Fokker-Planck equations for time-delayed systems via Markovian Embedding

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For stochastic systems with discrete time delay, the Fokker-Planck equation (FPE) of the one-time probability density function (PDF) does not provide a complete, self-contained probabilistic description, as it explicitly involves the two-time PDF. We here introduce a new approach to find a Fokker-Planck description by using a Markovian embedding technique and a subsequent limiting procedure. On this way, we derive a hierarchy of FPEs whose first member is the well-known FPE for the one-time PDF. Moreover, as second member we obtain a new equation for the two-time PDF. The latter gives the correlation between the present and the delayed time and is thus a central quantity in the description of these time-delayed, non-Markovian systems. From a conceptual point of view, our approach yields interesting insight into both, the physical meaning, and the mathematical structure of delayed processes. We further propose a possible approximation scheme basing on this new equation.

1 Introduction

Predicting stochastic dynamics far from thermal equilibrium is a major goal of statistical physics and a key step towards an understanding of realistic, fluctuation-dominated systems from biology, chemistry, or socio-economics, just to name a few of the many fields of application. An important mechanism that drives system out of equilibrium and, at the same time, renders the dynamics non-Markovian is time delay. Delays can have various origins, such as unavoidable signal transmission time lags (e.g., in laser systems [1, 2]), information processing times (as in neural systems [3–6]), or decision making times (e.g., in the context of financial markets [7, 8]). Moreover, they are omnipresent in systems subject to feedback control [9–18]. In many cases, it is sufficient and suitable to model such processes by including a single, discrete delay and a white noise. This is the situation considered in this paper. Discrete delays are known to induce complex behavior (e.g., delay-induced oscillations, chaos), and, on the other hand, to stabilize unstable orbits [19–21]. Therefore, they are often implemented intentionally, for example in the framework of Pyragas control [22]. We note that the time-delayed systems considered here are different from those modeled by generalized Langevin equations [23]. The latter involve a memory kernel in the deterministic (friction) force resulting from conservative interactions between a colloidal particle (or, more generally, a “slow” variable) and the bath particles (as well as among the bath particles). This delayed friction is related to the noise via a fluctuation-dissipation relation [24] (see, e.g., [25–28]). In contrast, the systems considered here involve a discrete delay within a deterministic force, and there is no relation to noise correlations.

While they have numerous applications, the mathematical description of time-delayed stochastic systems is still far from being complete. The Langevin equation (LE) is used to model such processes on a stochastic level, but it is infinite-dimensional due to the discrete delay. Exact analytical results based on the LE have, so far, been obtained only for linear systems [29]. On the other hand, the Fokker-Planck (FP) description for the probability density function (PDF), which we focus on in this paper, is given by an infinite hierarchy of coupled equations of increasing complexity [30–33]. As shown by Frank [30] (who only considered the first member), this hierarchy can be derived using Novikov’s theorem [34]. The first member of the FP hierarchy (originally derived by Guillouzic et al. [35]) is the FP equation (FPE) for the one-time PDF. It explicitly involves the two-time PDF for the spatio-temporal correlations between times \( t \) and \( t - \tau \), with \( \tau \) being the delay time. Although not being self-sufficient, the equation for the one-time PDF has proven itself to be quite useful for the analytical treatment. On the one hand, it is an important tool in the search for exact results [36–37]. Moreover, on the base of this FPE different approximation schemes have been developed in the past years (see [31] for

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an overview. Examples are the perturbation theory \[35\] and the “force-linearization closure” \[31, 37\], both of which yield reasonable approximations for the one-time PDFs in quite large parameter regimes. (As opposed to this, the so called small $\tau$ expansion \[35\], which is based on the LE, is only appropriate for very small values of the delay time, where the system behaves more or less like a Markovian one.)

While these analytical results have indeed contributed to an understanding of delayed processes, major challenges remain. In particular, the insights provided by the one-time PDF alone are admittedly limited as we deal with non-Markovian dynamics, which is crucially determined by memory, and, hence, temporal correlations. Having this in mind, it is not surprising that many non-Markovian effects are only captured by two-time PDFs (or higher PDFs). In fact, only by studying them, non-Markovian steady-states can be qualitatively distinguished from thermal equilibria at all \[31\]. Moreover, the two-time PDF is essential to obtain stochastic thermodynamical quantities like the fluctuating heat, work, or entropy \[39\]. As an example, the distinguished from thermal equilibria at all PDFs (or higher PDFs). In fact, only by studying them, non-Markovian steady-states can be qualitatively

This paper is organized as follows. First, we review earlier derivations of the FPE known from the literature. Then, we discuss the Markovian embedding and show how the delayed FPE can be derived from it by marginalization. We further discuss the higher members stemming from this approach, particularly focusing on the second member, which are different from those obtained by earlier approaches. In the appendix, we show how the second member of our hierarchy can be transformed into the one obtained from Novikov’s theorem, \[34\]. Explicitly considering the second member, we show how the two hierarchies can be converted into each other.

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2 Langevin equation and Fokker-Planck equation for delayed systems

We consider a system described by a stochastic delay differential equation, in particular, by the overdamped LE

$$dX(t) = F[X(t), X(t-\tau)]dt + \sqrt{2D_0}dW(t), \quad (1)$$

with $X \in \Omega = [\omega_1, \omega_2] \subset \mathbb{R}$ and time $t > 0$. $F$ denotes the deterministic force given by some (generally nonlinear) function depending on the instantaneous and on the delayed system state, $X(t)$ and $X(t-\tau)$, with $\tau \geq 0$ being the single discrete time delay. $W$ is a Wiener process with independent increments, $\langle W \rangle = 0$, and $\langle W(t)W(t') \rangle = \min(t,t')$, generated by the additive Gaussian white noise $\xi$, with $\langle \xi \rangle = 0$, $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$. Thereby, $\langle \ldots \rangle$ denotes the ensemble average (i.e., average over all noise realizations), w.r.t. a given initial condition. The latter is specified by a history function $\phi(\tau \leq t \leq 0)$, i.e., $X(t) = \phi(t), t \in [-\tau, 0]$, which can be fixed for the entire ensemble or be drawn from a distribution $P(\phi)$. $D_0$ is the (constant) strength of the noise. We further consider natural boundary conditions (details are given below).

\[\text{As an illustrative example, consider the following. Let } \rho_1^M(x) \text{ be the non-Markovian one-time PDF of an arbitrary nonequilibrium steady state. This PDF can in general not be distinguished from a PDF }\rho_1^M(x) \text{ of a Markovian (equilibrium) process in a (fictive) potential defined by } U_{\text{ fictive}}(x) \equiv k_B T \ln \rho_1^M(x), \text{ which would equally yield a distribution } \rho_1^M = Z^{-1} e^{-U_{\text{ fictive}}/k_B T} = \rho_1^M.\]
The FP description provides a complementary way to model the process on the probabilistic level. It is well-known that the FPE for the one-time PDF related to (1) reads \[\rho_N(x,t) = \int_{\mathbb{R}} \frac{1}{(2\pi)^{D/2}} e^{-\frac{1}{2} \sum_{j=1}^D (x_j - \mu_j(t))^2} \, dx_0 \bigg|_{x_0 = x} \] where \(\rho_N(x,t)\) is the \(N\)-time PDF (with normalization \(\int_{\mathbb{R}^N} \rho_N(x,t) \, dx = 1\)). As opposed to Markovian dynamics, the FPE is not self-sufficient. In the following, we briefly review earlier work, in particular Refs. [30, 50, 51], in order to better understand the technical and conceptual difference of our approach.

