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Microdynamics and Time-Evolution of Macroscopic Non-Markovian Systems

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The time evolution of the single event probability of macroscopic variables is studied from a microscopic point of view. The explicit consideration of the preparation of the initial microdistribution leads to a unique decomposition of the macrodynamics into two parts, a local and instantaneous one and a nonlocal and retarded one. In this retarded, i.e., non-Markovian master equation no inhomogeneity occurs in contrast to previous approaches. It is shown that the retarded master equation can exactly be transformed into a time-convolutionless and homogeneous form $\dot{p}(t)=\Gamma(t)\,p(t)$, which generates a substitutive Markov process with the same single event behaviour as the process in question.

1. Introduction

The time evolution of macrovariables of a system can be described successfully within the theory of stochastic processes. The Markov approximation obtained through a coarse graining in time has been used extensively in this field, e.g., in the theory of collective phenomena [1]. Loosely speaking the Markov property states that the process has no memory of the past for a known present. This fact yields that, in general, the sample functions are not differentiable [2]. Therefore, realistic physical processes are, in general, at best approximative Markov processes.

The non-Markovian behaviour becomes important in transport problems in solids and fluids for short times [3–5] as well as in the theory of critical phenomena [6], in problems of quantum optics [7, 8] and for the study of initial condition effects [9, 10]. Even the long time behaviour of certain correlation functions is influenced by non-Markovian effects [5, 10].

The stochastic properties of systems are characterized by a probability distribution $p(a,t)$ in the space Σ of macrovariables $a=(a_1,a_2\ldots)$ and by higher joint probabilities. The non-Markovian time evolution of these probabilities has been treated in a recent paper [11] with interesting results. In this paper we investigate the time evolution of $p(a,t)$ from a microscopic point of view.

As the stochastic process of the macrovariables depends on the microscopic dynamics together with the initial microscopic distribution we introduce in Section 2 a concept of preparation classes (π) specifying the essential information about the initial microscopic state $\rho(0)$, that means about the preparation procedure of this state. Every preparation class corresponds to a different stochastic process of the macrovariables a.

In Section 3 we derive an exact generalized master equation for the single-event probability $p(a,t)$ by means of the projection operator method [12, 13]. So far several generalized master equations have been derived using different projection operators [12–17]. All these equations lead, in general, to an inhomogeneity and thus have not the form expected from the theory of stochastic processes [11]. We introduce a projection operator leading to a master equation without an inhomogeneity. By this property the projection operator is uniquely defined and depends on the preparation class (π), hence, manifesting explicitely the dependence of the stochastic process on the preparation.

In Section 4 properties of the operators occurring in the derived master equation are discussed. We obtain an integral equation for the memory function which is useful for perturbative evaluations. In Section 5 we transform the master equation into an equivalent time-convolutionless form

$$\dot{p}(t)=\Gamma_\pi(t)\,p(t), \tag{1.1}$$

where the stochastic operator $\Gamma_\pi(t)$ is the generator of a substitutive Markov process with the same single event behaviour as the process in question. This property of the stochastic operator does not hold for time-convolutionless master equations containing inhomogeneities [18–20].

In Section 6, we summarize the important features of the results obtained.

2. Initial Distribution and Preparation Classes

In this paper we restrict ourselves to classical statistical mechanics. On the microscopic level the system is described by a microdistribution $\rho(q)$, where $q=(q_1,\ldots,q_\alpha,\ldots)$ is a point in the phase space Γ. $\rho(q)$ is an element of the linear manifold $\Pi(\Gamma)$ of absolutly integrable functions. On the macroscopic level the system is characterized by a set of macrovariables $a=(a_1,\ldots,a_n,\ldots)$ forming the state space Σ. These macrovariables are phase functions $A(q)$ and define hyper-surfaces $S(a)$ with fixed values $A(q)=a$ in Γ. The macrodistribution $p(a)$ is an element of $\Pi(\Sigma)$ and is obtained from $\rho(q)$ by means of a coarse graining operator

