

Monte Carlo study of the Spin-1 Baxter-Wu model in a crystal field

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Abstract. The two-dimensional Baxter-Wu model with spin-1, in the presence of a crystal field, 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. Single histogram techniques are used to get the results close to the phase transitions. The finite-size scaling procedure is employed in order to obtain the critical behavior. The simulations have shown that the critical exponents are different from the spin-1/2 case and are crystal field dependent.

1. Introduction

The Baxter-Wu model was first introduced by Wood and Griffiths [1] as a model which does not exhibit invariance by a global inversion of all spins. It is defined on a triangular lattice and can be described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ijk \rangle} s_i s_j s_k, \quad (1)$$

where the exchange interaction 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 $k_B T_c / J = 2 / \ln(1 + \sqrt{2})$, $\alpha = \nu = \frac{2}{3}$ and $\gamma = \frac{7}{6}$ [2], where k_B is the Boltzmann constant, T_c is the critical temperature, and α , ν and γ are the critical exponents of the specific heat, correlation length, and susceptibility, respectively. 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 results. It is the purpose of this work to study the Baxter-Wu model



for the spin-1 case by using Monte Carlo simulations, where the variables s_i take now the values $s_i = -1, 0, 1$, and the Hamiltonian can be written as

$$\mathcal{H} = -J \sum_{\langle ijk \rangle} s_i s_j s_k + \Delta \sum_i s_i^2, \quad (2)$$

where Δ is the crystal field interaction. This model has been treated by conformal invariance, finite-size scaling and mean-field renormalization group approaches, [8] and Monte Carlo simulations at zero crystal field [9]. It has been shown that the system belongs to a different universality class with exponents that depend on the value of Δ .

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. (2) 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 for some values of the reduced crystal field $D = \Delta/J$, namely $D = -1$ and $D = +1$.

2. Simulation background

The simulations have been carried out by employing the single-spin-flip Metropolis algorithm [10, 11]. 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 $L = 21, 48, 60, 90, 108, 156, 210$. 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 with spins up, and spins down on the other two sublattices), the allowed values of L must be always a multiple of 3. In this way, all ground states of the infinite lattice would fit on any finite lattice. Following equilibration runs comprising up to 10^8 MCS (Monte Carlo steps per spin) were performed (each equilibration comprised 3×10^5 MCS). Histogram reweighting [12, 13] and finite-size scaling (FSS) techniques were used to precisely locate the second-order phase transition. Regarding the histograms, great care has been taken in order to assure the reliability of the extrapolated results for all lattice sizes.

The thermodynamic quantities that have been measured in our simulations are the order parameter, defined as the root mean square average of the magnetization of the three sublattices

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

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

$$\chi = \beta L^2 \left(\langle m^2 \rangle - \langle m \rangle^2 \right), \quad (4)$$

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

$$C = \beta^2 L^{-2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right), \quad (5)$$

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

In the case of a second-order phase transition, we then expect, for large system sizes, an asymptotic FSS behavior of the form

$$C = C_{reg}(T) + L^{\alpha/\nu} f_C(x) [1 + A_C(x) L^{-\omega}], \quad (6)$$

$$\chi = \chi_{reg}(T) + L^{\gamma/\nu} f_\chi(x) [1 + A_\chi(x) L^{-\omega}], \quad (7)$$

$$\frac{d \ln [\langle m^p \rangle]}{dT} = L^{1/\nu} f_p(x) [1 + A_p(x) L^{-\omega}], \quad (8)$$

where $C_{reg}(T)$ and $\chi_{reg}(T)$ are regular temperature dependent background terms, ν , α , and γ are the usual critical exponents, and $f_i(x)$, with $i = C, \chi, p$, are FSS functions with $x = (T - T_c)L^{1/\nu}$ being the scaling variable. The second term in the brackets approximate all the corrections to scaling by a single term, where ω is the leading correction-to-scaling exponent and $A_i(x)$ are non-universal functions (see, for instance, reference [14]). One should still emphasize that Eq. (6) is valid for $\alpha > 0$ only. Eq. (8) gives the maximum value of temperature derivative of logarithm of the mean value of the p power of the order parameter.

