Time Evolution, Correlations, and Linear Response of Non-Markov Processes *

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We investigate the time evolution of stochastic non-Markov processes as they occur in the coarse-grained description of open and closed systems. We show that semigroups of propagators exist for all multivariate probability distributions, the generators of which yield a set of time-convolutionless master equations. We discuss the calculation of averages and time-correlation functions. Further, linear response theory is developed for such a system. We find that the response function cannot be expressed as an ordinary time-correlation function. Some aspects of the theory are illustrated for the two-state process and the Gauss process.

1. Introduction

The stochastic behaviour of the coarse-grained variables of a system is described in general as a stochastic process with memory (non-Markov process) [1-3]. The Markov approximation, obtained by a coarse-graining in time, has been extensively used in the theory of collective phenomena far from thermodynamic equilibrium (see e.g. [4]). The interest in non-Markov behaviour has been renewed because of its relevance to certain non-equilibrium phase-transition phenomena [5, 6], and to transport problems in solids and fluids [7-9]. This question has been discussed in particular in context with the long-time behaviour of certain time-correlation functions in fluids [8-10].

The stochastic properties of the system are characterized by a probability distribution $p(\mathbf{x}\,t)$ in the space Σ of coarse-grained macrovariables $\mathbf{x} = (x_1, x_2 \,...)$ of the system. The microscopic degrees of freedom as well as the bath variables are eliminated by applying projector methods to the microscopic Liouville-von Neumann equation [1-3]. If the system is prepared at an initial time $t = t_0$ with probability distribution $p_0(\mathbf{x})$ without any correlations between the macrovariables $\mathbf{x}$ and the rest of the system, the rate of change of the probability distribution $p(t)$ is found

to be given by the stochastic equation

$$\frac{dp(t)}{dt} = \int_{t_0}^{t} A(t|s)\, p(s)\, ds. \qquad (1.1)$$

Here, the "retarded kernel" $A(t|s)$ is an operator acting on the space Π of probability distributions*. It describes the memory effect of the distribution at time s on the rate of change at time t, and may contain a Markov contribution $A^{\text{Markov}}(t|s) = \Gamma(t)\,\delta(t - s - 0^+)$. This equation has the formal solution

$$p(t) = G(t|t_0)\, p_0 \qquad (t \geq t_0) \qquad (1.2)$$

where the Green's function $G(t|t_0)$ is defined by the equation

$$\frac{dG(t|t_0)}{dt} = \int_{t_0}^{t} A(t|t')\, G(t'|t_0)\, dt' \qquad (1.3)$$

with the initial condition $G(t_0^+|t_0) = \mathbb{1}$.

* Here and in the following, we use the following notation: $p(t)$ denotes an element of function space Π with values $p(\mathbf{x}\,t)$. Elements like $A(t|s)$ are operators acting on Π, with integral kernel $A(\mathbf{x}\,t|\mathbf{y}\,s)$ which may contain δ-functions and their derivatives. Application of an operator to an element of function space, and operator multiplication are written in the usual way as products $A(t|s)\, p(s)$ and $A(t|s)\, A(s|t_1)$, respectively:

$$[A(t|s)\, p(s)]_{\mathbf{x}} = \int A(\mathbf{x}\,t|\mathbf{y}\,s)\, p(\mathbf{y}\,s)\, dy$$

$$[A(t|s)\, A(s|t_1)]_{\mathbf{x},\,\mathbf{x}_1} = \int A(\mathbf{x}\,t|\mathbf{y}\,s)\, A(\mathbf{y}\,s|\mathbf{x}_1\,t_1)\, dy$$

The Green's function $G(t|t_0)$ contains the effects of the initial preparation of the system. In most cases, however, one is interested in the behaviour of an aged system, in which the effects of initial preparation have died out. Therefore, the following problem suggests itself: Can one construct a general evolution equation

$$p(t) = G(t|s) \, p(s) \qquad (t \geq s) \tag{1.4}$$

for arbitrary times t, s? The existence of such an equation is not self-evident, because the corresponding equation for a Markov process is usually derived from the Chapman-Kolmogorov equation [11] which does not hold in the non-Markov case. In the present paper, this question is investigated in detail. We find that such an evolution equation always exists, independent of the validity of the Chapman-Kolmogorov equation. However, in contrast to the Markov case, the propagator $G(t|s)$ has in general not the significance of a conditional probability $R(t|s)$, with the exception of the solution $G(t|t_0)$ of Equation (1.3) relating back to the time t_0 of preparation of the system, which is indeed identical to the conditional probability $R(t|t_0)$. But neither $G(t|s)$ nor $G(t|t_0)$ can be used to compute joint probabilities $p^{(2)}(t, s)$ and time-correlation functions of an aged system. This restriction has not been observed in some recent work on non-Markov processes [12–15].

In Sections 2 and 3 we study the general problem of the time evolution of non-Markov systems. A set of stochastic equations for the rate of change of the single-event and the multivariate distributions is derived, the solutions of which can be expressed in terms of propagators forming semigroups. These propagators must not be identified with the corresponding conditional probabilities. We also discuss the calculation of mean values and of time-correlation functions. Further, we investigate the asymptotic behaviour for large times. In Section 4, we present the linear-response theory for a Markovian perturbation. In contrast to the Markov case, the response tensor cannot be related by a generalized fluctuation theorem [16] to a stationary time-correlation function. Some aspects of the theory are illustrated in the Appendix for the two-state process and for the Gauss process.

