Fractional diffusion equation in a confined region: Surface effects and exact solutions

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Surface effects on a diffusion process governed by a fractional diffusion equation in a confined region with spatial and time dependent boundary conditions are investigated. First, we consider the one-dimensional case with the boundary conditions $\rho(0,t)=\Phi_0(t)$ and $\rho(a,t)=\Phi_a(t)$. Subsequently, the two-dimensional case in the cylindrical symmetry with $\rho(a,\theta,t)=\tilde{\Phi}_a(\theta,t)$ and $\rho(b,\theta,t)=\tilde{\Phi}_b(\theta,t)$ is investigated. For these cases, we also obtain exact solutions for an arbitrary initial condition by using the Green's function approach.

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I. INTRODUCTION

Several physical situations including relaxation to equilibrium in systems (such as polymers chains and membranes) with long temporal memory [1,2], the transport of a substance in a solvent from one vessel to another across a thin membrane [3], diffusion on fractals [4], asymmetry of DNA translocation [5], random compressible flows [6], tumor development [7], and anomalous transport in disordered systems [8], present a strange dynamical behavior which has been successfully investigated by several approaches, in particular, by fractional diffusion equations [9–12]. This variety of applications of these equations has also motivated the study of their solutions [13–24] by taking several scenarios into account: the analysis of the behavior at the origin [25], the investigation of the changes produced by the presence of reaction terms [26–28], and the fractional Kramers equation [29] related to them. In this context, we work out the surface effects on a diffusive process governed by a fractional diffusion equation which occurs in a limited region. This problem is interesting and may find applications, for example, in the adsorption phenomena where the memory effect plays an important role [30,31], in the presence of a reactive boundary [32], and first passage time in confined regions [33]. Our analysis of this question is performed by considering the fractional diffusion equation

$$\frac{\partial^\gamma}{\partial t^\gamma}\rho(\bar{r},t) = \mathcal{D}\nabla^2\rho(\bar{r},t) + \int_0^t d\bar{t}\bar{\mathcal{K}}(t-\bar{t})\nabla^2\rho(\bar{r},t), \qquad (1)$$

where $\mathcal{D}$ is a dimensionless diffusion coefficient, the fractional derivative considered here is the Caputo definition [34], $\bar{\mathcal{K}}(t)$ is a time dependent kernel which we consider given by $\bar{\mathcal{K}}(t)=\mathcal{D}_\alpha t^{\alpha-1}/\Gamma(\alpha)$. The boundary conditions of Eq. (1) are spatial time dependent and the initial condition is $\rho(\bar{r},0)=\tilde{\rho}(\bar{r})$. Equation (1) is analyzed focusing the case $0<\gamma\leq 1$ with $0<\alpha+\gamma\leq 1$ $(0<\alpha)$, i.e., on the subdiffusive behavior. However, this equation could be analyzed by considering other ranges for the parameters γ and α, for example, $0<\gamma\leq 1$, with $0<\alpha$ or $1<\gamma<2$, with $0<\alpha$. In this direction, it is interesting to mention that the results found for the subdiffusive case may be extended to $1<\gamma<2$ by incorporating the condition $\partial_t\rho|_{t=0}=0$. Another aspect of Eq. (1) is the presence of different regimes which, by a suitable choice for $\mathcal{K}(t)$, may be used to investigate particle diffusion in a quasi-two-dimensional bacterial bath [35], enhanced diffusion in active intracellular transport [36], and Hamiltonian systems with long range interactions [37]. In addition, it can be related to the continuous time random walk (CTRW) formalism [10] for the probability density function $\psi(k,s)=\phi(s)\lambda(k)$ with the waiting time distribution in the Laplace space given by $\phi(s)=(\mathcal{D}+\mathcal{K}(s))/(\mathcal{D}+\mathcal{K}(s)+\tau s^\gamma)$ (τ is a characteristic waiting time) and the jumping probability distribution $\lambda(k)=1-\tau k^2$ in the Fourier space.

