

A novel approach to the determination of equilibrium properties of classical Hamiltonian systems with long-range interactions

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2009 J. Phys. A: Math. Theor. 42 165001

(<http://iopscience.iop.org/1751-8121/42/16/165001>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.153

The article was downloaded on 03/06/2010 at 07:36

Please note that [terms and conditions apply](#).

A novel approach to the determination of equilibrium properties of classical Hamiltonian systems with long-range interactions

T M Rocha Filho, M A Amato and A Figueiredo

Instituto de Física, Universidade de Brasília, CP 04455, 70919-970-Brasília, Brazil

E-mail: marciano@fis.unb.br

Received 31 December 2008, in final form 26 February 2009

Published 25 March 2009

Online at stacks.iop.org/JPhysA/42/165001

Abstract

A novel approach to computing the entropy of classical Hamiltonian systems with long-range interactions is presented. The one-particle distribution function is explicitly given in closed form depending only on numerical constants obtained from solutions of purely algebraic equations. Comparison of microcanonical and canonical forms for the entropy shows that they are always the same, thus implying that both ensembles are fully equivalent unless the heat capacity is negative in some energy range. Our approach is illustrated with the Hamiltonian mean field (HMF) and a mean-field model in two spatial dimensions.

PACS numbers: 05.70.-a, 05.20.Dd, 05.90.+m

1. Introduction

In thermodynamics the study of systems with long-range interactions presents challenging problems. This fact is well illustrated by the existence of quasi-stationary non-Gaussian states (which become stationary in the $N \rightarrow \infty$ limit), temperature jumps at critical temperatures, negative heat capacity and inequivalence of microcanonical and canonical ensembles [1, 2]. Examples of systems with long-range forces are self gravitating systems [3], non-neutral plasmas [4, 5] and some simplified models such as the Hamiltonian mean field (HMF) [6], free electron laser [7] and plasma single-wave models [8]. An interaction potential is long ranged if it decays for long distances as $r^{-\alpha}$ with $\alpha < d$, where d is the spatial dimension.

In order to understand how a negative heat capacity arises, let us consider an isolated system of N particles with arbitrary masses interacting through their mutual gravitational forces. For a stationary state of an isolated system in a three-dimensional space, the virial theorem yields [9]

$$E = K + W = (\alpha - 2)K, \quad (1)$$

where K and W are the kinetic and potential energies, respectively. For the gravitational case $\alpha = 1$ and hence $E = -K$, which results in a negative heat capacity for all energy values. Other examples of negative heat capacity in systems with long-range interactions are discussed by Lynden-Bell [10]. For $2 < \alpha < 3$, there is no negative heat capacity. Consequently, a long-range force is not a sufficient condition for a negative heat capacity. For instance Barré *et al* have shown that for the HMF model the microcanonical and canonical ensembles are fully equivalent, and therefore the heat capacity is always positive [11].

For short-range interactions canonical and microcanonical ensembles are equivalent [12]; this is not always the case for long-range interactions. The possibility for ensemble inequivalence has provided a profusion of work on the subject over the last decade (see, [13–25] and references therein). Microcanonical and canonical ensemble properties can be determined from the entropy and the free energy, respectively. The free energy in the canonical ensemble is the Legendre–Fenchel transform of the microcanonical entropy. The latter is the inverse transform of the free energy provided that the entropy is strictly concave. This condition is violated (for S is a non-concave function of the energy) in systems with negative heat capacity. The explicit computation, when feasible, of either the entropy or the free energy of long-range interacting systems is in many cases performed using large deviation techniques or a generalized canonical ensemble, which are rather cumbersome [11, 20, 26].

In this paper, we present a simpler and straightforward approach to computing the entropy for a class of classical Hamiltonian systems. We show that for a class of classical Hamiltonian long-range interacting systems, the microcanonical entropy and the one-particle distribution function can be obtained, after the determination of purely numerical constants, using an approach based on the direct solution of the maximum entropy principle. Once the properties of the system in the microcanonical ensemble are known, those in the canonical ensemble can be inferred as discussed above.

The paper is structured as follows. In section 2 we present our approach to compute equilibrium statistical mechanical properties of classical Hamiltonian systems with long-range interactions. We also discuss some implications to ensemble inequivalence. We illustrate our approach with two examples given in section 3: the HMF model and the two-dimensional mean-field system of [27, 28]. We close the paper with some concluding remarks in section 4.

