Extended phase-space dynamics for the generalized nonextensive thermostatistics

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We apply a variant of the Nosé thermostat to derive the Hamiltonian of a nonextensive system that is compatible with the canonical ensemble of the generalized thermostatistics of Tsallis. This microdynamical approach provides a deterministic connection between the generalized nonextensive entropy and power-law behavior. For the case of a simple one-dimensional harmonic oscillator, we confirm by numerical simulation of the dynamics that the distribution of energy H follows precisely the canonical q statistics for different values of the parameter q. The approach is further tested for classical many-particle systems by means of molecular dynamics simulations. The results indicate that the intrinsic nonlinear features of the nonextensive formalism are capable of generating energy fluctuations that obey anomalous probability laws. For $q<1$ a broad distribution of energy is observed, while for $q>1$ the resulting distribution is confined to a compact support.

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I. INTRODUCTION

Since the pioneering work of Tsallis in 1988 [1], where a nonextensive generalization of the Boltzmann-Gibbs (BG) formalism for statistical mechanics has been proposed, intensive research [2] has been dedicated to develop the conceptual framework behind this new thermodynamical approach and to apply it to realistic physical systems. In order to justify the generalization of Tsallis, it has been frequently argued that the BG statistical mechanics has a domain of applicability restricted to systems with short-range interactions and non(multi)fractal boundary conditions [3]. Moreover, it has been recalled that anomalies displayed by mesoscopic dissipative systems and strongly non-Markovian processes represent clear evidence of the departure from BG thermostatistics. These types of arguments have been duly reinforced by recent convincing examples of physical systems that are far better described in terms of the generalized formalism than in the usual context of the BG thermodynamics (see [3] and references therein). It thus became evident that the intrinsic nonlinear features present in the Tsallis formalism, which lead naturally to power laws, represent powerful ingredients for the description of complex systems.

In the majority of studies dealing with the thermostatistics of Tsallis, the starting point is the expression for the generalized entropy S_q,

$$S_q=\frac{k}{q-1}\left\{1-\int [f(x)]^q dx\right\}, \tag{1}$$

where k is a positive constant, q a parameter, and f is the probability distribution. Under a different framework, some interesting studies [4] have shown that the parameter q can be somehow linked to the system sensibility on initial conditions. Few works have been committed to substantiate the form of entropy (1) in physical systems based entirely on first principles [5,6]. For example, it has been demonstrated that it is possible to develop dynamical thermostat schemes, which are compatible with the generalized canonical ensemble [7]. In a recent study by one of us [8], a derivation of the generalized canonical distribution is presented from first principle statistical mechanics. As a consequence, it is shown that the particular features of a macroscopic subunit of the canonical system, namely, the heat bath, determines the nonextensive signature of its thermostatistics and, therefore, its power law behavior. More precisely, it is exactly demonstrated in [8] that if one specifies the capacity of the heat bath as

$$\frac{dE}{d(1/\beta)}\propto\frac{1}{q-1}, \tag{2}$$

where q is a constant, $1/\beta\propto kT$, and T is the temperature, the generalized canonical distribution maximizing Eq. (1) for the Hamiltonian H of the system is recovered,

$$f(H)\propto[1+\beta(q-1)(E-H)]^{1/(q-1)}. \tag{3}$$

Here, E is a conserved quantity and denotes the energy of the extended system (system+heat bath). Equation (2) provides a very simple but meaningful connection between the generalized q statistics and the thermodynamics of nonextensive systems. It is analogous to state that, if the condition of an infinite heat bath capacity is violated, the resulting canonical distribution can no longer be of the exponential form and, therefore, should not follow the traditional BG thermostatistics. In the present study, we will show how the conjecture proposed in [8] can be used to develop a variant of the original Nosé thermostat [9] that is consistent with the q thermostatistics. We will then validate the technique by applying it to the cases of a simple harmonic oscillator and a classical many-particle system.

