Relationship between a Non-Markovian Process and Fokker-Planck Equation

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Abstract

We demonstrate the equivalence of a Non–Markovian evolution equation with a linear memory–coupling and a Fokker–Planck equation (FPE). In case the feedback term offers a direct and permanent coupling of the current probability density to an initial distribution, the corresponding FPE offers a non-trivial drift term depending itself on the diffusion parameter. As the consequence the deterministic part of the underlying Langevin equation is likewise determined by the noise strength of the stochastic part. This memory induced stochastic behavior is discussed for different initial distributions. The analytical calculations are supported by numerical results.

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I. INTRODUCTION

One century after Einstein’s explanation of Brownian motion [1], compare also [2], stochastic processes are ubiquitous in almost every branch of physics [3] and beyond it like in economics [4], chemistry [5] and biology [6]. The notion “Brownian motion” not only stands for the movement of pollens suspended in water, but is a generic term for the Wiener process [7], see also the textbooks [8, 9, 10]. Two main approaches in describing stochastic processes has been developed, related to the Langevin and to the Fokker-Planck equation, respectively. The underlying basic for the stochastic description is the ability of a separation of time scales leading to an evolution equation with a deterministic part supplemented by a stochastic force. In this Langevin equation the probability of the stochastic force is in general an input. An alternative way is the treatment of the stochastic process by the Fokker-Planck equation (FPE) [8, 9, 10], where a parabolic partial differential equation for a probability density is the basis of calculation. As already known both description are equivalent for special stochastic forces [9, 10, 11]. In the last decades there is an increasing effort in generalization of the Langevin equation respectively the Fokker-Planck equation by including memory effects [12, 13, 14, 15]. In the framework of investigation of anomalous diffusion [15] and fractional diffusion [13] the descriptive equations are non-Markovian (non-local in time). The combination of diffusion with feedback couplings has not only an influence on the long time behavior, for the stationary state, but on the dynamics in an intermediate time regime. Such a memory dominated behavior is well established in analyzing the freezing processes in undercooled liquids [16, 17, 18, 19], where the underlying mathematical representation is based on a projector formalism proposed by Mori [20]. In [21] two of us studied a simple model, which still includes the dynamical features of evolution models as conservation of the relevant quantity $p(\vec{r}, t)$, which could be interpreted as probability density for a particle and moreover, a time delayed feedback coupling. Due to this coupling the generic behavior may be changed by the additional delay effects and could lead to non-stationary steady state solutions.

The aim of the present paper is to show the equivalence between a special non-Markovian equation [21] and the standard FPE with a non-trivial drift term. Firstly we present the non-Markovian model and its main features which consists of the occurrence of a non-trivial stationary solution and the dependence of the solution on the initial distribution.
\( p_0(\vec{r}) \equiv p(\vec{r}, t = 0) \). As the result the underlying FPE reveals a drift term which is itself determined by the strength of the stochastic force. The corresponding potential are discussed in detail. The analytical results are supported by numerical simulations.

II. THE NON-MARKOVIAN FOKKER-PLANCK EQUATION

In media with a spatial–temporal accumulation process transport phenomena should be described by a stochastic approach based on probabilities. The time evolution of the probability density could depend on the history of the sample to which it belongs, i.e. the changing rate of the probability should be influenced by the changing rate in the past and so the evolution equation of the probability has to be supplemented by memory terms. A recent overview is given in [8]. The obvious modification of the FPE by memory effects is to replace the conventional equation by

\[
\partial_t p(\vec{r}, t) = \mathcal{M}(\vec{r}; p, \nabla p) + \int_0^t dt' \int_{-\infty}^\infty d^d \vec{r}' K(\vec{r} - \vec{r}', t - t'; p, \nabla p) \mathcal{L}(\vec{r}', t'; p, \nabla p). \tag{1}
\]