2. Time-Evolution of Single-Event Probability

In this section, we investigate the basis for the existence of time-evolution equations of the form (1.4). In the case of a Markov process, there exists a conditional probability $R(\mathbf{x}\,t|\mathbf{x}_1 t_1)$ with $t \geq t_1$ which may be used for two different purposes: It is the integral kernel of the propagator $R(t|t_1)$ of the single-event probability $p(t)$, such that

$$p(t) = R(t|t_1) \, p(t_1) \qquad (t \geq t_1), \tag{2.1}$$

and it allows to compute the two-event joint probability

$$p^{(2)}(\mathbf{x}\,t; \mathbf{x}_1 t_1) = R(\mathbf{x}\,t|\mathbf{x}_1 t_1) \, p(\mathbf{x}_1 t_1). \tag{2.2}$$

The simplicity of the Markov theory arises from the Chapman-Kolmogorov equation [11],

$$R(t|t_1) = R(t|s) \, R(s|t_1) \qquad (t \geq s \geq t_1) \tag{2.3}$$

indicating that the elements $R(t|t_1)$ form a semigroup which can be generated from the infinitesimal propagator $R(t + dt|t) = \mathbb{1} + \Gamma(t) \, dt$ where

$$\Gamma(t) = \frac{d}{ds} R(s|t)\big|_{s = t^+}. \tag{2.4}$$

In the non-Markov case, however, the conditional probability is a very complicated object, because it depends on previous history. The balance equation for the conditional probability

$$R(t|t_1) = R(t|s, t_1) \, R(s|t_1) \tag{2.5}$$

relates the time evolution of $R(t|t_1)$ to the higher-order conditional probability $R(t|s, t_1)$, and one can construct an infinite hierarchy of coupled evolution equations. This "memory" of the conditional probability, which is due to the fact that the sample functions passing through state $\mathbf{y}$ at time s remember which states they traversed at previous times, is illustrated in Figure 1. For the special case of an initially sharp distribution $p_0(x_0) = \delta(x_0 - x_0')$, we find for instance

$$R(x_2 \, t_2 | x_1 \, t_1)$$

$$= \frac{\int R(x_2 \, t_2 | x_1 \, t_1, x_0 \, t_0) \, R(x_1 \, t_1 | x_0 \, t_0) \, p_0(x_0) \, dx_0}{\int R(x_1 \, t_1 | x_0 \, t_0) \, p(x_0) \, dx_0}$$

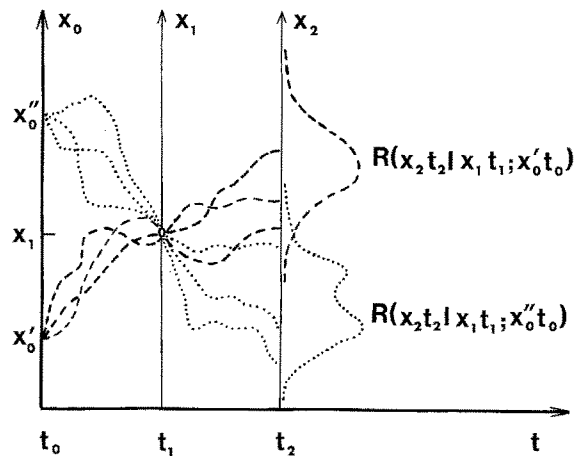$$= R(x_2 \, t_2 | x_1 \, t_1, x_0' \, t_0) \tag{2.6}$$

Fig. 1. Sample functions of a non-Markov process passing through x_1 at time t_1 remember at time t_2 which point (x_0' or x_0'') they started from at time t_0. For a Markov process, the two conditional distributions would be equal

which shows that $R(t_2|t_1)$ depends on the initial state x'_0. Note that $R(t|t_0)$, on the other hand, is always independent of the initial distribution p_0.

Thus, the elements $R(t|s)$ do not form a semigroup, and can therefore not be generated from an infinitesimal propagator. However, a significant simplification arises from the following theorem: Any stochastic process (Markov or non-Markov) satisfies

$$p(t) = R(t|s) R(s|t_1) p(t_1). \tag{2.7}$$

Thus, although the Chapman-Kolmogorov Equation (2.3) does not hold for a non-Markov process, one obtains an equality if both sides are applied to the single-event probability $p(t_1)$. The proof of Equation (2.7) is evident from the definition of the conditional probability.

Using theorem (2.7) one may construct a whole class of semigroups of propagators $G(t|t_1)$ for the single-event probability such that

$$p(t) = G(t|t_1) p(t_1) \tag{2.8}$$

with

$$G(t^+|t) = \mathbb{1} \tag{2.9}$$

and

$$\int G(\mathbf{x} t|\mathbf{x}_1 t_1) dx = 1. \tag{2.10}$$

The propagators $G(t|t_1)$ of each semigroup are the conditional probabilities of a Markov process which has the same single-event probabilities $p(t)$ (but different multivariate probabilities $p^{(n)}$) as the non-Markov process under consideration.

