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Particular solution for anomalous diffusion equation with source term

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Abstract: In literature the phenomenon of diffusion has been widely studied, however for nonextensive systems which are governed by a nonlinear stochastic dynamic, there are a few soluble models. The purpose of this study is to present the solution of the nonlinear Fokker-Planck equation for a model of potential with barrier considering a term of absorption. Systems of this nature can be observed in various chemical or biological processes and their solution enriches the studies of existing nonextensive systems.

1. Introduction

A large number of phenomena can be related to kinetic processes, this is the case, for example, of electrochemical reactions in metals or in membranes. In these cases, the atoms or particles that interact are in the interface between the environments, the medium and the interior of the material. In many cases, this difference between the environments leads to a diffusion process in which particles of the medium are absorbed into the structure. This absorption can occur at a constant rate or, in some cases it can present temporal dependence [1].

The Fokker-Planck equation is widely used in literature to study stochastic processes of diffusion, where it is possible to consider the presence of forces acting on the interaction between the bodies [2]. Its representation is:

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x} [f(x) \cdot P(x,t)] + Q \frac{\partial^2 P(x,t)}{\partial x^2}, \quad (1)$$

where $P(x,t)$ is the distribution of probabilities or a density of particles depending on the problem concerned. Q is the coefficient of diffusion and $f(x)$ is the external force that acts in the environment.

The distribution of probability obtained from equation (1) maximizes the entropy of Gibbs-Boltzmann $S = -\sum_i P_i \ln(P_i)$ and offers a very good description of the behavior of systems characterized by fluctuations which are proportional to the time variation, where there are short-range interactions among particles [3].

When considering anomalous systems, where the fluctuations are disproportionate to the time and where there is the presence of long-range interactions among particles, the common Fokker-Planck equation (1) is not able to describe well the model [4,5]. In order to solve this problem, the Fokker-Planck equation must be rewritten as:

$$\frac{\partial P(x,t)^\mu}{\partial t} = -\frac{\partial}{\partial x} [f(x) \cdot P(x,t)^\mu] + Q \frac{\partial^2 P(x,t)^\nu}{\partial x^2} \quad (2)$$

As it can be observed, the difference between (1) and (2) is the presence of the indexes μ and ν in $P(x,t)$ [6]. These indexes are real constants that must be adjusted according to the system analyzed and are constantly related to the process of anomalous diffusion in biological systems [7 – 10]. When $\mu = 1$, the probability provided by (2) is intimately associated with nonextensive systems, because it maximizes the entropy proposed by Tsallis [11, 12],

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} [f(x) \cdot P(x,t)] + Q \frac{\partial^2 P(x,t)^\nu}{\partial x^2}. \quad (3)$$

In the problem addressed, we will make a brief review of nonlinear diffusion in a simple system consisting of two regions separated by a barrier of potential. In section 2 we present the solution of the nonlinear Fokker-Planck equation (NLFP) with an additional term, which is interpreted as a source term or absorption term that favors the passage of particles through the potential barrier. In section 3 we discuss about the results obtained and, finally, we present the conclusions.

2. PURPOSE

In this paper, the function $P(x,t)$ is interpreted as a density of particles of a medium. An additional term, proportional to the function $\mu(t)$ is included in equation (3) and is related to the absorption rate of the model. This way, we obtain:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} [P(x,t)f(x)] + Q \frac{\partial^2 P(x,t)^\nu}{\partial x^2} - \mu(t)P(x,t) \quad (4)$$

The nonlinearity of the Fokker-Planck equation is due to the exponent ν present in the second derivative. Equation (1) is employed in the study of nonextensive systems, where there are long-range interactions and the thermodynamic relations meet the proposal introduced by Tsallis [5, 13].

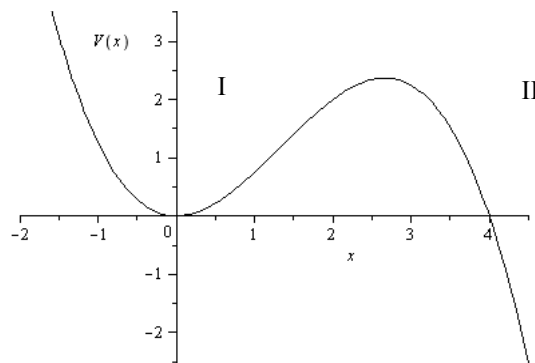


Figure 1: Representation of the potential considered with $k_1 = 1$ and $k_2 = 0.25$.

