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Diffusion equations and different spatial fractional derivatives

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ABSTRACT. We investigate for the diffusion equation the differences manifested by the solutions when three different types of spatial differential operators of noninteger (or fractional) order are considered for a limited and unlimited region. In all cases, we verify an anomalous spreading of the system, which can be connected to a rich class of anomalous diffusion processes.

Keywords: diffusion equation, fractional derivative, anomalous diffusion.

Equações de difusão e diferentes derivadas espaciais fracionárias

RESUMO. Investigamos para a equação de difusão as diferenças manifestadas pelas soluções quando três tipos diferentes de operadores diferenciais espaciais de ordem não inteiras (ou fracionárias) são considerados para regiões limitadas ou não limitadas. Em todos os casos, verificamos um espalhamento anômalo do sistema que pode ser conectado a uma rica classe de processos difusivos.

Palavras-chave: equação de difusão, derivada fracionária, difusão anômala.

Introduction

Actually, the fractional calculus represents an important tool which has been successfully applied to several contexts (DAS; MAHARATNA, 2013; DEBNATH, 2003; MACHADO et al., 2014; GLÖCKLE; NONNENMACHER, 1995; HILFER, 2000; SHLESINGER et al., 1994). For example, electrical response (LENZI et al., 2013; SANTORO et al., 2011), biological systems (CASPI et al., 2000; PLOTKIN; WOLYNES, 1998), finance, viscoelasticity (GLÖCKLE; NONNENMACHER, 1991) and anomalous diffusion (PEKALSKI; SZNAJD-WERON, 1999). In particular, the last point has received much attention since that the usual approach (RISKEN, 1989; GARDINER, 2009) does not provide a suitable description of the experimental results and, consequently, requires extensions. In this sense, by using fractional calculus, the diffusion equation (or Fokker - Planck equation) and the Langevin equation have been extended and, consequently, used to investigate several situations such as the ones present in Refs. (HILFER, 2000; METZLER; KLAFTER, 2000; LENZI et al., 2009; METZLER et al., 1994; SOKOLOV, 2012). However, there is more than one definition of the fractional (or noninteger) differential operators which have been used to investigate these situations. In this sense, our goal is to investigate the

differences manifested by the solutions when three representative fractional operators are incorporated to in the diffusive term, i.e., the usual spatial derivative is replaced by a fractional differential operator. The operators analyzed here are the Riemann - Liouville (PODLUBNY, 1999), Caputo (PODLUBNY, 1999), and the one proposed by Qianqian et al. (2010) which reminds us the usual case. For these operators, we consider the situations characterized by a limited and no limited regions in order to establish the differences. Analysis is performed next, followed by discussion and conclusion.

Material and methods

Diffusion equations and different fractional operators

Let us start our analysis about the differences of these operators by investigating the behavior of the solutions when these fractional differential operators are incorporated in the diffusive term. The first spatial differential operator considered here is the Riemann - Liouville, defined as (PODLUBNY, 1999)

$${}_x^R D_x^\alpha \rho(x, t) = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dx^n} \int_{x_0}^x \rho(x', t) dx' \quad (1)$$

where:

n is a integer and $n-1 < \alpha < n$. Using this definition for the spatial derivative the usual diffusion equation can be extended to

$$\frac{\partial}{\partial t} \rho(x, t) = (\mathcal{K}_{\alpha, a} {}^{RL}D_x^\alpha + \mathcal{K}_{\alpha, b} {}^{RL}D_b^\alpha) \rho(x, t) \quad (2)$$

to describe, for simplicity, a system defined in the interval $[a, b]$ and subjected to boundary and initial conditions. The usual diffusion equation can also be extended by incorporating the fractional differential operators in the Caputo (PODLUBNY, 1999) sense. In this case, the diffusion equation is modified to

$$\frac{\partial}{\partial t} \rho(x, t) = (\mathcal{K}_{\alpha, a} {}^CD_x^\alpha + \mathcal{K}_{\alpha, b} {}^CD_b^\alpha) \rho(x, t) \quad (3)$$

