Wang-Landau Monte Carlo simulation of the Blume-Capel model

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We carry out a study of the two-dimensional Blume-Capel model using the Wang-Landau Monte Carlo method which estimates the density of states $g(E)$ directly. This work validates the applicability of this method to multiparametric systems, since only one computer run is needed for all range of macroscopic parameters (temperature, anisotropy, etc.). The location of the tricritical point is determined as $k_BT_t/J=0.609(3)$, $D_t/J=1.966(2)$ and is in excellent agreement with previous estimates. The free energy and the entropy, which are not directly accessible by conventional Monte Carlo simulations, are obtained simply using $g(E)$.

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I. INTRODUCTION

The study of phase transitions and critical phenomena [1] has been enriched in recent years by the development of new algorithms that improve the efficiency of the computer simulations. The standard Metropolis Monte Carlo (MC) method [2] due to long time scales in both first-order and continuous phase transitions problems suffers from the slow dynamics which requires very long simulations. Several attempts to overcome these problems have been suggested, like the cluster algorithms proposed by Swendsen and Wang [3] and extended by Wolff [4], which have been used to reduce the critical slowing down at continuous transitions, or the multicanonical ensemble method [5], which reduces the tunneling time between coexisting phases in first-order transitions. Other approaches such as the histogram method of Ferrenberg and Swendsen [6], the entropic sampling [7], and the flat histogram method [8] also represented important improvements to circumvent problems of scalability for large systems.

Most conventional MC algorithms generate an unnormalized canonical distribution $P(E,T)=g(E)e^{-E/k_BT}$ at a given temperature T and then multiple runs are usually needed to describe thermodynamic quantities over a significant range of temperatures. However, a new, general, and efficient MC algorithm known as the Wang-Landau algorithm [9,10] offers substantial advantages over existing approaches since it estimates directly the density of states $g(E)$, the number of all possible states (or configurations) for an energy level E of the system. With an accurate estimate of $g(E)$ for all energies, one can construct canonical distributions at any temperature and calculate the partition function as

$$Z(T)=\sum_X e^{-E(X)/k_BT}=\sum_E g(E)e^{-E/k_BT}, \tag{1}$$

where the sum in X runs over all possible configurations and the sum in E runs over all the existing energy levels. Most thermodynamic quantities can therefore be calculated from Z.

The Wang-Landau method estimates $g(E)$ via a random walk in energy space that produces histograms locally flat and makes $g(E)$ converge quickly to the real value improving it at each step of the random walk using a carefully controlled modification factor. This method, initially proposed to study classical spin models [9,10], has proven to be very useful and efficient in many different applications, like systems with continuous degrees of freedom [11] and quantum systems [12], including systems with rough energy landscapes. Some generalizations have also been carried out to cluster dynamics [13] and N-fold way dynamics [14], and in order to avoid boundary effects in the algorithm itself [15].

In this paper, we apply the Wang-Landau method to the two-dimensional spin-1 Blume-Capel model [16] which exhibits a line of continuous phase transitions, a line of first-order phase transitions, and a tricritical point. The motivation behind this model is that it has a rich phase diagram and, since the density of states is independent of any macroscopic parameters, the study of such a diagram can be performed accurately by a single simulation. Using the background presented in [17], we also estimate directly the tricritical point, which characterizes the thermodynamic behavior of this model, and compare our value with some previously available results [18,19].

The rest of this paper is organized as follows. In Sec. II, we present the model. In Sec. III, we describe the simulation procedure employed in this study and the details of the Wang-Landau algorithm. In Sec. IV we show our results for the density of states, the thermodynamic properties, and both second- and first-order lines of the phase diagram and, in addition, the estimate of the tricritical point. Finally, in Sec. V we detail our conclusions.

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II. THE MODEL

The Blume-Capel model is the spin-1 generalization of the Ising model defined by the Hamiltonian

$$\mathcal{H} = -J\sum_{\langle ij\rangle} \sigma_i\sigma_j + D\sum_i \sigma_i^2, \tag{2}$$

where the spin variables σ_i take on the values -1, 0, $+1$, and the notation $\langle ij\rangle$ implies summation over all pairs of nearest-neighbor spins on a two-dimensional lattice. Here, J is the coupling constant and D is the single-spin anisotropy parameter. A wide variety of techniques have been employed to study this model, including mean-field theory [16], Monte Carlo simulations [20], series expansion methods [21], and renormalization group theory [22]. The model exhibits a phase diagram with ordered ferromagnetic and disordered paramagnetic phases separated by a transition line that changes from an Ising-like continuous phase transition to a first-order transition at a tricritical point. Most of the techniques cited above predict the existence of this tricritical point. A precise and conclusive result for the tricritical point was obtained by using conformal invariance and finite-size scaling in Ref. [19]. In this work the authors found the tricritical point at $k_BT_t/J=0.609(4)$ and $D_t/J=1.965(5)$. This is until now a well-established result and may be compared with a previous finite-size scaling calculation [18] that gives $k_BT_t/J=0.610(5)$ and $D_t/J=1.965(5)$.