This equation is of convolution type and consists of two competing parts standing for processes on different timescales. The first part manifested by the operator \( \mathcal{M} \) characterizes the instantaneous and local process, whereas the second part with the operators \( \mathcal{K} \) and \( \mathcal{L} \) represent the delayed processes, the memory. In general all the operators may be non-linear in \( p(\vec{r}, t) \) and \( \nabla p(\vec{r}, t) \). Physically it means that the time scale of the memory is determined by the relevant probability \( p \) itself. The specification of the operators has to be according to the physical situation, which one deals with. However the main feature of the probability density \( p(\vec{r}, t) \) is its conservation in time:

\[
\frac{dP(t)}{dt} = \frac{d}{dt} \int_{-\infty}^\infty d^d \vec{r} p(\vec{r}, t) = 0. \tag{2}
\]

To preserve \( p \) the instantaneous term \( \mathcal{M} \) has to be related to a probability current, e.g., \( \mathcal{M} \propto \nabla \cdot \vec{j} \). For an arbitrary polynomial kernel \( \hat{K}(\vec{r}, t) \) the conservation law (2) is not fulfilled in general. Using Laplace transformation one can show directly, compare for details [21], that the choice \( \mathcal{L} \equiv -\partial_t p(\vec{r}, t) \) guarantees conservation. Thus our starting equation is written in the form

\[
\partial_t p(\vec{r}, t) = D \nabla^2 p(\vec{r}, t) - \int_0^t dt' \int_{-\infty}^\infty d^d \vec{r}' K(\vec{r} - \vec{r}', t - t') \partial_t p(\vec{r}', t'). \tag{3}
\]
as a special realization of Eq. (1). This Fokker-Planck equation relates \( p(\vec{r}, t) \) to \( p(\vec{r}, t') \) with \( 0 < t' < t \) unlike to a conventional one, where the evolution is only dependent on the probability at present time. Moreover (3) offers a coupling between \( \partial_t p(\vec{r}, t) \) and \( \partial_t p(\vec{r}, t') \). The mixing of time scales leads to a substantial modification of the long time limit. To demonstrate the modification let us consider a very simple choice by a strictly spatial local, but time independent kernel

\[
K(\vec{r}, t) = \mu \delta(\vec{r}),
\]  

(4)

where parameter \( \mu > 0 \) characterizes the strength of the memory. By this choice the spatial and temporal variables are decoupled. Inserting the kernel in (3) one gets

\[
\partial_t p(\vec{r}, t) = D \nabla^2 p(\vec{r}, t) - \mu \left[ p(\vec{r}, t) - p_0(\vec{r}) \right] \quad \text{with} \quad p_0(\vec{r}) \equiv p(\vec{r}, t = 0).
\]  

(5)

The time independence of the kernel means that all times \( t' \) \( (0 < t' < t) \) in the past have the same weight and so there is a very strong memory with a direct coupling of the instantaneous value to the initial value. The memory induced feedback to the initial value appears as a driving force. Without this coupling one can interpret the equation as a description of a particle, which performs a diffusive motion, where the probability density \( p(\vec{r}, t) \) decays on a time scale \( \mu^{-1} \). As (5) is a linear equation and so the solution of it could be found analytically for arbitrary initial conditions

\[
p(\vec{r}, t) = e^{-\mu t} \int_{-\infty}^{\infty} d^d r' \ p_0(\vec{r}') \left[ G(\vec{r} - \vec{r}', t) + \mu \int_0^t dt' \ G(\vec{r} - \vec{r}', t - t') e^{\mu t'} \right],
\]  

(6)

where \( G(\vec{r}, t) \) is the Green’s function of the conventional diffusion equation

\[
G(\vec{r}, t) = \frac{\Theta(t)}{(4\pi Dt)^{d/2}} \exp(-\vec{r}^2/4Dt).
\]

From the general solution, some properties could be followed easily such as if the initial distribution is non-negative \( p_0(\vec{r}) \), so the \( p(\vec{r}, t) \) does provided \( \mu > 0 \). The second moment \( s(t) \) could be calculated

\[
s(t) \equiv \int_{-\infty}^{\infty} r^2 \ p(\vec{r}, t) \ d^d r = \frac{2 d D (1 - e^{-\mu t})}{\mu} \int_{-\infty}^{\infty} p_0(\vec{r}) \ d^d r + \int_{-\infty}^{\infty} r^2 \ p_0(\vec{r}) \ d^d r.
\]  

(7)

Notice that for the limit of vanishing memory \( \mu \to 0 \) one can easily verify that the last equation shows conventional diffusive behavior. The selection of the initial distribution is
the essential point in our model and so three example are given to illustrate the solution of (5). Without lack of generality we concentrate our calculation on the one-dimensional case. It can be generalized to higher dimensions.