which is very similar to Equation (2), however the differential operator, to be considered in this case, is given by

$${}^CD_x^\alpha \rho(x, t) = \frac{1}{\Gamma(n-\alpha)} \int_{x_0}^x \frac{\rho^{(n)}(x', t) dx'}{(x-x')^{\alpha+1-n}} \quad (4)$$

with $n-1 < \alpha < n$ where n is an integer number and $\rho^{(n)}(x, t)$ is the n^{th} - spatial derivative of the distribution $\rho(x, t)$. Note that for α integer Equation (2) and (3) recover the usual diffusion equation and the presence of the constants $\mathcal{K}_{\alpha, a}$ and $\mathcal{K}_{\alpha, b}$ permit us, from the form point of view, to work out the operators present in the diffusive term in the asymmetric and symmetric form. In addition, it is interesting to mention that the presence, in the diffusive term, of these differential operators can related to a long-tailed behavior of the jump probabilities which characterize the diffusive process manifested by the system.

For these operators when the system is defined in a infinite interval, i.e., $(-\infty, \infty)$, both equations lead us to the same solution since that the operators in this limit are equivalent as discussed in Ref. (PODLUBNY, 1999). This feature may be observed from the numerical from point of view. In fact, by using the discrete form of these operators known as the L2 method (QIANQIAN et al., 2010), we obtain, for the Grünwald-Letnikov fractional differential operator,

$$\begin{aligned} {}^{GL}D_x^\alpha u(x_i) \approx & \frac{h^{-\alpha}}{\Gamma(3-\alpha)} \left\{ \frac{(1-\alpha)(2-\alpha)u(-L)}{(i+N)^\alpha} + \frac{2-\alpha}{(i+N)^{\alpha-1}} \right. \\ & \times (u(-L+h) - u(-L)) \\ & \left. + \sum_{k=0}^{i-1} (u_{i-k+1} - 2u_{i-k} + u_{i-k-1}) [(k+1)^{2-\alpha} - (k-N)^{2-\alpha}] \right\} \end{aligned}$$

with the interval $[-L, L]$ divided in N parts, $h = L/N$, such that $-N < i < N$ and $x_i = ih$. Whereas, the discrete form of the Caputo's operator, using the same procedure, can be written as follows

$$\begin{aligned} {}^CD_x^\alpha u(x_i) \approx & \frac{h^{-\alpha}}{\Gamma(3-\alpha)} \sum_{k=0}^{i-1} (u_{i-k+1} - 2u_{i-k} + u_{i-k-1}) \\ & \times [(k+1)^{2-\alpha} - (k-N)^{2-\alpha}] \end{aligned}$$

Notice that equations for ${}^{GL}D_x^\alpha u(x_i)$ and ${}^CD_x^\alpha u(x_i)$ only differ by the first two terms before the sum, and these terms are inversely proportional to L . Therefore their discrepancies become smaller if we increase the size of the system, as illustrated in Figure 1.

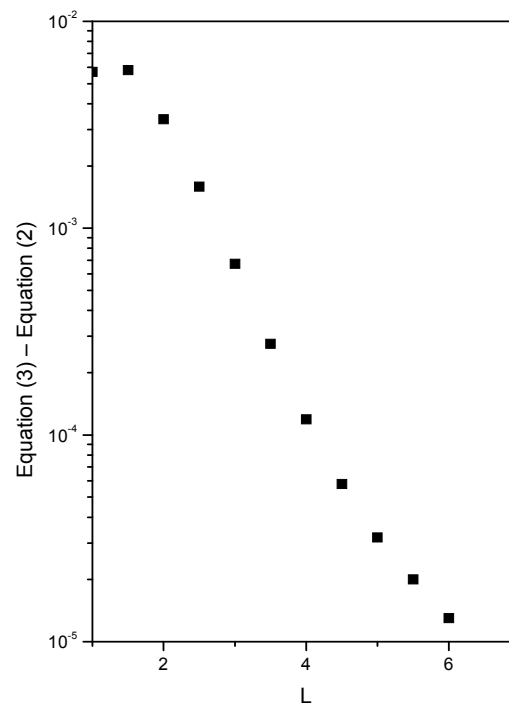


Figure 1. This figure illustrates the difference between the solutions of Equation (2) and (3) obtained in the interval $[-L, L]$ as a function of L for $t = 0.1$ and $x = 0$. We consider, for simplicity, $\alpha = 1.8$ and absorbent boundary conditions. Note that difference decrease by increasing the value of L .

