ON THE EQUIVALENCE OF TIME-CONVOLUTIONLESS MASTER EQUATIONS
AND GENERALIZED LANDÉGREN EQUATIONS

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For Langevin equations with colored random noise in either a retarded (Markov) form or in a time-instantaneous form we derive an exact closed time-convolutionless master equation. 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 Kramer-Moyal expression 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 even non-Markovian noise may be a better modeling.

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

\[
\dot{z}(t) = a(z, t) + f(t),
\]

or a Markov-type equation

\[
\dot{z}(t) = - \int_{t}^{\infty} \gamma(t-s) \dot{z}(s) ds + f(t),
\]

where \( \gamma(t) \) may contain an instantaneous contribution \( \delta(t-t') \). 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. \( f(t) \sim b(z, t) \Psi(t) \)) so that its stochastic properties may depend on the choice of the initial probability \( p_{0}(z) \).

We note that the solution for \( x(t) \) are themselves functions of the random force \( f(t) \), \( 0 < t \leq T \).

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 master equation the following correlation plays an important role

\[
\langle f(t) r(t') \rangle, \quad 0 < t < T,
\]

with \( \langle z(t) \rangle = \Psi(t), \quad 0 < t < T \) some functional of the random process \( z(t) \).

By use of the cumulants \( K_{n}(t_{1}, ..., t_{n}) \) of the random force \( f(t) \) one obtains for eq. (3) [3]
\[ \langle \psi | \hat{H} | \psi \rangle = \sum_{\mathbf{r}} \langle \mathbf{r} | \hat{H} | \mathbf{r} \rangle = \sum_{\mathbf{r}} \langle \mathbf{r} | \hat{V} | \mathbf{r} \rangle + \sum_{\mathbf{r} \neq \mathbf{s}} \langle \mathbf{r} | \hat{V} | \mathbf{s} \rangle, \]

where \( \hat{V} \) is the interaction Hamiltonian.

With the auxiliary functional \( \Omega_{\rho}[\psi] \)
\[ \Omega_{\rho}[\psi] = \int \psi \hat{V} \psi \, d^3 \mathbf{r}, \quad \rho > 0 < \tau, \]

where \( \rho \) denotes the characteristic functional
\[ \rho[\psi] = \left\{ \exp \left[ \int \frac{1}{2} \psi \hat{V} \psi \, d^3 \mathbf{r} \right] \right\}, \]

the result in eq. (4) can be rewritten in the compact form
\[ \langle \psi | \hat{H} | \psi \rangle = \left\{ \int \frac{1}{2} \psi \hat{V} \psi \, d^3 \mathbf{r} \right\} \rho[\psi], \quad \rho > 0. \]

The case with \( \rho = \tau \) needs special treatment. With the auxiliary functional \( \Sigma_{\rho}[\psi] \)
\[ \Sigma_{\rho}[\psi] = \int \frac{1}{2} \psi \hat{V} \psi \, d^3 \mathbf{r}, \quad \rho > 0 < \tau, \]

it is shown in eq. (9) that
\[ \langle \psi | \hat{H} | \psi \rangle = \left\{ \int \frac{1}{2} \psi \hat{V} \psi \, d^3 \mathbf{r} \right\} \rho[\psi], \]

Wiring for the probability \( p(\psi, t) \) the expectation
\[ \langle \psi, t | \hat{H} | \psi, t \rangle = \langle \psi | \hat{H} | \psi \rangle, \]

which is the meaning of all realizations of \( \hat{H} \) and the initial probability \( p(\psi, 0) \).

The relation of eq. (9) for a bosonic system with \( \Delta(\mathbf{r}, t) = \Delta(\mathbf{r}) \)

Using the dynamical nature of \( \Delta(\mathbf{r}, t) \) we obtain with eq. (9) and the relation
\[ \langle \Delta(\mathbf{r}, t) \rangle = \langle \Delta(\mathbf{r}) \rangle \]

The closed maxima for the \( \Delta(\mathbf{r}, t) \)

Note that for potentials \( \mathcal{F} \), the subsequent result of eq. (12) can be obtained if we rewrite eq. (7) with the symmetrical force \( \mathcal{F}(\mathbf{r}) + \mathcal{F}(\mathbf{r}) = \mathcal{F}(\mathbf{r}) + \mathcal{F}(\mathbf{r}) \) and \( \rho > 0 < \tau \). Generally, eq. (12) depends on the cumulants of \( \mathcal{F}(\mathbf{r}) \) on the initial probability \( \rho[\psi] \). This shows clearly the non-Markovian character of the process \( \hat{H} \) under consideration. If the noise \( \mathcal{F}(\mathbf{r}) \) is independent, we obtain a closed maximization with \( \rho[\psi] \) independent and bosonic Green function \( \tilde{\rho}(\mathbf{r}, t) = \tilde{\rho}(\mathbf{r}) \).

