


Partial equivalence of statistical ensembles in a simple spin model with discontinuous phase transitions

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In this paper, we draw attention to the problem of phase transitions in systems with locally affine microcanonical entropy, in which partial equivalence of (microcanonical and canonical) ensembles is observed. We focus on a very simple spin model, that was shown to be an equilibrium statistical mechanics representation of the biased random walk. The model exhibits interesting discontinuous phase transitions that are simultaneously observed in the microcanonical, canonical, and grand canonical ensemble, although in each of these ensembles the transition occurs in a slightly different way. The differences are related to fluctuations accompanying the discontinuous change of the number of positive spins. In the microcanonical ensemble, there is no fluctuation at all. In the canonical ensemble, one observes power-law fluctuations, which are, however, size dependent and disappear in the thermodynamic limit. Finally, in the grand canonical ensemble, the discontinuous transition is of mixed order (hybrid) kind with diverging (critical-like) fluctuations. In general, this paper consists of many small results, which together make up an interesting example of phase transitions that are not covered by the known classifications of these phenomena.

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I. INTRODUCTION

Classic ideal gas has the same properties regardless of whether it is studied in the formalism of the microcanonical, canonical, or grand canonical ensemble [1–3]. Many other models of statistical physics also show such a correspondence. Because of that time, over time, the feature began to be considered as a kind of paradigm of statistical physics. However, the truth is that the so-called equivalence of ensembles does not hold in general and the prominent counterexamples are nonadditive systems, which include systems with long range interactions [4,5].

The first mentions of nonequivalent ensembles began to appear about 50 years ago (e.g., [6–8]), and they concerned astrophysical self-gravitating systems. Over time, however, the problem was also noticed in other physical systems and models (to name a few examples, see [9–19]). Some time ago, systematic research on these phenomena started, which, in addition to studying specific models, laid the foundations for the general theory of nonequivalent ensembles [20–24].

Among the references just mentioned, two contributions [20,21] deserve special attention. The first one, entitled “Large deviation principles and complete equivalence and nonequivalence results for pure and mixed ensembles” by Ellis *et al.* [20], provides the basis for a complete mathematical theory of the problem. The authors show there that the issue of nonequivalent ensembles can be resolved by examining the concavity of entropy as a function of energy, $S(U)$. In short, in [20] (see also [22,23]), the authors show that microcanonical and canonical ensembles are *equivalent* when $S(U)$ is strictly concave. *Nonequivalence* is observed when $S(U)$ is convex. Finally, the *partial equivalence* is referred to systems with locally affine $S(U)$.

In turn, [21], entitled “Classification of phase transitions and ensemble inequivalence in systems with long range interactions,” by Bouchet and Barre, takes up an important issue of phase transitions in nonequivalent ensembles. By combining the singularity and concavity analysis of the entropy $S(U)$, the authors present a kind of thermodynamic classification of the phase transitions in nonequivalent ensembles.

To be concrete, in the case of equivalent ensembles, microcanonical macrostates with the fixed energy U and microcanonical temperature given by $\beta_m = \partial S / \partial U$ directly correspond to canonical macrostates with the fixed temperature and average energy satisfying $\beta = \beta_m$ and $\langle U \rangle = U$, respectively. The equivalence of ensembles holds whenever entropy is a concave function, regardless of whether the considered system is additive or not. The case of macrostates for which $S(U)$ is a convex function is much more complicated. In general, convex macrostates have less entropy than states represented by the concave envelope of $S(U)$. Therefore, such envelope states are realized in additive systems, where they correspond to phase separation. They are, however, forbidden in nonadditive systems. Thus, the lack of additivity forces the system to realize convex states, which (surprisingly) make the microcanonical ensemble much more interesting than the canonical one. An immediate consequence of such states is, for example, negative specific heat or negative magnetic susceptibility. Other noncommon behaviors arising from ensemble nonequivalence relate to the entire spectrum of microcanonical phase transitions, which are not visible in other ensembles.

In particular, a number of generic situations, regarding concave and convex entropies, and having the hallmarks of microcanonical phase transitions, were discussed in [21]. Many of these possible generic situations have not yet been observed in any models, not to mention real systems. Clearly,

there is a lot of work to be done in this field, especially since so far little attention has been paid to the partial equivalence of ensembles [25]. To be honest, the preliminary classification of phase transitions in nonadditive [26] systems developed in [21] completely ignores the cases with locally affine entropy and focuses only on singularities arising in its concave and convex regions. This paper aims to make a small contribution to this omitted area.

In what follows, we study the partial equivalence of ensembles in the so-called minimal diffusion-based spin model, which has been introduced in [27]. It was already shown that the model exhibits very interesting critical-like behavior (i.e., Thouless effect [27] and hybrid phase transition [28]), when it is analyzed in the canonical and grand canonical ensemble. In this paper, we confront microcanonical and canonical properties of the model. Our paper reveals that in this simple model a unique first order transition in both ensembles emerges, which results from affine thermodynamic potentials. Not so long ago, the possibility of such a behavior was predicted theoretically [29]. Such a generic situation, however, has not been raised in the context of phase transitions in partially equivalent ensembles [21], which we are doing here.

