

# Novel order parameter to describe the critical behavior of Ising spin glass models

F. Romá<sup>a</sup>, F. Nieto<sup>a</sup>, A.J. Ramirez-Pastor<sup>a,\*</sup>, E.E. Vogel<sup>b</sup>

<sup>a</sup>*Departamento de Física, Universidad Nacional de San Luis - CONICET, Chacabuco 917, 5700 San Luis, Argentina*

<sup>b</sup>*Departamento de Física, Universidad de La Frontera, Casilla 54-D, Temuco, Chile*

Received 11 May 2005; received in revised form 13 July 2005

Available online 19 September 2005

## Abstract

A novel order parameter  $\Phi$  for spin glasses is defined based on topological criteria and with a clear physical interpretation.  $\Phi$  is first investigated for well known magnetic systems and then applied to the Edwards–Anderson  $\pm J$  model on a square lattice, comparing its properties with the usual  $q$  order parameter. Finite size scaling procedures are performed. Results and analyses based on  $\Phi$  confirm a zero temperature phase transition and allow to identify the low temperature phase. The advantages of  $\Phi$  are brought out and its physical meaning is established.

© 2005 Elsevier B.V. All rights reserved.

*Keywords:* Lattice theory and statistics; Spin-glass and other random models; Phase transitions

## 1. Introduction

Despite over three decades of intensive work, the nature of the low temperature phase of two-dimensional Edwards–Anderson (EA) [1] model for spin glasses remains controversial. It is agreed that a phase transition occurs at zero temperature for a Gaussian distribution of bonds (GD) [2–5]. Similarly, for a symmetric  $\pm J$  distribution or bimodal distribution (BD) of bonds, very convincing numerical evidence has been found that there is no transition at finite temperature [5–11]. In most of these references, the authors do not use an order parameter for characterizing the phase transition. On the other hand, data arising from other contributions, which are based on the behavior of a standard overlapping order parameter, support the existence of a finite critical temperature [12–14].

In this context, the main purposes of this paper are the following: (a) to show that the disagreement pointed out in previous paragraph is related to the non-zero overlap of site-order parameters obtained for quite distinct energy valleys; (b) to overcome this situation by proposing here a novel order parameter  $\Phi$ , which is quite drastic to characterize phases but still is general enough to coincide with usual descriptions of ferromagnetic (F) and antiferromagnetic (AF) systems; (c) to apply  $\Phi$  to do a scaling analysis for

\*Corresponding author. Fax +54 2652 430224.

*E-mail addresses:* [froma@unsl.edu.ar](mailto:froma@unsl.edu.ar) (F. Romá), [fnieto@unsl.edu.ar](mailto:fnieto@unsl.edu.ar) (F. Nieto), [antorami@unsl.edu.ar](mailto:antorami@unsl.edu.ar) (A.J. Ramirez-Pastor), [ee\\_vogel@ufro.cl](mailto:ee_vogel@ufro.cl) (E.E. Vogel).

two-dimensional EA systems including Binder cumulant [15]; (d) to confirm the assumption of the zero-temperature phase transition for two-dimensional BD, thus reinforcing this result obtained by previously quoted authors; and (e) to give a physical meaning to this finding by using the grounds on which  $\Phi$  is based on.

The present work is organized as it follows. In Section 2, we introduce the model and define a novel order parameter,  $\Phi$ , very useful for spin glasses and other frustrated systems. Results of the simulation are presented in Section 3. Finally, our conclusions are drawn in Section 4.

## 2. Model and basic definitions

Let us begin by very briefly introducing the system under study. Ising spin  $s_i$  occupies  $i$ th site of a two dimensional (square for simplicity) lattice. The interaction with the spin at site  $j$  is mediated by exchange interaction  $J_{ij}$ . In the absence of magnetic field (which is the case for the scope of the present paper) the Hamiltonian of such system can then be written as

$$H = \sum_{\langle i,j \rangle} J_{ij} s_i s_j, \quad (1)$$

where interactions  $\{J_{ij}\}$  are restricted to nearest neighbor couplings. In the F Ising model,  $J_{ij} = -J \forall \langle i,j \rangle$ . For the EA model, we will consider half of the bonds F, while the other half will be described by AF bonds of the same magnitude, namely,  $J_{ij} = +J$  ( $J > 0$ ). A sample is one of the possible random distributions of these mixed bonds. For simplicity spins take values  $s_j = \pm 1$ , which can be equally denoted by their signs.