The kernel of the initial Green function \( \tilde{\rho}(t, 0) \)

\[ \tilde{\rho}(t, 0) = \int \exp \left\{ \int_0^t \mathcal{F}(\mathbf{r}, t) \, dt \right\} \tilde{\rho}(0) \]

concludes with the initial non-Markovian conditional probability \( \rho[\psi, t, 0] \) of the process [1]. As an example for eq. (13) we consider a 2-dependent Gaussian random force \( \mathcal{F}(\mathbf{r}) \) with \( \mathcal{F}(\mathbf{r}) = \mathcal{F}(\mathbf{r}) \) and \( \mathcal{F}(\mathbf{r}, t) = \mathcal{F}(\mathbf{r}, t) + \mathcal{F}(\mathbf{r}, t) \) and \( \tilde{\rho}(t, 0) = \tilde{\rho}(t, 0) \) and \( \tilde{\rho}(t, 0) = \tilde{\rho}(t, 0) \). Noting that the operator \( \Sigma_{\rho} \) breaks off after the second cumulant we obtain for the generator \( \mathcal{E}(t) \) the Fokker–Planck-type result

\[ \mathcal{E}(t) = \frac{3}{2} \mathcal{F}(t) + \int \mathcal{F}(t) a(x, t) \, dx, \quad \mathcal{F}(t) = \mathcal{F}(t) \]

Note that \( \tilde{\rho}(t) \) in eq. (12) is composed of all time-independent functions. Omitting this in the solution of eq. (12) results in a Markov process [3], an important fact to which has not been paid attention in recent related papers [4]. A particular case is considered in the random force \( \mathcal{F}(\mathbf{r}, t) \) in eq. (13) two-state dependent random

\[ \mathcal{F}(\mathbf{r}, t) = \mathcal{F}(\mathbf{r}) \tilde{\rho}(t, 0) + \mathcal{F}(\mathbf{r}) \tilde{\rho}(t, 0) \]

with \( \tilde{\rho}(t, 0) \) a normalized white Gaussian process and \( \tilde{\rho}(t, 0) \) is a white Gaussian Poisson process. By using of the functional \( \Sigma_{\rho} \) of these processes [3], we obtain for the non-Markov process of the Markov process \( \tilde{\rho}(t) \)
Here λ denotes the parameter in Poisson’s law and \( \gamma(t) \) are the higher moments of the statistically independent jump variables with varying mean in the generalized Poisson process. Eq. (17) can be cast in the form of the Kramers–Moyal expansion \[ \gamma(t) \] with the moments \( \alpha_r(t) \) given by

\[ \alpha_r(t) = n \frac{\partial}{\partial t} \gamma(t, t) + \frac{n^2}{2} \frac{\partial^2}{\partial t^2} \gamma(t, t) \]

(18)

\[ \alpha_r(t) = \alpha_r(t) + \frac{n^2}{2} \frac{\partial^2}{\partial t^2} \gamma(t, t) \]

(19)

Hence we use the function \( D' \) introduced by Baxandall [12].

\[ D'[\gamma(t, t)] = \sum_{n=1}^{\infty} \frac{n}{n!} \gamma(t, t) \frac{\partial}{\partial t} \gamma(t, t) \]

(20)

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

For the important case of the Kramers-Moyal equations, Eq. (2), the solution can be written in terms of the Greens function \( G(x) \) satisfying

\[ \frac{d}{dx} G(x) + x G(x) = 0 \]

(21)

Noting that

\[ \frac{d}{dx} G(x) + x G(x) = 0 \]

(22)

one can set up a closed master equation which with \( n \alpha_r(t) + \frac{n^2}{2} \alpha_r(t) \) explicitly depends on the initial condition \( \gamma(0) \). Here we restrict the discussion to the case that the “correlation” \( \gamma(t) \) after a partial course growing in time takes on only positive values. Eq. (22) can then be transformed into an exact time-convolutionless form

\[ \phi(t) = \int_0^t \frac{d\tau}{X(\tau)} \phi(\tau) G(x) \frac{d}{dx} X(\tau) \]

(23)

In terms of the operators \( \Phi_0(x) \) and \( \Sigma_0(x) \) one can derive again a closed master equation. For example, using the stationary \( z \)-independent Gaussian noise with \( \langle q(t) \rangle = 0 \) which fulfills the 2nd fluctuation dissipation theorem

\[ \langle q(t) q(t - \tau) \rangle = c \tau \]

(24)

we obtain for the linear generator \( G(\tau) \) in presence of an external deterministic force \( K(x) \) coupled additively into eq. (2) after a somewhat laborious but straightforward calculation the simple result

\[ \Gamma(\tau) = -\frac{\partial}{\partial x} \left( \frac{d}{dx} \right) \]

(25)

Note that the effect of the perturbation is given only by the last term \( \langle f(t) \rangle \) does not depend on \( K(x) \) by assumption in form of a linear functional which involves in contrast to the Markov case \( \langle f(t) \rangle = c \tau \) the whole prehistory of \( K(x) \) at well.

References