Non-Markovian Fokker-Planck equation: Solutions and first passage time distribution

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We investigate the solutions and first passage time distribution for an anomalous diffusion process governed by a generalized non-Markovian Fokker-Planck equation. In our analysis, we also consider the presence of external forces and absorbent (source) terms. In addition, we show that a rich class of diffusive processes, including normal and anomalous ones, can be obtained from the solutions found here.

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I. INTRODUCTION

A large class of physical phenomena related to relaxation processes in complex systems may be usually described by the non-Markovian Fokker-Plack equation [1]

$$\frac{\partial}{\partial t}\rho(r,t) = \int_0^t d\bar{t}\mathcal{K}(t-\bar{t})\mathcal{L}\{\rho(r,\bar{t})\},\tag{1}$$

where $\mathcal{K}(t)$ is a kernel which takes a memory effect into account and $\mathcal{L}\{\cdots\}$ is a linear operator, acting on the spatial variable, which we considered, without loss of generality, given by

$$\mathcal{L}\{\rho\} \equiv \mathcal{D}\widetilde{\nabla}^2 \rho - \nabla \cdot [\bar{F}(r)\rho] + \alpha(r)\rho, \qquad (2)$$

where \mathcal{D} is a diffusion coefficient, $\nabla^2 \equiv r^{1-\mathcal{N}}\partial_r \{r^{\mathcal{N}-1-\theta}\partial_r [r^{-\beta}\cdots]\}$ $(\theta=\beta=0$ recovers the usual La- $\widetilde{\nabla}^2$ placian operator for the N-dimensional case within radial symmetry), $\overline{F}(r) = F(r)\hat{r}$ represents an external force applied to the system, and $\alpha(r)$ is an absorbent (source) term related to a reaction diffusion process. Particular cases of this operator have been used in the analysis of a rich variety of scenarios such as diffusion on fractals [2-4], systems with finite boundary conditions [5], the first passage time related to anomalous diffusion processes [6,7], fast electrons in a hot plasma in the presence of a electric field [8], and turbulence [9,10]. The reaction term present in Eq. (2) may be applied to several scenarios such as catalytic processes in regular, heterogeneous, or disordered systems [11] and in irreversible first-order reactions of the transported substance whose rate of removal equals $\bar{\alpha}\rho$ [12]. Equation (1) may also be used to investigate subdiffusion-limited reactions [13], and by suitable changes it may correspond to a Schrödinger-like equation for $\mathcal{K}(t) \propto \delta(t)$ with mass depending on the position, similarly to the one investigated in [14]. Equation (1) recovers the usual N-dimensional diffusion equation within radial symmetry without memory effect for $\mathcal{K}(t) = \delta(t)$ and $\theta = \beta = 0$. The fractional diffusion equation used to investigate physical phenomena related to anomalous diffusion [15-20] may be obtained from Eq. (1). By employing a suitable kernel with $\beta=0$ and by choosing the kernels $\mathcal{K}(t) \propto \int d\gamma p(\gamma) t^{\gamma-1}$, it is possible to study slow processes lacking scaling [21]. Also, by using Eq. (1), a well-known limitation of the description of diffusion processes with the diffusion equation-i.e., the infinite velocity of information

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propagation inherent to a parabolic equation—can be avoided by choosing a suitable kernel [22].

From the previous discussion, we note the importance of this kind of equation not only due to the broad range of scenarios which can be successfully described, but also due to the growing interest in the feasibility of covering new situations. Thus, the present work intends to establish some classes of solutions for this non-Markovian Fokker-Planck equation. In connection with these solutions, we investigate the first passage time distribution (FPTD), since only in few cases does one have an explicit analytical expression for the FPTD distribution as is pointed out in [23]. Notice that knowledge of the FPT distribution $\mathcal{F}(t)$ is essential to obtain the mean first passage time (MFPT). Examples of the MFPT are the escape time from a random potential, intervals between neural spikes [24], stochastic resonance [25], and fatigue failure [26].