Now, let us consider a configuration  $\alpha$  defined by a collection of ordered spin orientations  $\{s_j^\alpha\}$ . The usual EA order parameter  $q$  is built up by means of overlaps between two configurations  $\alpha$  and  $\beta$  and takes the form

$$q_{\alpha\beta} = \frac{1}{N} \sum_{j=1}^N s_j^\alpha s_j^\beta, \quad (2)$$

where  $N$  ( $\equiv L \times L$ ) is the total number of spins.

For models in which the ground state is non degenerate after breaking ergodicity, such as the pure F case, the distribution of  $q_{\alpha\beta}$  values for the ground manifold ( $T = 0$ ) is trivial and it is given by delta functions at  $q_{\alpha\beta} = 1.0$  and  $q_{\alpha\beta} = -1.0$ . This also happens in general for all systems with non-degenerate ground level. But this also applies to GD, where local fields have all different values at different sites, leading to a true minimum energy for just one pair of opposite ground states. However, for the BD the local field assumes a few discrete values only, which necessarily means highly degenerate ground manifolds leading to  $|q_{\alpha\beta}| < 1.0$ , for a large number of possible pairs of ground states. This distribution will have two broad symmetric maxima but it will not vanish in the intermediate region [13].

On the other hand, a more detailed description based on a topological picture of the ground state of BD was presented [16,17]. This framework allows us to define a state function with a clear physical meaning, which is a good candidate to be a new order parameter for a phase transition. In fact, it has been reported an important feature of the ground state, namely, at  $T = 0$  there exist clusters of solidary spins (CSS) preserving the magnetic memory of the system (solidary spins maintain their relative orientation for all states of the ground manifold) [18]. The main idea of this work is to characterize the nature of the low temperature phase through the CSS.

Let us consider a particular sample of any given size  $N$ . We denote by  $\Gamma_\kappa$  any of the  $n$  CSS of the sample ( $\kappa$  runs from 1 to  $n$ ). Calculations begin recognizing all of the CSS of each sample belonging to a set of 2000 randomly generated samples of each size. This process is closely related to finding the so-called “diluted lattice” that prevails after removing all frustrated bonds [19], so the algorithms designed for that purpose can also be used here.

Let us first pick any arbitrary ground state configuration denoted by an asterisk (\*) fixing one of the possible relative orientations of the CSS, thus becoming a reference configuration. Then a local overlap

corresponding to the configuration  $\alpha$  in the  $\kappa$ th cluster, of size  $N_\kappa$ , can be defined as

$$\phi_\kappa^\alpha = \frac{1}{N_\kappa} \sum_{j \in \Gamma_\kappa} s_j^* s_j^\alpha, \tag{3}$$

where the sum runs over all spins in the cluster  $\Gamma_\kappa$  only. Thus,  $|\phi_\kappa^\alpha| = 1$  indicates a fully ordered cluster; otherwise  $|\phi_\kappa^\alpha| < 1$ . The magnetic order of the sample is characterized by the set of overlaps, namely,  $\{\phi_\kappa^\alpha\}$ . Under the occurrence of a phase transition, the new set  $\{\phi_\kappa^\alpha\}$  will determine uniquely the ergodic component of the reached phase. This fact is a required characteristic for a well behaved order parameter [20].

We are now ready to define the new order parameter introduced in this paper. It is given by

$$\Phi_\alpha = \sum_{\kappa=1}^n f_\kappa |\phi_\kappa^\alpha|, \tag{4}$$

where  $f_\kappa = N_\kappa/N_I$ , being  $N_I = \sum_{\kappa=1}^n N_\kappa$ , ( $N_I \leq N$ ). From the definition it flows that for  $T \geq T_c$  the average value of  $\Phi_\alpha$ , namely,  $\Phi$ , should be 0. Similarly, for  $T < T_c$  it should hold that  $0 < \Phi \leq 1$ , being  $\Phi = 1$  for  $T = 0$  only. It is important to emphasize that  $\Phi_\alpha$  is a state function, which is an advantage over  $q_{\alpha\beta}$  defined in Eq. (2) as an overlap between two configurations of the system.

