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HARMONIC OSCILLATOR DRIVEN BY GENERALIZED NOISES: OVERDAMPED BEHAVIOR

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Abstract. An analytical treatment of a generalized Langevin equation for a harmonic oscillator driven by generalized noises is presented. The overdamped limit (cases of high viscous damping) as a model of conformational dynamics of proteins is considered. The behavior of the oscillator is analyzed by calculation of the mean square displacement and normalized displacement correlation function. The results are expressed in terms of Mittag-Leffler type functions. Standard Brownian motion is a special case of the considered model. It is shown a good agreement with some experimental results.

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1. INTRODUCTION

The standard Brownian motion, which represents a random process driven by Gaussian white noise, can be analyzed either by standard diffusion equation for the probability distribution function or by stochastic Langevin equation for a Markov process, where the consecutive displacements are independent. Analysis lead to Gaussian form of the probability distribution function $u(x,t)=(1/\sqrt{4\pi K_1 t})\exp\left(-x^2/4K_1 t\right)$, where K_1 is the diffusion coefficient of dimension $[K_1]=\mathrm{m}^2/\mathrm{s}$, and linear dependence of the mean square displacement (MSD) on time, i.e. $\langle x^2(t)\rangle = 2K_1 t$. Normal diffusion appears when the microscopic time scale is short comparing with the observation time. Contrary, one may observe deviations from Brownian diffusion. Thus, MSD has a power law dependence on time $\langle x^2(t)\rangle = 2K_\alpha t^\alpha/\Gamma(1+\alpha)$ [1], where K_α is the generalized diffusion coefficient of dimension $[K_\alpha]=\mathrm{m}^2/\mathrm{s}^\alpha$, and α is the anomalous diffusion exponent. Such diffusion is the so-called anomalous diffusion (subdiffusion if $0<\alpha<1$ and superdiffusion if $1<\alpha$), which is a characteristic for non-Markovian processes, and can be observed in different systems [1-4]. This means that the evolution of the system in a given moment of time t depends on the past; the time domain of the memory is long comparing with the characteristic time scale of the motion. Anomalous diffusion can be studied either by fractional differential equations for the probability distribution function [1,5,6] or by stochastic equations, such as the generalized Langevin equation (GLE). GLE for a particle of mass in a given potential $V(x)$ is given by [7]:

$$m\ddot{x}(t)+\int_0^t \gamma(t-t')\dot{x}(t)\mathrm{d}t'+\frac{\mathrm{d}V(x(t))}{\mathrm{d}x}=\xi(t),$$
$$\dot{x}(t)=v(t), \tag{1}$$

where $x(t)$ is the particle displacement, $v(t)$ is the particle velocity, $F(x)=-\mathrm{d}V(x(t))/\mathrm{d}x$ is the external force acting on the particle due to the potential $V(x)$, $\gamma(t)$ is the frictional memory kernel, and $\xi(t)$ is a stationary random force with a zero mean $\langle\xi(t)\rangle=0$. Its correlation is given by:

$$\langle\xi(t)\xi(t')\rangle=C(t'-t). \tag{2}$$

The notation $\langle\cdot\rangle$ means an ensemble averages, i.e. statistical averaging over an ensemble of particles at a given moment of time *t*. In case when fluctuation and dissipation come from same source then correlation (2) is related with $\gamma(t)$ via the second fluctuation-dissipation theorem [7]:

$$C(t)=k_B T\gamma(t) \tag{3}$$

where k_B is the Boltzmann constant and T is the absolute temperature of the environment in which the particle is immersed. Otherwise, relation (3) does not hold. GLE (1) can be derived from the Hamiltonian representing the physical microscopic interactions between the particle and the surrounding complex environment [7].

The case of large friction (high damping) in GLE (1) usually is analyzed to model experimental data related to the movements within proteins. Large friction means that the acceleration of the particle $\ddot{x}(t)$ is negligible. Due to the liquid environment of proteins frictional term usually is very high, so the overdamped behavior of the particle is of importance [2,8,9]. When the movement is confined to a short range, which is a case for movement within proteins, the potential function can be well approximated by a harmonic potential $V(x)=m\omega^2x^2/2$, where ω is the oscillator frequency. Thus, GLE (1) in which appears a term of form $m\omega^2x(t)$ represents a suitable model of anomalous dynamics within proteins [2,8,9].