The plan of this work is to investigate, in Sec. II, the solutions of Eq. (1). We start by considering the kernel $\mathcal{K}(t) = \mathcal{K}_0 \delta(t) + \mathcal{K}_1 t^{\gamma-2} / \Gamma(\gamma-1)$, the external force $F(r) = \mathcal{K}_{\nu} / r^{1+\nu}$ ($\nu = \theta + \beta$), and the absorbent term $\alpha(r) = -\alpha/r^{\eta}$ ($\eta = 2 + \theta + \beta$). Afterwards, we discuss the first passage time distribution related to this process by employing $\mathcal{K}_1 = 0$ and $\alpha = 0$. In this context, we first study situations characterized by the boundary conditions defined in a finite interval and after we extend our analysis to a semi-infinite interval. In particular, for the case characterized by a semi-infinite interval. In particular, for simplicity, $\mathcal{K}_0 = 0$. Subsequently, we consider the external force $F(r) = -kr + \mathcal{K}_{\nu} / r^{1+\nu}$ and the absorbent (source) term $\alpha(r) = -\alpha_1 r^{\eta} - \alpha_2 / r^{\eta}$. Finally, we present our conclusions in Sec. III.

II. NON-MARKOVIAN FOKKER-PLANCK EQUATION

Let us start our discussion by considering Eq. (1) in the presence of the external force $F(r) = \mathcal{K}_{\nu}/r^{1+\nu}$ ($\nu = \theta + \beta$), subjected to the boundary condition $\rho(a,t)=0$ and the presence of the absorbent (source) term $\alpha(r)=-\alpha/r^{\eta}$ ($\eta=2+\theta+\beta$). Note that the potential related to this external force extends the logarithmic potential used, for instance, to establish a connection between the fractal diffusion coefficient and the generalized mobility [27]. Now, we employ the Laplace transform to solve Eq. (1) subjected to these conditions. Thus, by taking the Laplace transform and by using the Green's function approach [28], we obtain

$$\rho(r,s) = \int_{0}^{a} d\xi \xi^{\mathcal{N}-1-\beta-\mathcal{K}_{1}/\mathcal{D}} \widetilde{\rho}(\xi) \mathcal{G}(r,\xi,s),$$

$$\mathcal{G}(r,\xi,s) = \frac{\omega}{a^{\omega}} \sum_{n=1}^{\infty} \frac{(\xi r)^{(\omega+\beta+\mathcal{K}_{1}/\mathcal{D}-\mathcal{N})/2}}{\{J_{p+1}(\bar{\lambda}_{n}a^{\omega/2})\}^{2}}$$

$$\times J_{p}(\bar{\lambda}_{n}\xi^{\omega/2}) J_{p}(\bar{\lambda}_{n}r^{\omega/2}) \Phi_{n}(s),$$

$$\Phi_{n}(s) = \frac{1}{s + \mathcal{K}(s)\mathcal{D}\lambda_{n}^{2}},$$
(3)

in Laplace space, where $\omega = 2 + \theta + \beta$, $p = \{ [\mathcal{N} - \omega + \beta] \}$ $+\mathcal{K}_{\nu}/\mathcal{D}]^{2}+4\alpha/\mathcal{D}^{1/2}/\omega, \,\overline{\lambda}_{n}=2\lambda_{n}/\omega, \,J_{\nu}(x)$ is the Bessel function, λ_n (eigenvalue) is obtained from $J_n(\overline{\lambda}_n a^{\omega/2}) = 0$ and the initial condition is given by $\rho(r,0) = \tilde{\rho}(r)$. To obtain the inverse of Laplace transform of Eq. (3) is a hard task if we consider a general kernel $\mathcal{K}(s)$. However, for some cases such as $\mathcal{K}(s) = \mathcal{K}_0$ and $\mathcal{K}(s) = \mathcal{K}_1 s^{1-\gamma}$, it is possible to obtain the inverse of the Laplace transform. In particular, these cases play an important role in the analysis of the relaxation process of a complex system. In fact, the first case corresponds to the usual relaxation-i.e., an exponential behavior-and the second one is related to an anomalous relaxation [15], whose behavior is given in terms of the Mittag-Leffler function $[E_{\gamma}(x) = \sum_{n=0}^{\infty} x^n / \Gamma(1 + \gamma n)]$. In order to unify these cases, we consider $\mathcal{K}(s) = \mathcal{K}_0 + \mathcal{K}_1 s^{1-\gamma}$, which leads us to

