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Dynamic Approach to the Thermodynamics of Superdiffusion

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We address the problem of relating thermodynamics to mechanics in the case of microscopic dynamics without a finite time scale. The solution is obtained by expressing the Tsallis entropic index q as a function of the Lévy index α , and using dynamic rather than probabilistic arguments. [S0031-9007(99)09030-4]

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The problem of establishing a connection between dynamics and thermodynamics is still the object of wide interest among physicists. Recently rather than deriving Brownian diffusion from statistical mechanics, and consequently from thermodynamics, the inverse procedure was applied, of deriving Brownian motion from merely dynamic arguments [1,2]. It was also shown that this is equivalent to deriving thermodynamics from mechanics. However, this mechanical derivation of thermodynamics rests on the assumption that a finite microscopic time scale exists. In the past few years an increasing interest has been devoted to generalized forms of Brownian motion that are incompatible with the existence of a finite microscopic time scale, notably the processes of superdiffusion, and especially the Lévy diffusion [3–5]. We aim at unifying thermodynamics and mechanics without using the assumption of time scale separation, and in so doing we also aim at relating these two areas of research.

It is well known [6] that the anomalous diffusion processes, in the one-dimensional case, are characterized by probability distributions $p(x, t)$ whose Fourier transform in the symmetric case reads

$$\hat{p}(k, t) = \exp(-b|k|^\alpha t), \quad (1)$$

where α is the Lévy index ranging, in principle, in the interval $0 < \alpha < 2$, and b denotes the diffusion intensity. Note that according to the analysis of [7,8], the processes corresponding to the more restricted range

$$1 < \alpha < 2 \quad (2)$$

are compatible with dynamic derivations, including those of deterministic and Hamiltonian nature [9]. The work of Ref. [8] illustrates a dynamic derivation resting on a stationary correlation function of the microscopic fluctuation, $\Psi_W(t) \propto 1/t^\beta$ with $0 < \beta < 1$, namely, with an infinite time scale, thereby making it impossible to derive thermodynamics along the lines of Ref. [2]. Here we show that in spite of this limitation, these dynamics are not incompatible with thermodynamics, provided that a nonextensive rather than an extensive entropy is adopted.

Note that the diffusing system of Ref. [8] has a finite velocity with only two possible values, W and $-W$, corresponding to two distinct states of the system, and the time duration of these two states, t , is characterized by the probability distribution $\psi(t)$. The function $\psi(t)$, in turn, is proportional to the second time derivative of $\Psi_W(t)$ and, consequently, $\psi(t) \propto 1/t^{1+\alpha}$ with $1 < \alpha < 2$. A jump of a given length $|x|$, with probability density $\Pi(x)$, is not instantaneously made, but it takes place through a time interval proportional to the distance $|x|$ traveled by the particle. Consequently, the correlation function with an infinite lifetime $\Psi_W(t)$ results in $\Pi(x) \propto 1/|x|^{1+\alpha}$.

A crucial aspect of this dynamic approach is that the distribution is characterized by finite moments, in spite of the fact that the moments of the Lévy diffusion, from that of the second order on, are divergent. The apparent conflict between these dynamically derived diffusion processes and

the traditional Lévy processes is settled by noticing that the dynamic derivation implies the existence of a propagation front, characterized by ballistic peaks [10,11], and that the probability distribution of x between these peaks takes the shape of a truncated Lévy process. The shape of an ideal Lévy process is reached, instead, in the time asymptotic limit, as a consequence of the fact that the intensity of these peaks tends to zero, although very slowly.

It has to be pointed out that the historical foundation of the Lévy processes is probabilistic in nature [12]. We note that, according to the perspective established by Jaynes [13], there is a close connection between the second principle of thermodynamics and a probabilistic approach to statistical mechanics. This means that the thermodynamic foundation of the Lévy diffusion should be more natural than its dynamic foundation. On the contrary, as recently pointed out by a group of authors [14–16], the moment divergencies raise problems also to this thermodynamic foundation. These authors proved that if a proper use is made of the Tsallis entropy [17]

$$S_q[\Pi(x)] = -\frac{1 - \int_{-\infty}^{\infty} \Pi(x)^q dx}{(1 - q)}, \quad (3)$$