Different frictional memory kernels $\gamma(t)$ have been introduced. In [10] we introduced an internal noise with correlation of form:

$$C(t)=\frac{C_{\alpha,\beta,\delta}}{\tau^{\alpha\delta}}t^{\beta-1}E_{\alpha,\beta}^{\delta}\left(-\frac{t^\alpha}{\tau^\alpha}\right), \tag{4}$$

where τ is the characteristic memory time, $C_{\alpha,\beta,\delta}$ is a coefficient independent on time and which may depends on $\alpha>0$, $\beta>0$, $\delta>0$. Here $E_{\alpha,\beta}^{\delta}(\cdot)$ is the three parameter Mittag-Leffler (M-L) function $E_{\alpha,\beta}^{\delta}(z)=\sum_{k=0}^{\infty}(\delta)_k/\Gamma(\alpha k+\beta)\cdot z^k/k!$, $(\beta,\ \delta,\ z\ \in\ \mathbb{C},\ \Re(\alpha)>0)$, $(\delta)_k$ is the Pochhammer symbol, $(\delta)_0=1$, $(\delta)_k=\Gamma(\delta+k)/\Gamma(\delta)$.

For $\delta=1$ it becomes a two parameter M-L function $E_{\alpha,\beta}^{1}(z)=E_{\alpha,\beta}(z)$ and for $\beta=\delta=1$ – one parameter M-L function $E_{\alpha,1}^{1}(z)=E_{\alpha}(z)$. By using asymptotic expansion formula [12], $E_{\alpha,\beta}^{\delta}(z)=(-z)^{\delta}/\Gamma(\delta)\sum_{k=0}^{\infty}\Gamma(\delta+k)/\Gamma(\beta-\alpha(\delta+k))\cdot(-z)^{-k}/k!$, $|z|>1$, for large values of z, it can be shown that $\gamma(t)$ satisfies $\lim_{t\to\infty}\gamma(t)=\lim_{t\to\infty}s\hat{\gamma}(s)=0$ [10], where $\hat{\gamma}(s)=L[\gamma(t)]=\gamma_{\alpha,\beta,\delta}\,s^{\alpha\delta-\beta}/(s^{\alpha}+\tau^{-\alpha})^{\delta}$ is the Laplace transform of $\gamma(t)$, $\gamma_{\alpha,\beta,\delta}=C_{\alpha,\beta,\delta}/k_BT\tau^{\alpha\delta}$ [10]. The case $\tau\to 0$, $\alpha\neq 1$, $\beta=\delta=1$ yields the power law frictional memory kernel $C(t)=C_{\alpha}t^{-\alpha}/\Gamma(1-\alpha)$, which has been used to model anomalous diffusive processes [13-15]. Note that the standard Brownian motion is a special case of the considered problem and can be obtained in case when $\alpha=\beta=\delta=1$ and $\tau\to 0$ (noise term becomes the Dirac delta or white noise). In [10,16-19] M-L frictional memory kernels were used as generalizations of the one of power law form. In [19-21] fractional GLEs with different noise terms were analyzed and used for modeling generalized diffusive processes.

This paper is organized as follows. In section 2 formal solution of the GLE is given. The asymptotic behavior of the oscillator in the long time limit is analyzed. Exact results for the MSD, and normalized displacement correlation function in case of generalized internal noises, in the overdamped limit, are derived. Some possible applications of the considered model are discussed. Conclusions are given in section 3.

2. GLE FOR A HARMONIC OSCILLATOR. SOLUTION AND RESULTS

Let us solve the GLE (1) for a harmonic oscillator. By Laplace transform one obtains:

$$\hat{X}(s)=x_0\left[s^{-1}-\omega^2\hat{I}(s)\right]+\left[v_0+\frac{1}{m}\hat{F}(s)\right]G(s) \tag{5}$$

$$\hat{V}(s)=\left[v_0+\frac{1}{m}\hat{F}(s)\right]\hat{g}(s)-\omega^2x_0\hat{G}(s) \tag{6}$$

where $\hat{X}(s)=L[x(t)]$, $\hat{V}(s)=L[v(t)]$, $x_0=x(0)$ and $v_0=v(0)$ are initial particle displacement and initial particle velocity, respectively, $\hat{F}(s)=L[\xi(t)]$,

$$\hat{I}(s)=\frac{s^{-1}}{s^2+s\hat{\gamma}(s)/m+\omega^2}, \tag{7}$$

$\hat{G}(s)=s\hat{I}(s)$, $\hat{g}(s)=s\hat{G}(s)$. The inverse Laplace transform of relations (5) and (6) yields:

