Eur. Phys. J. B **48**, 87–93 (2005)
DOI: 10.1140/epjb/e2005-00372-3

THE EUROPEAN PHYSICAL JOURNAL B

Dynamical thermostatting and statistical ensembles

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Received 23 May 2005 / Received in final form 31 August 2005
Published online 9 December 2005 –

Abstract. Dynamical thermostatting constitutes a procedure for computing thermodynamical mean values of classical dynamical systems that is of interest both from the practical and from the conceptual points of view. Here we extend and unify previous partial results, showing that the dynamical thermostatting approach can be implemented in order to simulate a wide family of statistical ensembles of general dynamical systems with a vanishing divergence and admitting an integral of motion. As a particular illustration, the thermostatting procedure is applied to power law-like maximum entropy ensembles.

PACS. 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion – 05.20.Gg Classical ensemble theory

1 Introduction

Dynamical thermostats [1–8] (also referred to as deterministic thermostats [9]) constitute useful tools for computing thermodynamic properties of classical Hamiltonian systems. The gist of the dynamical thermostatting method consists of extending the original dynamical system, the new degrees of freedom representing a heat bath, in such a way that the time mean values of the original phase space variables coincide with the desired ensemble averages. The main ideas of this method were originally advanced by Nosé [1,2] and Hoover [3,4]. An interesting and versatile extension of this approach was later developed by Kusnezov, Bulgac and Bauer (KBB) [5,6]. By recourse to an appropriate choice of the coupling with the heat bath variables, it is possible to obtain a highly ergodic dynamics leading to the alluded equivalence between time and ensemble averages. The KBB method provides a powerful alternative to the Monte Carlo method for computing thermal properties of classical systems. In a previous work Plastino and Anteneodo [7] adapted this method to simulate generalized non-extensive (power-law) canonical ensembles of classical Hamiltonian systems [10].

There are many interesting dynamical systems in physics, theoretical biology, and other areas, that are not Hamiltonian, or that have their most natural description in terms of a noncanonical set of variables. Therefore, it is of great importance to extend the methods of Statistical Mechanics to nonhamiltonian systems [11]. Plastino et al. [8] have considered the thermostatting approach to standard, exponential, canonical ensembles within the context of general dynamical systems exhibiting a phase space flow of vanishing divergence. The aim of the present work is to unify and generalize these previous results, implementing the Dynamical Thermostatting procedure for a wide family of statistical ensembles of dynamical systems of zero divergence endowed with an integration constant C. The alluded statistical ensembles can be obtained from a maximum entropy principle based upon an appropriate entropic functional [12]. The thermo-statistical formalisms associated with these maximum entropy prescriptions have arose a considerable amount of interest in recent years [13–21]. In particular, power-law statistical ensembles, and their associated thermo-statistics, are nowadays the focus of intensive research efforts because they are very useful in order to describe many systems and processes in physics, biology, economics, and other related fields [19–21]. Parameterizing the power-law distributions in terms of Tsallis q-distributions (that is, distributions maximizing Tsallis' non-extensive information measure) it is possible to recover the standard exponential canonical distribution in the limit $q \to 1$. As an example of the general thermostatting method that is advanced here, we implement a thermostatting scheme for systems of vanishing divergence described by a non-extensive (power-law) thermostatistics. Numerical illustrations are provided for two specific cases: a Lotka-Volterra [22,23] system with three species, and a Nambu system.

This paper is organized as follows. The formalism advanced here for the thermostatting approach to general statistical ensembles of dynamical systems of zero

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divergence is analyzed in Section 2. In Section 3 it is shown how the general formalism reduces to the original KBB one in the case of Gibbs' ensembles associated with Hamiltonian systems. In Section 4 the general approach is applied to power law-like ensembles parameterized as Tsallis' distributions. Numerical illustrations are discussed in Section 5. Finally, some conclusions are drawn in Section 6.

2 Dynamical thermostats for general statistical ensembles

The KBB Dynamical Thermostatting approach, as originally formulated in [5], is a dynamical procedure for the evaluation of thermal mean values corresponding to the canonical ensemble associated to a dynamical system with Hamiltonian $H(\mathbf{x}, \mathbf{p})$. The main idea of this method consists in enlarging the system by incorporating two new dynamical variables, ϵ and η , representing the heat bath. In this Section we are going to generalize the thermostatting procedure in order to treat general statistical ensembles of dynamical systems with vanishing divergence admitting an integral of motion C. Let us consider an autonomous dynamical system

$$\dot{\mathbf{z}} = \mathbf{w}(\mathbf{z}), \mathbf{z}, \mathbf{w} \in \mathcal{R}^{\mathbf{N}}, \tag{1}$$

where the vector $\mathbf{z}$ represents a point in the system's phase space. It is going to prove convenient to separate the phase space variables in two-subsets,

$$\mathbf{z} = (\mathbf{x}, \mathbf{y}), \tag{2}$$

with

$$\begin{aligned} \mathbf{x} &\in \mathcal{R}^{N_1}, \\ \mathbf{y} &\in \mathcal{R}^{N_2}, \quad N_1 + N_2 = N. \end{aligned} \tag{3}$$