III. RESULTS

Obviously the results for a system with memory should be sensitive with respect to the initial distribution or at least from configurations in the past. Therefore, we study different realizations for $p_0(\vec{r})$ separately.

A. Stationary solution

The first example is the delta–starting distribution $p_0(x) = p_0 \delta(x)$. Substituting this in (6) the following solution is calculated

$$p(x, t) = \frac{p_0}{\sqrt{4\pi D t}} e^{-\left(\frac{\mu t + x^2}{4 D t}\right)} + \frac{p_0 \kappa}{4} \left[f_+(x; D, \mu) + f_-(x; D, \mu)\right]$$

$$f_\pm = e^{\pm\kappa x} \left[\text{erf}\left(\frac{\pm x}{\sqrt{4 D t}} + \sqrt{\mu t}\right) - \text{sgn}(\pm x)\right],$$

where erf(x) is the error function [23] and $\kappa = \sqrt{\mu/D}$. The first part is the solution of the homogeneous equation showing temporal decay with time constant $\mu^{-1}$. In the long time limit the system shows a non-trivial stationary solution

$$\lim_{t \to \infty} p(x, t) \equiv p_s(x) = \frac{p_0 \kappa}{2} e^{-\kappa |x|}.$$  

Such a stationary solution is due to the permanent coupling to the initial distribution and the greater $\mu > 0$ the stronger is this effect and more pronounced are the deviations from the pure diffusive behavior ($\mu = 0$). The generalization to higher dimensions $0 < d < 5$ and arbitrary initial condition can be directly calculated. It results in

$$p_s(\vec{r}) = \frac{\kappa^{\frac{d+2}{2}}}{(2\pi)^{d/2}} \int d^{d}r' \frac{p_0(\vec{r}')}{|\vec{r} - \vec{r}'|^{\frac{d-2}{2}}} K_{\frac{d-2}{2}}(\kappa |\vec{r} - \vec{r}'|),$$

with $\kappa^2 = \mu/D$ and $K_{\nu}(x)$ is a modified Bessel function [23].
Using the last result in Eq. (11) we get for the Gaussian distribution \(p_0(x) = p_0 e^{-\lambda x^2}\), the following result

\[
p_s(x) = \frac{p_0 \kappa}{4} \sqrt{\frac{\pi}{\lambda}} e^{\beta^2} [g_+(x; \beta, \lambda, \kappa) + g_-(x; \beta, \lambda, \kappa)]
\]

with

\[
g_\pm (x; \beta, \lambda, \kappa) = e^{\pm \kappa x} \text{erfc} \left( \beta \pm x \sqrt{\lambda} \right) \quad \text{and} \quad \beta = \sqrt{\frac{\mu}{4 \lambda D}} = \frac{\kappa}{2 \sqrt{\lambda}}.
\]

Here \(\text{erfc}(x)\) is the complementary error function [23]. In case of an exponential decreasing initial distribution \(p_0(x) = p_0 e^{-\lambda |x|}\) the calculation leads to

\[
p_s(|x|) = \begin{cases} 
  \frac{\lambda \kappa^2}{\kappa^2 - \lambda^2} \left[ \frac{e^{-\lambda |x|}}{\lambda} - \frac{e^{-\kappa |x|}}{\kappa} \right] & \text{for } \lambda \neq \kappa \\
  \frac{1+\kappa |x|}{2} e^{-\kappa |x|} & \text{for } \lambda = \kappa
\end{cases}
\]

Let us note that the stationary distribution depends on all cases on the initial conditions.