$$\begin{aligned}x(t)&=x_0\left[1-\omega^2I(t)\right]+v_0G(t)+\frac{1}{m}\int_0^t G(t-t')\xi(t')\mathrm{d}t'=\\&=\langle x(t)\rangle+\frac{1}{m}\int_0^t G(t-t')\xi(t')\mathrm{d}t'.\end{aligned} \tag{8}$$

$$v(t) = v_0 g(t) - \omega^2 x_0 G(t) + \frac{1}{m}\int_0^t g(t-t')\xi(t')\mathrm{d}t' = \\ = \langle v(t)\rangle + \frac{1}{m}\int_0^t g(t-t')\xi(t')\mathrm{d}t' \tag{9}$$

where $\langle x(t)\rangle = x_0[1-\omega^2 I(t)] + v_0 G(t)$, $\langle v(t)\rangle = v_0 g(t) - \omega^2 x_0 G(t)$ are mean particle displacement and mean particle velocity, respectively, and $I(t) = L^{-1}[\hat{I}(s)]$, $G(t) = L^{-1}[\hat{G}(s)]$ and $g(t) = L^{-1}[\hat{g}(s)]$ are the so-called relaxation functions. They are related to the MSD $\langle x^2(t)\rangle$, time-dependent diffusion coefficient $D(t) = (1/2)\,\mathrm{d}\langle x^2(t)\rangle/\mathrm{d}t$, velocity autocorrelation function (VACF) $C_V(t) = \langle v(t)v(0)\rangle/\langle v^2(0)\rangle$. In the long time limit ($t\to\infty$), one obtains $\langle x^2(t)\rangle = (2k_BT/m)I(t)$, $D(t) = (k_BT/m)G(t)$ and $C_V(t) = g(t)$ [14,16,17].

2.1. Asymptotic behavior

Sometimes, finding the relaxation functions is very complicated problem. Since we are interested to analyze the anomalous diffusive behavior of the oscillator, we investigate the asymptotic behavior of relaxation functions in the long time limit by using Tauberian theorem [22]. It stands that if the asymptotic behavior of a given non negative and monotone function $r(t)$ for $t\to\infty$ is $r(t)\simeq t^{-\alpha}$, then its corresponding Laplace transform pair $\hat{r}(s) = L[r(t)]$, has the behavior $\hat{r}(s)\simeq\Gamma(1-\alpha)s^{\alpha-1}$, for $s\to 0$. Thus, for $\beta-1<\alpha\delta<\beta+1$, it is obtained:

$$I(t) = \sum_{k=0}^{\infty}\left(-\omega^2\right)^k t^{2k+2} E^{k+1}_{2-(1+\alpha\delta-\beta),2k+3}\left(-\frac{C_{\alpha,\beta,\delta}}{k_BTm}t^{2-(1+\alpha\delta-\beta)}\right) \\ \simeq \frac{k_BTm}{C_{\alpha,\beta,\delta}}t^{1+\alpha\delta-\beta}E_{1+\alpha\delta-\beta,2+\alpha\delta-\beta}\left(-\frac{k_BTm\omega^2}{C_{\alpha,\beta,\delta}}t^{1+\alpha\delta-\beta}\right) \quad \text{for} \quad t\to\infty. \tag{10}$$

By using $E_{\alpha,\beta}(z) = zE_{\alpha,\alpha+\beta}(z) + 1/\Gamma(\beta)$, relaxation function (10) yields the MSD:

$$\langle x^2(t)\rangle = \frac{2k_BT}{m\omega^2}\left[1 - E_{1+\alpha\delta-\beta}\left(-\frac{k_BTm\omega^2}{C_{\alpha,\beta,\delta}}t^{1+\alpha\delta-\beta}\right)\right], \tag{11}$$

from where we find $D(t)$ and $C_V(t)$. Relation (11) turns to $\langle x^2(t)\rangle \simeq t^{1+\alpha\delta-\beta}/\Gamma(2+\alpha\delta-\beta)$ in case of a free particle ($V(x)=0$) [10], from where one concludes that anomalous diffusion occurs (subdiffusion if $\beta-1<\alpha\delta<\beta$ and superdiffusion if $\beta<\alpha\delta<\beta+1$). Relation (11) gives the equilibrium value $\langle x^2(t)\rangle_{t\to\infty} = 2k_BT/m\omega^2$. Note that relation (10) is the exact expression for the case $\tau\to 0$. The result for $C_V(t)\simeq t^{\alpha\delta-\beta-1}/\Gamma(\alpha\delta-\beta)$ can be used, for example, in the description of experimental data for VACF in the motion of atoms in liquid argon [23]. For $\alpha=\beta=\delta=1$ it is obtained the result for the standard Brownian motion, i.e. a linear dependence of the MSD on time.