2. Statistical ensembles of long-range interacting systems

For long-range interacting systems starting from an arbitrary initial condition, it is observed that its statistical state undergoes, in a short time, a violent relaxation into a quasi-stationary state [1, 2, 4, 5, 9, 29]. Persistent collective oscillations have also been reported [30]. Quasi-stationary states relax very slowly with a life-time diverging with the number N of particles, into the true thermodynamical equilibrium, with a Gaussian distribution of velocities. A satisfactory theory predicting the resulting quasi-stationary state from the initial distribution is still lacking [17, 31, 32]. In this paper, we are only interested in the thermodynamical properties of the system at the final stage of its evolution, after reaching the true thermodynamical equilibrium.

Here we consider systems with the Hamiltonian of the form

$$H = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{1}{2N} \sum_{i,j=1}^N v(\mathbf{r}_i - \mathbf{r}_j), \quad (2)$$

where $v(\mathbf{r}_i - \mathbf{r}_j)$ is the interparticle potential, and the $1/N$ factor in the second term on the right-hand side was introduced using the Kac prescription [34] and is equivalent to a change in

the unit of time. In this form, the energy is extensive though not necessarily additive. Consider an ensemble formed by a large number of identical copies of the system, in mutual thermal contact, and with an average energy E [35]. Each system is coupled to the thermal bath formed by all the other (identical) systems in the ensemble. The state of each individual system is specified by a point in the N -particle phase space, and the ensemble is hence represented by the N -particle distribution function $f_N(\mathbf{r}_1, \mathbf{p}_1, \dots, \mathbf{r}_N, \mathbf{p}_N)$. The most probable state at equilibrium corresponds to the maximum of the Gibbs entropy,

$$S = - \int f_N \ln f_N \, d\mathbf{r}_1 \dots d\mathbf{r}_N \, d\mathbf{p}_1 \dots d\mathbf{p}_N, \quad (3)$$

satisfying the normalization and average energy constraints:

$$\int f_N \, d\mathbf{r}_1 \dots d\mathbf{r}_N \, d\mathbf{p}_1 \dots d\mathbf{p}_N = 1, \quad (4)$$

$$\int H(\mathbf{r}_1, \mathbf{p}_1, \dots, \mathbf{r}_N, \mathbf{p}_N) f_N \, d\mathbf{r}_1 \dots d\mathbf{r}_N \, d\mathbf{p}_1 \dots d\mathbf{p}_N = E. \quad (5)$$

In equation (3), by choice of units, we set the Boltzmann constant equal to 1 for simplicity of notation. It is important to stress that the total energy of the ensemble is fixed, but not the energy of any given individual system. The average energy of a system in the ensemble is E . This situation hence corresponds to the canonical ensemble. For long-range interactions in the limit $N \rightarrow \infty$, the equilibrium distribution function is fully factored (see [33] and references therein):

$$f_N(\mathbf{p}_1, \dots, \mathbf{p}_N, \mathbf{r}_1, \dots, \mathbf{r}_N, t) = \prod_{i=1}^N f(\mathbf{p}_i, \mathbf{r}_i, t), \quad (6)$$

and the entropy in equation (3) assumes the form

$$S = -N \int f \ln f \, d\mathbf{r} \, d\mathbf{p}, \quad (7)$$

where f is the one-particle distribution function.

Any square integrable function $u(\mathbf{r})$ on a finite domain can be expanded as a convergent series using a basis of orthonormal functions $\{\varphi_k(\mathbf{r})\}$ as [36]

$$u(\mathbf{r}) = \sum_{k=1}^M c_k \varphi_k(\mathbf{r}) + R(\mathbf{r}), \quad (8)$$

where the norm of the rest function R can be made arbitrarily small by increasing M . Divergent potentials for $\mathbf{r} \rightarrow 0$ can be regularized by introducing a softening parameter ϵ such that $v(\mathbf{r}) \rightarrow v(\mathbf{r} + \mathbf{e})$ (\mathbf{e} is a vector with components ϵ). With these considerations, we can expand v as

$$v(\mathbf{r} - \mathbf{r}') \approx \frac{1}{N} \sum_{k=1}^M a_k(\mathbf{r}) b_k(\mathbf{r}'). \quad (9)$$