III. SIMULATION PROCEDURE

The Wang-Landau algorithm performs random walks in the energy space by changing randomly the states of the spins, where the new configurations are accepted with a probability that is proportional to $1/g(E)$, the reciprocal of the density of states. As a result a flat histogram is generated for the energy distribution. We accumulate this histogram $H(E)$ during the random walk and the current density of states is modified by a multiplicative factor f, and the new (updated) density of states is used to perform a further random walk. Since the density of states is not known *a priori* in the beginning of the simulations we set all entries to $g(E)=1$ for all energy levels. In an ideal case, when the density of states would reach its true value, the simulation would be finished and the modification factor should be the unit.

The random walk is then performed considering that if E_i and E_f are energies before and after a spin is flipped, the transition probability from energy level E_i to E_f is

$$p(E_i \to E_f) = \min\left(\frac{g(E_i)}{g(E_f)}, 1\right). \tag{3}$$

The density of states is modified by f using

$$g(E) \to g(E)f, \tag{4}$$

whenever a state with energy E is accepted. In addition the energy histogram is updated as $H(E)\to H(E)+1$. In practice, we use

$$\ln[g(E)] \to \ln[g(E)] + \ln(f). \tag{5}$$

In choosing the initial modification factor one should have in mind that all possible energy levels must be reached quickly even for a large system. A reasonable choice is $f=f_0=e=2.718\,28\ldots$. To reduce the modification factor we use a function like $f_{i+1}=\sqrt{f_i}$. This reduction is accomplished whenever the energy histogram becomes flat during the random walk.

In our simulations, the flatness criterion for the histogram $H(E)$ is about 80% of the average histogram $\langle H(E)\rangle$, and this is generally checked about each 10 000 Monte Carlo sweeps. For the multiparametric case a higher percentage of $\langle H(E)\rangle$ would take long simulation times. Afterward the histogram is always reset $[H(E)=0]$ for all values of E. Finally the simulation comes to an end when the modification factor is smaller than $f_{final}=1+10^{-8}$.

Specifically for the Blume-Capel model we may define, from Eq. (2),

$$E_1 = \sum_{\langle ij\rangle} \sigma_i\sigma_j \tag{6}$$

and

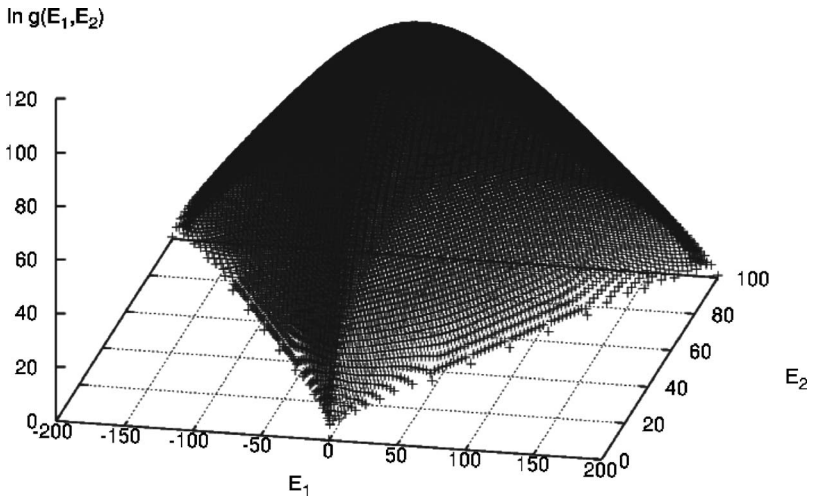

FIG. 1. Logarithm of the density of states of the two-dimensional (2D) Blume-Capel model for $L=10$.

