Thermodynamics of Anomalous Diffusion

Damián H. Zanette and Pablo A. Alemany
Consejo Nacional de Investigaciones Científicas y Técnicas, Centro Atómico Bariloche and Instituto Balseiro, 8400 Bariloche, Río Negro, Argentina
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It is pointed out that the generalized statistical mechanics introduced by Tsallis [J. Stat. Phys. **52**, 479 (1988)] provides a natural frame for developing a thermodynamical formalism of anomalous diffusion. Within such a frame, we calculate the mean square displacement as a function of time and generalize the Einstein relation of diffusivity and temperature for random walks of the Lévy-flight type.

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In recent years, much attention has been paid to physical systems driven by transport mechanisms other than ordinary diffusion. In particular, anomalous diffusion has been shown to play a fundamental role in the dynamics of a wide class of systems [1]. Turbulent flows [2], phase-space motion in chaotic dynamics [3], and transport in highly heterogeneous media, such as porous materials or gels [1,4], are some of the main instances where anomalous diffusion underlies transport processes.

Ordinary diffusion is characterized by a mean square displacement proportional to the time, $\langle x^2 \rangle \propto t$, whereas anomalous diffusion can exhibit a variety of alternative behaviors. Depending on the physical system under study, they can range from generalized diffusion laws, $\langle x^2 \rangle \propto t^\alpha$ ($\alpha \neq 1$), to situations in which $\langle x^2 \rangle$ is not a well defined quantity. These anomalies are related with the appearance of unusual topological features, such as fractal structure [2,5].

Two somewhat different approaches can be used to model anomalous diffusion by means of random walks. The first one, in the frame of the continuous time formulation of random walks, makes use of long tailed waiting-time distributions [4,6]. The other approach considers long tailed distributions for the jump length probability and discrete time steps [7]. Both approaches can be combined to account for complex scaling laws, as in turbulence problems [2]. Discrete time random walks with long tailed jump distributions are paradigmatically represented by Lévy flights [1–6,8].

Lévy flights are defined by a jump probability $p(\mathbf{x})$ whose Fourier transform reads $p(\mathbf{k}) = \exp(-ak^\gamma)$, with $k = |\mathbf{k}|$ and $\gamma < 2$. For $\gamma = 2$, an ordinary diffusive random walk—with a well defined mean square displacement—is recovered. Since it is not possible to find an analytical closed form for the corresponding $p(\mathbf{x})$, it is usually replaced by a function with the same asymptotic properties which, ultimately, determine the global features of the process. A possible alternative form for the jump probability is

$$p(\mathbf{x}) = N_x(x_0^2 + x^2)^{-(d+\gamma)/2}, \qquad (1)$$

where $x = |\mathbf{x}|$, d is the spatial dimension, and N_x is a proper normalization constant. The distance x_0 measures the length scale above which the fractal features—exhibited by Lévy flights at all scales—appear for the alternative form (1).

We associate now the random walk defined by Eq. (1) with the transport mechanism of a set of independent particles in a background at a well defined temperature T, and try to describe this system in the frame of equilibrium statistical thermodynamics, as is usually done with ordinary diffusion [9]. In generic diffusion problems—as seen from the thermodynamical viewpoint—the possibility of exploiting the ergodic hypothesis to replace the ensemble by temporal averages requires one to assume that the mean time between collisions of the diffusing particles with the background is finite. Here, we suppose that the time between collisions is a constant τ, but remark that the extension of our formulation to the case of a well defined mean time should be straightforward. Certainly, this is not the case for the so-called Lévy walks [2,4]—or any other representation of anomalous diffusion in terms of waiting-time distributions with divergent first-order moment—which would require a much more complex mathematical treatment.

Supposing that during the time between collisions the velocity v of each particle is essentially constant, a jump of length x is performed with velocity $v = x/\tau$ and, therefore, with energy $\epsilon = mv^2/2$, with m the particle mass. This connection between the jump length and the energy makes it possible to obtain, from Eq. (1), the probability distribution of ϵ along the trajectory of a single particle. By virtue of the ergodic hypothesis, this distribution can then be associated with the equilibrium probability $p(\epsilon)$ of a one-particle state of energy ϵ. Taking into account that $g(\epsilon)p(\epsilon)\,d\epsilon = p(x)\,dx$, where $g(\epsilon)$ is the free-particle density of states in d dimensions, we obtain

$$p(\epsilon) = N_\epsilon\left(1 + \frac{2\tau^2}{mx_0^2}\,\epsilon\right)^{-(d+\gamma)/2}, \qquad (2)$$

where N_ϵ is a normalization constant. It is apparent that this form of $p(\epsilon)$ does not correspond to the exponential energy distribution obtained from Boltzmann-Gibbs statistics. Instead, it coincides in form with the energy distribu-

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tion derived in the frame of a generalization of statistical thermodynamics recently proposed by Tsallis [10].

