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Nonlinear effects in the dynamics governed by non-Markovian stochastic Langevin-like equations

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Abstract.

The influence of nonlinear effects in stochastic equations of motion with both additive and multiplicative noises is studied. Non-Markovian stochastic dynamics are compared with their corresponding Markovian (local approximations). Non-Markovian effects are implemented through Ornstein-Uhlenbeck and exponential damped harmonic dissipative kernels.

1. Introduction

In nature, almost as a rule, most systems behave as open ones, interacting with an environment (e.g., a thermal bath). Interactions with an environment lead, as a consequence, to dissipative as well-stochastic effects. Nonlinear stochastic dynamical systems are of interest in many different areas of investigation with applications in diverse fields, like in the study of double quantum dot systems (1; 2; 3), in fundamental aspects of biological systems (4; 5; 6), in studies concerning domain growth processes (7) and in the context of field theory models (8; 9). In double quantum dot systems, for instance, the importance resides in their possible applications in nanotechnology and quantum information processing (10; 11). Fluctuation and dissipation appear in these systems due to quantum operations and measurements and these can change the physics of the system's coherent evolution. Recently, many investigations have been performed using different forms of noises and interactions that can change the coherent evolution of electrons in the double dot quantum system.

Another area of interest is the application of stochastic models in biological systems. In this case, for example, one of the aspects studied is the issue of how cooperative behavior may emerge. The competition among different growth and death processes and the inclusion of external mechanisms can influence the global properties of these systems. Many efforts have been dedicated to provide a theoretical framework for understanding the cooperative behavior. Another example that has been a focus of attention in recent years is the analysis of tumor growth. In this case, a population of proliferating cells can be considered as a stochastic dynamical system far from equilibrium. To obtain a better understanding of the behavior of this type of phenomenon is necessary to include stochastic effects and, ideally, spatial correlations (12).

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Journal of Physics: Conference Series 246 (2010) 012029	doi:10.1088/1742-6596/246/1/012029

Nonlinear stochastic dynamical systems also appear in the context of field theory models (8; 9). It has been shown in that case how generalized equations of motion can be derived microscopically, resulting is a complicated structure depending on the form of the couplings involved between the fields, like between some background configuration we are interested in the dynamics and other fields and degrees of freedom taken as an environment or (quantum or thermal) bath fields.

One common way for describing all the above mentioned forms of evolution is by means of generalized stochastic Langevin-like equations of motion. These non-deterministic equations of motion are used in many applications of interest, including, e.g., for the study the system mentioned above. These equations, for example, can simulate Brownian motion in (classical and quantum) statistical mechanics and in other areas of physical interest (13; 14).

A classical example of a system whose dynamics is modeled by a Langevin equation of motion is the one that describes the Brownian motion of a classical particle described by a coordinate q, unitary mass and subjected to a potential V(q) (as usual dots mean derivative with respect to time and $V'[q(t)] \equiv dV/dq$),

$$\ddot{q}(t) + \eta \dot{q}(t) + V'[q(t)] = \xi(t) , \qquad (1)$$

where η is a Markovian (local) dissipation term and $\xi(t)$ is a stochastic term describing a white noise with Gaussian properties, satisfying (throughout this work we consider the Boltzmann constant $k_B = 1$)

$$\langle \xi(t) \rangle = 0 , \quad \langle \xi(t)\xi(t') \rangle = 2T\eta\delta(t-t') . \tag{2}$$

Approaches with Langevin equations like Eq. (1) and their generalizations, are used in different contexts, e.g. in classical statistical mechanics to study problems with dissipation and noise, to determine how order parameters equilibrate and in the studies like dynamic scaling and dynamic critical phenomena (15; 16). Though extensively used, equations of the form of Eq. (1) and with noise properties as given by Eq. (2), can only be considered phenomenologically. This is because it implicitly assumes that the environment interacts instantaneously with the system. This is a physically unacceptable situation that violates causality, since the environment bath has no memory time.

In a microscopic description, the effects of the environment on some select variable, taken as the system, dissipation and stochastic noise terms are expected to originate from scattering events, thus giving origin to finite interaction times that reflect in the system's equation of motion as being nonlocal, *i.e.*, they have non-Markovian terms with finite memory. The simplest archetype of this is the description of the system-environment as being modeled by linearly coupled harmonic oscillators (17) (for a general review, see, e.g., Ref. (18)), which also become to be known as Caldeira-Leggett type of models (19; 20; 21).

