ON THE EQUIVALENCE OF TIME-CONVOLUTIONLESS MASTER EQUATIONS AND GENERALIZED LANGEVIN EQUATIONS ☆

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For Langevin equations with colored random noise in either a retarded (Mori) form or in a time-instantaneous form we derive an exact closed time-convolutionless masterequation. We show the equivalence of an extension of the usual Markovian nonlinear Langevin equation with both, white Gaussian noise and white generalized Poisson noise to the Kramers–Moyal expansion and derive the fluctuation induced drift.

In the last years an ever increasing interest is paid to the modelling of statistical systems in terms of stochastic differential equations for macrovariables. By use of the projector method there have been many attempts to derive exact generalized Langevin equations starting from first principles [1,2]. In practice, however, these exact equations involve many difficulties connected with the evaluation of the microscopic expressions for e.g. memory kernels, transport coefficients etc. To overcome these difficulties one usually sets up phenomenological equations retaining the main structures of exact equations. In this context, a well known procedure is the description of collective variables in terms of a continuous Markov process either by Langevin equations driven with white Gaussian noise or equivalently by the corresponding Fokker–Planck equation. However the physical justification for such an approximation is often dubious and not well understood. Because of the large variety of factors responsible for the fluctuations an approach implying continuous and discontinuous sample paths generated from Markovian or even non-Markovian noise may be a better modelling.

The aim of this letter is to present the derivation of an exact closed time-convolutionless masterequation for the probability $p(z, t)$ of the process $z(t)$ described either by an equation of the form

$$\dot{z}(t) = a(z, t) + f(t) , \quad (1)$$

or a Mori-type equation

$$\dot{z}(t) = -\int_0^t \gamma(t-s)\, z(s)\, ds + f(t) , \quad (2)$$

where $\gamma(t-s)$ may contain an instantaneous contribution $a\delta(t-s^+)$. It is worth emphasizing that the random force in eq. (1) and eq. (2) may depend in general on the collective variable $z(t)$ (e.g. $f(t) = b(z, t)\,\xi(t)$) so that its stochastic properties may depend on the choice of the initial probability $p_0(z)$. We note that the solution for $z(t)$ are themselves functionals of the random force $f(s)$, $0 \leqslant s \leqslant t$.

In this letter we present only some main results. The details of the calculations and more general results will be presented elsewhere [3]. For the derivation of the masterequation the following correlation plays an important role

$$\langle f(r)\, g_t[z] \rangle , \quad 0 \leqslant r \leqslant t , \quad (3)$$

with $g_t[z] = g(z(\tau), 0 \leqslant \tau \leqslant t)$ some functional of the random process $z(\tau)$.

By use of the cumulants $K_n(t_1, ..., t_n)$ of the random force $f(t)$ one obtains for eq. (3) [3]

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$$\langle f(r)g_t[z]\rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^t ds_1 \dots \int_0^t ds_n K_{n+1}(r, s_1, ..., s_n)$$

$$\times \left\langle \frac{\delta^n g_t[z]}{\delta z(s_1) \dots \delta z(s_n)} \right\rangle . \tag{4}$$

With the auxiliary functional $\Omega_{t,r}[v]$

$$\Omega_{t,r}[v] = \frac{\delta \ln \phi_t[v]}{i\delta v(r)}, \quad 0 \le r < t , \tag{5}$$

where $\phi_t[v]$ denotes the characteristic functional

$$\phi_t[v] = \left\langle \exp i \int_0^t f(s) v(s) ds \right\rangle , \tag{6}$$

the result in eq. (4) can be rewritten in the compact form

$$\langle f(r)g_t[z]\rangle = \left\langle \Omega_{t,r}\left[\frac{\delta}{i\delta f}\right] g_t[z] \right\rangle, \quad 0 \le r < t . \tag{7}$$

