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# Microdynamics and Time-Evolution of Macroscopic Non-Markovian Systems. II*

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We study the time-evolution of the joint and the conditional probability of macroscopic variables of a closed system from a microscopic point of view. We derive an exact generalized master equation for their time rate of change which consists of two parts, one instantaneous and local in state space, the other retarded and nonlocal in state space. It is represented by stochastic operators depending both on the initial preparation and on the initial macrodistribution, which reflects the non-Markovian character of the process. The connection with the time-evolution of the single-event probability is discussed.

## Introduction

In the last two decades there has been considerable progress by the attempt to deduce the macroscopic properties of large physical systems from first principles. Especially the projection-operator technique originated by Nakajima [1] and Zwanzig [2] proved to be very useful in this field. In the first paper of this series [3] (referred to as I) we have used this technique to derive an exact equation of motion for the single-event probability $p^{(1)}(a,t)$ of a set of macrovariables $a$. By taking the preparation of the initial distribution explicitly into account, we obtained a homogeneous master equation with uniquely defined stochastic operators.

It has been pointed out in I that the Greens function of the master equation for $p^{(1)}(a,t)$ allows for the calculation of *initial* time-correlation functions of macrovariables. To determine correlation functions for arbitrary times, however the $p^{(1)}(a,t)$-level of description is not sufficient, but one has to look for an evolution equation for the joint probability $p^{(2)}(a',t';a,t)$. In this paper, we derive an exact equation of motion for the macroscopic joint probability by means of extended projection-operator techniques in the framework of classical statistical mechanics. To our knowledge, up to now the time-evolution of the multivariate probability distributions has not been considered starting from first principles. The interest in this problem arises not only from the wellknown importance of time-correlation functions in non-equilibrium statistical mechanics [4] but multivariate probability distributions are also important for the investigation of the nature of the stochastic process of macrovariables. For instance, a satisfactory discussion of the Markovian limit cannot be given on the $p^{(1)}(a,t)$-level of description.

The paper is organized as follows. In the next Section we give a detailed discussion of the microscopic joint probability $\rho^{(2)}(q',t';q,t)$ and the conditional probability $\rho(q',t'|q,t)$. Although the properties of $\rho^{(2)}(q',t';q,t)$ are well-known, a comparison with the properties of the macroscopic joint probability $p^{(2)}(a',t';a,t)$ is very informative as the micrody-

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namics is a Markovian process whereas the macrodynamics is non-Markovian if no approximation is made. In Section 3, the macroscopic probabilities $p^{(2)}(a',t';a,t)$ and $p(a',t'|a,t)$ are related to the microscopic ones by the coarse-graining operation. The connection is given in terms of the probability distribution $w_\sigma(q,t)$ of macroscopically equivalent microstates $q$ corresponding to a given macrostate $a$. The time-evolution of this distribution is obtained as a preparation-dependent functional of the past history of the macroscopic single-event distribution $p^{(1)}(t)$. In Section 4 which contains the main results of this work, the time-evolution of the macroscopic joint and conditional probabilities is expressed completely in terms of the macroscopic motion by means of extended projection-operator techniques. We derive exact generalized master equations for $p(t'|t)$ and $p^{(2)}(t',t)$ with stochastic operators depending explicitly not only on the initial preparation but also on the initial macrodistribution $p^{(1)}(0)$. In Section 5, we finally discuss the connection with the time-evolution of the macroscopic single-event probability $p^{(1)}(t)$ and establish the connection with the results of I.

## 2. The Microscopic Joint and Conditional Probabilities

Throughout this paper we use the notation of I. In this Section we consider the time-evolution of the microscopic joint probability $\rho^{(2)}(t',t)$ which determines time-correlation functions $\langle F(t')G(t)\rangle$ of arbitrary phase functions $F(q)$, $G(q)$, where $q=(q_1,\dots,q_\alpha,\dots)$ is a point in the phase space $\Gamma$.
Let $\rho^{(1)}(q,0)$ be the initial microdistribution of the ensemble of systems considered. The mean value $\langle F(t)\rangle$ of a phase function $F(q)$ at time $t$ is given by

$$\langle F(t)\rangle=\int dq\,F(q(t))\,\rho^{(1)}(q,0), \tag{2.1}$$

where $q(t)$ is the solution of Hamilton's equations of motion with the initial condition $q(0)=q$. The time-correlation function of two phase functions $F(q)$, $G(q)$ reads

$$\langle F(t')\,G(t)\rangle=\int dq\,F(q(t'))\,G(q(t))\,\rho^{(1)}(q,0). \tag{2.2}$$