II. PARTIAL EQUIVALENCE OF ENSEMBLES: CASE STUDY

A. The model

The spin model we deal with is completely defined by the Hamiltonian:

$$\mathcal{H}_N(\Omega) = -N_+(\Omega) \ln a + \ln \binom{N}{N_+(\Omega)}, \quad (1)$$

where $\Omega = (s_1, s_2, \dots, s_N)$ represents microscopic configuration of the system of N distinguishable spins $s_i = \pm 1$, with $N_+(\Omega)$ standing for the number of positive spins, and $a > 0$ being the model external parameter [with the notion from [27] we take $a = (1 - q)/q$]. Although in [27] the model was designed to provide theoretical explanation for certain critical-like phenomena observed in a dynamic social network [30,31], and although it was shown there that its dynamical properties can be one-to-one related to the phenomenon of the biased random walk, in this paper, we cut ourselves off from the question of whether the model is physically realistic or not. We just treat it as a toy model having some nontrivial properties resulting from the lack of additivity (i.e., $\mathcal{H}_N + \mathcal{H}_R \neq \mathcal{H}_{N+R}$).

B. Microcanonical ensemble

In textbooks on statistical physics, the discussion of the microcanonical ensemble usually precedes the discussion of the canonical ensemble. In this paper, we also uphold this habit. Our first goal is to draw up the microcanonical phase diagram of the considered model and to identify phase transition points on it.

In the microcanonical ensemble, one assumes that the energy U of the system as a whole is fixed. In this paper, however, since we study systems in the thermodynamic limit, $N \rightarrow \infty$, instead of the total energy U , as the control parameter, we use the energy per spin, u , which is given by [cf.

Eq. (1)]

$$u = \frac{U}{N} = -\ln a n_+ - n_+ \ln n_+ - n_- \ln n_-, \quad (2)$$

where

$$n_+ = N_+/N, \quad n_- = 1 - n_+. \quad (3)$$

Equation (2) defines energy as a function of the number of positive spins n_+ and the parameter a , i.e., $u(n_+, a)$. Since the variable n_+ belongs to the range $[0, 1]$, the energy per spin is not arbitrary, but it meets certain restrictions [see Figs. 1(a)–1(c)]. In particular,

$$\begin{aligned} \text{for } a < 1: & \quad u \in [u(0), u_{\max}] = [0, \ln \frac{1+a}{a}], \\ \text{for } a = 1: & \quad u \in [u(0), u_{\max}] = [u(1), u_{\max}] = [0, \ln 2], \\ \text{for } a > 1: & \quad u \in [u(1), u_{\max}] = [-\ln a, \ln \frac{1+a}{a}], \end{aligned}$$

where $u_{\max} = u(n_+^*, a) = \ln \frac{a+1}{a}$ is the maximum energy value obtained for $n_+^* = \frac{1}{a+1}$. A few realizations of $u(n_+, a)$, for various representative values of the parameter a are shown in Figs. 1(a)–1(c). In this figure, one can see that certain energy values can be realized in one way and others can be realized in two ways. In the first case, microcanonical entropy of the system is simply given by

$$S = \ln \binom{N}{N_+}. \quad (4)$$

The second case, with two different macroscopic realizations of the system, $n_+^{(1)}$ and $n_+^{(2)}$ [see Figs. 1(a)–1(c)], is a bit more complicated. Now, microcanonical entropy of the system is given by

$$S = \ln \left[\binom{N}{N_+^{(1)}} + \binom{N}{N_+^{(2)}} \right], \quad (5)$$

where $N_+^{(i)} = N n_+^{(i)}$ for $i = 1, 2$. In the thermodynamic limit $N \rightarrow \infty$, Eq. (5) reduces to Eq. (4) with N_+ standing for the macrostate with higher entropy among the two considered, i.e.,

$$\binom{N}{N_+} = \max \left\{ \binom{N}{N_+^{(1)}}, \binom{N}{N_+^{(2)}} \right\}. \quad (6)$$

In Figs. 1(a) and 1(c), the bold parts of the $u(n_+, a)$ curves represent those system realizations (macrostates) that have greater entropy and therefore they are more likely to occur. Correspondingly, in the thermodynamic limit, microcanonical entropy per spin underlying ergodic dynamics of the system can be written as

$$s = \frac{S}{N} = \frac{\ln \binom{N}{N_+}}{N} = -n_+ \ln n_+ - n_- \ln n_- \quad (7)$$

$$= u + n_+ \ln a, \quad (8)$$

where n_+ refers to the most entropic state satisfying the energy constraint, Eq. (2).