$$\mathbf{C}\colon\ \Pi(\Gamma)\to\Pi(\Sigma)$$

$$p(a)=(\mathbf{C}\rho)(a)=\int dq\, C(a;q)\,\rho(q) \tag{2.1}$$

where

$$C(a;q)=\delta(A(q)-a). \tag{2.2}$$

$p(a)$ yields correct mean values for functions of the macrovariables

$$\int dq\, f(A(q))\,\rho(q)=\int da\, f(a)\,p(a). \tag{2.3}$$

We introduce the conditional probability

$$w(q|A(q))=\frac{\rho(q)}{p(A(q))}\equiv w(q) \tag{2.4}$$

which gives the distribution of the microstates q on a known hyper-surface $S(A(q))$. $w(q|A(q))$ is normalized on every surface $S(a)$

$$\int dq\,\delta(A(q)-a)\,w(q|A(q))=1. \tag{2.5}$$

The initial microdistribution $\rho(0)$ at time $t_0=0$ is a result of the preparation procedure; its determination is, in general, itself a complicated problem of statistical mechanics. To prepare an ensemble of physical systems in a reproducible way one usually has to start with a time-translation invariant state characterized by a set of parameters λ, e.g., temperature of reservoirs, external fields, etc. Afterwards, one breaks this symmetry by a well defined external operation at time t_0, e.g., by switching on or off an interaction.

Using the conditional probability defined in (2.4) we may decompose the initial microdistribution $\rho(0)$ according to

$$\rho(q,0)=w_\pi(q|A(q))\,p(A(q),0). \tag{2.6}$$

The macrodistribution p represents the information controlled by the experiment for times $t\geqq t_0$, whereas the initial conditional probability w_π contains the additional information about the preparation (π) and therefore depends on the parameters λ.

Let us now introduce preparation classes (π) of initial microdistributions $\rho(0)$ leading to the same conditional probability. As a first example we consider a physical system which is initially in a thermodynamic equilibrium state described by

$$\rho_\beta(q,0)=Z^{-1}\,e^{-\beta(H(q)+H'(A(q)))}, \tag{2.7}$$

where $H'(A(q))$ describes the coupling of the macrovariables to external fields. At time $t_0=0^-$ these fields are switched off.

From Equation (2.7) we derive using (2.4)

$$w_\pi(q)=\frac{e^{-\beta H(q)}}{\int dq'\,\delta(A(q)-A(q'))\,e^{-\beta H(q')}}. \tag{2.8}$$

We see that this preparation class includes all types of couplings to external fields via macrovariables and depends only on the temperature.

Considering a subsystem described by the variables $A(q)$ which is brought at time t_0 into interaction with reservoirs with steady distributions $\phi_j(B_j(q))$ we get for the conditional probability $w_\pi(q)$ from

$$\rho(q,0)=p(A(q),0)\prod_j\phi_j(B_j(q)) \tag{2.9}$$

$$w_\pi(q)=\prod_j\phi_j(B_j(q)). \tag{2.10}$$

This preparation class depends only on the parameters fixing the steady reservoir distributions.

3. Equation of Motion for $p(a,t)$

In this section we derive an exact generalized master equation for the macrodistribution $p(a,t)$ by means of the projection operator technique [12–14]. For every preparation class (π) we introduce an operator

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

$$(\mathbf{K}_\pi f)(q)=\int da\, K_\pi(q;a)\,f(a) \tag{3.1}$$

where

$$K_\pi(q;a)=w_\pi(q)\,\delta(A(q)-a). \tag{3.2}$$

From Equation (2.6) we derive the relation

$$\rho(0)=\mathbf{K}_\pi\,p(0) \tag{3.3}$$

which holds for the initial distributions. The operator $\mathbf{K}_\pi$ blows up the coarse-grained initial distribution $p(0)$ to the correct initial microdistribution $\rho(0)$.
Together with (2.1) this equation yields

$$\rho(0)=\mathbf{P}_\pi\,\rho(0) \tag{3.4}$$

where we have introduced the projection operator

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

$$\mathbf{P}_\pi=\mathbf{K}_\pi\mathbf{C};\quad \mathbf{P}_\pi^2=\mathbf{P}_\pi. \tag{3.5}$$

The second relation follows from

$$\mathbf{C}\mathbf{K}_\pi=\mathbf{1}. \tag{3.6}$$

The projection operator $\mathbf{P}_\pi$ maps the space $\Pi(\Gamma)$ of microdistributions onto the subspace of distributions belonging to the preparation class (π) in question and is *uniquely* determined by the initial microdistribution. For special preparation classes (π) the projectors introduced by several authors [14–17] are obtained.
From the Liouville equation

$$\dot\rho(t)=\{H,\rho(t)\}\equiv\mathbf{L}\rho(t) \tag{3.7}$$

$$\rho(t)=e^{\mathbf{L}t}\,\rho(0) \tag{3.8}$$

for the microdistribution $\rho(t)$ where H is the Hamiltonian and $\{\,,\}$ denotes the Poisson bracket we have

$$\dot p(t)=\mathbf{C}\dot\rho(t)=\mathbf{C}\mathbf{L}\,e^{\mathbf{L}t}\,\rho(0). \tag{3.9}$$