3. Results

In the limit $D = \Delta/J \rightarrow -\infty$ one recovers the spin-1/2 model and we have the results $k_B T_c/J = 2.269185\dots$, $1/\nu = 1.5$, $\alpha/\nu = 1$, and $\gamma/\nu = 1.75$. So, let us start discussing the case $D = -1$. Independent evaluation of the critical exponent ν , as obtained from Eq. (8), 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).

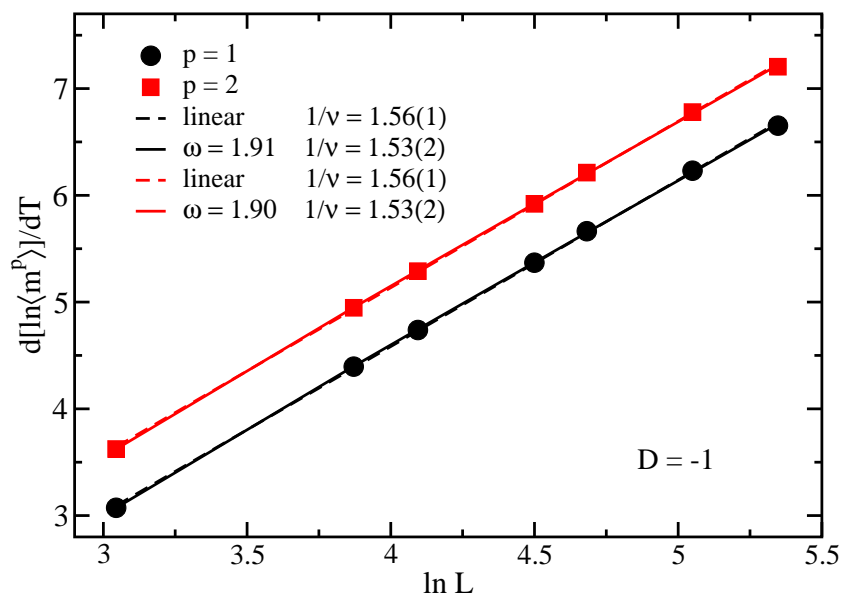


Figure 1. Logarithm of the maximum values of the derivatives of $\ln \langle m \rangle$ and $\ln \langle m^2 \rangle$ as a function of the logarithm of the size L for $D = -1$. The dashed lines are linear fits and the full lines are fits taken into account corrections to scaling. The errors are smaller than the symbol sizes.

The logarithms of the maximum values of the order parameter susceptibility and specific heat, as functions of the logarithm of L , are shown in Figs. 2 and 3, respectively.

From Figs. 1-3 one can see that for this value of the crystal field there is a slight deviation from the critical exponents of the spin-1/2 model. The results are still almost the same whether we take into account corrections to scaling or not. In most of the figures one cannot distinguish the linear fit from the one taking the corrections to scaling. We also note that there is not a strong dependence of the final fittings on the correction-to-scaling exponent, and in general the correction-to-scaling exponent remains close to the expected value of the spin-1/2 case, which is $\omega = 2$. The values of the critical exponents are, however, still closer to the expected results at the limit $D \rightarrow -\infty$.