In this work our objective is to study the nonlinear effects on the dynamics governed by a non-Markovian generalized Langevin equation when compared to the approximated Markovian form. We will consider some of the most common forms for the dissipation kernels. These forms for the dissipation kernels include, for example, the one that describes an Ornstein-Uhlenbeck (OU) process (22) and the exponential damped harmonic (EDH) kernel (23; 24). We study both the cases of additive and multiplicative noises, including system dependent dissipation terms, according to the fluctuation dissipation theorem (for details see (25)). A detailed numerical analysis is made when the various regimes of non-linearity are considered.

2. Non-Markovian Generalized Langevin Equation (GLE)

Here we study a GLE describing the interaction of a system, denoted by a variable ϕ (which can be e.g. the coordinate of a particle) interacting with a thermal bath. The GLE studied here

has the generic form

$$\ddot{\phi}(t) + \phi^n(t) \int_{t_0}^t dt' \phi^n(t') K(t-t') \, \dot{\phi}(t') + V'(\phi) = \phi^n(t) \, \xi(t) \;, \tag{3}$$

where n = 0, 1, with n = 0 giving the standard GLE of additive noise, while for n = 1 gives a multiplicative form of GLE. The inclusion of multiplicative noise and system dependent dissipation is motivated from field theory calculations (for details, see e.g. Refs. (8; 9)). The potential in Eq. (3) is considered to be one with quadratic and quartic terms, given by

$$V(\phi) = \frac{m^2}{2}\phi^2 + \frac{\lambda}{4}\phi^4 , \qquad (4)$$

where m^2 and λ are parameters depending on the details of the system under study. The parameter m can be associated with the system's frequency and λ characterizes the degree of nonlinearity.

Non-Markovian and nonlinear GLEs of the form of Eq. (3) are very difficult to solve in general. Analytical methods can only be used in linear regimes (26), like in the additive noise case and when the quartic term in the potential can be neglected. In this case, the equation is in the form of a convolution, thus easily solvable through Laplace transform for instance (26). Otherwise, in more general cases, we must resort to numerical methods. This is the approach we follow in this paper in order to analyze the dynamics obtained from the full nonlinear Eq. (3). Though there are some specific numerical methods using e.g. Fourier transform that may apply for equations with non-Markovian kernels of generic form (27), we still would like to be able to solve equations like Eq. (3) through standard methods, which are less numerically expensive than other alternatives. Recently, the authors (26) have demonstrated the reliability of using a fourth-order Runge-Kutta method when solving GLE of the OU and EDH forms. The way this can be done stems from the fact that non-Markovian equations with kernels of those forms can be replaced by a system of completely local first-order differential equations, as described in details in (25; 26; 28).

The local version of the GLE that we will use to contrast the Markovian and the non-Markovian dynamics of the system is obtained by the following approximation (29; 30)

$$\phi^{n}(t) \int_{t_{0}}^{t} dt' D(t-t') \phi^{n}(t') \dot{\phi}(t') \simeq$$

$$\phi^{2n}(t) \dot{\phi}(t) \int_{-\infty}^{t} dt' D(t-t') \to \eta \phi^{2n}(t) \dot{\phi}(t) , \qquad (5)$$

where η is the local dissipation coefficient. Our local version of the GLE is then given by

$$\ddot{\phi}(t) + \eta \,\phi^{2n}(t) \,\dot{\phi}(t) + V'(\phi) = \phi^n(t) \,\xi(t) \,. \tag{6}$$

In this work we concentrate our study in equations like Eq. (3) with non-Markovian kernels of either the OU type (22),

$$D_{OU}(t-t') = \eta \,\gamma e^{-\gamma(t-t')} \,, \tag{7}$$

or with the EDH type (23; 24),

$$D_H(t-t') = \eta \, e^{-\gamma(t-t')} \frac{\Omega_0^2}{2\gamma} \left\{ \cos[\Omega_1(t-t')] + \frac{\gamma}{\Omega_1} \sin[\Omega_1(t-t')] \right\} \,, \tag{8}$$

doi:10.1088/1742-6596/246/1/012029

where in the equations above, η sets the magnitude of the dissipation, γ sets the relaxation time for the bath kernels, $\tau = 1/\gamma$, and Ω_0 gives the oscillation time scale in the case of the EDH kernel. In Eq. (8), $\Omega_1^2 = \Omega_0^2 - \gamma^2$, and so, in the EDH case the values of γ and Ω_0 are restricted such that $\Omega_1^2 \ge 0$.