### 2.1 Second member of the Fokker-Planck hierarchy from Novikov’s theorem

In this section, we briefly review the approach [30, 31] based on Novikov’s theorem [26] (a short derivation of the latter is given in the Appendix [3]). Besides leading to (2), this approach can also be used to obtain the FPE for \(\rho_2\) and, in general, \(\rho_N, N \in \mathbb{N}\). It renders an infinite hierarchy of coupled equations of increasing complexity, whose \(N\)th member involves both, the \(N\)-time (joint) PDF \(\rho_N(x,t; x_0, x_1, t-\tau; ...; x_N, t-N\tau)\) and the \((N+1)\)-time PDF \(\rho_{N+1}\). It should be noted, however, that the higher members (starting from the second one) contain functional derivatives w. r. t. the noise, which need to be obtained separately from the LE. For example, the second member reads

\[
\partial_t \rho_2(x,t; x_0, x_1, t-\tau) = -\partial_x \left\{ F(x_0, x_1) \rho_2(x_0, x_1, t-\tau) \right\} - \partial_{x_0} \left\{ F(x_0, x_1) \rho_3(x_0, x_1, t-\tau; x_2, t-2\tau) \right\} + D_0 \left( \partial_{x_0}^2 + \partial_{x_1}^2 \right) (\partial_t + \partial_{x_2}^2) \rho_2(x_0, x_1, t-\tau) \tag{3}
\]

(see [31] for a derivation). This equation resembles a Markovian FPE of a two-dimensional (or two-particle) process in the variables \(x, x_2\), with the exception of the term which involves a derivative w. r. t. the noise. For the special case of linear forces, the latter can be calculated using the method of steps [64], see Appendix [3]. However, to the best of our knowledge, this functional derivative is unknown for general nonlinear forces. We note that this term stems from the fact that if \(X(t)\) and \(X(t-\tau)\) are regarded as “two” random processes, then these processes are not only connected by the force \(F\) (via the LE), but additionally by the fact that the corresponding noise processes \(\xi(t)\) and \(\xi(t-\tau)\) are identical with time-shift \(\tau\). To elucidate this last point, we briefly review an alternative derivation of the FPE known from the literature, which does not yield this term, but instead imposes additional constraints on the solutions.

The mentioned approach is used in [50, 51] to derive a FPE for \(\rho_1\). Here we extended it towards the higher members of the hierarchy. The approach uses a description with two time arguments \(j, z\). In particular, an integer \(j = 0, 1, 2, \ldots\) counts the number of intervals of length \(\tau\) that have passed since the beginning \(t = 0\), and a continuous variable \(z \in [0, \tau]\) measures the time within the current interval. Then, auxiliary phase-space variables \(X_{j\tau}(z) := X(z + j\tau)\) are introduced, which, by construction, all follow a LE of the identical form

\[
dX_{j\tau}(z) = F[X_{j\tau}(z), X_{(j-1)\tau}(z)] \, dz + \sqrt{2D_0} \, dW_{j\tau}(z). \tag{4}
\]

(If one is interested in steady-state dynamics, \(j \to \infty\).) A sketch of the construction of the auxiliary variables is given in Fig. [1]. In the probability space belonging to the phase space \(\{X_0(z), \ldots, X_N(z)\}\), the process is Markovian, and the corresponding FPE reads

\[
\partial_z \rho_{N+1} + \sum_{j=1}^N \left[ -\partial_x \left\{ F(x_{j\tau}, x_{(j-1)\tau}) \rho_{N+1} \right\} + D_0 \partial_{x_{j\tau}}^2 \rho_{N+1} \right] = \partial_{x_{N\tau}} \left[ F(x_{N\tau}, x_{(N-1)\tau}) \rho_{N+1} \right] + D_0 \partial_{x_{N\tau}}^2 \rho_{N+1}, \tag{5}
\]

with \(\rho_{N+1}(x_{0\tau}, x_{1\tau}, \ldots, x_{N\tau}, z) = \int [\delta[x_{0\tau} - X(z)] \delta[x_{1\tau} - X(z + \tau)] \ldots \delta[x_{N\tau} - X(z + N\tau)] \, dx_{0\tau}] \). By integrating the equation over the entire domain of all variables but the first (and the last) one, this many-variable FPE can be used to derive the FPE (2) for \(\rho_1\), and a FPE for \(\rho_2\), reading

\[
\partial_t \rho_2 = -\partial_x \left\{ F(x, x_2) \rho_2 \right\} - \partial_{x_2} \int \left\{ F(x, x_2) \rho_2 \right\} \, dx_{2\tau} + D_0 \left( \partial_x^2 + \partial_{x_2}^2 \right) \rho_2. \tag{6}
\]
with \( \rho_2(x,t;x,\tau, t-\tau) \) and \( \rho_3(x,t;x,\tau, t-\tau; x_2 \tau, t-2\tau) \). As opposed to \( \rho_1 \) (from Novikov’s theorem), this equation lacks the term with the unknown functional derivative. This is because the stochastic set of equations \( \rho_3 \) is, in fact, only equivalent to the delayed process, if one further imposes additional constraints \( X_j(\tau)=X_{j+1}(0), \forall j \), ensuring that the end point of the stochastic trajectories on \([j\tau, (j+1)\tau]\) matches the starting point on \([j\tau, (j+2)\tau]\). Translating these constraints to the level of PDFs is a non-trivial task on its own, thus, the usefulness of these equations as a starting point for approximation schemes is very limited.

**Figure 1:** Sketch of the different ways to introduce auxiliary variables, left: within the approach based on two time arguments \( j \), right: within the Markovian embedding approach \( j \).

### 3 Markovian embedding

As an alternative approach to formulate a complete FP description and to derive the FPE \( \rho_2 \), we here employ the Markovian embedding technique \( \rho_4, \rho_5 \), as also suggested in earlier literature \( \rho_6 \). The key idea is to introduce \( n \in \mathbb{N} \) auxiliary variables \( X_j \) (with one of them replacing the delayed system state in the original equation), giving rise to a \((n+1)\)-dimensional Markovian system that generates the same dynamics as the original delay equation (which is hence “embedded” in that extended system). Specifically, we consider the set of dynamical equations given by \( \rho_7 \)

\[
\begin{align*}
\dot{X}_0(t) &= F(X_0(t), X_n(t)) + \sqrt{2D_0} \xi(t) \quad \text{(7a)} \\
\dot{X}_j(t) &= \left(\frac{n}{\tau}\right)[X_{j-1}(t)-X_j(t)] \quad \text{(7b)}
\end{align*}
\]

with \( j \in \{1,2,\ldots,n\}, \ t \geq -\tau, \ X_j \in \mathbb{R} \) and the initial conditions \( X_{j \in \{1,\ldots,n\}}(-\tau) \equiv 0 \) (see Appendix \( \rho_A \) for a discussion of the initial conditions). Projection of \( \rho_7 \) onto the variable \( X_0 \) (see Appendix \( \rho_A \) for details) yields

\[
\dot{X}_0(t) = F \left[ X_0(t), \int_{-\tau}^{t} K(t-s)X_0(s) \, ds \right] + \sqrt{2D_0} \xi(t) \label{8a},
\]

with the Gamma-distributed memory kernel

\[
K_n(t-s) = \left(\frac{n}{\tau}\right)^n \frac{(t-s)^{n-1}}{(n-1)!} e^{-n(t-s)/\tau}. \label{8b}
\]