Figures 1(d)–1(f) show a few realizations of $s(u, a)$, Eq. (7), for various representative values of the parameter a . By making simple calculations [32], one can show that these entropy curves are strictly concave for all values of the parameter $a \neq 1$. The case when $a = 1$ is an exception. Then, entropy becomes affine in the whole energy range: $s(u, a) = u$ for $u \in [0, \ln 2]$. According to what was said at the

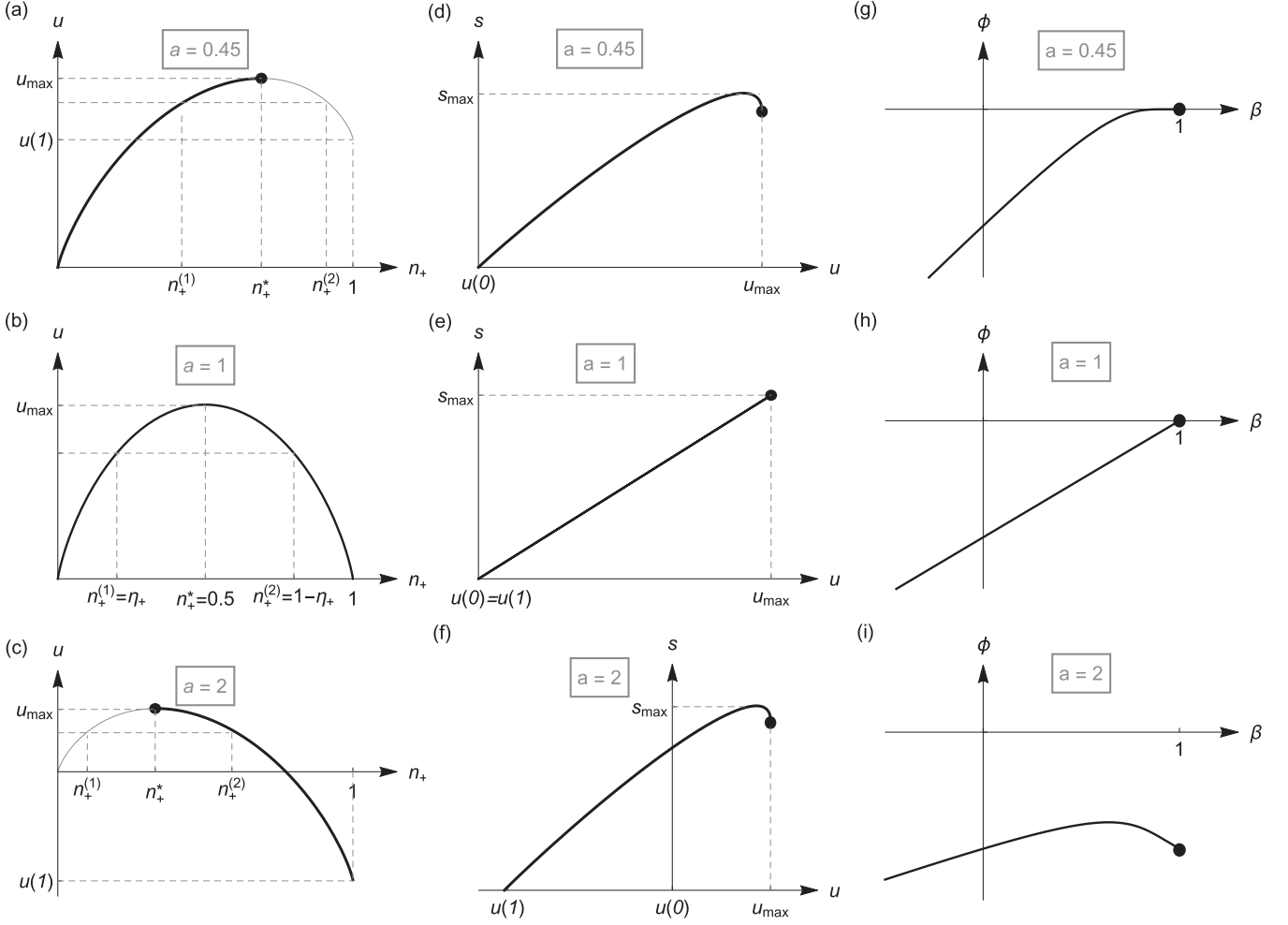


FIG. 1. A few realizations of different thermodynamic state functions characterizing the model for three representative values of the parameter $a = 0.45, 1.0, 2.0$. In the first column, in graphs (a)–(c), internal energy, u , as a function of the number of positive spins, n_+ , is shown [see Eq. (2)]. In the second column, in graphs (d)–(f), microcanonical entropy per spin, s , is presented as a function of the internal energy, u [see Eq. (7)]. In the third column, in graphs (g)–(i), free energy per spin ϕ characterizing the model in the canonical ensemble is drawn as a function of β [see Eq. (21)]. The meaning of bold parts of the $u(n_+, a)$ and $s(u, a)$ curves, and other symbols in this figure (e.g., u_{\max} , n_+^* , $n_+^{(1)}$, $n_+^{(2)}$, etc.), is explained in the main text.

beginning of this paper, the strict concavity of $s(u, a)$ proves the equivalence of statistical ensembles while affinity results in partial equivalence. Now, we will take a closer look at these issues. To this aim, we will compare phase diagrams, microcanonical and canonical, of the model.