$$\Phi_n(t) = \sum_{k=0}^{\infty} \frac{1}{k!} (-\mathcal{K}_0 \mathcal{D} \lambda_n^2 t)^k E_{\gamma, 1+(1-\gamma)k}^{(k)} (-\lambda_n^2 \mathcal{K}_1 \mathcal{D} t^{\gamma}), \quad (4)$$

with $E_{\lambda,\mu}^{(k)}(x) \equiv \sum_{n=0}^{\infty} (n+k)! x^n / [n! \Gamma(\lambda(n+k)+\mu)]$. By taking $\mathcal{K}_1 = 0$ in Eq. (4), we obtain the usual exponential behavior i.e., $\Phi_n(t) = e^{-\mathcal{K}_0 D \lambda_n^2 t}$ —and for $\mathcal{K}_0 = 0$, we have $\Phi_n(t) = E_{\gamma}(-\mathcal{K}_1 D \lambda_n^2 t^{\gamma})$. From these particular cases, we verify that the kernel $\mathcal{K}(s)$, as we mentioned above, corresponds to the mixing of the usual relaxation governed by exponential behavior and the anomalous relaxation governed by a Mittag-Leffler function. Thus, Eq. (4) presents two diffusive regimes. Similar situations characterized by two regimes may appear, for instance, in systems with long-ranged interaction Hamiltonians [29,30] and in active intracellular transport [31]. By using the definition present in [32], we may obtain the first passage time related to this process by considering, for simplicity, $\mathcal{K}_1 = 0$ and $\alpha = 0$. The last requirement is used to fix the number of particles present in the system. After some calculations, it is possible to show that

$$\mathcal{F}(\xi,t) = \frac{2\mathcal{K}_0 \mathcal{D}}{a^{\omega}} \int_0^a d\xi \xi^{\mathcal{N}-1-\beta-\mathcal{K}_v/\mathcal{D}} \widetilde{\rho}(\xi) \sum_{n=1}^\infty \frac{\xi^{(\omega+\beta+\mathcal{K}_v/\mathcal{D}-\mathcal{N})/2}}{\{J_{p+1}(\bar{\lambda}_n a^{\omega/2})\}^2} \\ \times J_p(\bar{\lambda}_n \xi^{\omega/2}) \lambda_n^2 e^{-\mathcal{K}_0 \mathcal{D} \lambda_n^2 t} \left[\frac{\omega^2}{2\lambda_n^2 \Gamma(p)} \left(\frac{\lambda_n}{\omega} \right)^p \right. \\ \left. - \frac{\omega a^{\omega(1-p)/2}}{2\lambda_n} J_{p-1} \left(\frac{2\lambda_n}{\omega} a^{\omega/2} \right) \right], \tag{5}$$

with $\omega > \beta + \mathcal{K}_{\nu} / \mathcal{D} + \mathcal{N}$ (see Fig. 1). In particular, this result



FIG. 1. Behavior of $\mathcal{F}(\xi,t)$ versus *t* for a typical values of β and \mathcal{K}_{ν} by considering, for simplicity, $\xi=1.0$, a=3.0, $\mathcal{N}=1.0$, $\theta=2$, $\mathcal{K}_{0}=3$, $\tilde{\rho}(r)=r^{1+\beta+\mathcal{K}_{\nu}/\mathcal{D}-\mathcal{N}}\delta(r-\xi)$, and $\mathcal{D}=1.0$.

found for the first passage time distribution extends the results obtained in [7].