The case with $r = t$ needs a special treatment. With the auxiliary functional $\Sigma_t[v]$

$$\Sigma_t[v] = \frac{1}{iv(t)} \frac{\partial}{\partial t} \ln \phi_t[v] \tag{8}$$

it is shown in [3] that

$$\langle f(t)g_t[z]\rangle = \left\langle \Sigma_t\left[\frac{\delta}{i\delta f}\right] g_t[z] \right\rangle . \tag{9}$$

Writing for the probability $p(z, t)$ the expectation

$$p(z, t) = \langle \delta(z(t) - z)\rangle , \tag{10}$$

where the averaging is over all realizations of $f(t)$ *and* the initial probability $p_0(z_0)$ we obtain the master-equation by differentiation with respect to the time t. For the sake of simplicity we first consider the processes described by eq. (1) for a linear system with $a(z(t), t) = \alpha z(t)$.

Observing the dynamical nature of $z(t)$ we obtain with eq. (9) and the relation

$$\frac{\delta}{\delta f(s)} \delta(z(t) - z) = -e^{\alpha(t-s)} \frac{\partial}{\partial z} \delta(z(t) - z) , \tag{11}$$

the closed masterequation for $p(z, t)$

$$\dot p(z, t) = -\alpha \frac{\partial}{\partial z} z p(z, t)$$

$$-\frac{\partial}{\partial z} \Sigma_t\left[i\, e^{\alpha(t-s)} \frac{\partial}{\partial z}\right] p(z, t) . \tag{12}$$

Note, that for nonlinear $a(z, t)$ the analogous result of eq. (12) can be obtained if we rewrite eq. (1) with the random force $f(t) \to \tilde f(t) = f(t) + a(z, t) - \alpha z$. Generally Σ_t in eq. (12) depends via the cumulants of $f(t)$ on the initial probability p_0. This shows clearly the non-Markovian character of the process $z(t)$ under consideration. If the noise $f(t)$ is z-independent we obtain a closed masterequation with a p_0-independent and hence linear generator $\Gamma(t)$ defined by eq. (12):

$$\dot p(t) = \Gamma(t) p(t) . \tag{13}$$

Then the kernal of the initial Greensfunction $G(t|0)$

$$G(t|0) = \mathcal{T} \exp \int_0^t \Gamma(s)\, ds \tag{14}$$

coincides with the initial non-Markovian conditional probability $R(z, t|z_0, 0)$ of the process [4]. As an example for eq. (13) we consider a z-independent Gaussian random force $f(t)$ with $\langle f(t)\rangle = a(t)$ and $\langle f(t)f(s)\rangle = c(t, s) + a(t)a(s)$. Noting that the operator Σ_t breaks off after the second cumulant we obtain for the generator $\Gamma(t)$ the Fokker–Planck-type result

$$\Gamma(t) = -\alpha\frac{\partial}{\partial z} z - a(t)\frac{\partial}{\partial z} + \int_0^t c(t, s)\, e^{\alpha(t-s)} ds \frac{\partial^2}{\partial z^2} . \tag{15}$$

Next we assume that $z(t)$ in eq. (1) is composed of in each timepoint independent increments. Only in this case it is guaranteed that the solutions of eq. (1) describe a Markov process [5], an important fact to which has not been paid attention in a recent related paper [6]. In particular we decompose the random force $f(t)$ in eq. (1) into two state dependent terms

$$f(t) = \gamma_G(z, t)\, \xi_G(t) + \gamma_P(z, t)\xi_P(t) , \tag{16}$$

with $\xi_G(t)$ a normalized white Gaussian process and $\xi_P(t)$ a white generalized Poisson process. By use of the functionals Σ_t of these processes [3] we obtain for the masterequation of the Markov process $z(t)$

$$\dot{p}(z,t) = -\frac{\partial}{\partial z} a(z,t) p(z,t) + \frac{1}{2}\left(\frac{\partial}{\partial z}\gamma_G(z,t)\right)^2 p(z,t)$$

$$+ \lambda \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} \langle x^n \rangle \left(\frac{\partial}{\partial z}\gamma_P(z,t)\right)^n p(z,t) . \quad (17)$$