In the limit \( n \to \infty \), the kernel collapses onto a delta peak centered at \( \tau \), i.e., \( K_n(t-s) \to \delta(t-s-\tau) \). Then, the projected equation \( \rho_8 \) becomes identical to the original, delayed LE \( \rho_1 \), with

\[
\begin{align*}
X_0(t) &= X(t), \quad \text{(9a)} \\
X_n(t) &= X(t-\tau). \quad \text{(9b)}
\end{align*}
\]

In addition to \( \rho_9 \), also the other auxiliary variables can be linked to the variable \( X \) of the delayed LE \( \rho_1 \). In particular, using the difference quotient to approximate \( \dot{X}_j \) in the dynamical Eqs. \( \rho_7 \), that is, \( [X_{j-1}(t)-X_j(t)](n/\tau) = \dot{X}_j(t) \approx [X_j(t+\Delta t)-X_j(t)]/\Delta t \), gives rise to the interpretations \( \Delta t = \tau/n \), and \( X_j(t+\Delta t) \approx X_j(t) \). Iteration implies \( X_j(t+j\tau/n) \approx X_{j-i}(t) \). In combination with Eq. \( \rho_{8a} \), this ultimately reveals

\[
X_j(t) = X(t-j\tau/n), \quad \forall j \in \{0,1,2,\ldots,n\}
\]

which becomes accurate in the limit \( n \to \infty \) (at \( \Delta t \to 0 \) the difference quotient equals the differential quotient).

The here presented scheme of rewriting the delayed differential equation as a set of non-delayed ones is called the linear chain trick \( \rho_7, \rho_{39} \). A schematic visualization of the system described by \( \rho_7 \) is given in Fig. \( \rho_2 \). Importantly, the \( n \) auxiliary variables generally follow linear Eqs. \( \rho_7 \), even if the delayed process itself involves nonlinear forces, \( F \). Furthermore, their dynamical equations are deterministic, as opposed to \( X_0 \) which is subject to the white noise term \( \xi \) [see \( \rho_{7a} \)]. We stress that the set of auxiliary variables \( \rho_{10} \) is different from the one \( \rho_1 \) used in the earlier approach. A direct comparison is provided in Fig. \( \rho_1 \).

Next, we will use the Markovian embedding to find a probabilistic description of the delayed system.

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\( \rho_i \): Various symbols and expressions used throughout the text.
3.1 Fokker-Planck equation of the Markovian \((n + 1)\)-dimensional system

The Markovian \((n + 1)\)-dimensional system given by the set of coupled LEs (7), can also be described by the FPE

\[
\frac{\partial \rho_{n+1}}{\partial t} = - \frac{\partial}{\partial x_0} [F(x_0, x_n)\rho_{n+1}] - \sum_{j=1}^{n} \frac{\partial}{\partial x_j} [(x_{j-1} - x_j)\rho_{n+1}] + D_0 \frac{\partial^2}{\partial x_{n+1}^2} \rho_{n+1}
\]

for the \((n + 1)\)-point (joint) PDF \(\rho_{n+1}(x_0, t; x_1, t; \ldots; x_n, t) = \langle \delta[x_0 - X_0(t)]\delta[x_1 - X_1(t)]\ldots\delta[x_n - X_n(t)] \rangle\). Importantly, \(n\) is considered to be a finite value here. Finding a mathematical framework in which the limit \(n \to \infty\) of Eq. (11) is meaningful and well-defined, is subject of ongoing work. Indeed, it is not clear how to formulate a Fokker-Planck equation on an infinite-dimensional space. Moreover, since one drift term is in fact proportional to \(n\) itself, this limit is highly non-trivial. Here, we can safely ignore this problem, since we focus on the equations for the marginalized (low-dimensional) PDFs. As shown in Secs. 4 and 5, they can be derived by keeping \(n\) finite and performing the limit only after the marginalization.

Equation (11) resembles the FPE of a many-particle system. However, in sharp contrast to a system of interacting (colloidal) particles, the “interactions” are here unidirectional (see Fig. 2), which means that the “particle” \(x_j\) only feels the “particle” \(x_{j-1}\) and not vice-versa. Hence, the forces between them are non-Newtonian (violating Newton’s 3rd law) and cannot be described by an interaction potential.

4 Derivation of first member of Fokker-Planck hierarchy via Markovian embedding

4.1 Marginalization

In the following, we show that the delayed FPE for \(\rho_1\) can be derived by a “coarse-graining” of (11) in the limit \(n \to \infty\). To be more specific, we marginalize the FPE (11) for the joint PDF, that is we integrate it over the whole domain of all \(n\) auxiliary variables, i.e., \(\int \int \ldots \int \Omega \, dx_1 dx_2 \ldots dx_n\), and, therewith obtain an equation for the marginal PDF. Importantly, we take the limit \(n \to \infty\) only after the marginalization. We further use natural boundary conditions at the endpoints of the domain \(\Omega = [\omega_1, \omega_2]\) specified by

\[
\lim_{x_j \to \omega_1, 2} \rho_m(x_j, \ldots) = \lim_{x_j \to \omega_1, 2} \partial_{x_j} \rho_m(x_j, \ldots) = 0, \quad \forall j, m,
\]

which are justified in most physical scenarios. For sake of a shorter notation, we will omit the time arguments of the PDFs in lengthy expressions. The terms (I – III) in Eq. (11) can be readily marginalized to

\[
(I) \to \partial_t \rho_1(x_0, t), \quad (II) \to - \frac{\partial}{\partial x_0} \int_{\Omega} [F(x_0, x_n)\rho_2(x_0, t; x_n, t)] \, dx_n, \quad (III) \to \frac{\partial^2}{\partial x_{n+1}^2} \rho_1(x_0, t).
\]

The remaining drift terms (IV) in Eq. (11) can be simplified by making use of their linearity w. r. t. the various \(x_j\) (please note that they are always linear as a result of the linearity in (11) despite of the fact that \(F\) is, in...
general, nonlinear). By application of the product rule and the natural boundary conditions, we first find

\[ (IV) \rightarrow \frac{n}{\tau} \left\{ n\rho_1(x_0) - \sum_{j=2}^{n} \int_{\Omega} x_j \partial x_j \rho_3(x_0; x_{j-1}; x_j) dx_j dx_{j-1} + \sum_{j=2}^{n} \int_{\Omega} x_j-1 \rho_3(x_0; x_{j-1}; x_j) \right\}_{x_0}^{x_j} dx_{j-1} \]

\[ - \int_{\Omega} x_1 \partial x_1 \rho_2(x_0; x_1) dx_1 + x_0 \left[ \rho_2(x_0; x_1) \right]_{x_0}^{x_2} \right\}. \]  