We may extend the above results found for Eq. (1) by considering $a \rightarrow \infty$ for the case characterized, for simplicity, by $\mathcal{K}(t) = \mathcal{K}_1 t^{\gamma-2} / \Gamma(\gamma-1)$, with $\mathcal{K}_1 = 1$. This choice of kernel leads us to a fractional diffusion like equation which may be useful to investigate several situations such as axial transport of granular materials [33], random compressible flows [34], transport of a substance in a solvent from one vessel to another across a thin membrane [35], and asymmetry of DNA translocation [36]. To obtain this extension, it is useful to use

$$\rho(r,t) = \int_0^\infty dk \mathcal{C}(k,t) \Psi(r,k),$$

$$\Psi(r,k) = r^{(\omega+\beta+\mathcal{K}_p/\mathcal{D}-\mathcal{N})/2} J_p\left(\frac{2}{\omega}kr^{\omega/2}\right),\tag{6}$$

where C(k,t) is the kernel to be found. By substituting Eq. (6) into Eq. (1) and taking the previous external force and absorbent terms into account, we obtain

$$\frac{d}{dt}\mathcal{C}(k,t) = -\mathcal{D}k^2 \int_0^t d\tilde{t}\mathcal{K}(t-\tilde{t})\mathcal{C}(k,\tilde{t}).$$
(7)

By solving Eq. (7), we found $C(k,t) = C(k,0)E_{\gamma}(-k^2Dt^{\gamma})$, where C(k,0) is determined by the initial condition. By using the initial condition $\rho(r,0) = \tilde{\rho}(r)$, we verify that

$$C(k,0) = \frac{2k}{\omega} \int_0^\infty d\xi \xi^{\mathcal{N}-1-\beta-\mathcal{K}_v/\mathcal{D}} \widetilde{\rho}(\xi) \Psi(\xi,k).$$
(8)

Thus, the solution is given by

$$\rho(r,t) = \int_0^\infty d\xi \xi^{\mathcal{N}-1-\beta-\mathcal{K}_\gamma/\mathcal{D}} \tilde{\rho}(\xi) \mathcal{G}(r,\xi,t),$$
$$\mathcal{G}(r,\xi,t) = \frac{2}{\omega} \int_0^\infty dk k \Psi(\xi,k) \Psi(r,k) E_\gamma(-k^2 \mathcal{D} t^\gamma). \tag{9}$$

Notice that if we have used $\mathcal{K}(t) = \mathcal{K}_0 \delta(t) + \mathcal{K}_1 t^{\gamma-2} / \Gamma(\gamma-1)$, the main change produced in Eq. (9) would be the presence of the function $\Phi(t)$, defined by Eq. (4), instead of the Mittag-Leffler function. From the above equation, two interesting cases emerge when we consider p=1/2 with an arbitrary γ and $\gamma=1$ with an arbitrary p. For the first case—i.e., p=1/2 with γ arbitrary—the Green function can be reduced to

$$\mathcal{G}(r,\xi,t) = \frac{(r\xi)^{(\omega/2+\beta+\mathcal{K}_{r}/\mathcal{D}-\mathcal{N})/2}}{\sqrt{4\mathcal{D}t^{\gamma}}} \\ \times \left(H_{11}^{10} \left[\left. \frac{2|r^{\omega/2} - \xi^{\omega/2}|}{\omega\sqrt{\mathcal{D}t^{\gamma}}} \right|_{(0,1)}^{(1-\gamma/2,\gamma/2)} \right] \\ - H_{11}^{10} \left[\left. \frac{2|r^{\omega/2} + \xi^{\omega/2}|}{\omega\sqrt{\mathcal{D}t^{\gamma}}} \right|_{(0,1)}^{(1-\gamma/2,\gamma/2)} \right] \right), \quad (10)$$

where $H_{pq}^{mn}[x|_{(b_1,B_1),\ldots,(a_p,A_p)}^{(a_1,A_1),\ldots,(a_p,A_p)}]$ is the Fox *H* function [37]. For the second case, $\gamma = 1$ with *p* arbitrary, we can simplify the Green function present in Eq. (9) by using the identity [38] $\int_{0}^{\infty} dkkJ_{\nu}(\widetilde{\alpha}k)J_{\nu}(\widetilde{\beta}k)e^{-\widetilde{\alpha}^2k^2} = e^{-(\beta^2+\widetilde{\alpha}^2)/(4\widetilde{\alpha}^2)}I_{\nu}(\widetilde{\alpha}\widetilde{\beta}/(2\widetilde{\alpha}^2))/(2\widetilde{\alpha}^2)$ in order to obtain