II. THE GENERALIZED EXTENDED SYSTEM

We consider a system of N particles having coordinates x_i', masses m_i and potential energy $\Phi(x')$. As in the extended system method originally proposed by Nosé, here we also introduce an additional degree of freedom through a variable s, which will play the role of an external heat bath, acting to keep the average of the kinetic energy at a constant value. In practice, this is achieved by simply rescaling the *real* variables in terms of a new set of *virtual* variables

$$\mathbf{x}_i' = \mathbf{x}_i, \quad \mathbf{p}_i' = \frac{\mathbf{p}_i}{s^{\lambda}}, \quad p_s' = \frac{p_s}{s^{\lambda}}, \quad t' = \int \frac{dt}{s}, \tag{4}$$

where λ is a rescaling exponent, and $(\mathbf{x}_i', \mathbf{p}_i', t')$ and $(\mathbf{x}_i, \mathbf{p}_i, t)$ are the real and virtual coordinates, momenta, and time, respectively. At this point, we postulate that a generalized Hamiltonian for the extended system can be written as

$$H_q(\mathbf{x}, \mathbf{p}, p_s, s) = \sum_{i=1} \frac{\mathbf{p}_i^2}{2 m_i s^{2\lambda}} + \Phi(\mathbf{x}) + \frac{p_s^2}{2Q} + \frac{1}{\alpha} \frac{s^{\gamma} - 1}{\gamma}, \tag{5}$$

where the first two terms on the right side represent the energy of the physical system that is free to fluctuate [10]. The virtual variable p_s also has a real counterpart, $p_s' = p_s / s^{\lambda}$, and has been introduced to allow for a dynamical description of the variable s. More precisely, the third term $p_s^2/2Q$ corresponds to the kinetic energy of the heat bath and the parameter Q is an inertial factor associated with the motion of the variable s. The last term of the Hamiltonian (5) is a power-law potential in s with α and γ as parameters. As we show next, it provides the essential link between the concept of extended phase-space dynamics and the generalized canonical ensemble.

We start by considering the quasiergodic hypothesis and writing the time average of a given quantity (in the virtual time scale) $A(\mathbf{x}, \mathbf{p})$ as

$$\overline{A} = \frac{1}{Z} \int \int \int \int d\mathbf{x}\, d\mathbf{p}\, dp_s\, ds\, A\, \delta(H_q - E) \tag{6}$$

with

$$Z = \int \int \int \int d\mathbf{x}\, d\mathbf{p}\, dp_s\, ds\, \delta(H_q - E),$$

where Z is analogous to a microcanonical normalization factor for the generalized Hamiltonian (5). Transforming the virtual momenta $\mathbf{p}$ and coordinates $\mathbf{x}$ back to real variables, changing the order of integration and rewriting the volume element as $d\mathbf{x} d\mathbf{p} = s^{g\lambda} d\mathbf{x}' d\mathbf{p}'$, where g is the number of degrees of freedom, we obtain

$$\overline{A} = \frac{1}{Z} \int \int d\mathbf{x}' d\mathbf{p}' A \int \int dp_s\, ds\, s^{g\lambda} \delta(H_q - E). \tag{7}$$

If we now make use of the property of the δ function, $\delta(h(s)) = \delta(s - s_0)/h'(s_0)$, where s_0 is the zero of h, it follows that

$$\overline{A} = \frac{1}{Z} \int \int d\mathbf{x}' d\mathbf{p}' A \int dp_s \alpha \times \left[1 + \alpha\gamma \left(E - H - \frac{p_s^2}{2Q} \right) \right]^{(g\lambda + 1)/\gamma - 1}, \tag{8}$$

where,

$$H = H(\mathbf{x}', \mathbf{p}') = \sum_{i=1} \frac{\mathbf{p}_i'^2}{2 m_i} + \Phi(\mathbf{x}'). \tag{9}$$

By integration with respect to p_s we get

$$\overline{A} = \frac{1}{Z} \left(\frac{\alpha Q}{2\gamma} \right)^{1/2} B\left(\frac{1}{2}, \frac{g\lambda + 1}{\gamma} \right) \int \int d\mathbf{x}' d\mathbf{p}' A \times [1 + \alpha\gamma(E - H)]^{(g\lambda + 1)/\gamma - 1/2}, \tag{10}$$

where B is the beta function, $B(z, w) = \int_0^1 t^{z-1}(1-t)^{w-1} dt$. Finally, if we define

$$\alpha \equiv \frac{\beta(q+1)}{2(g\lambda + 1)} \quad \text{and} \quad \gamma \equiv 2(g\lambda + 1) \frac{q-1}{q+1}, \tag{11}$$

the generalized canonical average is recovered,

$$\overline{A} = \frac{1}{Z'} \int \int d\mathbf{x}' d\mathbf{p}' A [1 + \beta(q-1)(E - H)]^{1/(q-1)}$$

with

$$Z' = \int \int d\mathbf{x}' d\mathbf{p}' [1 + \beta(q-1)(E - H)]^{1/(q-1)}, \tag{12}$$

and we have thus proved that, under conservation of the extended Hamiltonian Eq. (5), the fluctuations in the energy $H(\mathbf{x}', \mathbf{p}')$ of the physical system should be consistent with the canonical formulation of the nonextensive q thermostatistics [11,12]. To obtain the time average in the real time scale, it is necessary to replace everywhere $g\lambda$ by $(g\lambda - 1)$ [9].