To start with, let us note that the microcanonical temperature of the model is given by

$$\beta_m = \frac{\partial s}{\partial u} = \frac{\partial s}{\partial n_+} \frac{\partial n_+}{\partial u} = \frac{\ln \left(\frac{n_+}{n_-} \right)}{\ln a + \ln \left(\frac{n_+}{n_-} \right)}, \quad (9)$$

where n_+ , which stands for the most entropic macrostate, is not arbitrary but it depends on u and a , which are the control parameters in this ensemble. In particular, this makes the range of temperatures $\beta_m > 1$ unattainable in this model. To make this inaccessibility more understandable, let us concentrate, for example, on Fig. 1(a). For a given value of the energy u (marked by the intermediate horizontal dashed line), there are two possible states $n_+^{(1)} = 0.42$ and $n_+^{(2)} = 0.91$. According to Eq. (9), the first one corresponds to $\beta_m = 0.3$

and the second one corresponds to $\beta_m = 2$ (i.e., $\beta_m > 1$). However, for large systems, the number of microstates that could be realized for $n_+^{(1)}$ is of orders of magnitude larger than that for $n_+^{(2)}$ (e.g., the factor is 10^{164} for $N = 1000$). It means that the system will visit almost all the time the state characterized by $\beta_m = 0.3$. In this sense, the temperature $\beta_m > 1$ is inaccessible in the thermodynamic limit.

Furthermore, for $a = 1$, regardless of the energy value, the microcanonical temperature is always $\beta_m = 1$. It means that phase diagram points for which $a=1$ and $\beta_m \neq 1$ are forbidden [see Fig. 2(a)]. Correspondingly, for $a = 1$ and $\beta_m = 1$, discontinuous phase transition occurs for different values of u . It is due to the fact that for $a = 1$ (or $\ln a = 0$) and for the energy values $u \in [0, \ln 2)$ there are always two different macrostates [i.e., $n_+^{(1)} = \eta_+$ and $n_+^{(2)} = 1 - \eta_+$, see Fig. 1(b)] which have the same entropy. When $a \neq 1$, one of these states becomes more entropic [see the discussion that accompanies Eqs. (4)–(7)]. This leads to a discontinuous jump in n_+ . The size of this jump depends on the energy of

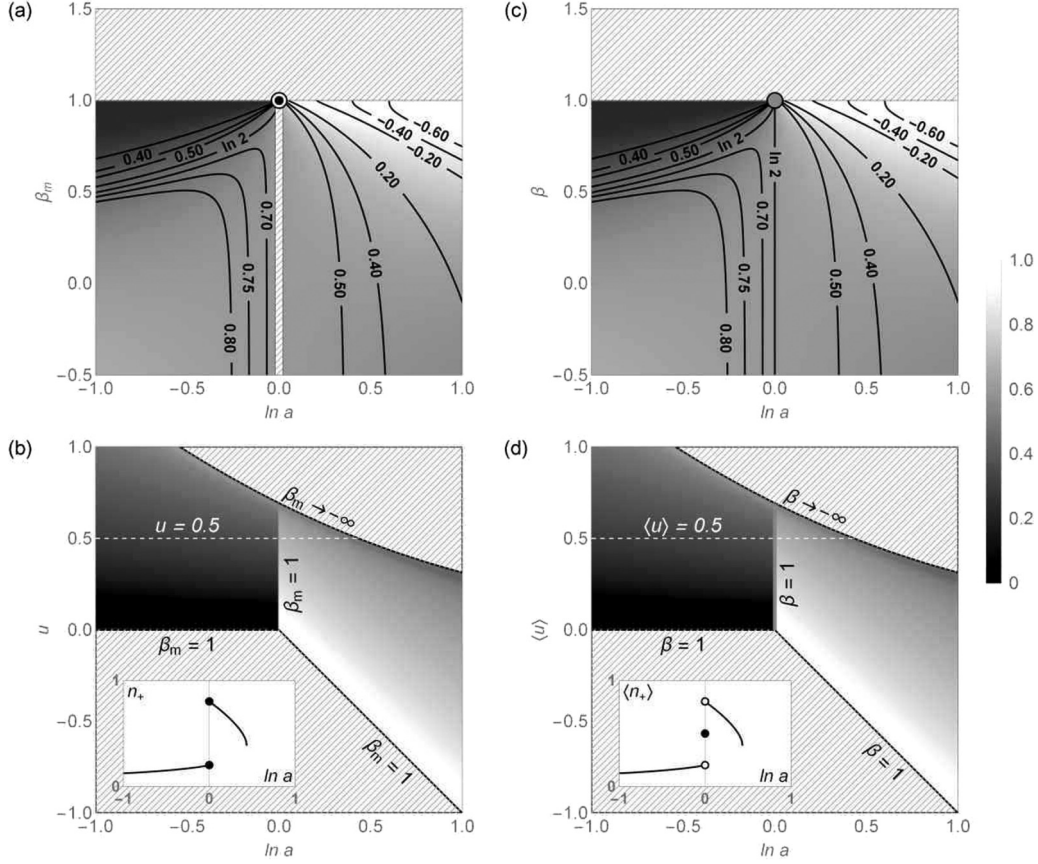


FIG. 2. Phase diagrams of the model in the microcanonical (a, b) and canonical ensemble (c, d). Two variants of phase diagrams are shown: (i) (a) and (c) present the number of positive spins [n_+ and $\langle n_+ \rangle$, cf. Eqs. (10) and (19)] as a function of the inverse temperature (β_m and β , respectively) and the parameter a , and (ii) (b) and (d) show the number of positive spins as a function of the internal energy (correspondingly, u and $\langle u \rangle$) and the parameter a . The grayscale bar on the right represents the average number of spins. The hatched areas indicate forbidden macrostates. The black contour lines in graphs (a) and (c) highlight states with a given value of the internal energy, u and $\langle u \rangle$, respectively. The phase transition points $a = 1$ and $\beta_m = \beta = 1$, in diagrams (a) and (c), correspond to straight line segments: $a = 1$ and $u, \langle u \rangle \in [0, \ln 2]$ in diagrams (b) and (d). Inset plots in (b) and (d) show cross sections of these diagrams for $u = \langle u \rangle = 0.5$, respectively.

the system. This is clearly visible in Fig. 2(b), where n_+ is depicted as a function of u and a .