The GLE equations with kernels of those forms can be replaced by a system of completely local first order differential equations (25; 26; 28). For the OU case,

$$\dot{\phi} = y,
\dot{y} = -V'(\phi) + \phi^n w_{OU} + \phi^n \xi_{OU},
\dot{w}_{OU} = -\gamma w_{OU} - D_{OU}(0)\phi^n y,
\dot{\xi}_{OU} = -\gamma \left[\xi_{OU} - \sqrt{2T\eta} \zeta\right],$$
(9)

while for the EDH case we obtain

$$\dot{\phi} = y,
\dot{y} = -V'(\phi) + \phi^{n}w_{H} + \phi^{n}\xi_{H},
\dot{w}_{H} = u - 2\gamma w_{H} - D_{H}(0) \phi^{n}y,
\dot{u} = -\Omega_{0}^{2}w_{H} + \dot{D}_{H}(0) \phi^{n}y - 2\gamma D_{H}(0) \phi^{n}y,
\dot{\xi}_{H} = z,
\dot{z} = -2\gamma z - \Omega_{0}^{2}\xi_{H} + \Omega_{0}^{2}\sqrt{2T\eta}\zeta.$$
(10)

In the above equations, $D_{OU}(0) = \eta \gamma$, $D_H(0) = \eta \Omega_0^2/(2\gamma)$ and $\dot{D}_H(0) = 0$, which follow from Eqs. (7) and (8). As before, the additive noise case is when n = 0 is used in Eqs. (9) and (10), while n = 1 is for the multiplicative noise case. ζ is a white Gaussian noise.

We take the initial time as $t_0 = 0$ and define new variables u(t) and w(t) by (25; 26):

$$w_{OU,H}(t) = -\int_0^t dt' \phi^n(t') D_{OU,H}(t-t') \dot{\phi}(t') , \qquad (11)$$

and

$$u(t) = \int_0^t dt' \left[\frac{dk_H(t-t')}{dt'} - \gamma D_H(t-t') \right] \frac{d\phi(t')}{dt'} \,. \tag{12}$$

In Ref. (25) we have studied how the variation of the various parameters of the noise and dissipation kernels affect the dynamics. Here, we study how the variation of the non-linearity parameter λ affects overall system dynamics and its effects in the applicability or not of the simpler Markovian approximation. Of course, we expect that both dynamics, the non-Markovian and the Markovian ones to have the same asyntoptic state because, by definition, the system reaches the equilibrium, but the question we want to address here is, given a set of model parameters representing the system and the thermal bath to which it is coupled to, for how long can we expect the memory effects due to the non-Markovian dynamics changes if we vary the λ parameter ? Since the representation of the dynamics in a local form as given by Eq. (6) represents a considerable simplification, for both a numerical point of view, or for analytical analysis (when it is possible), when compared, e.g., with the full nonlocal, nonlinear integro-differential stochastic equation (3), these then become important questions to be accessed for most practical studies that make use of nonlinear stochastic equations of motion.

In the following we will study how the non-linearity (when the quartic constant term in the potential is varied) change the equilibration and thermalization of the stochastic system.

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IOP Publishing doi:10.1088/1742-6596/246/1/012029

$\Delta \phi_{ m OU\ add}$	$\Delta \phi_{\rm OU\ mult}$	$\Delta \phi_{ m EDH \ add}$	$\Delta \phi_{ m EDH \ mult}$	
0.0	20	19	44	35
5.0	15	14	32	38
15.0	11	10	23	75

Table 1. The time scale (in units of 1/m), using $\eta = 1.0$, for the non-Markovian dynamics to approach the Markovian one, within a precision of 10^{-3} for the differences defined in Eq. (13).

3. Numerical Results

Let us now turn to our numerical results for the Markovian and non-Markovian dynamics of the system. Numerical simulations of the system of differential first-order equations, Eqs. (9) and (10), for the non-Markovian GLE with OU and EDH kernels, respectively, are compared with those obtained through the local approximation given by Eq. (6). All our simulations were performed with 300,000 realizations over the noise and we have integrated all differential equations using a standard fourth-order Runge-Kutta method with a time stepsize of $\delta t = 0.001$, which was found to be more than enough for both numerical stability and also for numerical precision (as determined in Ref. (26), these values already assure an overall numerical error always smaller than about one percent, which suffices for our comparison purposes set here). In all our simulations we have also used the initial conditions $\phi(0) = 1$ and $\dot{\phi}(0) = 0$. The time in all our evolutions is in units of the (inverse of the) frequency for the system (which is equivalent to consider m = 1 throughout). Comparisons between the Markovian and non-Markovian dynamics are made changing the degree of non-linearity of the system's potential. The other model parameters are kept fixed.

