Computation of Microcanonical Entropy at Fixed Magnetization Without Direct Counting

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Abstract

We discuss a method to compute the microcanonical entropy at fixed magnetization without direct counting. Our approach is based on the evaluation of a saddle-point leading to an optimization problem. The method is applied to a benchmark Ising model with simultaneous presence of mean-field and nearest-neighbour interactions for which direct counting is indeed possible, thus allowing a comparison. Moreover, we apply the method to an Ising model with mean-field, nearest-neighbour and next-nearest-neighbour interactions, for which direct counting is not straightforward. For this model, we compare the solution obtained by our method with the one obtained from the formula for the entropy in terms of all correlation functions. This example shows that for general couplings our method is much more convenient than direct counting methods to compute the microcanonical entropy at fixed magnetization.

1 Introduction

The determination of the entropy of a physical system is a major task in any thermodynamic calculation [1]. To compute the entropy, as notoriously carved on the Boltzmann tombstone, one has to compute the number of microscopic states consistent with the macroscopic quantities characterizing the system. The central problem is then the counting of the number of such states. When the system is simple, by means of combinatoric tools one can perform explicitly this calculation for any finite number N of the constituents of the system. In other cases one does not have the access to the exact number at finite N, but the correct limit for large N can be found by neglecting subleading contributions. We refer to the possibility of directly determining the number of states—in an exact or approximate form—as *direct*

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counting or enumeration, as it is also referred to in [2]. We stress that the problem of the difficulty of computing the entropy by direct counting is particularly relevant when dealing with non-additive systems, like systems with long-range interactions, since these systems present, most of the times, ensemble inequivalence, and thus the microcanical entropy is in general different from the canonical entropy [3].

When direct counting is not easy or possible, due to the difficulty of carrying out the corresponding full or approximate combinatoric calculation, one can anyway aim at calculating the entropy in the limit of large N resorting to other accessible thermodynamic quantities or using information from the equation of state of the system under consideration. A problem that is often encountered is represented by the difficulty of getting the needed expressions in presence of additional conserved quantities, consequence of specific physical constraints acting on the system. This issue is present, e.g., when, working in the microcanonical ensemble, the entropy at a given energy has to be determined in presence of other constraints. In this case the entropy, and therefore the number of states, has to be known as a function not only of the energy, but also of other macroscopic observables, such as order parameters and other correlation functions, characterizing the thermodynamic state.

Among the various physical systems in which the previous general considerations apply, a special attention is devoted to magnetic and spin systems, where the issue of determining the entropy from the counting of states is ubiquitously present [4]. The order parameter characterizing these systems is the magnetization. Then there are situations in which it could be necessary to compute the entropy as a function of the energy and magnetization, or, in other words, to find the entropy in presence of the constraint of fixed magnetization. Generally the natural physical setting of a magnetic system is one in which the fixed control parameter is the external magnetic field, with the (average) magnetization obtained as a derived quantity by the usual thermodynamic relation; also the spontaneous magnetization in absence of an external field in ferromagnetic systems falls into this scheme. However, there are cases in which the Hamiltonian of a magnetic system can be used to describe another type of system, meaning that it is possible to map the original system into a magnetic one; the magnetization would then represent, under this mapping, a control parameter of the original system. For example, the spin value could be associated to the presence or absence of a charged particle in the corresponding site, and the magnetization would be related to the density of the system [5]. It is clear that in such cases the magnetization is a natural control parameter. When ensembles are equivalent, the computation of the entropy could be done in the canonical ensemble, which is generally easier to deal with. But if equivalence does not hold, as in most non-additive systems, in particular those with long-range interactions, if one wants to study the system at given energy (and magnetization), it is necessary to compute the microcanonical partition function, i.e., to compute the number of states. In this circumstance, the interest of this computation is present also when the Hamiltonian represents a genuine magnetic system; in fact, inequivalence would be associated to a possible negative susceptibility in the microcanonical ensemble. To determine if this property occurs, one has to compute the microcanonical entropy at fixed magnetization.

Another typical situation in which one works at a fixed magnetization in magnetic systems is provided by spin models obtained in the strong coupling limit from lattice fermionic or bosonic systems, such as the Hubbard model [6] or its bosonic counterpart [7]. In that case, for large interactions one naturally obtains spin models [8] since in that limit the part of the Hilbert space contributing to the effective Hamiltonian for each lattice site is finite dimensional. When the number of particles in the original lattice model is fixed, the magnetization in the spin model is in turn fixed and therefore one is interested to work in sectors at a fixed magnetization.

Since the calculation of entropy at fixed magnetization without resorting to direct counting is in general a challenging problem, in this paper we aim at presenting a method that, starting from the *canonical* partition function, is able to give a useful expression for the microcanonical entropy at fixed magnetization. As a benchmark, we first apply the presented method to a model in which there is a long-range, mean-field coupling between all the spins of an Ising chain in presence of a nearest-neighbour term [9–11]. The rationale for this choice is that it may exhibit ensemble inequivalence when the long-range coupling is ferromagnetic and the short-range is antiferromagnetic, and one can study and compare both the canonical and microcanonical phase diagrams. Even more importantly for our purposes, in this model the direct counting is possible and one can compare the results obtained from the method presented here and direct counting findings. Moreover, the model has the merit that it is easily generalizable, and one can study the effect of additional couplings, such as finite-range terms. In a recent paper [12] the addition of a next-nearest-neighbour term was considered and the canonical phase diagram shown to exhibit a rich structure, with a large variety of different critical points. Since the direct counting in such a model is rather involved and cumbersome, it provides an ideal case study to give results for the microcanonical entropy at fixed magnetization in a case in which direct counting is not known in the literature.

The plan of the paper is the following. In Sect. 2 we derive formal expressions for the canonical and microcanonical partition functions at fixed magnetization. In Sect. 3 these expressions are used to obtain the procedure to compute the canonical and microcanonical entropies at fixed magnetization for a general spin system in which there are both long-range mean-field and short-range interactions. In this section we also discuss the issue of ensemble inequivalence. In Sect. 4 we apply the procedure to specific models; in particular we consider a model where the short-range interaction is only between nearest-neighbours and another model where also a next-nearest-neighbour interaction is present. We choose these models since they allow (with difficulty for the second case) a direct counting evaluation, and thus a comparison with the results of our procedure provides a test for it. In Sect. 5 a discussion and the conclusions are given. Some additional material is in the appendices.

2 Formal Expressions for the Partition Functions at Fixed Magnetization

In this paper we consider spin systems, for which the dynamical variables take discrete values; correspondingly, the sum over the configurations is denoted by a sum over the discrete values of the spins S_i. The constraint of fixed magnetization is a constraint on the sum of the S_i. However, the general expressions that we obtain in this section and in the following one are independent from the structure of the configuration space of the system. In particular, they are valid also for continuous dynamical variables (in that case the constraint would be, e.g., on the position of the center of mass of the system): in the derivation of the general expressions one would substitute the sum over the spin configurations $\{S_i\}$ with the integral over the continuous dynamical variables, obtaining at the end the same expressions.

As explained above, we focus on the entropy at fixed magnetization, which is defined by:

$$\hat{m} = \frac{1}{N} \sum_{i=1}^{N} S_i \, . \tag{1}$$

The use of the hat in the notation is justified by the necessity to distinguish the magnetization $\hat{m}$ as a function of the spin configuration from its fixed value m on which the thermodynamic quantities defined in the following will depend. Before proceeding, we find it convenient to begin by writing down the known expressions for the usual entropy and the free energy, i.e., for the case when there is no such constraint of fixed magnetization. In a system of N spins, the number of states (i.e., the microcanonical partition function) $\Omega(\epsilon, N)$ with fixed energy per particle equal to ϵ and the associated microcanonical entropy $s_{\mathrm{micr}}(\epsilon)$ are given by:

$$\Omega(\epsilon, N) \equiv \exp\left[N s_{\mathrm{micr}}(\epsilon)\right] = \sum_{\{S_i\}} \delta\left(N\epsilon - H(\{S_i\})\right) . \tag{2}$$

On the other hand, the partition function $Z(\beta, N)$ and the associated (rescaled) free energy $\phi(\beta)$ per particle are expressed by:

$$\begin{aligned} Z(\beta, N) \equiv \exp\left[-N\phi(\beta)\right] &= \sum_{\{S_i\}} \exp\left[-\beta H(\{S_i\})\right] \\ &= \int \mathrm{d}(N\epsilon) \exp\left\{-N\left[\beta\epsilon - s_{\mathrm{micr}}(\epsilon)\right]\right\} , \end{aligned} \tag{3}$$

where $\beta = 1/k_B T$ is proportional to the inverse of the temperature T, with k_B the Boltzmann constant. The last expression shows that in the thermodynamic limit, where the saddle-point approximation becomes exact, the rescaled free energy $\phi(\beta)$ is the Legendre-Fenchel transform of the microcanonical entropy $s_{\mathrm{micr}}(\epsilon)$:

$$\phi(\beta) = \min_{\epsilon}\left[\beta\epsilon - s_{\mathrm{micr}}(\epsilon)\right] . \tag{4}$$

To consider now the magnetization constraint, we need to modify the above expressions by adding a proper δ function. Precisely, the number of states (or microcanonical partition function) $\widetilde{\Omega}(\epsilon, m, N)$ with fixed energy per particle equal to ϵ and fixed magnetization per particle equal to m, and the associated microcanonical entropy per particle $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$ are obtained by:

$$\widetilde{\Omega}(\epsilon, m, N) \equiv \exp\left[N\widetilde{s}_{\mathrm{micr}}(\epsilon, m)\right] = \sum_{\{S_i\}} \delta\left(N\epsilon - H(\{S_i\})\right) \delta\left(\sum_i S_i - Nm\right) . \tag{5}$$

Analogously, the partition function $\widetilde{Z}(\beta, m, N)$ and the associated rescaled free energy $\widetilde{\phi}(\beta, m)$ per particle at fixed magnetization m are given by:

$$\begin{aligned} \widetilde{Z}(\beta, m, N) \equiv \exp\left[-N\widetilde{\phi}(\beta, m)\right] &= \sum_{\{S_i\}} \exp\left[-\beta H(\{S_i\})\right] \delta\left(\sum_i S_i - Nm\right) \\ &= \int \mathrm{d}(N\epsilon) \exp\left\{-N\left[\beta\epsilon - \widetilde{s}_{\mathrm{micr}}(\epsilon, m)\right]\right\} . \end{aligned} \tag{6}$$

As in the case of Eq. (4), the last expression shows that in the thermodynamic limit the rescaled free energy $\widetilde{\phi}(\beta, m)$ is the Legendre-Fenchel transform of the microcanonical entropy $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$:

$$\widetilde{\phi}(\beta, m) = \min_{\epsilon}\left[\beta\epsilon - \widetilde{s}_{\mathrm{micr}}(\epsilon, m)\right] , \tag{7}$$

(for brevity in the following we do not specify any more that the entropy and the free energy are to be intended per particle).

The above expressions can be transformed by using the representation of the δ function. Since the partition functions are given by sums over spin configurations that assume discrete values, in principle the δ functions should not be interpreted as Dirac δ, but as Kronecker

δ. This should be reflected in the corresponding representation. However, the distinction between Dirac and Kronecker δ is not relevant for the final expression, as will be clear in the following (besides, in the thermodynamic limit both ϵ and m become parameters assuming continuous values). We can therefore use the representation of the Dirac δ function. For the microcanonical partition function we thus have:

$$
\begin{aligned}
&\widetilde{\Omega}(\epsilon, m, N) \\
&= \sum_{\{S_i\}} \left(\frac{1}{2\pi}\right)^2 \int_{-\infty}^{+\infty} \mathrm{d}\lambda \int_{-\infty}^{+\infty} \mathrm{d}\varphi \, \exp\left\{ \mathrm{i}\lambda \left[N\epsilon - H(\{S_i\})\right] + \mathrm{i}\varphi \left[\sum_i S_i - Nm\right]\right\} \\
&= \sum_{\{S_i\}} \left(\frac{1}{2\pi \mathrm{i}}\right)^2 \int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty} \mathrm{d}\lambda \int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty} \mathrm{d}\varphi \, \exp\left\{ \lambda \left[N\epsilon - H(\{S_i\})\right] + \varphi \left[\sum_i S_i - Nm\right]\right\}. \qquad (8)
\end{aligned}
$$

For the canonical partition function we similarly have:

$$
\widetilde{Z}(\beta, m, N) = \sum_{\{S_i\}} \frac{1}{2\pi \mathrm{i}} \int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty} \mathrm{d}\varphi \, \exp\left\{ -\beta H(\{S_i\}) + \varphi \left[\sum_i S_i - Nm\right]\right\}. \qquad (9)
$$

The microcanonical entropy and the rescaled free energy, as shown in the defining equivalences at the beginning of Eqs. (5) and (6), are then obtained from the logarithm of Eqs. (8) and (9), respectively. We note that in both expressions (8) and (9) the sum over the configurations is the canonical partition function of the system with an added external magnetic field, in which φ is equal to the magnetic field multiplied by the inverse temperature.

In the next section we apply these general expressions to the case where long-range interactions are present.

3 Models with Long- and Short-Range Terms

We are interested in models that can exhibit ensemble inequivalence, arising from the presence of long-range interactions. In this framework and considering spin systems, the latter are defined as those in which the coupling constant between two spins has a decaying behaviour with distance as $J_{i,j} \sim 1/|i-j|^{\alpha}$, with α smaller than the spatial dimension of the system. When $\alpha = 0$ we have the case of mean-field terms. When long-range interactions are present, thermodynamic quantities are no more additive and ensemble inequivalence can arise. In particular, this generally occurs in presence of first order phase transitions in the canonical ensemble, so that the function $\phi(\beta)$ is not everywhere differentiable; it is known, in fact, that if $\phi(\beta)$ is everywhere differentiable, then Eq. (4) can be inverted [3], so that $s(\epsilon)$ is concave and ensembles are equivalent[1].

To have a concrete case of study, we consider models having general finite-range interactions plus long-range terms of the mean-field form. These models generally present first order phase transitions, due to the combined effect of the mean-field terms and of the short-range terms. We will derive our expressions by assuming a system with two mean-field terms plus unspecified short-range interactions. The dimensionality d of the lattice will also be left unspecified. Of course, as in any computational method, the computations in concrete models are easier for one-dimensional systems. In the following section, where we show the application to a specific model, we will then consider, as an example, a one-dimensional model

[1] We remind that the Legendre–Fenchel transform of any function is automatically concave.

that we have already studied within the framework of the canonical ensemble [12] and that, even with only one mean-field term, presents a very rich thermodynamic phase diagrams, with first and second order phase transitions, critical and tricritical points, and critical end points.