the challenge posed by the infinite moments can be successfully addressed, since the constraint on the moments is set using $\Pi(x)^q$ as a weighting function thereby ensuring convergence even where the standard weight would produce divergencies. Using this kind of weight, the Lévy process can be derived by means of the standard procedure of entropy maximization resting on the technique of Lagrange multipliers. Later on in this paper we shall give more details on this approach. For the time being, let us limit ourselves to noticing that the maximization of the nonextensive entropy of Eq. (3) led the authors of Refs. [14–16] to the conclusion that the entropic index q is related to α as follows:

$$q = \frac{3 + \alpha}{1 + \alpha}. \quad (4)$$

We are now forced to find a relation of the type of that of Eq. (4), using dynamic rather than probabilistic arguments. Our search is made easier by the recent results of Refs. [18–20]. In fact, these authors laid the foundation for the connection between the entropic index q and fractal dynamics. The Kolmogorov entropy, which is a sort of Gibbs entropy for unit time, is generalized [19] by expressing it in terms of the Tsallis entropy and is called K_q . This yields the generalization of the well-known Pesin identity [21] to

$$K_q = \lambda_q, \quad (5)$$

with λ_q playing the role of a generalized Lyapunov coefficient. This important result is obtained by studying the distance $\Delta y(t)$ between two trajectories departing from two distinct initial conditions, at the distance $\Delta y(0)$ the one

from the other, and assigning to $\delta(t) \equiv \lim_{|\Delta y(0)| \rightarrow 0} \left| \frac{\Delta y(t)}{\Delta y(0)} \right|$ the following form:

$$\delta(t) = [1 + (1 - q)\lambda_q t]^{1/(1-q)}. \quad (6)$$

It is evident that the traditional exponential sensitivity to the initial conditions is recovered from Eq. (6) by setting $q = 1$. Note that we adopt the symbol y to denote *microscopic* trajectories so as to avoid confusion with the *probabilistic* and *macroscopic* level of description, denoted by the symbol x .

In Refs. [7,8] it has been discussed how to derive superdiffusion on the basis of dynamic properties, with a procedure, valid also in the Hamiltonian case, which however recovers the results of the continuous random walk method of [10,11,22,23] when applied to the same dynamic systems. These dynamic systems are bimodal maps, with two laminar regions, derived from that of Geisel and Thomae [24]. With respect to the laboratory reference frame, the particles are characterized by the velocity W or $-W$, according to whether they move in the right or left laminar region. The analytical form of the map describing the motion in the left laminar region is given by [24]

$$y_{n+1} = y_n + ay_n^z, \quad (7)$$

with $a > 0$, $z > 1$. This map extends from $y = 0$ to $y = d$ with the parameter d defining the size of the laminar region. The right laminar region, with the same size d , is separated from the left by a chaotic layer and its analytical form is the same as that of Eq. (7) with y denoting in this case the distance from the right border of the map. The particles starting from an initial condition very close to $y = 0$ are assumed to be driven by the continuous time approximation to Eq. (7),

$$\frac{dy}{dt} = ay^z. \quad (8)$$

Thus it is possible to evaluate the distribution of waiting times in the interval $(0, d)$. The assumption that the trajectories are injected with uniform probability yields [24]

$$\psi(t) = d^{z-1} a [1 + d^{z-1} a (z-1)t]^{-z/(z-1)}. \quad (9)$$

The right laminar region yields for the corresponding waiting time distribution the same analytical form as that of Eq. (9). Note that the research work of Refs. [7,8,22] has established the connection between the index z and the Lévy index α to be given by

$$\alpha = \frac{1}{z-1}. \quad (10)$$

Note also that the value $z = 2$ is the border with the region where the first moment of $\psi(t)$ diverges and represents the limit of validity of the dynamic treatment [8]. For values of $z < 3/2$, on the contrary, the second moment of $\psi(t)$,

as well as the first, becomes convergent. Thus $z = 3/2$ is the border between the Lévy and the Gaussian region.