The dynamical equations of motion can now be written as

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{u}(\mathbf{x}, \mathbf{y}), \\ \dot{\mathbf{y}} &= \mathbf{v}(\mathbf{x}, \mathbf{y}), \end{aligned} \tag{4}$$

where $\mathbf{w} = (\mathbf{u}, \mathbf{v})$. As already mentioned, in [8] Plastino et al. proved that the only requirements that a dynamical system has to fulfill in order to be thermalizable by the KBB procedure (in the context of the standard Gibbs canonical ensemble) are to admit an integral of motion $C(\mathbf{x}, \mathbf{y})$,

$$\frac{dC}{dt} = \left(\sum_{i=1}^{N_1} u_i \frac{\partial C}{\partial x_i} \right) + \left(\sum_{j=1}^{N_2} v_j \frac{\partial C}{\partial y_j} \right) = 0 \tag{5}$$

and to exhibit a divergence free phase-space flow, that is,

$$\nabla \cdot \mathbf{w} = \left(\sum_{i=1}^{N_1} \frac{\partial u_i}{\partial x_i} \right) + \left(\sum_{j=1}^{N_2} \frac{\partial v_j}{\partial y_j} \right) = 0. \tag{6}$$

In [8] Plastino et al. considered a system verifying conditions (5) and (6), admitting an integral of motion $C(\mathbf{z})$. Hamiltonian systems fulfill condition (6), but there are other interesting systems within this family. Among others, the Lotka-Volterra predator-prey systems [22,23] and the Nambu systems [24] share the vanishing divergence property. The Lotka-Volterra predator-prey systems constitute some of the most important dynamical systems considered in theoretical biology [22]. Nambu systems have been the focus of a considerable research activity (see [25–33] and reference therein). The Nambu dynamical structures arise in a natural way in several contexts. For instance, Nambu dynamics has been applied to the relativistic dynamics of charged spinning particles [31], and to some hydrodynamical type systems [32].

Now we are going to propose a thermostatting scheme to dynamically simulate a statistical ensemble described by a phase-space probability distribution of the form

$$g\left[\gamma + \frac{C(\mathbf{x}, \mathbf{y})}{T}\right]. \tag{7}$$

These ensembles arise naturally from the maximum entropy principle when general entropic measures are considered [12]. The extremalization of an entropic measure under the constraints imposed by normalization and the mean value $\langle C \rangle$ of the integral of motion C leads to probability distributions of the form (7). The quantities γ and $(1/T)$ are, respectively, the Lagrange multipliers associated with the normalization and $\langle C \rangle$ constraints. Here C plays the same role played by the energy in the standard Gibbs ensemble (and T, of course, plays the role of the temperature). Even if C is a constant of motion, it is sometimes useful to consider statistical ensembles like equation (7), where phase space points with different values of C have finite values of the probability density $g(\mathbf{x}, \mathbf{y})$ (for an example in theoretical biology, see [22]). The system under consideration is usually not completely isolated: it is weakly interacting with another system playing the role of a "C-bath" (again, this situation is similar to the one associated with the standard Gibbs ensemble). Even for an isolated system, according to Jaynes' information theory approach to statistical mechanics [34–37], a maximum entropy statistical ensemble provides an appropriate description. If the only available information about the system is the mean value of C, it is reasonable to adopt a maximum entropy phase space probability distribution like equation (7). In point of fact, these kind of distributions, for various entropic measures, are widely used in the literature to describe diverse systems in physics, biology, and other fields [19,20].

Let us now consider the (extended) dynamical equations for the original system coupled with the bath (which are a set of $N + 2$ coupled differential equations). For the equations of motion of the system's phase space coordinates we propose,

$$\begin{aligned} \frac{dx_i}{dt} &= u_i - h_2(\epsilon)\ F_i(\mathbf{x}, \mathbf{y}), \qquad (i = 1, \ldots.N_1) \\ \frac{dy_j}{dt} &= v_j - h_1(\eta)\ G_j(\mathbf{x}, \mathbf{y}), \qquad (j = 1, \ldots.N_2), \end{aligned} \tag{8}$$

and for the equations of motion of the bath variables we propose,

$$\frac{d\epsilon}{dt} = -\beta \left\{ \left[\frac{g'\left(\gamma + \frac{C}{T}\right)}{g\left(\gamma + \frac{C}{T}\right)} \right] \sum_{i=1}^{N_1} F_i \frac{\partial C}{\partial x_i} + T \sum_{i=1}^{N_1} \frac{\partial F_i}{\partial x_i} \right\}$$
$$\frac{d\eta}{dt} = -\alpha \left\{ \left[\frac{g'\left(\gamma + \frac{C}{T}\right)}{g\left(\gamma + \frac{C}{T}\right)} \right] \sum_{j=1}^{N_2} G_j \frac{\partial C}{\partial y_j} + T \sum_{j=1}^{N_2} \frac{\partial G_j}{\partial y_j} \right\}. \quad (9)$$

The present developments formally hold for arbitrary forms of the functions F_i and G_j. The specific forms of F_i and G_j to be used in each case, in order to make the extended system ergodic, depend on the particular dynamical system under consideration. Specific examples are given in Section 5.