Hamilton's equations of motion lead to

$$F(q(t))=e^{-\mathbf{L}t}F(q), \tag{2.3}$$

where $\mathbf{L}$ denotes the Liouvillian which acts on a phase function $\varphi(q)$ as the Poisson bracket with the Hamilton function $H(q)$,

$$\mathbf{L}\varphi=\{H,\varphi\}. \tag{2.4}$$

This Poisson-bracket structure of the Liouvillian leads to the relations

$$\int dq\,\varphi(q)\,\mathbf{L}\psi(q)=-\int dq\,\psi(q)\,\mathbf{L}\varphi(q) \tag{2.5}$$

$$\mathbf{L}\varphi(q)\,\psi(q)=\varphi(q)\,\mathbf{L}\psi(q)+\psi(q)\,\mathbf{L}\varphi(q) \tag{2.6}$$

and

$$\int dq\,\varphi(q)\,e^{\mathbf{L}t}\psi(q)=\int dq\,\psi(q)\,e^{-\mathbf{L}t}\varphi(q) \tag{2.7}$$

$$e^{\mathbf{L}t}\varphi(q)\,\psi(q)=(e^{\mathbf{L}t}\varphi(q))(e^{\mathbf{L}t}\psi(q)). \tag{2.8}$$

Using (2.1), (2.3) and (2.7) we have

$$\langle F(t)\rangle=\int dq(e^{-\mathbf{L}t}F(q))\,\rho^{(1)}(q,0)$$
$$=\int dq\,F(q)\,\rho^{(1)}(q,t) \tag{2.9}$$

where

$$\rho^{(1)}(q,t)=e^{\mathbf{L}t}\rho^{(1)}(q,0) \tag{2.10}$$

denotes the single-event microdistribution at time $t$. With (2.3), (2.7) and (2.8) the time-correlation function (2.2) reads

$$\langle F(t')\,G(t)\rangle=\int dq(e^{-\mathbf{L}(t'-t)}F(q))\,G(q)\,e^{\mathbf{L}t}\rho^{(1)}(q,0). \tag{2.11}$$

This may be written as

$$\langle F(t')\,G(t)\rangle=\int dq'\,dq\,F(q')\,G(q)\,\rho^{(2)}(q',t';q,t), \tag{2.12}$$

where we have introduced the microscopic joint probability

$$\rho^{(2)}(q',t';q,t)=e^{\mathbf{L}'(t'-t)}\,\delta(q'-q)\,e^{\mathbf{L}t}\rho^{(1)}(q,0)$$
$$=\delta(q'-q(t'-t))\,\rho^{(1)}(q,t). \tag{2.13}$$

Here $\mathbf{L}'$ acts only on the $q'$-coordinate.
The probability distributions $\rho^{(1)}(t)$, $\rho^{(2)}(t',t)$ are elements of $\Pi(\Gamma)$ and $\Pi(\Gamma\otimes\Gamma)$, respectively, where $\Pi(\Omega)$ denotes the linear manifold of absolutely integrable real functions on $\Omega$. In spite of the fact that the single-event probabilities $\rho^{(1)}(t)$ at time $t$ are submitted to the constraints of positivity and normalization

$$\rho^{(1)}(q,t)\geqq 0$$
$$\int dq\,\rho^{(1)}(q,t)=1, \tag{2.14}$$

the linear closure of this set coincides with $\Pi(\Gamma)$. There is a uniquely defined group of time-evolution operators $\mathbf{U}(\tau)$ with the properties

$$\mathbf{U}(\tau)\colon\ \Pi(\Gamma)\to\Pi(\Gamma)$$
$$\mathbf{U}(\tau_1+\tau_2)=\mathbf{U}(\tau_1)\,\mathbf{U}(\tau_2)$$
$$\mathbf{U}(0)=\mathbf{1}$$
$$\mathbf{U}(-\tau)=\mathbf{U}^{-1}(\tau)$$
$$\rho^{(1)}(t')=\mathbf{U}(t'-t)\,\rho^{(1)}(t)\qquad\forall\rho^{(1)}(t) \tag{2.15}$$

which is given by

$$\mathbf{U}(\tau)=e^{\mathbf{L}\tau}. \tag{2.16}$$

The joint probability $\rho^{(2)}(t',t)$, $t'\geqq t$, and the single-event probability $\rho^{(1)}(t)$ are connected by the microscopic conditional probability $\rho(t'|t)$ defined by

$$\rho^{(2)}(q',t';q,t)=\rho(q',t'|q,t)\,\rho^{(1)}(q,t). \tag{2.17}$$

From (2.13) we see that

$$\rho(q',t'|q,t)=\delta(q'-q(t'-t)). \tag{2.18}$$

The microscopic conditional probability $\rho(q',t'|q,t)$ is identical with the kernel of the time-evolution operator $\mathbf{U}(t'-t)$ introduced in (2.15). Consequently, $\rho(t'|t)$ satisfies the Chapman-Kolmogorov equation. These properties express the wellknown fact that the microscopic process is Markovian.

