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# Continuous Time Random Walk and different diffusive regimes

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**ABSTRACT.** We investigate how it is possible to obtain different diffusive regimes from the Continuous Time Random Walk (CTRW) approach performing suitable changes for the waiting time and jumping distributions in order to get two or more regimes for the same diffusive process. We also obtain diffusion-like equations related to these processes and investigate the connection of the results with anomalous diffusion.

**Keywords:** random walk, anomalous diffusion, diffusive regimes.

## Caminhantes Aleatórios e diferentes regimes difusivos

**RESUMO.** Investigamos como é possível obter diferentes regimes difusivos do formalismo de caminhadas aleatórias com espaço-tempo contínuo fazendo mudanças adequadas na distribuição de tempos de espera e de saltos de forma a obter dois ou mais regimes para o mesmo processo difusivo. Também obtivemos equações tipo difusão para estes processos e investigamos a conexão desses resultados com a difusão anômala.

**Palavras-chave:** caminhates aleatórios, difusão anômala, diferentes regimes.

## Introduction

Since the first observations performed by Robert Brown on the random motion of particles suspended in a fluid and the explanation proposed by Einstein for this phenomenon, the diffusive processes have been widely investigated in several contexts. One of the main characteristics of this phenomenon is the behavior of the mean square displacement which is linear in time, i.e., $\left\langle \left(x-\langle x\rangle\right)^2\right\rangle \propto t$. This behavior for the mean square displacement accomplished by the Gaussian solution is essentially due to the Markovian nature of this process. The phenomena characterized by these properties are described by the usual diffusion $\partial_t \rho = \mathcal{D}\partial_x^2 \rho$, in which $\partial_t \rho + \nabla\cdot\vec{\jmath} = 0$ can be obtained by considering the continuity equation with the Fick law $\left(\vec{\jmath} = -\mathcal{D}\nabla\rho\right)$. It should be noted that this equation may be obtained by using other approaches, such as Langevin equations or random walks. However, there are several situations which are not conveniently described in terms of the usual form of the diffusion equation. For example, diffusion in a fractal medium (ACEDO; YUSTE, 1998; ANH et al., 2007; CAMPOS; MÉNDEZ, 2004; METZLER et al., 1994; O'SHAUGHNESSY; PROCACCIA, 1985), relaxation in systems with memory (CROTHERS et al., 2004; HILFER, 2000; SCHRIESSEL; BLUMEN, 1995), transport in porous media (MUSKAT, 1937; POLUBARINOVA-KOCHINA, 1962), fluctuation in financial markets (PLEROU et al., 2000), tumor development (FEDOTOV; IOMIN, 2007; IOMIN, 2006), micelles solvated in water (OTT et al., 1990). In these situations, the diffusive process is not normal but anomalous and the distribution which characterizes these processes is not the Gaussian one. In addition, the mean square displacement may be finite or not. For the finite case, in general, we have that $\left\langle \left(x-\langle x\rangle\right)^2\right\rangle \propto t^{\alpha}$ where $\alpha < 1$ and $\alpha > 1$ corresponds to the sub- and superdiffusive case. Situations characterized by different diffusive regimes are also verified in several contexts such as biological systems (GREGOIRE et al., 2001; ROGERS et al., 2008; WU; LIBCHABER, 2000), motion of colloidal particles (TIERNO et al., 2007), system with long range interactions (LATORA et al., 1999; LATORA et al., 2001), and adsorption-desorption processes (LENZI et al., 2009a). These physical situations have been investigated by several approaches such as fractional diffusion equations (BADINI et al., 2007; GONÇALVES et al., 2006; HILFER et al., 2004; ISFER et al., 2010; LENZI et al., 2011; LENZI et al., 2010; LENZI et al., 2009b; METZLER; KLAFTER, 2000; SANTORO et al., 2011; ROSSATO et al. 2007), nonlinear diffusion equations (FRANK, 2005), random walks (WEISS, 1994) and Langevin equations (COFFEY et al., 2004).

In this manuscript, we investigate how it is possible to get different diffusive regimes from the Continuous Time Random Walk (CTRW). We consider suitable choices to the waiting time distribution and jumping probability density in order to obtain different diffusive regimes for the same diffusive process. Depending on the choice of these functions, the system may exhibit two or more diffusive regimes which may present a finite or divergent (Lévy flights) second moment.