3.1. The dynamics of the system

Let us first consider the analysis of the dynamics for ϕ . In Fig. 1 we plot side by side, using $\eta = 1$, our results for the difference between the Markovian and non-Markovian dynamics, which can be estimated by defining the quantities below:

$$\Delta \varphi = \langle \phi \rangle_{\text{non-Markovian}} - \langle \phi \rangle_{\text{Markovian}} .$$
(13)

In Eq. 13, $\langle \phi \rangle$ is the ensemble averaged macroscopic system variable $\phi(t)$, where the average is over the noise realizations. In Fig. 2, we perform the same numerical computation, but using $\eta = 10.0$. The results from the plots shown in Figs. 1 and 2 are useful to determine within which time scale the Markovian and non-Markovian dynamics become sufficiently close (within to some given precision) and how the non-linearity of the system influences this time scale. The results for these time scales for the different simulations we have performed, for the Markovian dynamics and for the non-Markovian dynamics with the two types of memory kernels, are given in tables 1 and 2.

The effect of changing λ is clear: The larger is λ , the more pronounced are the memory effects, resulting in a strong difference with respect to the local approximation. As expected, at some sufficient long time, the two dynamics, Markovian and non-Markovian approximate each other. This can also be seen in the case where we have plotted the correlation $\langle \phi^2(t) \rangle$ for both OU and EDH cases. There is another interesting aspect of our results. If we look at Fig. 2, we can see that the larger is λ , the faster the difference between Markovian and non-Markovian dynamics seems to tend to zero. It occurs more explicitly in the EDH cases (top panels). However, note that the behavior shown in Fig. 1 is exactly the opposite: the larger is λ , the slower the difference between Markovian and non-Markovian and non-Markovian dynamics reduces.

doi:10.1088/1742-6596/246/1/012029



Figure 1. The time evolution for $\Delta \phi = \langle \phi \rangle_{\text{non-Markovian}} - \langle \phi \rangle_{\text{Markovian}}$ fixing $\eta = 1.0$ and varying the λ parameter for (a) EDH additive noise case, (b) EDH multiplicative noise case, (c) OU additive noise case and (d) OU multiplicative noise case. The other parameters used are: $T = 1.0, \Omega_0 = 1.0, m^2 = 1.0$ and $\gamma = 0.5$ (EDH case) or $\gamma = 5.0$ (OU case).

$\overline{\Delta\phi_{\rm OU\ add}}$	$\Delta \phi_{\rm OU \ mult}$	$\Delta \phi_{ m EDH \ add}$	$\Delta \phi_{ m EDH\ mult}$	
0.0	58	23	92	150
5.0	20	16	29	14
15.0	11	10	22	13

Table 2. The time scale (in units of 1/m), using $\eta = 10.0$, for the non-Markovian dynamics to approach the Markovian one, within a precision of 10^{-3} for the differences defined in Eq. (13).

3.2. The thermalization and nonlinear effects

It is also useful to determine how the parameter λ influences the thermalization time for the system when put in contact with the thermal bath at some temperature T. For this, let us define an effective time dependent temperature for the system according to the equipartition of kinetic energy:

$$T_{\rm eff}(t) = \langle \dot{\phi}^2(t) \rangle . \tag{14}$$

doi:10.1088/1742-6596/246/1/012029

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0.4

0.2

-0.2

-0.4

0

Φ





Figure 2. The time evolution for $\Delta \phi$ fixing $\eta = 10.0$ and varying the λ parameter for (a) EDH additive noise case, (b) EDH multiplicative noise case, (c) OU additive noise case and (d) OU multiplicative noise case. The other parameters used are: T = 1.0, $\Omega_0 = 1.0$, $m^2 = 1.0$ and $\gamma = 0.5$ (EDH case) or $\gamma = 5.0$ (OU case).

