Monte Carlo Study of the Spin-1 Baxter-Wu Model

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The two-dimensional spin-1 Baxter-Wu model is studied by using Monte Carlo simulations. The standard single-spin-flip Metropolis algorithm is used to generate the configurations from which the order parameter, specific heat and magnetic susceptibility are measured. The finite-size scaling procedure is employed in order to get the critical behavior. Extensive simulations show that the critical exponents are different from those of the spin-1/2 model suggesting that the spin-1 model is in a different universality class.

1 Introduction

The Baxter-Wu model is a system of spins defined on a two-dimensional triangular lattice with the classical spin variables s_i taking only integer values. It was first introduced by Wood and Griffiths [1] as a model which does not exhibit invariance by a global inversion of all spins. The system is described by the Hamiltonian

$$\mathcal{H} = -J \sum_{<ijk>} s_i s_j s_k, \qquad (1)$$

where the coupling constant J is positive and the sum is over all triangles made up of nearest-neighbor sites on the triangular lattice. For the spin-1/2 model, where $s_i = \pm 1$, the exact solution obtained by Baxter and Wu gives $k_B T_c/J = 2/\ln(1+\sqrt{2})$ and $\alpha = \nu = \frac{2}{3}$[2]. The system has also been studied with quenched impurities by Monte Carlo [3] and Monte Carlo renormalization group approaches [4]. Conformal invariance studies [5, 6] have shown that the pure spin-1/2 Baxter-Wu and the four-state Potts models have the same operator content and are in the same universality class. More recently, the short time critical dynamics has been investigated through the relaxation of the order parameter at the critical temperature by Monte Carlo simulations [7]. On the other hand, for spin values greater or equal to one there are neither exact solutions nor even much approximate approaches. It is the purpose of this work to study the model above for the spin-1 case by using Monte Carlo simulations, where the variables s_i take the values $s_i = -1, 0, 1$.

Monte Carlo methods [8, 9] form the largest and most important class of numerical methods used for solving statistical physics problems. The basic idea behind Monte Carlo simulation is to simulate the random thermal fluctuation of the system from state to state over the course of an experiment. Performing a high-precision finite-size scaling analysis using standard Monte Carlo techniques is very difficult due to constraints on the available computer resources. The introduction of histogram techniques to extract the maximum information from Monte Carlo simulation data at a single temperature enhances the potential resolution of Monte Carlo methods substantially [10, 11]. In this sense, we apply the histogram techniques together with the Metropolis simulation algorithm in order to investigate the thermal behavior of the spin-1 Baxter-Wu model defined by Eq. (1) by considering the specific heat, order parameter and magnetic susceptibility. Our main interest is to obtain, through a finite-size scaling analysis, the phase transition temperature as well as the critical exponents of the model.

In the next section we present the thermodynamic quantities and the details of the simulations. In section III we discuss the results and in section IV we summarize our conclusions.

2 Simulation background

The simulations have been carried out by using the single-spin-flip Metropolis algorithm. In the course of the simulations we considered triangular lattices with linear dimensions $L \times L$ and fully periodic boundary conditions for system sizes of length $18 \leq L \leq 108$. Due to the fact that the system has, in addition to the ferromagnetic phase (with all spins up), three different ferrimagnetic phases with three different sublattices (one sublattice up and spins on the other two sublattices down) the allowed values of L are always a multiple of 3. In this way, all ground states of the infinite lattice would fit on any finite lattice. Following equilibration (which comprised 6×10^4 MCS) runs comprising up to 5×10^6 MCS (Monte Carlo steps per spin) were performed. Histogram reweighting [10, 11] and finite-size scaling techniques were used to precisely locate the second-order phase transition. Regarding the histograms, great care has been taken in order to assure the reliabily of the extrapolated results for all lattice sizes.