### B. Relationship to Fokker-Planck Equation

The conventional form of the FPE including an external force, has in the one-dimensional case the following form

\[
\frac{\partial p(x, t)}{\partial t} = D \frac{\partial^2 p(x, t)}{\partial x^2} - \frac{\partial}{\partial x} \left[ f(x) p(x, t) \right],
\]

where \(D\) is the diffusion coefficient, supposed to be constant here, and \(f(x)\) is the drift force, for which \(f(x) = -dU(x)/dx\) with \(U(x)\) as corresponding potential. On the one hand, the diffusion coefficient \(D\) measures the intensity of the noise and represents the stochastic part of motion, whereas the drift coefficient \(f(x)\) corresponds to the force experienced by the system and so it describes the deterministic part of motion. In this subsection we calculate the force \(f(x)\) which corresponds to the potential \(U(x)\) for the different starting distributions \(p_0(x)\), in such a way that both Fokker-Planck equations (5) and (15) are equivalent. To do this deterministic parts of both equations are compared in the long time limit, in the stationary state. Provided \(p_s(x) \neq 0\) the formal solution is found by integration

\[
f(x) = \frac{\mu}{p_s(x)} \int_{-\infty}^{x} \left[ p_s(\xi) - p_0(\xi) \right] d\xi + \frac{C}{p_s(x)},
\]
where $C$ is an integration constant, which one could set to zero. To show the equivalence mathematically correct, one has to do this comparison in the following way. First take an arbitrary function $h(x)$ with bounded support, then integrate the product of $h$ and the deterministic part of (13) resp. (19) over the complete real line, and finally compare the results of these integrations. If both integrations are equal, then the functions are equal. In case of arbitrary dimension the $\alpha$- component of the drift force is given by

$$f_\alpha = \mu \int_{-\infty}^{\infty} \left[ p_s(\xi) - p_0(\xi) \right] d\xi.$$ 

Here the integration constant is assumed to be zero as in the one dimensional case. Finally we present the results for three different initial distributions, depicted in Fig. 1 the corresponding stationary solutions is shown in Fig. 2 the drift term and the corresponding potential in Fig. 3 and Fig. 4 respectively. For the delta-like starting distribution the drift term can be calculated to

$$f(x) = -\sqrt{\mu D} \text{sign}(x)$$

and so one can verify the following potential

$$U(x) = \sqrt{\mu D} |x| .$$

In case of a Gaussian initial distribution an analogue calculation leads to

$$f(x) = \sqrt{\mu D} \frac{g_+(x; \beta, \lambda, \kappa) - g_-(x; \beta, \lambda, \kappa)}{g_+(x; \beta, \lambda, \kappa) + g_-(x; \beta, \lambda, \kappa)},$$

whereas an exponential starting distributions yields to the drift term

$$f(x) = -\sqrt{\mu D} \text{sign}(x) \lambda \begin{cases} \frac{e^{-\lambda|x|} - e^{-\kappa|x|}}{\kappa e^{-\lambda|x|} - \lambda e^{-\kappa|x|}} & \text{for } \kappa \neq \lambda, \\ \frac{|x|}{1+\lambda|x|} & \text{for } \kappa = \lambda. \end{cases}$$
The underlying potentials can be obtained after an integration. The results are shown in Fig. 4. It should be noticed that the potential is likewise determined by the diffusion constant $D$ which is a measure of the stochastic force. This point will be discussed in the next section.
C. Deterministic motion in the potential

As discussed before the speciality of the present approach consists of including the diffusive parameter $D$ likewise into the force term $f(x)$ of the FPE. Insofar it seems to be reasonable to study the corresponding Langevin equation, especially in the small noise limit. The trajectories obey the equation

$$\frac{dx(t)}{dt} = f[x(t)] + \xi(t) \quad \text{with} \quad \langle \xi(t) \xi(t') \rangle = 2D \delta(t - t').$$

(21)

Firstly let us solve the deterministic equation of motion under the influence of the different potentials depicted in Fig. 4. All potentials offer their (global) minimum at $x \equiv 0$, so this is the fixed point of the equation

$$\frac{dx(t)}{dt} = f[x(t)].$$

For the Delta-starting distribution one can calculate the deterministic trajectory exactly

$$x(t; \mu, D, x_0) = \Theta(t - |x_0|/\sqrt{\mu D}) \left[ x_0 - \text{sign}(x_0) \sqrt{\mu D} t \right].$$

There is a linear decrease (increase) of $x$ to the fixed point $x \equiv 0$ in the time interval $0 \leq t \leq |x_0|/\sqrt{\mu D}$. After reaching the fixed point the particle stays there if no noise is present.