III. RESULTS AND DISCUSSION

It is possible to confirm the validity of this approach with a simple realization of the generalized thermostat scheme. We consider an extended system composed of a single one-dimensional harmonic oscillator coupled to a heat bath whose thermal capacity obeys essentially Eq. (2). From Eq. (5), such a system can be described by the following extended Hamiltonian:

$$H_q(x, p, p_s, s) = \frac{p^2}{2 s^{2\lambda}} + \frac{x^2}{2} + \frac{p_s^2}{2Q} + \frac{1}{\alpha} \frac{s^{\gamma} - 1}{\gamma}. \tag{13}$$

Here $m = 1$ for simplicity and we choose to set $\lambda = 2$ because the nonlinear dynamics for this case when $q = 1$ (i.e., for the BG thermostatistics) has been shown to be sufficiently chaotic to generate average properties of the canonical ensemble [13]. From Eq. (13) and the scaling relations (4), we obtain the equations of motion for the extended system in the real phase space

$$\frac{dx'}{dt'} = \frac{p'}{s},$$

$$\frac{dp'}{dt'} = -\frac{x'}{s} - \frac{2 s^2 p_s' p'}{Q},$$

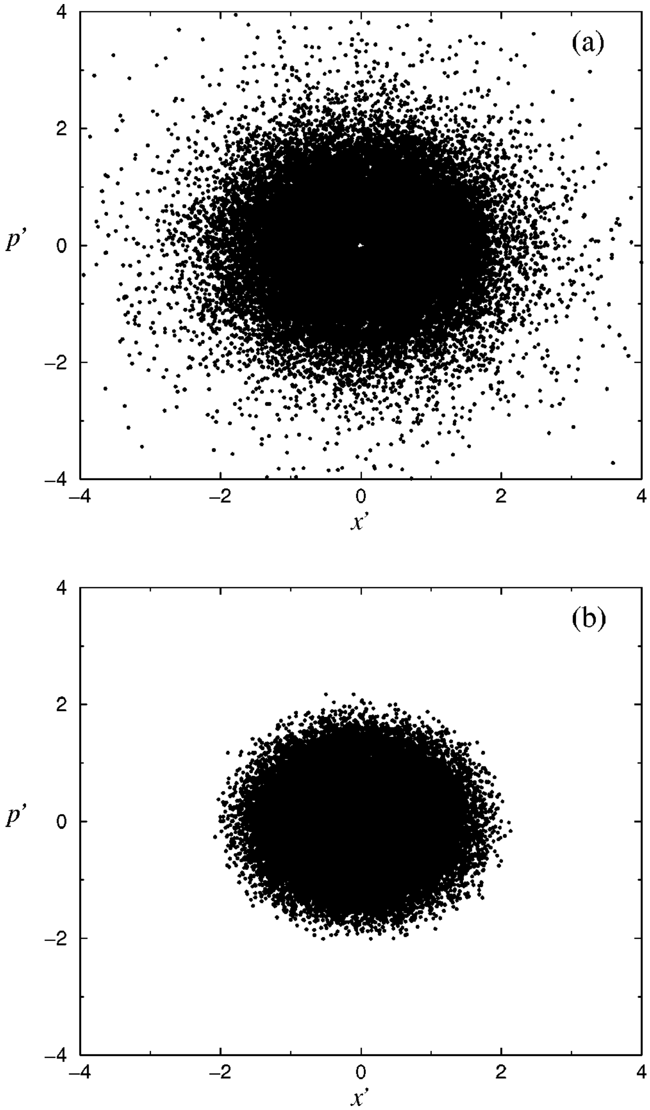

FIG. 1. (a) Density plot of the harmonic oscillator dynamics subjected to the generalized thermostat scheme for $q=0.8$. The initial conditions are $[x'(0)=0.5, p'(0)=0.5, s(0)=1.0, p_s'(0)=0.0]$ and the thermostat parameters have been set to $\alpha=1.0$ and $Q=1.0$. (b) Same as (a) but for $q=1.2$.

$$\frac{ds'}{dt'}=\frac{s^3 p_s'}{Q},$$

$$\frac{dp_s'}{dt'}=\frac{1}{s^2}\left(2p'^2-\frac{1}{\alpha}s^{\gamma}\right)-\frac{2s^2 p_s'^2}{Q}. \tag{14}$$