The approximation in equation (9) can be made as precise as needed. For some models in the literature equation (9) is in fact exact for a finite small M [6, 27, 28]. We identify the mean-field variables:

$$K = \frac{1}{N} \sum_{i=1}^N \frac{p_i^2}{2m}, \quad A_k = \frac{1}{N} \sum_{i=1}^N a_k(\mathbf{r}_i), \quad B_k = \frac{1}{N} \sum_{i=1}^N b_k(\mathbf{r}_i). \quad (10)$$

The Hamiltonian is then written as

$$H = N \left[K + \sum_{k=1}^M A_k B_k \right]. \quad (11)$$

From the factorization of the N -particle distribution function f_N , the canonical equilibrium distribution obtained by maximizing S in equation (3), with the normalization and energy constraints in equations (4) and (5), is equivalent to maximizing the entropy as given by equation (7), with the energy constraint,

$$\int f(\mathbf{p}, \mathbf{r}) \left(\frac{\mathbf{p}^2}{2m} + \frac{1}{2} U(\mathbf{r}) \right) d\mathbf{r} d\mathbf{p} = \epsilon \equiv \frac{E}{N}, \quad (12)$$

and the normalization constraint,

$$\int f(\mathbf{p}, \mathbf{r}) d\mathbf{r} d\mathbf{p} = 1. \quad (13)$$

In equation (12) the mean-field potential is given by

$$U(\mathbf{r}) = \int f(\mathbf{p}, \mathbf{r}, t) v(\mathbf{r} - \mathbf{r}') d\mathbf{p}' d\mathbf{r}'. \quad (14)$$

These expressions are those of an isolated system with fixed energy E as given by equation (12), and therefore also describe the microcanonical ensemble for this same system. As a consequence, both the canonical and microcanonical ensembles correspond to the same extremum solution. They can still be not equivalent as the stability of the equilibrium states is not necessarily the same, as we discuss in section 2.1. We now turn to the solution of the extremum problem for the entropy.

Equating to zero the first variation of S subject to the constraints given in equations (12) and (13) yields

$$-\ln f - 1 - \lambda - \beta e(\mathbf{p}, \mathbf{r}) = 0, \quad (15)$$

where λ and β are Lagrange multipliers and $e(\mathbf{p}, \mathbf{r})$ is the energy of a particle with momentum \mathbf{p} at position \mathbf{r} :

$$e(\mathbf{p}, \mathbf{r}) = \frac{\mathbf{p}^2}{2m} + U(\mathbf{r}). \quad (16)$$

Equation (15) is a self-consistent equation for f , as the potential $U(\mathbf{r})$ is a functional of f . To solve this equation we substitute equations (9) and (14) into equation (15), and define $W = \ln f$:

$$W(\mathbf{r}, \mathbf{p}) = -\beta \sum_{k=1}^M a_k(\mathbf{r}) \int b_k(\mathbf{r}') \exp[W(\mathbf{p}', \mathbf{r}')] d\mathbf{r}' d\mathbf{p}' + \phi(\mathbf{p}), \quad (17)$$

with

$$\phi(\mathbf{p}) = -\beta \frac{\mathbf{p}^2}{2m} - \lambda - 1. \quad (18)$$

This is a nonlinear integral equation of the Hammerstein type with a factored kernel for the unknown function W . Its solution can be obtained analogously to the linear case [36], as we proceed to show. We define the constants

$$\sigma_k = \int b_k(\mathbf{r}') \exp[W(\mathbf{p}', \mathbf{r}')] d\mathbf{r}' d\mathbf{p}', \quad (19)$$

such that equation (17) is rewritten as

$$W(\mathbf{r}, \mathbf{p}) = -\beta \sum_{k=1}^M a_k(\mathbf{r})\sigma_k + \phi(\mathbf{p}) \quad (20)$$

or equivalently

$$f(\mathbf{r}, \mathbf{p}) = C \exp \left[-\beta \left(\sum_{k=1}^M a_k(\mathbf{r})\sigma_k + \frac{\mathbf{p}^2}{2m} \right) \right], \quad (21)$$

where $C = \exp(-\lambda - 1)$ is the normalization constant. Finally, we insert equation (20) into the right-hand side of equation (19):

$$\sigma_k = \int \exp \left[-\beta \sum_{l=1}^M a_l(\mathbf{r})\sigma_l + \phi(\mathbf{p}) \right] b_k(\mathbf{r}) \, d\mathbf{r} \, d\mathbf{p}. \quad (22)$$

Performing the integration in the momenta one gets

$$\sigma_k = C \left(\frac{2m\pi}{\beta} \right)^{d/2} \int \exp \left[-\beta \sum_{l=1}^M a_l(\mathbf{r})\sigma_l \right] b_k(\mathbf{r}) \, d\mathbf{r}. \quad (23)$$

Equation (23) is an algebraic equation for the unknown constants σ_k . It can be solved analytically in some cases, as for the HMF model in section 3.1. If an analytical solution is not feasible, equation (23) can be solved numerically using a standard method for algebraic equations. Once the constants σ_k are known, the distribution function is given in closed form by equation (21).