As a preliminary step, we recall that, dealing with systems with long-range interactions, one often obtains an expression of the canonical partition function $Z(\beta, N)$ in the form

$$Z(\beta, N) = \int_{-\infty}^{+\infty} \mathrm{d}\mathbf{x} \exp\left[-N\psi(\beta, \mathbf{x})\right] , \tag{10}$$

where $\mathbf{x} \equiv (x_1, \ldots, x_M)$ is a M-dimensional auxiliary variable, and where $\psi(\beta, \mathbf{x})$ is a real analytic function of β and $\mathbf{x}$. This form is a multidimensional generalization [13] of an expression previously considered only for $M = 1$ [14]. As we will see shortly, one obtains an expression of this sort by using a Hubbard-Stratonovich transformation to perform the computation of the canonical partition function in presence of mean-field terms. Using a saddle-point evaluation, valid in the thermodynamic limit, one finds that the microcanonical entropy $s_{\mathrm{micr}}(\epsilon)$ is given by [3,13,14]:

$$s_{\mathrm{micr}}(\epsilon) = \max_{\mathbf{x}} \left\{ \min_{\beta} \left[\beta\epsilon - \psi(\beta, \mathbf{x})\right] \right\} . \tag{11}$$

On the other hand, the canonical entropy, computed from the rescaled free energy $\phi(\beta)$, is obtained from

$$s_{\mathrm{can}}(\epsilon) = \min_{\beta} \left\{ \max_{\mathbf{x}} \left[\beta\epsilon - \psi(\beta, \mathbf{x})\right] \right\} . \tag{12}$$

These two min-max expressions can give different results [3,13,14], and when this happens ensemble inequivalence occurs.

In this section we will consider the case with two auxiliary variables (i.e., $M = 2$), thus an expression of the form

$$Z(\beta, N) = \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}y \exp\left[-N\psi(\beta, x, y)\right] . \tag{13}$$

Let us then introduce the kind of models we consider. As mentioned above, we will work with a system with two mean-field terms, more precisely with a Hamiltonian given by:

$$H(\{S_i\}) = -\frac{J}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 - \frac{K}{2N}\left(\sum_{i=1}^{N} S_i^2\right)^2 + \sum_{i=1}^{N} U([S_i]) , \tag{14}$$

with positive coupling constants, $J > 0$, $K > 0$. We see that the first mean-field term is proportional to $-N\hat{m}^2$, with the magnetization $\hat{m}$ defined in Eq. (1), while the second mean-field term is proportional to $-N\hat{q}^2$, with $\hat{q}$ equal to the quadrupole moment

$$\hat{q} = \frac{1}{N}\sum_{i=1}^{N} S_i^2 . \tag{15}$$

As usual with mean-field terms, the coupling constants are normalized with the number N of spins. In the final term of the Hamiltonian the notation $U([S_i])$ denotes a function of the i-th spin S_i and its neighbours. Namely, $U([S_i])$ is a short-range term that could contain the interaction of the i-th spin with its nearest-neighbours, next-nearest-neighbours, next-to-next-nearest-neighbours, and so on. If the lattice is not one-dimensional, of course the index i stands for the set of indices used to identify the lattice point. In the implementation of the method to an one-dimensional lattice in section 4 we consider in detail Ising spins with $U([S_i]) = -(K_1/2)S_i S_{i+1}$ (only nearest-neighbour couplings) and $U([S_i]) = -(K_1/2)S_i S_{i+1} - (K_2/2)S_i S_{i+2}$ (including a next-nearest-neighbour term). However, the general expressions that we will derive are independent on the spin value. As a matter of fact, in order to have a nontrivial contribution to the Hamiltonian in correspondence of the quadrupole mean-field term, one has to consider non Ising spins[2].

We now make use of the Hubbard-Stratonovich transformation

$$\exp(ab^2) = \sqrt{\frac{a}{\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x \, \exp(-ax^2 + 2abx) \qquad (a > 0)\,, \tag{16}$$

applied, for positive β, once to the case where $a = \beta JN/2$ and $b = \left(\sum_i S_i/N\right) = \hat{m}$, and once to the case where $a = \beta KN/2$ and $b = \left(\sum_i S_i^2/N\right) = \hat{q}$. We then obtain:

$$\begin{aligned} &\exp\left[-\beta H(\{S_i\})\right] \\ &\quad = \frac{\beta N\sqrt{JK}}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}y \exp\Bigg[-\frac{N}{2}\beta J x^2 - \frac{N}{2}\beta K y^2 \\ &\qquad + \beta J x \sum_{i=1}^{N} S_i + \beta K y \sum_{i=1}^{N} S_i^2 - \beta \sum_{i=1}^{N} U([S_i]) \Bigg]. \end{aligned} \tag{17}$$

Inserting in Eq. (9) and performing the sum over the spin configurations we get

$$\begin{aligned} &\widetilde{Z}(\beta, m, N) \\ &\quad = \frac{1}{2\pi \mathrm{i}} \frac{\beta N\sqrt{JK}}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}y \int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty} \mathrm{d}\varphi \exp\Bigg\{ -N\Bigg[\frac{\beta J}{2} x^2 + \frac{\beta K}{2} y^2 \\ &\qquad + \hat{\psi}(\beta, \beta J x + \varphi, \beta K y) + m\varphi \Bigg]\Bigg\}, \end{aligned} \tag{18}$$

where the function $\hat{\psi}(\beta, \beta J x + \varphi, \beta K y)$ is defined by:

$$\begin{aligned} &\exp\left[-N\hat{\psi}(\beta, \beta J x + \varphi, \beta K y)\right] \\ &\quad = \sum_{\{S_i\}} \exp\left[(\beta J x + \varphi) \sum_{i=1}^{N} S_i + \beta K y \sum_{i=1}^{N} S_i^2 - \beta \sum_{i=1}^{N} U([S_i]) \right]. \end{aligned} \tag{19}$$

Then, we have an expression of the canonical partition function $Z(\beta, m, N)$ in which, besides the two auxiliary variables x and y, the other auxiliary variable φ, coming from the Fourier representation of the δ function that implements the constraint of fixed magnetization m, appears. We see that $\hat{\psi}$ is a real analytic function of its arguments. Thus, the dependence of $\hat{\psi}$ on $\beta J x + \varphi$ comes from the combination of the third term in the exponent of Eq. (17) and the second term in the exponent of Eq. (9), the dependence on $\beta K y$ comes from the fourth term in the exponent of Eq. (17), while the extra dependence on β comes from the short-range term, the last term in the exponent of Eq. (17). It might be difficult to obtain $\hat{\psi}$, for example the use of a transfer matrix evaluation could be necessary. Here we do not specify any particular form. Clearly, if $d > 1$ the determination of $\hat{\psi}$ becomes considerably more involved (one may resort to approximations for it), but for the purposes of the present discussion there are no changes in the argument. We remark that these difficulties would be

[2] For $S_i = -1, 0, 1$ and a function $U([S_i])$ given by just a term proportional to S_i^2 we would obtain the Hamiltonian of the Blume-Emery-Griffiths model; however, in this computation we are not assuming a specific spin model and a specific function $U([S_i])$.

present already in the calculation of the canonical partition function. Moreover, so far we did not explicitly use the values taken by the spins S_i. As remarked above, in the implementation we will consider Ising spins, $S_i = \pm 1$, but the application to more general cases is straightforward.

Furthermore, for the moment we consider only positive temperatures, i.e. $\beta \geq 0$, postponing the treatment of negative temperatures. In spin systems, where the energy is upper bounded, the latter are possible in the microcanonical ensemble. They occur for energies where the derivative of the entropy with respect to the energy is negative. Although physically we do not envisage a thermal bath at negative temperatures, it is possible to formally define a canonical partition function at negative temperatures, since the upper boundedness of the energy implies that this partition function is well defined. We remind that, thinking to the thermodynamic situations in which it is sensible to talk of negative temperatures, we are forced to consider them as "hotter" than the positive temperatures. More precisely, $T = +\infty$ and $T = -\infty$ coincide, while any negative temperature is "hotter" than $T = \infty$. Moreover, if $T_1 < T_2 < 0$, then T_2 is "hotter" than T_1. Finally, the "hottest" temperature is $T = 0^-$, although numerically it is infinitesimally close to the coldest temperature $T = 0^+$.

Before writing the expression for the microcanonical partition function (8) we remark the following. In (8) the integrals on λ and φ are made on the imaginary axis; however, we can perform the integration on a line parallel to the imaginary axis, adding a real part to both λ and φ, since this is allowed by the definition of the Dirac δ. Furthermore, as discussed in [3], the integrals in λ and φ can be limited to a finite segment parallel to the imaginary axis[3].

We then obtain:

$$\begin{aligned}\widetilde{\Omega}(\epsilon, m, N) \; &= \left(\frac{1}{2\pi \mathrm{i}}\right)^2 \frac{\beta N \sqrt{JK}}{2\pi} \\ &\times \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}y \int_{\sigma-\mathrm{i}\eta}^{\sigma+\mathrm{i}\eta} \mathrm{d}\lambda \int_{\mu-\mathrm{i}\nu}^{\mu+\mathrm{i}\nu} \mathrm{d}\varphi \exp\left\{N\Big[\lambda\epsilon - \frac{\lambda J}{2}x^2 - \frac{\beta K}{2}y^2 \right. \\ &\left. - \hat{\psi}(\lambda, \lambda J x + \varphi, \lambda K y) - m\varphi\Big]\right\}, \qquad (20)\end{aligned}$$

where σ and μ are the fixed real parts of λ and φ, respectively, while η and ν denote the respective limits of integration along the segments parallel to the imaginary axis. Analogously, the integration limits of φ in Eq. (18) can be changed in $(\mu - \mathrm{i}\nu, \mu + \mathrm{i}\nu)$. We note that, since Eq. (17) is valid for positive β, then the fixed real part σ in the integral in λ must be nonnegative.

From Eqs. (18) and (20) one can derive the expressions giving the rescaled free energy $\widetilde{\phi}(\beta, m)$ and the microcanonical entropy $\widetilde{s}(\epsilon, m)$. The integrals can be evaluated with the saddle point approximation. It can be shown [3] that the relevant saddle points in the variables λ and φ lie on the real axis. Let us first consider $\widetilde{\phi}(\beta, m)$. Since the real part of the exponent in Eq. (18) has a minimum on the real axis when φ varies on the line parallel to the imaginary axis, then it has a maximum, on the same point of the real axis, when φ varies along the real axis. We therefore have:

$$\widetilde{\phi}(\beta, m) = \min_{x,y}\left[\max_{\varphi}\left(\frac{\beta J}{2}x^2 + \frac{\beta K}{2}y^2 + \hat{\psi}(\beta, \beta J x + \varphi, \beta K y) + m\varphi\right)\right]. \qquad (21)$$

From this one can obtain the expression for the canonical entropy $\widetilde{s}_{\mathrm{can}}(\epsilon, m)$

$\widetilde{s}_{\mathrm{can}}(\epsilon, m)$

[3] This also shows why, as noted above, the use of the representation of the Dirac δ, instead of that of the Kronecker δ, has no importance in this computation.

$$= \min_{\beta \geq 0} \left\{ \max_{x,y} \left[\min_{\varphi} \left(\beta\epsilon - \frac{\beta J}{2} x^2 - \frac{\beta K}{2} y^2 - \hat{\psi}(\beta, \beta J x + \varphi, \beta K y) - m\varphi \right) \right] \right\} \quad (22)$$

An analogous saddle point evaluation of Eq. (20) allows to find the expression of the microcanonical entropy $\widetilde{s}_{\rm micr}(\epsilon, m)$, obtaining:

$$\widetilde{s}_{\rm micr}(\epsilon, m) = \max_{x,y} \left\{ \min_{\beta \geq 0} \left[\min_{\varphi} \left(\beta\epsilon - \frac{\beta J}{2} x^2 - \frac{\beta K}{2} y^2 - \hat{\psi}(\beta, \beta J x + \varphi, \beta K y) - m\varphi \right) \right] \right\} \quad (23)$$

From Eqs. (22) and (23) one can obtain the (β, x, y, φ) point satisfying the extremal problems. As in the case of $s_{\rm micr}(\epsilon)$ and $s_{\rm can}(\epsilon)$, given respectively in Eqs. (11) and (12), the different order in which minimization with respect to β and maximization with respect to x and y is performed can lead to different results, i.e., to different extremal points, and then to ensemble inequivalence. From the properties of min-max extremal problems [3] it follows that in general we will have $\widetilde{s}_{\rm micr}(\epsilon, m) \leq \widetilde{s}_{\rm can}(\epsilon, m)$.

We note that in Eqs. (22) and (23) it is possible to include $\beta = 0$. In fact, for $\beta = 0$ the partition function (9) reduces to the number of states with given magnetization, and no Hubbard-Stratonovich transformation is necessary. However, the function in round brackets in Eqs. (22) and (23) becomes equal to $(-\hat{\psi}(0, \varphi, 0) - m\varphi)$, and it is easy to see that this value[4] is reached continuously when $\beta \to 0^+$. Therefore, the two extremal problems (22) and (23) can be extended to $\beta = 0$, for which no maximization with respect to x and y has to be performed.

The study of the extremal problems (22) and (23) is performed by determining the stationarity and stability conditions that have to be satisfied by the (β, x, y, φ) point in each case. We emphasize that the relations we are going to derive have the purpose to find analytical expressions for the points, but in an actual computation concerning a given concrete model the most rapid way to proceed will be to numerically solve the extremization problems (22) and (23). Therefore, the somewhat cumbersome appearance of the expressions that we will obtain are not a hindrance for the applications. To ease the notation it is convenient to denote with u, v and w the three arguments (β, $\beta J x + \varphi$ and $\beta K y$) of $\hat{\psi}$, and, as customary, to use subscripts to denote partial derivatives with respect to an argument.