The thermodynamic quantities we measured in our simulations are the order parameter, defined as the root mean

square average of the magnetization of the three sublattices

$$m = \sqrt{\frac{{m_A}^2 + {m_B}^2 + {m_C}^2}{3}} \, , \tag{2}$$

where m_A, m_B and m_C are the magnetizations per spin of the different sublattices, the order parameter susceptibility defined as

$$\chi = \beta L^2 \left(\langle m^2 \rangle - \langle m \rangle^2 \right) \, , \tag{3}$$

where $\beta = 1/k_B T$ (with k_B the Boltzmann constant and $\langle ... \rangle$ means an average over the generated Monte Carlo configurations), and the specific heat

$$C = \beta^2 L^{-2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \, , \tag{4}$$

where $\langle E \rangle$ is the mean value of the energy.

According to finite-size scaling theory the critical temperature scales as

$$T_L = T_c + \lambda L^{-1/\nu} \, , \tag{5}$$

where λ is a constant, T_c is the critical temperature of the infinite system, and T_L is the effective transition temperature for the lattice of linear size L. This effective temperature can be given by the position of the maximum of any of the following quantities: the temperature derivative of m, $\ln m$ or $\ln m^2$, the order parameter susceptibility or the specific heat. The above temperatures are given in units of J/k_B. An independent estimate of ν, however, can be made through the evaluation of the maximum logarithmic derivative of any power of the order parameter m^n since one has

$$\left(\frac{dU}{dT} \right)_{max} = a L^{1/\nu} \, , \tag{6}$$

where a is a constant and U is either $\ln m$ or $\ln m^2$ (or, in general, $\ln m^n$). In addition, the specific heat and the magnetic susceptibility scale, at the transition temperature, as

$$C \propto L^{\alpha/\nu}, \quad \chi \propto L^{\gamma/\nu} \, , \tag{7}$$

where α and γ are the critical exponents of the specific heat and susceptibility, respectively. From Eqs. (2-7) one can obtain the critical temperature and critical exponents of the model.

3 Results

The independent evaluation of the critical exponent ν, as obtained from Eq. (6) without any consideration of the critical temperature T_c, is shown in Fig. 1 for the maximum derivative of the logarithm of m and m^2 (although other powers of m can also be used). From both cases one has $\nu = 0.617(4)$, which is different from $\nu = 0.666$ for the spin-1/2 model.

With ν determined quite accurately we proceed to estimate the position of T_c. As discussed in the previous section, the location of the maxima of the various thermodynamic derivatives, namely the maximum of the specific heat, susceptibility, and the derivatives of m and $\ln m$ and $\ln m^2$, provide estimates for the transition temperature which scale with system size as Eq. (5). A plot of these estimates is given in Fig. 2. The results from the linear fit are listed in Table 1. One can note that they are indeed quite close to each other and a final estimate is $T_c = 1.6607(3)$.

The logarithm of the maximum value of the specific heat and order parameter susceptibility as a function of the logarithm of L is shown in Fig. 3. From these data one has $\alpha = 0.692(8)$ and $\gamma = 1.13(1)$.

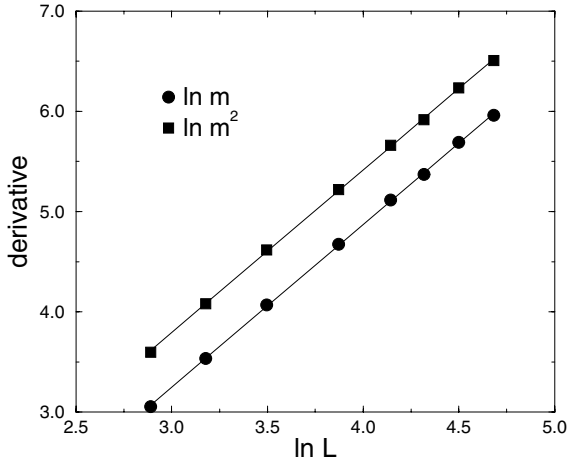

Figure 1. Logarithm of the maximum values of the derivatives of $\ln m$ and $\ln m^2$ as a function of the logarithm of the size L. The straight lines, with slopes corresponding to $\nu = 0.617(3)$ in both cases, show the asymptotic behavior of the fits. The errors are smaller than the symbol sizes.