The Gibbs entropy is obtained by rewriting equation (23) using the definition of $\phi(\mathbf{p})$ and the normalization constant C from equation (21),

$$\begin{aligned} \sigma_k &= \int b_k(\mathbf{r}) \exp \left[-\beta \sum_{k=1}^M a_k(\mathbf{r})\sigma_k \right] d\mathbf{r} \times \left\{ \int \exp \left[-\beta \sum_{k=1}^M a_k(\mathbf{r})\sigma_k \right] d\mathbf{r} \right\}^{-1} \\ &= -\frac{1}{\beta\alpha_l} \frac{\partial}{\partial \sigma_l} \ln Q = B_k, \end{aligned} \quad (24)$$

where we used that for every k there is a unique l such that $a_k = \alpha_l b_l$ (this is always the case for a symmetric potential $v(\mathbf{r} - \mathbf{r}')$ for α_l constant, and

$$Q = \int \exp \left[-\beta \sum_{k=1}^M a_k(\mathbf{r})\sigma_k \right] d\mathbf{r}. \quad (25)$$

Finally, from equations (7), (21) and (24) we obtain

$$s \equiv \frac{S}{N} = \ln \int \exp \left[-\beta \sum_{k=1}^M a_k(\mathbf{r})B_k \right] d\mathbf{r} + \beta \sum_{k=1}^M A_k B_k + \frac{d}{2} + \frac{d}{2} \ln(2m\pi/\beta). \quad (26)$$

Once the values of the constants B_k are known and since K can be determined by usual means, the internal energy $E = H$ is obtained from equation (11) as a function of the Lagrange multiplier β . The entropy as a function of the energy is then obtained in a parametric form. If for a given value of E or β there is more than one solution for the entropy S in equation (26), then only the maximal value corresponds to the true thermodynamical entropy at equilibrium. The remaining solutions are associated with unstable or meta-stable states.

2.1. Stability of the canonical ensemble

The only possibility for classical systems with the Hamiltonian (2) of having non-equivalent microcanonical and canonical ensembles is the presence of a convex dip in the entropy in some energy interval:

$$\partial E / \partial \beta > 0. \quad (27)$$

Using the mean-field variables K , A_k and B_k , the energy per particle ($\epsilon = E/N$) is then given by

$$\epsilon = K + \frac{1}{2} \sum_{k=1}^M A_k B_k. \quad (28)$$

From equations (21) and (24) we obtain

$$-\frac{\partial K}{\partial \beta} = \frac{d}{2\beta^2} \quad (29)$$

and

$$\frac{\partial A_k}{\partial \beta} = A_k \sum_{k'=1}^M A_{k'} B_{k'} - \sum_{k'=1}^M \langle a(\mathbf{r}) b_{k'}(\mathbf{r}) \rangle A_{k'}, \quad (30)$$

$$\frac{\partial B_k}{\partial \beta} = B_k \sum_{k'=1}^M A_{k'} B_{k'} - \sum_{k'=1}^M \langle b_k(\mathbf{r}) a_{k'}(\mathbf{r}) \rangle B_{k'}. \quad (31)$$

In equation (29) d is the dimension of the physical space. By differentiation of the energy in equation (28) and using equations (29)–(31) and from the symmetric properties of the potential one has

$$\frac{\partial \epsilon}{\partial \beta} = -\frac{d}{2\beta^2} + \left[\sum_{k=1}^M A_k B_k \right]^2 - \sum_{k,k'=1}^M A_k \langle b_k(\mathbf{r}) a_{k'}(\mathbf{r}) \rangle B_{k'}. \quad (32)$$

From this expression it is easy to see why the presence of the kinetic energy term is important in many situations to ensure ensemble equivalence, as discussed in [14].

