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A Dynamical Thermostatting Approach to Nonextensive Canonical Ensembles

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We treat Tsallis generalized nonextensive thermostatistics through the method developed by Kusnezov, Bulgac, and Bauer (1990) to simulate the canonical ensemble. Given a Hamiltonian system with a $2N$-dimensional phase space, the introduction of two additional dynamical variables allows us to mimic the coupling of the original system to a thermal bath, yielding ergodic behavior. In this way, ensemble averages within the generalized nonextensive canonical ensemble can be obtained as temporal mean values evaluated on a trajectory of the extended dynamical system. We illustrate these ideas with some 1D and 2D examples.
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1. INTRODUCTION

Increasing attention is being devoted to a new development in statistical physics generalizing Boltzmann–Gibbs (BG) thermostatistics. This generalization, based upon the Tsallis entropy functional [3], was introduced in order to deal with systems where non-extensivity plays an important rôle and, therefore, the standard BG treatment fails. The new formalism has been shown to either preserve or suitably generalize the relevant properties of the BG statistics [4–9] and a huge number of interesting physical applications has already been worked out [10–26]. Since classical many body systems are concerned, it is of interest to explore numerical methods to evaluate the thermodynamical properties of these systems.

Recently, Kusnezov *et al.* (KBB) [1, 2] introduced a procedure for computing thermodynamic properties of $2N$-dimensional classical systems governed by a Hamiltonian.

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The method consists in extending by two the phase space dimension, in order to mimic the coupling of the original system to the infinite degrees of freedom of a heat bath. KBB obtained a stationary solution of the Liouville equation for the enlarged dynamical system. The projection of this probability distribution onto the original $2N$-dimensional phase space coincides with the Gibbs canonical distribution. If the trajectories are truly ergodic in the extended phase space, averages within the canonical ensemble may be replaced by time averages, which are computed by simply following the time evolution of the system for some time interval.

It is the aim of the present work to adapt the KBB method for the simulation of the generalized nonextensive canonical ensemble. Following KBB, given a Hamiltonian system, we extend its phase space dimension by two, in order to simulate the coupling to a thermal bath. For different values of the parameter q that characterizes the statistics of the nonextensive system and for various potentials, we show that, with an appropriate coupling scheme, good agreement can be obtained between thermal distributions evaluated along an orbit of the expanded system and those resulting from the generalized canonical ensemble associated with the original Hamiltonian system.

The KBB method was developed as an alternative to the Monte Carlo approach [1, 2]. The application of the dynamical thermostatting procedure to nonextensive thermostatistics may play the same rôle within this generalized context.

2. NONEXTENSIVE THERMOSTATISTICS

Boltzmann–Gibbs (BG) thermostatistics is unable to satisfactorily describe systems where extensivity does not hold such as those with a fractal space-time structure or where interactions or microscopic memory are long-range. Then, the BG formalism fails in describing, for instance, self-gravitating systems [27, 28], Lévy-like diffusion [29] or two dimensional turbulence [16] (see reference [29] for a more complete list).

Recently, Tsallis [3] introduced a new entropy functional that has attracted great interest in statistical physics and related fields. It has been the basis of an entire generalization of Jaynes' information theoretical approach to statistical mechanics [4, 5]. This new statistical formalism has been shown to have many elegant mathematical properties [6–9] and interesting physical applications. Among the latter, we find the statistical mechanics principles for Lévy-flights [10, 11] and for the ubiquity of Lévy distributions in nature [12]. The generalized statistics also provides a method for generating exact time dependent solutions of correlated anomalous diffusion equations [13, 14]. The formalism offers, as well, a description of the meta-equilibrium state of the two-dimensional Euler-like turbulence of electron plasma [15–17]. Non-extensive statistical mechanics appears to be a useful tool in the description of self-gravitating systems [18, 19], that has inspired, in turn, a possible solution to the solar neutrino problem [20]. Interesting cosmological aspects of Tsallis statistics have been recently addresed [21]. The formalism has also been applied to the study of self organization in biological systems [22]. Furthermore, Tsallis entropy was employed to improve the simulated annealing and other optimization procedures [23–26].

The generalized entropy, S_q, is defined as

$$S_q = \frac{k}{q-1} \int (f(\mathbf{x}, \mathbf{p}) - [f(\mathbf{x}, \mathbf{p})]^q) \, d\Omega, \tag{1}$$

where k is a positive constant (from here on, we will take $k=1$), q is a real parameter related to the degree of non-extensivity and $f(\mathbf{x}, \mathbf{p})$ stands for a probability distribution in phase space fulfilling the appropriate normalization condition

$$\int f(\mathbf{x}, \mathbf{p}) \, d\Omega = 1. \tag{2}$$

Note that in the limit $q \to 1$, S_q tends to the standard logarithmic entropy $-\int f \ln f \, d\Omega$. S_q possesses the usual properties of non-negativity, equiprobability, concavity and irreversibility, but, it is non-additive for $q \neq 1$.

By defining q-generalized mean values of any dynamical quantity $A(\mathbf{x}, \mathbf{p})$

$$\langle A \rangle_q = \int [f(\mathbf{x}, \mathbf{p})]^q \, A(\mathbf{x}, \mathbf{p}) \, d\Omega, \tag{3}$$

it can be shown that the entire Legendre transform connection between statistical mechanics and thermodynamics is q-invariant [4, 5, 30].