We will proceed step by step for each of the two extremal problems, since this is convenient to determine the stability conditions, expressed by inequalities to be satisfied at the extremal points (β, x, y, φ). On the other hand, the stationarity conditions can be easily written all together, and they are the same for both problems, and we anticipate them here. They are given by:

$$\hat{\psi}_v + m = 0 \quad (24)$$

$$\hat{\psi}_v + x = 0 \quad (25)$$

$$\hat{\psi}_w + y = 0 \quad (26)$$

$$\epsilon - \frac{J}{2} x^2 - \hat{\psi}_u - J x \hat{\psi}_v - K y \hat{\psi}_w = 0 \,. \quad (27)$$

The first three equations are also those that must be verified in the extremal problem (21). The first two equations imply that at the extremal points we have $x = m$. The fact that at the extremal point one has $x = m$ is consistent with what obtained in the study of the unconstrained problem, i.e., in the computation of $\phi(\beta)$ and $s(\epsilon)$ (canonical or microcanonical),

[4] It is also not difficult to realize from Eq. (19) that $\exp\left[-N\hat{\psi}(0, \varphi)\right]$ is equal to the partition function of N independent spins subject to a magnetic field h with φ playing the role of βh.

where one derives the equilibrium magnetization and finds that it is equal to the extremal value of x [3].

Let us know complete the analysis, obtaining for each one of the stationarity conditions summarized in Eqs. (24–27) the corresponding stability condition. We begin with the problem (22). Minimizing with respect to φ one has:

$$\hat{\psi}_v + m = 0 \tag{28}$$

$$\hat{\psi}_{vv} < 0\,. \tag{29}$$

Eq. (28) gives φ as a function of (β, x, y, m), and one obtains the following relations:

$$\varphi_x = -\beta J \tag{30}$$

$$\varphi_y = -\beta K \frac{\hat{\psi}_{vw}}{\hat{\psi}_{vv}} \tag{31}$$

$$\varphi_\beta = -\frac{\hat{\psi}_{uv}}{\hat{\psi}_{vv}} - Jx - Ky\frac{\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\,, \tag{32}$$

useful for the successive steps. Then we have now:

$$\begin{aligned}\widetilde{s}_{\rm can}(\epsilon, m) &= \min_{\beta\geq 0}\left\{\max_{x,y}\left[\beta\epsilon - \frac{\beta J}{2}x^2 - \frac{\beta K}{2}y^2\right.\right.\\ &\left.\left.-\hat{\psi}(\beta, \beta J x + \varphi(\beta, x, y, m), \beta K y) - m\varphi(\beta, x, y, m)\right]\right\}.\end{aligned} \tag{33}$$

The maximization with respect to x and y leads to the following stationarity and stability conditions:

$$\hat{\psi}_v + x = 0 \tag{34}$$

$$\hat{\psi}_w + y = 0 \tag{35}$$

$$1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right) > 0\,, \tag{36}$$

where use has been made of Eqs. (30) and (31). Equation (36) will be compared with the corresponding one obtained below in the study of $\widetilde{s}_{\rm micr}(\epsilon, m)$, to see how inequivalence can arise. Eqs. (34) and (35) define in principle x and y as a function of (β, m). However, the former one, taken together with Eq. (28), shows that at the extremum one has $x = m$. Consistently, computing the derivative of x and y with respect to β, used in the following step, we find, with the help of (32):

$$x_\beta = 0 \tag{37}$$

$$y_\beta = -\frac{\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)}{1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)}\,. \tag{38}$$

Then we are left with:

$$\begin{aligned}\widetilde{s}_{\rm can}(\epsilon, m) &= \min_{\beta\geq 0}\left\{\beta\epsilon - \frac{\beta J}{2}x^2(\beta, m) - \frac{\beta K}{2}y^2(\beta, m)\right.\\ &-\hat{\psi}(\beta, \beta J x(\beta, m) + \varphi(\beta, x(\beta, m), y(\beta, m), m), \beta K y(\beta, m))\\ &\left.-m\varphi(\beta, x(\beta, m), y(\beta, m), m)\right\},\end{aligned} \tag{39}$$

where in this expression we have left the formal dependence of x and y on (β, m). Without writing explicitly anymore this dependence, minimization with respect to β leads to the stationarity condition:

$$\epsilon - \frac{J}{2}x^2 - \frac{K}{2}y^2 - \hat{\psi}_u - Jx\hat{\psi}_v - Ky\hat{\psi}_w = 0\,, \tag{40}$$

where use has been made of Eqs. (28), (37) and (38). This equation gives β as a function of ϵ and m. The stability condition requires some algebra. Using Eq. (32) the stability is obtained as:

$$\begin{aligned}&\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) + (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right)\\ &+\beta K\hat{\psi}_{vv}\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]y_\beta > 0\,.\end{aligned} \tag{41}$$

Substituting the expression of y_β given by Eq. (38) we have:

$$\begin{aligned}&\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) + (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right)\\ &-\beta K\hat{\psi}_{vv}\frac{\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)} > 0\,.\end{aligned} \tag{42}$$

From Eqs. (29) and (36) it follows that the second line of Eq. (42) (including the minus sign) is positive. This is to be taken into account in the comparison with the corresponding stability condition in the following study of $\widetilde{s}_{\rm micr}(\epsilon, m)$.

It is convenient to summarize the stability conditions of the problem (22). They are:

$$\hat{\psi}_{vv} < 0 \tag{43}$$

$$1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right) > 0 \tag{44}$$

$$\begin{aligned}&\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) + (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right)\\ &-\beta K\hat{\psi}_{vv}\frac{\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)} > 0\,.\end{aligned} \tag{45}$$

We now consider the extremal problem (23), concerning the microcanonical entropy. The first step is the same of the canonical case, so that the corresponding stationarity and stability conditions are given by (28) and (29), respectively, and also Eqs. (30), (31) and (32) are the same. Then we have:

$$\begin{aligned}\widetilde{s}_{\rm micr}(\epsilon, m) &= \max_{x,y}\left\{\min_{\beta\ge 0}\left[\beta\epsilon - \frac{\beta J}{2}x^2 - \frac{\beta K}{2}y^2\right.\right.\\ &\qquad\left.\left. -\hat{\psi}(\beta, \beta Jx + \varphi(\beta, x, y, m), \beta Ky) - m\varphi(\beta, x, y, m)\right]\right\}.\end{aligned} \tag{46}$$

The minimization with respect to β gives the stationarity condition:

$$\epsilon - \frac{J}{2}x^2 - \frac{K}{2}y^2 - \hat{\psi}_u - Jx\hat{\psi}_v - Ky\hat{\psi}_w = 0\,, \tag{47}$$

where Eq. (28) has been used. As we know, it is the same as that of the other extremal problem. It gives β as a function of (ϵ, x, y, m). From this function we obtain, using (32):

$$\beta_x = 0 \tag{48}$$

$$\beta_y = -\beta K \frac{\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)}{\hat{\psi}_{uu} - \frac{\hat{\psi}_{uv}^2}{\hat{\psi}_{vv}} + 2Ky\left(\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\right) + (Ky)^2\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)}\,. \tag{49}$$

We point out that in writing the last expressions we have also used the stationarity conditions that are obtained in the following and last step, the maximization with respect to x and y. Making use of Eq. (32), we find that the stability condition is given by:

$$\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) + (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right) > 0\,. \tag{50}$$

We see that this is different from the corresponding stability condition (42). The latter requires the positivity of an expression given by the left hand side of (50) plus the second line of (42), that we have noted is always positive at the extremal point. We come back to this later. The final step is given by:

$$\begin{aligned}\widetilde{s}_{\mathrm{micr}}(\epsilon, m) \;&= \max_{x,y}\Big\{\beta(\epsilon, x, y, m)\epsilon - \frac{\beta(\epsilon, x, y, m)J}{2}x^2 - \frac{\beta(\epsilon, x, y, m)K}{2}y^2 \\ &\quad -\hat{\psi}(\beta(\epsilon, x, y, m), \beta(\epsilon, x, y, m)Jx + \varphi(\beta(\epsilon, x, y, m), x, y, m), \beta(\epsilon, x, y, m) \\ &\quad \times Ky) - m\varphi(\beta(\epsilon, x, y, m), x, y, m)\Big\}\,. \end{aligned} \tag{51}$$

The stationarity conditions are:

$$\hat{\psi}_v + x = 0 \tag{52}$$

$$\hat{\psi}_w + y = 0\,, \tag{53}$$

equal respectively to (34) and (35), as expected. But the stability condition is not equal to (36), being instead given by, using (30) and (31):

$$\begin{aligned}&1 + \beta K\left[\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right] \\ &\quad + \left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]\beta_y > 0\,. \end{aligned} \tag{54}$$

Substituting β_y from Eq. (49) we obtain:

$$\begin{aligned}&1 + \beta K\left[\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right] \\ &-\beta K \frac{\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{\hat{\psi}_{uu} - \frac{\hat{\psi}_{uv}^2}{\hat{\psi}_{vv}} + 2Ky\left(\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\right) + (Ky)^2\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)} > 0\,. \end{aligned} \tag{55}$$

Furthermore, from Eqs. (29) and (50) we have that the denominator in the fraction in the second line is negative; therefore the second line (including the minus sign) is positive. On the other hand, we had noted, in the study of the canonical problem, that the corresponding stability condition [see Eq. (36)] required that the first line alone be positive. After treating the case of negative temperatures we come back to the differences between the stability conditions and the associated possibility of ensemble inequivalence.

The summary of the stability conditions of the problem (23) is:

$$\hat{\psi}_{vv} < 0 \tag{56}$$

$$\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) + (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right) > 0 \tag{57}$$

$$1 + \beta K\left[\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right] - \beta K \frac{\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{\hat{\psi}_{uu} - \frac{\hat{\psi}_{uv}^2}{\hat{\psi}_{vv}} + 2Ky\left(\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\right) + (Ky)^2\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)} > 0\,. \tag{58}$$

3.1 Negative Temperatures

We noted above that spin systems can have negative temperatures, since the energy is upper bounded. As a consequence, we should expect that, if in Eqs. (22) or (23) we choose values of ϵ and m for which the corresponding temperature is negative, then the extremal problems will not be satisfied for any $\beta \geq 0$. Then we have to extend the analysis to negative values of β. The treatment of negative temperatures requires some changes in the expressions. However, we will see below that, considering the two cases together, we can obtain a procedure that has the double advantage to be shorter and to include at the same time temperatures of both signs.

When $\beta < 0$ we have to use a different form of the Hubbard-Stratonovich transformation, i.e.

$$\exp(ab^2) = \sqrt{\frac{-a}{\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x\ \exp(ax^2 + 2\mathrm{i}abx)\,, \tag{59}$$

which is valid for $a < 0$. For the following analysis it is useful to note that this equality is valid also if we add fixed imaginary parts to x and to y , i.e., if we perform the x and y integral on a line parallel to the real x axis and the real y axis, respectively. The expression for the canonical partition function that replaces (18) is then

$$\widetilde{Z}(\beta, m, N) = \frac{1}{2\pi\mathrm{i}} \frac{|\beta| N\sqrt{JK}}{2\pi} \int_{-\infty}^{+\infty}\mathrm{d}x \int_{-\infty}^{+\infty}\mathrm{d}y \int_{\mu-\mathrm{i}\nu}^{\mu+\mathrm{i}\nu}\mathrm{d}\varphi \exp\Big\{ - N\Big[-\frac{\beta J}{2}x^2 - \frac{\beta K}{2}y^2 + \hat{\psi}(\beta, \mathrm{i}\beta Jx + \varphi, \mathrm{i}\beta Ky) + m\varphi\Big]\Big\}\,, \tag{60}$$

where we have already taken into account that the integral over φ can be on a line parallel to the imaginary axis, with real part equal to μ, and that the integration limits of φ can be changed in $(\mu - \mathrm{i}\nu, \mu + \mathrm{i}\nu)$. The function $\hat{\psi}(\beta, \mathrm{i}\beta Jx + \varphi, \mathrm{i}\beta Ky)$ is defined as in Eq. (19), therefore by the right hand side of that expression with β substituted by $\mathrm{i}\beta$. In the same way, the expression of the microcanonical partition function replacing (20) is

$$
\begin{aligned}
\widetilde{\Omega}(\epsilon, m, N) \ &= \left(\frac{1}{2\pi \mathrm{i}}\right)^2 \frac{|\beta| N \sqrt{JK}}{2\pi} \\
&\quad \times \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}y \int_{\sigma-\mathrm{i}\eta}^{\sigma+\mathrm{i}\eta} \mathrm{d}\lambda \int_{\mu-\mathrm{i}\nu}^{\mu+\mathrm{i}\nu} \mathrm{d}\varphi \exp\left\{ N \Big[\lambda\epsilon + \frac{\lambda J}{2} x^2 + \frac{\beta K}{2} y^2 \right. \\
&\quad \left. - \hat{\psi}(\lambda, \mathrm{i}\lambda J x + \varphi, \mathrm{i}\lambda K y) - m\varphi \Big] \right\}, \qquad (61)
\end{aligned}
$$

where σ is the fixed real parts of λ, and we have taken into account that the integration limits of λ can be taken as $(\sigma - \mathrm{i}\eta, \sigma + \mathrm{i}\eta)$. We note that, since Eq. (59) is valid for negative β, then the fixed real part σ in the integral in λ must be nonpositive.

Then, we obtain the following expressions replacing Eqs. (21), (22) and (23):

$$
\widetilde{\phi}(\beta, m) = \min_{x,y} \left[\max_{\varphi} \left(-\frac{\beta J}{2} x^2 - \frac{\beta K}{2} y^2 + \hat{\psi}(\beta, \mathrm{i}\beta J x + \varphi, \mathrm{i}\beta K y) + m\varphi \right) \right], \qquad (62)
$$

for the rescaled free energy,

$$
\begin{aligned}
&\widetilde{s}_{\mathrm{can}}(\epsilon, m) \\
&\quad = \min_{\beta \le 0} \left\{ \max_{x,y} \left[\min_{\varphi} \left(\beta\epsilon + \frac{\beta J}{2} x^2 + \frac{\beta K}{2} y^2 - \hat{\psi}(\beta, \mathrm{i}\beta J x + \varphi, \mathrm{i}\beta K y) - m\varphi \right) \right] \right\}, \qquad (63)
\end{aligned}
$$

for the canonical entropy, and

$$
\begin{aligned}
&\widetilde{s}_{\mathrm{micr}}(\epsilon, m) \\
&\quad = \max_{x,y} \left\{ \min_{\beta \le 0} \left[\min_{\varphi} \left(\beta\epsilon + \frac{\beta J}{2} x^2 + \frac{\beta K}{2} y^2 - \hat{\psi}(\beta, \mathrm{i}\beta J x + \varphi, \mathrm{i}\beta K y) - m\varphi \right) \right] \right\}, \qquad (64)
\end{aligned}
$$

for the microcanonical entropy. For the same argument given before, the value $\beta = 0$ can be included in the analysis. Depending on the values of ϵ and m we expect that it is possible to satisfy either the extremal problem (22) or the extremal problem (63), but not both (except when they are both satisfied for $\beta = 0$); the same for the couple of problems (23) and (64).

