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Integrodifferential diffusion equation for continuous-time random walk

Kwok Sau Fa[1,*] and K. G. Wang[2]
[1]*Departamento de Física, Universidade Estadual de Maringá, Av. Colombo 5790, 87020-900 Maringá, PR, Brazil*
[2]*Department of Physics & Space Sciences, Materials Science and Nanotechnology Institute, Florida Institute of Technology, Melbourne, Florida 32901, USA*

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In this paper, we present an integrodifferential diffusion equation for continuous-time random walk that is valid for a generic waiting time probability density function. Using this equation, we also study diffusion behaviors for a couple of specific waiting time probability density functions such as exponential and a combination of power law and generalized Mittag-Leffler function. We show that for the case of the exponential waiting time probability density function, a normal diffusion is generated and the probability density function is Gaussian distribution. In the case of the combination of a power law and generalized Mittag-Leffler waiting probability density function, we obtain the subdiffusive behavior for all the time regions from small to large times and probability density function is non-Gaussian distribution.

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I. INTRODUCTION

Diffusion is a ubiquitous phenomenon and it is one of the fundamental mechanisms for transport of materials in physical, chemical, and biological systems. The well-known example of a diffusion process is the Brownian motion. Diffusion processes are classified according to their mean-square displacements. The normal diffusion is that the mean-squared displacement grows linearly with time and in other situations, the processes are said to exhibit anomalous diffusion. Nowadays, there are several approaches to describe anomalous diffusion processes and they can be applied to many situations of natural systems [1–9]. One of the most interesting features incorporated into these approaches is the memory effect. In particular, the memory effect incorporated into the Langevin approach, referred to as generalized Langevin equation (GLE) [9], can be associated to the retardation of friction and fractal media [10,11]. Moreover, according to the fluctuation-dissipation theorem [1], the internal friction is directly related to the correlation function of the random force.

In many situations, a finite correlated noise is necessary for describing the real systems in equilibrium states. However, in order to describe anomalous diffusion, a nonlocal friction should be employed so that it satisfies the fluctuation-dissipation theorem. For instance, anomalous diffusion processes have been observed in a variety of systems such as bacterial cytoplasm motion [12], conformational fluctuations within a single protein molecule [13], and fluorescence intermittency in single enzymes [14]. These processes have been described by the GLE and the memory effect has also been shown in the generalized Fokker-Planck equations (GFPE) [9].

The continuous-time random walk (CTRW) of Montroll and Weiss [15] has been employed to describe anomalous diffusion [16–22]. The CTRW with a power-law waiting time probability density function (pdf) [23,24] was also linked to the following fractional Fokker-Planck equation:

$$\frac{\partial \rho(x,t)}{\partial t} = {}_0D_t^{1-\alpha} K_\alpha \frac{\partial^2}{\partial x^2}\rho(x,t), \tag{1}$$

where

$${}_0D_t^{1-\alpha}\rho(x,t) = \frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t \frac{\rho(x,t_1)}{(t-t_1)^{1-\alpha}}dt_1 \tag{2}$$

is the Riemann-Liouville fractional derivative and $\Gamma(z)$ is the Gamma function. $\rho(x,t)dx$ is the probability for finding particle in position between x and $x+dx$ at time t.

The CTRW model may be described by a set of Langevin equations [4,25,26] or an appropriate generalized master equation [19,27,28]. The pdf $\rho(x,t)$ obeys the following equation in Fourier-Laplace space [4]:

$$\rho(k,s) = \frac{1-g(s)}{s}\frac{\rho_0(k)}{1-\psi(k,s)}, \tag{3}$$

where $\rho_0(k)$ is the Fourier transform of the initial condition $\rho_0(x)$, $\psi(x,t)$ is the jump pdf, and $g(t)$ is the waiting time pdf defined by

$$g(t) = \int_{-\infty}^{\infty}\psi(x,t)dx. \tag{4}$$

Moreover, from the jump pdf, we also have the jump length pdf defined by

$$\phi(x) = \int_0^{\infty}\psi(x,t)dt. \tag{5}$$

The continuous-time random-walk model can be simplified through the decoupled jump pdf $\psi(k,s)=\phi(k)g(s)$. Furthermore, jump length pdf can be approximated as following [4]:

$$\phi(k) \sim 1 - Dk^2 + O(k^4). \tag{6}$$

Different types of the CTRW models are specified through specifying the waiting time pdf. The CTRW model is also

*kwok@dfi.uem.br

connected to a class of Fokker-Planck equations [4,29]. Furthermore, in the CTRW model, solutions for $\rho(x,t)$ under the condition of long-tailed waiting time pdf can be found in Refs. [30–32].