(12b)

The remaining integrals can be treated by partial integration and then, again, application of the boundary conditions, resulting in

\[ (IV) \rightarrow \frac{n}{\tau} \left\{ n\rho_1(x_0) - \sum_{j=2}^{n} \int_{\Omega} \rho_2(x_0; x_j) dx_j - \int_{\Omega} \rho_2(x_0; x_1) dx_1 \right\} = 0. \]  

(12c)

Hence, the contribution to the drift term of the entire sum vanishes, and we obtain in total from (12a) and (12c)

\[ \partial_t \rho_1(x_0, t) = -\partial_{x_0} \int_{\Omega} F(x_0, x_n) \rho_2(x_0; x_n) dx_n + D_0 \partial_{x_0}^2 \rho_1(x_0, t). \]  

(13)

So far, the marginalized FPE (13) still pertains to a finite (but arbitrary) value of \( n \in \mathbb{N} \). As a last step, we take the limit. To this end, we recall the meaning of the respective stochastic variables in this limit [Eq. (9)]. Based on that we perform the phase space transformation \( \{x_0, t\} \rightarrow \{x, t\} \) and \( \{x_n, t\} \rightarrow \{x, t - \tau\} \). Therewith, we finally obtain the delayed FPE for the one-time PDF \( \rho(2) \). Next, we demonstrate that our procedure can also be applied to find higher members of the FP hierarchy.

5 Derivation of higher members via Markovian embedding

In the following, we use the Markovian embedding procedure to derive a FPE for the two-time PDF \( \rho_2(x, t; x_\tau, t - \tau) \). This is a particularly important quantity in the description of delayed processes, as it explicitly describes the correlation between the delayed and present time. To this end, we again start from the FPE (11) of the \( n \)-variable system. This time, we marginalize w.r.t. all auxiliary variables but the last one, keeping \( n \) again finite until the marginalization is completed. We do not integrate over \( x_n \) as this variable represents \( X(t - \tau) \) in the limit \( n \rightarrow \infty \). In a second step, we will perform a coordinate transformation to take the limit.

5.1 Marginalization

It is easily seen that the marginalization of (I–III) in Eq. (11) yields

\[ (I) \rightarrow \partial_t \rho_2(x_0; x_n), \quad (II) \rightarrow -\partial_{x_0} \left[ F(x_0, x_n) \rho_2(x_0; x_n) \right], \quad (III) \rightarrow D_0 \partial_{x_0}^2 \rho_2(x_0; x_n). \]  

(14)

For the remaining part of the drift term,

\[ (IV) \rightarrow \frac{n}{\tau} \sum_{j=1}^{n} \int_{\Omega} \cdots \int_{\Omega} \partial_{x_j} \left\{ (x_j - x_{j-1}) \rho_{j+1}(x_0; x_1; \ldots; x_n) \right\} dx_j \cdots dx_{n-1}, \]  

(15a)

it is easiest to treat the summands \( j = 1, 1 < j < n \), and \( j = n \) separately. The summand with \( j = 1 \) can be simplified by partial integration and subsequent application of the boundary conditions, yielding

\[ \int_{\Omega} \cdots \int_{\Omega} \left\{ \rho_{n+1} + (x_1 - x_0) \partial_{x_1} \rho_{n+1} \right\} dx_1 \cdots dx_{n-1} = \rho_2(x_0; x_n) + \int_{\Omega} x_1 \partial_{x_1} \rho_3(\ldots) dx_1 - x_0 \left[ \rho_3(x_1, \ldots) \right]_{x_0}^{x_2} \]

\[ = \rho_2(x_0; x_n) + \left[ x_1 \rho_3(x_1, \ldots) \right]_{x_0}^{x_2} - \rho_2(x_0; x_n) = 0. \]  

(15b)

Analogously, we find for the summands \( 1 < j < n \),

\[ (n - 2) \rho_2(x_0, x_n) + \sum_{j=2}^{n-1} \int_{\Omega} \left\{ x_j \rho_4(\ldots) \right\} dx_j - \int_{\Omega} \rho_4(\ldots) dx_j - x_{j-1} \left[ \rho_4(x_j, \ldots) \right]_{x_0}^{x_2} \]  

\[ dx_{j-1} = 0. \]  

(15c)
While the summands \( j < n \) vanish \((15b, 15a)\), the summand \( j = n \) in \((15a)\) gives a contribution to \((IV)\), yielding

\[
(IV) \rightarrow \partial_{x_n} \left[ \int_{\Omega} \frac{n}{\tau} (x_n - x_{n-1}) \rho_3(x_0, x_n - 1, x_n)dx_{n-1} \right].
\]

(15d)

Recalling \((14)\), we therewith finally obtain the marginalized FPE

\[
\partial_t \rho_2(x_0, t; x_n, t) = -\partial_{x_0} \left[ F(x_0, x_n) \rho_2(x_0, t; x_n, t) \right] + D_0 \partial^2_{x_0} \rho_2(x_0, t; x_n, t)
\]

\[
+ \partial_{x_n} \int_{\Omega} \frac{n}{\tau} (x_n - x_{n-1}) \rho_3(x_0, t; x_n-1, t; x_n, t)dx_{n-1}.
\]

(16)

Please note that integrating over \( x_n \in \Omega \) yields the first member of the hierarchy \((13)\), which shows the consistency of our calculation. The higher-order members can be obtained in an analogous manner, yielding an infinite hierarchy of coupled equations

\[
\partial_t \rho_m(x_0; x_{n-m+2}, \ldots, x_n) = -\partial_{x_0} \left[ F(x_0, x_n) \rho_m(x_0; x_{n-m+2}, \ldots, x_n) \right]
\]

\[
+ \sum_{l=0}^{m-3} \frac{n}{\tau} \partial_{x_{n-l}} \left[ (x_{n-l} - x_{n-l-1}) \rho_m(x_0; x_{n-m+2}, \ldots, x_n) \right]
\]

\[
+ \frac{n}{\tau} \partial_{x_{n-m+2}} \int_{\Omega} (x_{n-m+2} - x_{n-m+1}) \rho_{m+1}(x_0; x_{n-m+1}, x_n)dx_{n-m+1}
\]

\[
+ D_0 \partial^2_{x_0} \rho_m(x_0, t; x_{n-m+2}, t, \ldots, x_n, t),
\]

(17)

for \( m \geq 3 \). Note that in contrast to the FPE \((13)\) for \( \rho_1 \), all higher members of the FP hierarchy \((16, 17)\) explicitly contain the linear forces stemming from the auxiliary variable Eqs. \((7b)\).

We now inspect in more detail the second member \((16)\) in the limit \( n \rightarrow \infty \), to recover the system with discrete delay. Similar to the first member, we again need to transform the probability space, hence, the phase space and the PDFs defined on it.