We can now follow the same steps as above to obtain the stationarity and stability conditions of the problems (63) and (64). We will make a shorter presentation than for positive β, in particular we will not mention explicitly the equations used to obtain the stability conditions. In both cases the first step, i.e., the minimization with respect to φ, is the same as before. We then have the same stationarity and stability conditions, namely

$$
\hat{\psi}_v + m = 0 \qquad (65)
$$

$$
\hat{\psi}_{vv} < 0\,. \qquad (66)
$$

In writing, here and in the following, an inequality like (66) for a quantity that in principle is complex, we are assuming that it is actually real. In fact, as it can be verified a posteriori, both $\mathrm{i}x$ and $\mathrm{i}y$ at the extremal points are real quantities. Eq. (65), defining φ as a function of (β, x, y, m), now gives:

$$
\varphi_x = -\mathrm{i}\beta J \qquad (67)
$$

$$
\varphi_y = -\mathrm{i}\beta K \frac{\hat{\psi}_{vw}}{\hat{\psi}_{vv}} \qquad (68)
$$

$$\varphi_\beta = -\frac{\hat{\psi}_{uv}}{\hat{\psi}_{vv}} - \mathrm{i}Jx - \mathrm{i}Ky\frac{\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\,. \tag{69}$$

Thus, in the second step for the canonical case we have

$$\begin{aligned}\widetilde{s}_{\mathrm{can}}(\epsilon, m) &= \min_{\beta\leq 0}\left\{\max_{x,y}\left[\beta\epsilon + \frac{\beta J}{2}x^2 + \frac{\beta K}{2}y^2\right.\right.\\ &\left.\left. -\hat{\psi}(\beta, \mathrm{i}\beta Jx + \varphi(\beta, x, y, m), \mathrm{i}\beta Ky) - m\varphi(\beta, x, y, m)\right]\right\}.\end{aligned} \tag{70}$$

The maximization with respect to x and y leads to the following stationarity and stability conditions:

$$-\mathrm{i}\hat{\psi}_v + x = 0 \tag{71}$$

$$-\mathrm{i}\hat{\psi}_w + y = 0 \tag{72}$$

$$1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right) > 0\,. \tag{73}$$

This stationarity condition (71), defining x as a function of (β, m), shows, together with Eq. (65), that $\mathrm{i}x = m$, that we substitute in the next and final step. Then, as before, $x_\beta = 0$. We note that the application of the saddle point requires that the integral in x be performed on a line parallel to the real axis with imaginary part equal to $-\mathrm{i}m$. Furthermore, as mentioned above, Eq. (72) shows that at the stationary point $\mathrm{i}y$ is real, and, as for the integration in x, the saddle point application requires that the integral in y be performed on a line parallel to the real axis. The third and final step for the canonical case is:

$$\begin{aligned}\widetilde{s}_{\mathrm{can}}(\epsilon, m) &= \min_{\beta\leq 0}\left\{\beta\epsilon - \frac{\beta J}{2}m^2 + \frac{\beta K}{2}y^2\right.\\ &\left. -\hat{\psi}(\beta, \beta Jm + \varphi(\beta, y(\beta, m), m)) - m\varphi(\beta, y(\beta, m), m)\right\}.\end{aligned} \tag{74}$$

The stationarity and stability conditions are given by

$$\epsilon - \frac{J}{2}m^2 + \frac{K}{2}y^2 - \hat{\psi}_u - Jm\hat{\psi}_v - \mathrm{i}Ky\hat{\psi}_w = 0 \tag{75}$$

$$\begin{aligned}&\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2\mathrm{i}Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) - (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right)\\ &-\beta K\hat{\psi}_{vv}\frac{\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + \mathrm{i}Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)} > 0\,.\end{aligned} \tag{76}$$

We write for convenience, as before, the stability conditions of the problem (63). They are:

$$\hat{\psi}_{vv} < 0 \tag{77}$$

$$1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right) > 0 \tag{78}$$

$$\begin{aligned}&\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2\mathrm{i}Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) - (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right)\\ &-\beta K\hat{\psi}_{vv}\frac{\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + \mathrm{i}Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{1 + \beta K\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)} > 0\,.\end{aligned} \tag{79}$$

Going now to the microcanonical entropy, the second step for the problem (64) is:

$$\begin{aligned}\widetilde{s}_{\mathrm{micr}}(\epsilon, m) &= \max_{x,y}\left\{\min_{\beta\le 0}\left[\beta\epsilon + \frac{\beta J}{2}x^2 + \frac{\beta K}{2}y^2\right.\right.\\ &\left.\left. -\hat{\psi}(\beta, \mathrm{i}\beta J x + \varphi(\beta, x, y, m), \mathrm{i}\beta K y) - m\varphi(\beta, x, y, m)\right]\right\}. \qquad (80)\end{aligned}$$

Minimization with respect to β leads to the following stationarity and stability conditions:

$$\epsilon + \frac{J}{2}x^2 + \frac{K}{2}y^2 - \hat{\psi}_u - \mathrm{i}Jx\hat{\psi}_v - \mathrm{i}Ky\hat{\psi}_w = 0 \qquad (81)$$

$$\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2\mathrm{i}Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) - (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right) > 0\,. \qquad (82)$$

As we know, the stationarity condition is the same of the other extremal problem, and it gives β as a function of (ϵ, x, y, m). On the other hand, as for $\beta > 0$ the stability condition is different. From the stationarity condition we obtain, in particular:

$$\beta_y = -\mathrm{i}\beta K \frac{\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + \mathrm{i}Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)}{\hat{\psi}_{uu} - \frac{\hat{\psi}_{uv}^2}{\hat{\psi}_{vv}} + 2\mathrm{i}Ky\left(\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\right) - (Ky)^2\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)}\,. \qquad (83)$$

We can now write the final step, given by:

$$\begin{aligned}\widetilde{s}_{\mathrm{micr}}(\epsilon, m) &= \max_{x,y}\left\{\beta(\epsilon, x, y, m)\epsilon + \frac{\beta(\epsilon, x, y, m)J}{2}x^2 + \frac{\beta(\epsilon, x, y, m)K}{2}y^2\right.\\ &-\hat{\psi}(\beta(\epsilon, x, y, m), \mathrm{i}\beta(\epsilon, x, y, m)Jx\\ &+\varphi(\beta(\epsilon, x, y, m), x, y, m), \mathrm{i}\beta(\epsilon, x, y, m)Ky)\\ &\left.-m\varphi(\beta(\epsilon, x, y, m), x, y, m)\right\}. \qquad (84)\end{aligned}$$

The stationarity conditions are:

$$-\mathrm{i}\hat{\psi}_v + x = 0 \qquad (85)$$

$$-\mathrm{i}\hat{\psi}_w + y = 0\,, \qquad (86)$$

equal respectively to (71) and (72), as expected. But the stability condition is not equal to (73), being instead given by:

$$\begin{aligned}&1 + \beta K\left[\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right]\\ &-\beta K\frac{\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + \mathrm{i}Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{\hat{\psi}_{uu} - \frac{\hat{\psi}_{uv}^2}{\hat{\psi}_{vv}} + 2\mathrm{i}Ky\left(\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\right) - (Ky)^2\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)} > 0\,. \qquad (87)\end{aligned}$$

The summary of the stability conditions of the problem (64) is:

$$\hat{\psi}_{vv} < 0 \qquad (88)$$

$$\begin{aligned}&\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2\mathrm{i}Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right)\\ &-(Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right) > 0 \qquad (89)\end{aligned}$$

$$1+\beta K\left[\hat{\psi}_{ww}-\frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right]$$

$$-\beta K\frac{\left[\hat{\psi}_{uw}-\frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}+\mathrm{i}Ky\left(\hat{\psi}_{ww}-\frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{\hat{\psi}_{uu}-\frac{\hat{\psi}_{uv}^2}{\hat{\psi}_{vv}}+2\mathrm{i}Ky\left(\hat{\psi}_{uw}-\frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\right)+(Ky)^2\left(\hat{\psi}_{ww}-\frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)}>0\,. \tag{90}$$

3.2 Unified Treatment of Temperatures of Both Signs

From the above computations we see that it is possible to treat at the same time both positive and negative temperatures. It is sufficient to put from the start $x=m$ for $\beta>0$ and $\mathrm{i}x=m$ for $\beta<0$, and identifying y for $\beta>0$ with $\mathrm{i}y$ for $\beta<0$. Since in this way it is not necessary to optimize with respect to x, the numerical procedure would be shorter. Thus, the extremal problems to study would be:

$$\widetilde{\phi}(\beta,m)=\min_y\left[\max_\varphi\left(\frac{\beta J}{2}m^2+\frac{\beta K}{2}y^2+\hat{\psi}(\beta,\beta Jm+\varphi,\beta Ky)+m\varphi\right)\right], \tag{91}$$

for the rescaled free energy,

$$\widetilde{s}_{\mathrm{can}}(\epsilon,m)$$
$$=\min_\beta\left\{\max_y\left[\min_\varphi\left(\beta\epsilon-\frac{\beta J}{2}m^2-\frac{\beta K}{2}y^2-\hat{\psi}(\beta,\beta Jm+\varphi,\beta Ky)-m\varphi\right)\right]\right\}, \tag{92}$$

for the canonical entropy, and

$$\widetilde{s}_{\mathrm{micr}}(\epsilon,m)$$
$$=\max_y\left\{\min_\beta\left[\min_\varphi\left(\beta\epsilon-\frac{\beta J}{2}m^2-\frac{\beta K}{2}y^2-\hat{\psi}(\beta,\beta Jm+\varphi,\beta Ky)-m\varphi\right)\right]\right\}, \tag{93}$$

for the microcanonical entropy. The search for the extremal points would proceed as before, with the stationary conditions summarized by:

$$\hat{\psi}_v+m=0 \tag{94}$$

$$\hat{\psi}_w+y=0 \tag{95}$$

$$\epsilon-\frac{J}{2}m^2-\hat{\psi}_u-Jm\hat{\psi}_v-Ky\hat{\psi}_w=0\,, \tag{96}$$

while the stability conditions would be

$$\hat{\psi}_{vv}<0 \tag{97}$$

$$1+\beta K\left(\hat{\psi}_{ww}-\frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)>0 \tag{98}$$

$$\hat{\psi}_{uu}\hat{\psi}_{vv}-\hat{\psi}_{uv}^2+2Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv}-\hat{\psi}_{uv}\hat{\psi}_{vw}\right)+(Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww}-\hat{\psi}_{vw}^2\right)$$

$$-\beta K\hat{\psi}_{vv}\frac{\left[\hat{\psi}_{uw}-\frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}+Ky\left(\hat{\psi}_{ww}-\frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{1+\beta K\left(\hat{\psi}_{ww}-\frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)}>0\,, \tag{99}$$

for the canonical problem (92), and

$$\hat{\psi}_{vv} < 0 \tag{100}$$

$$\hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 + 2Ky\left(\hat{\psi}_{uw}\hat{\psi}_{vv} - \hat{\psi}_{uv}\hat{\psi}_{vw}\right) + (Ky)^2\left(\hat{\psi}_{vv}\hat{\psi}_{ww} - \hat{\psi}_{vw}^2\right) > 0 \tag{101}$$

$$1 + \beta K\left[\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right] - \beta K \frac{\left[\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}} + Ky\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)\right]^2}{\hat{\psi}_{uu} - \frac{\hat{\psi}_{uv}^2}{\hat{\psi}_{vv}} + 2Ky\left(\hat{\psi}_{uw} - \frac{\hat{\psi}_{uv}\hat{\psi}_{vw}}{\hat{\psi}_{vv}}\right) + (Ky)^2\left(\hat{\psi}_{ww} - \frac{\hat{\psi}_{vw}^2}{\hat{\psi}_{vv}}\right)} > 0\,, \tag{102}$$

for the microcanonical problem (93). However, now the search could be extended also to $\beta < 0$.

At this point we can discuss the issue of ensemble inequivalence, on the basis of the comparison between the stability conditions of the two problems. We start by noting what can be deduced from the expression of $\hat{\psi}(\beta, \beta Jx + \varphi, \beta Ky)$ given in Eq. (19). In fact, $\hat{\psi}(\beta, \beta Jx + \varphi, \beta Ky)$ is proportional to minus the logarithm of the right hand side of that equation, and then it is easy to see that for any x, y and φ the total second derivative of $\hat{\psi}$ with respect to β is negative. From this, in turn, one obtains that the left hand side of Eq. (101) is always positive, i.e., it is a stability condition of the microcanonical problem that is always satisfied. The consequences are the following, taking into account that for both problems the first stability condition is $\hat{\psi}_{vv} < 0$. Let us first suppose to have a solution of the canonical problem, i.e., to have a stationary point where the three stability conditions (97)-(99) are satisfied[5]. Then also the microcanonical stability condition (102) is satisfied. This can be seen, e.g., in the following way: the left hand side of (102) is equal to the left hand side of (99) multiplied by the ratio of the left hand side of (98) and the left hand side of (101); since this ratio is positive, this implies that (102) is satisfied. In other words, any stable canonical equilibrium state is also a stable microcanonical equilibrium state. This is consistent with a general result obtained, e.g., through large deviation techniques [3]. On the other hand, it is possible to satisfy the stability condition (102) of the microcanonical problem without satisfying the stability condition (98) of the canonical problem (and then, for what we have seen, neither (99) would be satisfied); namely, there can be stable microcanonical equilibrium states that are not stable canonical equilibrium states. Nevertheless, although for the values of (ϵ, m) where the latter situation is verified there are not stable canonical equilibrium states, still the extremal problem (92) can be satisfied. This occurs since in that case the function $y(\beta)$ defined by the stationarity condition (95) has a point of discontinuity in its derivative with respect to β, given by Eq. (38), and for a range of ϵ values the minimization problem (92) is satisfied by the β value of the point of discontinuity. This is associated with the occurrence of a first order phase transition in the canonical ensemble: there are not stable canonical equilibrium states for the ϵ values in that range (but only for the two values at the extremes of the range), and the computed canonical entropy $\widetilde{s}_{\mathrm{can}}(\epsilon, m)$ has a straight line segment for that ϵ range. In that range we have strictly $\widetilde{s}_{\mathrm{micr}}(\epsilon, m) < \widetilde{s}_{\mathrm{can}}(\epsilon, m)$[6].