## Material and methods

### Continuous Time Random Walk

Let us start our discussion about Continuous Time Random Walk (CTRW) and different regimes by performing a review of some aspects of the CTRW approach. Following the discussion presented by Metzler and Klafter (2000), we start by introducing a jump probability distribution function (pdf) $\psi(x,t)$ which contains the characteristics of the system in analysis. From $\psi(x,t)$, we can obtain

$$\omega(t) = \int_{-\infty}^{\infty} \psi(x,t)dx \tag{1}$$

and

$$\lambda(x) = \int_{0}^{\infty} \psi(x,t)dt \tag{2}$$

As such, the quantity $\lambda(x)dx$ is the probability for a jump length in the interval $(x, x+dx)$ and $\omega(t)dt$ the probability for a waiting time in the interval $(t, t+dt)$. If the jump length and waiting time are independent random variables, one finds the decoupled form $\psi(x,t) = \omega(t)\lambda(x)$ for the jump pdf $\psi(x,t)$. If both are coupled, a jump of a certain length involves a time cost or, vice versa; i.e., in a given time span the walker can only travel a maximum distance. By using these definitions, a CTRW process can be described by the following equation

$$\eta(x,t) = \delta(x)\delta(t) + \int_{-\infty}^{\infty}\int_{0}^{t} \eta(\bar{x},\bar{t})\psi(x-\bar{x}, t-\bar{t})d\bar{t}d\bar{x} \tag{3}$$

which connects the (pdf) $\eta(x,t)$ of just having arrived at position $x$ at time $t$, with the event of having just arrived at $x'$ at time $t'$, $\eta(x',t')$ . The first term in the above equation is the initial condition for the random walk. Consequently, the distribution $\rho(x,t)$ of being at point $x$ at time $t$ is given by

$$\rho(x,t) = \int_{0}^{t} \eta(x,\bar{t})\Psi(t-\bar{t})d\bar{t} \tag{4}$$

where:

$$\Psi(t) = 1 - \int_{0}^{t} \omega(\bar{t})d\bar{t} \tag{5}$$

is the cumulative probability. In addition, by using the Fourier-Laplace transform, Equation (4) can be written as

$$\rho(k,s) = \frac{1-\omega(s)}{s}\frac{1}{1-\psi(k,s)} \tag{6}$$

The previous discussion essentially characterizes the CTRW approach that we use to investigate the situations characterized by different diffusive regimes.

## Results and discussion

Before analyzing a complex situation, let us study a usual diffusive process within this approach, in order to gain some insight on the changes we have to make. The usual diffusive process may be obtained from the above formalism by an appropriate choice of $\psi(k,s)$. To do this, it is necessary to note that the usual diffusion has a variance, i.e., the second moment is finite, and the average of the waiting time distribution is defined. These features are related to the Markovian characteristic of this process in which we are interested. These characteristics lead us to choose the jumping probability and waiting time distributions function with the following behavior $\lambda(k) \approx 1 - \mathcal{D}k^2 + O(k^4)$ and $\omega(s) \approx 1 - s\tau + O(s^2)$, to assure the previous assumptions. In order to check our choices and the relation to the usual diffusion, we may directly relate Equation (6) with the distribution that emerges from the diffusion equation

$$\frac{\partial}{\partial t}\rho(x,t)=\mathcal{D}\frac{\partial^2}{\partial x^2}\rho(x,t) \tag{7}$$

after applying the Fourier and Laplace transforms. This enables us to compare Equation (6) with the distribution obtained from Equation (7). Performing some calculations, it is possible to show that

$$\rho(k,s)=\frac{1}{s+(\mathcal{D}/\tau)k^2} \tag{8}$$

for the diffusion equation with the initial condition $\rho(x,0)=\delta(x)$ and the boundary conditions $\rho(\pm\infty,t)=0$. By comparing Equation (8) with Equation (6) we can find $\lambda(x)$ and $\omega(t)$, which for this case in the Fourier-Laplace space are given by $\lambda(k)\approx 1-\mathcal{D}k^2$. Note that the solution is $\omega(s)=1/(1+s\tau)$ in agreement with our previous choice for these functions.