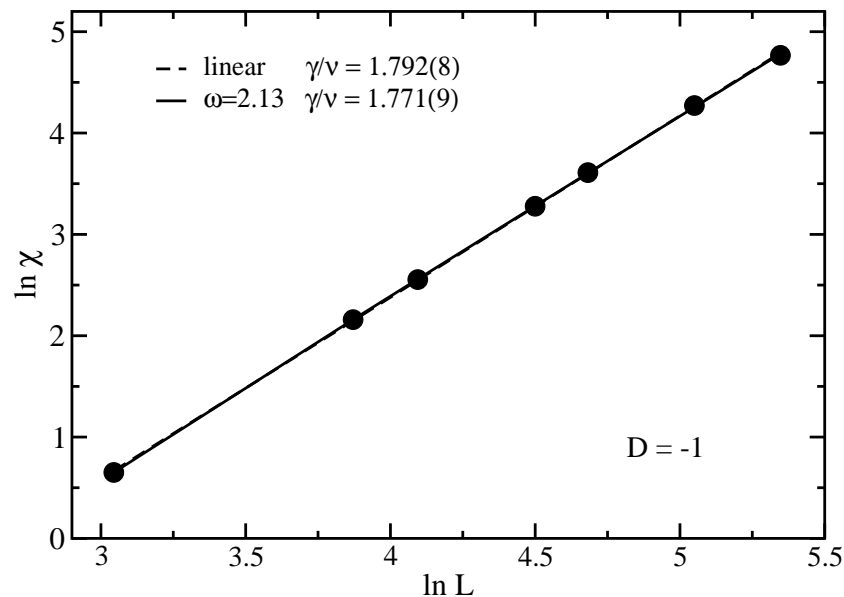


Figure 2. Logarithm of the maximum values of the order parameter susceptibility χ as a function of the logarithm of L for $D = -1$. The dashed line is a linear fit and the full line is a fit taken into account corrections to scaling. The errors are smaller than the symbol sizes.

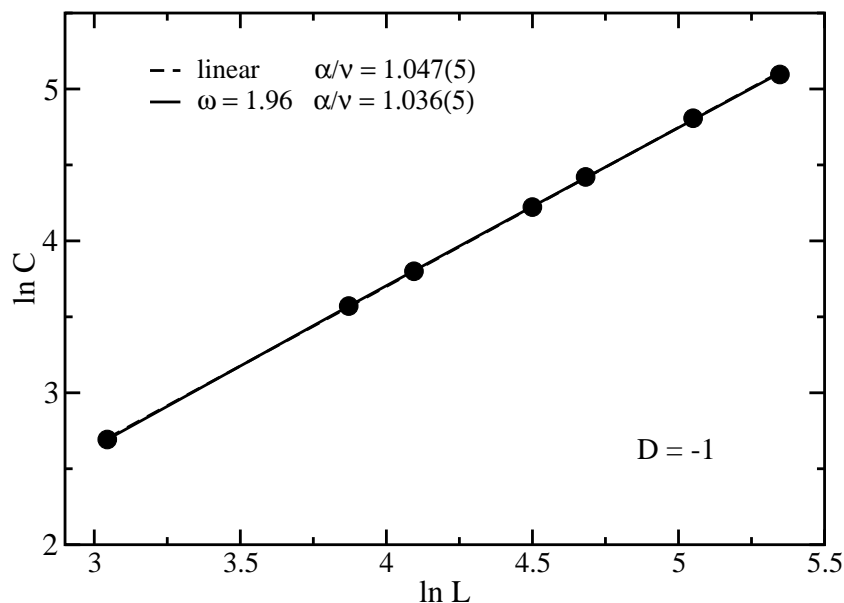


Figure 3. The same as Fig. 2 for the logarithm of the maximum values of the specific heat.

Having ν been determined quite accurately, we can proceed to estimate the position of T_c . As is well known, the location of the maxima of the various thermodynamic derivatives, namely the maximum of the specific heat, susceptibility, and the derivatives of $\ln \langle m \rangle$ and $\ln \langle m^2 \rangle$, provide estimates for the transition temperature itself. As the critical exponents have similar values by either considering or not corrections to scaling, in order to estimate the critical temperature we can use the simpler finite-size scaling relation

$$T_L = T_c + \lambda L^{-1/\nu}, \quad (9)$$

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 . A plot of these estimates is given in Fig. 4 for the four largest lattices we have studied and ν obtained from Fig. 1 by taking into account corrections to scaling. We can note that the critical temperature from the different quantities are indeed quite close to each other.