The semigroup G can be generated from the infinitesimal propagator $G(t+dt|t) = \mathbb{1} + \Gamma(t) dt$ with the generator $\Gamma(t) = dG(s|t)/ds|_{s=t^+}$. The most obvious choice consists in using the conditional probability $R(t+dt|t)$ itself as infinitesimal propagator, whence

$$\Gamma(t) = \frac{d}{ds} R(s|t)|_{s=t^+}. \tag{2.11}$$

However, this construction has the disadvantage that $R(s|t)$ depends on the initial distribution p_0 (see Fig. 1 and Eq. (2.6)). Thus, to every initial preparation of the system there will correspond a different substitutive Markov process. A propagator independent of p_0 is obtained by going back to the initial time t_0 at each infinitesimal step:

$$\Gamma(t) = \frac{d}{ds} R(s|t_0) R(t|t_0)^{-1}|_{s=t^+}. \tag{2.12}$$

The significance of the time instant t_0 lies in the fact that at this time the system is prepared without any correlations between the macrovariables $\mathbf{x}$ and the rest of the system, i.e. without any memory of previous times $t < t_0$.

The generator $\Gamma(t)$ determines the rate of change of the single-event distribution by the time-convolutionless stochastic equation

$$\frac{dp(t)}{dt} = \Gamma(t) p(t) \tag{2.13}$$

and of the propagator by the "forward equation"

$$\frac{dG(t|t_1)}{dt} = \Gamma(t) G(t|t_1). \tag{2.14}$$

The formal solution of this differential equation can be written

$$G(t|t_1) = \mathscr{T} \exp \int_{t_1}^{t} \Gamma(s) ds \tag{2.15}$$

where $\mathscr{T}$ is the time-ordering operator. Equation (2.15) guarantees the semigroup property

$$G(t|t_1) = G(t|s) G(s|t_1). \tag{2.16}$$

The propagator determined by the generator (2.12) has the simple properties

$$G(t|t_0) = R(t|t_0) \tag{2.17}$$

and

$$G(t|t_1) = R(t|t_0) R(t_1|t_0)^{-1}. \tag{2.18}$$

It can be obtained by Equation (1.3) in conjunction with the semigroup property (2.16) from the retarded kernel $\Lambda(t|s)$ which is directly related to the microscopic dynamics of the system.

The use of the reciprocal operator $R(t|t_0)^{-1}$ in (2.12) and (2.18) requires some comments. In the case of a finite number of states, the probability distributions are ordinary vectors and the operators are ordinary matrices, and there will be no problem to define G^{-1} for a "connected" system. For a countable set of states, however, there is the possibility that the eigenvalues of G converge to zero, and for a continuous state space, G will in general have a continuous spectrum extending down to 0^+. In these cases, G^{-1} will not exist for all functions of function space Π. However, $G^{-1}(t|t_1)$ will always exist for functions $p(t)$ which have evolved out of a probability distribution $p(t_1)$, and only to such functions will operators like (2.12) and (2.18) be applied.[*]

With the help of the propagator $G(t|t_1)$, the statistical expectation of any state function $\phi(t)$ can be calculated from the statistical distribution $p(t_1)$ at an arbitrary fixed time $t_1 \leq t$,

$$\langle \phi(\mathbf{x} t) \rangle = \iint \phi(\mathbf{x}, t) G(\mathbf{x} t|\mathbf{x}_1 t_1) p(\mathbf{x}_1, t_1) dx_1 dx. \tag{2.19}$$

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[*] The same remark applies to the use of the reciprocal propagator $R(t|t_0)^{-1}$ of a Markov process in Reference 16

This includes all averages $\langle x_\alpha(t) \rangle$ of the state variables, all moments $\langle x_\alpha^n(t) \rangle$, and all equal-time correlations $\langle x_\alpha^m(t) \, x_\beta^n(t) \rangle$.

Up to this point, we have made no assumption about the behaviour against time-translations. We now assume time-translation invariance of the underlying microscopic process. It is important to note that even in this case the process is always nonstationary, in contrast to the Markov case. This is so because the effects of the preparation at time t_0 influence the evolution of the system for a finite time. Time-translation symmetry requires invariance with respect to a shift of all times, including t_0. Consequently, the single-event probability depends on $t - t_0$, and equations like (2.8) should be written more fully as

$$p(t - t_0) = G(t - t_0 | t_1 - t_0) \, p(t_1 - t_0) \tag{2.20}$$

in order to show the dependence on t_0 explicitly. — This nonstationarity which is due to the breaking of time-translation symmetry by the initial preparation of the system, should be distinguished from an explicitly nonstationary process controlled by time-dependent external parameters, such as has been discussed for the Markov case in Reference 16.