2.2. High viscous damping

Next we investigate the behavior of oscillator in case of high friction. Neglecting the inertial term, by applying an inverse Laplace transform [24] of relation (7), relaxation function becomes:

$$I_0\left(t\right)=L^{-1}\left[\frac{s^{-1}}{s\hat{\gamma}\left(s\right)/m+\omega^2}\right]=\frac{1}{\omega^2}\sum_{k=0}^{\infty}\left(-\frac{\gamma_{\alpha,\beta,\delta}}{m\omega^2}\right)^k t^{(\beta-1)k}E_{\alpha,(\beta-1)k+1}^{\delta k}\left(-\frac{t^\alpha}{\tau^\alpha}\right). \qquad (12)$$

From the asymptotic expansion formula for the three parameter M-L function, $I_0\left(t\right)$ becomes:

$$\begin{aligned}I_0\left(t\right)&=\frac{k_BTm}{C_{\alpha,\beta,\delta}}t^{1+\alpha\delta-\beta}E_{1+\alpha\delta-\beta,2+\alpha\delta-\beta}\left(-\frac{k_BTm\omega^2}{C_{\alpha,\beta,\delta}}t^{1+\alpha\delta-\beta}\right)=\\&=\frac{1}{\omega^2}\left[1-E_{1+\alpha\delta-\beta}\left(-\frac{k_BTm\omega^2}{C_{\alpha,\beta,\delta}}t^{1+\alpha\delta-\beta}\right)\right],\end{aligned} \qquad (13)$$

in the long time limit. Thus, MSD has the form (11). Thus, the anomalous diffusive behavior of the oscillator may be investigated by considering high viscous damping, instead of the GLE (1).

2.3. Results and discussion

Let us now consider the following initial conditions: $\langle x_0^2\rangle=k_BT/m\omega^2$, $\langle x_0v_0\rangle=0$, $\langle\xi(t)x_0\rangle=0$ [15]. Thus, for the normalized displacement correlation function given by $C_X(t)=\langle x(t)x_0\rangle/\langle x_0^2\rangle$, which is an experimentally measured quantity, one obtains:

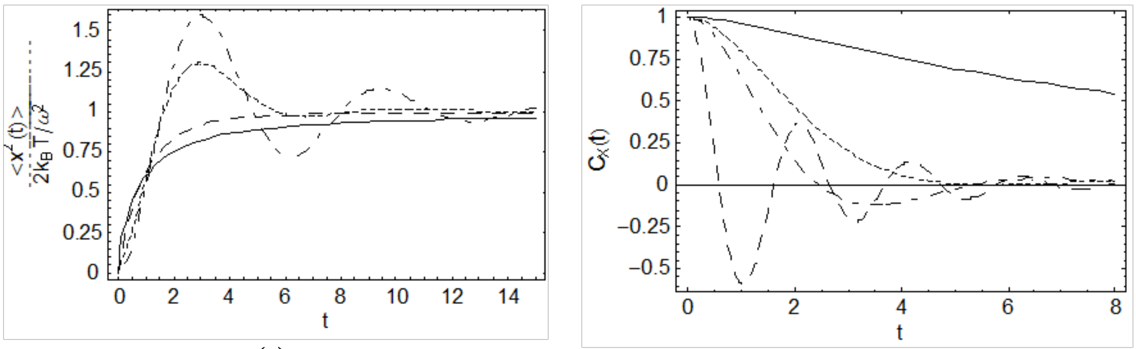
$$C_X\left(t\right)=L^{-1}\left[\frac{1}{s}-\frac{\omega^2s^{-1}}{s\hat{\gamma}\left(s\right)/m+\omega^2}\right]=1-\omega^2I_0\left(t\right) \qquad (14)$$

where $I_0(t)$ is given by (13). For $\tau\to 0$ it follows $C_X(t)=E_{1+\alpha\delta-\beta}\left(-(k_BTm\omega^2/C_{\alpha,\beta,\delta})t^{1+\alpha\delta-\beta}\right)$, which is in agreement with experimental results for the fluctuations of the distance between fluorescein-tyrosine pair within a single protein [9].