For the Gaussian distribution the drift term is highly nonlinear and the deterministic equation is not solvable exactly. In Fig. 5 the direction field of the solution of the deterministic motion is illustrated for different starting values, where the numerical calculation is done with the Runge-Kutta 4th order algorithm with a step length $h = 0.05$. As seen from Fig. 4 (b) the potential exhibits two different regimes, namely a parabolic one if $|x| \ll 1$ and linear regime for $|x| \gg 1$. Assuming a piecewise approximation for the drift term as shown in Fig. 6 the trajectories could be calculated exactly. Both pieces are merged together at the new parameter $x_0$

$$x_a(t) = \begin{cases} 
  x_0 + \sqrt{\mu D} t & \text{for } t \leq t_1 \\
  \sqrt{\mu D} e^{s(t-t_1)} & \text{for } t > t_1
\end{cases} \quad \text{if} \quad x_0 < \sqrt{\mu D} \frac{s}{s},$$

$$x_a(t) = \begin{cases} 
  x_0 e^{s t} & \text{if } \frac{s}{s} < x_0 < -\sqrt{\mu D} \frac{s}{s} \\
  x_0 - \sqrt{\mu D} t & \text{for } t \leq t_2 \\
  -\sqrt{\mu D} e^{s(t-t_2)} & \text{for } t > t_1
\end{cases} \quad \text{if} \quad x_0 > -\sqrt{\mu D} \frac{s}{s},$$

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FIG. 5: Numerical calculated trajectory for $p_0(x) = \exp(-x^2)$, $D = 1$, $\mu = 1$ and $x_0 = -2; -1; 0; 1; 2$

FIG. 6: Comparison between the drift term $f(x)$ (solid) and the piecewise approximative drift term $f_a(x)$ (dashdotted) for $\lambda = 1, \mu = 1, D = 1$

where $t_1 = s^{-1} - x_0/\sqrt{\mu D}$ and $t_2 = s^{-1} + x_0/\sqrt{\mu D}$. In the outer area the decrease of $x(t)$ is linear, whereas after the cross-over it is exponential in the inner area. Because the piecewise approximation is quite rough we have studied a better one by replacing the drift term by

$$f(x) = \sqrt{\mu D} \tanh \left( \frac{s}{\sqrt{\mu D}} x \right), \tag{22}$$

where both regimes are matched, the long distance regime $x \to \pm \infty$ as well as the short distance regime $x \to 0$. The approximative drift term leads to the following solution for the trajectories

$$x_a(t) = \frac{\sqrt{\mu D}}{s} \text{arsinh} \left[ \sinh \left( \frac{s}{\sqrt{\mu D}} x_0 \right) e^{st} \right],$$

which are plotted in comparison to the numerically calculated trajectories in Fig. 8. Approximation (22) underestimates the exact drift term that leads to an overestimated absolute
FIG. 7: The drift term $f(x)$ and the approximative one $f_a(x)$ and the relative error (percentage) for $\lambda = 1, \mu = 1$ and $D = 1$

FIG. 8: Trajectories $x(t)$ (solid) and the approximative trajectories $x_a(t)$ (dashdotted) $\lambda = 1, \mu = 1, D = 1$ and $-4 \leq x_0 \leq 4$

value of $x(t)$ in the intermediate regime, whereas for the piecewise approximation the drift term is overestimated and (the absolute value of) the deviation between $x(t)$ and $x_a(t)$ in the cross-over area is underestimated. A similar situation is observed for the exponential decreasing initial condition. Therefore, we skip this part.

Concluding our paper we have discussed a simple evolution equation with a long-range memory. Due to the permanent coupling to the initial distribution the system offers a stationary solution which depends on the special choice of the initial distribution. Then we have demonstrated that this evolution equation is fully related to a FPE with non-trivial deterministic forces. As a new feature it results that the deterministic part is also characterized by the
diffusion constant $D$, with other word the memory induces a stochastic behavior also within the deterministic part. As the consequence already the deterministic part of the underlying Langevin equation exhibits special trajectories.

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