The calculation of the new order parameter  $\Phi_\alpha$  requires the previous determination of the set of CSS for each considered sample. This procedure which was performed by using the numerical scheme introduced in Ref. [21], is a computational limitation for going to larger system sizes. Once the ground manifold of each sample is completely characterized after this procedure, the numerical calculations converge very quickly by flipping the spins not present in the largest CSS only. The second run on each sample takes much less time than the first one that is needed to find all CSS.

In the F Ising model there is a unique cluster of  $N$  solidary parallel spins at  $T = 0$ . As it can be trivially demonstrated, Eq. (4) leads to the magnetization per spin, which is the natural order parameter of such system. Similarly, for the AF case we get the well-known order parameter defined as the magnetization difference between the two possible interpenetrating sublattices. Finally, for GD, there also exists a unique CSS in the ground state and the phase transition occurring in the system is completely described by the new order parameter, Eq. (4), as well. So the new parameter retains all the properties of the well-known non-degenerate systems.

Finally, the reduced fourth-order cumulant, introduced by Binder [15], can be calculated as

$$U_L = 1 - \frac{[\langle m^4 \rangle]}{3[\langle m^2 \rangle]^2}, \tag{5}$$

where  $m$  is a given order parameter, and  $\langle \dots \rangle$  and  $[\dots]$  mean the spin configuration (thermal) average and the bond configuration (sample) average, respectively. In general, the structure of the distribution of  $m$  affects the behavior of the fourth-order Binder cumulant. Thus, for a trivial distribution, both  $|m| \rightarrow \pm 1$  and  $U_L \rightarrow \frac{2}{3}$ , as  $T$  goes to zero. On the other hand, if the distribution is nontrivial,  $|m|$  tends to a value  $m^o$  lower than 1, while  $U_L$  tends to a value  $U_L^o$  lower than  $\frac{2}{3}$  upon decreasing temperature.

### 3. Results

Distribution functions for  $q_{\alpha\beta}$  and  $\Phi_\alpha$ , were obtained for BD by using a standard simulated-tempering procedure<sup>1</sup> [22,23] along with the well known Glauber's dynamics [24]. For illustration purposes, we perform calculations on 1000 samples of size 64 ( $8 \times 8$ ) at different temperatures ranging from  $T = 0.2$  to  $T = 1.0$ . (throughout this paper,  $k_B/J = 1$  without any loss of generality). The results corresponding to  $T = 0.31$ ,  $T = 0.53$  and  $T = 0.69$  are presented in Fig. 1. As it is shown in part (a), the distribution of the new order parameter,  $R(\Phi_\alpha)$ , exhibits a drastic behavior as  $T$  decreases. In part (b) it is shown how the corresponding curves for  $r(q_{\alpha\beta})$  have a broad maximum over the plotted range and  $r(0) > 0$ . These undesired characteristics for this order parameter remain even at low temperatures.

<sup>1</sup>It must be emphasized that it is not necessary a simulated-tempering scheme for calculating the new order parameter,  $\Phi$ .