Interesting characteristics of Equation (2) and (3) appear when they are considered in a finite interval

where the surface effects may play an important role. In order to face this point, we investigate the differences between Equation (2) and (3) when the system is considered, without loss of generality, in a limited interval, i.e., $[0, L]$, with $\mathcal{K}_{\alpha, b} = 0$. We also assume that $\rho(x, t)$ is $(n-1)$ times continuously differentiable and that $\rho^{(n)}(x, t)$ is integrable in the interval $[0, L]$. Using these assumptions, it is possible to show that

$${}^{RL}_0 D_x^\alpha \rho(x, t) = \frac{\rho(0, t)}{\Gamma(1-\alpha)x^\alpha} + \frac{x^{1-\alpha}}{\Gamma(2-\alpha)} \times \left(\frac{\partial}{\partial x} \rho(x, t) \Big|_{x=0} \right) + {}^C_0 D_x^\alpha \rho(x, t) \quad (5)$$

for $1 < \alpha < 2$. Equation 5 shows a connection between the Riemann - Liouville and Caputo differential operators which implies in the presence of the addition terms. These terms related to the boundary conditions, imposed by the problem under consideration, may behave as a source or sink by introducing or removing particles of the system such as adsorption and/or desorption process. Thus, the extensions of the diffusion equation given by Equation (2) and (3) have different solutions and, consequently, are not equivalent. This feature is also verified for a semi-infinity interval, i.e., $[0, \infty)$.

Now, let us consider the fractional differential operator proposed in Ref. [2]. This fractional operator is defined as $\nabla^\alpha \psi_n(x) = \lambda_n \psi_n(x)$ with $\nabla^\alpha = -(-\nabla^2)^{\alpha/2}$ which brings the usual differential operator raised to a noninteger exponent. The eigenfunctions and eigenvalues may be represented by $\psi_n(x)$ and λ_n , respectively. Incorporating this operator in the usual diffusion equation, we obtain that

$$\frac{\partial}{\partial t} \rho(x, t) = \mathcal{K}_\alpha \nabla^\alpha \rho(x, t) \quad (6)$$

The solution for this equation can be formally written as:

$$\rho(x, t) = \sum_{n=0}^{\infty} \mathcal{B}_n \psi_n(x) e^{-\lambda_n t} \quad (7)$$

for a system defined in an interval $[a, b]$ with

$$\mathcal{B}_n = \int_a^b \psi_n(x) \rho(x, 0) dx \Big/ \int_a^b \psi_n^2(x) dx \quad (8)$$

and $\psi_n(x)$ subjected to boundary conditions. From this previous development, we verify that the definition of fractional operator present in Ref. [2] is very interesting since that it allows us to use some the properties of the integer differential operator and introduces a noninteger index.

To investigate a possible equivalence with the previous fractional diffusion equations, we consider the solutions of Equation (6) in a limited region. In particular, we analyze the behavior of the solutions of these equations in two situations, when the system is subjected to absorbing boundary conditions ($\rho(0, t) = \rho(L, t) = 0$). The first of them is to consider, for simplicity, the initial condition $\rho(x, 0) = (\pi/2) \sin(\pi x)$ and $\mathcal{K}_{\alpha, b} = 0$ for Equation. (2), (3), and (6). For this case, the results shown in Figure 2 illustrate the differences evidencing the nonequivalence of the fractional diffusion equations. In the second case, we restrict our analysis, without loss of generality, to Equation (3) and (6) by taking into account the initial condition $\rho(x, 0) = J x E_{\alpha, 2}(-kx^\alpha)$ with k obtained from the equation $E_{\alpha, 2}(-kx^\alpha) = 0$ and $J = 1 / \int_0^L \rho(x, 0) dx$. By