In the framework of the information theory approach to statistical mechanics we assume that partial prior information about the system is given by the q-generalized mean values $(\langle A_i \rangle_q, i = 1, ...M)$ of M relevant quantities. We can then construct a MaxEnt distribution f_q^{ME} that maximizes the entropy functional (1), subject to the constraints imposed by the M generalized mean values plus the normalization prescription. The solution of this variational problem is given by the Tsallis MaxEnt [5] probability distribution

$$f_q^{ME}(\mathbf{x}, \mathbf{p}) = \frac{1}{Z_q} \left[1 - (1-q) \sum_{i=1}^{M} \lambda_i A_i(\mathbf{x}, \mathbf{p}) \right]^{1/(1-q)}, \tag{4}$$

where the generalized partition function Z_q is

$$Z_q = \int \left[1 - (1-q) \sum_{i=1}^{M} \lambda_i A_i(\mathbf{x}, \mathbf{p}) \right]^{1/(1-q)} d\Omega \tag{5}$$

and λ_i is the Lagrange multiplier associated to the constraint imposed by the value $\langle A_i \rangle_q$. It is convenient to introduce the q-generalization of $\ln Z$

$$\lambda_0 = \frac{Z_q^{1-q} - 1}{1-q}. \tag{6}$$

The generalized entropy S_q, the mean values $\langle A_i \rangle_q$, the parameter λ_0 and the Lagrange multipliers λ_i, all satisfy the usual thermodynamical (Legendre transform) relations [5]

$$S_q = \lambda_0 + \sum_{i=1}^{M} \lambda_i \langle A_i \rangle_q, \tag{7}$$

$$\frac{\partial \lambda_0}{\partial \lambda_i} = -\langle A_i \rangle_q \quad (i = 1, ..., M), \tag{8}$$

and

$$\frac{\partial S_q}{\partial \langle A_i \rangle_q} = \lambda_i, \quad (i = 1, ..., M). \tag{9}$$

In the particular case when the only relevant information is provided by the generalized mean value of the Hamiltonian, one obtains the q-generalization of the standard Gibbs canonical ensemble [4]. The corresponding MaxEnt probability distribution reads

$$f_q^{ME}(\mathbf{x}, \mathbf{p}) = \frac{1}{Z_q} \left[1 - \frac{1-q}{T} H(\mathbf{x}, \mathbf{p}) \right]^{1/(1-q)}, \tag{10}$$

where the generalized partition function Z_q is

$$Z_q = \int \left[1 - \frac{1-q}{T} H(\mathbf{x}, \mathbf{p}) \right]^{1/(1-q)} d\Omega. \tag{11}$$

In this case, the parameter λ_0 is related to the generalized free energy by $F_q = -T\lambda_0$.

When parameter q lies in the range $q < 1$, we must require that the concomitant probability distribution vanish if

$$H < H_c = \frac{T}{(1-q)}, \tag{12}$$

the so called Tsallis cut-off condition.

At this point, it is opportune to make some comments with regard to the unusual kind of generalized nonlinar mean values (3). The main original motivation for introducing these expectation values was to preserve, within the generalized thermostatistics, the Legendre transform structure existing between the Lagrange multipliers and the relevant mean values. This Legendre structure provides, within Jaynes approach to statistical mechanics, the connection with thermodynamics. However, a clear physical interpretation for the generalized mean values is still lacking. Particularly problematic is how, by recourse to some kind of ergodic hypothesis, these generalized mean values can be related to time averages. Despite these difficulties, *there is plenty of evidence that Tsallis generalized canonical distribution appears in many physical scenarios such as Lévy flights, plasma physics, astrophysical self-gravitating systems and cosmology. Moreover, Tsallis distributions proved to be very useful in optimization problems.* With the exception of Lévy flights, the generalized mean values do not play a fundamental rôle in any of these applications. In the case of Lévy flights and Lévy distributions, the relevant linear mean values diverge, while the generalized ones are well defined. Hence, they constitute good quantities in order to characterize Lévy distributions. However, it is not clear that they admit a physical interpretation. Moreover, one of us recently proved that there are other kinds of mean values that preserve the Legendre structure [31]. In particular, the usual linear ones.

In the present work, we will not address this "mean value issue". Given the fact that Tsallis distributions seem to be quite useful in many physical problems, we will try to answer just the following question: Are Tsallis distributions compatible with the dynamical thermostatting approach? It is worth mentioning that ours constitute the first attempt to obtain Tsallis distributions, in a direct fashion, from the detailed behaviour of a particular dynamical system (in our approach, a Hamiltonian system interacting with a thermostat). We think that this line of research might eventually be useful in order to clarify some aspects of Tsallis formalism.

3. KBB METHOD

According to the KBB formulation, the Hamilton equations of motion are coupled to a heat bath as follows

$$\begin{aligned} \dot{x}_i &= \frac{\partial H}{\partial p_i} - h_2(\xi)\, F_i(\mathbf{x}, \mathbf{p}), \\ \dot{p}_i &= -\frac{\partial H}{\partial x_i} - h_1(\zeta)\, G_i(\mathbf{x}, \mathbf{p}) \quad (i = 1, ..., N), \end{aligned} \tag{13}$$

where $\boldsymbol{x} = (x_1, ..., x_N)$ and $\mathbf{p} = (p_1, ..., p_N)$ stand for the N canonical coordinates and their conjugate momenta, respectively. The new variables ζ and ξ represent the heat bath and the functions h_1, h_2, F_i and G_i characterize the coupling to the thermal bath. KBB chose the form

$$\mathcal{F}(\mathbf{x}, \mathbf{p}, \zeta, \xi) = \mathcal{N} \exp\left(-\frac{1}{T}\left[H(\mathbf{x}, \mathbf{p}) + \frac{1}{\alpha} g_1(\zeta) + \frac{1}{\beta} g_2(\xi) \right]\right) \tag{14}$$