One expects that in systems of physical interest the effects of initial preparation die out after some time, and the distribution tends to a stationary distribution

$$p_{\mathrm{as}} = \lim_{t_0 \to -\infty} p(t - t_0)$$

independent of the initial distribution p_0. This asymptotic stability of the single-event distribution is a consequence of the general ergodicity requirement discussed in Section 3. In the case of definition (2.11), there will exist a stationary asymptotic propagator

$$G_{\mathrm{as}}(t - t_1) = \lim_{t_0 \to -\infty} G(t - t_0 | t_1 - t_0) \tag{2.22}$$

which has p_{as} as eigenvector. In the case of definition (2.12), on the other hand, $G(t | -\infty)$ exists and represents a time-independent singular operator with kernel

$$G(\mathbf{x}\,t | \mathbf{y}, -\infty) = R(\mathbf{x}\,t | \mathbf{y}, -\infty) = p_{\mathrm{as}}(\mathbf{x}). \tag{2.23}$$

However, no such statements can be made for $G_{\mathrm{as}}(t | t_1)$ in case of (2.12) and for $G(t | -\infty)$ in case of (2.11).

We have thus obtained an understanding of the existence of a propagator for the single-event probability in the non-Markov case. We stress again that the propagator $G(t | t_1)$ is not identical with the conditional probability $R(t | t_1)$ except for $t_1 = t_0$ in the case of definition (2.12).

3. Multivariate Distributions and Time-Correlation Functions

The considerations of Section 2 can be generalized easily to the multivariate case. The multivariate distribution $p^{(n)}(\mathbf{X}\,T)$ for the sequence of states $\mathbf{X} \equiv (\mathbf{x}^{(1)} \dots \mathbf{x}^{(n)})$ at the time sequence $T \equiv (t^{(1)} \dots t^{(n)})$ is an element $p^{(n)}(T)$ of Π^n, and the conditional probability $R^{(n)}(\mathbf{X}\,T | \mathbf{X}_1 T_1)$ is the kernel of an operator $R^{(n)}(T | T_1)$ acting on Π^n such that

$$p^{(n)}(T) = R^{(n)}(T | T_1) \, p^{(n)}(T_1), \tag{3.1}$$

where the smallest $t \in T$ is assumed to be larger than or equal to the largest $t_1 \in T_1$, symbolically $T \geq T_1$. For a non-Markov process, the balance equation

$$R^{(n)}(T | T_1) = R^{(n)}(T | S, T_1) \, R^{(n)}(S | T_1) \tag{3.2}$$

relates the time evolution of $R^{(n)}(T | T_1)$ to the higher-order conditional probability $R^{(n)}(T | S, T_1)$. Thus, the elements $R^{(n)}(T | T_1)$ do not form a semigroup and can therefore not be generated from an infinitesimal propagator. The simplification arises from the generalization of theorem (2.7): Any stochastic process satisfies

$$p^{(n)}(T) = R^{(n)}(T | S) \, R^{(n)}(S | T_1) \, p^{(n)}(T_1). \tag{3.3}$$

This shows that n-parameter semigroups of propagators $G^{(n)}(T | T_1)$ for the multivariate distribution $p^{(n)}(T)$ can be constructed such that

$$p^{(n)}(T) = G^{(n)}(T | T_1) \, p^{(n)}(T_1). \tag{3.4}$$

The semigroup $G^{(n)}$ can be generated from the vector generator

$$\Gamma^{(n)}(T) = \frac{\partial}{\partial S} G^{(n)}(S | T)|_{S = T^+}$$

$$\frac{\partial}{\partial S} \equiv \left(\frac{\partial}{\partial s^{(1)}}, \dots, \frac{\partial}{\partial s^{(n)}} \right), \tag{3.5}$$

and there is again a multitude of choices for $\Gamma^{(n)}(T)$. One can generate the semigroup as in (2.11) by taking the conditional probability $R^{(n)}(T + dT | T)$ itself as infinitesimal propagator,

$$\Gamma^{(n)}(T) = \frac{\partial}{\partial S} R^{(n)}(S | T)|_{S = T^+}, \tag{3.6}$$

but this has the disadvantage that it depends on the initial distribution p_0. In order to obtain a semigroup independent of the initial distribution, one has to relate back to the initial time t_0 as in (2.12),

$$\Gamma^{(n)}(T) = \frac{\partial}{\partial S} R^{(n)}(S | t_0 D) \, R^{(n)}(T | t_0 D)^{-1}|_{S = T^+} \tag{3.7}$$

where $D = (1, 1 \dots 1)$ such that $t_0 D$ denotes the n-tupel of initial times $(t_0, \dots t_0)$.

The stochastic equation

$$\frac{\partial}{\partial T} p^{(n)}(T) = \Gamma^{(n)}(T) \, p^{(n)}(T) \tag{3.8}$$

can be integrated along a curve $T = T(\theta)$ in the space of n times $T = (t^{(1)}, \ldots t^{(n)})$ passing through the points $T_1 = T(\theta_1)$ and $T_2 = T(\theta_2)$ to give a solution of the form (3.4) with

$$G^{(n)}(T_2|T_1) = \mathscr{T} \exp \int_{\theta_1}^{\theta_2} \Gamma^{(n)}(T(\theta)) \cdot \frac{dT(\theta)}{d\theta} \, d\theta \qquad (3.9)$$

where the ordering operator $\mathscr{T}$ acts on the curve parameter θ. The semigroup property

$$G^{(n)}(T|T_1) = G^{(n)}(T|S) \, G^{(n)}(S|T_1) \qquad (3.10)$$

follows immediately from (3.9) by choosing a curve which passes through S.