using this initial condition is possible to show that a solution of Equation (3), satisfying the required boundary condition, is given by

$$\rho(x, t) = J x E_{\alpha, 2}(-kx^\alpha) e^{-\mathcal{K}_\alpha k^2 t} \quad (9)$$

where $\alpha = 2$ recovers the usual solution connected to the initial condition. Figure 3 illustrates Equation (9) for different values of α in order to illustrate the effect of the noninteger index of the differential operator and the time evolution of the solution.

The solution for Equation (6), by considering the previous absorbent boundary condition, can be written as follows:

$$\rho(x, t) = \sum_{n=0}^{\infty} \mathcal{B}_n \sin(n\pi x) e^{-(n\pi/L)^\alpha t} \quad (10)$$

with

$$\mathcal{B}_n = \frac{2J}{L} \int_0^L x \sin(n\pi x/L) E_{\alpha, 2}(-kx^\alpha) dx \quad (11)$$

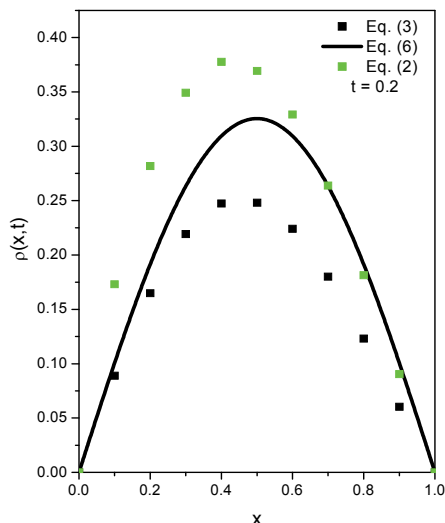


Figure 2. This figure illustrates the solution of Equation (2), (3), and (6), for simplicity, by considering $\alpha = 1.8$ and $L = 1$.

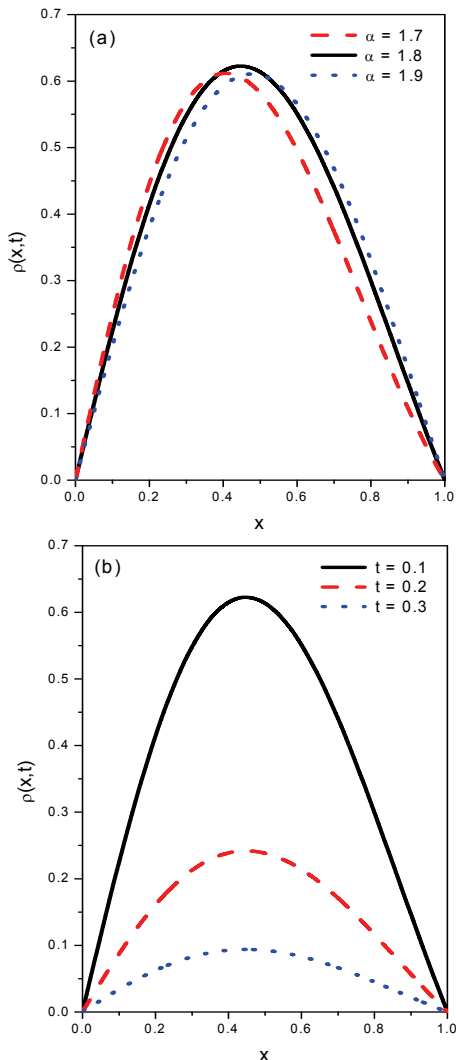


Figure 3. The figures, (a) and (b), illustrate the behavior of Equation (9) for different values of α and t , for simplicity, by considering $L = 1$.

Equation (10) is illustrated in Figure 4 in order to show the effect of the index α on the solution and the time evolution. From Figures 3 and 4, we observe that solutions obtained from Equation (3) and (6), subject to the certain initial condition, are different when the system is defined in a limited region. This point is illustrated in Figure 5 and shows the nonequivalence of these spatial differential operators for the conditions considered here.