A fifth-order Runge-Kutta subroutine is then used to numerically solve this set of nonlinear differential equations. To ensure the conservation of energy H_q and the stability of integration, all runs have been performed with 10^8 time steps of $\Delta t'=10^{-4}$ each. The density maps shown in Figs. 1(a) and 1(b) for $q=0.8$ and 1.2, respectively, provide clear evidence that the dynamics of both systems fills space. For $q>1$ [see Fig. 1(b)], the accessible phase space lies in a compact set, whereas the phase-space support for $q<1$ [see Fig. 1(a)] is infinite. The former situation is compatible with the necessary cutoff condition on energy for $q>1$ [3]. In Fig. 2 we show the logarithmic plot of the distributions of the transformed variable $\chi=1+\beta(q-1)(E-H)$, where $H=p'^2/2+x'^2/2$, for three different values of the parameter $\gamma=4(q-1)/(q+1)$ corresponding to $q=0.7$, 0.8, and 0.9. Indeed, we observe in all cases that the fluctuations in χ follow very closely the prescribed power-law behavior, $\rho(\chi)\propto\chi^{1/(q-1)}$, and therefore confirm the validity of our dynamical approach to the generalized canonical ensemble. As shown in Fig. 3, the simulations performed for $q>1$ are also compatible with

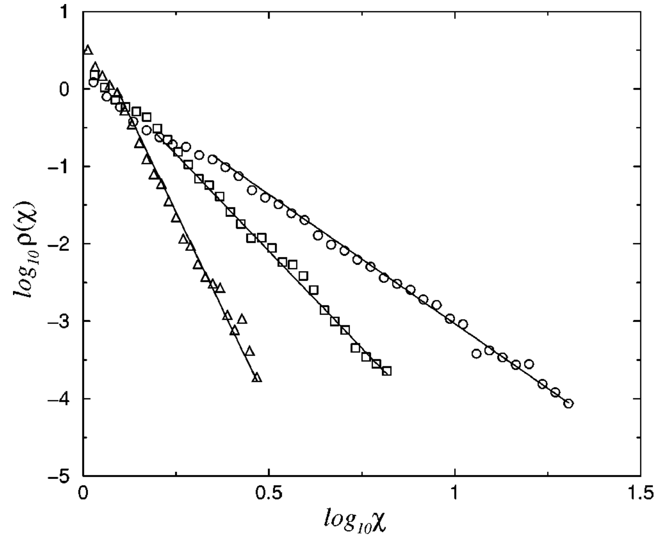

FIG. 2. Logarithmic plot of the distributions of the transformed variable χ for $q=0.7$ (circles), 0.8 (squares), and 0.9 (triangles). From right to left, the three straight lines with slopes -3.33, -5.0, and -10.0 correspond to the expected power-law behavior $\rho(\chi)\propto\chi^{1/(q-1)}$.

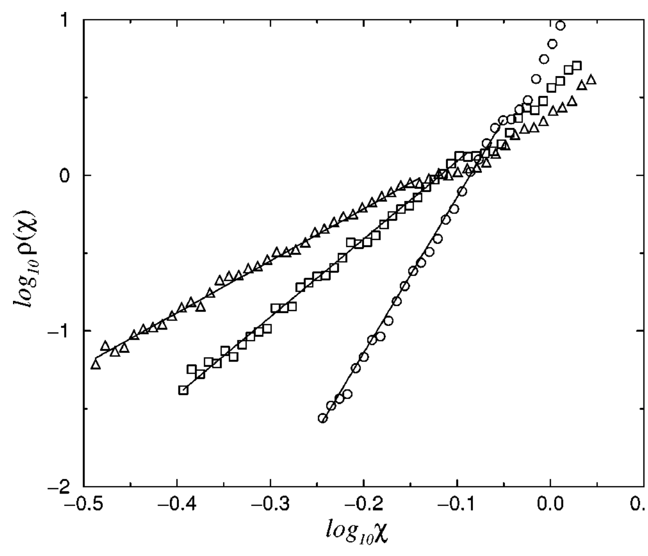

FIG. 3. Logarithmic plot of the distributions of the transformed variable χ for $q=1.1$ (circles), 1.2 (squares), and 1.3 (triangles). From right to left, the three straight lines with slopes 10.0, 5.0, and 3.33 correspond to the expected power-law behavior $\rho(\chi)\propto\chi^{1/(q-1)}$.

the expected scaling behavior. However, instead of the long-range tail obtained for the case $q<1$, a rather unusual power law with positive exponent is observed.