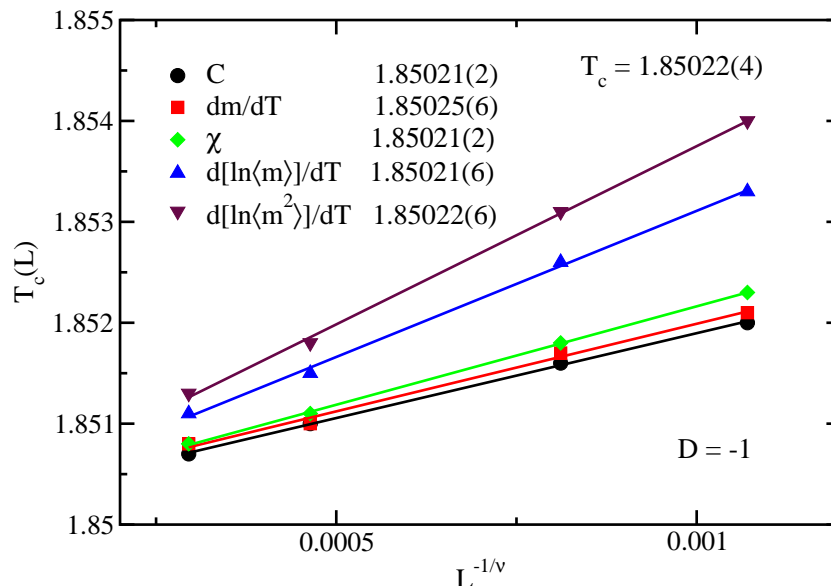


Figure 4. Size dependence of the effective critical temperatures (in units of J/k_B) estimated from several thermodynamic quantities. The lines are fits to Eq. (9) with ν obtained from Fig. 1 with corrections to scaling. The errors are smaller than the symbol sizes.

Now, Figs. 5, 6, and 7 show the corresponding results for the critical exponents for the case $D = +1$. One can see that the same behavior regarding the corrections to scaling is happening in this case, however, the critical exponents are now farther from the corresponding ones of the spin-1/2 model. Fig. 8 depicts the critical temperature obtained from several quantities for $D = +1$ and the four largest lattices considered.

Table 1. Estimated critical exponents and critical temperatures for different values of the crystal field. The results for $D = 0$ are from reference [9] and the exact ones for $D \rightarrow -\infty$ from reference [2]

D	$1/\nu$	γ/ν	α/ν	T_c
$-\infty$	1.5	1.75	1	2.269185..
-1	1.53(2)	1.771(9)	1.036(5)	1.85022(4)
0	1.621(5)	1.83(3)	1.12(1)	1.6607(3)
1	1.864(8)	1.951(5)	1.53(2)	1.35966(3)

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 with critical exponents which are indeed different from the spin-1/2 case. This means that this three-spin interaction model has exponents which depend not only

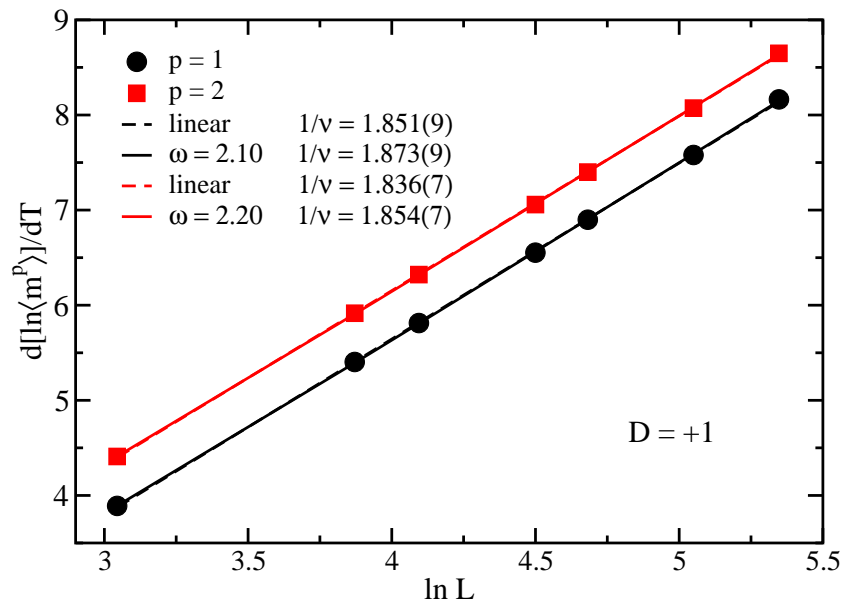


Figure 5. The same as Fig. 1 for $D = 1$.