Using the identity

$$e^{\mathbf{L}t}=\mathbf{P}_\pi\,e^{\mathbf{L}t}+(\mathbf{1}-\mathbf{P}_\pi)\;e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)t}(\mathbf{1}-\mathbf{P}_\pi)$$
$$+\int_0^t ds(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)(t-s)}(\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{P}_\pi\,e^{\mathbf{L}s} \tag{3.10}$$

which can be verified by differentiation, Equation (3.9) yields for the rate of change of the macrodistribution

$$\dot p(t)=\mathbf{C}\mathbf{L}\mathbf{K}_\pi\,p(t)$$
$$+\int_0^t ds\,\mathbf{C}\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)(t-s)}(\mathbf{1}-\mathbf{P}_\pi)\,\mathbf{L}\mathbf{K}_\pi\,p(s). \tag{3.11}$$

Here we have used

$$\mathbf{P}_\pi\,e^{\mathbf{L}t}\,\rho(0)=\mathbf{K}_\pi\,p(t) \tag{3.12}$$

and (3.4) which has the consequence that in the master equation (3.11) no inhomogeneity occurs.

Introducing the stochastic operator defined on $\Pi(\Sigma)$

$$\boldsymbol{\Omega}_\pi=\mathbf{C}\mathbf{L}\mathbf{K}_\pi \tag{3.13}$$

$$\boldsymbol{\Lambda}_\pi(t)=\mathbf{C}\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)t}(\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{K}_\pi. \tag{3.14}$$

Equation (3.11) reads

$$\dot p(t)=\boldsymbol{\Omega}_\pi\,p(t)+\int_0^t ds\,\boldsymbol{\Lambda}_\pi(t-s)\,p(s). \tag{3.15}$$

This equation is an exact master equation for the single-event distribution of the non-Markov process in consideration. To stochastic operators $\boldsymbol{\Omega}_\pi$, $\boldsymbol{\Lambda}_\pi(t)$ depend on the preparation class (π) thus showing explicitly the dependence of the stochastic process on the preparation. $\boldsymbol{\Omega}_\pi$ gives the instantaneous contribution to the rate of change of $p(t)$ whereas $\boldsymbol{\Lambda}_\pi(t-s)$ describes the influence of the memory for former times s.

4. Properties of the Stochastic Operators

In this section an exact integral equation for $\boldsymbol{\Lambda}_\pi(t)$ is derived. More explicit expressions for the stochastic operators are given.
From the definition (3.14) of the stochastic operator $\boldsymbol{\Lambda}_\pi(t)$ we see that its calculation involves the solution of a problem with the unusual propagator $e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)t}$. Often, this is one of the main problems of a microscopic approach. In such a case one might overcome this difficulty by means of an exact integral equation for the memory function following from the identity

$$(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)t}(\mathbf{1}-\mathbf{P}_\pi)=(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}t}(\mathbf{1}-\mathbf{P}_\pi)$$
$$-\int_0^t ds(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)(t-s)}(\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{P}_\pi\,e^{\mathbf{L}s}(\mathbf{1}-\mathbf{P}_\pi). \tag{4.1}$$

Using (3.14) this relation yields

$$\boldsymbol{\Lambda}_\pi(t)=\boldsymbol{\Lambda}_\pi^0(t)-\int_0^t ds\,\boldsymbol{\Lambda}_\pi(t-s)\,\boldsymbol{\Xi}_\pi(s) \tag{4.2}$$

where

$$\boldsymbol{\Lambda}_\pi^0(t)=\mathbf{C}\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)\,e^{\mathbf{L}t}(\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{K}_\pi \tag{4.3}$$

$$\boldsymbol{\Xi}_\pi(t)=\mathbf{C}\,e^{\mathbf{L}t}(\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{K}_\pi. \tag{4.4}$$