Finally, from Eq. (9), the expression for n_+ as a function of β_m and $a \neq 1$ can be obtained:

$$n_+(\beta_m, a) = \frac{1}{1 + a^{\kappa_m}}, \quad \text{where } \kappa_m = \frac{\beta_m}{\beta_m - 1}, \quad (10)$$

which is useful in drawing up the microcanonical phase diagram of the model. In Fig. 2(a), forbidden macrostates are marked as hatched areas. As already said, in addition to states for which $a = 1$ and $\beta_m \neq 1$, all macrostates with $\beta_m > 1$ are also unavailable. The solid lines in Fig. 2(a) indicate states with the same energy (numbers placed on these curves correspond to different values of u). The point $a = \beta_m = 1$, at which all these curves converge, is the point of the first order microcanonical transition. From Eqs. (2) and (10) one can show that

$$\lim_{\beta_m \rightarrow 1^-} n_+(\beta_m, a) = \begin{cases} 0 & \text{for } \ln a < 0 \\ \eta_+ & \text{for } \ln a \rightarrow 0^- \\ 1 - \eta_+ & \text{for } \ln a \rightarrow 0^+ \\ 1 & \text{for } \ln a > 0 \end{cases}, \quad (11)$$

where $\eta_+ \leq \frac{1}{2}$ and $1 - \eta_+ \geq \frac{1}{2}$ represent the allowed macrostates of equal entropy in the system for which $a = 1$ [see Fig. 1(b) and Fig. 2(b) inset].

Below we show that the canonical phase diagram differs from the just described microcanonical one.

C. Canonical ensemble

As mentioned at the beginning of this paper, some canonical analysis of the considered model has already been carried out. Namely, in [27], properties of the model at fixed temperature, $\beta = 1$, have been studied. It was shown there that, when the parameter a approaches unity, an interesting discontinuous phase transition with diverging response function is observed.

To be concrete, for $\beta = 1$, the partition function was shown to be given by

$$Z_N(a) = \sum_{\Omega} e^{-\mathcal{H}_N(\Omega)} = \frac{1 - a^{N+1}}{1 - a}. \quad (12)$$

Resulting from the above expression, Helmholtz free energy per spin has a singularity at $a = 1$. This singularity leads to a

discontinuous jump in the average number of positive spins:

$$\langle n_+ \rangle = \lim_{N \rightarrow \infty} \frac{\langle N_+ \rangle}{N} = \begin{cases} 0 & \text{for } \ln a < 0 \\ \frac{1}{2} & \text{for } \ln a = 0, \\ 1 & \text{for } \ln a > 0 \end{cases} \quad (13)$$

which is accompanied by diverging susceptibility:

$$\chi = \frac{\partial \langle n_+ \rangle}{\partial a} \sim \frac{1}{N} |a - 1|^{-2}. \quad (14)$$

Although further in this section a more extensive canonical analysis of this model for any temperature value is performed, already at this moment, we highlight that at the transition point $\beta = \beta_m = 1$ and $a = 1$ both (microcanonical and canonical) ensembles differ from each other at the level of macrostates [cf. Eqs. (11) and (13)].

For arbitrary temperature, in the continuum limit, the partition function of the model can be written as

$$Z_N(\beta, a) = \sum_{\Omega} e^{-\beta \mathcal{H}_N(\Omega)} \quad (15)$$

$$= \sum_{N_+=0}^N \binom{N}{N_+}^{1-\beta} a^{\beta N_+} \quad (16)$$

$$= N \int_0^1 e^{-N\phi(n_+; \beta, a)} dn_+, \quad (17)$$

where

$$\phi(n_+; \beta, a) = (1 - \beta)(n_+ \ln n_+ + n_- \ln n_-) - \beta n_+ \ln a. \quad (18)$$

It is easy to check that for $\beta < 1$ the function $\phi(n_+; \beta, a)$ is strictly convex with respect to n_+ on the interval $[0, 1]$. Furthermore, in this interval, it has a minimum at

$$n_+^c = \frac{1}{1 + a^\kappa}, \quad \text{where } \kappa = \frac{\beta}{\beta - 1}. \quad (19)$$

Therefore, for $\beta < 1$, the Laplace method of steepest descents (also known as the saddle-point method) can be used to calculate the integral (17). In this way one gets

$$Z_N(\beta, a) \asymp e^{-N\phi(\beta, a)}, \quad (20)$$

where

$$\phi(\beta, a) \stackrel{\text{Eq. (18)}}{=} \phi(n_+^c; \beta, a) = (1 - \beta) \ln \left(\frac{a^\kappa}{1 + a^\kappa} \right). \quad (21)$$

The symbol “ \asymp ” in Eq. (20) means that, as $N \rightarrow \infty$, the dominant part of the partition function, $Z_N(\beta, a)$, scales exponentially with the system size.