5.2 Transformation of phase space, limiting procedure

In order to take the limit \( n \rightarrow \infty \) of Eq. \((16)\), we will transform the phase space and the PDFs defined on it. We perform the transformation in two steps. First we replace the phase space variable \( x_{n-1} \) by \( \tilde{x} = (n/\tau)(x_{n-1} - x_n) \), which will later in the limit \( n \rightarrow \infty \) receive the meaning of a velocity. In a second step, we transform back to the original variables of the delayed LE \((1)\), whereby mainly the time arguments will be affected.

As first step, we change the phase space from \( \{x_0, t; x_{n-1}, t; x_n, t\} \) to \( \{x_0, t; \tilde{x}, t; x_n, t\} \). To this end, we start with performing the substitution \( x_{n-1} \rightarrow \tilde{x} = (n/\tau)(x_{n-1} - x_n) \) to rewrite the integral \( \int dx_{n-1} \) as \( (\tau/n) \int d\tilde{x} \). The drift term then becomes

\[
\frac{n}{\tau} \partial_{x_n} \int_{\Omega} (x_n - x_{n-1}) \rho_3(x_0, t; x_{n-1}, t; x_n, t)dx_{n-1} = \frac{\tau}{n} \partial_{x_n} \int_{\Omega} \tilde{x} \rho_3 \left( x_0, t; \frac{\tau}{n} \tilde{x} + x_n, t; x_n, t \right) d\tilde{x}.
\]

(18a)

In the next step, we need to transform the PDF \( \rho_3 \rightarrow \tilde{\rho}_3 \), where \( \tilde{\rho}_3 \) is a normalized (joint) PDF of the new phase space variables \( \{x_0, \tilde{x}, x_n\} \). The relation between both PDFs can be found by comparing the normalizations. In particular,

\[
\int_{\Omega} \rho_3(x_0, t; x_{n-1}, t; x_n, t) dx_0 dx_{n-1} = \frac{\tau}{n} \int_{\Omega} \int_{\Omega} \rho_3(\tilde{x}, t; x_n, t) d\tilde{x} dx_n = 1
\]

(18b)

and, on the other hand, by definition, \( \int_{\Omega} \tilde{\rho}_3(x_0, t; \tilde{x}, t; x_n, t) d\tilde{x} dx_n = 1 \). Combining both conditions yields

\[
\rho_3 \left( x_0, t; \frac{\tau}{n} \tilde{x} + x_n, t; x_n, t \right) \leq \frac{\tau}{n} \tilde{\rho}_3(x_0, t; \tilde{x}, t; x_n, t).
\]

(18c)

Therewith, we obtain the drift term

\[
\frac{n}{\tau} \partial_{x_n} \int_{\Omega} (x_n - x_{n-1}) \rho_3(x_0, t; x_{n-1}, t; x_n, t)dx_{n-1} \rightarrow \frac{\tau}{n} \partial_{x_n} \int \tilde{x} \tilde{\rho}_3 \left( x_0, t; \tilde{x}, t; x_n, t \right) d\tilde{x}.
\]

(18d)

Now, we recall the meaning of the respective stochastic variables in the limit \( n \rightarrow \infty \), i.e., \( X_0(t) = X(t) \),
\[ X_n(t) = X(t - \tau) \] from \([9]\), and \( \dot{X}_n(t) = \frac{\alpha}{\tau} [X_{n-1}(t) - X_n(t)] \) from \([71]\). Based on this, we perform the transformation

\[
\begin{align*}
\{x_0, t\} &\rightarrow \{x, t\}, \\
\{x_n, t\} &\rightarrow \{x_r, t - \tau\}, \\
\{\dot{x}, t\} &\rightarrow \{\dot{x}, t - \tau\}, \\
\hat{\rho}_3(x_0, t; \tilde{x}, t; x_n, t) &\rightarrow \rho_3(x, t; \tilde{x}, t - \tau; x_r, t - \tau),
\end{align*}
\]

with \( \tilde{x} \in \tilde{\Omega} = \mathbb{R} \). With these steps, we finally obtain from \([16]\), which is the FPE for the two-point PDF of the (artificial) Markovian system, the second member of the FP hierarchy for the delayed system

\[
\begin{align*}
\partial_t \rho_2(x, t; x_r, t - \tau) &= -\partial_x [F(x, x_r) \rho_2(x, t; x_r, t - \tau)] + D_0 \partial^2_x \rho_2(x, t; x_r, t - \tau) \\
&\quad + \partial_{x_r} \int \dot{x}_r \rho_3(x, t; \tilde{x}, t - \tau; x_r, t - \tau) d\tilde{x}_r,
\end{align*}
\]

with the three-point (joint) PDF \( \rho_3(x, t; x_r, t - \tau, \tilde{x}, t - \tau) = \langle \delta[x - X(t)] \delta[x_r - X(t - \tau)] \delta[\tilde{x}_r - \tilde{X}(t - \tau)] \rangle \) and the improper integral \( \lim_{\tau \to \infty} \int_{-\infty}^{\infty} \) denoted by \( \int \). Comparison with the corresponding FPE \((3)\) obtained from Novikov's theorem reveals that Eq. \((19)\) is in fact quite different. However, we show in the Appendix \([3]\) that one can indeed transform \((19)\) into \((3)\). Our approach thus yields an alternative representation of the second member. This novel representation is potentially a new starting point to approximate or calculate the two-time PDF, \( \rho_3(x, t; x_r, t - \tau) \), for which, so far, no approaches have been found.

The main difference of Eq. \((19)\) as compared to \((3)\) (from Novikov's theorem), is that it involves the three-point PDF \( \rho_3(x, t; x_r, t - \tau, \tilde{x}, t - \tau) \), and not the three-time PDF \( \rho_3(x, t; x_r, t - \tau, x_{2\tau}, t - 2\tau) \). This means, instead of going back even further into the past with every member [by first taking into account \( X(t - \tau) \), then \( X(t - 2\tau) \), then \( X(t - 3\tau) \) ...], the here derived hierarchy rather collects more and more information about the dynamics at time \( t - \tau \) [by taking into account \( X(t - \tau) \), then \( \tilde{X}(t - \tau) \)]. Both representations are valid and describe the same process. This shows that (probabilistically) predict the future after a time \( t \), either knowledge of the system states at all times \( t, t - \tau, t - 2\tau, ... \) would be needed, or, complete knowledge about the preceding interval \( [t - \tau, t] \) would suffice. On the stochastic level of description, the process which underlies the non-Markovian one, can either be considered as a process of the state vector \( (X(t), X(t - \tau), X(t - 2\tau), X(t - 3\tau), ...) \), or, equivalently, of the state vector of all \( X(t - \tau \leq s \leq t) \in \mathbb{R}^\infty \).

A major technical advantage of Eq. \((19)\) is that it does not involve unknown functional derivatives w.r.t. the noise, as opposed to \((3)\). Moreover, the equation is much simpler, as it only contains one diffusion term w.r.t. \( x \) (and no additional diffusion term in \( x_r \)). A new feature of \((19)\) is that it involves a correlation between the position and the velocity. This is somewhat unusual, in particular, since we consider overdamped dynamics.