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[5] It is not difficult to see that for $\beta > 0$ the conditions (97) and (98), taken together, imply the condition (99); this is not true for $\beta < 0$.

[6] In a system with only short-range interactions, where ensembles are equivalent and the two entropies are always equal, $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$ would have the same straight line segment, and for the values of ϵ inside the range of

In Appendix A we provide an alternative derivation of the expression of the maximization problem (93) for the microcanonical entropy, using a procedure based on large deviation techniques.

3.3 The Limit $J \to 0$ and $K \to 0$

We want to show that in the limit $J \to 0$ and $K \to 0$ our expressions go continuously to those one would expect for the Hamiltonian (14) in absence of mean-field terms, i.e., when the system becomes a short-range one. We first note that the Hubbard-Stratonovich equality (16) is valid also in the limit $a \to 0$, as it can be easily checked. This implies that for $J \to 0$ and $K \to 0$ the expressions (18) and (20) remain valid by simply removing, on the right hand side, the integrations over x and y with the corresponding prefactors, and by putting $J = 0$ and $K = 0$ in the integrand. In particular, now the function $\hat{\psi}$ would appear as $\hat{\psi}(\beta, \varphi, 0)$, with $\exp\left[-N\hat{\psi}(\beta, \varphi, 0)\right]$ being equal to the partition function of the short-range system subject to a magnetic field h with φ playing the role of βh. Correspondingly, in the expressions (21), (22) and (23) for the rescaled free energy and the entropy, the variables x and y would disappear, and we would get:

$$\widetilde{\phi}(\beta, m) = \max_{\varphi} \left(\hat{\psi}(\beta, \varphi, 0) + m\varphi\right) \tag{103}$$

and

$$\widetilde{s}(\epsilon, m) = \min_{\beta} \left[\min_{\varphi} \left(\beta\epsilon - \hat{\psi}(\beta, \varphi, 0) - m\varphi\right)\right]. \tag{104}$$

The latter equation holds for both the canonical and microcanonical cases.

Then, we can conclude this subsection by observing that the method presented in this paper works then both for short-range interactions (when both J and K are equal to 0) and for long-range interactions. For the former the problem of determining the entropy at fixed magnetization is solved once that the partition function in a magnetic field is known, as expected. However, in short-range models there is not the issue whether the microcanonical entropy and the canonical one are different: they are the same in the thermodynamical limit [15]. Similarly, one can see that microcanonical and canonical entropies at fixed magnetization are also the same in short-range models. For this reason, we devote the section of the implementation to models with $J \neq 0$, where ensemble inequivalence can occur and it is interesting to compute and compare canonical and microcanonical entropies at fixed magnetization. As anticipated, in the implementation we consider systems with only one mean-field term, thus with $K = 0$.

3.4 The Model with Only One Mean-Field Term

In the next section we will implement the method in a model where the Hamiltonian contains only one mean-field term, the one proportional to $-N\hat{m}^2$. The corresponding expressions would be obtained by the ones derived above by putting $K = 0$ and in which there would be no integration over the y auxiliary variable and the corresponding optimization with respect to it.

(Footnote 6 continued)
the segment the equilibrium states, in both ensembles, would be realized with a phase separation, something that does not occur in long-range systems.

However, we write in the following the optimizations problems and the corresponding stationarity and stability conditions, since an interesting issue arises. From Eq. (91) with $K = 0$ and with no optimization with respect to y, we obtain

$$\widetilde{\phi}(\beta, m) = \max_{\varphi} \left(\frac{\beta J}{2} m^2 + \hat{\psi}(\beta, \beta J m + \varphi, 0) + m\varphi \right) . \tag{105}$$

In the same way, for the entropies, from Eqs. (92) and (93) we obtain in both cases

$$\widetilde{s}(\epsilon, m) = \min_{\beta} \left[\min_{\varphi} \left(\beta\epsilon - \frac{\beta J}{2} m^2 - \hat{\psi}(\beta, \beta J m + \varphi, 0) - m\varphi \right) \right] , \tag{106}$$

expression which is then valid for both ensembles. The stationarity and stability conditions of the latter problem are

$$\hat{\psi}_v + m = 0 \qquad \hat{\psi}_{vv} < 0 \tag{107}$$

$$\epsilon - \frac{J}{2} m^2 - \hat{\psi}_u - J m \hat{\psi}_v = 0 \qquad \hat{\psi}_{uu}\hat{\psi}_{vv} - \hat{\psi}_{uv}^2 > 0 . \tag{108}$$

The fact that now we have the same optimization problem for both ensembles, allows to make the following interesting observation. For the class of systems where the long-range interaction is given only by a term proportional to $-N\hat{m}^2$, the entropy at fixed magnetization is the same for the canonical and the microcanonical case. From the equality $\widetilde{s}_{\rm micr}(\epsilon, m) = \widetilde{s}_{\rm can}(\epsilon, m)$, one might superficially conclude that there is ensemble equivalence. However, equivalence occurs when we have $s_{\rm micr}(\epsilon) = s_{\rm can}(\epsilon)$, and it is not automatically guaranteed that this latter equality is verified when the former equality, $\widetilde{s}_{\rm micr}(\epsilon, m) = \widetilde{s}_{\rm can}(\epsilon, m)$, holds. In a moment we provide a concrete example of this fact, but first we describe the mathematical reason that can explain why it is possible to have $s_{\rm micr}(\epsilon) < s_{\rm can}(\epsilon)$ for one or more ranges of the energy[7] even when $\widetilde{s}_{\rm micr}(\epsilon, m) = \widetilde{s}_{\rm can}(\epsilon, m)$. The microcanonical entropy $s_{\rm micr}(\epsilon)$ is obtained by maximizing $\widetilde{s}_{\rm micr}(\epsilon, m)$ with respect to m, i.e., $s_{\rm micr}(\epsilon) = \max_m [\widetilde{s}_{\rm micr}(\epsilon, m)]$; however, the canonical entropy $s_{\rm can}(\epsilon)$ is not obtained performing the analogous maximization of $\widetilde{s}_{\rm can}(\epsilon, m)$. In fact, $s_{\rm can}(\epsilon)$ is given by the general thermodynamic relation $s_{\rm can}(\epsilon) = \min_\beta [\beta\epsilon - \phi(\beta)]$, where, in our case, $\phi(\beta) = \min_m \widetilde{\phi}(\beta, m)$, with the latter function obtained in turn from $\widetilde{s}_{\rm micr}(\epsilon, m)$ through the minimization problem in Eq. (7). These different extremization procedures to obtain $s_{\rm micr}(\epsilon)$ and $s_{\rm can}(\epsilon)$ can thus lead to different functions. An example can be found in the Blume-Capel model. It is a simplified version of the model cited in footnote 2, and in which the general Hamiltonian (14) has $K = 0$ (i.e., the only mean-field term is the one proportional to $-N\hat{m}^2$) and the function $U([S_i])$ simply given by ΔS_i^2 (Δ is a positive parameter); the spins take the values $-1, 0, 1$. For this simple model direct counting can easily be performed, and in Ref. [16] it is shown that ensemble inequivalence occurs, since there are ranges of the energy where $s_{\rm micr}(\epsilon) < s_{\rm can}(\epsilon)$. However, it is also easy to see explicitly that $\widetilde{s}_{\rm micr}(\epsilon, m) = \widetilde{s}_{\rm can}(\epsilon, m)$. In fact, a direct computation allows to obtain

$$\begin{aligned}\widetilde{s}_{\rm micr}(\epsilon, m) = &- [1 - b(\epsilon, m)] \ln [1 - b(\epsilon, m)] - \frac{1}{2} [b(\epsilon, m) + m] \ln [b(\epsilon, m) + m] \\ &- \frac{1}{2} [b(\epsilon, m) - m] \ln [b(\epsilon, m) - m] + b(\epsilon, m) \ln 2 ,\end{aligned} \tag{109}$$

where $b(\epsilon, m) \equiv \frac{\epsilon}{\Delta} + \frac{m^2}{2\Delta}$. Obviously, ϵ and m can vary in ranges for which the argument of all the logarithms in (109) are non-negative. For any allowed value of ϵ and m, this function

[7] We remind that, because of the properties of min–max extremal problems [3], in general one has $s_{\rm micr}(\epsilon) \le s_{\rm can}(\epsilon)$.

is concave in ϵ. Therefore the Legendre-Fenchel transform (7) is invertible, assuring that $\widetilde{s}_{\text{micr}}(\epsilon, m) = \widetilde{s}_{\text{can}}(\epsilon, m)$, in agreement with the general result of this section, i.e., that in models with only the mean-field term proportional to $-N\hat{m}^2$ we have, for both ensembles, the same entropy $\widetilde{s}(\epsilon, m)$ given in Eq. (106).

In conclusion, ensemble inequivalence can occur even when $\widetilde{s}_{\text{micr}}(\epsilon, m)$ and $\widetilde{s}_{\text{can}}(\epsilon, m)$ are equal; even when $\widetilde{s}_{\text{micr}}(\epsilon, m)$ is concave in ϵ for any m, so that the Legendre-Fenchel transform (7) is invertible, $s_{\text{micr}}(\epsilon)$ can be non-concave, so that the Legendre-Fenchel transform (4) is not invertible.

4 Implementation of the Method

As anticipated above, we implement here our computational method to an Ising spin model ($S_i = \pm 1$) on a one-dimensional lattice, described by a Hamiltonian of the type (14) in which the short-range term is given by $U([S_i]) = -(K_1/2)S_i S_{i+1} - (K_2/2)S_i S_{i+2}$. Furthermore, the coefficient of the quadrupole term, K, is set equal to zero (in any case, the quadrupole term for Ising spins would give a constant trivial contribution). Therefore, we are going to treat a system with only the mean-field term proportional to $-N\hat{m}^2$. For convenience, we write the explicit form of the Hamiltonian, i.e.:

$$H = -\frac{J}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 - \frac{K_1}{2}\sum_{i=1}^{N} S_i S_{i+1} - \frac{K_2}{2}\sum_{i=1}^{N} S_i S_{i+2}\,, \tag{110}$$

where periodic boundary conditions are assumed. Thus, the short-range part of this Hamiltonian has a nearest-neighbour interaction term (with coefficient K_1) and next-nearest-neighbour interaction term (with coefficient K_2). It is the simplest Hamiltonian having a long-range interaction term and a short-range part with an internal structure, with the K_1 and K_2 parts of the model possibly competing.

To show the intricacies of the calculation of microcanonical entropy at fixed magnetization using direct counting, also in relatively simple models like this one, and the convenience of the implementation of the method presented in this work, we adopt the following strategy. Using the results given in Ref. [17], we will first describe, in Sect. 4.1, what would be the procedure to follow to obtain a direct counting evaluation of $\widetilde{s}_{\text{micr}}(\epsilon, m)$. From this description and the expressions to use in such a procedure (the interested reader can find in Appendix B a summary of the results of Ref. [17] and of the relevant expressions), it will be evident that the actual numerical computations are quite cumbersome, so that the optimization method introduced in Sect. 3 has to be preferred. Then, in Sect. 4.2 we will show the evaluation of $\widetilde{s}_{\text{micr}}(\epsilon, m)$ with the method of this work. This will be done first for the case with $K_2 = 0$; in this case, the direct counting is simple, and it was done in Ref. [11], a work that was primarily devoted to the study of ensemble inequivalence. Thus, we will also show the comparison of our computation with that obtained with direct counting. Afterwords, we will show our results for some selected values of $K_2 \neq 0$. In this case the direct counting becomes rather involved, and has not been done up to now. In order to provide a comparison, we have performed the direct counting evaluation; this is shown in Appendix C.

4.1 The Procedure for the Direct Counting Evaluation

Reference [17] gives a general procedure for a computation of the microcanonical entropy of translationally invariant one-dimensional Ising spin systems with short-range interactions. Restricting to models with only two-spin interactions, a short-range Hamiltonian should have the form:

$$H_{SR} = -\frac{1}{2}\sum_{r=1}^{R} K_r \sum_i S_i S_{i+r} \,. \tag{111}$$

The subscript (SR) denotes that the Hamiltonian describes a short-range system. The procedure can be extended to models where also a long-range interaction, like the first term in the Hamiltonian (110), is present. For convenience we will denote this long-range part of the Hamiltonian with H_{LR}. Therefore in (110) we have $H = H_{LR} + H_{SR}$, where in this case H_{SR} is a particular form of (111) having $R = 2$. Despite the simplicity of the model (110), it displays a remarkably rich phase diagrams in the canonical ensemble [12].

While more details for the case with generic R are given in Appendix B, let us here consider the direct counting procedure for the Hamiltonian (110). We begin with the simple case in which $K_2 = 0$.

4.1.1 $K_2 = 0$

It is possible to compute the number of spin configurations that have given values m and g_1 of, respectively, the magnetization $\hat{m}$ and the nearest-neighbour correlation function $\hat{g}_1$:

$$\hat{m} = \frac{1}{N}\sum_{i=1}^{N} S_i \tag{112}$$

$$\hat{g}_1 = \frac{1}{N}\sum_{i=1}^{N} S_i S_{i+1} \,. \tag{113}$$

The logarithm, divided by N, of such number of spin configurations can be denoted with $s(m, g_1)$, and called the entropy as a function of m and g_1. In the thermodynamic limit it is given by [17]:

$$\begin{aligned} s(m, g_1) = &-\frac{1+2m+g_1}{4}\ln\frac{1+2m+g_1}{4} - \frac{1-2m+g_1}{4}\ln\frac{1-2m+g_1}{4} \\ &-\frac{1-g_1}{2}\ln\frac{1-g_1}{4} + \frac{1+m}{2}\ln\frac{1+m}{2} + \frac{1-m}{2}\ln\frac{1-m}{2} \,. \end{aligned} \tag{114}$$

It follows that $s(m, g_1)$ is defined within the convex polytope (polygon) defined by the following constraints:

$$1+2m+g_1 > 0, \qquad 1-2m+g_1 > 0, \qquad 1-g_1 > 0 \,. \tag{115}$$

As noted above, the expression for $s(m, g_1)$ was obtained already in Ref. [11]. It must be emphasized that, although $s(m, g_1)$ is naturally called an entropy, being given by the logarithm of a number of configurations, it is not the usual thermodynamic entropy, that has to depend on the energy ϵ, like the function of our interest, $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$. To obtain the latter from $s(m, g_1)$, one has to express the energy as a function of m and of the correlation g_1, as we now explain (obviously the same remark is valid also for the more complex case with $K_2 \neq 0$, discussed below).