In this study, the function $f(x)$ is given by the derivative of the potential:

$$V(x) = k_1 x^2 - k_2 x^3, \quad (5)$$

whose characteristic graph is shown in Figure 1. The solution for this system is the form:

$$P(x,t) = D(t) \left\{ 1 - (\nu - 1) \beta(t) \left[x^2 - M(x,t) \right] \right\}^{1/(\nu-1)}, \quad (6)$$

where $D(t)$, $\beta(t)$ and $M(x,t)$ are functions dependent on the time to be defined later. For a long time, the *ansatz* above indicates the distribution of the stationary probability of the Fokker-Planck equation. As we are considering a nonextensive system, the solution needs to be given this way, because this function maximizes the Tsallis' entropy and allows us to obtain a good description of the environment through relevant thermodynamic information as, for example, the free energy.

Applying (6) in (4) we obtain a system of equations,

$$\left\{ \begin{array}{l} i) \quad \frac{dD(t)}{dt} - 2D(t)k_1 + 2\nu QD(t)^\nu \beta(t) + \mu(t)D(t) = 0 \\ ii) \quad -6k_2 D(t)x - \nu QD(t)^\nu \beta(t) \frac{\partial^2 M}{\partial x^2} = 0 \\ iii) \quad x^2 \left[\frac{1}{\beta(t)} \frac{d\beta(t)}{dt} - 4k_1 + 4\nu QD(t)^{\nu-1} \beta(t) \right] = 0 \\ iv) \quad -\frac{\partial M}{\partial t} - \frac{M}{\beta(t)} \frac{d\beta(t)}{dt} + (2k_1 x - 3k_2 x^2) \frac{\partial M}{\partial x} - 6k_2 x^3 - Q\nu \beta(t) D(t)^{\nu-1} \left\{ 4x \frac{\partial M}{\partial x} + \left(\frac{\partial M}{\partial x} \right)^2 \right\} = 0 \end{array} \right.$$

Disregarding the relations *ii*) and *iv*), we go back to the system presented in [14], when the force is proportionate to x , only less than the source term $\mu(t)$. By isolating the term $2\nu Q\beta(t)D(t)^\nu$ from *i*) and substituting in *iii*), we find the following expression:

$$\frac{1}{\beta(t)} \frac{d\beta(t)}{dt} - \frac{2}{D(t)} \frac{dD(t)}{dt} - 2\mu(t) = 0. \quad (7)$$

By integrating (7) with respect to t , we observe that $\beta(t)$ is defined as:

$$\beta(t) = \frac{\beta_0}{D_0^2} D(t)^2 e^{2T(t)}, \quad (8)$$

where the function $T(t)$ is equal to the integration of $\mu(t)$ in a determined time interval.

The equation *ii*) provides the function $M(x, t)$, which satisfies the problem. To that effect, integrating twice over x is enough. To facilitate, we will replace the function $\beta(t)$ by definition (8). Therefore, the expression is:

$$M(x, t) = \frac{-k_2 x^3 e^{-2T(t)}}{\gamma D(t)}, \quad (9)$$

where γ is a constant equal to $Q\nu\beta_0/D_0$, adopted to facilitate the notation.

Thus, after some manipulations we obtain the following expression:

$$-\frac{k_2(\nu+1)x^3 e^{-2T(t)}}{\gamma D(t)^{\nu+2}} \frac{dD}{dt} + \frac{k_2 x^3 e^{-2T(t)}}{\gamma D(t)^{\nu+1}} \frac{2}{D(t)} \frac{dD(t)}{dt} - \frac{6k_1 k_2 x^3 e^{-2T(t)}}{\gamma D(t)^{\nu+1}} - 6k_2 x^3 + 12k_2 x^3 = 0, \quad (10)$$

or:

$$-\frac{(\nu-1)}{3} \frac{dD}{dt} - 2k_1 D(t) + 2\gamma D(t)^{\nu+2} e^{2T(t)} = 0. \quad (11)$$

Until now, from a system of four equations (*i*, *ii*, *iii* and *iv*), we have defined $\beta(t)$ and $M(x, t)$ in terms of $D(t)$ and $\mu(t)$, which were not found yet. In order to obtain these expressions, it is necessary to compare equations (11) and *i*):

$$\begin{cases} \frac{dD(t)}{dt} - 2D(t)k_1 + 2\gamma D(t)^{\nu+2} e^{2T(t)} + \mu(t)D(t) = 0 \\ -\frac{(\nu-1)}{3} \frac{dD}{dt} - 2k_1 D(t) + 2\gamma D(t)^{\nu+2} e^{2T(t)} = 0 \end{cases} \quad (12)$$