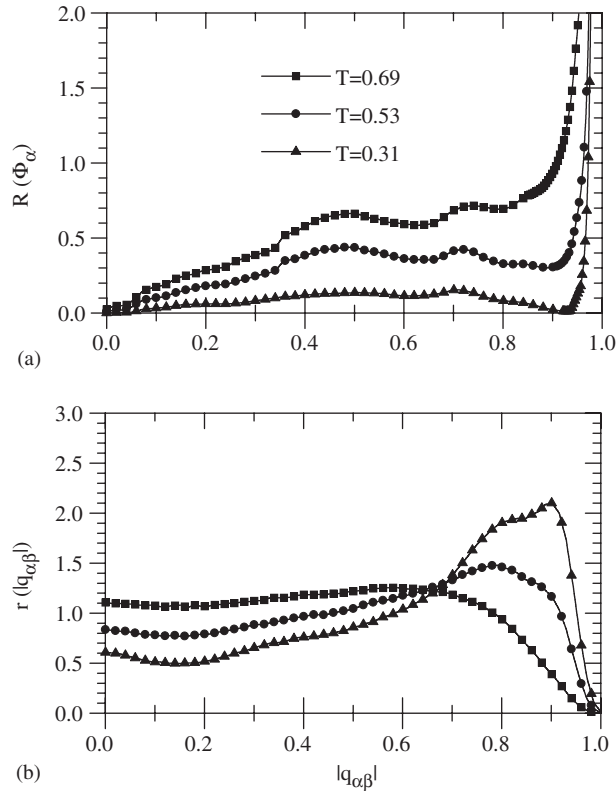


Fig. 1. Distributions of the order parameters (a)  $\Phi_x$  and (b)  $|q_{z\beta}|$ , at 3 different temperatures as indicated.

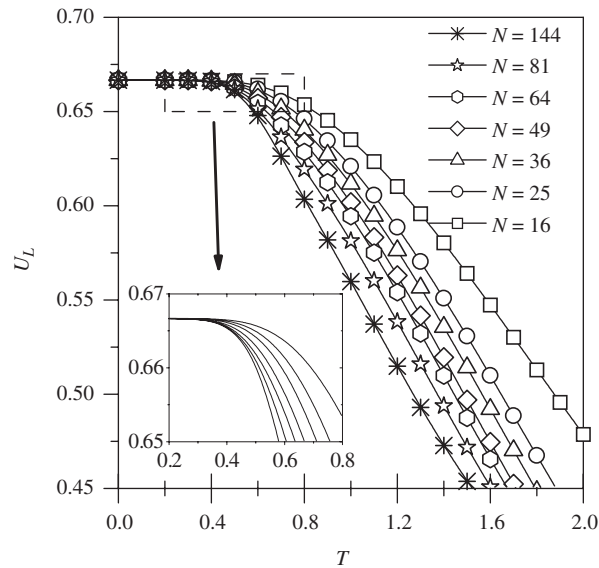


Fig. 2. Cumulant  $U_L(T)$  plotted versus  $T$  for various lattice sizes as indicated. The inset zooms the area indicated by a dashed frame.

In Fig. 2,  $U_L(T)$ , built up from  $R(\Phi_x)$  distribution, is presented for different lattice sizes ranging from  $N = 16$  to 144 and each point was calculated by averaging over a set of 2000 samples. With the help of the inset, it is observed that the curves do not intersect each other as a direct indication of the absence of a phase

transition for finite temperature, at least for the sizes considered here. Eventually we are not free from finite size considerations yet as it has been recently proposed that at least samples with  $L = 50$  should be reached when conventional parameters are used [25]. However, using a more drastic parameter like the one proposed here, a faster convergence towards large  $L$  values is expected. It is clear that all curves go to  $\frac{2}{3}$  as  $T \rightarrow 0$ , which reinforces the robustness of Eq. (4). On the other hand, this property is not followed by cumulants obtained from other overlapping order parameters. This is the case of Fig. 7 in Ref. [13], where it is possible to think that the reported crossing of the cumulants of  $q$  arises from the dependence of  $U_L^q$  on size. In this contribution, the authors reported a critical temperature different from zero,  $T_c \approx 0.23$ .

Finite-size scaling [15] predicts that all curves in a figure such as Fig. 2, should collapse onto a single one when using  $(T - T_c)L^{1/\nu}$  as independent variable, being  $T_c$  the critical temperature for the transition and  $\nu$  an appropriate critical exponent. Upon choosing  $T_c = 0$  and the exponent  $\nu$  is taken as  $\nu = 2.63 \pm 0.20$ , the standard universal behavior for  $U_L(T)$  is obtained as shown in Fig. 3. This is an independent confirmation of previously reported results [6,26–28].

The following two parameters were also measured as each sample was solved exactly: (a) The mean fraction of spins,  $P \equiv [N_I]/N$ , belonging to any CSS; and (b) The fraction of spins in the largest CSS  $p \equiv [N_\ell]/N$ , where  $N_\ell$  is the number of spins in the largest CSS. Fig. 4(a) shows that while  $P$  remains rather constant,  $p$  clearly decreases with size and the stabilizing role of the largest CSS is lost. The average number of CSS  $[n]$  as function of size was also measured, finding that  $[n]$  grows linearly with  $N$ , as it is shown in Fig. 4(b). For  $N > 49$ , say (when small size effects do not play an important role), the following approximate law is obtained  $[n] \approx 0.03N + 0.60$ .