To assess the validity of the entropic prediction (6) we calculate $\delta(t)$ using the dynamics of Eq. (7) and we prove

$$\delta(t) = [1 - a(z - 1)y_0^{z-1}t]^{-z/(z-1)}, \quad (11)$$

where y_0 is the initial condition of one of the two trajectories under study. As done in [24], this initial condition is set so close to $y = 0$ as to make it possible to adopt the continuous time representation of Eq. (8). Furthermore the assumption is made that $|\Delta y_n/y_n| \ll 1$. Notice that d is finite ($d = 1/2$ in [11]). Thus the divergence of $\delta(t)$ of Eq. (11) occurs at times much larger than the escape time from the laminar region. By comparing Eq. (11) with the general property of Eq. (6), and using also Eq. (10), we obtain

$$q = \frac{2 + \alpha}{1 + \alpha} \quad (12)$$

and

$$\lambda_q = a \frac{\alpha + 1}{\alpha} y_0^{1/\alpha}. \quad (13)$$

This is an important result. However, to realize the main purpose of this paper, Eq. (12) must be made compatible with thermodynamics, in apparent conflict with the fact that it is seemingly at variance with Eq. (4), which results, in fact, from the adoption of thermodynamical arguments. As a matter of fact, to establish a connection between the dynamic and the thermodynamic approach in the same spirit as that leading all the current attempts at unifying dynamics and thermodynamics, we must move from the canonical condition of [1,2] to the microcanonical condition [25].

To prove this interesting conclusion, let us give details on the variational approach of [15]. Let us consider the functional form $F_q(\Pi)$ defined by

$$F_q(\Pi) \equiv \frac{1 - \int_{-\infty}^{\infty} \Pi(x)^q dx}{(1 - q)} - \beta \int_{-\infty}^{\infty} |x|^\nu \Pi(x)^q dx + \alpha \int_{-\infty}^{\infty} \Pi(x) dx. \quad (14)$$

This means that, according to the spirit of the technique of Lagrange multipliers, we plan to look for the entropy maximum under the constraint of keeping constant the ν -th moment, second term on the right-hand side (rhs) of Eq. (14), and the norm of the distribution $\Pi(x)$, third term on the rhs of Eq. (14). The authors of Refs. [14–16] made the choice $\nu = 2$. This choice was dictated by the fact that in their picture the diffusing particle undergoes a collision process at regular time intervals, of duration τ , making the velocity variable v fluctuate. Since $x = v\tau$, the constraint on the second moment of x is actually a constraint on the first moment of the energy distribution.

To establish a connection between entropic and dynamic arguments we are led to make a different choice. The space variable is made to change by the fluctuating velocity, which, as earlier pointed out, has only two possible values, W and $-W$. During the motion in a laminar region, corresponding to the map of Eq. (7), the velocity variable keeps the same value, either W or $-W$. Consequently the space x traveled is rigorously proportional to the time t spent in a given laminar region, and the transition probability $\Pi(x)$ is related to the waiting time distribution $\psi(t)$ by the crucial relation

$$\Pi(x) = \psi(x/W)/W. \quad (15)$$

This means that within the dynamic approach of this Letter, the constraint has to be established on the first moment of $\Pi(x)$, this being essentially a constraint on the mean time spent in a given laminar region. In other words, this physical condition implies $\nu = 1$.

By means of the entropy maximization, carried out by differentiating Eq. (14) with respect to Π , we get (A is a function of α and both Lagrange parameters are determined by the corresponding moment values)

$$\Pi(x) = \frac{A}{[1 + \beta(q - 1)|x|^\nu]^{1/(q-1)}}. \quad (16)$$

As argued by the authors of [16], we note that the Lévy diffusion process is obtained for $N \rightarrow \infty$ from $\Pi(x, N)$ defined as the N -fold convolution product $\Pi(x) * \Pi(x) * \dots * \Pi(x)$ [26]. We notice that it is not necessary to assume the point of view that a transition controlled by $\Pi(x)$ takes place at any time step. In the dynamic case of the intermittent map of Eq. (7), we can also follow a different approach. We define the mean waiting time in a laminar region, using as a weight the distribution $\psi(t)$. We call this time T and we assume it to be finite. This is possible only if $\alpha > 1$, and this is the reason why our dynamic approach is confined to the interval $1 < \alpha < 2$. Then we consider a time $t \gg T$. It is evident that for $t \rightarrow \infty$, the distribution $p(x, t)$ becomes very close to the N -fold convolution product $\Pi(x) * \Pi(x) * \dots * \Pi(x)$ with N given by the integer approximating the quantity t/T . As done by the authors of [16], we apply the Lévy-Gnedenko generalized central limit theorem [26] and we get a Lévy diffusion with the Lévy index α determined by the condition that the transition probability $\Pi(x)$ fulfills the asymptotic limit,

$$\lim_{t \rightarrow \infty} \Pi(x) \propto \frac{1}{|x|^{1+\alpha}}. \quad (17)$$

