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Note on Time Evolution of Non-Markov Processes

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We discuss the question of the construction of a linear semigroup for the time evolution of the single-event probabilities of general non-Markov processes. It is shown that such a linear semigroup may not exist for all finite times. The consequences are sketched for the description of equilibrium and nonequilibrium systems. Further, the relationship with nonstationary Markov processes is investigated, and some confusion in recent works is cleared up using the example of free Brownian motion.

KEY WORDS: Non-Markov processes; nonstationary Markov processes; master equation; generalized Langevin equation; semigroup approach.

There has recently been a remarkable interest in the time-convolutionless formulation of the stochastic properties of non-Markov processes.[1–9] In particular, the time evolution of probabilities in non-Markovian systems has been investigated both from the theory of stochastic processes[5] and from the underlying microscopic point of view.[6] The question has also been discussed on the basis of transformation techniques that remove the memory from the usually accepted generalized Langevin equations.[7–9] In this context it has been claimed[9] that the original process with a memory kernel description is not non-Markovian but actually nonstationary Markovian, and all the memory kernel really does is produce a nonstationary Markovian process. Unfortunately, no useful strict theorems presently exist for the condition under which the Markov property is inherited on contraction or projection. It is generally believed that without any coarse-graining in time, or without any limiting procedures, the process obtained by a coarse-graining in phase space is always non-Markovian. Some rigorous derivations of Markovian

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subdynamics, using limiting procedures, have been discussed recently.[10–12] Since we have been bombarded during the last years with papers on the subject of "non-Markovian" versus time-convolutionless descriptions, the authors think it is worthwhile to point out the relationships among the different approaches and clear up a possible confusion in this context.

To discuss the relationships, the following problem suggests itself: Can one construct for non-Markov processes a linear propagator $G(t/s)$ (independent of the initial probability function p_0) satisfying

$$p(t) = G(t/s)p(s), \qquad t \geqslant s \tag{1}$$

for *arbitrary* times t and s? Such a construction then yields from the underlying semigroup property of G the time-convolutionless master equation for the non-Markov process

$$\dot{p}(t) = \Gamma(t)p(t) \tag{2}$$

where

$$\Gamma(t) = (d/dr)G(r/t)|_{r=t^+} \tag{3}$$

It is worth emphasizing at this stage the following[5]: From the knowledge of the single-time master equation it is not possible to decide whether the process is Markovian or not Markovian. Further, given the information that the process *is* non-Markovian, it is also, in general, not possible to determine the conditional probability $R(t/s)$ for given times t and s via the Green's function solution of Eq. (2). The exception is given for the time set (t/t_0) where the time t_0 denotes the time of initial preparation so that the system has *no* memory for previous times $t \leqslant t_0$.[5,6] [See also Eq. (4b).] In recent works,[5,6] the linear generator $\Gamma(t)$ was obtained by going back to the initial time t_0 of preparation

$$\Gamma(t) = (d/dr)R(r/t_0)R(t/t_0)^{-1}|_{r=t^+} \tag{4a}$$

so that we get

$$G(t/s) = R(t/t_0)R(s/t_0)^{-1} \tag{4b}$$

The construction makes use of the conditional probability $R(t/t_0)$, which is always independent of the initial probability p_0 and is obtained in principle as the Green's function solution of the integrodifferential equation derived within the framework of projector methods.[6]

The use of the inverse operator $R(t/t_0)^{-1}$ in Eqs. (4) requires some further comments. For a non-Markov system, one cannot in general assume that the conditional probability $R(t/t_0)$ is invertible for all finite times t, and as a consequence, the linear generator $\Gamma(t)$ does not exist for some times t, possibly even for a whole range of parameter values of t.[4]

As an illustration, we consider a one-dimensional *stationary* Gaussian non-Markov process whose conditional probability is given by the Gaussian (free Brownian motion)

$$R^{st}(xt/y0) = \left\{\frac{2\pi kT}{M}[1 - \xi^2(t)]\right\}^{-1/2} \exp\frac{-[x - y\xi(t)]^2}{(2kT/M)[1 - \xi^2(t)]} \tag{5}$$

with

$$\xi(t) = \langle x(t)x(0)\rangle/\langle x^2\rangle, \qquad \lim_{t\to+\infty} \xi(t) = 0 \tag{6}$$

where $t_0 = 0$ has been chosen.

This stationary conditional probability does not form a semigroup except in the Markov case, where

$$\xi(t + s) = \xi(t)\xi(s) = \exp[-\gamma(t + s)], \qquad \gamma > 0 \tag{7}$$

By differentiating with respect to the time t, one obtains the linear generator $\Gamma(t)$ for non-Markov processes with the initial conditional probability $R(t/0)$ given by Eq. (5):

$$\Gamma(t) = -\frac{\dot{\xi}(t)}{\xi(t)}\left(\frac{d}{dx}x + \frac{kT}{M}\frac{d^2}{dx^2}\right) \tag{8}$$