$$E_2 = \sum_i \sigma_i^2. \tag{7}$$

These quantities are independent of the set of parameters J, D, and T. The energy of the system is then reduced to $-JE_1+DE_2$. At a temperature T the partition function may be written as

$$Z(T,D) = \sum_X e^{[JE_1(X)-DE_2(X)]/k_BT} \tag{8}$$

or

$$Z(T,D) = \sum_{E_1,E_2} g(E_1,E_2)e^{[E_1-(D/J)E_2]/(k_BT/J)}. \tag{9}$$

In this case, D/J varies from $-\infty$ to 2. Thus, if the function $g(E_1,E_2)$, which is independent of the temperature and the anisotropic parameter, can be calculated precisely, one may therefore estimate all thermodynamic properties of the system. For example, the internal energy $U(T,D)$ can be calculated as

$$U(T,D) = \frac{\sum_{E_1,E_2} (-JE_1 + DE_2)P(E_1,E_2,T,D)}{\sum_{E_1,E_2} P(E_1,E_2,T,D)} \equiv \langle E \rangle, \tag{10}$$

where

$$P(E_1,E_2,T,D) = g(E_1,E_2)e^{[E_1-(D/J)E_2]/(k_BT/J)} \tag{11}$$

is the canonical distribution. The specific heat $C(T,D)$ can be estimated from the fluctuations in the internal energy

$$C(T,D) = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_BT^2}. \tag{12}$$

Furthermore, one can also calculate quantities that are not available from conventional Monte Carlo simulation, such as the Helmholtz free energy and the entropy. The free energy $F(T,D)$ can be calculated directly from the partition function Z using

$$F(T,D) = -k_B \ln(Z), \tag{13}$$

and the entropy as

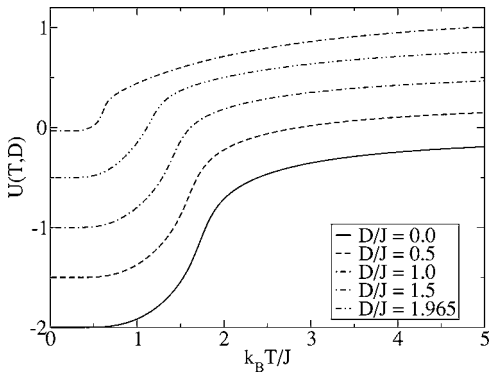

FIG. 2. Internal energy calculated from the density of states of the Blume-Capel model for $L=12$ and some values of D/J.

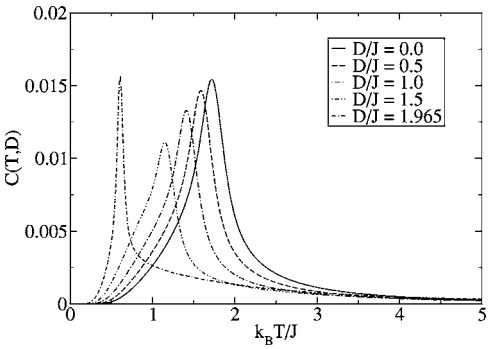

FIG. 3. Specific heat calculated from the density of states of the Blume-Capel model for $L=12$ and some values of D/J.

$$S(T,D) = \frac{U(T,D) - F(T,D)}{T}. \tag{14}$$

IV. RESULTS

The estimate of the density of states for $L=10$ using Wang-Landau sampling is shown in Fig. 1. Similar results are obtained for other values of L. Note that the macrostate space E_1 vs E_2 is not completely covered because some pairs (E_1,E_2) do not correspond to existing states. We also note that the energy space of the Blume-Capel model has a huge number of levels. This increases the simulation time and restricts the applicability of the Wang-Landau method to multiparametric systems as well as to large lattices L. Although the random walk can be done over several energy windows independently, this causes considerable fluctuations in the thermodynamic properties when the windows are joined together [14]. Also, this does not reduce the simulation time noticeably. Thus, our random walk is made over the entire energy space without windows. Since $g(E_1,E_2)$ is now obtained, we can calculate any thermodynamic quantity without resorting again to computer simulations. We have calculated the internal energy, the specific heat, the free energy, and the entropy as continuous functions of temperature T for some values of the anisotropy parameter D/J. Our results for the internal energy, the specific heat, the free energy and the entropy are shown in Figs. 2, 3, 4, and 5, respectively.