(α and β are free parameters; $\mathcal{N}$ is a normalization constant) for the stationary solution to the (extended) Liouville equation

$$\frac{\partial \mathcal{F}}{\partial t}+\sum_{i=1}^{N}\left\{\frac{\partial(\mathcal{F}\dot{x}_i)}{\partial x_i}+\frac{\partial(\mathcal{F}\dot{p}_i)}{\partial p_i}\right\}+\frac{\partial(\mathcal{F}\dot{\zeta})}{\partial \zeta}+\frac{\partial(\mathcal{F}\dot{\xi})}{\partial \xi}=0. \tag{15}$$

Assuming that

$$\frac{\partial \dot{\zeta}}{\partial \zeta}=0 \qquad \text{and} \qquad \frac{\partial \dot{\xi}}{\partial \xi}=0, \tag{16}$$

the requirement that the distribution given by Eq. (14) be a time independent solution of the Liouville equation (15) is fulfilled if the heat bath variables evolve according to [1]

$$\dot{\zeta}=\alpha\sum_i\left\{G_i\frac{\partial H}{\partial p_i}-T\frac{\partial G_i}{\partial p_i}\right\}, \tag{17}$$

$$\dot{\xi}=\beta\sum_i\left\{F_i\frac{\partial H}{\partial x_i}-T\frac{\partial F_i}{\partial x_i}\right\} \quad (i=1, ..., N), \tag{17}$$

and, self-consistently with Eqs. (16), the following relations hold

$$h_1=\frac{dg_1}{d\zeta}, \qquad h_2=\frac{dg_2}{d\xi}. \tag{18}$$

KBB showed that for a suitable choice of coupling functions and parameters α and β, the extended dynamical system may exhibit ergodic behavior. In that case, thermal distributions obtained from the time evolution of the extended dynamical system are in good agreement with canonical ensemble distributions, as exemplified for several 1D and 2D Hamiltonian systems. Kusnesov and Bulgac have extended this method to constrained dynamical systems [32] and also developed, along similar lines, a deterministic and time reversal invariant description of Brownian motion (i.e., normal diffusion) [33].

The KBB method was inspired on the pioneer work of Nosé, who first discovered a dynamics consistent with Gibbs canonical ensemble [34–36]. The main difference between KBB and Nosé approaches is that the former extends the phase space dimension by two instead of only one as the latter does. Nose's dynamical approach to the canonical ensemble was further developed in many directions. Hoover clarified several aspects of Nose's approach by introducing a simpler, but equivalent, set of differential equations for the enlarged system [37]. Jellinek and Berry [38–40] considered, under quite general assumptions, Hamiltonian extensions of the equations of motion yielding the canonical ensemble. Also, Evans and Holian [41] extended the thermostatting approach to situations far from thermodynamical equilibrium (see ref. [42] for a complete list of references on previous work in this field).

4. GENERALIZED DYNAMICAL THERMOSTATTING SCHEME

We will show that adopting the following form for the coupling with the heat bath

$$\dot{x}_i = \frac{\partial H}{\partial p_i} - h_2(\xi)\left[1 - \frac{1-q}{T}H\right] F_i(\mathbf{x}, \mathbf{p}), \tag{19}$$

$$\dot{p}_i = -\frac{\partial H}{\partial x_i} - h_1(\zeta)\left[1 - \frac{1-q}{T}H\right] G_i(\mathbf{x}, \mathbf{p}) \quad (i = 1, ..., N), \tag{19}$$

the concomitant Liouville equation admits as stationary solutions distributions of the form

$$\mathscr{F}_q(\mathbf{x}, \mathbf{p}, \zeta, \xi) = \mathscr{N}\left[1 - \frac{1-q}{T}H\right]^{1/(1-q)} \exp\left(-\frac{1}{T}\left[\frac{1}{\alpha}g_1(\zeta) + \frac{1}{\beta}g_2(\xi)\right]\right). \tag{20}$$

Since we are interested in reproducing the generalized canonical ensemble for the physically relevant dynamical variables $(\mathbf{x}, \mathbf{p})$ and a detailed physical interpretation of the thermal variables is still lacking (even for $q = 1$), the exponential dependence of $\mathscr{F}_q$ on the heat bath variables was preserved.

By substitution of the equations of motion (19) and the distribution (20) into the time independent form of the Liouville equation (15), we get

$$\frac{2-q}{T}\sum_i \left\{h_2 F_i \frac{\partial H}{\partial x_i} + h_1 G_i \frac{\partial H}{\partial p_i}\right\} - \left[1 - \frac{1-q}{T}H\right]\sum_i \left\{h_2 \frac{\partial F_i}{\partial x_i} + h_1 \frac{\partial G_i}{\partial p_i}\right\}$$
$$+ \frac{\partial \dot{\zeta}}{\partial \zeta} + \frac{\partial \dot{\xi}}{\partial \xi} - \frac{\dot{\zeta}}{T\alpha}\frac{dg_1}{d\zeta} - \frac{\dot{\xi}}{T\beta}\frac{dg_2}{d\xi} = 0. \tag{21}$$

Following KBB, we impose that Eqs. (16) hold. Again, analogously as in the case $q = 1$ (BG), Eq. (21) is satisfied when Eqs. (18) hold and the heat bath variables evolve according to

$$\dot{\zeta} = \alpha\left\{(2-q)\sum_i G_i \frac{\partial H}{\partial p_i} - T\left[1 - \frac{1-q}{T}H\right]\sum_i \frac{\partial G_i}{\partial p_i}\right\},$$
$$\dot{\xi} = \beta\left\{(2-q)\sum_i F_i \frac{\partial H}{\partial x_i} - T\left[1 - \frac{1-q}{T}H\right]\sum_i \frac{\partial F_i}{\partial x_i}\right\} \quad (i = 1, ..., N). \tag{22}$$

Thus, the full set of $2N + 2$ differential equations for the extended system (Eqs. (19) and (22)) has been obtained.