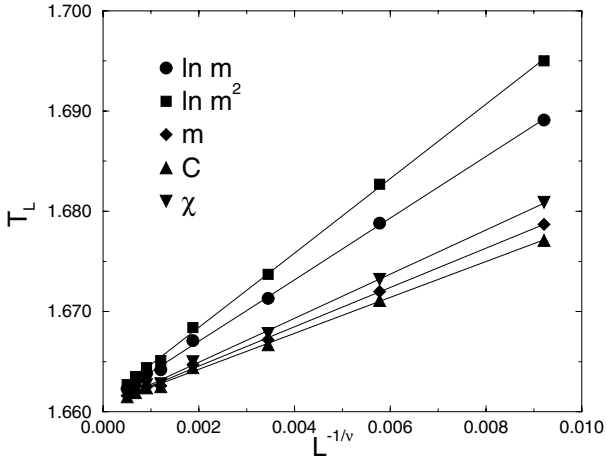

Figure 2. Size dependence of the effective critical temperatures (in units of J/k_B) estimated from several thermodynamic quantities. The lines are fits to Eq. (5) with $\nu = 0.617$ obtained from Fig. 1 and the intercepts are given in Table 1. The errors are smaller than the symbol sizes.

TABLE 1. Estimated critical temperatures from different thermodynamic quantities according to the linear fit shown in Fig. 2.

Quantity	T_c
C	1.6607(1)
χ	1.6605(1)
$\left(\frac{dm}{dT}\right)_{max}$	1.6606(1)
$\left(\frac{d\ln m}{dT}\right)_{max}$	1.6609(1)
$\left(\frac{d\ln m^2}{dT}\right)_{max}$	1.6610(2)

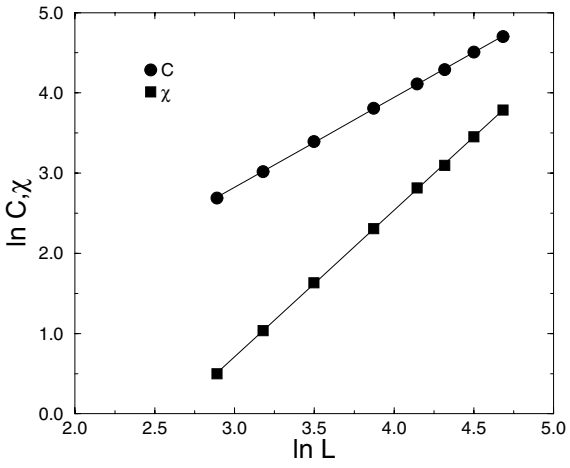

Figure 3. Logarithm of the maximum values of the specific heat C and order parameter susceptibility χ as a function of the logarithm of L. The straight lines are fits to Eqs. (7) with $\alpha/\nu = 1.121(6)$ and $\gamma/\nu = 1.829(9)$. The errors are smaller than the symbol sizes.

4 Conclusions

It is clear, from the quality of the above results, that a well defined second order phase transition takes place in the model at $T_c = 1.6607(3)$ with critical exponents $\nu = 0.617(3)$, $\alpha = 0.692(6)$ and $\gamma = 1.13(1)$, which are indeed different from the spin-1/2 case, namely $\nu = 2/3$, $\alpha = 2/3$ and $\gamma = 7/6$. This means that this three spin interaction model has exponents which depend on the spin value. It is worth saying that the present model can also have an extra interaction with a crystal field of the form $D\sum_i {s_i}^2$. This is a generalization in the direction of the so-called Blume-Capel model [12]. What we have done here is studied the special case $D = 0$. However, in the limit $D \to -\infty$ one recovers the spin-1/2 model. From the present results we then expect that along the second-order transition line for different values of D one has a line with varying critical exponents. In addition, as we have shown, a second-order phase transition takes place at $D = 0$ in contrast with the conjecture that the spin-1 Baxter-Wu model is critical only in the limit $D \to -\infty$ [13]. Some preliminary results, agreeing with the picture of a line of second-order phase transition with varying exponents and the presence of a multicritical point, for the present system with crystal field interaction, have already been obtained from conformal invariance with finite-size scaling theory and the mean field renormalization group approach [14]. Work in this direction using Monte Carlo simulations is now in progress.

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