Rephrasing the remark closing the last paragraph, one could say that for $\beta < 1$ the considered system is extensive. This is because its free energy [33]

$$\Phi_N(\beta, a) = -\ln Z_N(\beta, a) \stackrel{N \gg 1}{\asymp} N\phi(\beta, a) \quad (22)$$

is linear with respect to N . This confirms the known fact that extensiveness is not in contradiction with the lack of additivity. On the other hand, for $\beta > 1$, due to strict concavity of $\phi(n_+; \beta, a)$ with respect to n_+ , the model is nonextensive. We will not bother with this case here.

In what follows, we discuss thermodynamic properties of the model in the canonical ensemble. These properties can be easily obtained from the bulk free energy, $\phi(\beta, a)$ (21), which is an analytic and concave function for all $\beta < 1$ and $a > 0$ [see Figs. 1(g)–1(i)]. For these parameter ranges, the average number of positive spins is also an analytic function,

$$\langle n_+ \rangle = -\frac{1}{\beta} \frac{\partial \phi(\beta, a)}{\partial \ln a} = \frac{1}{1 + a^\kappa}, \quad (23)$$

just like the average energy

$$\langle u \rangle = \frac{\partial \phi(\beta, a)}{\partial \beta} = -\langle n_+ \rangle \ln(a \langle n_+ \rangle) - \langle n_- \rangle \ln \langle n_- \rangle, \quad (24)$$

where $\langle n_- \rangle = 1 - \langle n_+ \rangle$. It is remarkable that Eqs. (23) and (24) have the same form as the corresponding Eqs. (10) and (2) in the microcanonical ensemble. The difference, however, arises when ranges of their applicability are taken into account. Namely, in the canonical ensemble, when $a = 1$, for the entire temperature range, $\beta \leq 1$, one has $\langle n_+ \rangle = \frac{1}{2}$ and $\langle u \rangle = \ln 2$. On the other hand, in the microcanonical ensemble, when $a = 1$, the states with $\beta_m < 1$ are forbidden, whereas for $\beta_m = 1$ the number of positive spins, η_+ , depends on $u \in [0, \ln 2]$ [see Eq. (11)]. The above properties of the model are illustrated in Fig. 2, where the canonical phase diagram is shown in comparison to its microcanonical version.

D. Partial equivalence and phase transitions

The equivalence of microcanonical and canonical ensembles of the model studied, which holds for $\beta \leq 1$ and $a \neq 1$, is in agreement with theoretical predictions of [20]. It is due to strict concavity of the microcanonical entropy as a function of u . For $a = 1$, when entropy becomes affine in u , partial equivalence is observed in the model, again in agreement with [20].

As emphasized in [25], in a situation of partial equivalence, a whole set of values of the control parameter in one ensemble corresponds to a single value of the control parameter in the other ensemble. In particular, the same value of the average energy can be obtained for the whole set of canonical temperatures, or the whole set of energies characterizing microcanonical systems may show the same microcanonical temperature. In our case study, both behaviors are observed, which make the considered model interesting, because in the systems studied so far at most one (usually the first one) of these behaviors was observed.

Another valuable feature of the model studied is a unique phenomenology of the observed first order transition that occurs simultaneously in both ensembles. In additive systems, the commonly known cause of such simultaneous transitions is the bimodal shape of the microcanonical entropy as a function of the energy. In nonadditive systems, when only strict nonequivalence of ensembles is taken into account, much richer phenomenology comes into play [21], which, however, in any of the possible scenarios, does not lead to simultaneous (in both ensembles) first order transitions. Our paper shows that such a scenario is possible in partially equivalent ensembles.

In our model, the microcanonical transition arises as a result of singularity in entropy $s(u, a)$ (7) that appears at $a = 1$