Equations (19) were cast in a way that explicitly puts into evidence the dependence on parameter q. A cursory glance at Eqs. (19) may suggest that our new dynamical system is equivalent to the KBB one, arising just from a redefinition of functions F_i and G_i. However, if one considers *the complete set of extended equations of motion* (19) and (22), it is easy to see that they can not be obtained from the corresponding equations (13) and (17) by a simple redefinition procedure. Hence, our generalized equations of motion (19) and (22) have a different structure from that exhibited by KBB equations, although the latter are recovered in the limit $q \to 1$. However, it is worth mentioning that the present formulation is not unique. For example, we can define a temperature dependent effective Hamiltonian

$$H_{eff} = -\frac{T}{1-q} \ln \left[1 - \frac{1-q}{T} H \right] \tag{23}$$

and substitute H by H_{eff} in Eqs. (13) and (17). In that case, we obtain a dynamical system characterized by the same phase space probability distributions although yielding different trajectories. The present formulation has the virtue of expliciting some features of the generalized canonical distribution such as the cut-off condition (we will come back to this point later).

Finally, returning to the discussion at the end of Section 2, let us stress that this generalized thermostatting scheme will provide linear mean values evaluated upon Tsallis canonical distribution. Hence, non linear generalized mean values do not play any essential rôle here.

4.1. *Fixed Points Stability*

The equations of motion may be written in the form

$$\dot{\mathbf{z}} = \mathbf{Z}_q(\mathbf{z}), \tag{24}$$

where $\mathbf{z} = (x_1, ..., x_N, p_1, ..., p_N, \zeta, \xi)$. The trace of the stability matrix $\partial \mathbf{Z}_q / \partial \mathbf{z}$ is

$$\mathrm{Tr} \frac{\partial \mathbf{Z}_q}{\partial \mathbf{z}} = \sum_i \frac{\partial Z_i}{\partial z_i} = \sum_i \left\{ \frac{\partial \dot{x}_i}{\partial x_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right\} + \frac{\partial \dot{\zeta}}{\partial \zeta} + \frac{\partial \dot{\xi}}{\partial \xi}. \tag{25}$$

Taking into account conditions (16) and the concerned derivatives of Eqs. (19), we get

$$\mathrm{Tr} \frac{\partial \mathbf{Z}_q}{\partial \mathbf{z}} = \frac{1-q}{T} \sum_i \left\{ h_2 F_i \frac{\partial H}{\partial x_i} + h_1 G_i \frac{\partial H}{\partial p_i} \right\} - \left[1 - \frac{1-q}{T} H \right] \sum_i \left\{ h_2 \frac{\partial F_i}{\partial x_i} + h_1 \frac{\partial G_i}{\partial p_i} \right\}. \tag{26}$$

Considering the time independent form of Eqs. (19) and (22), straightforwardly, we have that, at a fixed point $\mathbf{z} \equiv FP$ (where $\dot{\mathbf{z}} = 0$),

$$\mathrm{Tr} \left. \frac{\partial \mathbf{Z}_q}{\partial \mathbf{z}} \right|_{FP} \equiv 0. \tag{27}$$

This means that the sum of eigenvalues of $\partial \mathbf{Z}_q/\partial \mathbf{z}$ is always identically zero, i.e., for arbitrary Hamiltonians and heat bath couplings, there are no stable fixed points. Hence, the most simple kind of non ergodic behavior is lacking if the stability matrix had at least one eigenvalue with non-vanishing real part. A more detailed analysis of stability will depend on each particular case.

4.2. *Cut-Off Condition*

In order to clarify the meaning of the cut-off prescription (12) within our approach, we will consider the behavior of $H(t)$ (recall that H is not a constant of motion of the extended dynamical system) on the hypersurface $\sum_c$ given by $H(\mathbf{x}, \mathbf{p}) = H_c$. The nth time derivative of the Hamiltonian is given by the recurrence relation

$$H^{(n)} = \left[1 - \frac{1-q}{T} H\right] J^{(n-1)} - \frac{1-q}{T} \sum_{k=1}^{n-1} \binom{n-1}{n-k-1} J^{(n-k-1)} H^{(k)}, \tag{28}$$

where

$$J(t) = \sum_i \left\{ h_1(\zeta)\, G_i \frac{\partial H}{\partial p_i} + h_2(\xi)\, F_i \frac{\partial H}{\partial x_i} \right\}. \tag{29}$$

It is clear from the two above expressions and the cut-off condition (12), that, on the hypersurface Σ_c, the nth time derivative of the Hamiltonian vanishes for all n. From the particular case $n = 1$, it follows that Σ_c is invariant under the dynamical evolution of our extended system. Therefore, an orbit of this system can not cross Σ_c: if the system is initially inside Σ_c, i.e. if $H < H_c$, it will remain there forever.