Therefore, if the entropy is convex part in an energy interval $E_1 < E < E_2$, this same interval is forbidden for the canonical ensemble, resulting in a first-order phase transition with an energy jump in the canonical ensemble. As discussed in the previous section, those microcanonical states with a negative heat capacity are also the extrema of the canonical entropy, but with a different stability character. This type of result was observed in some models of long-range forces [19, 27, 28, 37]. For classical Hamiltonian systems of form (2), there is no other source of ensemble inequivalence in the present situation.

3. Applications

In this section, we illustrate our approach with two examples: the HMF model, and a two-dimensional mean-field system displaying first- and second-order phase transitions, and negative heat capacity.

3.1. HMF model

Here we present a new derivation for the entropy of the HMF model using our approach in section 2. The Hamiltonian for the model is given by [6]:

$$H = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^N [1 - \cos(\theta_i - \theta_j)]. \quad (33)$$

We define the mean-field variables

$$M_x(\theta) = \frac{1}{N} \sum_{i=1}^N \cos(\theta_i), \quad M_y(\theta) = \frac{1}{N} \sum_{i=1}^N \sin(\theta_i) \quad (34)$$

and

$$K = \frac{1}{N} \sum_{i=1}^N \frac{p_i^2}{2}. \quad (35)$$

Thus equation (33) can be written in the form

$$H = N \left[K - \frac{1}{2} (M_x^2 + M_y^2) \right], \quad (36)$$

where we dropped out a constant additive term. Without loss of generality, in determining the equilibrium state, we consider the case with $M_x = 0$, which amounts to a choice of origin for the angles. The canonical equilibrium is determined by solving equation (23) with the identifications $\sigma_1 \equiv M_y \equiv A_1 = -B_1$ and $b_1(\theta) = -a_1(\theta) \equiv \sin(\theta)$, and $\sigma_2 = M_x = 0$:

$$M_y = D \int_0^{2\pi} e^{\beta M_y \sin(\theta)} \sin(\theta) d\theta = 2\pi D I_1(\beta M_y), \quad (37)$$

where I_n is the modified Bessel function of the first kind with index n ,

$$D = (2\pi/\beta)^{1/2} \exp(-\lambda - 1),$$

and λ is determined from the normalization condition:

$$\begin{aligned} e^{-\lambda-1} \int f(p, \theta) dp d\theta &= e^{-\lambda-1} \left(\frac{2\pi}{\beta} \right)^{1/2} \int_0^{2\pi} e^{\beta M_y \sin(\theta)} d\theta \\ &= e^{-\lambda-1} \left(\frac{2\pi}{\beta} \right)^{1/2} 2\pi I_0(\beta M_y) = 1. \end{aligned} \quad (38)$$

From equations (37) and (38) we finally obtain

$$M_y = \frac{I_1(\beta M_y)}{I_0(\beta M_y)}, \quad (39)$$

which is the result obtained in [6, 38], but derived in a somewhat simpler way, without resorting to a saddle-point approximation or a Hubbard–Stratonovich transformation.

As shown in [11], both ensembles are fully equivalent for the HMF model. We retrieve now explicitly this result. Equation (32) is written here as

$$\frac{\partial \epsilon}{\partial \beta} = -\frac{1}{2\beta^2} + M_y^2 [M_y^2 - \langle \sin^2 \theta \rangle]. \quad (40)$$

Considering that $M_y^2 = \langle \sin^2 \theta \rangle$, the second term on the right-hand side of equation (39) is also negative, then

$$-\frac{1}{2\beta^2} + M_y^4 - \langle \sin^2 \theta \rangle M_y^2 < 0,$$

implying a positive heat capacity for all energy values. Hence both canonical and microcanonical ensembles are equivalent.

3.2. Two-dimensional mean-field system

Here we consider a two-dimensional system in a torus with the Hamiltonian [27, 28]:

$$H = \frac{1}{2} \sum_{i=1}^N (p_{x,i}^2 + p_{y,i}^2) + V(x, y), \quad (41)$$

$$V(x, y) = \frac{1}{2N} \sum_{i,j=1}^N [2 + a - \cos(x_i - x_j) - \cos(y_i - y_j) - a \cos(x_i - x_j) \cos(y_i - y_j)], \quad (42)$$

where $x_i, y_i \in [0, 2\pi)$ and p_{x_i} and p_{y_i} are the momenta conjugate to x_i and y_i , respectively. This system presents two or three phases depending on the value of the parameter a . For small a it has two phases, with a first-order transition from a Homogeneous phase (HP) to a single-cluster phase (SCP). For higher values of this parameter, it presents an intermediate two-cluster phase (TCP), with first- and second-order transitions connecting it to the SCP and HP phases, respectively. For an interval of values of a the system also presents, inside the negative heat-capacity region, a temperature jump [27]. We show now how this can be obtained straightforwardly within our approach.