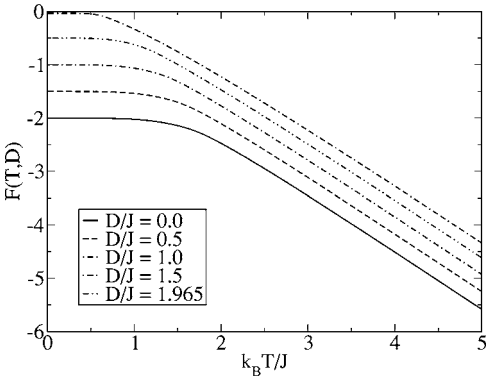

FIG. 4. Helmholtz free energy calculated from the density of states of the Blume-Capel model for $L=12$ and some values of D/J.

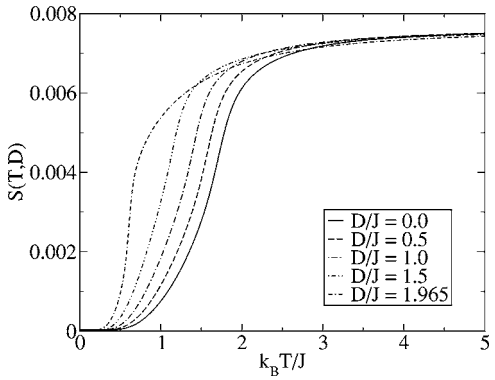

FIG. 5. Entropy calculated from the density of states of the Blume-Capel model for $L=12$ and some values of D/J.

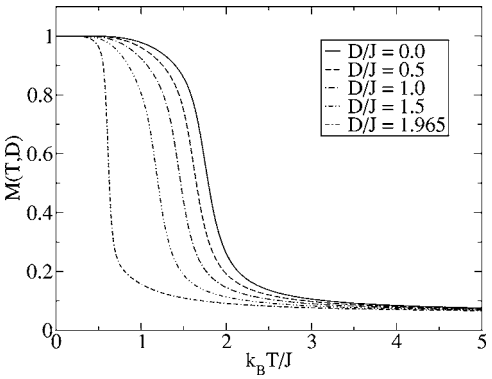

FIG. 6. Canonical average of the magnetization obtained from the density of states of the Blume-Capel model for $L=12$ and some values of D/J.

In Fig. 6 we show the magnetization of the Blume-Capel model as a function of temperature for some values of D/J. This quantity is obtained from the canonical average

$$M(T,D) = \frac{\sum_{E_1,E_2} \langle M(E_1,E_2)\rangle P(E_1,E_2,T,D)}{\sum_{E_1,E_2} P(E_1,E_2,T,D)} \equiv \langle m \rangle, \quad (15)$$

where $\langle M(E_1,E_2)\rangle$ is a microcanonical average of the magnetization which is calculated simultaneously with the energy histogram $H(E_1,E_2)$. Similar results are obtained for other values of L.

A. The phase diagram

Because of the huge number of energy levels of the Blume-Capel model, we have chosen to study four system sizes corresponding to $L=8,10,12,16$. Our attempts at simulating the system for $L=32$ have shown that it would take a prohibitive computer time for our available facilities. Problems with large system sizes are also present in other Monte Carlo estimates for the same model [18,19] and our work reveals some limitations for the Wang-Landau sampling as well. Nevertheless, we have obtained very good results as will become clear farther on. First, we have investigated the second-order line of the phase diagram. From the peaks of the specific heat the transition temperature $k_B T_c/J$ in the thermodynamic limit was estimated for each value of anisotropy parameter D/J. Some of these points are shown in Table I, where our results are compared with some previous estimates obtained in Refs. [18,19], when available. One can see that there is an overall good agreement between them.

To examine the first-order line we have computed the probability distribution which should have a double-peak picture at a first-order transition. Following the prescription of Wilding and Nielaba [17] we have located the first-order transition temperatures. In this work, the authors calculate the distribution of a new variable defined as

$$\mathcal{D} = E_1 - sE_2, \quad (16)$$

where s is an arbitrary field mixing parameter [23].

TABLE I. Comparison between our results of the second- and first-order lines with the previous results obtained by the finite size scaling technique.