Substituting Eq. (6) into Eq. (3), we have

$$\rho(k,s) = \frac{1-g(s)}{s}\frac{\rho_0(k)}{1-(1-Dk^2)g(s)}. \quad (7)$$

When Cakir *et al.* [33] studied trajectory and density memory, Eq. (43) in their paper is same as our Eq. (7) with consideration of $\rho_0(k)=1$. In their study, the initial condition is that when $t=0$, particle is at origin and therefore $\rho_0(k)=1$. However, Eq. (7) can be applied to cases without requirement of $\rho_0(k)=1$ that appeared in the paper of Cakir *et al.* [33]. In particular, the CTRW model can be classified by the characteristic waiting time T and the jump length variance Σ^2 defined by

$$T = \int_0^\infty t g(t) dt \quad (8)$$

and

$$\Sigma^2 = \int_{-\infty}^{\infty} x^2 \phi(x) dx. \quad (9)$$

For finite T and Σ^2, the long-time limit corresponds to the Brownian motion [4]. Although Eq. (7) is valid for a finite jump length variance, anomalous diffusion can be produced by Eq. (7) with appropriate choices of waiting time pdf.

The aim of this work are (1) from Eq. (7) to investigate general behavior of particle's diffusion without any specified waiting time pdf and (2) study the effects of different waiting time pdfs on the behavior of particle's diffusion in the framework of CTRW. This paper is organized as follows. In Sec. II, we study CTRW under a general waiting time pdf and two specific waiting time pdfs. In Sec. III, we show the exact solutions for pdf $\rho(x,t)$. Finally, conclusions are presented in Sec. IV.

II. CONTINUOUS TIME RANDOM WALK AND INTEGRODIFFERENTIAL EQUATION FOR GENERAL WAITING TIME PROBABILITY DENSITY FUNCTION

Equation (7) was already employed to study diffusion behavior when the form of waiting time pdf $g(t)$ was first specified such as exponential function or a power-law function in the long-time limit [4]. However, for a generic form of $g(t)$, Eq. (7) is not convenient to be used to study diffusion behavior due to the difficulty in the inverse transformations of Fourier and Laplace in Eq. (7). In this paper, we will derive an integrodifferential equation for CTRW, which is valid for general waiting time probability density function. The details of derivation can be found in the Appendix. This integrodifferential equation for CTRW is written by

$$\frac{\partial\rho(x,t)}{\partial t} - \int_0^t g(t-t_1)\frac{\partial\rho(x,t_1)}{\partial t_1}dt_1 = D\frac{\partial}{\partial t}\int_0^t g(t-t_1)\frac{\partial^2\rho(x,t_1)}{\partial x^2}dt_1. \quad (10)$$

For the case of $g(t)=t^{\alpha-1}/\Gamma(\alpha)$, it is noted that the Caputo fractional derivative appears on the left side of Eq. (10) and the Riemann-Liouville fractional derivative appears on the right side of Eq. (10). The Caputo fractional derivative requires the integrability of the derivative and contains the initial value of the function. Therefore, the Caputo fractional derivative is more restrictive than the Riemann-Liouville fractional derivative is. It should be pointed out that the use of these operators may lead to different behaviors including unphysical behavior in different systems [34,35]. Equation (10) is derived from a well-defined physical process and no ambiguities and unphysical behaviors are expected. The left side of Eq. (10) shows the variation of $\rho(x,t)$ with respect to time, which does not depend only on the ordinary derivative operator but also the difference between ordinary and nonlocal integral operators.

Our Eq. (10) is different from the fractional Fokker-Planck Eq. (1) in the structure because the fractional Fokker-Planck Eq. (1) does not have the second term of the left side of Eq. (10). Substituting $g(t)=t^{\alpha-1}/\Gamma(\alpha)$ into Eq. (10) cannot directly obtain Eq. (1). In order to exclude the second term of the left side of Eq. (10), the asymptotic behavior for $g(t)$ must be carefully treated.

