A Broad Histogram study of a two-dimensional Blume-Capel model

C. J. Silva* and A. A. Caparica†
Instituto de Física, Universidade Federal de Goiás, 74.001-970, Goiânia (GO), Brazil

The generalization of the Broad Histogram Method for systems with multiparametric Hamiltonians enable us to calculate the density of states of a two-dimensional Blume-Capel model in zero field. The full density of states is calculated as a function of the two spin summations which appear in the Hamiltonian. This permits any thermodynamics functions to be evaluated for any temperature and any single site anisotropy with only one computer run. With the density of states one can explore the entire parameter of space in detail and the region near the tricritical point would be investigated with more accuracy.

Keywords: Blume-Capel model; Microcanonical Monte Carlo simulations

I. INTRODUCTION

To calculate the density of states for classical spin systems has been a major task of computer simulation in last years. Several methods have been developed in this sense, like Flat Histogram method[1], Wang-Landau Sampling[2], and so on. In this work we study the Broad Histogram Method (BHM)[3] and its applicability to the Blume-Capel model. This method was proposed by Oliveira *et al.* in 1996 to calculate the density of states directly using a relation between the density of states for the energy and a quantity that has relation to transition of energy. In that work, the author paid attention to the number of potential moves for energy transitions, or the number of the possible energy change, $N(\mathbf{E}, \mathbf{\Delta E})$, for a given microstate $\mathbf{X}$ and a fixed $\mathbf{\Delta E}$.

The density of states is related to the number of potential moves as

$$\langle N(\mathbf{E}, \mathbf{\Delta E})\rangle g(\mathbf{E}) = \langle N(\mathbf{E} + \mathbf{\Delta E}, -\mathbf{\Delta E})\rangle g(\mathbf{E} + \mathbf{\Delta E}), \tag{1}$$

where $\langle N(\mathbf{E}, \mathbf{\Delta E})\rangle$ is a microcanonical average. For the multiparametric case $\mathbf{E}$ is a vector in the space of macrostates with values $(E_1, E_2, ..., E_n)$ if we have a Hamiltonian with n parameters. The movements that are realized in the space of microstates are only allowed if each movement $\mathbf{X_{old}} \rightarrow \mathbf{X_{new}}$ is reversible, this means that the movement $\mathbf{X_{new}} \rightarrow \mathbf{X_{old}}$ is also possible. The number $N(\mathbf{E}, \mathbf{\Delta E})$ counts the movements that change the macrostate $\mathbf{E}$ to another $\mathbf{E} + \mathbf{\Delta E}$. Analogously, $N(\mathbf{E} + \mathbf{\Delta E}, -\mathbf{\Delta E})$ is the number of movements from $\mathbf{E} + \mathbf{\Delta E}$ to $\mathbf{E}$. This can be seen in Eq. (1), which has been proven to be exact for any energy spectrum. This equation can be rewritten as

$$\ln g(\mathbf{E} + \mathbf{\Delta E}) - \ln g(\mathbf{E}) = \ln \frac{\langle N(\mathbf{E}, \mathbf{\Delta E})\rangle}{\langle N(\mathbf{E} + \mathbf{\Delta E}, -\mathbf{\Delta E})\rangle}, \tag{2}$$

since $g(\mathbf{E})$ is a monotonically fast increasing function.

In this work we show preliminary results on the density of states of the two dimensional Blume-Capel model calculated using the relation (1).

II. THE MODEL

The Blume-Capel (BC) model which was first introduced by *Blume*[4] is an extension of the spin-1 Ising model. The Hamiltonian has an additional single-ion anisotropy factor and the model exhibits first order and continuous phase transitions. The continuous phase transition joins the first order transition at the so-called **tricritical point** (see Fig. 1). Its Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j + D \sum_i \sigma_i^2, \tag{3}$$

*Electronic address: claudius_fis@yahoo.com.br
†Electronic address: caparica@if.ufg.br

where, σ_i are the spin variables, which are coupled by J, and takes the values $-1, 0$ and $+1$, D denotes the single-ion crystal field anisotropy, and the summation $\langle ij \rangle$ is made over nearest-neighbor pairs of spins. Here, we consider the ferromagnetic case ($J > 0$).

FIG. 1 shows a schematic phase diagram of the Blume-Capel model. The solid curve is a line of continuous, the dashed curve of first-order phase transitions. They separate the spin-ordered from the disordered phase, and meet at the tricritical point.

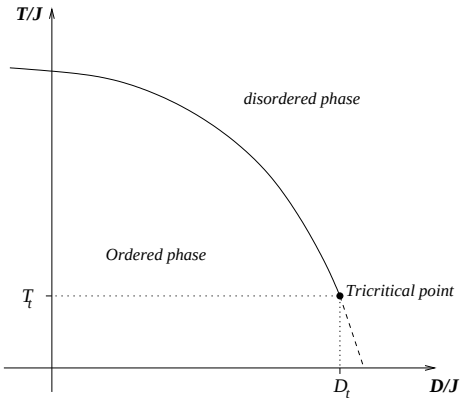

FIG. 1: Phase diagram of the Blume-Capel model.