These stochastic operators do not contain the unusual propagator $e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)t}$.
By differentiation we see that $\boldsymbol{\Xi}_\pi(t)$ obeys the differential equation

$$\dot{\boldsymbol{\Xi}}_\pi(t)=\mathbf{C}\mathbf{L}\,e^{\mathbf{L}t}(\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{K}_\pi$$
$$=\boldsymbol{\Lambda}_\pi^0(t)+\boldsymbol{\Omega}_\pi\boldsymbol{\Xi}_\pi(t) \tag{4.5}$$

with the initial condition

$$\boldsymbol{\Xi}_\pi(0)=\mathbf{C}(\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{K}_\pi=\mathbf{0}, \tag{4.6}$$

where we have used Equations (3.5), (3.6) and (3.13). Introducing the free propagator

$$\mathbf{G}_\pi^0(t) = e^{\mathbf{\Omega}_\pi t} \tag{4.7}$$

the solution of the inhomogeneous Equation (4.5) reads

$$\mathbf{\Xi}_\pi(t) = \int_0^t ds\, \mathbf{G}_\pi^0(t-s) \mathbf{\Lambda}_\pi^0(s). \tag{4.8}$$

The kernels of the stochastic operators $\mathbf{\Omega}_\pi$ and either $\mathbf{\Lambda}_\pi(t)$ or $\mathbf{\Lambda}_\pi^0(t)$ have to be calculated within the microscopic theory in an appropriate approximation. Afterwards, the remaining stochastic operators may be evaluated by means of the purely macroscopic relations (4.2), (4.7) and (4.8).

Now we give expressions for $\mathbf{\Omega}_\pi$, $\mathbf{\Lambda}_\pi(t)$ and $\mathbf{\Lambda}_\pi^0(t)$ which are more useful both for physical interpretations and for approximative evaluations. The Poisson-bracket structure of the Liouvillian $\mathbf{L}$ leads to

$$\int dq\, \psi(q) \mathbf{L} \varphi(q) = -\int dq\, \varphi(q) \mathbf{L} \psi(q). \tag{4.9}$$

Inserting the definitions (2.1), (3.1) into Equation (3.13) we find

$$(\mathbf{\Omega}_\pi f)(a) = \int dq\, \delta(A(q)-a) \mathbf{L} w_\pi(q) f(A(q)) \tag{4.10}$$

which holds for every $f \in \Pi(\Sigma)$.

With the help of (4.9) and the relation

$$\mathbf{L}\delta(A(q)-a) = -\sum_j \frac{\partial}{\partial a_j} \delta(A(q)-a) \mathbf{L} A_j(q) \tag{4.11}$$

we derive

$$(\mathbf{\Omega}_\pi f)(a) = -\sum_k \frac{\partial}{\partial a_k} v_k(a) f(a). \tag{4.12}$$

The drift vector is given by

$$v_j(a) = \int dq\, \delta(A(q)-a) w_\pi(q) \dot{A}_j(q) \tag{4.13}$$

where

$$\dot{A}_j(q) = -\mathbf{L} A_j(q) = \{A_j(q), H(q)\}. \tag{4.14}$$

Transforming $\mathbf{\Lambda}_\pi(t)$ in the same manner we derive the following expression

$$(\mathbf{\Lambda}_\pi(t) f)(a) = \sum_j \frac{\partial}{\partial a_j} \int da' \cdot \left\{ \sum_k D_{jk}(a, a'; t) \frac{\partial}{\partial a_k'} + D_{j0}(a, a'; t) \right\} f(a'). \tag{4.15}$$

The same expression holds for $\mathbf{\Lambda}_\pi^0(t)$ if D_{jk} is replaced by D_{jk}^0.

The details of the calculation and the definitions of the matrices D and D^0 are outlined in the Appendix.

The free propagator defined in (4.7) fulfills the forward equation

$$\dot{\mathbf{G}}_\pi^0(t) = \mathbf{\Omega}_\pi \mathbf{G}_\pi^0(t). \tag{4.16}$$

This equation can easily be solved if the solutions of the pure drift-motion

$$\dot{a}_j(t) = v_j(a(t)) \tag{4.17}$$

are known leading to

$$(\mathbf{G}_\pi^0(t) f)(a) = \int da'\, \delta(a - a'(t)) f(a'). \tag{4.18}$$

Obviously this propagator describes fluctuations only by randomness contained in the initial distribution. Hence, it is the deterministic part of the exact propagator $\mathbf{G}_\pi(t)$ treated in the next section. The fluctuating motion is due to the memory effects described by the stochastic operator $\mathbf{\Lambda}_\pi(t)$.