As we can observe, both expressions are similar except for the derivative in relation to $D(t)$ and the product $\mu(t) \cdot D(t)$. By subtracting one from the other, we have:

$$\frac{dD(t)}{dt} + \frac{(\nu-1)}{3} \frac{dD}{dt} + \mu(t)D(t) = 0 \quad (13)$$

and by rearranging the terms of (13), we obtain a relation for $\mu(t)$ in function of $D(t)$:

$$\mu(t) = -\frac{(\nu+2)}{3D(t)} \frac{dD}{dt}. \quad (14)$$

Through the relation found above, we can rewrite $T(t)$ as

$$T(t) = \ln(D(t))^{-(\nu+2)/3}. \quad (15)$$

By using (15), the exponential term is replaced by,

$$e^{2T(t)} = e^{\ln(D(t))^{-2(\nu+2)/3}} = D(t)^{-2(\nu+2)/3}. \quad (16)$$

and by substituting the relation above in (11) we obtain an equation which is only dependent on the function $D(t)$, which, being solved provides the other functions: $\beta(t)$, $M(x, t)$ and $\mu(t)$. Due to the simplicity, we will work with the second equation of system (12) and, for this reason, we have rewritten it as:

$$\frac{dD^{-(\nu-1)/3}}{dt} - 2k_1 D^{-(\nu-1)/3} + 2\gamma = 0. \quad (17)$$

The expression of $D(t)$ that satisfies the above is

$$D(t) = \left\{ \frac{Q\nu\beta_0}{k_1 D_0^2} + \left(1 - \frac{Q\nu\beta_0}{k_1 D_0^2} \right) e^{2k_1 t} \right\}^{-3/(\nu-1)}. \quad (18)$$

Accordingly with the relations (8), (9) and (14), the functions $\beta(t)$, $M(x,t)$ e $\mu(t)$ are represented as:

$$\beta(t) = \frac{\beta_0}{D_0^2} \left\{ \frac{Q\nu\beta_0}{k_1 D_0^2} + \left(1 - \frac{Q\nu\beta_0}{k_1 D_0^2} \right) e^{2k_1 t} \right\}^2, \quad (19)$$

$$\mu(t) = -2 \frac{(\nu+2)}{(\nu-1)} \left(k_1 - \frac{Q\nu\beta_0}{D_0^2} \right) \left\{ 1 - \left(e^{-2k_1 t} - 1 \right) \frac{Q\nu\beta_0}{k_1 D_0^2} \right\}^{-1}, \quad (20)$$

and

$$M(x,t) = \frac{-k_2 k_1 D_0^2}{Q\nu\beta_0} \left\{ \frac{Q\nu\beta_0}{k_1 D_0^2} + \left(1 - \frac{Q\nu\beta_0}{k_1 D_0^2} \right) e^{2k_1 t} \right\} x^3. \quad (21)$$

Having defined all the expressions of *ansatz* (6) the probability is expressed as:

$$P(x,t) = \left\{ \frac{Q\nu\beta_0}{k_1 D_0^2} + \left(1 - \frac{Q\nu\beta_0}{k_1 D_0^2} \right) e^{2k_1 t} \right\}^{-3/(\nu-1)} \cdot \left\{ 1 - (\nu-1) \frac{\beta_0}{D_0^2} \left[\frac{Q\nu\beta_0}{k_1 D_0^2} + \left(1 - \frac{Q\nu\beta_0}{k_1 D_0^2} \right) \cdot e^{2k_1 t} \right] \right\}^2 \cdot \left[x^2 - \frac{k_2 k_1 D_0^2}{Q\nu\beta_0} \left\{ \frac{Q\nu\beta_0}{k_1 D_0^2} + \left(1 - \frac{Q\nu\beta_0}{k_1 D_0^2} \right) \cdot e^{2k_1 t} \right\} x^3 \right]^{1/(\nu-1)}. \quad (22)$$

3. RESULTS AND DISCUSSION

Figures 2 and 3 present the graphs of the distribution $P(x,t)$ obtained in different time intervals, with x ranging from -1.5 to 2, which corresponds to the region of stable potential minimum (region I). The values assigned to constants were $Q = 0,5$ and $k_1 = 1$, $k_2 = 0.25$, $\nu = 1.5$ for Figure 2 and $k_1 = 0.2$, $k_2 = 0.05$, $\nu = 0.5$ for Figure 3.

The time taken by the particles density to reach zero, considering these values of the constants, was of approximately 1 unit, when ν is 1.5 and 2 units for ν equal 0,5.