By adopting the definition (3.7) one obtains a propagator with the simple properties

$$G^{(n)}(T|t_0 D) = R^{(n)}(T|t_0 D) \qquad (3.11)$$

and

$$G^{(n)}(T|T_1) = R^{(n)}(T|t_0 D) \, R^{(n)}(T_1|t_0 D)^{-1}. \qquad (3.12)$$

The use of the reciprocal operator in (3.7) and (3.12) is subject to the same remarks as stated after Equation (2.18). In contrast to the single-event case, no method has been worked out yet to compute the multivariate distribution from the microscopic dynamics of the system.

With the help of the n-event propagator $G^{(n)}(T|T_1)$ one can calculate the n-event joint probability $p^{(n)}(T)$ and therefore any n-time correlation function from the single-event probability at an arbitrary fixed time $t_1 \leq T$. Because of $p^{(n)}(X_1, t_1 D) = p^{(1)}(x_1 \, t_1) \, \delta(x_1^{(2)} - x_1) \ldots \delta(x_1^{(n)} - x_1)$ one finds

$$p^{(n)}(XT) = \int G^{(n)}(XT|x_1 D, t_1 D) \, p^{(1)}(x_1 \, t_1) \, dx_1 \qquad (3.13)$$

and

$$\langle \phi_1(x^{(1)} \, t^{(1)}) \ldots \phi_n(x^{(n)} \, t^{(n)}) \rangle$$
$$= \int \phi_1(x^{(1)}, t^{(1)}) \ldots \phi_n(x^{(n)}, t^{(n)})$$
$$\times G^{(n)}(XT|x_1 D, t_1 D) \, p^{(1)}(x_1 \, t_1) \, d^n X \, dx_1. \qquad (3.14)$$

If the n-event propagator $G^{(n)}$ is known, all lower-order propagators can be calculated. It is not difficult to prove that the $(n-1)$-event propagator $G^{(n-1)}$ can be obtained from $G^{(n)}$ by the same procedure as the $(n-1)$-event conditional probability $R^{(n-1)}$ is obtained from $R^{(n)}$: In order to eliminate the ν-th event from $G(XT|X_1 T_1)$, set $t^{(\nu)} = t^{(\mu)}$, $t_1^{(\nu)} = t_1^{(\mu)}$, $x_1^{(\nu)} = x_1^{(\mu)}$, where $t^{(\mu)}$ and $t_1^{(\mu)}$ are time instants adjacent to $t^{(\nu)}$ and $t_1^{(\nu)}$, respectively, and integrate over $x^{(\nu)}$. We illustrate this procedure for the case $n = 2$:

$$\int G^{(2)}(x^{(1)} \, t^{(1)}, x^{(2)} \, t^{(1)} | x_1^{(1)} \, t_1^{(1)}, x_1^{(1)} \, t_1^{(1)}) \, dx^{(2)}$$
$$= G^{(1)}(x^{(1)} \, t^{(1)} | x_1^{(1)} \, t_1^{(1)}). \qquad (3.15)$$

It is also possible to keep all times of the sequence T except the latest time $t^{(1)}$ fixed, and study propagation with respect to this $t^{(1)}$ alone. The corresponding propagator can be viewed as an operator acting on Π^1 which depends parametrically on the other events.

Time-translation symmetry of the underlying microscopic process requires invariance with respect to a shift of all times, including t_0. Consequently, the multivariate distributions depend on $T - t_0 D$, and this dependence can be exhibited explicitly by writing equations like (3.4) in the form

$$p^{(n)}(T - t_0 D) = G^{(n)}(T - t_0 D|T_1 - t_0 D) \, p^{(n)}(T_1 - t_0 D). \qquad (3.16)$$

In systems of physical interest, the effects of initial preparation of the system are expected to die out after some time. We call the process *ergodic* if

$$\lim_{t_0 \to -\infty} p^{(n)}(T - t_0 D) = p_{as}^{(n)}(T) \qquad (3.17)$$

exists for all n and is independent of the initial preparation. Then, in the case of definition (3.7), $G^{(n)}(T| -\infty D)$ exists and represents a singular operator

$$G^{(n)}(XT|Y, -\infty) = p_{as}^{(n)}(XT). \qquad (3.18)$$

In the case of (3.6), no statement can be made on $G^{(n)}(T| -\infty D)$.

Time-translation symmetry requires that the process is asymptotically stationary, i.e. that $p_{as}^{(n)}(T)$ is invariant under a shift of time

$$p_{as}^{(n)}(T + \tau D) = p_{as}^{(n)}(T). \qquad (3.19)$$

In the case of definition (3.6), there will exist an asymptotic propagator $G_{as}^{(n)}(T|T_1)$ which is stationary in the sense

$$G_{as}^{(n)}(T + \tau D|T_1 + \tau D) = G_{as}^{(n)}(T|T_1), \qquad (3.20)$$

and $p_{as}^{(n)}(T)$ will be eigenvector of $G_{as}^{(n)}(T + \tau D|T)$. In the case of (3.7), no statement can be made on $G_{as}^{(n)}(T|T_1)$.