This result obtained for the diffusion equation indicates that to model another diffusive process, we have to choice a suitable $\psi(k,s)$ accomplishing the characteristic of the diffusive process. In the previous discussion, the first situation that we can consider is the mixing between a long and short tailed behavior for the waiting time distribution. The previous choice to $\omega(s)$, i.e., $\omega(s)\approx 1-s\tau+O(s^2)$, gives a short tailed behavior. A long tailed behavior for $\omega(s)$ may be obtained by considering, e.g., $\omega(s)\approx 1-s^\gamma\tau_\gamma^\gamma+O(s^{2\gamma})$, with $0<\gamma<1$. By incorporating these two behaviors in $\omega(s)$, we obtain $\omega(s)\approx 1-(s\tau+s^\gamma\tau_\gamma^\gamma)$. Note that the different diffusive behaviors manifested by this choice to $\omega(s)$ are exhibited in accordance with a characteristic time determined by $\tau$ and $\tau_\gamma$; i.e., depending on the time scale considered, we may have an usual or anomalous behavior. In this context, a typical choice to the waiting time distribution is given by

$$\omega(s)=\frac{1}{1+s\tau+(s\tau_\gamma)^\gamma} \tag{9}$$

This waiting time distribution has two different behaviors which may be evidenced by considering $s\to 0$ $(t\to\infty)$ and $s\to\infty$ $(t\to 0)$. For the first case, the behavior of $\omega(s)$ is essentially governed by

$$\omega(s)=\frac{1}{1+(s\tau_\gamma)^\gamma} \tag{10}$$

which has as inverse Laplace transform

$$\omega(t)=\frac{1}{\tau_\gamma^\gamma}\left(\frac{t}{\tau_\gamma}\right)^{\gamma-1}\mathrm{E}_{\gamma,\gamma}\left(-\frac{t^\gamma}{\tau_\gamma^\gamma}\right) \tag{11}$$

where $\mathrm{E}_{\alpha,\beta}(x)$ is the generalized Mittag-Leffler function (PODLUBNY, 1999). For the other limit, the behavior of $\omega(s)$ is essentially governed by

$$\omega(s)=\frac{1}{1+s\tau} \tag{12}$$

which has as inverse Laplace transform

$$\omega(t)=\frac{1}{\tau}e^{-t/\tau} \tag{13}$$

The inverse Laplace transform of Equation (9) is given by

$$\omega(t)=\frac{1}{\tau}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{\tau_\gamma^\gamma}{\tau}t^{1-\gamma}\right)^n\mathrm{E}_{\alpha,\beta}^{(n)}\left(-\frac{t}{\tau}\right) \tag{14}$$

with $\alpha=1$ and $\beta=1-\gamma n$, where: $\mathrm{E}_{\alpha,\beta}^{(n)}(x)\equiv\frac{d^n}{dx^n}\mathrm{E}_{\alpha,\beta}(x)$. Similar to the case worked out for the usual diffusion process, it is possible to relate this diffusive process to a diffusion-like equation. In particular, it is given by

$$\tau\frac{\partial}{\partial t}\rho(x,t)+\tau_\gamma^\gamma\frac{\partial^\gamma}{\partial t^\gamma}\rho(x,t)=\mathcal{D}\frac{\partial^2}{\partial x^2}\rho(x,t) \tag{15}$$

The behavior considered for the $\omega(t)$ may be verified from Equation (15) by analyzing the mean square displacement $\sigma_x^2=\left\langle(x-\langle x\rangle)^2\right\rangle$ which for the initial conditions considered here is equal to the second moment. The second moment for this case is give by Lenzi et al. (2003)

$$\left\langle x^2\right\rangle=2\mathcal{D}\frac{t}{\tau}\mathrm{E}_{1-\gamma,2}\left(-\frac{\tau_\gamma^\gamma}{\tau}t^{1-\gamma}\right) \tag{16}$$

see Figure 1. By taking the previous limits into account, it is possible to show $\left\langle x^2\right\rangle\approx t^\gamma$ and $\left\langle x^2\right\rangle\approx t$ characterizing two different regimes for the spreading of the system, as expected. It also is possible to extend the previous analysis by considering the waiting time distribution

$$\omega(s)=\frac{1}{1+s\tau+\Lambda(s)} \quad (17)$$

where:

$\Lambda(s)$ is the Laplace transform of a time-dependent function $\Lambda(t)$. Equation (16) may present different behaviors depending on the choice performed for $\Lambda(s)$.