The Hamiltonian can be written using the mean-field variables [28]:

$$\begin{aligned} a_1 &= -b_1 = \cos x, & a_2 &= -b_2 = \sin x, \\ a_3 &= -b_3 = \cos y, & a_4 &= -b_4 = \sin y, \\ a_5 &= -\frac{2}{a} b_5 = \cos(x + y), & a_6 &= -\frac{2}{a} b_6 = \sin(x + y), \\ a_7 &= -\frac{2}{a} b_7 = \cos(x - y), & a_8 &= -\frac{2}{a} b_8 = \sin(x - y). \end{aligned} \quad (43)$$

Following [28], due to the symmetry of the Hamiltonian, choosing the origin of the variables x and y and without loss of generality we have $A_1 = A_3, A_5 = A_7$ and $A_2 = A_4 = A_6 = A_8 = 0$, where A_i are defined in equation (10). Thus we have at equilibrium

$$H = N [K + A_1 B_1 + A_5 B_5]. \quad (44)$$

The algebraic system in equation (23) is here given by

$$\begin{aligned} B_1 &= -\frac{\pi}{Q} \int_0^\infty dy e^{-\beta B_1 \cos y} \{\cos y I_0(\beta[B_1 + 2B_5 \cos y]) \\ &\quad - I_1(\beta[B_1 + 2B_5 \cos y])\}, \\ B_5 &= \frac{\pi a}{Q} \int_0^\infty dy e^{-\beta B_1 \cos y} \cos y I_1(\beta[B_1 + 2B_5 \cos y]), \end{aligned} \quad (45)$$

where

$$Q = 2\pi \int_0^\infty dy e^{-\beta B_1 \cos y} \cos y I_0(\beta[B_1 + 2B_5 \cos y]), \quad (46)$$

and I_0 and I_1 are Bessel functions of the first kind.

In order to illustrate our approach, we consider the parameter value $a = 2$, where both negative heat capacity and temperature jump occur. The solutions to equations (45) are determined numerically using a globally convergent Broydn method [39], and are shown in figure 1. The figure clearly shows a back-bending of the curves $B_1(\beta)$ and $B_5(\beta)$ corresponding

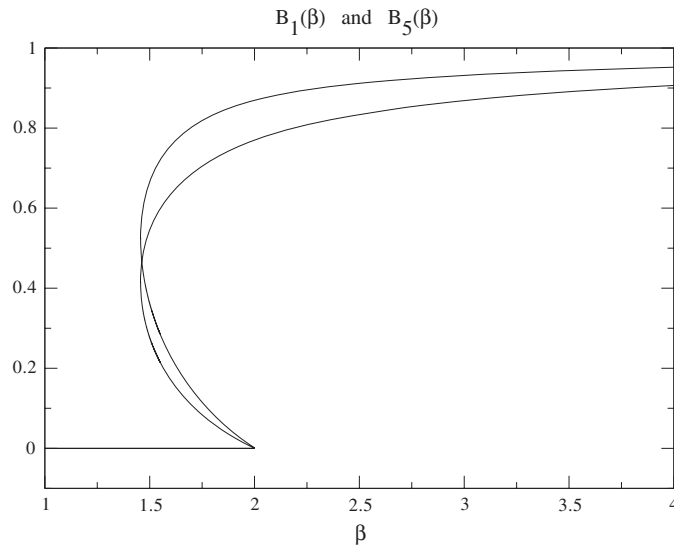


Figure 1. Numerical solutions of equation (45). The curve with the highest value at $\beta = 4$ is the function $B_1(\beta)$, and the one with lower value $B_5(\beta)$.