Let us consider a Hamiltonian $H = \frac{1}{2}\mathbf{p}^2 + V(\mathbf{x})$. In the one-dimensional case, Σ_c is given by the following curve on the (x_1, p_1)-plane

$$\tfrac{1}{2}p_1^2 + V(x_1) = H_c. \tag{30}$$

In the bi-dimensional case, we will consider the $2D$-projection of Σ_c onto the configurational space (x_1, x_2)

$$V(x_1, x_2) = H_c. \tag{31}$$

4.3. *Energy Shift Invariance*

Within Tsallis' statistics, the generalized canonical ensemble is not invariant under a constant energy shift (ΔE) of the Hamiltonian. If one replaces the Hamiltonian H by a new shifted Hamiltonian H^* given by

$$H^* = H + \Delta E, \tag{32}$$

the phase space probability distribution associated with Tsallis canonical ensemble (10) does not remain unchanged. The distribution admits this invariance property only in the limiting case $q \to 1$. However, for any value of q, the generalized canonical ensemble distribution is invariant under the simultaneous transformations

$$\begin{cases} H \to H^*, \\ T \to T^*, \end{cases} \tag{33}$$

where

$$T^* = \nu T, \tag{34}$$

with

$$\nu = \left[1 - \frac{1-q}{T} \Delta E \right]. \tag{35}$$

This invariance law is related to an invariance law of the motion equations of the extended dynamical system ((19) and (22)). It is easy to see that those motion equations are invariant under the transformation (33) together with

$$h_i^* = \nu h_i \quad (i = 1, 2). \tag{36}$$

5. NUMERICAL EXAMPLES

We examined thermal distributions for several simple 1D and 2D systems characterized by the potential energies $V(\mathbf{x})$ listed below

	$V(\mathbf{x})$
1D	$\frac{1}{2}x_1^2$
	x_1^3
	$\frac{1}{2}(x_1^2 - 1)^2$
	$\begin{cases} \frac{1}{2}(x_1^2-1)^2, & \text{if} \quad x_1 \geqslant 0 \\ \frac{1}{2}(1-x_1^3), & \text{if} \quad x_1 < 0 \end{cases}$
	$\cosh x_1$
	$-(x_1^2+\varepsilon^2)^{-1/2} + 1/\varepsilon, \quad \varepsilon > 0$
2D	$x^4 - x^2 \qquad (x^2 = x_1^2 + x_2^2)$
	$x^4 + x^2 - 3x_1^2$

Although nonextensive effects are relevant in complex many body systems, the thermosttating treatment of such systems is beyond the scope of the present work. Here, we apply the method to simple examples in order to study its general properties and feasibility.

The thermostatting was implemented through the following coupling schemes

$$F_i(\mathbf{x}, \mathbf{p}), G_i(\mathbf{x}, \mathbf{p}) = \begin{cases} 0 \\ x_i^n p_i^m \\ \sin(x_i^n p_i^m) \\ \cos(x_i^n p_i^m) \\ \exp(x_i^n p_i^m), \qquad \text{for} \quad n, m = 0, ..., 4 \quad 1, ..., N \end{cases}$$

and

$$h_1(\zeta) = \begin{cases} \zeta^n, n = 1, 3 \\ \zeta\ |\zeta| \end{cases} \qquad h_2(\xi) = \begin{cases} \xi^n, n = 1, 3 \\ \xi\ |\xi| \end{cases}$$

Functions h_1 and h_2 are chosen in such a way that, according to relations (18), the exponential factor in the stationary distribution (20) allows appropriate normalization.

Numerical integration of the equations of motion (19) and (20) was performed using a fourth-order Runge–Kutta method. The evolution was computed with double precision by means of a Pascal program run in a 486-PC (100 MHz). Simulated thermal distributions do not change significantly under reduction of the selected time step.

Theoretical distributions were obtained by projection of the generalized distribution (20) on the concerning variable z_i,

$$f_{q,\,exact}^{(i)}(z_i) = \int \cdots \int \mathscr{F}_q(\mathbf{z})\, d\mathbf{z}', \tag{37}$$

where integration is performed over the $2N+1$ variables z_j with $j \neq i$. We computed the time evolution of the deviation between simulated and theoretical distributions defined by

$$\Delta_{q,\,z_i}(t) = 100 \int |f_{q,\,exact}^{(i)}(z_i) - f_{q,\,numeric}(z_i, t)|\, dz_i \qquad (i = 1, ..., 2N+2). \tag{38}$$

Fig. 1 exhibits the trajectories in the (x_1, p_1)-plane for the asymmetric 1D potential when the thermal bath is modeled by the following cubic coupling scheme

$$\begin{aligned} F_1 &= x_1^3, \\ G_1 &= p_1, \\ h_1 &= \zeta^3, \\ h_2 &= \xi. \end{aligned} \tag{39}$$

The orbits in Fig. 1 followed during a longer time interval yield the plots displayed in Fig. 2 where, for $q < 1$, the cut-off condition (12) is clearly evidenced.

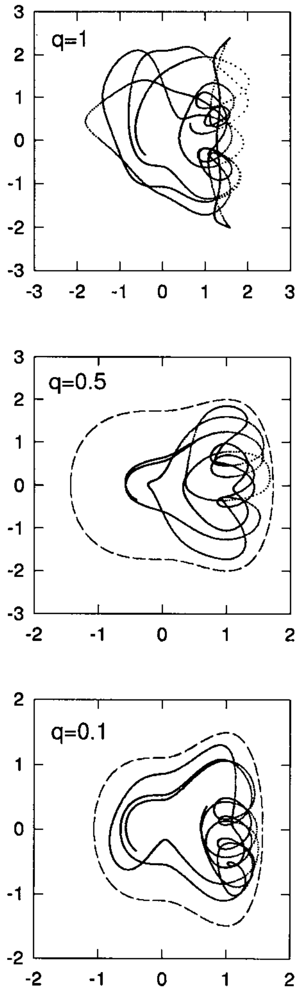

FIG. 1. (x_1, p_1) trajectories for the asymmetric 1D potential, for different values of parameter q, with $\alpha = \beta = T = 1$ and the cubic coupling scheme. The initial condition was $\mathbf{z} = (-0.4,\ -0.34,\ 0.5,\ 0.0)$. Dashed lines represent the cut-off condition. Integration step is $\Delta t = 0.01$ and $t = 30$ (3000 points).