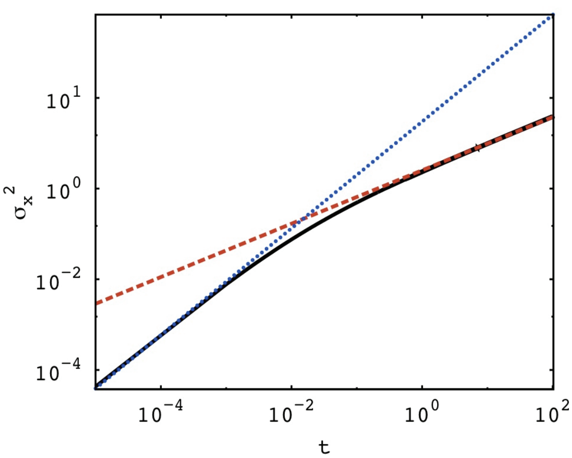


**Figure 1.** The continuous line is the variance versus time when considering Equation (16) with $\gamma=0.5$, $\mathcal{D}=1$, $\tau=0.1$ and $\tau_\gamma=0.1$. The dotted line is the asymptotic expansion for small times, $\sigma_x^2\sim t$, and the dashed line for long times, $\sigma_x^2\sim t^\gamma$.

The inverse Laplace transform to Equation (17) may be obtained and it is given by

$$\omega(t)=\frac{1}{\tau}e^{-t/\tau}+\frac{1}{\tau}\sum_{n=1}^{\infty}\left(-\frac{1}{\tau}\right)^n\int_0^t dt'(t-t')^n e^{-(t-t')/\tau}\int_0^{t'}dt_n\Lambda(t'-t_n)$$
$$\times\int_0^{t_n}dt_{n-1}\Lambda(t_n-t_{n-1})\cdots\int_0^{t_3}dt_2\Lambda(t_3-t_2)\int_0^{t_2}dt_1\Lambda(t_2-t_1)$$

In addition, the diffusion-like equation related to this choice for the waiting time distribution is given by

$$\int_0^t\Phi(t-t')\frac{\partial^\gamma}{\partial t'^\gamma}\rho(x,t')d\tilde{t}=\mathcal{D}\frac{\partial^2}{\partial x^2}\rho(x,t) \quad (18)$$

with $\Phi(t)=\tau\delta(t)+\Lambda'(t)$ and $\Lambda'(t)=\int_0^t\Lambda(t')dt'$. From this equation, is also possible to obtain the mean square displacement, for simplicity, by considering the initial condition $\rho(x,0)=\delta(x)$ which simplifies our calculation for the second moment. After some calculations, it is possible to show that it formally can be written as

$$\langle x^2\rangle=\frac{2\mathcal{D}}{\tau}t+\frac{2\mathcal{D}}{\tau}\sum_{n=1}^{\infty}\left(-\frac{1}{\tau}\right)^n\int_0^t dt'(t-t')\int_0^{t'}dt_n\Lambda(t'-t_n)$$
$$\times\int_0^{t_n}dt_{n-1}\Lambda(t_n-t_{n-1})\cdots\int_0^{t_3}dt_2\Lambda(t_3-t_2)\int_0^{t_2}dt_1\Lambda(t_2-t_1)\ .$$

The previous analysis was performed by considering the changes obtained by incorporating different situations to the waiting time distribution. Now, we investigate the changes produced by modifying the jumping probability $\lambda(k)$ in order to incorporate, for example, long tailed behavior. A typical change to be performed in $\lambda(k)$, which accomplishes long tailed behavior, is to add the term $\mathcal{D}_\mu|k|^\mu$. Thus, the jumping probability in the Fourier space is given by $\lambda(k)\approx 1-\mathcal{D}_\mu|k|^\mu$. This choice for $\lambda(k)$ has two behaviors, one of them governed by a Gaussian distribution and the other by a Levy distribution, since $\omega(s)=1/(1+s\tau)$. In this case, the diffusion-like equation is given by

$$\tau\frac{\partial}{\partial t}\rho(x,t)=\mathcal{D}\frac{\partial^2}{\partial x^2}\rho(x,t)+\mathcal{D}_\mu\frac{\partial^\mu}{\partial|x|^\mu}\rho(x,t)$$