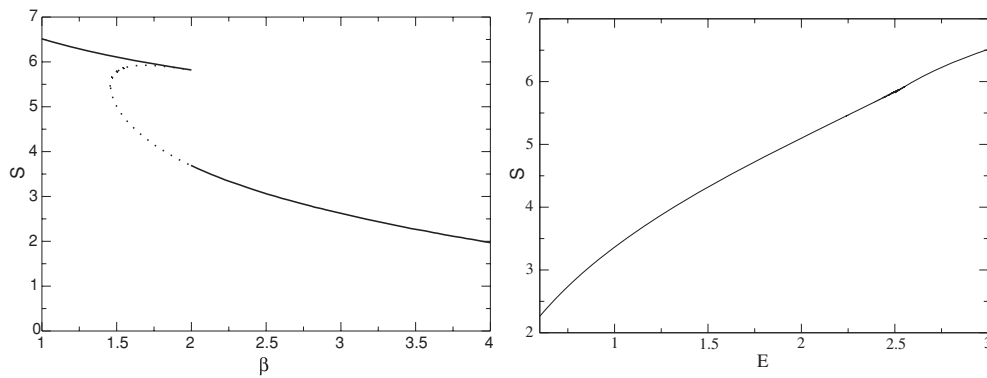


Figure 2. Left panel: entropy S as a function of β . Near the phase transition there is more than one solution for equation (23). The continuous lines correspond to the true (equilibrium) entropy and the dotted line to unstable or meta-stable states. Right panel: entropy as a function of energy per particle E . The convex dip is slightly visible here.

to the negative specific energy region. In the left panel of figure 2 we show the entropy as a function of the inverse temperature of β , and in the right panel the entropy as a function of energy E , obtained using the prescription in section 2. The curve $S(E)$ has a shallow convex dip, but still visible in the figure. The left panel of figure 2 shows that in the energy interval with a negative heat capacity the entropy has one global and two local maxima, which are respectively stable and meta-stable states in the microcanonical ensemble. The stable and meta-stable solution branches intersect transversely at $\beta \approx 2.548$ as shown in the enlarged graph of $S(\beta)$ in figure 3, leading to a temperature jump in the microcanonical ensemble. This temperature jump can only occur inside the negative heat-capacity region, which is also the condition for the existence of meta-stable states. Correspondingly in the

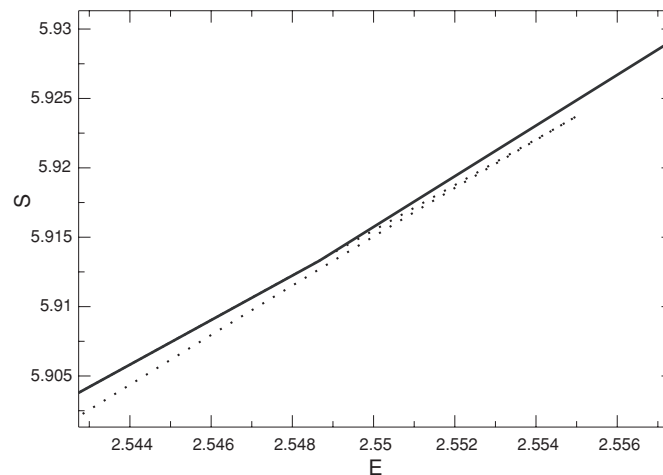


Figure 3. Graph of $S(E)$ showing the crossing of two solution branches. The continuous line corresponds to stable equilibrium states and the dotted line to unstable in meta-stable states.

canonical ensemble a first-order phase transition with an energy jump occurs, corresponding to the negative heat-capacity region, thus hiding the temperature jump.

4. Concluding remarks

We presented a new approach to computing the entropy of a class of long-range interacting systems by reducing the extremum principle for the entropy to the solution of a set of algebraic equations for the equilibrium values of global variables. For classical Hamiltonian systems with long-range interactions, our approach is simpler than large deviation techniques or the saddle-point approximation. The one-particle distribution function is obtained in closed form, depending on numerical constants which are solutions of purely algebraic equations (23). The microcanonical entropy is a more fundamental function, since other thermodynamic potentials can be obtained from it, though the opposite is not always true for long-range interacting systems. Besides being a more simple calculation procedure for the determination of the entropy, as illustrated by the HMF and two-dimensional systems in section 3, our approach is well suited for discussed ensemble inequivalence in classical Hamiltonian systems. It can also be used as a starting point for new approximate numerical methods. Its extension to systems including discrete variables, as the Colson–Bonifacio [7] or the Blume–Emery–Griffiths models [40], is straightforward.

Acknowledgments

TMRF and AF acknowledge financial support from CNPq (Brazil).