From the Hamiltonian (110) with $K_2 = 0$ one obatins the energy per spin at fixed values m and g_1. It is given by:

$$e(m, g_1) = -\frac{J}{2}m^2 - \frac{K_1}{2}g_1 . \tag{116}$$

To find $\widetilde{s}_{\rm micr}(\epsilon, m)$ one has to fix $e(m, g_1) \equiv \epsilon$, express from (116) g_1 as a function of ϵ and m, and then substitute $g_1(\epsilon, m)$ in Eq. (114). This can be done producing results in agreement with those presented in [11].

We now go to the model with $K_2 \neq 0$, i.e., the complete Hamiltonian (110); the direct counting procedure becomes much more involved.

4.1.2 $K_2 \neq 0$

Using the procedure described in Appendix B, one finds the number of spin configurations having given values m, g_1, g_2 and t of, respectively, the already defined magnetization $\hat{m}$ and nearest-neighbour correlation function $\hat{g}_1$, and of the other correlation functions $\hat{g}_2$ and $\hat{t}$; they are given by:

$$\hat{m} = \frac{1}{N}\sum_{i=1}^{N} S_i \qquad\qquad \hat{g}_1 = \frac{1}{N}\sum_{i=1}^{N} S_i S_{i+1} \tag{117}$$

$$\hat{g}_2 = \frac{1}{N}\sum_{i=1}^{N} S_i S_{i+2} \qquad\qquad \hat{t} = \frac{1}{N}\sum_{i=1}^{N} S_i S_{i+1} S_{i+2} . \tag{118}$$

The fixed value of one of this quantity can conveniently be denoted with the average of the corresponding spin correlation, e.g., $g_2 = \langle S_i S_{i+2}\rangle$, where translational invariance assures that the average actually does not depend on i. The logarithm, divided by N, of the number of the configurations at fixed (m, g_1, g_2, t), i.e., the entropy as a function of these variables, in the thermodynamic limit is obtained as the following long expression:

$$\begin{aligned} s(m, g_1, g_2, t) = &-\frac{1+m-g_2-t}{4}\ln\frac{1+m-g_2-t}{8} - \frac{1+m-2g_1+g_2-t}{8} \\ &\times \ln\frac{1+m-2g_1+g_2-t}{8} - \frac{1-3m+2g_1+g_2-t}{8} \\ &\times \ln\frac{1-3m+2g_1+g_2-t}{8} - \frac{1-m-g_2+t}{4}\ln\frac{1-m-g_2+t}{8} \\ &- \frac{1-m-2g_1+g_2+t}{8}\ln\frac{1-m-2g_1+g_2+t}{8} \\ &- \frac{1+3m+2g_1+g_2+t}{8}\ln\frac{1+3m+2g_1+g_2+t}{8} + \frac{1+2m+g_1}{4} \\ &\times \ln\frac{1+2m+g_1}{4} + \frac{1-2m+g_1}{4}\ln\frac{1-2m+g_1}{4} + \frac{1-g_1}{2}\ln\frac{1-g_1}{4} . \end{aligned} \tag{119}$$

From this entropy, which is a function of the four quantities (m, g_1, g_2, t), we can obtain the entropy as a function of (m, g_1, g_2) by maximizing $s(m, g_1, g_2, t)$ with respect to t, i.e.

$$\begin{aligned} s(m, g_1, g_2) &= s(m, g_1, g_2, t_0) \\ \frac{\partial s(m, g_1, g_2, t)}{\partial t} &= 0\Big|_{t=t_0} . \end{aligned} \tag{120}$$

An explicit expression for this entropy is still obtainable, involving the real solution of the third order equation in t_0:

$$
\begin{aligned}
&t_0^3 - m(2g_1+g_2)t_0^2 + [(1-2g_1^2+2g_1^2 g_2 - g_2^2) + m^2(-3+4g_1+2g_2)]t_0 \\
&\quad + m[-2g_1+2g_1^2-g_2+4g_1 g_2 - 2g_1^2 g_2 - 2g_1 g_2^2 + g_2^3 + m^2(2-2g_1-g_2)] = 0\,,
\end{aligned}
\tag{121}
$$

maximizing $s(m, g_1, g_2, t)$.

One finds from (119) that $s(m, g_1, g_2)$ is defined within the convex polytope (polyhedron) defined by the following constraints:

$$1+2m+g_1>0 \qquad 1-2m+g_1>0 \qquad 1-g_1>0 \tag{122}$$

$$1+2m+g_2>0 \qquad 1-2m+g_2>0 \qquad 1-g_2>0 \tag{123}$$

$$1+2g_1+g_2>0 \qquad 1-2g_1+g_2>0\,. \tag{124}$$

Notice that for certain ranges of the parameters m, g_1, g_2 there are three real roots of (121), but in these ranges direct inspection shows that for only one of these three roots the entropy is defined – i.e., all arguments of the logarithms in (119) are positive.

The energy per spin at fixed values of m, g_1, g_2 and t is given by:

$$e(m, g_1, g_2, t) = -\frac{J}{2}m^2 - \frac{K_1}{2}g_1 - \frac{K_2}{2}g_2\,, \tag{125}$$

that actually does not depend on t, since the Hamiltonian (110) has no contribution coming from three spin terms $\propto S_i S_{i+1} S_{i+2}$ (the extension to this case is straightforward). At this point, to find $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$ one has to fix $e \equiv \epsilon$ where $e = e(m, g_1, g_2, t = t_0)$. Then from (125) one has to express, say, g_2 [or, if one wants so, g_1] as a function of ϵ, m and g_1 [or, respectively, as a function of ϵ, m and g_2]. Then one has to substitute $g_2(\epsilon, m; g_1)$ in Eq. (119). The entropy will now depend on ϵ, m and g_1: maximizing with respect to g_1 will give $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$.

It is then clear that, despite the expression of the entropy is known, already in this simple case one can (painfully) realize that the computations from expression (119) is quite cumbersome. The analysis also clearly shows how difficult is to generalize it to more complicated forms of coupling, where the equations fixing the further correlation functions and the expression of the entropy become rapidly very involved, e.g. when a next-to-next-nearest-neighbour coupling is added. For example, assuming an Hamiltonian of the form

$$H = -\frac{J}{2N}\sum_{i,j} S_i S_j - \frac{K_1}{2}\sum_i S_i S_{i+1} - \frac{K_2}{2}\sum_i S_i S_{i+2} - \frac{K_3}{2}\sum_i S_i S_{i+3}\,,$$

one has an energy $e = e(m, g_1, g_2, g_3)$ with $g_3 = \langle S_i S_{i+3}\rangle$. The entropy $s = s(m, g_1, g_2, g_3, t, q_1, q_2, q_3)$ is a function of the already introduced quantities m, g_1, g_2, g_3 and t, and of the other quantities $q_1 = \langle S_i S_{i+1} S_{i+3}\rangle$, $q_2 = \langle S_i S_{i+2} S_{i+3}\rangle$, and $q_3 = \langle S_i S_{i+1} S_{i+2} S_{i+3}\rangle$, Despite having a quite convoluted expression, it can be determined using the method of Appendix B. Now, to arrive at $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$, one has first to fix t, q_1, q_2, q_3 by maximizing $s(m, g_1, g_2, g_3, t, q_1, q_2, q_3)$ with respect to these variables from the conditions $\partial s/\partial t = \partial s/\partial q_1 = \partial s/\partial q_2 = \partial s/\partial q_3 = 0$. Then fixing the energy to a certain value ϵ, from $\epsilon = e(m, g_1, g_2, g_3)$ one gets, say, $g_3 = g_3(m, g_1, g_2)$ and then an entropy s as a function of (m, g_1, g_2). Maximizing with respect to g_1 and g_2 one finally obtains the microcanonical entropy at fixed magnetization, $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$. So, one sees that increasing the range of the couplings and/or adding multi-spin interactions, one has first to eliminate

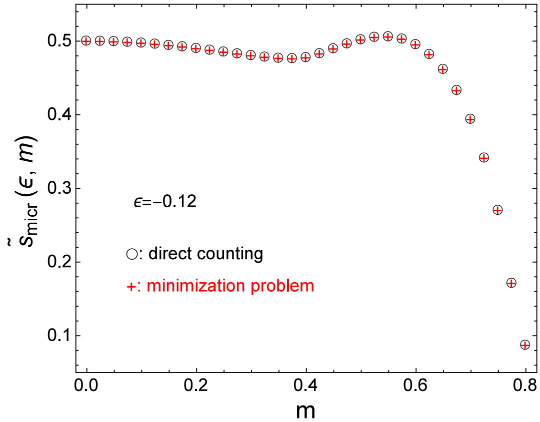


Fig. 1 $\widetilde{s}_{\rm micr}(\epsilon, m)$ vs. m at the fixed value of the energy $\epsilon = -0.12$ (in units of $J = 1$) for $K_1 = -0.4$ and $K_2 = 0$. We plot the results from the minimization procedure discussed in Sects. 2 and 3 and from the direct counting [11] (see as well Sect. 4.1.1)

the couplings not present in the Hamiltonian, and then – after using the expression of the energy – maximize over the remaining, which is of course a complicated task. This can be seen as a "direct counting", since the explicit expression of the entropy is used; but one concludes that the method presented in the Sect. 3 is more practical, since it involves only the extremization with respect to a given number of variables (depending on the number of auxiliary variables), independent from the range of the short-range interactions. What is actually increasing when more couplings are included is the size of the transfer matrix, whose only the largest eigenvalue is needed. Of course, the use of the transfer matrix would be present also in the computation of only canonical quantities. At variance, in the direct counting one has to maximize with respect to a growing number of variables, as the example now discussed shows. We have however to observe that the direct counting, as shown in Appendix B, gives not only the microcanonical entropy at fixed magnetization but also the values – at given energy and magnetization – of all independent correlation functions in the unit cell, e.g., in the considered case with K_1, K_2, the correlation functions $g_1(\epsilon, m) = \langle S_i S_{i+1}\rangle$, $g_2(\epsilon, m) = \langle S_i S_{i+2}\rangle$, and $t(\epsilon, m) = \langle S_i S_{i+1} S_{i+2}\rangle$.

After this exposition of the reasons that make the method presented in in Sect. 3 much more preferable with respect to a direct counting, already for a simple Hamiltonian like (110), in the next subsection we give the results obtainable with our method for this Hamiltonian. We find it useful to begin with the simple case with $K_2 = 0$, and then to proceed with the results obtained for selected values of $K_2 \neq 0$. The comparison with the direct counting evaluation will also be shown, although, as anticipated above, for $K_2 \neq 0$ the comparison is deferred to Appendix C.

4.2 Results for the Microcanonical Entropy $\widetilde{s}_{\rm micr}(\epsilon, m)$

As a first benchmark, in Fig. 1 we plot the microcanonical entropy for the model with $K_2 = 0$ discussed in Sect. 4.1.1. The comparison of the method presented in Sect. 3 with the findings obtained by direct counting confirms the validity of our results. Notice that in this section for simplicity we will set $J = 1$. Indeed, our interest as previously discussed is on the case $J \neq 0$ and moreover we remind that the model (110) does not exhibit magnetic order at finite temperature if J is negative (see [12] and references therein).

Let us pass now to the model with $K_2 \neq 0$. First, we remind that as a consequence of the nonadditivity of systems with long-range interactions, intermediate values of the extensive

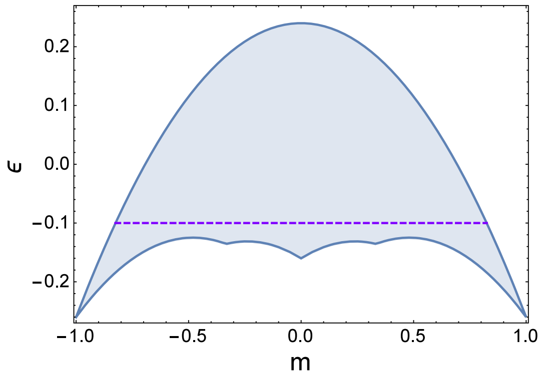


Fig. 2 Accessible region in the $m - \epsilon$ plane for $K_1 = -0.4$ and $K_2 = -0.08$. Blue dashed line shows the value of the energy at which the first-order transition takes place ($\epsilon \simeq -0.100$)

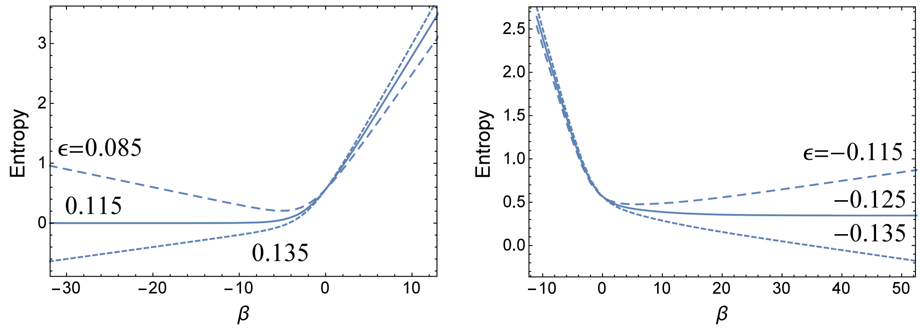
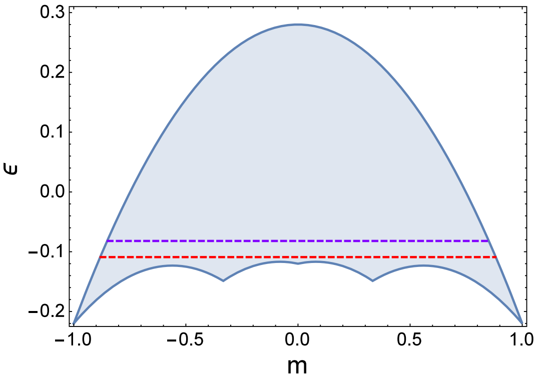


Fig. 3 Entropy from Eq. (106) as a function of β after minimizing only with respect to φ at $K_1 = -0.4$, $K_2 = -0.08$ and $m = 0.5$ for different values of ϵ. The left and right panels show that for values of the energy outside the allowed range for this value of m (see Fig. 2), the entropy function has no minimum as a function of β

variables may be not accessible. So a first important information is to determine the accessible region in the $m - \epsilon$ plane. This is done in Fig. 2 for fixed values of K_1 and K_2, chosen to be $K_1 = -0.4$, $K_2 = -0.08$. Note that this pair of values corresponds in the K_1-K_2 plane to a point in a region which, despite the presence of a non-vanishing K_2, has a phase diagram in the canonical ensemble in the space $K_1 - T$ at fixed K_2 qualitatively similar to the phase diagram in the space $K_1 - T$ with $K_2 = 0$. Since for $K_1 = -0.4$, $K_2 = -0.08$ one knows that in the canonical ensemble there is a first order phase transition line, as one can see from Fig. 2(left) of [12], we also plot in Fig. 2 the value of the energy at which the first-order phase transition occurs. More details on the behaviour of the entropy function at fixed magnetization after the minimization on the variable φ are given in Fig. 3, where the same values of K_1, K_2 of Fig. 2 are chosen. As seen in Fig. 2, for $m = 0.5$ the possible energy values are in the range $[-0.125, 0.115]$. Correspondingly, in Fig. 3 we see that for energy values outside this range, i.e., 0.135 in the left panel and -0.135 in the right panel, the entropy function (precisely, the function of β obtained from Eq. (106) after minimizing only with respect to φ) does not have a minimum as a function of β, i.e., the microcanonical extremal problem has no solution.