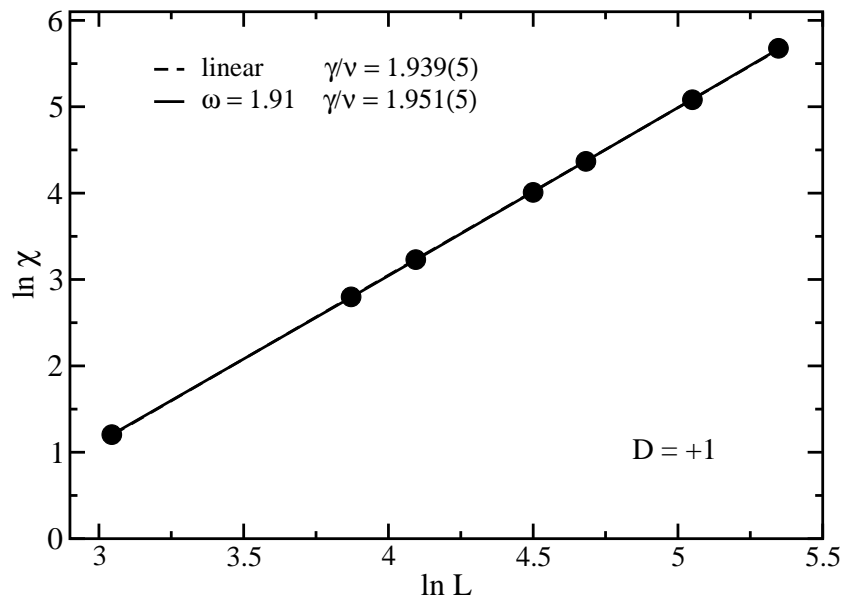


Figure 6. The same as Fig. 2 for $D = 1$.

on the spin value, but also on the crystal field. Table 1 shows the results for the present case in comparison to the values of the spin-1/2 model.

From the present results we then expect a second-order transition line whose critical temperature decreases as the crystal field increases, with varying critical exponents. This is indeed in contrast with the conjecture that the spin-1 Baxter-Wu model is critical only in the limit $D \rightarrow -\infty$ [15]. Moreover, the present results are in agreement with the picture of a line of second-order phase transition with varying critical exponents and the presence of a multicritical point, as has already been obtained from conformal invariance with finite-size scaling theory and the mean-field renormalization group approach [8]. Work in the direction of getting the

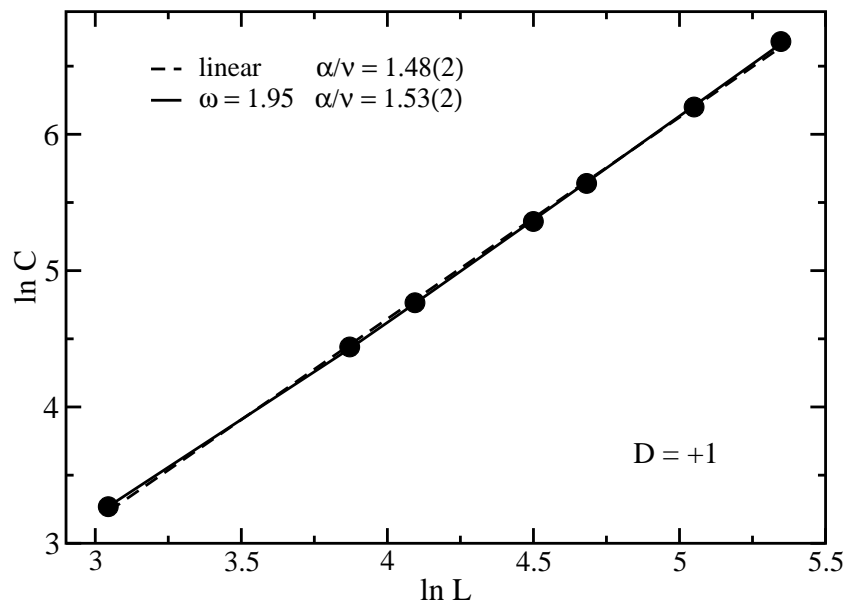


Figure 7. The same as Fig. 3 for $D = 1$.