$$\mathcal{G}(r,\xi,t) = (\xi r)^{(\omega+\beta+\mathcal{K}_{\nu}/\mathcal{D}-\mathcal{N})/2} \frac{e^{-(r^{\omega}+\xi^{\omega})/\omega^{2}\mathcal{D}t}}{\omega\mathcal{D}t} I_{p} \left[\frac{2(\xi r)^{\omega/2}}{\omega^{2}\mathcal{D}t}\right], \quad (11)$$

where $I_{\nu}(x)$ is a modified Bessel function. The asymptotic behavior for the second moment associated with this process is $\langle r^2 \rangle \sim t^{2/\omega}$ for long time, where $\omega > 2$, =2, or <2 corresponds, respectively, to a subdiffusive, normal, or superdiffusive process. In particular, for this case the first passage time distribution is given by $\mathcal{F}(\xi,t) = \xi^{\omega-\mathcal{N}} e^{-\xi^{\omega}/\mathcal{D}t\omega^2} / [t\Gamma(1 - \widetilde{\alpha})(\mathcal{D}\omega^2 t)^{1-\widetilde{\alpha}}]$ where $\widetilde{\alpha} = (\mathcal{N} + \mathcal{K}_{\nu}/\mathcal{D} + \beta)/\omega$, $\alpha = 0$, and $\omega > \mathcal{N} + \mathcal{K}_{\nu}/\mathcal{D} + \beta$ (see Fig. 2). Note that this result for the first passage time distribution recovers the result present in [7] for $\mathcal{N} = 1$, $\beta = 0$, and $\mathcal{K}_{\nu} = 0$.

Now, let us extend the external force and the absorbent term worked out above by incorporating a linear term in the external force and the positive power-law term in the absorbent term. More precisely, we consider the external force $F(r)=-kr+\mathcal{K}_{\nu}/r^{1+\nu}$ and the source term $\alpha(r)=-\alpha_1r^{\eta}-\alpha_2/r^{\eta}$. In order to obtain the solution for Eq. (1) taking these conditions into account, we expand $\rho(r,t) = \sum_n \Psi_n(r) \widetilde{\Phi}_n(t)$ with $\Psi_n(r)$ (eigenfunction) determined by the spatial equation

$$\frac{\mathcal{D}}{r^{\mathcal{N}-1}} \frac{d}{dr} \left\{ r^{\mathcal{N}-1} \left[r^{-\theta} \frac{d}{dr} [r^{-\beta} \Psi_n(r)] - F(r) \Psi_n(r) \right] \right\} + \alpha(r) \Psi_n(r)$$
$$= -\bar{\lambda}_n \Psi_n(r) \tag{12}$$

and $\Phi_n(t)$ obtained from the time equation $d\Phi_n(t)/dt =$



FIG. 2. Behavior of $\mathcal{F}(\xi, t)$ versus *t* for a typical values of ω , \mathcal{N} , and \mathcal{K}_{ν} by considering, for simplicity, $\xi=1.0$, $\beta=1$, $\tilde{\rho}(r) = r^{1+\beta+\mathcal{K}_{\nu}/\mathcal{D}-\mathcal{N}}\delta(r-\xi)$, and $\mathcal{D}=1.0$.

 $-[\overline{\lambda}_n/\Gamma(\gamma-1)]\int_0^t d\widetilde{t}(t-\widetilde{t})^{\gamma-2}\widetilde{\Phi}_n(\widetilde{t})$. Thus, after some calculation, it is possible to show that

$$\rho(r,t) = \int_{0}^{\infty} d\xi \xi^{N-1-\beta-\mathcal{K}_{\eta}/\mathcal{D}} \widetilde{\rho}(\xi) \mathcal{G}(r,\xi,t), \mathcal{G}(r,\xi,t)$$