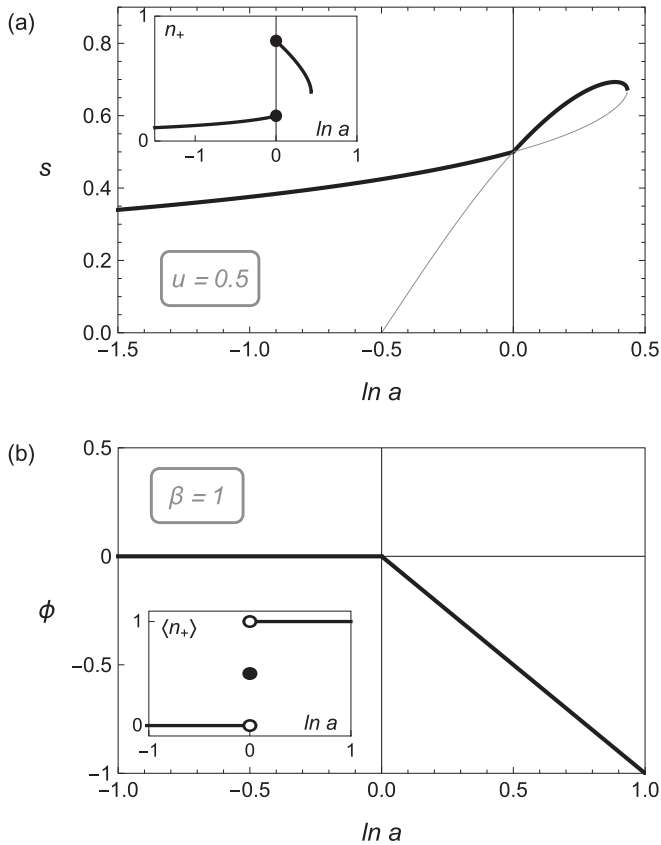


FIG. 3. Thermodynamic state functions in the vicinity of the transition point: (a) the microcanonical entropy per spin, $s(u, a)$ (8), as a function of the parameter a for $u = 0.5$, and (b) the free energy per spin, $\phi(\beta, a)$ (21), as a function of the parameter a for $\beta = 1$. These state functions have nonanalytical points for $a = 1$ and $u \in [0, \ln 2)$, in the microcanonical ensemble, and for $a = \beta = 1$, in the canonical ensemble, respectively. These nonanalytical points are seen as discontinuities of the corresponding derivatives: $n_+ = \partial s / \partial \ln a$ and $\langle n_+ \rangle = -\partial \phi / \partial \ln a$ (see inset plots).

(and correspondingly $\beta_m = 1$) when energy of the system is in the range $u \in [0, \ln 2)$. At this point, the right- and left-sided derivatives of $s(u, a)$ with respect to $\ln a$, which give the average number of positive spins, $n_+ = \partial s / \partial \ln a$, differ from each other [see Eq. (11) and Fig. 3(a)]. On the other hand, the canonical first order transition, that appears for the same parameter values as in the microcanonical ensemble, $a = 1$ and $\beta = 1$, results from the free energy (21) composed of two parts, flat [i.e., $\phi(1, a) \stackrel{a < 1}{=} 0$] and affine [i.e.,

$\phi(1, a) \stackrel{a \geq 1}{=} -\ln a$], at the interface of which a nonanalytical point develops [see Eq. (13) and Fig. 3(b)]. Not so long ago, purely theoretical considerations about such a canonical transition were put forward in [29]. The model studied in this paper is one in which such a transition was observed as resulting from the affine microcanonical entropy which is defined on a limited energy range.

III. CONCLUDING REMARKS

In this paper, we draw attention to the problem of phase transitions in partially equivalent ensembles. We focus on a very simple spin model which shows interesting discontinuous phase transitions that are simultaneously observed in all three basic statistical ensembles (microcanonical, canonical, and grand canonical), although in each of these three ensembles they occur in a slightly different way.

In the microcanonical ensemble (see Sec. II B), the transition is associated with a discontinuous change in the average number of positive spins (which is the order parameter of the transition), that is not accompanied by any fluctuations. In the canonical ensemble (see Sec. II C and [27]), the average number of spins also changes discontinuously, but this change is accompanied by power-law fluctuations, which are, however, size dependent and disappear in the thermodynamic limit. Finally, in the grand canonical ensemble (see [28]), the phase transition is mixed order (hybrid), because the discontinuous change of the order parameter is accompanied by diverging (i.e., critical-like) fluctuations.

The unique nature of phase transitions observed in this model escapes the existing classifications of these phenomena. (Here, we mean not only the well-established “modern” classification of phase transitions, which applies to additive systems, but also the recent attempt to generalize this classification into nonadditive systems that was introduced in [21]). In a broader context, results reported in this paper show that existing classifications must be refined. Particularly, the issue of phase transitions in partially equivalent ensembles (with locally affine microcanonical entropy) needs deeper insight. It also needs to be clarified whether the coexistence of affine microcanonical entropy and hybrid transition (see also [34–36]) that is observed in this model is accidental or not.

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- [1] J. W. Gibbs, *Elementary Principles in Statistical Mechanics with Especial Reference to the Rational Foundation of Thermodynamics* (Dover, New York, 1960).
- [2] K. Huang, *Statistical Mechanics* (Wiley, New York, 1987).
- [3] L. E. Reichl, *A Modern Course in Statistical Physics* (Wiley, New York, 1998).
- [4] A. Campa, T. Dauxois, and S. Ruffo, Statistical mechanics and dynamics of solvable models with long-range interactions, *Phys. Rep.* **480**, 57 (2009).
- [5] A. Campa, T. Dauxois, D. Fanelli, and S. Ruffo, *Physics of Long-Range Interacting Systems* (Oxford University, New York, 2014).
- [6] D. Lynden-Bell and R. Wood, The gravo-thermal catastrophe in isothermal spheres and the onset of red-giant structure for stellar systems, *Mon. Notic. R. Astron. Soc.* **138**, 495 (1968).
- [7] W. Thirring, Systems with negative specific heat, *Z. Physik.* **235**, 339 (1970).