## 3. The Macroscopic Joint and Conditional Probabilities

On the macroscopic level, the system is characterized by a set of macrovariables $a=(a_1,\ldots,a_n,\ldots)$ which form the state space $\Sigma$. These macrovariables are the values of phase functions $A\colon \Gamma\to\Sigma$. The reciprocal mapping associates with every point $a\in\Sigma$ a hypersurface $S(a)$ of macroscopically equivalent microstates in $\Gamma$ corresponding to fixed values $A(q)=a$ of the macrovariables.
The mean value of an arbitrary state space function $f(a)$ at time $t$ is given by

$$\langle f(t)\rangle=\int dq\, f(A(q))\,\rho^{(1)}(q,t)$$
$$=\int da\, f(a)\,p^{(1)}(a,t), \tag{3.1}$$

where $p^{(1)}(a,t)$ is the macroscopic single-event probability obtained from $\rho^{(1)}(q,t)$ by means of the coarse-graining operator

$$\mathbf{C}\colon\ \Pi(\Gamma)\to\Pi(\Sigma)$$
$$(\mathbf{C}\,\rho^{(1)}(t))\,(a)=\int dq\,\delta(A(q)-a)\,\rho^{(1)}(q,t)$$
$$=p^{(1)}(a,t). \tag{3.2}$$

This operator averages the microdistribution on every hypersurface $S(a)$.
The time-correlation function of two state space functions $f(a)$, $g(a)$ is given by

$$\langle f(t')\,g(t)\rangle=\int dq'\,dq\, f(A(q'))\,g(A(q))\,\rho^{(2)}(q',t';q,t)$$
$$=\int da'\,da\, f(a')\,g(a)\,p^{(2)}(a',t';a,t) \tag{3.3}$$

where we have introduced the macroscopic joint probability

$$p^{(2)}(a',t';a,t)$$
$$=\int dq'\,dq\,\delta(A(q')-a')\,\delta(A(q)-a)\,\rho^{(2)}(q',t';q,t). \tag{3.4}$$

The macrodistributions $p^{(1)}(t)$ and $p^{(2)}(t',t)$ are elements of the linear manifolds $\Pi(\Sigma)$ and $\Pi(\Sigma\otimes\Sigma)$, respectively. The macroscopic joint probability $p^{(2)}(t',t)$, $t'\geqq t$ and the macroscopic single-event probability $p^{(1)}(t)$ are connected by the macroscopic conditional probability $p(t'|t)$ which is defined for values $a$ with $p^{(1)}(a,t)\neq 0$ by

$$p^{(2)}(a',t';a,t)=p(a',t'|a,t)\,p^{(1)}(a,t). \tag{3.5}$$

In contrast to the microscopic conditional probability $\rho(t'|t)$ given by (2.18), the macroscopic conditional probability is a complicated quantity which depends on the history of the system between the time of preparation $t_0=0$ and the first time of observation $t$, as well as on the preparation itself. To make this explicit, we write (3.4) in the form

$$p^{(2)}(a',t';a,t)=\int dq'\,\delta(A(q')-a')\int dq\,\rho(q',t'|q,t)$$
$$\cdot\,\delta(A(q)-a)\,\rho^{(1)}(q,t), \tag{3.6}$$

where we have used (2.17). Equations (3.5) and (3.6) yield for the conditional probability

$$p(a',t'|a,t)=\int dq'\,\delta(A(q')-a')\int dq\,\rho(q',t'|q,t)$$
$$\cdot\,\delta(A(q)-a)\,w_\sigma(q,t) \tag{3.7}$$

where $w_\sigma(q,t)$ is defined by

$$\rho^{(1)}(q,t)=w_\sigma(q,t)\,p^{(1)}(A(q),t). \tag{3.8}$$

$w_\sigma(q,t)$ is the probability distribution of the microstates $q$ on the hypersurfaces $S(a)$ and is normalized on every hypersurface by

$$\int dq\,\delta(A(q)-a)\,w_\sigma(q,t)=1. \tag{3.9}$$

It will be seen below that $w_\sigma(q,t)$ generally is a different distribution for every stochastic process $(\sigma)$. In this context, the stochastic process is determined by both the Hamiltonian and the initial microdistribution.
Our next aim is an expression for $w_\sigma(q,t)$ in terms of macroscopic quantities. At the initial time $t_0=0$, $w_\sigma(q,0)$ is the statistical weight of macroscopically equivalent microstates resulting from the preparation procedure. $w_\sigma(q,0)$ is identical with $w_\pi(q)$ introduced in (I2.4) and characterizes the preparation classes $(\pi)$.