It is possible to prove, after some algebra, that the Liouville equation governing the evolution of the (extended) phase-space probability distribution $F(\mathbf{x}, \mathbf{y}, \epsilon, \eta)$,

$$\frac{\partial F}{\partial t} + \left[\sum_{i=1}^{N_1} \frac{\partial(\dot{x}_i F)}{\partial x_i} \right] + \left[\sum_{j=1}^{N_2} \frac{\partial(\dot{y}_j F)}{\partial y_j} \right] + \frac{\partial(\dot{\epsilon} F)}{\partial \epsilon} + \frac{\partial(\dot{\eta} F)}{\partial \eta} = 0, \quad (10)$$

admits a stationary solution of the form

$$F(\mathbf{x}, \mathbf{y}, \epsilon, \eta) = g\left[\gamma + \frac{C(\mathbf{x}, \mathbf{y})}{T}\right] \times \exp\left\{ -\frac{1}{T} \left[\frac{1}{\alpha} g_1(\eta) + \frac{1}{\beta} g_2(\epsilon) \right] \right\}, \quad (11)$$

where the functions $g_{1,2}$ and $h_{1,2}$ are related by

$$h_1(\eta) = \frac{dg_1}{d\eta},$$
$$h_2(\epsilon) = \frac{dg_2}{d\epsilon}. \quad (12)$$

When verifying that the probability distribution (11) is a solution to equation (10), notice that

$$\frac{\partial \dot{\eta}}{\partial \eta} = 0 \qquad \text{and} \qquad \frac{\partial \dot{\epsilon}}{\partial \epsilon} = 0, \quad (13)$$

and also

$$\left(\sum_{i=1}^{N_1} \frac{\partial u_i}{\partial x_i} \right) + \left(\sum_{j=1}^{N_2} \frac{\partial v_j}{\partial y_j} \right) - \frac{1}{T} \left(\sum_{i=1}^{N_1} u_i \frac{\partial C}{\partial x_i} \right) - \frac{1}{T} \left(\sum_{j=1}^{N_2} v_j \frac{\partial C}{\partial y_j} \right) = 0. \quad (14)$$

As we shall presently see, it is sometimes convenient to re-write the equations of motion (8) and (9) in the form,

$$\frac{dx_i}{dt} = u_i - h_2(\epsilon) k \left[\gamma + \frac{C}{T}\right] F_i(\mathbf{x}, \mathbf{y}), \quad (i = 1, \dots N_1)$$
$$\frac{dy_j}{dt} = v_j - h_1(\eta) k \left[\gamma + \frac{C}{T}\right] G_j(\mathbf{x}, \mathbf{y}), (j = 1, \dots N_2), \quad (15)$$

and

$$\frac{d\epsilon}{dt} = -\beta \left\{ \left[k'\left(\gamma + \frac{C}{T}\right) + k\left(\gamma + \frac{C}{T}\right) \frac{g'\left(\gamma + \frac{C}{T}\right)}{g\left(\gamma + \frac{C}{T}\right)} \right] \times \sum_{i=1}^{N_1} F_i \frac{\partial C}{\partial x_i} + Tk\left(\gamma + \frac{C}{T}\right) \sum_{i=1}^{N_1} \frac{\partial F_i}{\partial x_i} \right\}$$
$$\frac{d\eta}{dt} = -\alpha \left\{ \left[k'\left(\gamma + \frac{C}{T}\right) + k\left(\gamma + \frac{C}{T}\right) \frac{g'\left(\gamma + \frac{C}{T}\right)}{g\left(\gamma + \frac{C}{T}\right)} \right] \times \sum_{j=1}^{N_2} G_j \frac{\partial C}{\partial y_j} + Tk\left(\gamma + \frac{C}{T}\right) \sum_{j=1}^{N_2} \frac{\partial G_j}{\partial y_j} \right\}. \quad (16)$$

where $k\left[\gamma + \frac{C(\mathbf{x},\mathbf{y})}{T}\right]$ (as well as $g\left[\gamma + \frac{C(\mathbf{x},\mathbf{y})}{T}\right]$) is a general function of the argument $[\gamma + \frac{C(\mathbf{x},\mathbf{y})}{T}]$. Notice that the equations (15–16) are equivalent to the equations (8–9). The transformation from equations (8–9) to equations (15–16) only involves a redefinition of the functions F_i and G_j,

$$F_i(\mathbf{x}, \mathbf{y}) \rightarrow k\left[\gamma + \frac{C}{T}\right] F_i(\mathbf{x}, \mathbf{y}),$$
$$G_j(\mathbf{x}, \mathbf{y}) \rightarrow k\left[\gamma + \frac{C}{T}\right] G_j(\mathbf{x}, \mathbf{y}). \quad (17)$$