These plots are qualitatively independent of the initial conditions, as expected for a truly ergodic system.

It is worth remarking that, in the cases $q < 1$ (where the cut-off condition is involved), the orbits thoroughly fill the region bounded by Σ_c, as illustrated in Figs. 2b and 2c, in contrast to the case $q = 1$, illustrated in Fig. 2a, where the accessible phase space region to be filled is infinite. For $q > 1$, not only the accessible region is infinite but the generalized probability distribution (10) has

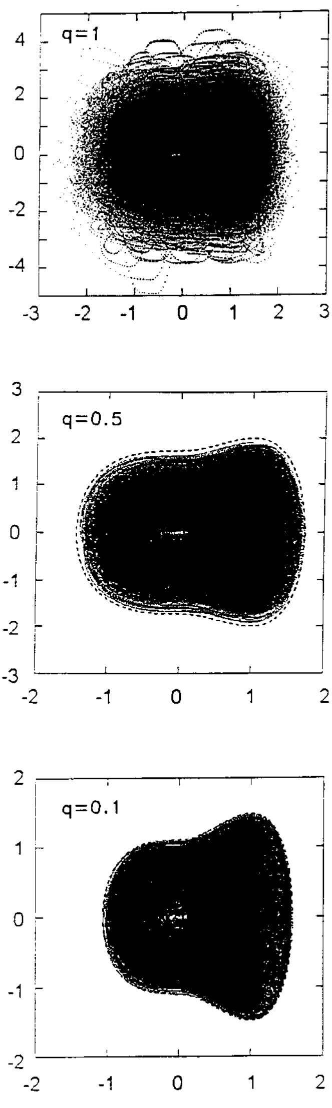

FIG. 2. The same as Fig. 1 but for $t = 10^4$.

a power law decay instead of the exponential one shown by Gibbs canonical ensemble. Therefore, for $q \geqslant 1$, the probability of an "overflow" during the trajectory evolution increases with q for a given potential. However, even if trajectories do not remain computationally tractable (due to numerical overflows) for long time intervals, we observed that the resulting histograms, although noisy, are in agreement with the corresponding theoretical distributions. This fact suggests that a more elaborated thermostatting scheme may allow to deal with the $q > 1$ scenario. This would be particularly interesting since the case $q > 1$ is associated to Lévy flights [12]. A possibility is to consider a representation of the thermal bath in terms of more than two variables [33].

In Fig. 3, we show the histograms that represent the thermal distributions corresponding to the trajectories depicted in Fig. 2 together with the respective theoretical distributions. Figure 4 displays the time behavior of the deviation between simulated and theoretical distributions according to Eq. (38). For any q, deviations decrease as $t^{-1/2}$. For the other 1D potential listed above, a good agreement between simulated and exact distributions was also obtained, for a suitable choice of the coupling scheme. In all analyzed cases the $t^{-1/2}$-law seems to set an upper bound to convergence speed.

As a further illustration of 1D potentials we show, in Fig. 5, results obtained for the softened Keplerian potential. This potential is of special interest in the context of the generalized statistics given that the associated standard partition function

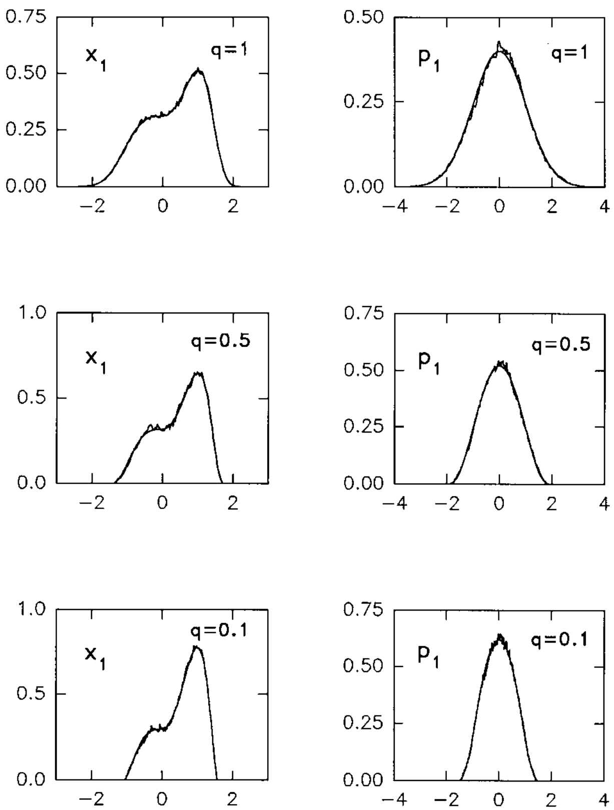

FIG. 3. Histograms representing the thermal distributions of the canonical variables x_1 and p_1, corresponding to the trajectories shown in Fig. 2. Smooth lines correspond to exact distributions.