Now we focus on a more complex application of the thermostat scheme introduced here. The basic idea is to simulate, through molecular dynamics (MD), the nonextensive behavior of a classical many-particle system. For completeness, we start by rewriting the expression for the extended Hamiltonian (5) in terms of the usual q-thermostatistics parameters (i.e., q and β),

$$H_q(\mathbf{x},\mathbf{p},p_s,s)=\sum_{i=1} \frac{p_i^2}{2m_i s^{2\lambda}}+\Phi(\mathbf{x})+\frac{\mathbf{p}_s^2}{2Q} + \frac{1}{\beta}\ln_q(s^{[2(g\lambda+1)/(q+1)]}), \tag{15}$$

where $\ln_q(s)\equiv(s^{q-1}-1)/(q-1)$ [3]. From Eq. (15), it is then possible to derive the equations of motion for any value of q and any type of effective potential of interaction. We consider a cell containing 108 identical particles that interact through the Lennard-Jones potential, $\Phi(\Delta x_{ij}) =4\epsilon[(\sigma/\Delta x_{ij})^{12}-(\sigma/\Delta x_{ij})^6]$, where Δx_{ij} is the distance between particles i and j, ϵ is the minimum energy, and σ the zero of the potential. The distance, energy, and time are measured in units of σ, ϵ, and $(m\sigma)^2/\epsilon$, respectively, and the equations of motion are numerically integrated using a predictor-corrector algorithm [14]. In all the simulations we performed, the relative fluctuation around the average of the total energy of the system has always been smaller than 10^{-6}.

Compared to the previous example of a single harmonic oscillator, the complexity of the many-particle system hinders a quantitative prediction of the statistical behavior of its energy fluctuations. Because the exact form or even a plausible approximation of the density of states $\Omega(H)$ is difficult to obtain in this case, we restrict ourselves to the qualitative analysis of the resulting energy distribution $\rho(H) \propto\Omega(H)f(H)$. Furthermore, we performed additional simulation tests with different number of particles and physical conditions to confirm that the MD system is always led to unstable trajectories in phase space whenever the value of q is set to be smaller than a given threshold $q_{\min}$. In spite of these limitations, however, the results shown in Fig. 4 clearly indicate the tendency for a broader distribution of energy when $q<1$ (we set q to be slightly larger than $q_{\min}$ ≈0.9940 in this case). For $q>1$, on the other hand, the resulting distribution of energy is notably more confined than the Gaussian-like distribution obtained for $q=1$ (see Fig. 4).

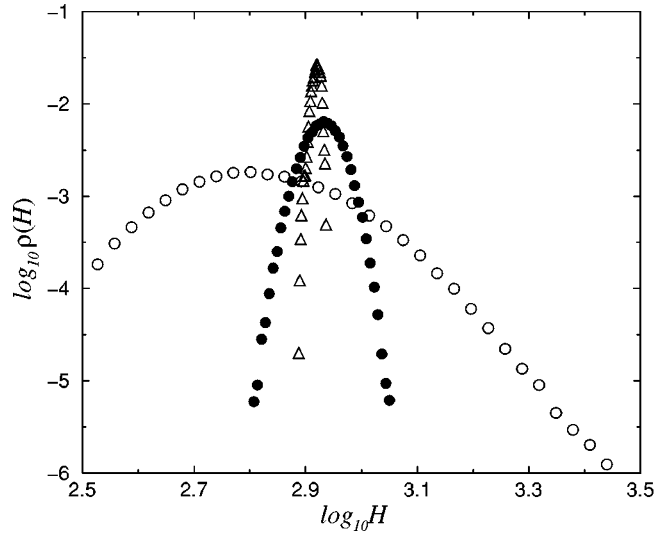

FIG. 4. Logarithmic plot of the energy distributions for $q=0.9941$ (circles), 1.0 (full circles), and 1.1 (triangles). In all three cases, the MD simulations have been performed with 108 particles, $\beta=0.2$, and a density of 0.1 particles/σ^3.

IV. CONCLUSION

In summary, we have shown that the essential features of the generalized canonical distribution can be captured with a proper extension of the standard Nosé thermostat. To the best of our knowledge, this is the first time that a Hamiltonian approach to the nonextensive q thermostatistics leads explicitly to the observation of a power-law behavior $(q<1)$. We thus believe that the microdynamical formalism presented in this work can provide a deterministic link between the generalized entropy conjecture Eq. (1) and the concept of Lévy flights [7,15]. Finally, the methodology introduced here is flexible enough to accommodate the description of other nonextensive systems of physical significance.

ACKNOWLEDGMENT

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