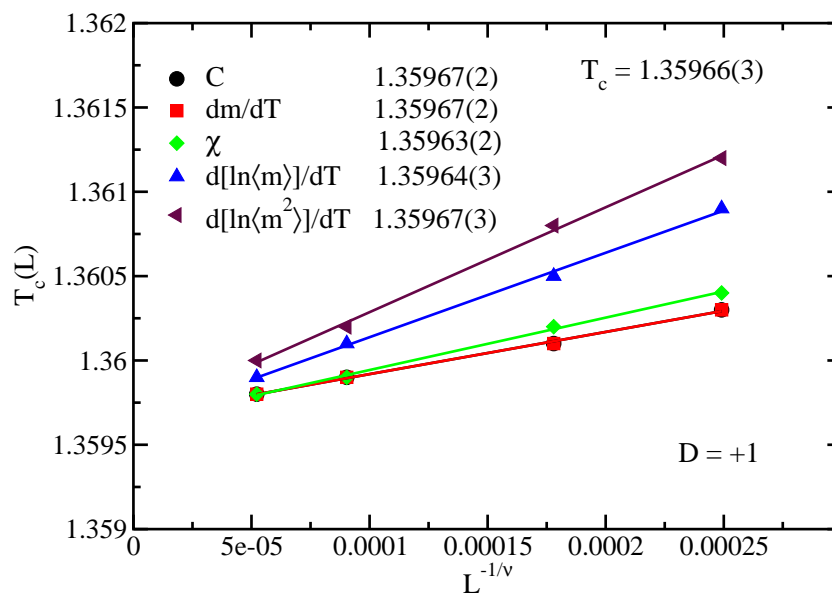


Figure 8. The same as Fig. 4 for $D = 1$.

multicritical point using Monte Carlo simulations is now in progress.

5. Acknowledgments

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References

- [1] Wood D W and Griffiths H P 1972 *J. Phys. C* **5** L253
- [2] Baxter R and Wu F 1973 *Phys. Rev. Lett.* **31** 1294
- [3] Novotny M A and Landau D P 1985 *Phys. Rev. B* **32** 5874
- [4] Novotny M A and Landau D P 1985 *Phys. Rev. B* **32** 3112

- [5] Alcaraz F C and Xavier J C 1997 *J. Phys. A* **30**, L203
- [6] Alcaraz F C and Xavier J C 1999 *J. Phys. A* **32** 2041
- [7] Santos M and Figueiredo W 2001 *Phys. Rev. E* **63** 042101
- [8] Costa M L M, Xavier J C and Plascak J A 2004 *Phys. Rev. B* **69** 104103
- [9] Costa M L M and Plascak J A 2004 *Braz. J. Phys.* **34** 419
- [10] Landau D P and Binder K 2014 *A Guide to Monte Carlo Simulation in Statistical Physics*, (4th edition, Cambridge University Press, Cambridge, England).
- [11] Newman M E J and Barkema G T 1999 *Monte Carlo Methods in Statistical Physics*, Oxford University Press
- [12] Ferrenberg A M and Swendsen R W 1988 *Phys. Rev. Lett.* **61** 2635; 1989 **63** 1195
- [13] Ferrenberg A M 1991 in *Computer Simulation Studies in Condensed Matter Physics III*, edited by D. P. Landau, K. K. Mon, and H. -B. Schuttler (Springer-Verlag, Heidelberg)
- [14] Landau D P 1994 *Physica A* **205** 41
- [15] Kinzel W, Domany E, and Aharony A 1981 *J. Phys. A: Math. Gen.* **14** L417