Another choice that can be performed for $\lambda(k)\approx 1-\mathcal{D}k^2-\mathcal{D}_\mu|k|^\mu$, where $\mathcal{D}_\mu(k)$ is a spatial dependent function that admits an inverse of the Fourier transform. For this general case, the diffusion equation is given by

$$\tau\frac{\partial}{\partial t}\rho(x,t)=\mathcal{D}\frac{\partial^2}{\partial x^2}\rho(x,t)+\int_{-\infty}^{\infty}\mathcal{D}_\mu(x-x')\rho(x',t)dx' \quad (19)$$

Figure 2 illustrates the behavior of the $[1/\rho(0,t)]^2$ obtained from Equation (19) versus $t$ by considering $\mathcal{D}_\mu(k)=\mathcal{D}_1|k|+\mathcal{D}_{3/2}|k|^{\frac{3}{2}}$. Note that the presence of different diffusive regimes, which may be detected by considering an appropriated time scale. In order to evidence these different diffusive regimes, which are manifested by a previous choice of $\mathcal{D}_\mu(k)$, we plot straight lines to indicate the dominant time dependence in such time scale.

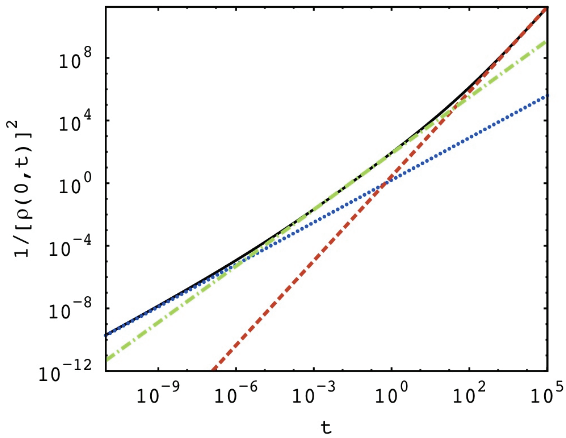


**Figure 2.** Behavior of the $[1/\rho(0,t)]^2$ versus $t$ by considering $\mathcal{D}_\mu(k)=\mathcal{D}_1|k|+\mathcal{D}_{3/2}|k|^{\frac{3}{2}}$. For simplicity, we choose, without loss of generality, $\mathcal{D}=1$, $\mathcal{D}_1=1$, and $\mathcal{D}_{3/2}=10$. The dotted line represents $[1/\rho(0,t)]^2\sim t^{4/3}$, the dotted – dashed line corresponds to the behavior $[1/\rho(0,t)]^2$ and the dashed line is the asymptotic behavior $[1/\rho(0,t)]^2\sim t^2$.

Another possibility to model situations with different diffusive regimes by using the CTRW approach is to consider simultaneous changes to the waiting time distribution and the jumping probability in order to produce the suitable behavior to describe the diffusive process under investigation. In this direction, it is possible to consider the waiting time distribution given by

$$\omega(s)=\frac{1}{1+s\tau+s^{\gamma-1}\Lambda(s)}$$

and the jumping probability given by $\lambda(k)\approx 1-\mathcal{D}_\mu(k)$ which yields,

$$\frac{\partial}{\partial t}\rho(x,t)+\int_0^t \Lambda(t-\tilde{t})\frac{\partial^\gamma}{\partial\tilde{t}^\gamma}\rho(x,\tilde{t})d\tilde{t}=\int_{-\infty}^{\infty}\mathcal{D}_\mu(x-x')\rho(x',t)dx' \quad (20)$$

The previous equation may exhibit different regimes depending on the choices performed for $\Lambda(t)$, $\mathcal{D}_\mu(x)$ and $\gamma$.

## Conclusion

We have investigated the diffusive regimes which can be obtained from the Continuous Time Random Walk formalism when suitable changes are considered. We first analyzed the CTRW by performing several choices for the waiting time or jumping distributions. The changes considered for the waiting time distribution led us to situations with finite mean square displacement and different regimes for the same processes, which are detected in different time scales. A typical example is given by Equation (16), which has two different regimes; one of them is manifested for small times and the other for long times. Finally, we expect that the results found here may be useful to investigate anomalous diffusion.

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