The equations of motion (8, 9) of the extended system do not exhibit, in general, a Hamiltonian form (not even the equations of motion (4) of the original system were assumed to have a Hamiltonian form). However, any dynamical system can be cast into a Hamiltonian form by appropriately enlarging the phase space (see, for example, [38,39]). Consequently, it is in principle possible to perform a further extension of the phase space in order to endow the equations of motion of the extended system with a Hamiltonian structure. This would allow for the exploration of possible connections of the present formalism with other, Hamiltonian-based thermostatting approaches, like the Poincare-Nosé scheme [40]. However, the alluded extension of the phase space seems (at least in the context of the present formalism) a rather artificial procedure. In point of fact, one of the aims of the present article is to show that the equations of motion of a system do not need a Hamiltonian structure in order to implement a KBB-like thermostatting scheme to simulate general statistical ensembles.

3 Hamiltonian systems and Gibbs canonical ensemble

The equations of motion originally proposed by KBB were intended to simulate Gibbs' canonical ensemble for Hamiltonian systems. Those equations of motion are a particular instance of our general equations. For a Hamiltonian system with n degrees of freedom we have $N = 2n$,

$N_1 = N_2 = n$, and $y_i = p_i, (i = 1, \ldots n)$. Furthermore, we have,

$$u_i = \partial H/\partial p_i$$
$$v_i = -\partial H/\partial x_i, (i = 1, \ldots n). \tag{18}$$

The integral of motion $C(\mathbf{x}, \mathbf{y})$ of the system is the Hamiltonian H. If we now set

$$g\left[\gamma + \frac{H}{T}\right] = \exp\left[-\gamma - \frac{H}{T}\right], \tag{19}$$

and

$$k\left[\gamma + \frac{C(\mathbf{x}, \mathbf{y})}{T}\right] = 1, \tag{20}$$

it can be verified that the general thermostatting equations reduce to the KBB ones,

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i} - h_2(\epsilon)F_i(\mathbf{x}, \mathbf{p}), (i = 1, ...N)$$
$$\frac{dp_i}{dt} = \frac{\partial H}{\partial x_i} - h_1(\eta)G_i(\mathbf{x}, \mathbf{p}), (i = 1, ...N) \tag{21}$$

$$\frac{d\epsilon}{dt} = \beta \sum_{i=1}^{N} \left(F_i \frac{\partial H}{\partial x_i} - T \frac{\partial F_i}{\partial x_i} \right)$$
$$\frac{d\eta}{dt} = \alpha \sum_{i=1}^{N} \left(G_i \frac{\partial H}{\partial p_i} - T \frac{\partial G_i}{\partial p_i} \right). \tag{22}$$

The Liouville equation associated with the extended dynamical system admits as stationary solution the probability distribution

$$F(\mathbf{x}, \mathbf{p}, \epsilon, \eta) = \frac{1}{Z} \times \exp\left\{ -\frac{1}{T} \left[H(\mathbf{x}, \mathbf{p}) + \frac{1}{\alpha} g_1(\eta) + \frac{1}{\beta} g_2(\epsilon) \right] \right\}, \tag{23}$$

where

$$\frac{1}{Z} = \exp[-\gamma]. \tag{24}$$

is an appropriate normalization factor.

4 Nonextensive canonical ensembles of general dynamical systems with vanishing divergence

There are many systems in nature that are described by power-law like distributions [19,20]. In many situations, these distributions are conveniently parameterized in terms of q-maximum entropy distributions maximizing Tsallis q-entropy [10],

$$S_q = \frac{1}{q-1} \int (f(\mathbf{z}) - [f(\mathbf{z})]^q) d\mathbf{z}, \tag{25}$$

where the entropic index q is any real number and $f(\mathbf{z})$ is a probability distribution in the relevant phase space, fulfilling the normalization condition,

$$\int f(\mathbf{z})\, d\mathbf{z} = 1. \tag{26}$$

The generalized entropy Sq is nonextensive such that

$$Sq(A + B) = Sq(A) + Sq(B) + (1 - q)Sq(A)Sq(B), \tag{27}$$

where A and B are two systems statistically independent in the sense that

$$f^{(A+B)}(\mathbf{z}, \mathbf{z}') = f^{(A)}(\mathbf{z})\, f^{(B)}(\mathbf{z}'). \tag{28}$$

We can construct a MaxEnt distribution f_q^{ME} that maximizes the entropy functional (25), subject to the constraints imposed by the mean value of the energy plus the normalization prescription (26). The solution of this variational problem is given by the Tsallis MaxEnt probability distribution [41]. When the only relevant information is provided by the generalized mean value of an integration constant C, the corresponding MaxEnt probability distribution reads

$$f_q^{\mathrm{ME}}(\mathbf{z}) = \frac{1}{Z_q} \left[1 - \frac{1-q}{T} C(\mathbf{z}) \right]^{\frac{1}{(1-q)}} \tag{29}$$

where Z_q is the generalized partition function

$$Z_q = \int \left[1 - \frac{1-q}{T}\, C(\mathbf{z}) \right]^{\frac{1}{(1-q)}} d\mathbf{z}. \tag{30}$$