The plan of this paper is initially to analyze Eq. (1) by considering the one-dimensional case subjected to the boundary condition $\rho(0,t)=\Phi_0(t)$ and $\rho(a,t)=\Phi_a(t)$, where $\Phi_0(t)$ and $\Phi_a(t)$ are two arbitrary time dependent functions. This result shows us how the time dependence on a surface may change the diffusion of a system subjected to a one-dimensional limited region. Following, the two-dimensional case accomplishing the cylindric symmetry with the boundary conditions $\rho(a,\theta,t)=\tilde{\Phi}_a(\theta,t)$ and $\rho(b,\theta,t)=\tilde{\Phi}_b(\theta,t)$ is investigated. This case incorporates a spatial dependence on the boundary condition and makes it possible to investigate the diffusion of a system limited by two inhomogeneous time dependent surfaces. For these cases, we also obtain exact solutions by using the Green's function approach which may be useful to calculate physical quantities such as the time evolution of the system for an arbitrary initial condition and the correlations functions. These developments are performed in Sec. II, and in Sec. III we present our conclusions.

II. FRACTIONAL DIFFUSION EQUATION

Let us start our analysis by considering Eq. (1) in one dimension with the time dependent boundary conditions $\rho(0,t)=\Phi_0(t)$ and $\rho(a,t)=\Phi_a(t)$, and the initial condition $\rho(x,0)=\tilde{\rho}(x)$. For this case, Eq. (1) can be written as follows:

$$\frac{\partial^\gamma}{\partial t^\gamma}\rho(x,t) = \mathcal{D}\frac{\partial^2}{\partial x^2}\rho(x,t) + \frac{\mathcal{D}_\alpha}{\Gamma(\alpha)}\int_0^t dt'(t-t')^{\alpha-1}\frac{\partial^2}{\partial x^2}\rho(x,t'), \qquad (2)$$

with $0<\gamma\leq 1$ and $0\leq\alpha+\gamma\leq 1$ $(\alpha>0)$. This equation extends the usual diffusion equation by the presence of the fractional derivative and the convolution integral present in the diffusive term.

In order to study the surface effects on the relaxation of the system and solve Eq. (2), we use the Laplace transform and the Green's function approach [38]. By applying the Laplace transform and employing this approach, we may obtain the solution in the Laplace space as follows:

$$\hat{\rho}(x,s) = -s^{\gamma-1}\int_0^a dx'\hat{\mathcal{G}}(x,x';s)\tilde{\rho}(x') + \left[\bar{\Phi}_a(s)\frac{\partial}{\partial x'}\hat{\mathcal{G}}(x,x';s)\bigg|_{x'=a} - \bar{\Phi}_o(s)\frac{\partial}{\partial x'}\hat{\mathcal{G}}(x,x';s)\bigg|_{x'=0}\right], \tag{3}$$

with $\tilde{\Phi}_{o,a}(s)=(\mathcal{D}+\mathcal{D}_\alpha s^{-\alpha})\Phi_{o,a}(s)$ and $\mathcal{G}(x,t;x',t')$ governed by the equation

$$\left(\mathcal{D}+\frac{\mathcal{D}_\alpha}{s^\alpha}\right)\frac{d^2}{dx^2}\hat{\mathcal{G}}(x,x';s) - s^\gamma\mathcal{G}(x;x',s) = \delta(x-x'), \tag{4}$$

subjected to the conditions $\mathcal{G}(0,x';s)=0$ and $\mathcal{G}(a,x';s)=0$. By using the eigenfunctions of the Sturm-Liouville problem related to spatial operator of Eq. (4), it is possible to show that

$$\hat{\mathcal{G}}(x,x';s) = -\frac{2}{a}\sum_{n=1}^{\infty}\frac{\sin(n\pi x'/a)\sin(n\pi x/a)}{s^\gamma+(\mathcal{D}+\mathcal{D}_\alpha s^{-\alpha})(n\pi/a)^2}. \tag{5}$$

Applying the inverse of Laplace transform in Eq. (2), we obtain

$$\rho(x,t) = -\frac{1}{\Gamma(1-\gamma)}\int_0^t d\bar{t}\frac{1}{(t-\bar{t})^\gamma}\int_0^a dx'\hat{\mathcal{G}}(x,x';t)\tilde{\rho}(x') + \int_0^t d\bar{t}\left[\bar{\Phi}_a(t-\bar{t})\frac{\partial}{\partial x'}\mathcal{G}(x,x';\bar{t})\bigg|_{x'=a} - \bar{\Phi}_o(t-\bar{t})\frac{\partial}{\partial x'}\mathcal{G}(x,x';\bar{t})\bigg|_{x'=0}\right], \tag{6}$$