Comparing (17) to (16), we are led to

$$q = 1 + \frac{\nu}{1 + \alpha}. \quad (18)$$

Note that setting $\nu = 1$ we recover the result of the dynamic treatment of Eq. (12), while the choice $\nu = 2$

yields Eq. (4). As earlier pointed out, in the original work of [15], the assumption was made that the energy of the diffusing particle fluctuates as a result of the interaction with a bath. This physical condition corresponds to that of Ref. [27], a work based on the joint use of Tsallis generalized thermodynamics [17], and Nse-Hoover (NH) dynamics [28–31]. In the case of ordinary thermodynamics, the NH dynamics generates, with the minimum number of auxiliary equations, the canonical equilibrium distribution. The work of [27] applies the NH dynamics to the case of nonordinary statistical mechanics, so as to make energy fluctuate as in the picture adopted by Alemany and Zanette [14].

A final issue to discuss is now the thermodynamical significance of the generalized version of the Kolmogorov entropy, namely, the trajectory entropy. We note that the function $\delta(t)$ of Eq. (11) fits very well the corresponding prediction of Eq. (6). We have also seen that the function $\psi(t)$ of Eq. (9) agrees, through Eq. (15), with the maximization of the Tsallis entropy, namely, the distribution entropy. From the comparison of Eq. (9) with Eq. (11) we obtain

$$\psi(t) = \kappa \delta[-\sigma(y_0)t] \quad (t > 0), \quad (19)$$

with $\sigma(y_0) = d^{z-1}/y_0^{z-1}$ and $\kappa = ad^{z-1}$. A connection of this kind, between $\psi(t)$ and $\delta(t)$, with σ independent of y_0 , is expected on an intuitive ground. In fact, the lifetime of a laminar region is determined by the time making the distance between two trajectories, initially very close to one another, infinitely large and so exceeding the size of the laminar region. Note however that $\psi(t)$ is independent of y_0 and that $\delta(t)$ depends on it. This is not surprising, since K_q , as the conventional Kolmogorov entropy K_1 , is a trajectory property. To make K_q compatible with thermodynamics, a process forcing the single trajectory to lose its dependence on its initial condition should be considered. The adoption of the distribution entropy seems to be more appropriate, to establish a connection between dynamics and mechanics, as a consequence of the fact that it explicitly involves a statistical average over many distinct trajectories, in accordance with the fact that also the dynamic derivation of the function $\psi(t)$ is obtained [24] by making averages over the trajectories injected with uniform probability into a given laminar region. This explains why the function $\psi(t)$ can be successfully determined using the entropic argument, namely, from Eq. (16) through Eq. (15), with no dependence on the initial conditions.

We conclude noticing that the microcanonical treatment of this Letter implies [25] the mechanical energy to be kept fixed [32]. The condition with the mechanical energy fluctuating, even if this is realized according to nonstandard statistical mechanical prescriptions [15], is equivalent to introducing probabilistic arguments, into a picture that, in principle, should remain mechanical at any step. In the present treatment the adoption of a stochastic assumption is confined to the chaotic transition from one laminar re-

gion to the other, and it is made apparently unnecessary by the adoption of distributions rather than trajectories.

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mechanics. According to [2], the derivation of ordinary Brownian motion from dynamics is equivalent to the dynamical derivation of canonical equilibrium. The ordinary thermal baths of the conventional derivation of Brownian motion are replaced by dynamical systems, assumed to be in a microcanonical condition determined by strong-chaos properties. Jarzynski [1] adopts a theoretical perspective close to that of Ref. [2]. The dynamic approach to anomalous diffusion of Refs. [8,10,11] is compatible with this microcanonical condition, and the search for the dynamic derivation of the entropic index $q \neq 1$ illustrated in this Letter is inspired by the microcanonical perspective of [1] and [2] as well as by the recent theoretical developments of [18–20].

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