Physica A 453 (2016) 327–335

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Connecting complexity with spectral entropy using the Laplace transformed solution to the fractional diffusion equation

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HIGHLIGHTS

- Laplace transformed fractional diffusion equation is formulated via Fox's H-function.
- The derived solution is equivalent with the existing Lévy stable solution.
- The overall spectral entropy increases with the decreasing derivative orders α and β.
- Spectral entropy is considered a measure to characterize the complexity of diffusion.

ARTICLE INFO

Article history:
Received 5 November 2015
Received in revised form 26 January 2016
Available online 22 February 2016

Keywords:
Fractional derivative
Spectral entropy
Diffusion equation
Laplace transform
Fourier transform
Long range correlation

ABSTRACT

Analytical solutions to the fractional diffusion equation are often obtained by using Laplace and Fourier transforms, which conveniently encode the order of the time and the space derivatives (α and β) as non-integer powers of the conjugate transform variables (s, and k) for the spectral and the spatial frequencies, respectively. This study presents a new solution to the fractional diffusion equation obtained using the Laplace transform and expressed as a Fox's H-function. This result clearly illustrates the kinetics of the underlying stochastic process in terms of the Laplace spectral frequency and entropy. The spectral entropy is numerically calculated by using the direct integration method and the adaptive Gauss–Kronrod quadrature algorithm. Here, the properties of spectral entropy are investigated for the cases of sub-diffusion and super-diffusion. We find that the overall spectral entropy decreases with the increasing α and β, and that the normal or Gaussian case with $\alpha = 1$ and $\beta = 2$, has the lowest spectral entropy (i.e., less information is needed to describe the state of a Gaussian process). In addition, as the neighborhood over which the entropy is calculated increases, the spectral entropy decreases, which implies a spatial averaging or coarse graining of the material properties. Consequently, the spectral entropy is shown to provide a new way to characterize the temporal correlation of anomalous diffusion. Future studies should be designed to examine changes of spectral entropy in physical, chemical and biological systems undergoing phase changes, chemical reactions and tissue regeneration.

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http://dx.doi.org/10.1016/j.physa.2016.02.056

1. Introduction

The study of diffusion in complex systems has expanded into many different fields [1–5] as investigators seek more accurate models to account for the movement of materials between and across multi-scale interfaces. The initial observation that diffusion should obey classical Brownian motion as derived from the classical Fick's first and second laws has not proven successful in complex materials, such as biological tissues for describing the movement of water or tracers in either the intracellular or the extracellular compartments [6–8]. There are many different models that have been used to describe non-Gaussian (i.e., anomalous) diffusion [3,6,8,9]. A recent review summarized the most popular anomalous diffusion models and discussed their properties [10]. In particular, the mean squared displacement (MSD) is shown in Table 1 of Ref. [10] to provide a common denominator for all models of anomalous diffusion. Despite this similarity, the physical foundations of these models are very different from each other. In this paper we present another way to establish a connection between different forms of anomalous diffusion by expressing the solution to the space–time fractional diffusion equation in terms of the spectral entropy.

In this model a random variable, $x(t)$, describes the movement of molecules in a heterogeneous and tortuous system. The space–time fractional diffusion equation describes the probability of finding this molecule at position, x, at time, t, in terms of $p(x, t)$, its probability density function (pdf). This model when extended using fractional order derivative can be expressed as [11,12],

$$\frac{\partial^{\alpha} p(x,t)}{\partial t^{\alpha}} = D_{\alpha,\beta} \frac{\partial^{\beta} p(x,t)}{\partial |x|^{\beta}}, \tag{1}$$

where the initial value $p(x, 0) = \delta(x)$, $D_{\alpha,\beta}$ is the generalized diffusion coefficient (m^{β}/s^{α}), the Caputo fractional derivative in time with the order $0 < \alpha \le 1$ is expressed as [13],

$$\frac{\partial^{\alpha} p(x,t)}{\partial t^{\alpha}} = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\tau)^{-\alpha} \frac{\partial p(x,\tau)}{\partial \tau} \mathrm{d}\tau. \tag{2}$$

The Fourier transform of the Reisz fractional derivative in space with the order $0 < \beta \le 2$ is expressed as [14],

$$F\left(\frac{\partial^{\beta} p(x,t)}{\partial |x|^{\beta}}\right) = |k|^{\beta} p(k,t), \tag{3}$$

where F represents the Fourier transform, $p(k, t)$ is the Fourier transform of $p(x, t)$. It is noted that the MSD of the pdf diverges when $\beta \neq 2$, and the scaling relation only exists for the rescaled fractional order moments, which is stated as,

$$\langle |x|^{q} \rangle \sim t^{q/\beta}, \tag{4}$$

where $0 < q < \beta \le 2$ for the space fractional diffusion equation [6]. Here, we use the pseudo or imaginary MSD of the pdf, which is a power law of time as [6,15]:

$$\langle x^2 \rangle_L \sim t^{2\alpha/\beta}. \tag{5}$$

The statistical process is the classical Brownian motion when $2\alpha/\beta = 1$, while if $2\alpha/\beta < 1$, the process is classified as sub-diffusion, and if $2\alpha/\beta > 1$, the process is described as super-diffusion. The detailed properties of rescaled fractional order moments of the pdf can be found in Ref. [6]. The solution of Eq. (1) can be obtained via the Fox's H-function, which has a heavy tail [16,17],

$$p(x,t) = \frac{1}{\beta |x|} H^{2,1}_{3,3}\left[\frac{-|x|}{(D_{\alpha,\beta} t^{\alpha})^{1/\beta}} \middle| \begin{matrix} (1, 1/\beta), (\alpha, \alpha/\beta)(1, 1/2) \\ (1, 1), (1, 1/\beta), (1, 1/2) \end{matrix} \right]. \tag{6}$$

Simpler algebraic solutions of Eq. (6) for special choices of α and β are given in Ref. [18].

It is known that the Fourier transform of $p(x, t)$, i.e., the characteristic function $p(k, t)$ follows the Mittag-Leffler function [17]. Recently, this technique has been expressed in terms of the spectral entropy $H_k(p)$ as a measure of spatial correlation in complex system, for example biological tissue [19]. Fig. 1 gives a schematic diagram of the strategy to measure the uncertainty in a diffusion process, in which FT and IFT respectively represent the Fourier transform and its inverse, LT and ILT respectively mean the Laplace transform and its inverse, FLT is the Fourier–Laplace transform, p^* is the complex conjugate of p, and H is the spectral entropy, which is calculated by the Shannon entropy (SE). In order to measure the temporal correlation of the diffusion process, we need to acquire the formula of $p(x, s)$ first. Previously, Mainardi gave an expression of $p(x, s)$ for the special case $\beta = 2$ [17], and Barkai introduced a general Lévy stable solution for $0 < \alpha \le 1$, $0 < \beta \le 2$ [20], in which the standard symmetric Lévy stable distribution is addressed [21]. In the present work, a more succinct solution for the Laplace transformed fractional diffusion equation is formulated with the Fox's H-function.

Furthermore, it has been recognized that entropy conveys more information about the dynamics of heterogeneous and multi-scale systems [22,23]. Higher entropy indicates more complexity of the underlying movement of molecules in the heterogeneous environment [16]. To detect the temporal correlation of anomalous diffusion in complex systems, the individual contributions of the frequency to the total spectral entropy $H_s(p)$ are illustrated, and the properties of spectral entropy in terms of the formula $p(x, s)$ are investigated both for the sub-diffusion and super-diffusion.