$$= \left(\frac{\overline{k}}{\omega \mathcal{D}}\right)^{\overline{\alpha}+1} (r\xi)^{\beta+\mu} e^{-(k/2\omega\mathcal{D})(r^{\omega}-\xi^{\omega})} e^{-(\overline{k}/2\omega\mathcal{D})(r^{\omega}+\xi^{\omega})}$$

$$\times \sum_{n=0}^{\infty} \frac{\omega\Gamma(n+1)}{\Gamma(1+\overline{\alpha}+n)} L_{n}^{(\overline{\alpha})} \left(\frac{\overline{k}\xi^{\omega}}{\omega \mathcal{D}}\right) L_{n}^{(\overline{\alpha})} \left(\frac{\overline{k}r^{\omega}}{\omega \mathcal{D}}\right) E_{\gamma}(-\overline{\lambda}_{n}t^{\gamma}),$$
(13)

with $\overline{k} = \sqrt{k^2 + 4D\alpha_1}$, $\mu = (\mathcal{K}_\nu/\mathcal{D} + 2 + \theta - \mathcal{N} + \omega\overline{\alpha})/2$, $\overline{\alpha} = \sqrt{4D\alpha_2 + [\mathcal{K}_\nu + \mathcal{D}(\mathcal{N} - 2 - \theta)]^2/(\omega \mathcal{D})}$, where $L_n^{(\overline{\alpha})}(x)$ are associated Laguerre polynomials, and $\overline{\lambda}_n = \omega \overline{k} \{(1 + \overline{\alpha})/2 + n - k[\mathcal{K}_\nu + \mathcal{D}(\mathcal{N} + \beta)]/(2\omega \mathcal{D}\overline{k})\}$. This result extends the result found in [16] for a linear external force, and for $\gamma = 1$, $\mathcal{N} = 1$, and $\beta = \theta = 0$, we recover the solution for the Rayleigh process presented in [32]. Another interesting feature concerning this case is that for long time, in the absence of absorbent (source) terms, the usual stationary solution may be recovered and is given by $\rho(r) \sim r^{\mathcal{K}_\nu/\mathcal{D} + \beta} e^{-kr^{\omega}/(\omega \mathcal{D})}$. This feature is in agreement with the results previously reported in [16,39].

III. SUMMARY AND CONCLUSIONS

We have worked a non-Markovian Fokker-Planck equation by considering radial symmetry. We have first analyzed

the case characterized by the presence of the external force $F(r) = \mathcal{K}_{\nu}/r^{1+\nu}$ ($\nu = \theta + \beta$), taking the absorbent term $\alpha(r) = \alpha(r)$ $-\alpha/r^{\eta}$ ($\eta=2+\theta+\beta$) into account, by considering a finite interval. We have also obtained the first passage time distribution for the $\mathcal{K}_1=0$ and $\alpha=0$. After, we have extended the results obtained for a semi-infinite interval. In particular, in this context we considered two particular cases from Eq. (9). Following, we have investigated the solutions to the external force $F(r) = -kr + \mathcal{K}_{\nu}/r^{1+\nu}$ and the absorbent (source) term $\alpha(r) = -\alpha_1 r^{\eta} - \alpha_2 / r^{\eta}$. For these cases, we have obtained an exact solution given in terms of the Fox H function, Bessel functions, or the associated Laguerre polynomial and Mittag-Leffler function. The presence of these functions—the Fox Hfunction and the Mittag-Leffler function-is due to the fractional derivative present in the diffusion equation. In fact, the presence of a fractional derivative in the diffusion equation changes the waiting time probability density function. Therefore, we have an anomalous relaxation for this case that differs from the usual case characterized by an exponential relaxation. We have pointed out that the stationary solution for Eq. (13) is equal to the usual one in the absence of the absorbent (source) term. In particular, this result is in agreement with the results presented in [39] concerning the fractional diffusion equations and thermodynamics. We have extended the results presented in [4] for a fractional diffusion equation, the Rayleigh process [32], and the asymptotic results reported in [16] for homogeneous and isotropic random walk models. Finally, we expect that the results presented here will be useful to discuss situations where anomalous diffusion is present.

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