Tsallis' generalized statistical mechanics (TGSM) is based on an alternative definition for the equilibrium entropy of a system whose ith microscopic state has probability p_i. It reads

$$S_q = k \frac{1 - \sum_i p_i^q}{q - 1}, \tag{3}$$

where k is a positive constant and the index q defines a particular statistics. In the limit $q \to 1$—and for $k = k_B$, the Boltzmann constant—the usual Boltzmann-Gibbs formulation is reobtained. To find the probability p_i as a function of the energy ϵ_i of the ith state, the entropy S_q is maximized with respect to p_i, taking into account the constraint of probability normalization, $\sum_i p_i = 1$, and a generalized constraint

$$\sum_i p_i^q \epsilon_i = E_q = \text{const}, \tag{4}$$

which defines the generalized mean energy E_q. Under such constraints, the maximization of the generalized entropy S_q produces

$$p_i = p(\epsilon_i) = A[1 + \beta(q - 1)\epsilon_i]^{-1/(q-1)}, \tag{5}$$

where the constants A and β play the role of Lagrange multipliers, respectively, associated with the partition function and the temperature [10].

Probably, the main difference between TGSM and the Boltzmann-Gibbs formulation lies in the fact that S_q is a nonadditive quantity. This suggests a connection between TGSM and nonextensive physics [11]. In fact, a major success of this generalization has been to give a solution for the divergent mass of the polytropic model of gravitational systems [12]. Suitable generalizations of the Ehrefest theorem and Jaynes duality relations [13], von Neumann equation [14], fluctuation-dissipation theorem [15], Bogolyubov inequality [16], Langevin and Fokker-Planck equations [17], and Callen identity [18] are consistent with TGSM, which also exhibits a Legendre-transformation structure [10] and can be extended to treat quantum problems [19]. A connection between TGSM and fractals, through the maximum-entropy formalism for random walks, has been found for the first time in [5].

Now, from the comparison of Eqs. (2) and (5), it clearly results that TGSM provides a natural frame for a thermodynamical treatment of anomalous diffusion. For a given value of the Lévy exponent γ the proper statistics correspond to the index

$$q = 1 + \frac{2}{d + \gamma}. \tag{6}$$

Note that $q > 1$. In fact, according to Eq. (5), a statistics index lower than unity would imply—in the present framework—an unphysical energy distribution. Moreover, in our particular picture of the diffusion process, it is possible to identify the temperature parameter as

$$\beta = \frac{2\tau^2}{(q - 1)mx_0^2}. \tag{7}$$

We observe that in the context of TGSM the one-step mean square displacement of a Lévy flight, which—according to Eq. (4)—should be defined as

$$\langle x^2 \rangle_q = \int x^2 p(\mathbf{x})^q \, d\mathbf{x}, \tag{8}$$

is finite [5]. In fact, according to Eq. (6), $x^2 x^{d-1} p(\mathbf{x})^q \sim x^{2+d-1} x^{-2-d-\gamma} \sim x^{-(1+\gamma)} < x^{-1}$ for large x. On the other hand, usual statistics produces a divergent mean square displacement for Lévy flights.

This observation implies that, in constrast with usual statistics, TGSM makes it possible to compute the mean square displacement of an n-step Lévy flight, $\langle x_n^2 \rangle_q$, and to relate it with the time elapsed during the flight, as usually done with ordinary diffusion. This mean value should be given by

$$\langle x_n^2 \rangle_q = \int x^2 p_n(\mathbf{x})^q \, d\mathbf{x}, \tag{9}$$

where $p_n(\mathbf{x})$ is the probability density of finding the walker at point $\mathbf{x}$ after the n-step flight. This probability density is easily defined in the Fourier representation as $p_n(\mathbf{k}) = p(\mathbf{k})^n$, where $p(\mathbf{k})$ is the Fourier transform of $p(\mathbf{x})$.

Since for $k \to 0$ the Fourier transform of Eq. (1) behaves as $p(\mathbf{k}) \approx 1 - ak^{\gamma_0}$ with $\gamma_0 = \min(\gamma, 2)$ [6,20] and a constant, its nth power satisfies

$$p^n(\mathbf{k}) \approx 1 - ank^{\gamma_0} \approx \tilde{p}(n^{1/\gamma_0}\mathbf{k}), \tag{10}$$

where the scaling function $\tilde{p}(\mathbf{k})$ is expected to have the same asymptotic properties as $p(\mathbf{k})$. Antitransforming this scaled form of $p_n(\mathbf{k})$ we obtain, for large x,

$$p_n(\mathbf{x}) \approx n^{-d/\gamma_0} \tilde{p}(n^{-1/\gamma_0}\mathbf{x}). \tag{11}$$

Taking into account Eq. (9), this implies

$$\langle x_n^2 \rangle_q \approx n^{[2-(q-1)d]/\gamma_0} \langle \tilde{x}^2 \rangle_q, \tag{12}$$

where $\langle \tilde{x}^2 \rangle_q$ is the mean square displacement associated with the scaling function $\tilde{p}(\mathbf{x})$. This approximate equation should become an identity for long times, when only the asymptotic properties of the distributions are relevant.