### 6 Conclusions

In this work, we have discussed the probabilistic description of delayed stochastic systems. As a starting point, we have reviewed an earlier approach based on Novikov's theorem, from which a Fokker-Planck description can be derived in the form of an infinite hierarchy \([30,32]\). The first member is the well-known FPE for the one-time PDF, which contains the two-time PDF and is thus not closed. Still, this equation has in the past been shown to be an important tool in the search for exact results \([36,37]\) and a valuable starting point for approximations \([31,33]\). The main purpose of our work was to shed light onto the higher members of this hierarchy, which have rarely been discussed in earlier literature.

To this end, we introduced an alternative FP description basing on a Markovian embedding technique, where the delayed process is represented as the dynamics of one variable of an \( (n + 1) \)-variable Markovian system, in the limit \( n \to \infty \). By projecting the corresponding closed, Markovian FPE onto lower-dimensional subspaces (and taking the limit only in the projected equations), we derive a hierarchy of FPEs. While the first member is identical, we showed that the higher members differ from those obtained by Novikov’s theorem. Therefore, the here derived equations might serve as a new starting point for approximation schemes. In particular, the second member, which we focused on in this paper, could be used to develop an approach aiming for the two-time PDF.

The benefit of such an approximation scheme, as compared to an approach operating on the first member (like the ones known from the literature), would indeed be twofold. First, an approximate two-time PDF could be used directly to estimate various quantities of interest, such as the distribution of the fluctuating heat production in nonlinear systems with delay \([37,40]\). Furthermore, an approach which works on the level of the
second member (instead of the first), is expected to yield an improved approximation of the one-time PDF. Indeed, it has been shown that all approximations for the one-time PDF known so far break down in parameter regions, where non-Markovian effects are especially prominent \cite{31}, e.

g., in the vicinity of coherence-resonance in a bistable delayed system \cite{37}.

The development of such an approximation scheme based on Eq. (19) is beyond the scope of the present paper. However, we still would like to give an idea for a possible approach. Using a type of mean field argument, one could assume \( p_3(x; \bar{x}_m, x_0) \approx p_2(x; \bar{x}_m) p_1(x_0) \). Inserting this into (19) and considering the non-equilibrium steady state (i.e., \( \partial_s \rho_2 = 0 \)), one would obtain

\[
- \langle \dot{X} \rangle \partial_s \rho_2 (x; x_0, x_m, t - \tau) = - \partial_s \left[ F(x; x_0) \rho_2 (x; x_0, x_m, t - \tau) \right] + D_0 \partial_x^2 \rho_2 (x; x_0, x_m, t - \tau),
\]

(20)

involving the particle current \( \langle \dot{X} \rangle \). In order to find an ansatz for the latter, one could proceed by utilizing the framework \cite{35} (developed for Markovian systems), which gives a connection between \( \langle \dot{X} \rangle \) and the probability current \( J \) via \( \langle \dot{X} \rangle = \int \Omega J(x, t) dx \), where \( J \) is found from the FPE \( \partial_t \rho_1 = \partial_x J \) (written in the form of a continuity equation). For the delayed systems considered here \( J(x, t) = \int \Omega F(x, x_0) \rho_2 (x, x_0) dx_0 - D_0 \partial_x \rho_1 (x) \).

These assumptions give rise to the approximate, closed FPE (20) with \( \langle \dot{X} \rangle = \int \Omega F(x, x_0) \rho_2 (x, x_0) dx_0 dx \).

Furthermore, using the Markovian embedding approach, another, quite different, type of approximation is in fact readily given, by directly considering the extended Markovian system with a finite number of auxiliary variables \( n \) \cite{19}. Then, Eq. (11) is a well-defined, closed FPE, which can be used to calculate the \( n \)-point PDF by means of standard techniques for Markovian FPEs (at least numerically). By marginalization of the resulting PDFs, one would recover the corresponding (approximate) PDFs of the delayed process. On the level of the stochastic delay differential equation (the LE), this is in fact a common method \cite{6} \cite{54} \cite{55}. It amounts to approximating the discrete delay by a Gamma-distributed memory kernel \cite{56} with finite width. However, a systematic investigation of this approximation (including an error estimate), has, to the best of our knowledge, not been performed yet. A similar finite-dimensional approximation for linear systems is discussed in \cite{57}. A more detailed study of these approximations is subject of ongoing work.

Finally, we would like to reconsider the Markovian embedding from a conceptional point of view. Non-Markovianity, in general, and specifically the discrete time delay considered here, is a consequence of an incomplete description of a system, i.e., missing degrees of freedom. The delayed force might either stem from a specifically designed external agent, a feedback controller, or, more generally, from any part of a more complex system (the “super-system”), which is not explicitly modeled within the considered description, but interacts with the system at hand in form of delayed forces. The Markovian auxiliary system, in which we here embed the delayed process, allows us to mimic the external agent (or other parts of the “super-system”) without explicitly modeling it in detail. In this sense, the auxiliary variables can be interpreted as a “substitute” of the hidden degrees of freedom in the system. On the other hand, it is well-known that hidden degrees of freedom have a significant impact on the entropy production and other thermodynamical notions, see for example \cite{58} \cite{59}. Therefore, a study of the consequences of our treatment of delayed systems from a stochastic thermodynamical (and information-theoretical) perspective would be very interesting. This will be a future work of focus.

Acknowledgements
This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Projekt Nummer 163436311 - SFB 910. We further thank Christian Kühn for fruitful discussions.

A APPENDIX: The discrete delayed case as limit of the coarse-grained dynamics

In this appendix, we show how the dynamical equation of the delayed system \cite{1} can be recovered by taking the limit \( n \rightarrow \infty \) of the corresponding equation for the embedded system \cite{3}. To this end, we project onto the the dynamics of the delayed process, allows us to mimic the external agent (or other parts of the “super-system”) without explicitly modeling it in detail. In this sense, the auxiliary variables can be interpreted as a “substitute” of the hidden degrees of freedom in the system. On the other hand, it is well-known that hidden degrees of freedom have a significant impact on the entropy production and other thermodynamical notions, see for example \cite{58} \cite{59}. Therefore, a study of the consequences of our treatment of delayed systems from a stochastic thermodynamical (and information-theoretical) perspective would be very interesting. This will be a future work of focus.