It also determines the operator $\mathbf{K}_\pi$ defined in (I3.1) by

$$\mathbf{K}_\pi:\ \Pi(\Sigma)\to\Pi(\Gamma)$$

$$(\mathbf{K}_\pi p)(q)=w_\pi(q)\int da\,\delta(A(q)-a)\,p(a) \tag{3.10}$$

as well as the projection operator

$$\mathbf{P}_\pi:\ \Pi(\Gamma)\to\Pi(\Gamma)$$

$$\mathbf{P}_\pi=\mathbf{K}_\pi\mathbf{C},\qquad \mathbf{P}_\pi^2=\mathbf{P}_\pi. \tag{3.11}$$

The operator $\mathbf{K}_\pi$ associates with every macrodistribution $p(a)$ a microdistribution $p(A(q))\,w_\pi(q)$, whereas the operator $\mathbf{P}_\pi$ projects all microdistributions that yield the same macrodistribution $p(a)$ onto a single microdistribution $p(A(q))\,w_\pi(q)$.

We now make use of the representation for $\rho^{(1)}(t)$,

$$\rho^{(1)}(t)=\mathbf{K}_\pi p^{(1)}(t)$$
$$+\int_0^t ds(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)(t-s)}(\mathbf{1}-\mathbf{P}_\pi)\,\mathbf{L}\mathbf{K}_\pi\,p^{(1)}(s) \tag{3.12}$$

which is a consequence of the operator identity (I3.10) and the property (I3.4) of the projection operator $\mathbf{P}_\pi$.

By comparing (3.12) with (3.8) we find

$$w_\sigma(q,t)=w_\pi(q)$$
$$+\frac{\int_0^t ds(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)(t-s)}(\mathbf{1}-\mathbf{P}_\pi)\,\mathbf{L}\,w_\pi(q)\,p^{(1)}(A(q),s)}{p^{(1)}(A(q),t)}. \tag{3.13}$$

This equation determines $w_\sigma(q,t)$ as a functional of the past history of the macroscopic single-event distribution $p^{(1)}(t)$ where the form of the functional depends explicitly on the preparation $(\pi)$. For every initial macrodistribution $p^{(1)}(0)$ we obtain $p^{(1)}(t)$ as a solution of the master equation (I3.15). Hence, $w_\sigma(q,t)$ depends not only on the preparation class $(\pi)$ but also on the initial macrodistribution $p^{(1)}(0)$, i.e. to every stochastic process $(\sigma)$ there will correspond a different function $w_\sigma(q,t)$. There is one exception: For the initial time of preparation $t_0=0$, we have $w_\sigma(q,0)=w_\pi(q)$ which is independent of the initial macrodistribution $p^{(1)}(0)$ and thus depends only on the preparation class $(\pi)$.

From (3.7) we see that the macroscopic conditional probability $p(t'|t)$ depends also on the initial macrodistribution $p^{(1)}(0)$. Consequently, Equation (3.5) which gives the connection between the joint and the single-event probabilities is not a linear relation with respect to $p^{(1)}(t)$. This shows clearly that the Markov property of the microscopic process has been lost by the coarse-graining operation.

With the use of (2.18), Equation (3.7) may be written as

$$p(a',t'|a,t)$$
$$=\int dq\,\delta(A(q)-a')\,e^{\mathbf{L}(t'-t)}\,\delta(A(q)-a)\,w_\sigma(q,t). \tag{3.14}$$

In this equation, part of the irrelevant microscopic dynamics is already eliminated as the dependence of $p(t'|t)$ on the first time of observation $t$ comes solely from the past history of $p^{(1)}(t)$, i.e. from a macroscopic quantity which obeys the master equation (I3.15). In contrast to this, the dependence of $p(t'|t)$ on $(t'-t)$ is still expressed in terms of the microscopic propagator $e^{\mathbf{L}(t'-t)}$. It is the aim of the next Section to eliminate the irrelevant microscopic dynamics completely.