4. Linear-Response Theory

In this Section, we study the linear response of the system to an external perturbation. The perturbed single-event distribution $\hat{p}(t)$ satisfies the stochastic equation

$$\frac{d\hat{p}(t)}{dt} = \int_{t_0}^{t} \hat{\Lambda}(t|s) \, \hat{p}(s) \, ds \qquad (4.1)$$

with the kernel

$$\hat{\Lambda}(t|s) = \Lambda(t - s) + \Lambda^{\text{ext}}(t|s). \qquad (4.2)$$

Here, we assume that the unperturbed system is time-translation invariant, such that its Green's function

determined by Equation (1.3) depends only on the time difference $t - t_0$,

$$G(t|t_0) \equiv R(t|t_0) = G(t - t_0). \tag{4.3}$$

The stochastic equation (4.1) is equivalent to the integral equation

$$\hat{p}(t) = p(t) + \int_{t_0}^{t} G(t - s) \int_{t_0}^{s} \Lambda^{\mathrm{ext}}(s|s') \, \hat{p}(s') \, ds' \, ds. \tag{4.4}$$

From this equation, the perturbed distribution can be found by iteration. The first-order change is obtained by replacing $\hat{p}(s')$ by $p(s')$ under the integral.

For the further discussion we assume that the perturbation can be described by a Markov kernel, and write the perturbation in terms of time-dependent external forces $F_i(t)$,

$$\Lambda^{\mathrm{ext}}(t|s) = \sum_i F_i(t) \Omega_i \, \delta(t - s^+) = \mathbf{F}(t) \cdot \mathbf{\Omega} \delta(t - s^+) \tag{4.5}$$

where the Ω_i are linear operators acting on Π. Then, the first-order change of the single-event distribution is given by

$$\delta \hat{p}(t) = \int_{t_0}^{t} G(t - s) \, \mathbf{F}(s) \cdot \mathbf{\Omega} p(s) \, ds. \tag{4.6}$$

The linear-response tensor $\chi(t|s)$ is defined by the relation of the response of the state variables

$$\langle \delta \mathbf{x}(t) \rangle \equiv \langle \mathbf{x}(t) \rangle^{\mathrm{perturbed}} - \langle \mathbf{x}(t) \rangle^{\mathrm{unperturbed}}$$

$$= \int \mathbf{x} \, \delta \hat{p}(\mathbf{x}t) \, dx \tag{4.7}$$

to the external forces,

$$\langle \delta \mathbf{x}(t) \rangle = \int_{t_0}^{t} \chi(t|s) \cdot \mathbf{F}(s) \, ds. \tag{4.8}$$

We find

$$\chi(t|s) = \theta(t - s) \iint \mathbf{x} \, \phi(\mathbf{y}s) \, G(\mathbf{x}, \mathbf{y}; t - s) \, p(\mathbf{y}s) \, dx \, dy \tag{4.9}$$

where we have introduced the vector-valued state function ϕ as in Reference 16

$$\phi(\mathbf{x}t) = [\mathbf{\Omega} p(t)]_{\mathbf{x}} / p(\mathbf{x}t). \tag{4.10}$$

Since the perturbation cannot change the normalization of the system, $\phi(\mathbf{x}t)$ has zero average,

$$\langle \phi(\mathbf{x}t) \rangle = \int [\mathbf{\Omega} p(t)]_{\mathbf{x}} \, dx = 0, \tag{4.11}$$

and represents thus a fluctuation (in general nonlinear) from the unperturbed state. Therefore, the state variable $\mathbf{x}$ may be replaced by its fluctuation $\boldsymbol{\xi} = \mathbf{x} - \langle \mathbf{x} \rangle^{\mathrm{unperturbed}}$ in Equation (4.9).

It is important to note that in Equation (4.6) the perturbation $\mathbf{F}(s) \, ds$ applied at time s is not, as one might have expected, propagated to time t by the propagator

$G(t|s)$ corresponding to this time intervall, but rather by the propagator $G(t - s) \equiv G(t_0 + t - s|t_0)$, i.e. in the same way as an initial distribution is propagated from t_0 to $t_0 + t - s$. For the same reason, in contrast to the Markov case, the response tensor (4.9) is not given as a true two-time correlation function (generalized fluctuation theorem), but as a pseudo-correlation function

$$\chi(t|s) = \theta(t - s) \langle\!\langle \boldsymbol{\xi}(t) \, \phi(\mathbf{y}s) \rangle\!\rangle \tag{4.12}$$

calculated with a joint probability

$$p_2^{\mathrm{pseudo}}(\mathbf{x}t, \mathbf{y}s) = G(\mathbf{x}, \mathbf{y}; t - s) \, p(\mathbf{y}s) \tag{4.13}$$

which is the joint probability $p_2(t_0 + t - s, t_0)$ of a system which was started with initial distribution $p(s)$.