Here the generator $\Gamma(t)$ has the form of a *nonstationary* Gaussian (pseudo-) Markov generator,[5] whose explicit Markovian nonstationary conditional probability $R_{GM}(t/t_1)$, $t \geqslant t_1$, reads

$$G(xt/yt_1) = R_{GM}(xt/yt_1) = \frac{\exp\{-\frac{1}{2}\alpha^{-1}(t/t_1)[x - \bar{\xi}(t, t_1)y]^2\}}{[2\pi\alpha(t, t_1)]^{1/2}} \tag{9}$$

with

$$\bar{\xi}(t, t_1) = \xi(t)/\xi(t_1), \qquad \xi(0) = 1 \tag{10}$$

$$\alpha(t, t_1) = \frac{kT}{M}\left[1 - \frac{\xi^2(t)}{\xi^2(t_1)}\right] \tag{11}$$

For $R_{GM}(t/0)$ we obtain from $\bar{\xi}(t, 0) = \xi(t)$ the expected result

$$R^{st}(xt/y0) = R_{GM}(xt/y0) \tag{12}$$

[4] This happens, for example, if the system is oscillating around the stationary probability function, or, more generally, whenever for a fixed time t two initially different probabilities coincide.

[5] In general, the diffusion coefficient may have negative values, indicating the existence of non-semipositive transition probabilities $G(xt/ys)$.

Furthermore, we explicitly see that if $\xi(t)$ in Eq. (8) is zero, $R^{st}(t/0)$ is singular and $\Gamma(t)$ therefore does not exist.[6] This behavior is physically realized if we consider the velocity $x(t)$ of a heavy isotropic impurity (mass M) in an infinite, one-dimensional harmonic lattice (masses m) with nearest neighbor interactions (spring constant k_s) in equilibrium.[13,14] If the mass ratio $m/M = \frac{1}{2}$, then as a function of the dimensionless time $\tau = 2(k_s/m)^{1/2}t$ the exact conditional probability $R(\tau/0)$ is the result in Eq. (5)[13,14] with

$$\xi(\tau) = 2J_1(\tau)/\tau \tag{13}$$

J_1 is the appropriate Bessel function, and the first zero of $\xi(\tau)$ occurs at $\tau = 3.83171\ldots$.

The generalized Langevin equation is found to be[14]

$$dx(\tau)/d\tau = -\int_0^\tau \beta(\tau - s)x(s)\,ds + f(\tau) \tag{14}$$

where $f(\tau)$ represents a stationary Gaussian stochastic driving force[14] with zero mean and with correlation

$$\langle f(\tau)f(s)\rangle = (kT/M)\beta(\tau - s) \tag{15}$$

The single-event probability of this stochastic equation has been shown to obey a time-convolutionless master equation with $\Gamma(\tau)$ given by Eq. (8)[8,9,15] and $\xi(\tau)$ given by Eq. (13). But again, one may not conclude that the process $x(\tau)$ is a nonstationary Gaussian Markov process. Different choices for the initial probability p_0 will define different non-Markov processes for which we have

$$R(t/t_1) \neq R_{GM}(t/t_1) \tag{16}$$

for $t_1 \neq t_0$. This can be seen more explicitly if, for example, one chooses for the initial probability p_0 the stationary Gaussian probability; then the conditional probability of the stationary Gaussian non-Markov Brownian motion process is given by the *stationary* conditional probability $R(t/t_1) = R^{st}(t - t_1/0)$ in Eq. (5), which differs from the *nonstationary* Gaussian Markovian conditional probability $R_{GM}(t/t_1)$ in Eq. (9) if $t_1 \neq t_0 = 0$. To obtain the detailed stochastic properties of the process defined by the generalized Langevin equation (14), one has to study the joint and higher multivariate probabilities for arbitrary time sets.

The fact that a non-Markov process may have a singular conditional probability $R(t/t_0)$ has further consequences. In recent works,[1-7] various time-convolutionless master equations containing, in general, an inhomogeneity have been derived. In most of these works one assumes the existence

[6] On the other hand, if $\xi(t)$ has no zeros for finite times, e.g., if $\xi(t) = 1/(1 + t)$, the linear generator $\Gamma(t)$ exists for the non-Markov processes for all finite times t.

of an inverse operator $\theta(t)$ to a certain expression obtained within the framework of projector techniques. It is easy to show that in all these cases the existence of the inverse operator $\theta(t)$ for all finite times t is equivalent to the existence of the linear generator $\Gamma(t)$, $t \in [t_0, \infty)$. However, if a so-called "partial coarse-graining in time" is performed by using a finite approximation of an infinite expansion of the exact operator $\theta(t)$ in terms of an effective coupling constant λ,

$$\theta(t) = \frac{1}{1 - \lambda A(t)} = 1 + \sum_{n=1}^{\infty} [\lambda A(t)]^n \tag{17}$$

one introduces additional "irreversibility terms," yielding a regular generator $\Gamma^{\mathrm{appr}}(t)$. Furthermore, in the description of equilibrium and nonequilibrium systems, a singularity in $R(t/t_0)$ means that no transformations exist that will remove the memory kernel terms from either the Langevin equations for macroscopic variables[16,17] or the deterministic evolution equations. In this context more detailed information about the exact structure of coarse-grained quantities obtained through a contraction or a projection is desirable.

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