## 4. Equations of Motion for the Macroscopic Joint and Conditional Probabilities

In this Section, we derive exact generalized master equations for the joint and conditional probabilities by means of extended projection-operator techniques. Equation (3.14) shows that the macroscopic conditional probability is the kernel of an operator

$$\mathbf{G}_\sigma(t',t)=\mathbf{C}\,e^{\mathbf{L}(t'-t)}\,\mathbf{K}_\sigma(t) \tag{4.1}$$

acting on $\Pi(\Sigma)$, where $\mathbf{C}$ is the coarse-graining operator (3.2), and $\mathbf{K}_\sigma(t)$ is defined by

$$\mathbf{K}_\sigma(t):\ \Pi(\Sigma)\to\Pi(\Gamma)$$

$$(\mathbf{K}_\sigma(t)\,p)(q)=w_\sigma(q,t)\int da\,\delta(A(q)-a)\,p(a). \tag{4.2}$$

The operator $\mathbf{K}_\sigma(t)$ associates with the macrodistribution $p^{(1)}(a,t)$ the microdistribution $\rho^{(1)}(q,t)=p^{(1)}(A(q),t)\,w_\sigma(q,t)$ of the actual process $(\sigma)$ at time $t$. It has the property

$$\mathbf{C}\mathbf{K}_\sigma(t)=\mathbf{1} \tag{4.3}$$

which allows the introduction of a time-dependent projection operator $\mathbf{P}_\sigma(t)$ defined by

$$\mathbf{P}_\sigma(t):\ \Pi(\Gamma)\to\Pi(\Gamma)$$
$$\mathbf{P}_\sigma(t)=\mathbf{K}_\sigma(t)\,\mathbf{C}$$
$$\mathbf{P}_\sigma(t)\,\mathbf{P}_\sigma(t')=\mathbf{P}_\sigma(t). \tag{4.4}$$

The operator $\mathbf{P}_\sigma(t)$ projects all microdistributions that yield the same macrodistribution $p(a)$ onto a single microdistribution $p(A(q))\,w_\sigma(q,t)$.

The operators $\mathbf{K}_\sigma(t)$ and $\mathbf{P}_\sigma(t)$ are defined in terms of the distribution $w_\sigma(q,t)$ of microstates on the hypersurfaces $S(a)$ which is determined by (3.13) as a preparation ($\pi$)-dependent functional of the past history of the macrodistribution $p^{(1)}(t)$. Thus, every stochastic process ($\sigma$) will in general determine different operators $\mathbf{K}_\sigma(t)$, $\mathbf{P}_\sigma(t)$.

From (4.1) we find

$$\frac{\partial}{\partial t'}\mathbf{G}_\sigma(t',t)=\mathbf{C}\mathbf{L}\,e^{\mathbf{L}(t'-t)}\mathbf{K}_\sigma(t). \tag{4.5}$$

Using

$$(\mathbf{1}-\mathbf{P}_\sigma(t))\,\mathbf{K}_\sigma(t)=0 \tag{4.6}$$

and the operator idendity

$$e^{\mathbf{L}(t'-t)}=\mathbf{P}_\sigma(t)\,e^{\mathbf{L}(t'-t)}+(\mathbf{1}-\mathbf{P}_\sigma(t))\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\sigma(t))(t'-t)}(\mathbf{1}-\mathbf{P}_\sigma(t))+\int_t^{t'} ds(\mathbf{1}-\mathbf{P}_\sigma(t))\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\sigma(t))(t'-s)}(\mathbf{1}-\mathbf{P}_\sigma(t))\,\mathbf{L}\mathbf{P}_\sigma(t)\,e^{\mathbf{L}s} \tag{4.7}$$

we easily get

$$\frac{\partial}{\partial t'}\mathbf{G}_\sigma(t',t)=\boldsymbol{\Omega}_\sigma(t)\,\mathbf{G}_\sigma(t',t)+\int_t^{t'} ds\,\boldsymbol{\Lambda}_\sigma(t'-s,t)\,\mathbf{G}_\sigma(s,t), \tag{4.8}$$

where we have introduced the time-dependent stochastic operators

$$\boldsymbol{\Omega}_\sigma(t)=\mathbf{C}\mathbf{L}\mathbf{K}_\sigma(t) \tag{4.9}$$

and

$$\boldsymbol{\Lambda}_\sigma(s,t)=\mathbf{C}\mathbf{L}(\mathbf{1}-\mathbf{P}_\sigma(t))\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\sigma(t))s}(\mathbf{1}-\mathbf{P}_\sigma(t))\,\mathbf{L}\mathbf{K}_\sigma(t). \tag{4.10}$$

Equation (4.8) determines the time rate of change of $\mathbf{G}_\sigma(t',t)$ in terms of macroscopic stochastic operators acting on $\Pi(\Sigma)$. It has to be solved with the initial condition

$$\mathbf{G}_\sigma(t,t)=\mathbf{1} \tag{4.11}$$

which follows from (4.1).