III. SIMULATION PROCEDURE

Since the BHM is not restricted to any specific dynamical rule, we adopted a non-biased random walk in the space of macrostates to obtain the macroscopic quantities $N(\mathbf{E}, \mathbf{\Delta E})$. The protocol of allowed movements we have chosen was the single spin-flip. Thus, for the BC model we have the allowed $\mathbf{\Delta E}$ as: $(-8,-1),(-8,0),(-8,1),...,(8,-1),(8,0),(8,1)$. We take a $L \times L$ square lattice and rewrite the Hamiltonian as

$$\mathcal{H} = -JE_1 + DE_2, \tag{4}$$

where we define each macrostate as $\mathbf{E} = (E_1, E_2)$.

We start our simulation dividing the space of macrostates into windows containing 12 energy levels for E_1 and 2 for E_2. Beginning inside the first window ($E_1 = 2L^2$ and $E_2 = L^2$), we flip a spin at random and a new macrostate is sampled if it is still inside the window. For each value of E_2 we sampled all values of E_1 and also the levels $E_2 \pm 1$ if it has any connection with the actual performed E_1. If the new macrostate is the actual $\mathbf{E}$ we store the numbers $N(\mathbf{E}, \mathbf{\Delta E})$ corresponding to energy jumps performed inside the window. After a certain number of visits in $\mathbf{E}$ we calculate the microcanonical average $\langle N(\mathbf{E}, \mathbf{\Delta E}) \rangle$ and the energy window is shifted to the not-yet-sampled lower-energy level and the simulation process continues while $E_1 \geq 0$. Then we continue from $E_2 = L^2$ to $E_2 = 0$. With the averages $\langle N(\mathbf{E}, \mathbf{\Delta E}) \rangle$ we calculate $g(\mathbf{E})$ using the Eq. (2). The value of $g(E_1, E_2)$ may be calculated exactly for some values of E_1 and E_2. The exact value used in this work is $g(2L^2, L^2) = 2$.

IV. RESULTS

Our estimation of the density of states is shown in FIG. 2 on a 8×8 lattice. The region for large E_1 and E_2 corresponds to the ordered ferromagnetic phase. The region of small E_1 and E_2 corresponds to the disordered, paramagnetic phase. Along the line $E_2 = L^2$ the system is effectively spin-1/2 and the density of states is only non-zero when E_1 is divisible by four. In this point the system has the same density of states of the two dimension Ising model.

This result is in agreement with ref. [5] in which the Blume-Capel model is study by a microcanonical Monte Carlo simulation.

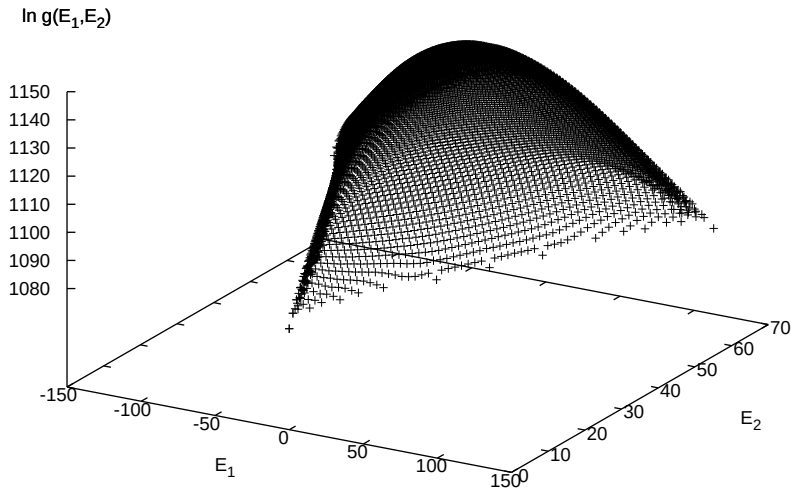

FIG. 2: Density of states $g(E_1, E_2)$ in the Blume-Capel model for a 8×8 lattice.

V. CONCLUSIONS

We presented a until now incomplete study on the density of states of the Blume-Capel model using the Broad Histogram Method. The ferromagnetic and paramagnetic regions are both explored and it is these two parts of the phase space which will contribute to the first-order behaviour. With this density of states any thermodynamic propertie can be obtained.

Acknowledgments

The authors would like to thank the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) and FUNAPE for financial support.

[1] J. S. Wang, Eur. Phys. J. B **8**, 287 (1998).
[2] F. Wang, D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
[3] P. M. C. de Oliveira, T. J. P. Penna and H. J. Hermann, Braz. J. Phys. **26**, 677 (1996).
[4] M. Blume, Phys. Rev. **141**, 517 (1966).
[5] C. M. Care, J. Phys. A: Math. Gen. **26**, 1481 (1993)