Here λ denotes the parameter in Poisson's law and $\langle x^n \rangle$ are the higher moments of the statistically independent jump variables with vanishing mean in the generalized Poisson process. Eq. (17) can be recast in the form of the Kramers–Moyal expansion [7] with the moments $\alpha_n(z,t)$

$$\alpha_1(z,t) = a(z,t) + \tfrac{1}{2}\gamma_G(z,t)\frac{\partial \gamma_G(z,t)}{\partial z}$$

$$+ \lambda \sum_{m=2}^{\infty} \frac{\langle x^m \rangle}{m!} \gamma_P(z,t) D^{m-1}[\gamma_P^{m-1}(z,t)] , \quad (18)$$

$$\alpha_n(z,t) = \gamma_G^2(z,t)\delta_{n,2}$$

$$+ n!\,\lambda \sum_{m=n}^{\infty} \frac{\langle x^m \rangle}{m!} \gamma_P(z,t) D^{m-n}[\gamma_P^{m-1}(z,t)] ,$$

$$n \geq 2 .$$

Here we made use of the function D^j introduced by Bedeaux [6]

$$D^j[\gamma_P^n(z,t)] = \sum_{\substack{i_1,\ldots,i_{j+1} \\ i_1+\ldots+i_{j+1}=n}} \gamma_P^{i_1}\frac{\partial}{\partial z}\gamma_P^{i_2}\frac{\partial}{\partial z}\cdots\gamma_P^{i_{j+1}} . \quad (19)$$

The first moment contains the fluctuation induced (Stratonovitch) drift divided up into two terms the well known part induced by white Gaussian noise and the one induced by white generalized Poisson noise.

For the important class of Mori-type Langevin equations, eq. (2), the solution can be written in terms of the Greens-function $\chi(t)$ satisfying

$$\dot{\chi}(t) = -\int_0^t \gamma(t-s)\,\chi(s)\,\mathrm{d}s , \quad \chi(0) = 1 . \quad (20)$$

Noting that

$$\frac{\delta}{\delta f(s)}\,\delta(z(t)-z) = -\chi(t-s)\frac{\partial}{\partial z}\delta(z(t)-z) \quad (21)$$

one can set up a closed masterequation which with $p_0(z) = \delta(z - z_0)$ explicitly depends on the initial condition z_0 [3]. Here we restrict the discussion to the case that the "correlation" $\chi(t)$ after a partial coarse graining in time takes on only positive values. Eq. (2) can then be transformed into an exact time-convolutionless form

$$\dot{z}(t) = \frac{\dot{\chi}(t)}{\chi(t)} z(t) + \chi(t)\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\chi(t-r)}{\chi(t)} f(r)\,\mathrm{d}r . \quad (22)$$

In terms of the operators $\Omega_{t,r}[\mathrm{i}\chi(t-s)(\partial/\partial z)]$ and $\Sigma_t[\mathrm{i}\chi(t-s)(\partial/\partial z)]$ one can derive again a closed masterequation. For example, using the stationary z-independent Gaussian noise with $\langle f(t) \rangle = 0$ which fulfills the 2nd fluctuation dissipation theorem [8]

$$\langle f(t) f(s) \rangle = c\gamma(|t-s|) , \quad (23)$$

we obtain for the linear generator $\Gamma(t)$ in presence of an external deterministic force $K(t)$ coupled additively into eq. (2) after a somewhat laborous but straight forward calculation the simple result

$$\Gamma(t) = -\frac{\dot{\chi}(t)}{\chi(t)}\left[\frac{\partial}{\partial z} z + c\frac{\partial^2}{\partial z^2}\right]$$

$$- \chi(t)\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\chi(t-s)}{\chi(t)} K(s)\,\mathrm{d}s\,\frac{\partial}{\partial z} . \quad (24)$$

Note that the effect of the perturbation is given only by the last term ($f(t)$ does not depend on $K(s)$ by assumption) in form of a linear functional which involves in contrast to the Markov case ($\chi(t) = e^{-\gamma t}$) the whole prehistory of $K(s)$ as well.

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