When the parameter q in the previous equations is such that $q < 1$, the concomitant probability distribution f vanishes if

$$C(\mathbf{z}) > C_c = \frac{T}{1-q}. \tag{31}$$

Equation (31) constitutes the Tsallis' cut-off condition, which constitutes an important feature of Tsallis' distributions. As a result of this condition we have that an orbit of a "thermalized" system cannot cross the hypersurface Σ_c defined by $C(\mathbf{z}) = C_c$. In other words, if the system is initially inside Σ_c, it will remain there forever. This kind of behavior of the thermalized system can be obtained by recourse to an appropriate choice for the function $k\left(\gamma + \frac{C}{T}\right)$.

The function $g\left(\gamma + \frac{C}{T}\right)$ associated with the nonextensive canonical ensemble is

$$g\left(\gamma + \frac{C}{T}\right) = \left[1 - \frac{1-q}{T} C(\mathbf{x}, \mathbf{y}) \right]^{\frac{1}{(1-q)}}, \tag{32}$$

and for the function $k\left(\gamma + \frac{C}{T}\right)$ we adopt

$$k\left(\gamma + \frac{C}{T}\right) = 1 - \frac{1-q}{T} C(\mathbf{x}, \mathbf{y}). \tag{33}$$

This form of k leads to a thermalizing dynamics in accord with Tsallis' cut-off prescription. The corresponding coupling with the heat bath is then described by the equations of motion

$$\frac{dx_i}{dt} = u_i - h_2(\epsilon)\left[1 - \frac{1-q}{T}C\right]F_i(\mathbf{x},\mathbf{y}),\ (i = 1, ...N_1)$$
$$\frac{dy_j}{dt} = v_j - h_1(\eta)\left[1 - \frac{1-q}{T}C\right]G_j(\mathbf{x},\mathbf{y}),\ (j = 1, ...N_2). \tag{34}$$

The equations of motion for the heat bath variables are,

$$\frac{d\epsilon}{dt} = \beta\left\{(2-q)\sum F_i\frac{\partial C}{\partial x_i} - T\left[1 - \frac{1-q}{T}C\right]\sum\frac{\partial F_i}{\partial x_i}\right\}$$
$$\frac{d\eta}{dt} = \alpha\left\{(2-q)\sum G_j\frac{\partial C}{\partial y_j} - T\left[1 - \frac{1-q}{T}C\right]\sum\frac{\partial G_j}{\partial y_j}\right\}. \tag{35}$$

Thus we have the full set of $N+2$ differential equations for the extended system (Eqs. (34) and (35)). In this case the Liouville equation of the extended system admits a stationary solution of the form,

$$F(\mathbf{x},\mathbf{y},\epsilon,\eta) = \frac{1}{Z_q}\left[1 - \frac{1-q}{T}C(\mathbf{x},\mathbf{y})\right]^{\frac{1}{(1-q)}} \times \exp\left\{-\frac{1}{T}\left[\frac{1}{\alpha}g_1(\eta) + \frac{1}{\beta}g_2(\epsilon)\right]\right\}. \tag{36}$$

The form of the equations (34) depends on parameter q. If we take $q \to 1$ we recover the KBB equations of motions derived in [8] for canonical ensembles distributions.

Due to the form (33) for the function k, it follows from the equations of motion (34) that

$$\frac{d^nC}{dt^n} = 0, n = 1, 2, 3\ldots, \tag{37}$$

for states of the system belonging to the hyper-surface Σ_c associated with Tsallis' cut-off. Consequently, the hyper-surface Σ_c constitutes an invariant set of the thermalized dynamics. That is, if the initial conditions are such that the system is within Σ_c the system stays in Σ_c forever. Moreover, the system's orbit cannot cross the hyper-surface Σ_c. Another convenient choice for the function k (instead of Eq. (33)) is

$$k\left(\gamma + \frac{C}{T}\right) = \left[1 - \frac{1-q}{T}C(\mathbf{x},\mathbf{y})\right]^f \tag{38}$$

where f is a real number. For $f = 1$ we recover equation (33).

5 Numerical illustrations

In this section we illustrate the dynamical thermostatting of a system of vanishing divergence for the case of nonextensive canonical ensembles. We work in a *Mathematica* environment (Wolfram Research), Version 4 [42]. In order to find the numerical solutions to the set of differential equations we use the function NDSolve. This function is based on the LSODE (Livermore Solver for Ordinary Differential Equations) which switches between a nonstiff Adams method and a stiff Gear method [42].