We note that

$$\frac{d\langle x^2\rangle}{dt} = \int_{-\infty}^{\infty} x^2\frac{\partial\rho(x,t)}{\partial t}dx. \quad (11)$$

Substituting Eq. (10) into Eq. (11) yields

$$\frac{d\langle x^2\rangle}{dt} = \int_0^t g(t-t_1)\frac{d\langle x^2\rangle}{dt_1}dt_1 + D\frac{\partial}{\partial t}\int_0^t g(t-t_1)\int_{-\infty}^{\infty} x^2\frac{\partial^2\rho(x,t)}{\partial x^2}dxdt_1. \quad (12)$$

After integrating the second term of the right side of Eq. (12) by parts twice, we have

$$\frac{d\langle x^2\rangle}{dt} = \int_0^t g(t-t_1)\frac{d\langle x^2\rangle}{dt_1}dt_1 + 2D\frac{\partial}{\partial t}\int_0^t g(t-t_1)\int_{-\infty}^{\infty}\rho(x,t)dxdt_1, \quad (13)$$

where we also consider that $\lim_{x\to\pm\infty}\rho(x,t)$ and it decreases faster than $1/x$. The normalization of the pdf $\rho(x,t)$ requires that $\int_{-\infty}^{\infty}\rho(x,t)dx=1$. Finally, Eq. (13) can be rewritten as

$$\frac{d\langle x^2\rangle}{dt} = \int_0^t g(t-t_1)\frac{d\langle x^2\rangle}{dt_1}dt_1 + 2D\frac{\partial}{\partial t}\int_0^t g(t-t_1)dt_1. \quad (14)$$

Employing the Laplace transform in Eq. (14), we obtain

$$\langle x^2\rangle_L = \frac{\langle x^2\rangle_0}{s} + \frac{2Dg(s)}{s[1-g(s)]} \tag{15}$$

in Laplace space. We have shown that from Eq. (10), even without the previous knowledge of the waiting time pdf, the second moment of displacement, i.e., the diffusion behavior, can also be obtained in Eq. (15). This is one of advantages of Eq. (10). Therefore, Eq. (15) is very general and valid for any waiting time pdf.

In fact, different diffusion behaviors can be found when substituting different waiting time pdfs into Eq. (15). Considering that the waiting time pdf must be positive and normalized, there exist only a few simple functions that can be used as waiting time pdfs. Now we study diffusion behaviors in two specific cases of waiting time pdfs.

First case: $g_1(t)=\lambda e^{-\lambda t}$. In this case, the characteristic waiting time is finite. The Laplace transform of $g_1(t)$ is given by

$$g_1(s) = \frac{\lambda}{\lambda + s}. \tag{16}$$

Substituting Eq. (16) into Eq. (15), we obtain

$$\langle x^2\rangle = \langle x^2\rangle_0 + 2D\lambda t. \tag{17}$$

Equation (17) shows the normal diffusion behavior. It has also shown that the generalized diffusion Eq. (10) can reduce to describe the normal diffusion process when the waiting time pdf is a simple exponential function.

Second case: $g_2(t)=\lambda_\alpha t^{\alpha-1}E_{\alpha,\alpha}(-\lambda_\alpha t^\alpha)$. $E_{\mu,\nu}(y)$ is the generalized Mittag-Leffler function defined by [36,37]

$$E_{\mu,\nu}(y) = \sum_{n=0}^{\infty}\frac{y^n}{\Gamma(\nu+\mu n)}, \quad \mu>0, \quad \nu>0. \tag{18}$$

We restrict the parameter α to $0<\alpha\le 1$ because $E_{\alpha,\alpha}(-\lambda_\alpha t^\alpha)$, in this interval, is completely monotone for $t>0$ [36]. We note that $g_2(t)$ can also be written as

$$g_2(t) = -\frac{d}{dt}E_{\alpha,1}(-\lambda_\alpha t^\alpha).$$

This waiting time pdf has been used to link the CTRW model and fractional master equation [38]. It has also been adopted as subordination function [39,40]. Fulger *et al.* [41] incorporated this waiting time pdf into Monte Carlo simulation of in uncoupled continuous-time random walks with a Lévy α-stable distribution of jumps. The Lévy α-stable distribution of jumps used in [41] has a diverging jump length variance in contrast to the finite jump length variance given by Eq. (6) in this paper.

The waiting time pdf $g_2(t)$ has the following asymptotic behavior:

$$g_2(t) \sim -\frac{1}{\lambda_\alpha t^{1+\alpha}\Gamma(-\alpha)}, \tag{19}$$

which has a power-law behavior. The characteristic waiting time is divergent. The Laplace transform of $g_2(t)$ is given by

$$g_2(s) = \frac{\lambda_\alpha}{\lambda_\alpha + s^\alpha}. \tag{20}$$

Substituting Eq. (20) into Eq. (15), we obtain

$$\langle x^2\rangle = \langle x^2\rangle_0 + \frac{2D\lambda_\alpha}{\Gamma(1+\alpha)}t^\alpha. \tag{21}$$

This result is the same as that one obtained in [4] for long-time limit using approximation of a long-tailed waiting time pdf. However, it should be noted that Eq. (21) describes the subdiffusive processes for the all time regions rather than only for long-time or short-time region. This point is different from the case of long-tailed waiting time pdf in Ref. [4].