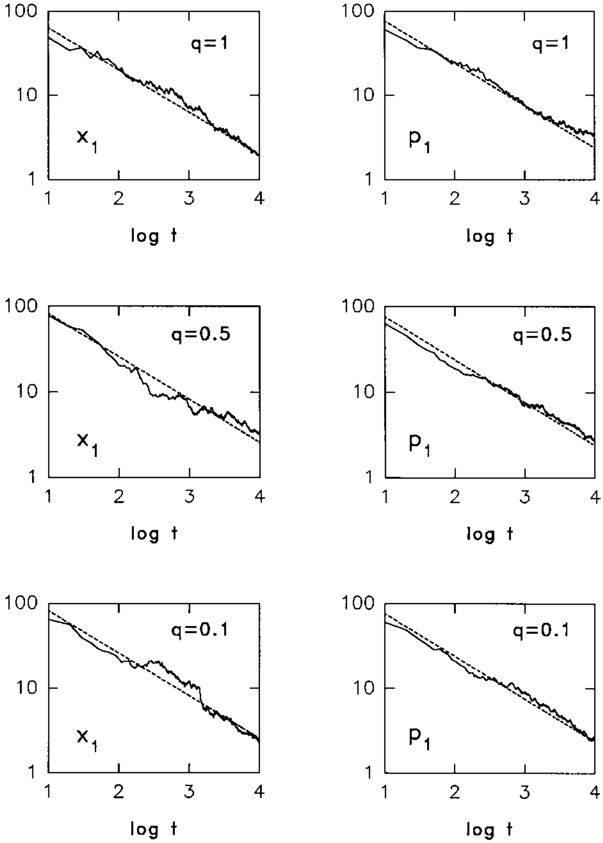

FIG. 4. Time evolution of the deviations between the simulated and theoretical distributions shown in Fig. 3, according to expression (38). Dashed lines have slope $-1/2$ in the log-log plots.

diverges. Such difficulties arise when considering the hydrogen atom and self-gravitating N-body systems (see [43] and references therein). Indeed, that potential has a form similar to that of the standard Keplerian one, but softened by a small parameter ε introduced in order to avoid the singularity at the origin. This procedure is commonly used in astrophysical numerical simulations of N-body systems [27]. Parameter ε implies an inferior energy bound, which plays a rôle similar to the fundamental level in the hydrogen atom. In fact, the generalized statistics was already shown to be the proper one for the treatment of the hydrogen atom [43]. The cut-off condition (12) restricts the values of q yielding normalizable distributions ($q < 1 - \varepsilon T$). Fig. 5 displays the cut-off boundaries in the (x_1, p_1)-plane for two allowed values of q. The same figure also exhibits the excellent agreement between simulated and analytical thermal distributions.

The thermostatting method was also applied to 2D potentials. As an illustration of those results, we consider the anisotropic 2D potential with the cubic coupling

$$
\begin{aligned}
F_i &= x_i^3 \\
G_i &= p_i \quad (i=1,2) \\
h_1 &= \zeta^3 \\
h_2 &= \xi.
\end{aligned}
\tag{40}
$$

The resulting 2D projected trajectories (not shown) are qualitatively similar to those in Figs. 1 and 2, i.e., they obey the cut-off condition and wholly fill the accessible region in phase space. The distributions of the canonical variables, for different values of q, are shown in Figs. 6-8.

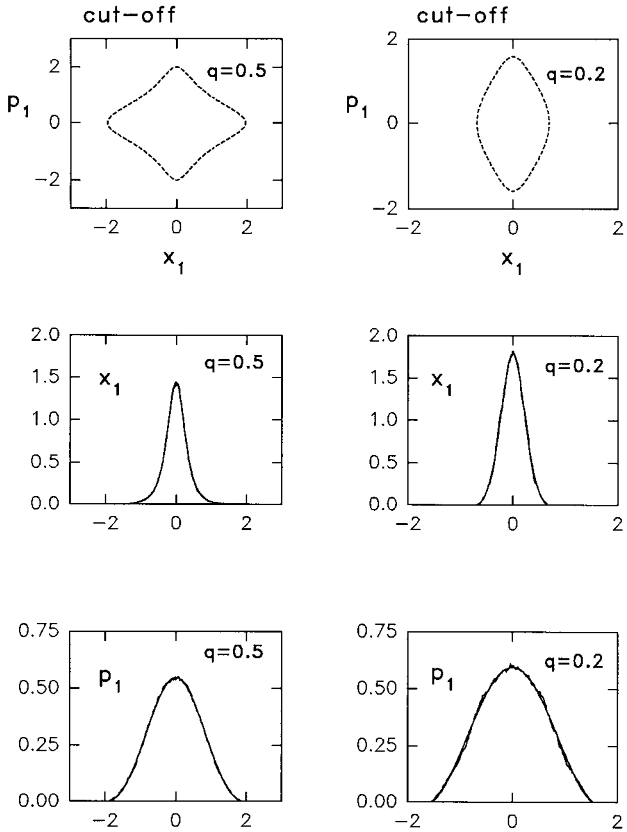

FIG. 5. Cut-off boundary (dashed lines) and histograms representing the thermal distributions of the canonical variables x_1 and p_1, corresponding to trajectories yield by the 1D softened Keplerian potential with $\varepsilon = 0.4$, for two values of parameter q and $T = 1$. We selected the cubic coupling scheme and $\alpha = \beta = 5$. The initial condition was $\mathbf{z} = (-0.4, -0.34, 0.5, 0.0)$ and $t = 10^4$. Smooth lines correspond to exact distributions.