First we consider a biological example given by the Lotka-Volterra differential equations describing predator-prey interactions. We apply equations (34) and (35) to a Lotka-Volterra model with three species described by the following set of coupled, ordinary differential equations

$$\begin{aligned}\frac{dz_1}{dt} &= e^{z_2} + 3e^{z_3} - 4,\\ \frac{dz_2}{dt} &= -e^{z_1} + 2e^{z_3} - 1,\\ \frac{dz_3}{dt} &= -3e^{z_1} - 2e^{z_2} + 5,\end{aligned} \tag{39}$$

where the variables z_i are given in terms of the populations N_i $(i = 1, 2, 3)$ of the three species by the following relation

$$z_i = \ln\left(\frac{N_i}{N_{i0}}\right), \tag{40}$$

where N_{i0} denotes the stationary values of those populations [22,23]. This system has a divergence free phase space flux,

$$\sum_{i=1}^{3}\frac{\partial}{\partial z_i}\left(\frac{dz_i}{dt}\right) = 0, \tag{41}$$

and admits the integral of motion

$$C(z_1, z_2, z_3) = \sum_{i=1}^{3}\left[e^{z_i} - z_i\right]. \tag{42}$$

We consider a thermalization scheme characterized by the functions

$$\begin{aligned}F_1 &= z_1\\ G_2 &= z_2^3\\ G_3 &= z_3^3\\ h_2(\epsilon) &= \epsilon\\ h_1(\eta) &= \eta.\end{aligned} \tag{43}$$

We use the k-function given by equation (33). We chose the parameter values $T = 4$ and $\alpha = \beta = 1$. the marginal ensemble probability distribution associated with one dynamical variable z_i is given by

$$P(z_i) = \int F(\mathbf{z},\epsilon,\eta)\, d\Omega', \tag{44}$$

where the complete stationary solution $F(\mathbf{z},\epsilon,\eta)$ (Eq. (36)) of the extended dynamical system's Liouville equation is integrated over all the dynamical variables with the exception of z_i. In Figure 1 we compare the marginal ensemble probability distribution $P(z_i)$ and the corresponding histogram obtained from a numerically computed orbit of the associated extended, thermalized system. The initial conditions used to generate the orbit of the extended dynamical system are $z_1(0) = 0.04$, $z_2(0) = -1.34$, $z_3(0) = 0.011$, $\epsilon(0) = 0$, and $\eta(0) = 0.5$.

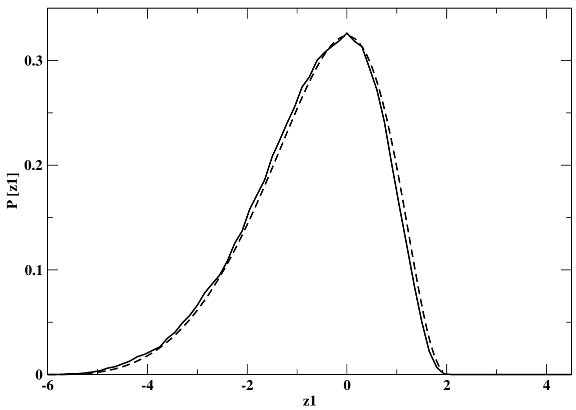

Fig. 1. The marginal ensemble distribution (dashed line) and the numerical histograms (solid line) for the variable z_1 of the Lotke-Volterra system (39) with $q = 0.5$ are plotted. All the depicted quantities are dimensionless.

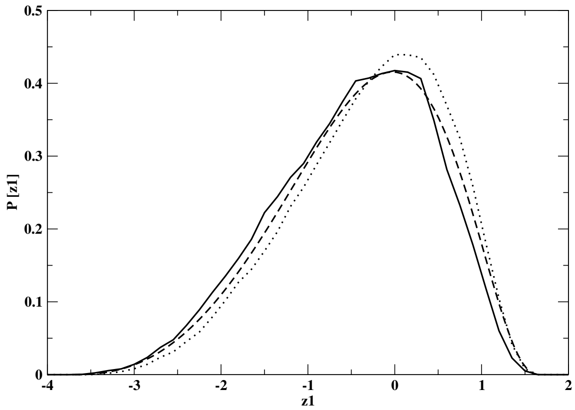

Fig. 2. The marginal ensemble distribution (dashed line) and the numerically computed histograms with $f = 1$ (dotted line) and with $f = 0.2$ (solid line) are plotted for the phase space coordinate z_1 of the Lotka-Volterra system (39) with $q = 0.3$. All the depicted quantities are dimensionless.

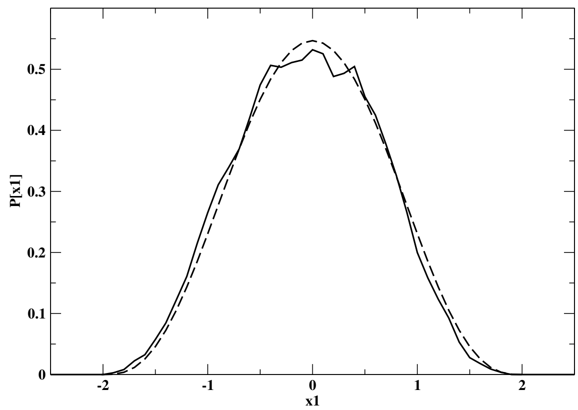

Fig. 3. The marginal ensemble distribution (dashed line) and the numerically computed histograms (solid line) for the dynamical variable x_1 of a Nambu system (Eq. (45)) with $q = 0.5$ are plotted. All the depicted quantities are dimensionless.