To illustrate the effectiveness of our method, let us consider a pair of values of K_1, K_2 for which the model (110) is known to have both a first-order and a second-order phase transitions in the canonical phase diagram. For this reason we consider $K_1 = -0.4$, $K_2 = -0.16$. As

Fig. 4 Accessible region in the $m - \epsilon$ plane at $K_1 = -0.4$ and $K_2 = -0.16$. Red (blue) dashed lines show the value of the energies at which the first-order (second-order) transition takes place: they are given respectively by $\epsilon \simeq -0.109$ ($\epsilon \simeq -0.082$)



one can see from Fig. 3(left) of [12], when the temperature T is increased at these particular values of K_1, K_2, one meets a first-order transition at a certain temperature, and then at a larger temperature a second-order transition. It is then very interesting to see what happens in the microcanonical ensemble when the energy is varied. Our main results are summarized in Figs. 4, 5, and 6. In Fig. 4 we plot the accessible region in the $m - \epsilon$ plane, and we mark the energies at which the first- and second-order transitions occur. One observes that the shape of the accessible region acquires further structure at low energies. Details on the behaviour of the microcanonical entropy near the first- and second-order transitions are given respectively in Figs. 5 and 6, from which one sees that the proposed method could be used to work out the phase diagram in the microcanonical ensemble. In order to have a comparison, in Appendix C we provide an explicit example of the determination of the microcanonical entropy at fixed magnetization corresponding to a particular point in Fig. 5 using direct counting, i.e. the expression of the entropy as a function of (m, g_1, g_2) for a given energy. Agreement is found with the results of Fig. 5.

5 Conclusions

In this paper we presented a method to determine the microcanonical entropy at fixed magnetization starting from the canonical partition function. We applied our results to the case of systems having long- and short-range (possibly competing) interactions. The rationale behind this choice is that for models with only short-range interactions the canonical and microcanonical entropies, and in particular the canonical and microcanonical entropies at fixed magnetization, do coincide, while this is not the case for models with long-range interactions, as our construction explicitly shows. We also discussed in the Appendix A the connection with large-deviation theory.

The presented method is based on the introduction of one (or more) auxiliary variables and on a min-max procedure, where the minimization is performed on the variable β, which can be both positive or negative. We emphasized that the method can be very useful where direct counting is not applicable or very difficult/convoluted.

We studied a model in which there is a long-range, all-to-all term in the presence of nearest-neighbour (K_1) and next-nearest-neighbour (K_2) couplings. Results for the microcanonical entropy at fixed magnetization of this model were presented, including a case in which the canonical phase diagram exhibits first- and second-order phase transitions. The discussion clearly shows that increasing the range of couplings (or including multi-spin interactions),

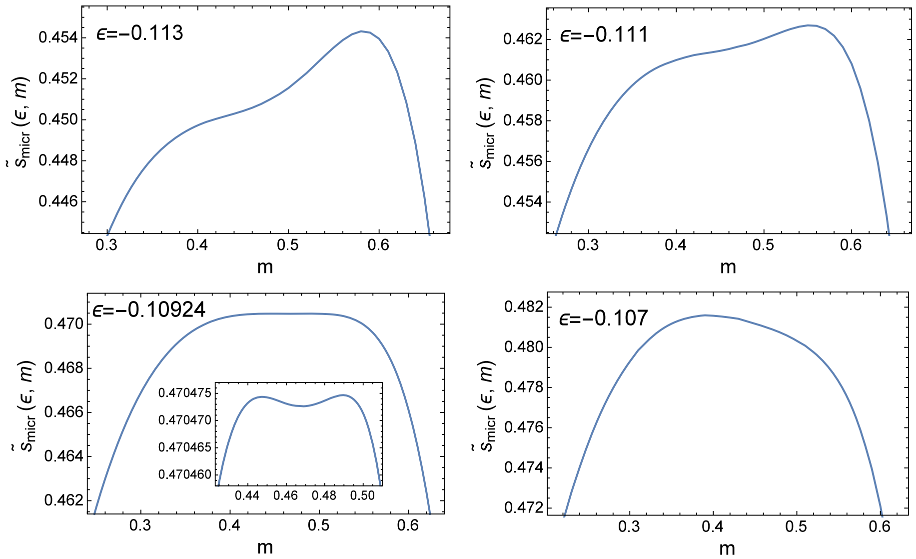


Fig. 5 $\widetilde{s}_{\text{micr}}(\epsilon, m)$ vs. m at the fixed value of the $K_1 = -0.4$, $K_2 = -0.16$ and few different values of ϵ near the first-order transition

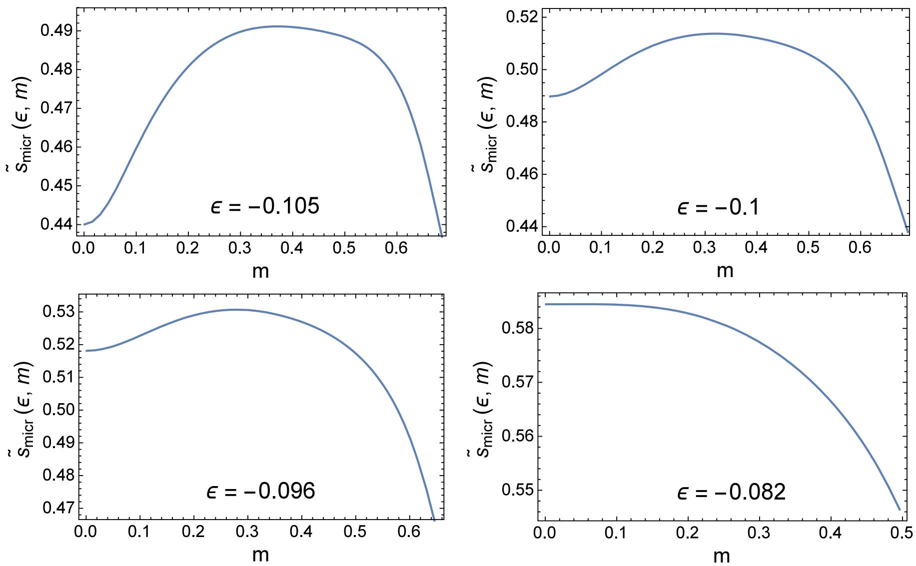


Fig. 6 $\widetilde{s}(\epsilon, m)$ vs. m at the fixed value of the $K_1 = -0.4$, $K_2 = -0.16$ and few different values of ϵ near the second-order transition

even though an expression for the entropy in terms of all possible couplings can be derived, the determination of the microcanonical entropy at fixed magnetization by direct counting requires the maximization over a number of variables increasing with the range of the short-range interaction, while the method presented in Sect. 3—once that one has determined the partition function, which can be done by determining the largest eigenvalue of the transfer matrix—requires the extremization on a given number of variables equal to one plus the number of auxiliary variables, which, e.g., is just one for the model (110), independently form the range of the short-range interaction. A discussion of advantages and disadvantages of the presented method with the direct counting has been provided and a comparison with direct counting both with $K_2 = 0$ and $K_2 \neq 0$ for illustration purposes has also been presented.

In the considered model the long-range interaction is of mean-field form, and it would be interesting as a future work to study the model in which the interaction decays in space as a power-law. One could also consider more complicated short-range terms, such as involving more than two spin interactions or couplings between spins up to a finite general R larger than 2. Moreover, our results show that the presented scheme can be used to determine the phase diagram in the microcanonical ensemble, and a deserving application would be to work out in detail the microcanonical phase diagram of Hamiltonian (110) in the whole $K_1 - K_2$ space, and compare it with the corresponding results in the canonical ensemble determined in [12].

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Declarations

Conflict of interest The authors declare that they have no conflict of interest.

Appendix A: Derivation Using Large Deviation Techniques

The basic expressions of this paper, i.e., Eqs. (21), (22) and (23), or equivalently Eqs. (91), (92) and (93), for the rescaled free energy and the canonical and microcanonical entropies, respectively, have been obtained starting from the formal expressions (8) and (9). The latter have been adapted to the models with Hamiltonian of the type (14) obtaining the expressions (18) and (20). In this Appendix we show how one can arrive at the basic expressions by using an approach based on large deviation techniques. Of course, since one arrives at the same basic expressions for the rescaled free energy and the entropies, the analysis presented in section 3 remains identical. Here, for brevity, we show the procedure by starting directly from models with Hamiltonian of the type (14), therefore, without writing the more general expressions and then adapting them to that kind of Hamiltonian.

Using the definitions (1) and (15) of the magnetization $\hat{m}$ and the quadrupole moment $\hat{q}$, respectively, and introducing the definition

$$\hat{r} = \frac{1}{N} \sum_{i=1}^{N} U([S_i]) \tag{126}$$

the Hamiltonian (14) can be written as

$$H(\{S_i\}) = N\left[-\frac{J}{2}\hat{m}^2 - \frac{K}{2}\hat{q}^2 + \hat{r}\right]. \tag{127}$$

At this point one formally defines

$$\begin{aligned}\widehat{\Omega}(m, q, r, N) &\equiv \exp\left[N\widehat{s}_{\text{micr}}(m, q, r)\right] \\ &= \sum_{\{S_i\}} \delta\left(N\hat{m} - Nm\right)\, \delta\left(N\hat{q} - Nq\right)\, \delta\left(N\hat{r} - Nr\right). \end{aligned} \tag{128}$$

One also defines the following kind of partition function

$$\begin{aligned}\widehat{Z}(\lambda_1, \lambda_2, \lambda_3, N) &\equiv \exp\left[-N\widehat{\phi}(\lambda_1, \lambda_2, \lambda_3)\right] \\ &= \sum_{\{S_i\}} \exp\left[-\lambda_1\hat{m} - \lambda_2\hat{q} - \lambda_3\hat{r}\right]. \end{aligned} \tag{129}$$

In analogy with what we have noted for β in the main text, the fact that the energy is upper bounded allows to consider both signs for the parameters λ_1, λ_2 and λ_3. It is not difficult to see that in the thermodynamic limit the function $\widehat{s}_{\text{micr}}(m, q, r)$ and $\widehat{\phi}(\lambda_1, \lambda_2, \lambda_3)$ are related by the Legendre-Fenchel transformation

$$\widehat{\phi}(\lambda_1, \lambda_2, \lambda_3) = \min_{m,q,r}\left[\lambda_1 m + \lambda_2 q + \lambda_3 r - \widehat{s}_{\text{micr}}(m, q, r)\right]. \tag{130}$$

In principle this transformation is not invertible. However, if $\widehat{\phi}$ is everywhere differentiable, the inversion is possible, so to have

$$\widehat{s}_{\text{micr}}(m, q, r) = \min_{\lambda_1,\lambda_2,\lambda_3}\left[\lambda_1 m + \lambda_2 q + \lambda_3 r - \widehat{\phi}(\lambda_1, \lambda_2, \lambda_3)\right]. \tag{131}$$

It can be seen, in analogy with the function $\hat{\psi}$ defined in Eq. (19), that the function $\widehat{\phi}(\lambda_1, \lambda_2, \lambda_3)$ is differentiable (basically, this is assured from the fact that the expressions in the exponent in the right hand side of Eq. (129) are sums of one-particle functions). Then, Eq. (131) is verified. Once $\widehat{s}_{\text{micr}}(m, q, r)$ is given, our function of interest, $\widetilde{s}_{\text{micr}}(\epsilon, m)$ is obtained from

$$\widetilde{s}_{\text{micr}}(\epsilon, m) = \max_{\left[q,r\,|\,-\frac{J}{2}m^2-\frac{K}{2}q^2+r=\epsilon\right]} \widehat{s}_{\text{micr}}(m, q, r). \tag{132}$$

It remains to see that from the last expression we can derive Eq. (93). Substituting Eq. (131) and expressing r as a function of ϵ, m and q, we have

$$\begin{aligned}&\widetilde{s}_{\text{micr}}(\epsilon, m) \\ &\quad = \max_q\left\{\min_{\lambda_1,\lambda_2,\lambda_3}\left[\lambda_1 m + \lambda_2 q + \lambda_3\left(\epsilon + \frac{J}{2}m^2 + \frac{K}{2}q^2\right) - \widehat{\phi}(\lambda_1, \lambda_2, \lambda_3)\right]\right\}. \end{aligned} \tag{133}$$

The four stationarity conditions of this problem are:

$$m - \frac{\partial\widehat{\phi}}{\partial\lambda_1} = 0 \tag{134}$$

$$q - \frac{\partial\widehat{\phi}}{\partial\lambda_2} = 0 \tag{135}$$

$$\epsilon + \frac{J}{2}m^2 + \frac{K}{2}q^2 - \frac{\partial\widehat{\phi}}{\partial\lambda_3} = 0 \tag{136}$$

$$\lambda_2 + \lambda_3 K q = 0\,. \tag{137}$$

Eliminating λ_2 from the problem by implementing immediately the last stationarity condition, we have

$$\widetilde{s}_{\mathrm{micr}}(\epsilon, m) = \max_q \left\{ \min_{\lambda_1, \lambda_3} \left[\lambda_1 m + \lambda_3 \left(\epsilon + \frac{J}{2} m^2 - \frac{K}{2} q^2 \right) - \widehat{\phi}(\lambda_1, -\lambda_3 K q, \lambda_3) \right] \right\}\,. \tag{138}$$

After the notation changes $\lambda_3 \to \beta$ and $q \to y$, and defining φ by $\lambda_1 = -\beta J m - \varphi$, the last expression becomes

$$\widetilde{s}_{\mathrm{micr}}(\epsilon, m) = \max_y \left\{ \min_{\beta, \varphi} \left[\lambda_1 m + \beta \epsilon - \beta \frac{J}{2} m^2 - \beta \frac{K}{2} q^2 - \widehat{\phi}(-\beta J m - \varphi, -\beta K y, \beta) \right] \right\}\,. \tag{139}$$

This is recognized to be the same as Eq. (93), once one realizes from the definitions (19) and (129) that $\widehat{\phi}(-\beta J m - \varphi, -\beta K y, \beta) = \hat{\psi}(\beta, \beta J m + \varphi, \beta K y)$.