Let us further analyze obtained results. Firstly, note that relaxation function (12) is represented in terms of infinite series of three parameter M-L functions. The long time limit yields relation (11) which is represented by one parameter M-L function. It is known that $f(t)=E_\alpha(-t^\alpha)$ is a completely monotone function for $0<\alpha<1$ [25], i.e. $(-1)^n f^{(n)}(t)\geq 0$ for all $t>0$ and all n = 0, 1, 2, ... The case $1<\alpha$ may show interesting oscillation-like behavior. By taking constants that appear in relation (11) equal to one and by using $\omega=1$, the MSD (11) is completely monotone for $0<1+\alpha\delta-\beta<1$. From Fig. 1(a) ($\omega=1$) we see that for $\alpha=3/2$, $\beta=1$, $\delta=1/2$ (solid line), and $\alpha=1/2$, $\beta=7/16$, $\delta=3/4$ (dashed line), MSD has monotonic behavior since $0 < 1 + \alpha\delta - \beta < 1$. For $\alpha = 5/4$, $\beta = 1/2$, $\delta = 1$ (dot-dashed line), and $\alpha = 3/4$, $\beta = 1/4$, $\delta = 1$ (dotted line), MSD shows oscillation-like behavior since $1 + \alpha\delta - \beta > 1$. In Fig. 1(b) graphical representation of $C_X(t) = 1 - \omega^2 I(t)$, where $I(t)$ is given by (10), for $\alpha = 1/2$, $\beta = 7/16$, $\delta = 3/4$, is presented. We see that for $\omega = 0.3$ (solid line), $C_X(t)$ has monotonic decay and does not cross the zero line. For $\omega = 3$ (dashed line) and $\omega = 1$ (dot-dashed line), $C_X(t)$ crosses the zero line and it has oscillation-like behavior. For $\omega = 0.74$ (dotted line), $C_X(t)$ has non monotonic decay. It approaches the zero line but does not cross it. These results are different than the ones for a classical damped oscillator, where only two types of motion may appear: overdamped motion when $\langle x(t) \rangle > 0$ for any time *t* when $\langle x_0 \rangle > 0$ and there are no oscillations, and underdamped motion when $\langle x(t) \rangle$ crosses the zero line and oscillates [15]. The frequency on which transition from overdamped to underdamped motion appears is so-called critical frequency. Here, in the considered GLE, there are additional definitions of critical frequencies [15] on which the oscillator changes its behavior, for example from monotonic to non monotonic decay of $C_X(t)$ without crossings of the zero line. They depend on parameters of the frictional memory kernel and their estimation is a nontrivial problem [15]. Such oscillations, as shown in Fig. 1(b), were observed in the molecular dynamic simulations of fluctuations of donor-acceptor distance for a single protein [26]. Furthermore, such oscillations and power law decay of the distance between fluorescein-tyrosine pair within a single protein have been observed experimentally [9].

3. CONCLUSIONS

It is shown that the GLE for a harmonic oscillator is a suitable model for anomalous dynamics within proteins. It is shown that the case of high friction, which is simpler, can be used for analyzing the anomalous diffusive behavior instead of the GLE (1). The obtained analytical results for the MSD and normalized displacement correlation function are in good agreement with some known experimental observations.



(a) (b)

Fig. 1: Graphical representation of: (a) MSD; (b) $C_X(t)$.

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ХАРМОНИСКИ ОСЦИЛАТОР ДВИЖЕН СО ГЕНЕРАЛИЗИРАНИ ШУМОВИ: ПОВЕДЕНИЕ ПРИ СИЛНО ТРИЕЊЕ

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Апстракт. Презентиран е аналитички третман на генерализирана равенка на Ланжевен за хармониски осцилатор движен со генерализирани шумови. Разгледан е случајот на силно вискозно триење како модел за конформациона динамика на протеини. Поведението на осцилаторот е анализирано со пресметување на средното квадратно поместување и нормираната корелациона функција на поместувањето. Резултатите се претставени со помош на функциите на Митаг-Лефлер. Стандардното Брауново движење претставува специјален случај на разгледаниот модел. Покажана е добра согласност со некои експериментални резултати.