Equation (4.8) can be written in a more explicit way if the stochastic operators $\boldsymbol{\Omega}_\sigma(t)$ and $\boldsymbol{\Lambda}_\sigma(s,t)$ are transformed in a manner completely analogous to our procedure in I, Section 4 with the stochastic operators $\boldsymbol{\Omega}_\pi$, $\boldsymbol{\Lambda}_\pi(t)$. We then find

$$(\boldsymbol{\Omega}_\sigma(t)\,p)\,(a)=-\sum_j\frac{\partial}{\partial a_j}v_j(a,t)\,p(a) \tag{4.12}$$

and

$$(\boldsymbol{\Lambda}_\sigma(s,t)\,p)\,(a)=\sum_j\frac{\partial}{\partial a_j}\int da'\cdot\left\{\sum_k D_{jk}(a,a';s,t)\frac{\partial}{\partial a'_k}+D_{j0}(a,a';s,t)\right\}p(a'). \tag{4.13}$$

The drift vector $v_j$ and the memory matrix $D_{jk}$ are defined by

$$v_j(a,t)=\int dq\,\delta(A(q)-a)\,w_\sigma(q,t)\,\dot{A}_j(q) \tag{4.14}$$

and

$$D_{jk}(a,a';s,t)=\int dq\,\delta(A(q)-a)\,(\dot{A}_j(q)-v_j(a,t))\cdot e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\sigma(t))s}\,w_\sigma(q,t)\,\delta(A(q)-a')\,(\dot{A}_k(q)-v_k(a',t)), \tag{4.15}$$

respectively, where

$$\dot{A}_j=\{A_j,H\}. \tag{4.16}$$

The memory functions $D_{j0}$ read

$$D_{j0}(a,a';s,t)=\int dq\,\delta(A(q)-a)\,(\dot{A}_j(q)-v_j(a,t))\cdot e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\sigma(t))s}\,w_\sigma(q,t)\,\delta(A(q)-a')\,(\dot{A}_0(q,t)-v_0(a',t)) \tag{4.17}$$

where

$$\dot{A}_0(t)=\{\ln w_\sigma(t),H\} \tag{4.18}$$

and

$$v_0(a,t)=\int dq\,\delta(A(q)-a)\,w_\sigma(q,t)\,\dot{A}_0(q,t)=\sum_k\frac{\partial}{\partial a_k}v_k(a,t). \tag{4.19}$$

With these relations, the equation of motion (4.8) may be written as an evolution equation for the kernel of $\mathbf{G}_\sigma(t',t)$, which coincides with the macroscopic conditional probability by construction. We find

$$\frac{\partial}{\partial t'}p(a',t'|a,t)=-\sum_j\frac{\partial}{\partial a'_j}v_j(a',t)\,p(a',t'|a,t)+\int_t^{t'} ds\sum_j\frac{\partial}{\partial a'_j}\int da''\left\{\sum_k D_{jk}(a',a'';t'-s,t)\frac{\partial}{\partial a''_k}+D_{j0}(a',a'';t'-s,t)\right\}p(a'',s|a,t). \tag{4.20}$$

This equation is the central result of the present work.

Equation (4.20) is an exact generalized master equation for the conditional probability of the non-Markov process under consideration. The initial condition reads

$$p(a', t|a, t)=\delta(a'-a). \qquad (4.21)$$

To deal with this equation, one first has to determine the single-event distribution $p^{(1)}(a,t)$ by solving the master equation (I3.15) for a given initial distribution $p^{(1)}(a,0)$.

The stochastic operators $\boldsymbol{\Omega}_\sigma(t)$, $\Lambda_\sigma(s,t)$ depend both on the preparation class ($\pi$) and the initial single-event probability $p^{(1)}(0)$, i.e. on the stochastic process ($\sigma$). $\boldsymbol{\Omega}_\sigma(t)$ gives an instantaneous contribution to the rate of change of $p(t'|t)$ whereas $\Lambda_\sigma(t'-s,t)$ describes the memory effect of the distribution $p(s|t)$ on the rate of change at time $t'$.

As the stochastic operators do not act on the variable $a$ at time $t$, it is clear that the joint probability $p^{(2)}(a',t';a,t)$ is also a solution of the master equation (4.20), however with the initial condition

$$p^{(2)}(a',t;a,t)=\delta(a'-a)\,p^{(1)}(a,t). \qquad (4.22)$$

The evolution equation (4.20) can be viewed as a generalized Fokker-Planck equation. It gives, depending on the initial condition, the evolution laws of both the joint and the conditional probability for a non-Markov process in the same way as the familiar Fokker-Planck equation does in the theory of Markov processes. There are two kinds of generalizations contained in (4.20), the retardation and the nonlocality in $\Sigma$-space. The retardation is a well-known characteristic of a non-Markov process. The nonlocality is not an additional independent property of (4.20), but is associated with the retardation. The generalized Fokker-Planck equation is nonstationary due to the nonstationarity of the single-event distribution. The special case of a stationary process will be considered in a separate paper.