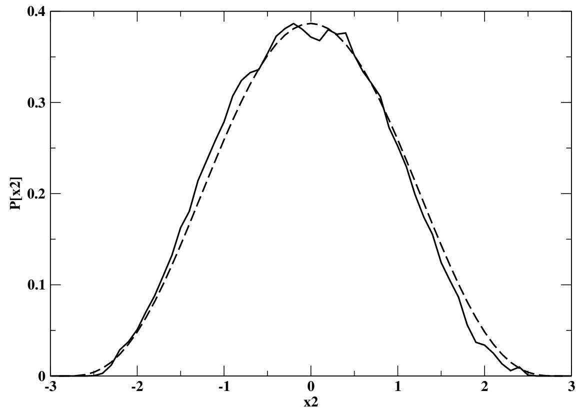

Fig. 4. The marginal ensemble distribution (dashed line) and the numerically computed histograms (solid line) for the dynamical variable x_2 of a Nambu system (Eq. (45)) with $q = 0.5$ are plotted. All the depicted quantities are dimensionless.

The time step is $0.0067 = 5/750$. The total sampling time is 10000. The histogram bin size is 0.15.

The three variables have all the same ensemble distribution. We can see from this figure that the histograms calculated following the Dynamical Thermostatting procedure for general divergence free dynamical systems accurately fit the corresponding ensemble distribution. We also considered the more general k-function given by equation (38). We found that the convergence of the method is improved if values $0 < f < 1$ are adopted for the exponent f appearing in k. In Figure 2, the marginal ensemble distribution (dashed line) for z_1 is compared with the numerically obtained distributions associated with $f = 1$ (dotted line) and with $f = 0.2$ (solid line). The initial conditions used in Figure 2 are the same as the ones used in Figure 1. The time step is $0.0033 = 5/1500$. The total sampling time is 5000. The histogram bin size is 0.15.

It transpires from Figure 2 that the histogram corresponding to $f = 0.2$ constitutes a better approximation to the marginal ensemble distribution than the histogram computed with $f = 1$.

We have also applied the thermalizing procedure to a three dimensional Nambu system [24], obtaining numerical results that fit very well with the corresponding ensemble distributions (see Figs. 3–5). The equations of motion of this system read

$$\frac{d\mathbf{x}}{dt} = (\nabla G) \times (\nabla H) \tag{45}$$

where G and H are the Hamiltonians

$$G = \frac{1}{2}\left(x_1^2 + x_2^2 + x_3^2\right) \tag{46}$$

and

$$H = \frac{1}{2}\left(\frac{x_1^2}{I_1} + \frac{x_2^2}{I_2} + \frac{x_3^2}{I_3}\right) \tag{47}$$

with $I_1 = 1$, $I_2 = 2$ and $I_3 = 3$. For this example we considered a Tsallis' distribution with $q = 0.5$. The initial conditions for the extended dynamical system used in

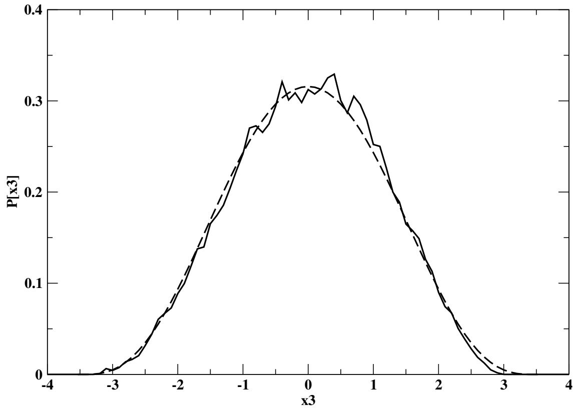

Fig. 5. The marginal ensemble distribution (dashed line) and the numerically computed histograms (solid line) for the dynamical variable x_3 of a Nambu system (Eq. (45)) with $q = 0.5$ are plotted. All the depicted quantities are dimensionless.

connection with Figures 3–5 are the same for the three figures: $x_1(0) = 0.4$, $x_2(0) = 0.34$, $x_3(0) = 0.11$, $\epsilon(0) = 0$, and $\eta(0) = 0.5$. The time step is $0.0167 = 1/60$. The total sampling time is 20000. The histogram bin size is 0.15.

6 Conclusions

We have shown that the Dynamical Thermostatting procedure can be successfully implemented in order to simulate general statistical ensembles of dynamical systems with vanishing divergence admitting an integral of motion. As an illustration of the present formalism, we have discussed in detail the case of power law-like ensembles, and have applied it to (i) the celebrated Lotka-Volterra equations for population dynamics and (ii) a Nambu system.