[see Fig. 1(a)] with $\bar{\Phi}_{o,a}(t)=\mathcal{D}\Phi_{o,a}(t)+\mathcal{D}_\alpha/\Gamma(\alpha)\int_0^t d\bar{t}(t-\bar{t})^{\alpha-1}\Phi_{o,a}(\bar{t})$,

$$\mathcal{G}(x,x';t) = -\frac{2}{a}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi}{a}x'\right)\sin\left(\frac{n\pi}{a}x\right)\Upsilon_n(t,k_n), \tag{7}$$

[see Fig. 1(b)] and

$$\Upsilon_n(t,k_n) = \sum_{m=0}^{\infty}(t^{\gamma-1}/m!) \times(-\mathcal{D}_\alpha t^{\gamma+\alpha}k_n^2)^m \mathrm{H}_{1\ 2}^{1\ 1}\left[\mathcal{D}k_n^2 t^\gamma\Big|_{(0,1)(1-(\gamma+\alpha)m-\gamma,\gamma)}^{(-m,1)}\right]$$

, where $k_n=n\pi/a$ and $\mathrm{H}_{p\ q}^{m\ n}\left[x\Big|_{(b_1,B_1),\cdots,(b_q,B_q)}^{(a_1,A_1),\cdots,(a_p,A_p)}\right]$ is the Fox H function [39]. Note that $\Upsilon_n(t,k_n)$ is essentially a mixing of two regimes, one of them governed by the fractional derivative and the other dominated by the kernel present in the diffusive term. In fact, $\Upsilon_n(t,k_n)=t^{\gamma-1}\mathrm{E}_{\gamma,\gamma}(-\mathcal{D}k_n^2t^\gamma)$, ($\mathrm{E}_{\gamma,\beta}(x)$ is the generalized Mittag-Leffler function [34]) for $\mathcal{D}\neq 0$ and $\mathcal{D}_\alpha=0$ with $\gamma\neq 1$ and $\Upsilon_n(t,k_n)=t^{\gamma-1}\mathrm{E}_{\gamma+\alpha,\gamma}(-\mathcal{D}_\alpha k_n^2 t^{\gamma+\alpha})$ for $\mathcal{D}=0$ and $\mathcal{D}_\alpha\neq 0$. The first term of Eq. (6) gives the time evolution of the system for an arbitrary initial condition and the second term represents the surface effect. In this direction, Fig. 1(a) shows that Eq. (6) presents a nonusual behavior (e.g, oscillations and accumulation near the boundaries) which may be useful, for example, to investigate systems with boundary condition governed by a kinetic equation related to an adsorption and desorption process [30,31]. This unexpected behavior in Eq. (6) is related to the presence of the fractional derivative, the kernel and the time dependence on the boundary conditions which change the dynamic as-