5. Stochastic Process and Substitutive Markov Process

It is shown that for any non-Markov process there exists a substitutive Markov process with the same single-event behaviour.

Let us introduce the propagator $\mathbf{G}_\pi(t)$ satisfying the integrodifferential equation

$$\dot{\mathbf{G}}_\pi(t) = \mathbf{\Omega}_\pi \mathbf{G}_\pi(t) + \int_0^t ds\, \mathbf{\Lambda}_\pi(t-s) \mathbf{G}_\pi(s) \tag{5.1}$$

with

$$\mathbf{G}_\pi(0) = \mathbf{1}.$$

Then the solution of (3.15) reads

$$p(t) = \mathbf{G}_\pi(t) p(0). \tag{5.2}$$

From this equation we derive for the rate of change of the macrodistribution $p(t)$ the time-convolutionless master equation

$$\dot{p}(t) = \mathbf{\Gamma}_\pi(t) p(t) \tag{5.3}$$

where

$$\mathbf{\Gamma}_\pi(t) = \dot{\mathbf{G}}_\pi(t) \mathbf{G}_\pi^{-1}(t). \tag{5.4}$$

Equation (5.3) is an exact transformation of the master equation with memory (3.15). Time-convolutionless master equations have yet been derived by several authors [18–20]. However, only the explicit consideration of the preparation (π) leads to the homogeneous form (5.3) and determines the generator $\mathbf{\Gamma}_\pi(t)$ of the infinitesimal time shift of the process.

$\mathbf{\Gamma}_\pi(t)$ defines a semigroup of time-ordered propagators $\mathbf{V}_\pi(t_2|t_1)$

$$\mathbf{V}_\pi(t_2|t_1) = \mathbf{T} \exp\left\{ \int_{t_1}^{t_2} ds\, \mathbf{\Gamma}_\pi(s) \right\} = \mathbf{G}_\pi(t_2) \mathbf{G}_\pi^{-1}(t_1) \tag{5.5}$$

where

$$t_2 \geqq t_1, \qquad \mathbf{V}_\pi(t^+|t) = \mathbf{1}.$$

This semigroup determines the macrodistribution $p(t_2)$ if $p(t_1)$ is known for an arbitrary time $t_1 \leqq t_2$ according to

$$p(t_2) = \mathbf{V}_\pi(t_2|t_1)\, p(t_1). \tag{5.6}$$

Formally, $\mathbf{V}_\pi(t_2|t_1)$ may be considered as the conditional probability of a substitutive* non-stationary Markov process [21]. By construction, the substitutive Markov process yields the same single-event behaviour as the process in question and its conditional probability $V_\pi(a_2 t_2|a_1 t_1)$ determines the time evolution of $p(a_1 t_1)$. However, this Markovian condition probability is, in general, not identical with the conditional probability of the non-Markov process under consideration [11].

In the non-Markovian system the conditional probability depends on the history. There is one exception: relating back to the initial time of preparation $t_0 = 0$ the system has no memory for previous times $t \leqq t_0$. Hence, $V_\pi(at|a't' = 0)$, which is identical with the kernel $G_\pi(a, a'; t)$ of the propagator $\mathbf{G}_\pi(t)$, coincides with the initial conditional probability of the process and allows for the calculation of initial correlation functions

$$\langle f_2(t)\, f_1(0)\rangle = \int da\, da' f_2 a)\, f_1(a')\, G_\pi(a, a'; t)\, p(a', 0). \tag{5.7}$$

In accordance with this interpretation the kernel of $\mathbf{G}_\pi(t)$ may be written as

$$G_\pi(a, a'; t) = \int dq\, \delta(A(q) - a)\, e^{\mathbf{L}t}\, \delta(A(q) - a')\, w_\pi(q). \tag{5.8}$$

Suppose that the class of initial distributions belonging to the preparation (π) contains a stationary microdistribution $\rho_{\mathrm{st}} = e^{\mathbf{L}t}\rho_{\mathrm{st}}$. In that case we have

$$w_\pi(q) = \frac{\rho_{\mathrm{st}}(q)}{p_{\mathrm{st}}(A(q))}. \tag{5.9}$$

Then, Equation (5.8) shows that $G_\pi(a, a'; t)$ is the stationary conditional probability. For instance, this is the case with the preparation (2.8), but not with the preparation (2.10).