In principle, this solution can be simplified using an appropriate initial condition for the auxiliary variables, for example \( X_j (0) = 0 \), \( \forall j \geq 0 \). However, we here proceed with the general case, i.e., without specifying the initial condition. As a next step (assuming \( n \geq 2 \)), we iteratively plug Eq. (21) into the corresponding solution for \( j + 1 \) [given by Eq. (21) with \( j + 1 \) instead of \( j \)]. For \( 1 \leq j < n \), we find

\[
X_{j+1} (t) = \left[ X_{j+1} (-\tau) \right] + \frac{2}{\tau} X_j (-\tau) t e^{-n (t + \tau) / \tau} + \frac{n^2}{\tau^2} \int_{-\tau}^{t} e^{-n (t - \tau') / \tau} X_{j-1} (\sigma) d\sigma.
\]

(22)

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\]

(22a)
Using the Heaviside function defined by $\Theta(z) = 1, \forall 0 \leq z$ and $\Theta(z) = 0, \forall z \geq 0$, we can simplify the double integral,

$$X_{j+1}(t) = \left[ X_{j+1}(-\tau) + \frac{n}{\tau} X_j(-\tau) t \right] e^{-n(t+\tau)/\tau} + \frac{n^2}{\tau^2} \int_{-\tau}^{t} \int_{-\tau}^{s} \Theta(s-s') ds' e^{-n(t-s')/\tau} X_{j-1}(s') ds', \tag{22b}$$

$$= \left[ X_{j+1}(-\tau) + \frac{n}{\tau} X_j(-\tau) t \right] e^{-n(t+\tau)/\tau} + \int_{-\tau}^{t} \frac{n^2}{\tau^2} [t-s'] e^{-n(t-s')/\tau} X_{j-1}(s') ds'. \tag{22c}$$

Repeating this iterative procedure, we finally obtain for $j = n$

$$X_n(t) = \left[ X_n(-\tau) + \frac{n}{\tau} X_{n-1}(-\tau) t + \frac{n^2}{\tau^2} X_{n-2}(-\tau) t^2 + \ldots \right] e^{-n(t+\tau)/\tau} + \int_{-\tau}^{t} K_n(t-s) X_0(s) ds, \tag{22d}$$

with the Gamma-distributed memory kernel defined in Eq. (8b). The first term in (22d) vanishes trivially, if the auxiliary variables satisfy the initial condition $X_{j\in\{1,2,\ldots,n\}}(-\tau) = 0$. Interestingly, this term also vanishes if the asymptotic behavior at $t \to \infty$ is considered, due to the exponential damping with time. Plugging (22d) into (8) [neglecting the initial condition term] then yields the projected Eq. (8a).

Now we consider the limit $n \to \infty$ of the memory kernel (8b). First, we find that the mean value of the kernel and the integral over it are, independently of the value of $n$, given by $\mu = \int_0^{\infty} K_n(T) T dT = \tau$ and $\int_0^{\infty} K_n(T) dT = 1$, respectively. Furthermore, for large $n$, the value of the kernel at $\tau$ can be estimated by using the Stirling formula $n! \approx \sqrt{2\pi n}(n/e)^n$, yielding $K_n(\tau) = \frac{n^e - n}{(n-1)^e} \approx \sqrt{2\pi} \frac{n}{\tau} \to \infty$. On the other hand, the variance of the kernel vanishes for $n \to \infty$, since $\int_0^{\infty} K_n(T) T^2 dT - \mu^2 = \tau^2/n \to 0$. This implies

$$\lim_{n \to \infty} K_n(\tau) = \delta(T - \tau). \tag{23}$$

Thus, the projected equation (8a) is indeed equal to Eq. (1) in the limit $n \to \infty$. We note that even the transient dynamics (i.e., finite $t$) is only equivalent for the initial conditions $X_{j\in\{1,2,\ldots,n\}}(-\tau) \equiv 0$, as mentioned above.

**B APPENDIX: Connection to Fokker-Planck hierarchy from Novikov’s theorem**

While the FPE for $\rho_1$ obtained by our approach is equivalent to the first member of the FP hierarchy from Novikov’s theorem (2), the second members differ. However, the apparent disagreement can be resolved. Indeed, as we show below, our result (12) can be transformed to the representation obtained from Novikov’s theorem [given in (3)]. We focus on the term which differs, i.e., the drift term involving $\rho_3$. To this end, we first use the definition of $\rho_3$ via delta-distributions, and perform the integration over $\dot{x}_\tau$, i.e.,

$$\partial_{\dot{x}_\tau} \int \dot{x}_\tau \rho_3(x,t;\dot{x}_\tau,t-\tau;x_\tau,t-\tau) d\dot{x}_\tau = \partial_{\dot{x}_\tau} \int \dot{x}_\tau \left\{ \delta[X(t) - x] \delta[X(t-\tau) - x_\tau] \delta[\dot{X}(t-\tau) - \dot{x}_\tau] \right\} d\dot{x}_\tau$$

$$= \partial_{\dot{x}_\tau} \left\{ \dot{X}(t-\tau) \delta[X(t) - x] \delta[X(t-\tau) - x_\tau] \right\}$$

$$= \partial_{\dot{x}_\tau} \left\{ \dot{X}(t-\tau) \delta[X(t) - x] \right\} \delta[X(t) - x_\tau]$$

$$\rightarrow \partial_{\dot{x}_\tau} \left\{ F[X(t-\tau),X(t-2\tau)] \delta[X(t) - x] \delta[X(t) - x_\tau] \right\}.$$ \hspace{1cm} (24a)

In the last step, we have plugged in the LE (3). At this point, we have two correlations to deal with. The first one (involving $F$) can easily be simplified by expressing the ensemble average with the help of the PDF $\rho_3$, i.e.,

$$\partial_{\dot{x}_\tau} \left\{ F[X(t-\tau),X(t-2\tau)] \delta[X(t) - x] \delta[X(t) - x_\tau] \right\}$$

$$= \partial_{\dot{x}_\tau} \int \int_\Omega F(x_\tau,x_{2\tau}) \delta[X(t) - x] \delta[X(t) - x_\tau] \rho_3(x,t;x_\tau,t-\tau;x_{2\tau},t-2\tau) dx_\tau dx_{2\tau}$$

$$= \partial_{\dot{x}_\tau} \int_\Omega F(x_\tau,x_{2\tau}) \rho_3(x,t;x_\tau,t-\tau;x_{2\tau},t-2\tau) dx_{2\tau}. \tag{24b}$$
The remaining term on the right side of (24a) (involving ξ) is simplified with the help of Novikov’s theorem (26) (see Appendix C). Specifically, we define Λ[ξ] := δ[x − X(t)]δ[xr − X(t−τ)], which yields

\[
\partial_{x_r} \left( \sqrt{2D_0} \xi(t−\tau) \delta[X(t−x)] \delta[X(t−x_r)] \right) = \sqrt{2D_0} \partial_{x_r} \left( \frac{\delta \Lambda[\xi]}{\delta \xi(t−\tau)} \right),
\]

\[
= \sqrt{2D_0} \partial_{x_r} \left( \frac{\delta \Lambda[\xi]}{\delta \xi(t−\tau)} \right) \delta X(t) + \frac{\delta}{\delta \xi(t−\tau)} \left[ \frac{\delta \Lambda[\xi]}{\delta \xi(t−\tau)} \right] \delta X(t−\tau) \frac{\delta \Lambda[\xi]}{\delta \xi(t−\tau)}
\]

\[
= - \sqrt{2D_0} \partial_{x_r} \left( \partial_{x} \delta[X(t)] \delta[x_r − X(t−\tau)] \right) \frac{\delta X(t−\tau)}{\delta \xi(t−\tau)}
\]

(24c)