The present results provide new evidence that the KBB approach is a robust and versatile method for simulating statistical ensembles and for computing the concomitant thermodynamical properties of a wide family of statistical ensembles and dynamical systems. Besides their possible practical applications, the generalized versions of the KBB approach are also of interest from a conceptual point of view. For instance, they provide a large family of dynamical systems leading to Tsallis' distributions. The study of these systems may contribute to the understanding of Tsallis' thermostatistics and its possible applications.

This work was partially supported by MEC grant BFM2002-03241 (Spain), CONICET (Argentina), and CNPq (Brazil).

References

1. S. Nosé, J. Chem. Phys. **81**, 511 (1984)
2. S. Nosé, Mol. Phys. **52**, 255 (1984)
3. W.G. Hoover, Phys. Rev. A **31**, 1695 (1985)
4. W.G. Hoover, *Molecular Dynamics*, Lecture Notes in Physics **258**, (Springer-Verlag, New York, 1986)
5. D. Kusnezov, A. Bulgac, W. Bauer, Annals of Physics **204**, 155 (1990)
6. A. Bulgac, D. Kusnezov, Phys. Rev. A **42**, 5045 (1990)
7. A.R. Plastino, C. Anteneodo, Ann. Phys. **255**, 250 (1997)
8. A.R. Plastino, A. Plastino, L.R. da Silva, M. Casas, Physica A **271**, 343 (1999)
9. D. Ruelle, Physics Today, May 2004, 48
10. C. Tsallis, Journ. of Stat. Phys. **52**, 479 (1988)
11. S. Smale, Annals of New York Academy of Sciencies **357**, (New York Academy of Sciencies, 1980)
12. A. Plastino, A.R. Plastino, Phys. Lett. A **226**, 257 (1997)
13. T. Yamano, Phys. Lett. A **308**, 364 (2003)
14. T. Yamano, Eur. Phys. J. B **18**, 103 (2000)
15. T. Yamano, Phys. Lett. A **264**, 276 (1999)
16. K.S. Fa, E.K. Lenzi, Chaos, Solitons, and Fractals **20**, 227 (2004)
17. E.K. Lenzi, R.S. Mendes, L.R. da Silva, Physica A **295**, 230 (2001)
18. E.K. Lenzi, R.S. Mendes, L.R. da Silva, Physica A **280**, 337 (2000)
19. *Nonextensive Statistical Mechanics and its Applications*, edited by S. Abe, Y. Okamoto (Springer-Verlag, Berlin, 2001)
20. *Nonextensive Entropy: Interdisciplinary applications*, edited by M. Gell-Mann, C. Tsallis (Oxford University Press, Oxford, 2004)
21. T.D. Frank, *Nonlinear Fokker-Planck Equations* (Springer-Verlag, Berlin, 2005)
22. E. Kerner, *Gibbs Ensemble, Biological Ensemble* (Gordon and Breach, 1972)
23. E.H. Kerner, Phys. Lett. A **151**, 401 (1990)
24. Y. Nambu, Phys. Rev. D **7**, 2405 (1973)
25. M. Razavy, F. Kennedy, Can. J. Phys. **52**, 1532 (1974)
26. W. Steeb, N. Euler, Nuovo Cimento B **106**, 263 (1991)
27. I. Bialynicki-Birula, P. Morrison. Phys. Lett. A **158**, 453 (1991)
28. S. Codriansky, C. Bernardo, A. Aglaee, F. Carrillo, J. Castellanos, G. Pereira, J. Perez, J. Phys. A **27**, 2565 (1994)
29. R. Chatterjee, Lett. Math. Phys. **36**, 117 (1996)
30. A.R. Plastino, A. Plastino, Physica A **232**, 458 (1996)
31. R.M. Yamaleev, Ann. Phys. **292**, 157 (2001)
32. P. Guha, J. Math. Phys. **43**, 4035 (2002)
33. H.W. Braden, A. Gorskyb, A. Odesskiid, V. Rubtsovb, Nuclear Physics B **633**, 414 (2002)
34. E.T. Jaynes, Phys. Rev. **106**, 620 (1957)
35. E.T. Jaynes, Phys. Rev. **108**, 171 (1957)
36. E.T. Jaynes, *Papers on Probability, Statistics and Statistical Physics*, edited by R.D. Rosenkrantz (Dordrecht, Reidel, 1987)
37. E.T. Jaynes, *Probability Theory: The Logic of Science* (Cambridge University Press, Cambridge, 2005)
38. G.E.O. Giacaglia, *Perturbation Methods in Non-Linear Systems* (Springer-Verlag, Berlin, 1972)
39. P.A.M. Dirac, Proc. Roy. Soc. London A **246**, 326 (1958)
40. S.D. Bond, B.J. Leimkuhler, B.B. Laird, J. Comp. Phys. **151**, 114 (1999)
41. A.R. Plastino, A. Plastino, Phys. Lett. A **177**, 177 (1993)
42. S. Wolfram, *The Mathematica Book*, 5th edn. (Wolfram Media, Champaign, 2003)