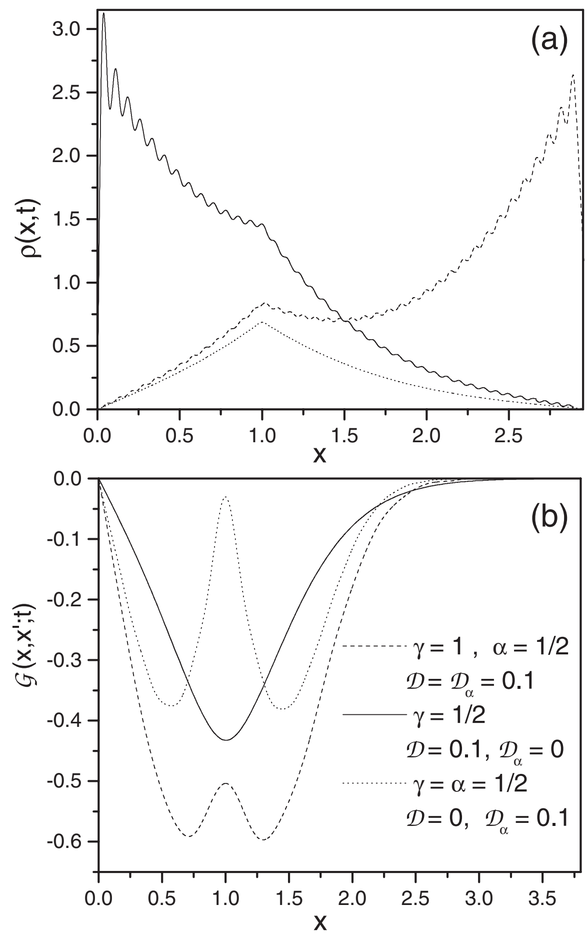

FIG. 1. (a) Behavior of $\rho(x,t)$ versus x, which illustrates Eq. (6) by considering, for simplicity, $\gamma=1/2$, $\mathcal{D}=1$, $\mathcal{D}_\alpha=0$, $a=3$, $t=0.1$, and $\rho(x,0)=\delta(x-1)$. The straight line corresponds to the solution of Eq. (6) subjected to the boundary conditions $\rho(0,t)=\Phi(1+t^{-\eta}/\Gamma(1-\eta))$ ($\Phi=1$ and $\eta=1/2$) and $\rho(a,t)=0$. The dotted line is the solution of Eq. (6) for $\rho(0,t)=\rho(a,0)=0$, and the dashed line corresponds to the solution with the boundary conditions $\rho(0,t)=0$ and $\rho(a,t)=\Phi(1+t^{-\eta}/\Gamma(1-\eta))$ ($\Phi=1$ and $\eta=1/2$). From this figure, it is possible to show that depending on the process, expressed by the boundary conditions, which occurs between the system limited in the confined region and the surface, the diffusion can be drastically modified and present an anomalous behavior. (b) Behavior of $\mathcal{G}(x,x';t)$ versus x, which illustrates Eq. (7) by considering, for simplicity, $a=5$, $x'=1$, and $t=1$.

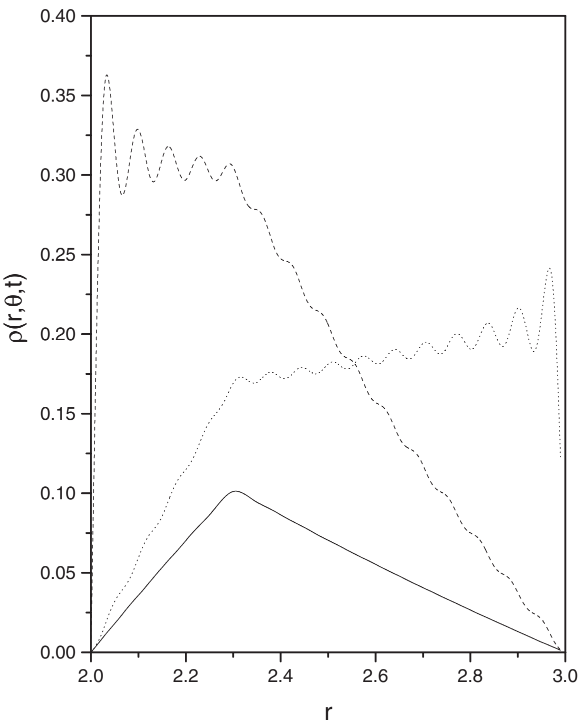

FIG. 2. Behavior of $\rho(r,\theta,t)$ versus r, which illustrates Eq. (8) by considering, for simplicity, $\gamma=1/2$, $\mathcal{D}=1$, $\mathcal{D}_\alpha=0$, $\rho(r,\theta,0)=(2/r)\delta(r-\tilde{r})$ with $\tilde{r}=2.3$, $a=2$, $b=3$, and $t=1$. The straight line corresponds to the solution of Eq. (8) subjected to the boundary conditions $\rho(a,\theta,t)=0$ and $\rho(b,\theta,t)=0$. The dotted line is the solution of Eq. (8) for $\rho(a,\theta,t)=0$ and $\rho(b,\theta,t)=2/(3\pi)$, and the dashed line corresponds to the solution with the boundary conditions $\rho(a,\theta,t)=1/\pi$ and $\rho(b,\theta,t)=0$.

pects of the system. For the special case in which $\Phi_o(t)=\Phi_a(t)=0$ the previous solution recovers the solution found in [18].

Let us analyze Eq. (1) by accomplishing the two-dimensional case with cylindric symmetry and subjected to the boundary conditions $\rho(a,\theta,t)=\tilde{\Phi}_a(\theta,t)$ and $\rho(b,\theta,t)=\tilde{\Phi}_b(\theta,t)$. In this manner, we extend the previous scenario for an inhomogeneous situation where boundary conditions has an angular dependence. By employing the above procedure, the solution of Eq. (1) for this case is given by