## 5. Connection with the Time-Evolution of the Macroscopic Single-Event Probability

If we make use of (3.5) and the compatibility relation

$$\int da\, p^{(2)}(a',t';a,t)=p^{(1)}(a',t') \qquad (5.1)$$

we find that the operator $\mathbf{G}_\sigma(t',t)$ has the property

$$p^{(1)}(t')=\mathbf{G}_\sigma(t',t)\,p^{(1)}(t), \qquad t \geqq t'. \qquad (5.2)$$

Thus, $\mathbf{G}_\sigma(t',t)$ is a propagator of the macroscopic single-event probability of the stochastic process. It should be noted, however, that (5.2) does not define $\mathbf{G}_\sigma(t',t)$ uniquely as there are many process-dependent propagators satisfying (5.2) [5]. The propagator $\mathbf{G}_\sigma(t',t)$ is distinguished by the property that its kernel coincides with the conditional probability of the process under consideration.

If we apply the operator relation (4.8) to the single event-probability $p^{(1)}(t)$ and take into account (5.2), we find an evolution equation for $p^{(1)}(t)$

$$\frac{\partial}{\partial t'}p^{(1)}(t')=\boldsymbol{\Omega}_\sigma(t)\,p^{(1)}(t')+\int_t^{t'}\Lambda_\sigma(t'-s,t)\,p^{(1)}(s)\,ds. \qquad (5.3)$$

For $t=0$, (5.3) coincides with the single-event master equation (I3.15), as the stochastic operators $\boldsymbol{\Omega}_\sigma(0)$, $\Lambda_\sigma(t,0)$ are identical with the stochastic operators $\boldsymbol{\Omega}_\pi$, $\Lambda_\pi(t)$ introduced in I. It is only in this special case $t=0$ that the stochastic operators in (5.3) become independent of the initial macrodistribution $p^{(1)}(0)$.

On the other hand, we find for $t'=t$

$$\frac{\partial}{\partial t}p^{(1)}(t)=\boldsymbol{\Omega}_\sigma(t)\,p^{(1)}(t). \qquad (5.4)$$

This is an exact time-convolutionless master equation for the single-event probability with a stochastic operator $\boldsymbol{\Omega}_\sigma(t)$ depending on the stochastic process ($\sigma$), i.e. in particular on the initial macrodistribution $p^{(1)}(0)$. In I we have derived a time-convolutionless master equation

$$\frac{\partial}{\partial t}p^{(1)}(t)=\boldsymbol{\Gamma}_\pi(t)\,p^{(1)}(t) \qquad (5.5)$$

with a stochastic operator $\boldsymbol{\Gamma}_\pi(t)$ depending only on the preparation class ($\pi$) but independent of the initial distribution $p^{(1)}(0)$. In deriving this equation we made use of the inverse of the operator $\mathbf{G}_\sigma(t,0)\equiv\mathbf{G}_\pi(t)$. In general, however, one cannot expect that $\mathbf{G}_\pi(t)$ is a regular operator for all times $t>0$, and the stochastic operator $\boldsymbol{\Gamma}_\pi(t)$ may therefore not always exist [6].

The stochastic operator $\boldsymbol{\Omega}_\sigma(t)$ defines a set of process-dependent time-ordered propagators

$$\Delta_\sigma(t',t)=T\exp\left\{\int_t^{t'}ds\,\boldsymbol{\Omega}_\sigma(s)\right\}, \qquad t'\geqq t \qquad (5.6)$$

satisfying

$$\Delta_\sigma(t'',t')\,\Delta_\sigma(t',t)=\Delta_\sigma(t'',t) \qquad t''\geqq t'\geqq t. \qquad (5.7)$$

From (5.4) we find

$$p^{(1)}(t')=\Delta_\sigma(t',t)\,p^{(1)}(t). \qquad (5.8)$$

The kernel of $\Delta_\sigma(t',t)$ satisfies a Chapman-Kolmogorov-equation according to (5.7) and may formally be considered as the conditional probability of a substitutive Markov process which yields the same single-event behaviour as the process in question. But this Markovian conditional probability has nothing to do with the true conditional probability of the non-Markov process under consideration. In general, the propagators $\mathbf{G}_\sigma(t', t)$ and $\Delta_\sigma(t', t)$ coincide only when they are applied to the single-event probability $p^{(1)}(t)$ of the considered process $(\sigma)$ according to (5.2) and (5.8), respectively.