The result obtained is the response of a nonstationary process, because it still contains the effects of initial preparation of the system. In the case of an ergodic process, the response of an aged system is obtained by performing the limit $t_0 \to -\infty$. Then, $p(s)$ is replaced by p_{as} in Equations (4.6) and (4.9), $\phi(\mathbf{x}t) = [\mathbf{\Omega} p_{\mathrm{as}}]_{\mathbf{x}} / p_{\mathrm{as}}(\mathbf{x}) \equiv \phi(\mathbf{x}(t))$ does not depend explicitly on time, and the response becomes stationary

$$\chi_{\mathrm{as}}(t - s) = \theta(t - s) \langle\!\langle \boldsymbol{\xi}(t) \, \phi(\mathbf{y}(s)) \rangle\!\rangle. \tag{4.14}$$

We stress again that it is important to distinguish the propagator $G(t - s)$ determining the linear response from the asymptotic conditional probability $R_{\mathrm{as}}(t - s)$ determining time-correlation functions of an aged system.

5. Conclusions

We have shown that semigroups of propagators $G^{(n)}$ for the n-time multivariate distributions $p^{(n)}$ exist for all n, which can be used to calculate averages and m-time correlation functions up to $m = n$ from the single-event distribution at an arbitrary fixed time. By going to the continuum limit, one may define a propagator $G(\mathbf{x}(t)|\mathbf{y}(s))$ which expresses the probability for a path $\mathbf{x}(t)$ as a path integral over paths $\mathbf{y}(s)$. The propagators $G^{(n)}$ of non-Markov processes are different from the conditional probabilities $R^{(n)}$ (except for conditions referring to the initial time t_0), and can therefore not be used to calculate m-time joint probabilities and correlation functions with $m > n$. The response to an external perturbation is given by the single-event propagator $G(t_0 + \tau|t_0)$, and can therefore not be expressed in the form of an ordinary generalized fluctuation theorem.

Appendix A. Two-State-Process

The single-event distribution and the conditional probability of a general two-state process can be

written in the form

$$p(t) = \frac{1}{2} \begin{pmatrix} 1+a(t) \\ 1-a(t) \end{pmatrix}, \quad |a(t)| \le 1 \tag{A.1}$$

and

$$R(t|t_1) = \frac{1}{2} \begin{pmatrix} 1+\rho(t,t_1)+\alpha(t,t_1) & 1-\rho(t,t_1)+\alpha(t,t_1) \\ 1-\rho(t,t_1)-\alpha(t,t_1) & 1+\rho(t,t_1)-\alpha(t,t_1) \end{pmatrix}$$

$$|\rho(t,t_1) \pm \alpha(t,t_1)| \le 1, \tag{A.2}$$

respectively. The time evolution of the single-event distribution is given by

$$a(t) = \alpha(t,t_1) + \rho(t,t_1) a(t_1). \tag{A.3}$$

The conditional probabilities (A.2) do not form a semigroup except in the Markov case

$$\rho(t,t_1) = \rho(t,s) \rho(s,t_1)$$

$$\alpha(t,t_1) = \alpha(t,s) + \rho(t,s) \alpha(s,t_1). \tag{A.4}$$

The generator of any semigroup has the form

$$\Gamma(t) = \frac{1}{2} \begin{pmatrix} \dot{P}(t)+\dot{A}(t) & -\dot{P}(t)+\dot{A}(t) \\ -\dot{P}(t)-\dot{A}(t) & \dot{P}(t)-\dot{A}(t) \end{pmatrix}, \tag{A.5}$$

and the propagator is given by

$$G(t|t_1) = \frac{1}{2} \begin{pmatrix} 1+P(t,t_1)+A(t,t_1) & 1-P(t,t_1)+A(t,t_1) \\ 1-P(t,t_1)-A(t,t_1) & 1+P(t,t_1)-A(t,t_1) \end{pmatrix} \tag{A.6}$$

where

$$P(t,t_1) = \exp[P(t)-P(t_1)]$$

$$A(t,t_1) = \int_{t_1}^{t} P(t,s) \dot{A}(s) ds. \tag{A.7}$$

The semigroup property of $G(t|t_1)$ follows immediately from the fact that $P(t,t_1)$ and $A(t,t_1)$ satisfy the Markov conditions (A.4).
In the case of definition (2.11) one has

$$\dot{P}(t) = \frac{d}{ds} \rho(s,t)|_{s=t^+} \le 0, \quad \dot{A}(t) = \frac{d}{ds} \alpha(s,t)|_{s=t^+} \tag{A.8}$$

which depend on the initial distribution.
In the case of definition (2.12) one finds

$$\dot{P}(t) = \dot{\rho}(t,t_0)/\rho(t,t_0)$$

$$\dot{A}(t) = \dot{\alpha}(t,t_0) - \dot{P}(t) \alpha(t,t_0) \tag{A.9}$$

whence

$$P(t,t_1) = \rho(t,t_0)/\rho(t_1,t_0)$$

$$A(t,t_1) = \alpha(t,t_0) - P(t,t_1) \alpha(t_1,t_0), \tag{A.10}$$

independent of the initial distribution. It is easy to verify that in this case $P(t,t_0) = \rho(t,t_0)$, $A(t,t_0) = \alpha(t,t_0)$ as required by (2.17).