$$\rho(r,\theta,t) = -\frac{1}{\Gamma(1-\gamma)}\int_0^t d\bar{t}\frac{1}{(t-\bar{t})^\gamma}\int_0^{2\pi} d\theta'\int_a^b dr' \times r'\mathcal{G}(r,\theta;r'\theta';t)\tilde{\rho}(r',\theta') + \int_0^t dt'\int_0^{2\pi} d\theta'\Bigg[b\bar{\tilde{\Phi}}_b(\theta',t-t') \times\frac{\partial}{\partial r'}\mathcal{G}(r,\theta;r',\theta';t')\bigg|_{r'=b} - a\bar{\tilde{\Phi}}_a(\theta',t') \times\frac{\partial}{\partial r'}\mathcal{G}(r,\theta;r',\theta';t-t')\bigg|_{r'=a}\Bigg], \quad (8)$$

with $\bar{\tilde{\Phi}}_{a,b}(t)=\mathcal{D}\tilde{\Phi}_{a,b}(t)+\mathcal{D}_\alpha/\Gamma(\alpha)\int_0^t d\bar{t}(t-\bar{t})^{\alpha-1}\tilde{\Phi}_{a,b}(\bar{t})$ and

$$\mathcal{G}(r,\theta;r',\theta';t) = -\frac{\pi}{2}\sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\mathcal{N}_{mn}\Psi_{mn}(r)\Psi_{mn}(r')\cos(m(\theta-\theta'))\Upsilon_{mn}(t,k_{mn}), \quad (9)$$

where $\Psi_{mn}(r)=\mathrm{J}_m(k_{mn}r)\mathrm{N}_m(k_{mn}a)-\mathrm{J}(k_{mn}a)\mathrm{N}_m(k_{mn}r)$ [$\mathrm{J}_m(x)$ and $\mathrm{N}_m(x)$ are the Bessel functions of first and second species], k_{mn} are solutions of the eigenvalue equation $\mathrm{J}_m(k_{mn}b)\mathrm{N}_m(k_{mn}a)-\mathrm{J}(k_{mn}a)\mathrm{N}_m(k_{mn}b)=0$, and $\mathcal{N}_{mn}=k_{mn}^2/(\varepsilon_m\{[\mathrm{J}_m(k_{mn}a)/\mathrm{J}_m(k_{mn}b)]^2-1\})$ with $\varepsilon_m=2$ for $m=0$ and $\varepsilon_m=1$ for $m\neq 0$ [see Fig. 2]. Similar to Eq. (6), the last term of Eq. (8) represents the surface effect on the first time which gives the time evolution of the system for an arbitrary initial condition.

An application of the above formalism can be found in those systems that involve liquid crystal samples confined between two concentric cylindrical surfaces. These problems have been investigated in connection with the flexoelectric instability [40], with the stability analysis of the orientational profile [41], and the Fréedericksz transition occurring in the absence of the external electric field [42]. The starting point of this analysis was the original problem proposed by Meyer, solved in a special case by Parodi, and then discussed by de Gennes [43]. Subsequently, the same problem was reexamined by Williams [44] by considering that the elastic constants of splay and bend are different, in the strong anchoring approximation. The formalism presented in this work represents the analytical solution for the diffusion problem of neutral particles in a liquid crystalline system confined in a cylindrical geometry of the kind described above. These neutral particles could be dyes doping the liquid crystalline material [45–49]. The boundary-value problem to determine the bulk density of particles has been solved by considering a temporal and an angular dependence for the orientation at the interface. This situation is physically relevant for a liquid-crystalline system for which the limiting surfaces are inhomogeneous and have a space and time distribution of easy directions. The situation in which the easy axes change direction continuously with time is relevant to investigate systems whose surfaces are covered with photopolymeric films [50]. In these systems, the orientational changes of the photochromic molecules promoted by incident light lead to remarkable changes in the molecular orientation.

III. SUMMARY AND CONCLUSIONS

We have investigated how the surface may modify the diffusive process of a system governed by a fractional diffusion equation. The first situation analyzed was the one-dimensional case characterized by time dependent boundary conditions. This scenario showed the influence of the time dependent boundary conditions on the diffusion of the system for an arbitrary initial condition. This fact is very interesting and changes other quantities related to this process, such as the first passage time which may have an anomalous behavior. Second, we considered the two-dimensional case with inhomogeneous and time dependent boundary conditions. Similarly to the one-dimensional case, the diffusive process and the quantities related to it were modified. Another interesting point concerning the results obtained here is the relation with other physical scenarios, such as the anchoring problem in liquid crystal in a cylindrical region and adsorption phenomena. Finally, we expect that the results found here may be useful to study the systems in which the anomalous diffusion is present and the surface (boundary condition) plays an important role.

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