III. EXACT SOLUTION FOR PROBABILITY DENSITY

Generally speaking, using Eq. (3), we can calculate the pdf in the framework of CTRW model. However, it is hard to obtain the exact pdf from Eq. (3). Now, we can obtain the exact solutions for $\rho(x,t)$ for the two waiting time pdfs in Sec. II from Eq. (7). In the following, we consider the initial condition as $\rho_0(k)=1$. After we do Fourier inverse for $\rho(k,s)$ in Eq. (7), we have

$$\rho(x,s) = \frac{1-g(s)}{2\pi Dsg(s)}\int_{-\infty}^{\infty}\frac{e^{ikx}}{k^2+\dfrac{1-g(s)}{Dg(s)}}dk. \tag{22}$$

We note that the denominator can have three different poles: $1-g(s)=0$ gives trivial result, $[1-g(s)]/g(s)<0$ gives the poles on the real axis, and $[1-g(s)]/g(s)>0$ gives the poles on the imaginary axis. For the waiting time pdfs given in the previous section, we can restrict to the case of the poles on the imaginary axis. Thus, the solution for $\rho(x,s)$ is given by

$$\rho(x,s) = \frac{1}{2\pi\sqrt{Ds}}\sqrt{\frac{1-g(s)}{g(s)}}\exp\left(-\frac{|x|}{\sqrt{D}}\sqrt{\frac{1-g(s)}{g(s)}}\right). \tag{23}$$

Before obtaining the exact solutions to $\rho(x,t)$, we can calculate the second moment in Laplace space which yields

$$\langle x^2\rangle_L = \frac{2Dg(s)}{s[1-g(s)]}. \tag{24}$$

This result is similar to Eq. (15), except the term of initial value $\langle x^2\rangle_0$. This indirectly shows that Eq. (23) is correct.

For the case of $g_1(t)=\lambda e^{-\lambda t}$, the solution for $\rho(x,t)$ is given by

$$\rho_1(x,t) = \frac{1}{\sqrt{4\pi D\lambda t}}\exp\left(-\frac{x^2}{4\lambda Dt}\right). \tag{25}$$

The pdf shows the Gaussian shape and it is exactly the solution of the normal diffusion equation [2,4].

For the case of $g_2(t)=\lambda_\alpha t^{\alpha-1}E_{\alpha,\alpha}(-\lambda_\alpha t^\alpha)$, the solution for $\rho(x,t)$ is given by

$$\rho_2(x,t) = \frac{1}{\sqrt{4D\lambda_\alpha t^\alpha}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\,\Gamma\left(1-\alpha\frac{1+n}{2}\right)} \left(\frac{x^2}{D\lambda_\alpha t^\alpha}\right)^{n/2}. \tag{26}$$

This result is exactly the solution of the fractional diffusion Eq. (1). The pdf (26) presents pronounced cusps in x coordinate for different times. This form is different from the Gaussian shape (25) which presents smooth shape in the same coordinate [4].

Equation (26) can also be expressed in terms of the Wright function $\Phi_{\eta,\delta}(y)$ [42] in the following form:

$$\rho_2(x,t) = \frac{1}{\sqrt{4D\lambda_\alpha t^\alpha}} \Phi_{-\alpha/2,1-\alpha/2}\left(-\frac{|x|}{\sqrt{D\lambda_\alpha} t^{\alpha/2}}\right), \tag{27}$$

where

$$\Phi_{\beta,\delta}(y) = \sum_{n=0}^{\infty} \frac{y^n}{n!\,\Gamma(\beta n+\delta)}, \quad \beta > -1, \quad \delta \in \mathbf{C}. \tag{28}$$

IV. CONCLUSION

In this work, we have investigated the CTRW model with the decoupled jump pdf. We have derived the integrodifferential Eq. (10). From Eq. (10), we have derived diffusion behavior that is explicitly related to the waiting time pdf. Equation (10) is more flexible to be used than Eq. (7) because using Eq. (10), we can avoid Laplace and Fourier transformations and their inverse operations, for instance, Eq. (14) is ready to be used for calculating the second moment numerically. Both Eqs. (10) and (15) are very general and valid for any waiting time pdf. To our knowledge, Eqs. (10) and (15) have not been published elsewhere. In fact, Eq. (7) or (10) describes random-walk model without external force. However, interesting physical problems involve external force. Generalization of Eq. (10) to include the effect of external force is a natural step. In addition, possible generalization of Eq. (10), e.g., using the master-equation approach [4], to include the effect of external force would be more convenient and appropriate than Eq. (7).