References

- [1] Dauxois T *et al* (ed) 2002 *Dynamics and Thermodynamics of Systems with Long-Range Interactions (Lecture Notes in Physics vol 602)* (New York: Springer)
- [2] Campa A *et al* (ed) 2008 *Dynamics and Thermodynamics of Systems with Long-Range Interactions: Theory and Experiments (AIP Conf. Proc. vol 970)* (New York: AIP)

- [3] Padmanabhan T 1990 *Phys. Rep.* **188** 285
- [4] Levin Y, Pakter R and Teles T N 2008 *Phys. Rev. Lett.* **100** 040604
- [5] Levin Y, Pakter R and Teles T N 2008 *Phys. Rev. E* **78** 021130
- [6] Antoni M and Ruffo S 1995 *Phys. Rev. E* **52** 2361
- [7] Bonifacio R, Casagrande F, Cerchioni G, De Salvo Souza L, Pierini P and Piovella N 1990 *Riv. Nuovo Cimento* **13** 1
- [8] Tennyson J L, Meiss J D and Morrison P J 1994 *Physica D* **71** 1
- [9] Binney J and Tremaine S 1987 *Galactic Dynamics* (Princeton, NJ: Princeton University Press)
- [10] Lynden-Bell D 1999 *Physica A* **263** 293
- [11] Barré J, Bouchet F, Dauxois T and Ruffo S 2005 *J. Stat. Phys.* **119** 677
- [12] Lebowitz J L and Lieb E H 1969 *Phys. Rev. Lett.* **22** 631
- [13] Barré J, Mukamel D and Ruffo S 2002 *Ensemble Inequivalence in Mean-Field Models of Magnetism (Lecture Notes in Physics vol 602)* ed T Dauxois (New York: Springer)
- [14] Casetti L and Kastner M *et al* 2007 *Physica A* **384** 318
- [15] Bouchet F and Barré J 2005 *J. Stat. Phys.* **118** 1073
- [16] Ellis R S, Touchette H and Turkington B 2004 *Physica A* **335** 518
- [17] Arad I and Lynden-Bell D 2005 *Mon. Not. R. Astron. Soc.* **361** 385A
- [18] Leyvraz F and Ruffo S 2002 *J. Phys. A: Math. Gen.* **35** 285
- [19] Antoni M, Ruffo S and Torcini A 2004 *Eur. Phys. Lett.* **66** 645
- [20] Ellis R S, Haven K and Turkington B 2000 *J. Stat. Phys.* **101** 999
- [21] Leyvraz F and Ruffo S 2002 *Physica A* **305** 58
- [22] Touchette H, Ellis R S and Turkington B *Physica A* **340** 138
- [23] Costeniuc M, Ellis R S, Touchette H and Turkington B 2006 *Phys. Rev. E* **73** 026105
- [24] Costeniuc M, Ellis R S, Touchette H and Turkington B 2005 *J. Stat. Phys.* **119** 1283
- [25] Costeniuc M, Ellis R S and Touchette H 2006 *Phys. Rev. E* **74** 010105
- [26] Ellis R S 1985 *Entropy, Large Deviations and Statistical Mechanics* (New York: Springer)
- [27] Antoni M, Ruffo S and Torcini A 2002 *Phys. Rev. E* **66** 025103
- [28] Torcini A and Antoni M 1999 *Phys. Rev. E* **59** 2746
- [29] Lynden-Bell D 1967 *Mon. Not. R. Astron. Soc.* **136** 101
- [30] Jeong D, Choi J and Choi M Y 2006 *Phys. Rev. E* **74** 056106
- [31] Arad I and Johansson P H 2005 *Mon. Not. R. Astron. Soc.* **362** 252
- [32] Rocha Filho T M, Figueiredo A and Amato M A 2005 *Phys. Rev. Lett.* **95** 190601
- [33] Chavanis P H 2006 *Physica A* **361** 55
- [34] Kac M, Uhlenbeck G E and Hemmer P C 1963 *J. Math. Phys.* **4** 216
- [35] Schrödinger E 1989 *Statistical Thermodynamics* (New York: Dover)
- [36] Tricomi F G 1985 *Integral Equations* (New York: Dover)
- [37] Tatekawa T, Bouchet F, Dauxois T and Ruffo S 2005 *Phys. Rev. E* **71** 056111
- [38] Latora V, Rapisarda A and Ruffo S 1999 *Physica D* **131** 38
- [39] Press W H, Teukolsky S A, Vetterling W T and Flannery P 1992 *Numerical Recipes* 2nd edn (New York: Cambridge University Press)
- [40] Blume M, Emery V J and Griffith R B 1971 *Phys. Rev. A* **4** 1071