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Correlation function induced by a generalized diffusion equation with the presence of a harmonic potential

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HIGHLIGHTS

- Calculation of the correlation function.
- The correlation function is connected to the survival probability.
- The model can be applied to the internal dynamics of proteins.

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ABSTRACT

An integro-differential diffusion equation with linear force, based on the continuous time random walk model, is considered. The equation generalizes the ordinary and fractional diffusion equations, which includes short, intermediate and long-time memory effects described by the waiting time probability density function. Analytical expression for the correlation function is obtained and analyzed, which can be used to describe, for instance, internal motions of proteins. The result shows that the generalized diffusion equation has a broad application and it may be used to describe different kinds of systems.

1. Introduction

The ordinary diffusion equation is an equation of motion for the probability density function (PDF) $\rho(x, t)$ in position space describing the Brownian motion of particles with the presence of external

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force $F(x)$ [1]. In one-dimensional space, it is given by

$$\frac{\partial\rho(x,t)}{\partial t}=\frac{1}{m\gamma}\left[-\frac{\partial}{\partial x}F(x)+k_BT\frac{\partial^2}{\partial x^2}\right]\rho(x,t), \tag{1}$$

where k_B, T, γ and m are the Boltzmann constant, the absolute temperature, the friction constant and the mass of Brownian particle, respectively. Eq. (1) describes normal diffusion for force-free case. An extension of the ordinary diffusion equation, the so-called fractional diffusion equation (originally called fractional Fokker–Planck equation) has been obtained from the continuous time random walk (CTRW) model for finite jump length variance and a long-tailed power-law waiting time PDF $g(t)\sim(\tau/t)^{1+\alpha}$ with $0<\alpha<1$ [2–4], and it is described by

$$\frac{\partial\rho(x,t)}{\partial t}={}_0D_t^{1-\alpha}\left[-\frac{\partial}{\partial x}\frac{F(x)}{m\eta_\alpha}+K_\alpha\frac{\partial^2}{\partial x^2}\right]\rho(x,t), \tag{2}$$

where K_α is the generalized diffusion constant. The operator ${}_0D_t^{1-\alpha}$ is the Riemann–Liouville fractional operator defined by

$${}_0D_t^{1-\alpha}f(t)=\frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t dt_1\frac{f(t_1)}{(t-t_1)^{1-\alpha}},\quad 0<\alpha<1, \tag{3}$$

where $\Gamma(z)$ is the Gamma function. Note that the fractional diffusion equation (2), for force-free case, describes subdiffusion. The CTRW model [5] was proved a useful tool for the description of nonequilibrium systems [4,6–14], from Biophysics to Geosciences. In fact, the CTRW has been used in a wide range of applications such as earthquake modeling [15,16], random networks [17], self-organized criticality [18], electron tunneling [19], electron transport in nanocrystalline films [20] and financial stock markets [21–25]; it has also been employed to describe the dynamic simulation data and neutron scattering experiments [26–28]. The CTRW model is based on the length of a given jump associated with the waiting time elapsing between two successive jumps, and these quantities are connected by a probability density function of jumps $\psi(x,t)$.

Recently, an extension of the fractional diffusion equation, based on the CTRW model, has been obtained, under the case of finite jump length variance, with any waiting time PDF and external force $F(x)$ [29,30], which is described by

$$\frac{\partial\rho(x,t)}{\partial t}-\int_0^t \mathrm{d}t_1 g(t-t_1)\frac{\partial\rho(x,t_1)}{\partial t_1}=\overline{C}\frac{\partial}{\partial t}\int_0^t \mathrm{d}t_1 g(t-t_1)L_{FP}\rho(x,t_1), \tag{4}$$

where $\sqrt{\overline{C}}$ has a dimension of length and the operator L_{FP} is given by

$$L_{FP}=-\frac{\partial}{\partial x}\frac{F(x)}{k_BT}+\frac{\partial^2}{\partial x^2}. \tag{5}$$

Eq. (4) includes short, intermediate and long-time memory effects given by the waiting time PDF. Some interesting results from Eq. (4) are also presented in [31]. Eq. (4) has also been used to describe the simulation data of hydrated proteins [28]. Besides, the compact form of Eq. (4) can be written as

$$\frac{\partial\rho(x,t)}{\partial t}=\overline{C}\frac{\partial}{\partial t}\int_0^t \mathrm{d}t_1\Lambda(t-t_1)L_{FP}\rho(x,t_1), \tag{6}$$

where $\Lambda(t)$ is defined through its Laplace transform as follows:

$$\Lambda_s(s)=\frac{g_s(s)}{1-g_s(s)}. \tag{7}$$

Eq. (6) is appropriate to obtain the limiting cases such as the ordinary diffusion equation, which can be recovered for the exponential waiting time PDF. Moreover, Eq. (6) can lead to the same fractional diffusion equation (2) for $g(t)$ described by the following function:

$$g_1(t)=-\frac{d}{dt}E_{\alpha,1}(-\lambda_\alpha t^\alpha)=\lambda_\alpha t^{\alpha-1}E_{\alpha,\alpha}(-\lambda_\alpha t^\alpha), \tag{8}$$