The process is ergodic if $\rho(t, -\infty) = 0$ and $\alpha_{as}(t, -\infty) = a_{as}(t)$ exist. Asymptotic stationarity requires that $\rho_{as}(t,t_1)$ and $\alpha_{as}(t,t_1)$ depend on $t-t_1$ only, and are related by

$$[1-\rho_{as}(t-t_1)] a_{as} = \alpha_{as}(t-t_1). \tag{A.11}$$

In the case of definition (2.11) it follows that

$$P_{as}(t,t_1) = \exp[-\gamma(t-t_1)]$$

$$A_{as}(t,t_1) = a_{as}\{1 - \exp[-\gamma(t-t_1)]\} \tag{A.12}$$

with $\gamma = -\dot{\rho}_{as}(0) > 0$, which shows the existence of a stationary asymptotic propagator (2.22).
In the case of definition (2.12), on the other hand, $G(t|t_0) = R(t|t_0)$ becomes singular for $t_0 \to -\infty$ because of $\rho(t|t_0) \to 0$, as required by (2.23).

Appendix B. Non-Markov-Gauss Process

The single-event distribution of a general Gauss process is determined by the mean $a(t)$ and the variance $s(t)$

$$p(xt) = [2\pi s(t)]^{-1/2} \exp\{-[x-a(t)]^2/2s(t)\} \tag{B.1}$$

and the conditional probability has the form

$$R(xt|yt_1) = \frac{\exp\{-[x-\rho(t,t_1)y-\alpha(t,t_1)]^2/2\sigma(t,t_1)\}}{[2\pi\sigma(t,t_1)]^{1/2}}. \tag{B.2}$$

The time evolution of the single-event distribution is given by

$$a(t) = \alpha(t,t_1) + \rho(t,t_1) a(t_1)$$

$$s(t) = \sigma(t,t_1) + \rho^2(t,t_1) s(t_1). \tag{B.3}$$

The conditional probabilities (B.2) do not form a semigroup except in the Markov case

$$\rho(t,t_1) = \rho(t,s) \rho(s,t_1)$$

$$\alpha(t,t_1) = \alpha(t,s) + \rho(t,s) \alpha(s,t_1)$$

$$\sigma(t,t_1) = \sigma(t,s) + \rho^2(t,s) \sigma(s,t_1). \tag{B.4}$$

The generator of the semigroup corresponding to Equation (2.11) is the "linear" Fokker-Planck operator

$$\Gamma(t) = \frac{\partial}{\partial x}\left[-\dot{\rho}(t)x - \dot{\alpha}(t) + \frac{1}{2}\dot{\sigma}(t)\frac{\partial}{\partial x}\right] \tag{B.5}$$

where

$$\dot{\rho}(t) = \frac{d}{ds}\rho(s,t)|_{s=t^+}$$

$$\dot{\alpha}(t) = \frac{d}{ds}\alpha(s,t)|_{s=t^+}$$

$$\dot{\sigma}(t) = \frac{d}{ds}\sigma(s,t)|_{s=t^+}. \tag{B.6}$$

$\Gamma(t)$ generates the general Gauss-Markov semigroup (see Ref. 16)

$$G(xt|yt_1) = \frac{\exp\{-[x - P(t, t_1)\,y - A(t, t_1)]^2 / 2\Sigma(t, t_1)\}}{[2\pi\,\Sigma(t, t_1)]^{1/2}}$$

(B.7)

where

$$P(t, t_1) = \exp[\rho(t) - \rho(t_1)]$$

$$A(t, t_1) = \int_{t_1}^{t} P(t, s)\,\dot\alpha(s)\,ds$$

$$\Sigma(t, t_1) = \int_{t_1}^{t} P^2(t, s)\,\dot\sigma(s)\,ds.$$

(B.8)

Calculation of the p_0-independent generator according to Equation (2.12) would require the inverse of $R(xt|yt_1)$ and is not carried out here.

For an ergodic process, $\rho(t, -\infty) = 0$, $\alpha(t, -\infty) = a_{as}(t)$ and $\sigma(t, -\infty) = s_{as}(t)$ exist. Asymptotic stationarity requires that $\rho_{as}(t, t_1)$, $\alpha_{as}(t, t_1)$ and $\sigma_{as}(t, t_1)$ depend on $t - t_1$ only, and satisfy

$$[1 - \rho_{as}(t - t_1)]\,a_{as} = \alpha_{as}(t - t_1)$$

$$[1 - \rho_{as}^2(t - t_1)]\,s_{as} = \sigma_{as}(t - t_1).$$

(B.9)

As a consequence,

$$P_{as}(t, t_1) = \exp[-\gamma(t - t_1)]$$

$$A_{as}(t, t_1) = a_{as}\{1 - \exp[-\gamma(t - t_1)]\}$$

$$\Sigma_{as}(t, t_1) = s_{as}\{1 - \exp[-2\gamma(t - t_1)]\}$$

(B.10)

where $\gamma = -\dot\rho_{as}(0) > 0$, which shows the existence of a stationary asymptotic propagator (2.22).

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