From the plots shown in both Figs. 3 and 4 we can see how the non-linearity of the system reflects in the thermalization of the system. Larger values of λ lead to a longer time for the system to thermalize. Typically, for comparable λ values, in the additive case the system tends to thermalize faster than in the multiplicative case. Also, we can see that the variation of λ produces more striking changes in the thermalization time of the EDH case, in both additive and multiplicative noise cases. In Tables 3 and 4 we give the approximate time (in units of 1/m) for thermalization for all the cases studied above. For comparative purposes, we show in Fig. 5 the additive and multiplicative Markovian dynamics for the effective temperature $T_{\rm eff}$ for both $\eta = 1.0$ and $\eta = 10.0$.

4. Conclusions

In this work we have studied how the variation of the nonlinear parameter λ of the system's quartic potential term affects the discrepancy between the dynamics of a GLE, given by Eq. (3), and the dynamics of its Markovian or local approximated form. We here have concentrated in two forms for the non-Markovian memory kernel, the OU and EDH cases, and we have analyzed



Figure 3. Time evolution for T_{eff} . (a) EDH additive noise case, (b) EDH multiplicative noise case, (c) OU additive noise case and (d) OU multiplicative noise case. The other parameters used are: $\eta = 1.0, T = 1.0, \Omega_0 = 1.0$ and $\gamma = 0.5$ (EDH case) or $\gamma = 5.0$ (OU case).

$\overline{ au_{ ext{markov add}}}$	$ au_{ m OU~add}$	$ au_{ m EDH~add}$	$ au_{ m markov\ mult}$	$ au_{ m OU\ mult}$	$ au_{ m EDH\ mult}$	
0.0	7	8	146	32	47	200
5.0	7	17	180	40	54	650
15.0	8	36	500	70	115	2500

Table 3. The approximate time for thermalization for $\eta = 1.0$, in units of 1/m, for the Markovian and non-Markovian dynamics, determined when (14) approaches the temperature of the thermal bath.

the cases of additive and multiplicative noises in both cases.

Our results show that the Markovian approximation becomes less applicable as the value of λ increases. Obviously, since these are all dissipative systems, we expect the two dynamics to tend to each other asymptotically. We have then analyzed how long it takes for the discrepancy between the non-Markovian and Markovian dynamics to tend to vanish. We have analyzed the time for the difference $\Delta \varphi$ and also the thermalization time for each of the dynamics by studying the behavior of the correlation function $\langle \phi^2 \rangle$, which is associated to the temperature of equilibration through the equipartition theorem. We have fixed the all other parameters and

doi:10.1088/1742-6596/246/1/012029



Figure 4. Time evolution for T_{eff} . (a) EDH additive noise case, (b) EDH multiplicative noise case, (c) OU additive noise case and (d) OU multiplicative noise case. The parameters used are: $\eta = 10.0, T = 1.0, \Omega_0 = 1.0$ and $\gamma = 0.5$ (EDH case) or $\gamma = 5.0$ (OU case).

$ au_{ m markov add}$	$ au_{ m OU~add}$	$ au_{ m EDH~add}$	$ au_{ m markov\ mult}$	$ au_{ m OU\ mult}$	$ au_{ m EDH\ mult}$	
0.0	6	10	120	9	27	150
5.0	5	10	125	10	28	320
15.0	6	10	420	13	25	2300

Table 4. The approximate time for thermalization for $\eta = 1.0$, in units of 1/m, for the Markovian and non-Markovian dynamics, determined when (14) approaches the temperature of the thermal bath.

then analyzed the system dynamics varying λ for two cases of dissipation coefficient η . By increasing λ , we have seen that in general, the larger is the λ parameter, the more important are the memory effects, resulting in a strong difference with respect to the local approximation. This difference is seen most notably at short times, obviously, but can last for considerable longer times.

Another interesting aspect of our results is the antagonistic behavior of the system dynamics face the variation of the magnitude of the dissipation parameter, η : looking at Fig. 2, we can see that the larger is λ , the faster the difference between Markovian and non-Markovian dynamics





Figure 5. Markovian time evolution for T_{eff} varying the λ parameter. (a) Additive noise case and (b) Multiplicative noise case for $\eta = 1.0$. (c) Additive noise case and (d) Multiplicative noise case for $\eta = 10.0$. The other parameters used are: T = 1.0 and $m^2 = 1.0$.

seems to tend to zero. The case we have shown in Fig. 1 is exactly the opposite. In general, the Markovian dynamics tend more and more to overestimate the time for thermalization as the value of λ increases. We can see that this behavior is more accentuated in both additive and multiplicative EDH cases. The results we have obtained here show that, in many cases, the local approximation is not a reliable description of the true non-Markovian dynamics and this becomes more accentuated as the dynamics becomes more nonlinear.

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