6. Conclusions

We considered the stochastic process of macrovariables from a microscopic point of view and took the preparation explicitly into account. To determine the stochastic process the preparation procedure is of the same importance as the underlying microdynamics. To describe the preparation effects we introduced a concept of preparation classes (π) characterized by an initial conditional probability w_π (2.4) which determines the statistical weight of macroscopically equivalent microstates.

We derived a master equation for the single-event probability $p(a, t)$ by means of well known projection-operator techniques. However, in contrast to usual exact equations of motion we obtained a decomposition of the rate of change of $p(a, t)$ into two parts only, an instantaneous and a memory contribution. The absence of a third contribution, the usually appearing inhomogeneity, leads to a unique decomposition of the macroscopic dynamics. We showed that the homogeneous master equation can exactly be transformed into a time-convolutionless form (5.3) where the new stochastic operator $\boldsymbol{\Gamma}_\pi(t)$ is the generator of a substitutive time-inhomogeneous Markov process.

So far we have been concerned with exact results only. The exact master equation may be written as

$$\frac{\partial}{\partial t} p(a, t) = -\sum_j \frac{\partial}{\partial a_j} v_j(a)\, p(a, t) + \int_0^t ds \sum_j \frac{\partial}{\partial a_j} \int da' \cdot \left\{ \sum_k D_{jk}(a, a', t-s) \frac{\partial}{\partial a'_k} + D_{j0}(a, a', t-s) \right\} p(a', s) \tag{6.1}$$

and approximations mainly concern the evaluation of the rather involved formal expression (A.8) for the matrix D. It should be noted that the quality of an approximation is strongly influenced by the preparation. For instance, in many cases we may neglect retardation effects in the master equation (usually referred to as Markov approximation), whereas this approximation cannot be adequate for the time-reversed process governed by the same master equation (6.1) with a different preparation (π), however. This preparation effect is apparent in our theory as the stochastic operators depend on the preparation explicitly.

The vast variety of conceivable initial microdistributions is reduced drastically if only experimentally accessible ones, i.e., reproducible preparations are taken into account. Then the preparation itself is a macroscopic process and, hence, the variable $A_0(q)$ introduced in Equation (A.3) usually has the property of a macrovariable that means it varies only slowly in time.

Considering the rates of change of the macrovariables (including A_0) as small one obtains a perturbative approach to the matrix D. To make this approach systematic we may split the Liouvillian $\mathbf{L}$

* It should be noted that, in general, the kernel $\mathbf{V}_\pi(a_2 t_2|a_1 t_1)$ may contain negative elements such that $\mathbf{V}_\pi(t_2|t_1)$ describes a pseudo-Markov process with negative transition probabilities. Nevertheless, $p(a, t)$ is a non-negative function

into two parts

$$\mathbf{L}=\mathbf{L}_0+\mathbf{L}_1 \tag{6.2}$$

so that $\mathbf{L}_0$ describes the fast motion within a surface of fixed values $A(q)=a$, $A_0(q)=a_0$ of the macrovariables, whereas $\mathbf{L}_1$ is the slow motion orthogonal to these surfaces. Afterwards one expands D into powers of $\mathbf{L}_1$.

D is at least of second order in $\mathbf{L}_1$ by definition. In the lowest approximation D coincides with D^0 and is local in Σ space,

$$D_{jk}(a,a';t)=D^0_{jk}(a,a',t)$$
$$=\delta(a-a')D^{\mathrm{L}}_{jk}(a,t). \tag{6.3}$$

Using the definition (A.10) of the matrix D^0, we see that an approximative locality in Σ space of D^0 can only be established if the macrovariables do not change appreciably within the memory time. On the other hand this is the property of macrovariables needed to justify the Markov approximation (locality in time). Hence, Equation (6.1) is approximated consistently in the lowest order by the Fokker-Planck equation. It seems that whenever memory effects are important the nonlocality of D has to be taken into account too. The derivation of an exact homogeneous master equation given in the present paper may easily be generalized to systems in interaction with time-dependent external forces or fields, governed by a time-dependent Liouville operator $\mathbf{L}(t)$. Furtheron, if one has already a description of a system by a reduced set of variables whose probability distribution obeys an instantaneous master equation, a further reduction of the set of variables (second coarse graining) may be done in principle by the same method.