If $\mathbf{G}_\pi(t)$ is a regular operator, there is another set of time-ordered propagators

$$\mathbf{V}_\pi(t', t) = \mathbf{G}_\pi(t')\,\mathbf{G}_\pi^{-1}(t) \qquad t' \geqq t \tag{5.9}$$

which is generated by $\Gamma_\pi(t)$ and is independent of the initial macrodistribution $p^{(1)}(0)$. In this case we have

$$p^{(1)}(t') = \mathbf{V}_\pi(t', t)\, p^{(1)}(t) \tag{5.10}$$

which holds for every stochastic process $(\sigma)$ belonging to the preparation class $(\pi)$. Again, the kernel of $\mathbf{V}_\pi(t', t)$ satisfies a Chapman-Kolmogorov equation, but has again nothing to do with the conditional probability of the non-Markov process under consideration, i.e. with the kernel of $\mathbf{G}_\sigma(t', t)$. This has not been observed in a recent work of Fox [7]. The propagators $\mathbf{G}_\sigma(t', t)$, on the other hand, do not satisfy an equation like (5.7). We only have

$$\mathbf{G}_\sigma(t'', t')\,\mathbf{G}_\sigma(t', t)\, p^{(1)}(t) = \mathbf{G}_\sigma(t'', t)\, p^{(1)}(t) \tag{5.11}$$

where $p^{(1)}(t)$ is the single-event probability of the considered process $(\sigma)$. In this equation, $p^{(1)}(t)$ cannot be canceled because of the dependence of $\mathbf{G}_\sigma(t', t)$ on $p^{(1)}(0)$. This fact shows the non-Markovian property of the process most clearly.

## Conclusions

We have studied the time-evolution of a closed macroscopic system from a purely microscopic point of view. Starting from hamiltonian microdynamics, we have derived an exact generalized master equation for the macroscopic conditional probability $p(t'|t)$ (4.8, 4.20) which is also satisfied by the macroscopic joint probability $p^{(2)}(t', t)$. The stochastic operators in this equation depend explicitly on the distribution $w_\sigma(t)$ over macroscopically equivalent microstates, which has been calculated in (3.13) as a preparation-dependent functional of the past history of the macroscopic single-event probability $p^{(1)}(t)$. Thus, in order to construct the master equation, one has first to solve the master equation for the macroscopic single-event probability $p^{(1)}(t)$ for a given process $(\sigma)$, i.e. for a given preparation class $(\pi)$ and a given initial condition $p^{(1)}(0)$ (Eq. (I3.15)), substitute the solution into (3.13) to obtain $w_\sigma(t)$, then form the operators $\mathbf{K}_\sigma(t)$ (4.2) and $\mathbf{P}_\sigma(t)$ (4.4), and finally the stochastic operators $\boldsymbol{\Omega}_\sigma(t)$ (4.9) and $\Lambda_\sigma(t, s)$ (4.10).

The dependence on the initial macrodistribution $p^{(1)}(0)$ reflects the non-Markovian character of the macroscopic stochastic process.

This procedure permits in principle the exact calculation of arbitrary macroscopic two-time correlation functions without solving the microscopic equations of motion, in the same way as the Nakajima-Zwanzig theory [1, 2] for the single-event probability $p^{(1)}(t)$ permits the calculation of arbitrary macroscopic single-time averages. It is evident that the calculation of higher-order correlation functions requires the construction of generalized master equations for higher-order joint probabilities, which will depend on the solution of all lower-order equations.

From the master equation for the joint probability $p^{(2)}(t', t)$, various forms for the time-evolution equation of the macroscopic single-event probability $p^{(1)}(t)$ can be obtained. In particular, there exist single-event propagators (process-dependent: $\Delta_\sigma(t', t)$ (5.6); under a regularity assumption even process-independent: $\mathbf{V}_\pi(t', t)$ (5.9)) with kernels satisfying the Chapman-Kolmogorov equation, in spite of the fact that the process is non-Markovian. Further, there exist single-event master equations with a memory kernel (5.3) and time-convolutionless master equations (5.4, 5.5). This illustrates again the fact stressed in [5] that the Markovian or non-Markovian character of a process cannot be decided on the basis of time-evolution equations for the single-event probability: Neither the existence of a single-event propagator with a kernel satisfying the Chapman-Kolmogorov equation nor the existence of a time-convolutionless single-event master equation imply a Markovian character of the process. Thus, the kernel of a single-event propagator should not be used for the calculation of time-correlation functions for general times $t', t > 0$ without independent proof that the process is (at least approximately) Markovian. A necessary condition for Markovian character is provided by the generalized master equation for the conditional probability $p(t'|t)$ derived in the present paper: In order for the process to be Markovian, the stochastic operators $\boldsymbol{\Omega}_\sigma(t)$ and $\Lambda_\sigma(s, t)$ must be independent of the process $(\sigma)$ in a given preparation class $(\pi)$. In this context, a quantitative measure for the deviation from Markovian behaviour would be very helpful.

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