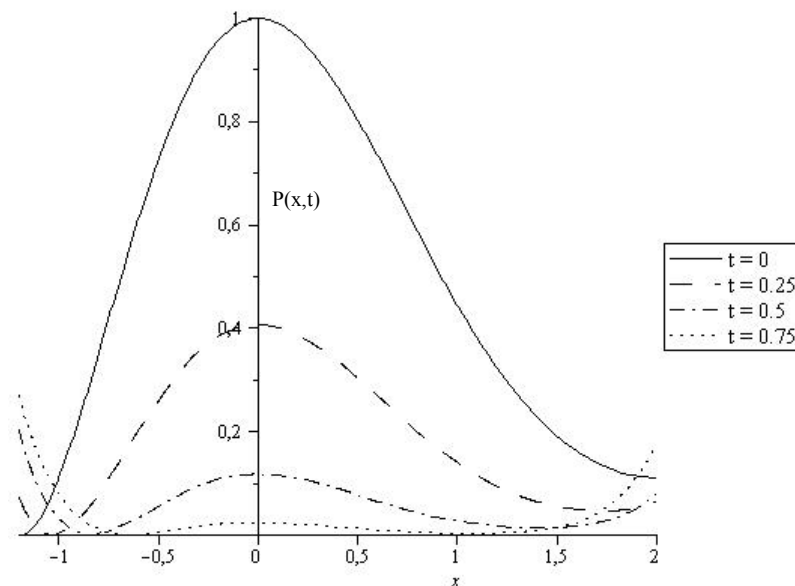


Figure 2: Density of particles vs. space and time for $k_1 = 1$, $k_2 = 0.25$ and $\nu = 1.5$.

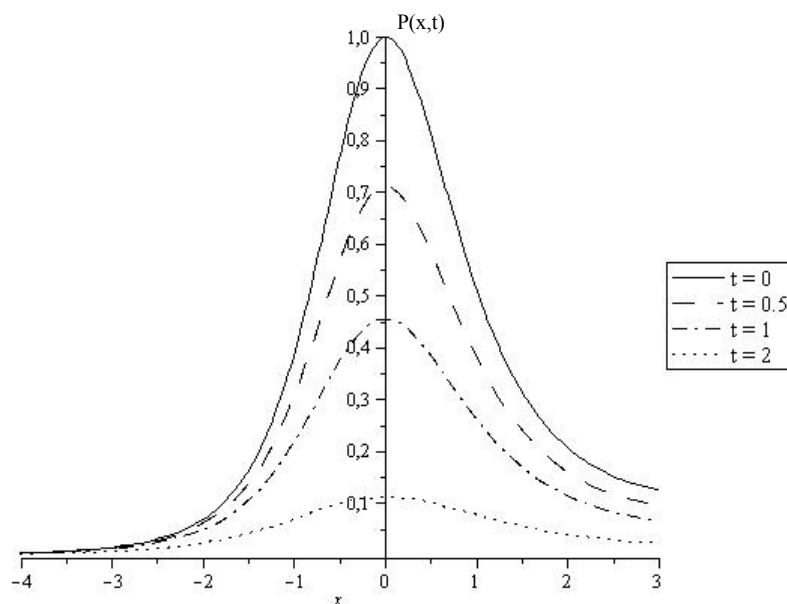


Figure 3: Density of particles vs. space and time for $k_1 = 0.2$, $k_2 = 0.05$ and $\nu = 0.5$.

The inclusion of a term referring to an absorption rate has been already discussed in some papers (see references [15] and [16]). However, in these cases, the function $f(x)$ corresponds to a harmonic potential. In this model, a disturbance term was inserted in the harmonic potential, creating a barrier and two state levels. This change has generated a specific temporal dependence for this case in the absorption rate (20).

Temporal dependences of the kind presented here (20) can be observed in many biochemical systems [17, 18] when analyzing the absorption rates, creating the possibility of approximating this theoretical model with data of reactions or interactions obtained in the laboratory. In these cases, the limitation consists of the necessity of adjusting the nonlinear parameter (ν) to the system being treated, as it can be seen when comparing Figures 2 and 3.

The values of k_1 and k_2 in Figure 3 are smaller than in Figure 2, reducing the size of the barrier and facilitating the diffusion between regions I and II of Figure 1. The value of nonlinear parameter is altered due to the change in the size of the barrier, guaranteeing a physically acceptable behavior of the solution.

4. CONCLUSION

The graphs made from *ansatz* have suggested an expected behavior of the system, i.e., as time passes there is a tendency for particles to go from a region of higher potential to a region of lower potential.

This diffusion process is favored not only by the nonlinear factor of the Fokker-Planck equation, but also by the addition of the source term $\mu(t)$, which helps the particles to transpose the barrier. The incorporation of this temporal function in the Fokker-Planck nonlinear equation led to the solution of a simple system of potential barrier.

In literature there are a few soluble models for NLFP, which hinders the application of the nonextensive formalism in the study of chemical or biological processes.

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