In the last step we have plugged in the definition of Λ and used the chain rule. Now, the term denoted ψ is calculated by replacing X(t−τ) with the integral form of the LE (1), i.e., X(t′) = ∫0t′ F[X(s), X(s−τ)] + √2D0ξ(s) ds, ∀t′ > 0, yielding

\[
\psi = \frac{\delta X(t−\tau)}{\delta \xi(t−\tau)} = \frac{\delta}{\delta \xi(t−\tau)} \left[ \int_0^{t−\tau} F[X(s), X(s−\tau)] + \sqrt{2D_0} \xi(s) \right] ds = \sqrt{2D_0} \frac{D_0}{2}, \tag{24d}
\]

independently from the specific form of F. We note that the other functional derivative in (24) cannot be treated analogously, since evaluation of the functional derivative of the trajectory X w.r.t. the earlier noise ξ requires the formal solution of (1), which is only known for linear systems. Indeed, for a LE with F = −c1X(t) − c2X(t−τ), one finds \( \frac{\delta X(t)}{\delta \xi(t−\tau)} = \sqrt{2D_0} e^{−c1τ} \) by using the method of steps, see [31]. For general nonlinear forces F, this term must be treated differently, e.g. by approximation methods, but a discussion of this goes beyond the scope of this paper. We therefore keep this functional derivative and only evaluate the delta-distributions. Based on these considerations, we can rewrite (24c) as

\[
\sqrt{2D_0} \partial_{x_r} \left( \xi(t−\tau) \Lambda[\xi] \right) = -\sqrt{2D_0} \partial_{x_r} \partial_t \left( \frac{\delta X(t)}{\delta \xi(t−\tau)} \right) \rho_2(x, t; x_r, t−\tau) − D_0 \partial_{x_r} \partial_t \rho_2(x, t; x_r, t−\tau) \tag{24e}
\]

In combination with (24a, 24b), we obtain the identity

\[
\partial_{x_r} \int \dot{x}_r \rho_3(x, t; \dot{x}_r, t−\tau; x_r, t−\tau) dx_r = -\sqrt{2D_0} \partial_{x_r} \partial_t \left( \frac{\delta X(t)}{\delta \xi(t−\tau)} \right) \rho_2(x, t; x_r, t−\tau)
\]

\[
- D_0 \partial_{x_r} \rho_2(x, t; x_r, t−\tau) + \partial_{x_r} \int_\Omega F(x_r, x_r) \rho_3(x, t; x_r, t−\tau; x_r, t−2\tau) dx_r, \tag{25}
\]

proving that the second member of the here presented FP hierarchy, Eq. (19), is identical to the one obtained from Novikov’s theorem (3).

C APPENDIX: Novikov’s theorem

In this section, we establish the relation [31]

\[
\langle \Lambda[\xi] \xi(t) \rangle = \left( \frac{\delta \Lambda[\xi]}{\delta \xi(t)} \right), \tag{26}
\]

for a functional Λ of a Gaussian white noise ξ. It links the functional derivative w.r.t. the noise to the cross-correlation between functional and noise. First, we consider the case where the ensemble is w.r.t. a fixed initial condition \( \phi = X(−τ ≤ t ≤ 0) \), yielding \( \Lambda(0) = \Lambda_0 \). In a second step we will generalize towards initial conditions drawn from an arbitrary distribution.

We express the ensemble average \( \langle \cdot \rangle_{\Lambda_0} \) of the left hand side of (26) via the path integral over all possible “paths” ξ between time 0 and t, accounting for all possible realizations of the random process ξ at each instant in time

\[
\langle \Lambda[\xi] \xi(t) \rangle_{\Lambda_0} = \int_{\xi_0}^{\xi_t} \Lambda[\xi] \Lambda_0 \xi \mathcal{P}[\xi] \mathcal{D}[\xi], \tag{27a}
\]
with arbitrary but fixed $\xi_0 := \xi(t_0)$ and $\xi_1 := \xi(t)$. Please note that specifying the noise process at the boundaries does not impose a restriction on the generality as we deal with white noise. The weight $P[\xi]$ of each white noise realization is given by the Gaussian path probability (for arbitrary $t > 0$)

$$P[\xi] = J e^{-\frac{1}{2} \int_{t_0}^{t} (\xi' \xi') dt'},$$

(27b)

with Jacobian $J$. Now, we rewrite the integrand in using that the functional derivative of $P[\xi]$ w.R.T. $\xi$ is simply $-\xi P[\xi]$, yielding

$$\langle \Lambda[\xi(t)] \rangle_{\Lambda_0} = - \int_{\xi_0}^{\xi_1} \frac{\delta \Lambda \{ P[\xi] \}}{\delta \xi} \left( e^{-\frac{1}{2} \int_{t_0}^{t} (\xi' \xi') \, dt'} \right) \, D[\xi]$$

$$= - \int_{\xi_0}^{\xi_1} \frac{\delta \{ \Lambda \{ P[\xi] \} \} \, D[\xi]}{\delta \xi} + \int_{\xi_0}^{\xi_1} \frac{\delta \Lambda \{ P[\xi] \} \, D[\xi]}{\delta \xi}.$$  

(27c)

In the last step we have used the product rule (and omitted the initial condition $A_0$ for sake of a shorter notation). The functional derivative in the first path integral yields

$$\int_{\xi_0}^{\xi_1} \frac{\delta \{ \Lambda \{ P[\xi] \} \} \, D[\xi]}{\delta \xi} = \int_{\xi_0}^{\xi_1} \Lambda[\xi + \xi_0] \, D[\xi] = - \int_{\xi_0}^{\xi_1} \Lambda[\xi] \, D[\xi].$$

(27d)

Now we use that the variations of the paths $\xi + \xi_0$ are already contained in the integral over all paths, and find

$$\int_{\xi_0}^{\xi_1} \frac{\delta \{ \Lambda \{ P[\xi] \} \} \, D[\xi]}{\delta \xi} = \int_{\xi_0}^{\xi_1} \Lambda[\xi] \, D[\xi] - \int_{\xi_0}^{\xi_1} \Lambda[\xi] \, D[\xi] = 0,$$

(27e)

(as long as $\int \Lambda[\xi] \, D[\xi] < \infty$), see also (on p. 273f). Hence, we obtain from (27c).

$$\langle \Lambda[\xi(t)] \rangle_{\Lambda_0} = \int_{\xi_0}^{\xi_1} \frac{\delta \Lambda \{ P[\xi] \} \, D[\xi]}{\delta \xi} = \left\langle \frac{\delta \Lambda \{ P[\xi] \} \, D[\xi]}{\delta \xi} \right\rangle_{\Lambda_0}.$$  

(27f)

This result can readily be generalized to ensembles where the initial conditions are instead drawn from an arbitrary, normalized distribution $P(\Lambda_0)$. In particular, Eq. (27f) implies

$$\langle \Lambda[\xi(t)] \rangle = \int \langle \Lambda[\xi(t)] \rangle_{\Lambda_0} P(\Lambda_0) \, d\Lambda_0 = \int \left\langle \frac{\delta \Lambda \{ P[\xi] \} \, D[\xi]}{\delta \xi} \right\rangle_{\Lambda_0} P(\Lambda_0) \, d\Lambda_0 = \left\langle \frac{\delta \Lambda[\xi]}{\delta \xi} \right\rangle.$$  

(28)

This is the relation (26), which is often referred to as 

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