Appendix B: General Expressions for the Entropy Obtained with Direct Counting

In this Appendix we provide a summary of the general expressions, obtained with direct counting, for the entropy of one-dimensional Ising spin models having the form $H = H_{LR} + H_{SR}$, where $H_{LR} = -\frac{J}{2N}\left(\sum_i S_i\right)^2$ is the long-range, mean-field term, and H_{SR} is the short-range part of the Hamiltonian. The interested reader can find full details in Ref. [17]. We emphasize that we are referring to the expressions of the entropy defined as the logarithm of the number of configurations for given values of the magnetization and of the spin correlations, like, e.g., the function $s(m, g_1, g_2, t)$ in (119). From these expressions one can obtain the microcanonical entropy $\widetilde{s}_{\mathrm{micr}}(\epsilon, m)$ with the long optimization procedure described in Sect. 4.1.

In the main text we confined ourselves to the form (111), where only two-spin terms are included. The short-range Hamiltonian (111) is a sub-case of the general one-dimensional short-range Ising model with multispin interactions defined by

$$\begin{aligned} H_{SR} = &- \sum_i j_i^{(1)} S_i - \sum_{i,j} j_{i,j}^{(2)} S_i S_j - \sum_{i,j,k} j_{i,j,k}^{(3)} S_i S_j S_k \\ &- \sum_{i,j,k,l} j_{i,j,k,l}^{(4)} S_i S_j S_k S_l - \dots \end{aligned} \tag{140}$$

where the sums run over distinct couples, triples, quartets and so on up to a certain finite range. Periodic boundary conditions are assumed and the couplings $j^{(n)}$ are assumed to be invariant under translation by ρ spins:

$$j_{i_1, i_2, \dots, i_n}^{(n)} = j_{i_1+\rho, i_2+\rho, \dots, i_n+\rho}^{(n)}. \tag{141}$$

As in the main text, N denotes the number of sites and R the finite-range of the interaction. For example, the Hamiltonian $H_{SR} = -(K_1/2)\sum_i S_i S_{i+1}$ has $\rho = 1$ and $R = 2$, while $H_{SR} = -(K_1/2)\sum_i S_i S_{i+1} - (K_2/2)\sum_i S_i S_{i+2}$ has $\rho = 1$ and $R = 3$. In the general case, for simplicity we assume N/ρ is an integer.

Following the notation and the procedure presented in [17], let us start from the case $J = 0$, for which $H = H_{SR}$. To simplify the notation let us rewrite (140) as

$$H_{SR} \equiv - \sum_{\mathrm{Rg}(\mu) \leq R}' \sum_{n=1}^{N/\rho} j_\mu O_{\mu+n\rho}(\{S_i\}), \tag{142}$$

where μ is a subset of $\{1, \ldots, R\}$. The notation $\mathrm{Rg}(\mu) \leq R$, stands for "the range of the interaction is less than or equal to R". Moreover, $O_{\mu+n\rho}$ is an operator associated to the subset $\mu \equiv \{n_1, n_2, \ldots n_{|\mu|}\}$, where $|\mu|$ is the number of elements of μ, and translated by $n\rho$ so that it acts on the spins as

$$O_{\mu+n\rho}(\{S_i\}) = S_{n_1+n\rho} S_{n_2+n\rho} \ldots S_{n_{|\mu|}+n\rho}. \tag{143}$$

For the null subset $\varnothing$ we define $O_\varnothing = 1$ and the prime $'$ in the sum over μ in (142) denotes that the null subset is not included and that the terms related by a translation of a multiple of ρ are counted only once. The correlation functions are denoted by g_μ. They are associated to the operator O_μ and defined according to

$$g_\mu = \langle O_\mu(\{S_i\}) \rangle = \langle S_{n_1} S_{n_2} \ldots S_{n_{|\mu|}} \rangle \tag{144}$$

(by definition, $g_\varnothing = 1$). For example, for the Hamiltonian considered in Sect. 4.1 we would have the correlation functions $g_{\{1\}}$, $g_{\{1,2\}}$, $g_{\{1,3\}}$ and $g_{\{1,2,3\}}$, that in the lighter notation of the main text were denoted, respectively, with m, g_1, g_2 and t.

The main result of Ref. [17] concerns the entropy $s(\{g_\mu\})$ for the model with interactions up to range R; it is given by:

$$s(\{g_\mu\}) = s^{(R)}(\{g_\mu\}) - s^{(R-\rho)}(\{g_\mu\}), \tag{145}$$

where in the left side and in the first term in the right hand side $\{g_\mu\}$ stands for the set of all possible correlations of range up to R, while in the seond term in the right hand side it stands for all correlations of range up to $(R - \rho)$. It is written in terms of the functions $s^{(Q)}(\{g_\mu\})$. The quantity $s^{(Q)}$ can be seen as the "entropy at range Q", and is given by

$$s^{(Q)}(\{g_\mu\}) = - \sum_{\tau_Q} p(\tau_Q) \ln p(\tau_Q), \tag{146}$$

where

$$p(\tau_Q) = 2^{-Q} \sum_{\mathrm{Rg}(\mu) \leq Q} g_\mu O_\mu(\tau_Q), \tag{147}$$

and $\tau_Q \equiv \{t_1, t_2, \ldots, t_Q\}$ denotes the configuration of Q Ising spins, with the sum over μ is on every subset (including the null one). Finally, from (142) one gets the energy per unit cell as:

$$e(\{g_\mu\}) = - \sum_{1 \leq \mathrm{Rg}(\mu) \leq R} g_\mu j_\mu. \tag{148}$$

When the mean-field term H_{LR} is turned on, only the energy e is affected, while the dependence of the entropy $s(\{g_\mu\})$ on the correlations g_μ is not. One then has to add the corresponding contribution to e. In this way one finds the results (114) and (116), respectively for s and for e, for the model (110) with $K_2 = 0$; and the results (119) and (125) for the same model with $K_2 \neq 0$. In particular, specializing (145) to our model with $K_2 = 0$ one has that Eq. (114) is obtained from $s(m, g_1) = s^{(2)}(m, g_1) - s^{(1)}(m)$, while Eq. (119) for the model with $K_2 \neq 0$ is obtained from $s(m, g_1, g_2, t) = s^{(3)}(m, g_1, g_2, t) - s^{(2)}(m, g_1)$.

Appendix C: Comparison of the Microcanonical Entropy at Fixed Magnetization for $K_2 \neq 0$

In this Appendix we consider an example of explicit determination of the microcanonical entropy at fixed magnetization directly from the entropy $s = s(m, g_1, g_2, t)$, given in Eq. (119), for the model (110). To compare the findings with the results obtained with the method presented in section 3, we choose the same values of K_1 and K_2 used in Fig. 5: $K_1 = -0.4$, $K_2 = -0.16$ (with $J = 1$). The energy is chosen as $\epsilon = -0.107$, as in the bottom right panel of Fig. 5.

As discussed in the main text, one has to determine t via Eqs. (120)–(121). Once this is done, one has to express g_2 as a function of m, g_1 using the energy expression (125). One has then s as a function of m and g_1 and it is possible to plot in the $m - g_1$ plane the allowed regions. Of course the same procedure can be performed by studying the entropy in the $m - g_2$ plane. The final point in both cases is to find the maximum of the microcanonical entropy maximizing with respect to, respectively, g_1 or g_2.

Notice that in this procedure finding the maximum with respect to g_1, g_2 and t is the easier part since the entropy is concave along these directions on the constant energy surface. In the remaining variable m instead, within the constant energy surface, the entropy is *not* concave and many entropy maxima can and do appear and compete resulting in the emergence of the different phases and transitions among them. This is obviously to be traced to the special role of m in the Hamiltonian, in which it appears nonlinearly and thus can spontaneously break the $m \to -m$ symmetry. Restricting to fixed magnetization indeed relieves many of the difficulties. The procedure is described in Figs. 7 and 8, where we consider the value $m = 0.55$, and one finds that the maximum entropy is $s \simeq 0.47828$, in agreement with the results presented in the bottom right panel of Fig. 5, obtained with the procedure described in section 3. Note that in the course of the process we also determine the macroscopic observables fully characterizing the thermodynamic state. Fig. 9 also shows that if we decide to eliminate g_2 in favour of (m, g_1) or, alternatively, g_1 in favour of (m, g_2), we obtain the same result for the microcanonical entropy at fixed magnetization when the maximum in, respectively, g_1 or g_2 is taken, as of course it has to be. For completeness we also plot the

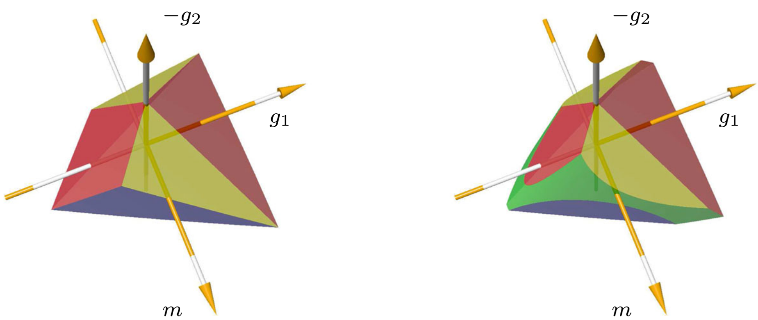


Fig. 7 Three-dimensional plot of the allowed region in the (m, g_1, g_2) space (left). On the right the allowed region has been cut with the constant energy surface (a parabolic cylinder) given by $\epsilon = -\frac{1}{2}(Jm^2 + K_1 g_1 + K_2 g_2)$. The green surface is thus the accessible region in the microcanonical ensemble. The chosen values are $\epsilon = -0.107$, $K_1 = -0.4$ and $K_2 = -0.16$. Please note that in order to improve visibility the g_2 axis has been reversed (Color figure online)

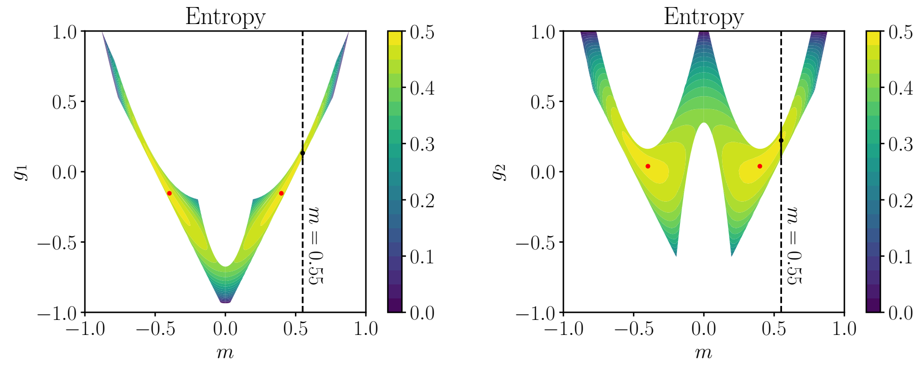
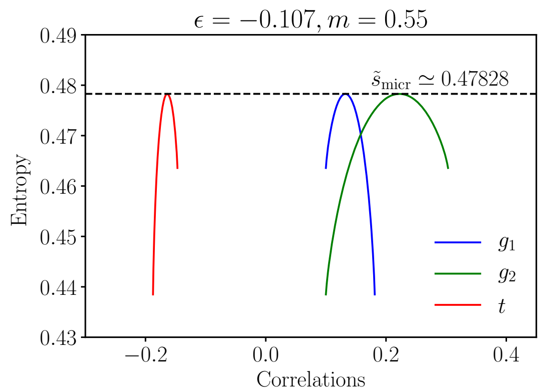


Fig. 8 Entropy as a function of m and g_1 (left) and m and g_2 (right) for the parameter values $\epsilon = -0.107$, $K_1 = -0.4$ and $K_2 = -0.16$. The line with magnetization $m = 0.55$ (chosen to have an example of comparison with Fig. 5) is denoted with a black line. The maximum of the entropy s in this fixed magnetization sector is denoted with a black dot. It is characterised by the observables $m = 0.55$, $g_1 \simeq 0.13235$, $g_2 \simeq 0.22226$ and $t \simeq -0.16384$. The global maxima of s are also shown with a red dot. These points are characterized by the following observables: $m \simeq \pm 0.39839$, $g_1 \simeq -0.15375$, $g_2 \simeq 0.03885$, and $t \simeq -0.46475$ (Color figure online)

Fig. 9 Entropy in the fixed energy ($\epsilon = -0.107$) and magnetization ($m = 0.55$) sector as a function of the three independent correlations g_1 (blue), g_2 (green) and t (red) when the other two are eliminated. Parameter values are $K_1 = -0.4$ and $K_2 = -0.16$. The maximum $\widetilde{s}_{\text{micr}}$ is denoted with a dashed line and it occurs at $g_1 \simeq 0.13235$, $g_2 \simeq 0.22226$, and $t \simeq -0.16384$. The value of the maximum, $\widetilde{s}_{\text{micr}} \simeq 0.47828$, corresponds to the value of $\widetilde{s}_{\text{micr}}(\epsilon, m)$ at $m = 0.55$ in the right bottom panel of Fig. 5 (Color figure online)



entropy as a function of the correlation t after maximizing with respect to one among g_1 and g_2.

The direct counting method outlined shows some technical difficulties due to the already moderately large number of variables over which the entropy has to be optimized. Of course these extra variables are interesting in their own right being macroscopic observables fully characterising the thermodynamic state. On the other hand direct counting possesses the virtue of making very clear the geometric origin of (microcanonical) phase transitions in long-range systems as the study of the maxima of the entropy restricted on the nonlinear energy surface. This makes interesting also short-range one-dimensional systems, whose entropy is concave in all variables, yielding normally no phase transition. The gained insight could prove useful in the understanding of and the hunt for the many exotic critical points expected in the microcanonical ensemble [18].

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