Using Eq. (10), we have studied diffusion behaviors for two cases: (1) in the case of $g_1(t)=\lambda e^{-\lambda t}$, a normal diffusion or normal Brownian motion is found; (2) in the case of $g_2(t)=\lambda_\alpha t^{\alpha-1}E_{\alpha,\alpha}(-\lambda_\alpha t^\alpha)$, we have discovered a subdiffusive behavior for the all time regions rather than only for long-time or short-time regions that appear in the literature. We have also obtained the exact solution for pdfs in the two cases. For the first case, the exact solution of pdf is Gaussian. For the second case, the exact solution of pdf is non-Gaussian, but it can reduce to Gaussian pdf when $\alpha=1$.

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APPENDIX: INTEGRODIFFERENTIAL EQUATION

In order to obtain the integrodifferential equation (10) from Eq. (7), we employ the Fourier and Laplace transforms of the following expressions:

$$\mathcal{F}\left[\frac{\partial^2\rho(x,t)}{\partial x^2}\right] = -k^2\rho(k,t) \tag{A1}$$

and the convolution theorem for Laplace transform

$$\mathcal{L}\left[\int_0^t g(t-t_1)\rho(x,t_1)dt_1\right] = g(s)\rho(x,s). \tag{A2}$$

First, we use the inverse Fourier transform and Eq. (A1) in Eq. (7) and we find

$$s\rho(x,s) - sg(s)\rho(x,s) - Dsg(s)\frac{\partial^2\rho(x,s)}{\partial x^2} = [1-g(s)]\rho(x,0). \tag{A3}$$

After both sides of Eq. (A3) are divided by s, we reorganize it as follows:

$$\rho(x,s) - \frac{1}{s}\rho(x,0) - g(s)\rho(x,s) + \frac{1}{s}g(s)\rho(x,0) = Dg(s)\frac{\partial^2\rho(x,s)}{\partial x^2}. \tag{A4}$$

Using Eq. (A2) and applying the inverse Laplace transform in Eq. (A4), we have

$$\rho(x,t) - \rho(x,0) - \int_0^t g(t-t_1)\rho(x,t_1)dt_1 + \rho(x,0)\int_0^t g(t_1)dt_1 = D\int_0^t g(t-t_1)\frac{\partial^2\rho(x,t_1)}{\partial x^2}dt_1. \tag{A5}$$

Using the Leibnitz theorem for integral, we have the following relationship:

$$\frac{\partial}{\partial t}\left[\int_0^t g(t-t_1)\rho(x,t_1)dt_1\right] = g(0)\rho(x,t) + \int_0^t \frac{\partial}{\partial t}g(t-t_1)\rho(x,t_1)dt_1. \tag{A6}$$

The integral on the right side of Eq. (A6) can be expressed as

$$\int_0^t \frac{\partial}{\partial t}g(t-t_1)\rho(x,t_1)dt_1 = -\int_0^t \frac{\partial}{\partial t_1}g(t-t_1)\rho(x,t_1)dt_1. \tag{A7}$$

The integral on the right side of Eq. (A7) can be integrated by parts and Eq. (A7) can be further written as

$$\int_0^t \frac{\partial}{\partial t} g(t-t_1)\rho(x,t_1)dt_1 = -g(0)\rho(x,t) + g(t)\rho(x,0) + \int_0^t g(t-t_1)\frac{\partial}{\partial t_1}\rho(x,t_1)dt_1. \tag{A8}$$

Substituting Eq. (A8) into Eq. (A6), Eq. (A6) can be rewritten as

$$\frac{\partial}{\partial t}\left[\int_0^t g(t-t_1)\rho(x,t_1)dt_1\right] = g(t)\rho(x,0) + \int_0^t g(t-t_1)\frac{\partial}{\partial t_1}\rho(x,t_1)dt_1. \tag{A9}$$

First employing the operator $\partial/\partial t$ to Eq. (A5) and then substituting Eq. (A9) into the equation, finally we have

$$\frac{\partial \rho(x,t)}{\partial t} - \int_0^t g(t-t_1)\frac{\partial \rho(x,t_1)}{\partial t_1}dt_1 = D\frac{\partial}{\partial t}\int_0^t g(t-t_1)\frac{\partial^2 \rho(x,t_1)}{\partial x^2}dt_1. \tag{A10}$$

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