(k_2-k_1)}) \cdots \chi(\lambda, \widetilde{L}^{(n-k_{r-1})}_{(k_r-k_{r-1})})\chi(\lambda, L^{(n-k_r)}), \tag{6.4}$$

i.e. in the form of the product of characteristic polynomials of corresponding sections of generators $L, \ldots, L^{(n-k_{r-1})}$ and the characteristic polynomial of the generator $L^{(n-k_r)}$. The spectra of $\widetilde{L}_{(k_1)}, \ldots, \widetilde{L}^{(n-k_{r-1})}_{(k_r-k_{r-1})}$ do not contain zero and the spectrum of $L^{(n-k_r)}$ is non-degenerate. Therefore, under the assumption that all b_i's are positive the one-step process has a unique stationary state in every case apart from $c_{n-1} = 0$. Obviously, the last statement remains true in the case of all c_i's positive and b_i's arbitrary apart from $b_0 = 0$.

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