D/J	$k_B T/J$			Order of transition
	Ref. [18]	Ref. [19]	Wang-Landau	
−0.5		1.794(7)	1.816(2)	Second
0.0	1.695	1.681(5)	1.714(2)	Second
0.5	1.567		1.584(1)	Second
1.0	1.398		1.413(1)	Second
1.5	1.150		1.155(1)	Second
1.87	0.800		0.800(3)	Second
1.9		0.764(7)	0.755(3)	Second
1.92	0.700		0.713(2)	Second
1.95	0.650		0.651(2)	Second
1.962	0.620		0.619(1)	Second
1.969	0.600		0.596(5)	First
1.99	0.550		0.555(2)	First
1.992	0.500		0.499(3)	First

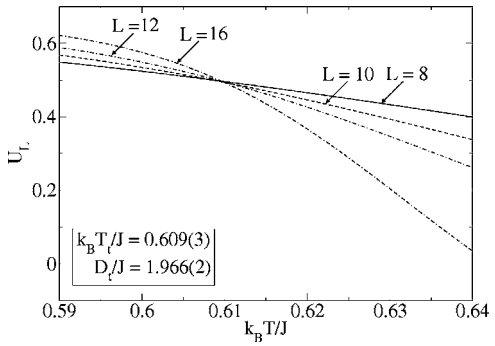

FIG. 7. The fourth-order cumulant U_L for the two-dimensional Blume-Capel model for a number of system sizes along the first-order line.

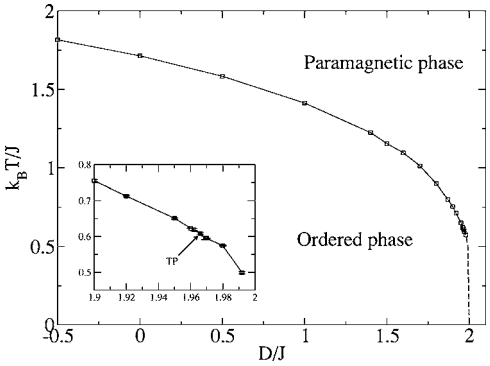

FIG. 8. Phase diagram of the Blume-Capel model in the plane of anisotropy parameter and temperature. The dashed curve is a first-order transition line and the solid curve is a second-order one. They separate the ordered from the paramagnetic phase, and join together at the tricritical point (TP). The inset shows an amplification of the region around the tricritical point.

For each value of D/J we adjust the values of s and k_BT/J that make the two peaks of the distribution to have the same height. This temperature corresponds to the first-order transition temperature k_BT_c/J. From theory we know that the first-order line is located close to 2; thus taking values of D/J in this region we obtain the corresponding transition temperatures. Some of our results for the first-order line are also shown in Table I.

To locate the tricritical point, we used the intersection of the fourth-order cumulant U_L [24], which is defined as

$$U_L = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}. \tag{17}$$

In our case, $\langle m^2 \rangle$ and $\langle m^4 \rangle$ are the canonical averages of the second and fourth moments of magnetization. Thus, we measured U_L for a number of temperatures and system sizes along the first-order line and at the tricritical point the curves U_L are expected to intersect one another. The cumulants were calculated in the range $D/J=1.96-1.97$ for each system size. Our result for the cumulant is presented in Fig. 7 as a function of the temperature. The common point of intersection have been estimated as $k_BT_t/J=0.609(3)$ with a corresponding tricritical anisotropy parameter $D_t/J=1.966(2)$. These values are in excellent agreement with the previous results mentioned before. In Fig. 8 we show the phase diagram of the Blume-Capel model in the plane of anisotropy parameter and temperature. The dashed curve is a first-order transition line and the solid curve is a second-order one. They separate the ordered from the paramagnetic phase, and join together at the tricritical point (TP). Our results confirm the great advantage of exploring the phase diagram using a microcanonical approach, since the simulation is independent of the macroscopic parameters.

V. CONCLUSIONS

In this work we have shown the applicability of the Wang-Landau method to the two-dimensional Blume-Capel model investigating its tricritical behavior. It is now clear that even though the method was originally proposed to study large systems, the simulation of systems with more than one macroscopic parameter (multiparametric Hamiltonians) is restricted to not very large lattice sizes because of the huge number of energy levels. Nevertheless by estimating with high accuracy the density of states, we succeeded in exploring the phase diagram of the present model with more precision then any previous simulational work.

Another advantage of our results is the calculation of the entropy and the Helmholtz free energy which are usually unreachable within the conventional Monte Carlo simulations. Finally, we have estimated the location of the tricritical point as $k_BT_t/J=0.609(3)$ and $D_t/J=1.966(2)$. This estimate is in excellent agreement with previous approaches and shows the great efficiency of the Wang-Landau method in estimating the density of states of any system like this.

ACKNOWLEDGMENTS

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