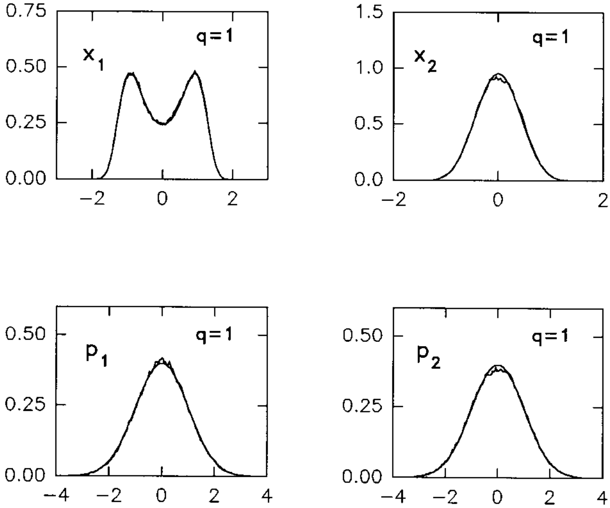

FIG. 6. Histograms representing the thermal distributions of the canonical variables for the 2D potential $V(\mathbf{x}) = x^4 + x^2 - 3x_1^2$ (where $x^2 = x_1^2 + x_2^2$), for $q = 1$ with $\alpha = \beta = T = 1$ and the cubic coupling scheme. The initial condition was $\mathbf{z} = (0.2, 0.21, -0.3, -0.37, 0.0, 0.0)$. Integration step is $\Delta t = 0.01$ and $t = 10^4$. Smooth lines correspond to exact distributions.

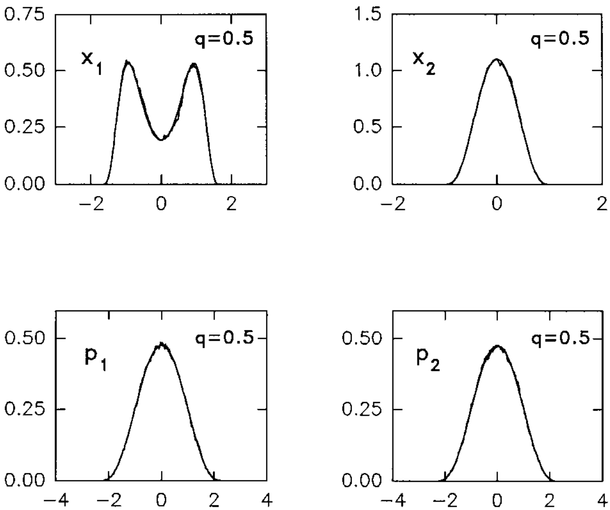

FIG. 7. The same as Fig. 5 with $q = 0.5$.

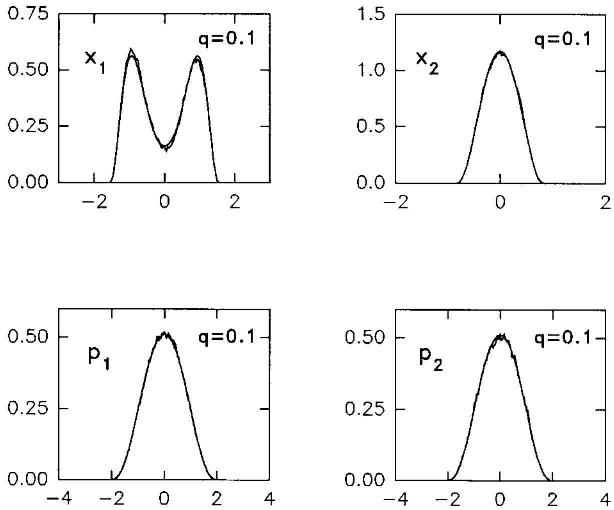

FIG. 8. The same as Fig. 5 with $q = 0.1$.

Both in 1D and 2D examples, the agreement between simulated and theoretical values is remarkable. However, given T and q, we found that not all coupling schemes yield equally good results and that, for a given coupling scheme, parameters α and β must be appropriately selected. These assertions were already shown to be true in the standard BG case ($q = 1$) [1, 2].

6. DISCUSSION

The main result of the present paper is to show the possibility of developing dynamical thermostatting schemes consistent with the generalized non-extensive canonical ensemble. To achieve this goal, we considered a generalization of the procedure that Kusnezov, Bulgac and Bauer introduced in order to simulate Gibbs canonical distribution.

We found that for certain coupling schemes and appropriate values of the parameters α, β and temperature T, the thermal distributions obtained by numerical integration of the extended equations of motion show a good agreement with the generalized ensemble distributions.

Since a good agreement is not found for any value of the parameters, then, in some cases, the extended dynamical system may not be fully ergodic. It is well known that similar problems arise in the Gibbs ($q = 1$) environment [42]. If the chaotic trajectories are only recurrent and not ergodic, only limited regions of the phase space are reached and the canonical ensemble can not be reproduced. Moreover, ergodicity may be temperature-dependent. In these situations, ergodicity can be achieved by recourse to thermostatting schemes with more than two heat bath variables, as showed by Bulgac *et al.* in [44, 45].

Our results suggest some possible further developments. It would be interesting to adapt other thermostatting procedures to the nonextensive thermostatistics, like the recently introduced kinetic-moment-method by Hoover and Holian [42]. It would be also worthwhile to consider, following Jellinek and Berry's beautiful analysis of the $q=1$ case, Hamiltonian approaches to the generalized ($q \neq 1$) canonical ensemble. Moreover, Lévy flights, that constitute generalizations of Brownian motion, were shown to be intimately connected with Tsallis generalized entropy [12], while Bulgac and Kusnezov [33] have obtained a deterministic time reversal model for Brownian motion. This suggests the possibility that q-generalized thermostatting could help in developing a deterministic approach to Lévy flights. To explore possible connections between the present thermostatting approach and the simulated annealing method would be also interesting. Some of these problems will be addressed elsewhere.

On the other hand, the fact that the thermostatting treatment works in the case of Tsallis generalized canonical distribution indicates that this approach may be implemented to describe more general distributions than the standard exponential one. This suggests that the method may be useful in connection with other physically relevant probability distributions.

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