So far, we have considered only the single-event probability $p(a,t)$. A microscopic derivation of the equations of motion for the multivariate probability distributions $p^{(n)}(t_1,\ldots,t_n)$ will be given in a forthcoming publication.

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Appendix

Derivation of Equation (4.15)

Using (4.9). (4.11–13) we get

$$(\mathbf{CL}(\mathbf{1}-\mathbf{P}_\pi)\phi)(a)=(\mathbf{CL}\phi)(a)-(\boldsymbol{\Omega}_\pi\mathbf{C}\phi)(a)$$
$$=-\sum_j\frac{\partial}{\partial a_j}\int dq\,\delta(A(q)-a)(\dot{A}_j(q)-v_j(a))\,\phi(q). \tag{A.1}$$

Furtheron, with definition (3.1) of $\mathbf{K}_\pi$ we derive

$$((\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{K}_\pi f)(q)=(\mathbf{L}\mathbf{K}_\pi f)(q)-(\mathbf{K}_\pi\boldsymbol{\Omega}_\pi f)(q)$$
$$=\int da'\left\{\mathbf{L}w_\pi(q)\,\delta(A(q)-a')\right.$$
$$\left.+\sum_k w_\pi(q)\,\delta(A(q)-a')\frac{\partial}{\partial a'_k}v_k(a')\right\}f(a'). \tag{A.2}$$

Introducing the variable

$$A_0(q)=\ln w_\pi(q) \tag{A.3}$$

we may write (A.2) by means of

$$\mathbf{L}w_\pi(q)\,\delta(A(q)-a')$$
$$=w_\pi(q)\left\{\sum_k\frac{\partial}{\partial a'_k}\delta(A(q)-a')\,\dot{A}_k(q)\right.$$
$$\left.-\delta(A(q)-a')\,\dot{A}_0(q)\right\} \tag{A.4}$$

in the form

$$((\mathbf{1}-\mathbf{P}_\pi)\mathbf{L}\mathbf{K}_\pi f)(q)=-\int da'\,w_\pi(q)\,\delta(A(q)-a')$$
$$\cdot\left\{\sum_k(\dot{A}_k(q)-v_k(a'))\frac{\partial}{\partial a'_k}+(\dot{A}_0(q)-v_0(a'))\right\}f(a') \tag{A.5}$$

where

$$v_0(a)=\sum_k\frac{\partial}{\partial a_k}v_k(a)$$
$$=\int dq\,\delta(A(q)-a)\,w_\pi(q)\,\dot{A}_0(q). \tag{A.6}$$

Here we have used Equations (4.11), (4.13) and (A.3). The definition (3.14) of $\Lambda_\pi(t)$ yields together with (A.1), (A.5)

$$(\Lambda_\pi(t)f)(a)=\sum_j\frac{\partial}{\partial a_j}\int da'\cdot\left\{\sum_k D_{jk}(a,a';t)\frac{\partial}{\partial a'_k}\right.$$
$$\left.+D_{j0}(a,a';t)\right\}f(a') \tag{A.7}$$

where the matrix D is determined by

$$D_{jk}(a,a';t)=\int dq\,\delta(A(q)-a)(\dot{A}_j(q)-v_j(a))$$
$$\cdot e^{\mathbf{L}(\mathbf{1}-\mathbf{P}_\pi)t}w_\pi(q)\,\delta(A(q)-a')(\dot{A}_k(q)-v_k(a')). \tag{A.8}$$

On the other hand the definition (4.3) of $\Lambda^0_\pi(t)$ leads in the same manner to

$$(\Lambda_\pi{}^0(t)f)(a)=\sum_j\frac{\partial}{\partial a_j}\int da'\left\{\sum_k D^0_{jk}(a,a';t)\frac{\partial}{\partial a'_k}\right.$$
$$\left.+D^0_{j0}(a,a',t)\right\}f(a') \tag{A.9}$$

where the matrix D^0 is defined by

$$D^0_{jk}(a,a';t)=\int dq\,w_\pi(q)\,\delta(A(q)-a')(\dot{A}_k(q)-v_k(a'))$$
$$\cdot e^{-\mathbf{L}t}\,\delta(A(q)-a)(\dot{A}_j(q)-v_j(a)). \tag{A.10}$$

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