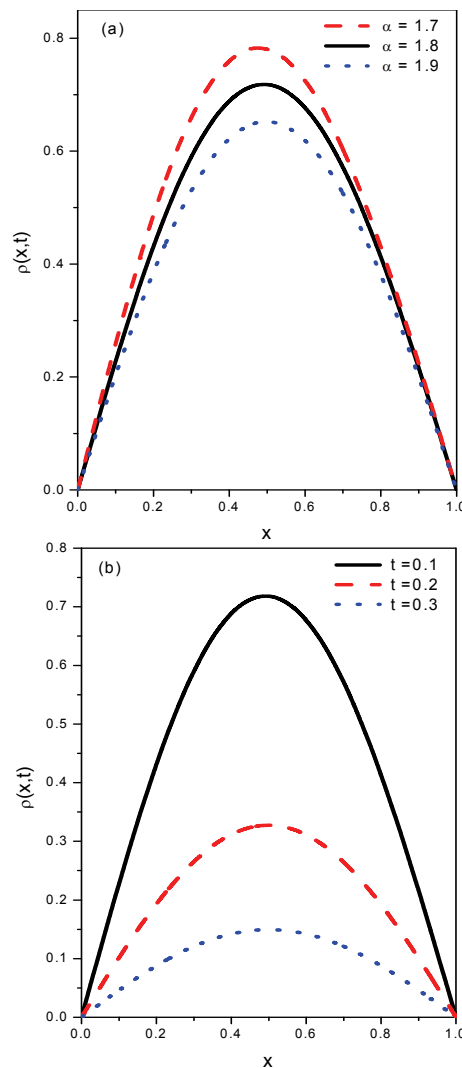


Figure 4. The figures, (a) and (b), illustrate the behavior of Equation (10) for different values of α and t , for simplicity, by considering the initial condition $\rho(x,0) = j x E_{2,\alpha}(-kx^\alpha)$ (where k is obtained from the equation $E_{2,\alpha}(-k)=0$) and $L = 1$.

Results and discussion

We have investigated the solutions of the fractional diffusion Equation (2), (3), and (6) by considering different situations in a finite interval.

The results found for these equations shown that the surface effects play an important role on the solutions of these equations. This point is shown, for example, by Equation (5) which implies that Equation (2) is equivalent to Equation (3) if additional terms connected to the surface are considered. Similar situation is evidenced in Figure 2 when Equation (2), (3), and (6) are compared for an initial condition. The equivalence is only found when the system is defined in the interval $(-\infty, \infty)$ where the surface effects are absent.

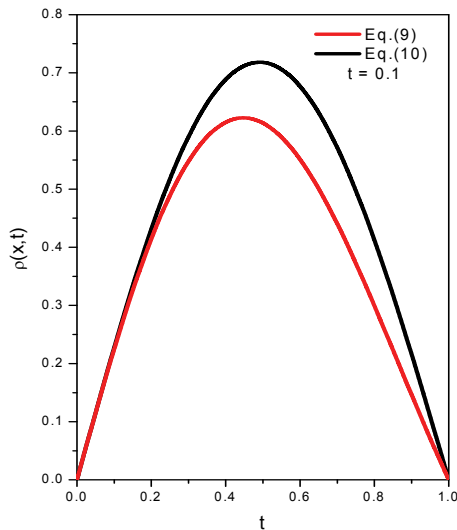


Figure 5. This figure illustrates the solution of Equation (9) and (10), for simplicity, by considering $\alpha = 1.8$, the initial condition $\rho(x,0) = j x E_{2,\alpha}(-kx^\alpha)$, and $L = 1$, for $t = 0.1$. Note the difference between the solutions evidencing the nonequivalence of the spatial differential operators.

Conclusion

The results presented here for a system subjected to a finite interval shows that the fractional operators are not equivalent. In this sense, it is interesting to note that the surface effects play an important role on these operators.

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