- [8] P. Hertel and W. Thirring, A soluble model for a system with negative specific heat, *Ann. Phys. (NY)* **63**, 520 (1971).
- [9] D. Lynden-Bell, Negative specific heat in astronomy, physics and chemistry, *Physica A* **263**, 293 (1999).
- [10] A. Torcini and M. Antoni, Equilibrium and dynamical properties of two-dimensional n-body systems with long-range attractive interactions, *Phys. Rev. E* **59**, 2746 (1999).
- [11] J. Barré, D. Mukamel, and S. Ruffo, Inequivalence of Ensembles in a System with Long-Range Interactions, *Phys. Rev. Lett.* **87**, 030601 (2001).
- [12] R. S. Ellis, H. Touchette, and B. Turkington, Thermodynamic versus statistical nonequivalence of ensembles for the mean-field Blume-Emery-Griffiths model, *Physica A* **335**, 518 (2004).
- [13] D. Mukamel, S. Ruffo, and N. Schreiber, Breaking of Ergodicity and Long Relaxation Times in Systems with Long-Range Interactions, *Phys. Rev. Lett.* **95**, 240604 (2005).
- [14] A. Campa, S. Ruffo, and H. Touchette, Negative magnetic susceptibility and nonequivalent ensembles for the mean-field φ^4 spin model, *Physica A* **385**, 233 (2007).
- [15] M. Kastner, Nonequivalence of Ensembles for Long-Range Quantum Spin Systems in Optical Lattices, *Phys. Rev. Lett.* **104**, 240403 (2010).
- [16] T. Mori, Phase transitions in systems with non-additive long-range interactions, *J. Stat. Mech.* (2013) P10003.
- [17] P. Kumar, B. N. Miller, and D. Pirjol, Thermodynamics of a one-dimensional self-gravitating gas with periodic boundary conditions, *Phys. Rev. E* **95**, 022116 (2017).
- [18] V. V. Hovhannisyanyan, N. S. Ananikian, A. Campa, and S. Ruffo, Complete analysis of ensemble inequivalence in the Blume-Emery-Griffiths model, *Phys. Rev. E* **96**, 062103 (2017).
- [19] M. Baldovin, Physical interpretation of the canonical ensemble for long-range interacting systems in the absence of ensemble equivalence, *Phys. Rev. E* **98**, 012121 (2018).
- [20] R. S. Ellis, K. Haven, and B. Turkington, Large deviation principles and complete equivalence and nonequivalence results for pure and mixed ensembles, *J. Stat. Phys.* **101**, 999 (2000).
- [21] F. Bouchet and J. Barre, Classification of phase transitions and ensemble inequivalence, in systems with long range interactions, *J. Stat. Phys.* **118**, 1073 (2005).
- [22] H. Touchette, Equivalence and nonequivalence of the micro-canonical and canonical ensembles: A large deviations study, Ph.D. thesis, McGill University, 2003.
- [23] H. Touchette, R. S. Ellis, and B. Turkington, An introduction to the thermodynamic and macrostate levels of nonequivalent ensembles, *Physica A* **340**, 138 (2004).
- [24] H. Touchette, The large deviation approach to statistical mechanics, *Phys. Rep.* **478**, 1 (2009).
- [25] L. Casetti and M. Kastner, Partial equivalence of statistical ensembles and kinetic energy, *Physica A* **384**, 318 (2007).
- [26] H. Touchette, When is a quantity additive, and when is it extensive? *Physica A* **305**, 84 (2002).
- [27] A. Fronczak, P. Fronczak, and A. Krawiecki, A minimal exactly solved model with the extreme Thouless effect, *Phys. Rev. E* **93**, 012124 (2016).
- [28] A. Fronczak and P. Fronczak, Mixed-order phase transition in a minimal, diffusion based spin model, *Phys. Rev. E* **94**, 012103 (2016).
- [29] H. Touchette, Comment on “First-order phase transitions: Equivalence between bimodalities and the Yang-Lee theorem”, *Physica A* **359**, 375 (2006).
- [30] W. Liu, B. Schmittmann, and R. K. P. Zia, Extraordinary variability and sharp transitions in a maximally frustrated dynamic network, *Europhys. Lett.* **100**, 66007 (2012).
- [31] K. E. Bassler, W. Liu, B. Schmittmann, and R. K. P. Zia, Extreme Thouless effect in a minimal model of dynamic social networks, *Phys. Rev. E* **91**, 042102 (2015).
- [32] The function $f(x)$ is strictly concave when $\frac{\partial^2 f}{\partial x^2} < 0$. It is strictly convex, when $\frac{\partial^2 f}{\partial x^2} > 0$. Finally, $f(x)$ is affine, when $\frac{\partial^2 f}{\partial x^2} = 0$.
- [33] It should be clarified that, in the canonical ensemble, the Helmholtz free energy is defined as $F_N(\beta, a) = \Phi_N(\beta, a)/\beta$. However, compared with $F_N(\beta, a)$, some features of $\Phi_N(\beta, a)$ make the latter function a better choice, especially when it comes to studies on the equivalence of statistical ensembles [21,24].
- [34] A. Bar and D. Mukamel, Mixed-Order Phase Transition in a One-Dimensional Model, *Phys. Rev. Lett.* **112**, 015701 (2014).
- [35] A. Bar and D. Mukamel, Mixed order transition and condensation in an exactly soluble one dimensional spin model, *J. Stat. Mech.* (2014) P11001.
- [36] R. Alert, P. Tierno, and J. Casademunt, Mixed-order phase transition in a colloidal crystal, *Proc. Natl. Acad. Sci. USA* **114**, 12906 (2017).