Now, assuming that $\tilde{p}(\mathbf{x}) \approx p(\mathbf{x})$ for large x, it is easily shown that $\langle \tilde{x}^2 \rangle_q = K(q,d)x_0^2$, where the coefficient $K(q,d)$ can depend on the index q and the dimension d but is independent of x_0. Moreover, the step number n can be put in terms of the time t elapsed during the flight as $n = t/\tau$. Introducing these expressions in Eq. (12) we find that the mean square displacement of the Lévy flight as a function of time reads

$$\langle x^2(t) \rangle_q = \frac{K(q,d)x_0^2}{\tau^{[2-(q-1)d]/\gamma_0}} t^{[2-(q-1)d]/\gamma_0}. \tag{13}$$

In order to relate this mean square displacement with the thermodynamical quantities—in particular, with the temperature parameter β—we replace x_0 from Eq. (7), obtaining

$$\langle x^2(t)\rangle_q = D_q t^\alpha, \tag{14}$$

where the generalized anomalous-diffusion coefficient D_q is given by

$$D_q = \frac{2K(q,d)}{q-1}\frac{\tau^{2-\alpha}}{m\beta}, \tag{15}$$

and

$$\alpha = \frac{2-(q-1)d}{\gamma_0} = \begin{cases} q-1 & \text{for } \gamma < 2, \\ 1-(q-1)d/2 & \text{for } \gamma > 2. \end{cases} \tag{16}$$

In Fig. 1 we show this anomalous-diffusion exponent α as a function of the statistics index q, for one, two, and three dimensions. We note that this exponent reduces to the ordinary value $\alpha = 1$ for $q \to 1$. In fact, γ diverges in this limit, and the second line of Eq. (16) holds. For other values of q, as shown in Fig. 1, this exponent can adopt a variety of values, representing both subdiffusive ($\alpha < 1$) and superdiffusive ($\alpha > 1$) regimes. We stress that for $\gamma < 2$—i.e., for sufficiently large values of q—α does not depend on the spatial dimension, as in the case of ordinary diffusion.

Equation (14) has the form of a typical relation between mean square displacement and time for anomalous diffusion. The coefficient D_q is related to the temperature through Eq. (15), which is nothing but a generalized form of the Einstein relation [9]. This generalized relation indicates that—as in ordinary diffusion—the diffusion coefficient is inversely proportional to the temperature parameter β. Recalling that in ordinary diffusion the product $\mu = \beta D$ defines the mobility of the diffusing particles [9], we can generalize this definition by taking $\mu_q \propto \tau^{2-\alpha}/m$. As the ordinary mobility, μ_q is proportional to a power of the mean time between collisions and depends inversely on the particle mass.

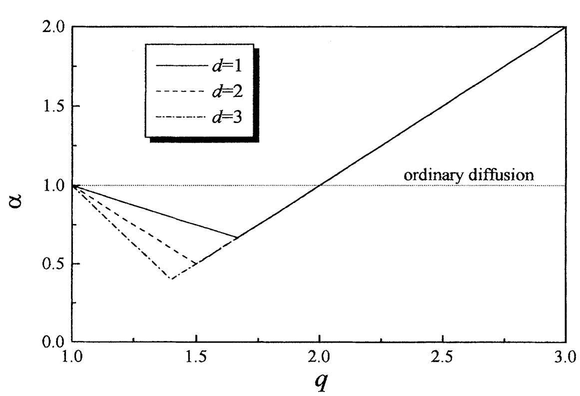

FIG. 1. The anomalous-diffusion exponent α as a function of the statistics index q, for one-, two-, and three-dimensional systems.

These results make evident a strong formal parallelism between the thermodynamical properties of ordinary diffusion as treated by means of the usual Boltzmann-Gibbs statistics, and those of anomalous diffusion with respect to the generalized statistical formulation. Such a parallelism suggests that TGSM is the natural statistical frame to deal with that transport process. Extending this conclusion to the physics of strongly interacting complex systems—which share with anomalous diffusion some bizarre features, such as the development of fractal structures—we can conjecture that TGSM can play a fundamental role in the description of a class of physical systems which are presently attracting increasing attention.

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