The size dependence of a possible spin-glass phase can be described in the following terms. For small sizes ( $N < 49$  say) most of solidary spins are grouped in one large cluster stabilizing a spin-glass phase. As size grows, the number of CSS increases linearly with  $N$  (or quadratically with  $L$ ), while the relative size of the largest CSS diminishes. This can be visualized as if the original lattice would break into portions of relatively smaller sizes, none of them large enough to stabilize a spin-glass phase. This is the reason for the numeric result of Fig. 2, showing no intersection of curves for different sizes.

If the same procedure used here for the symmetric case is applied to different concentrations of F and AF bonds, a stable phase is found in the extremes of high and low concentrations of F bonds in correspondence with results already reported in the literature [29,30]. As the relative concentration of F bonds varies the behavior of  $P$  and  $[n]$  is very similar to that shown in Fig. 4. However,  $p$  tends to be constant for very

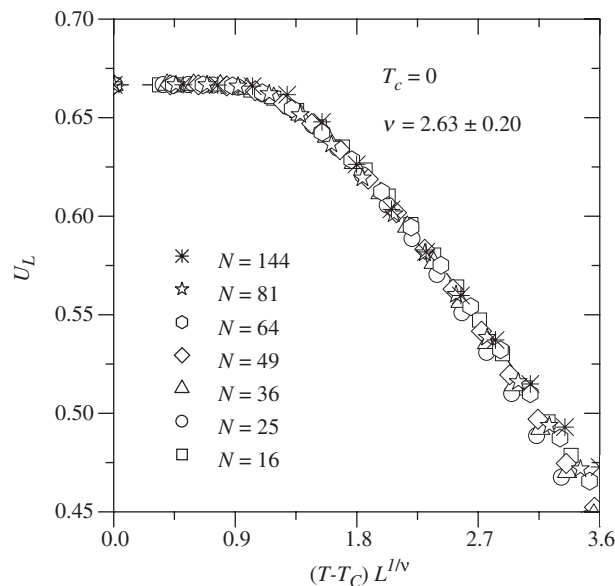


Fig. 3. Scaling plot of  $U_L$  against  $(T - T_c)L^{1/\nu}$ , with  $T_c = 0$  and  $\nu = 2.63 \pm 0.20$ .

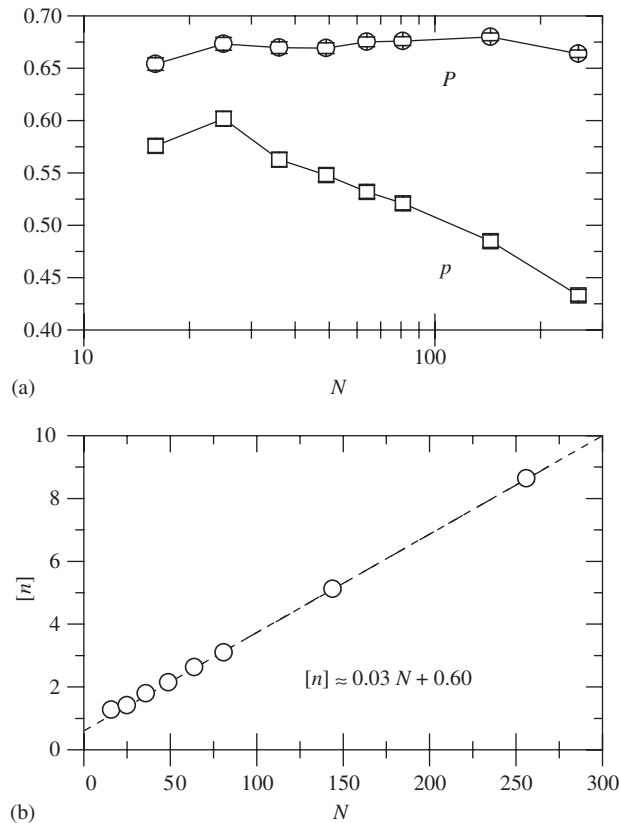


Fig. 4. (a)  $P$  and  $p$  and (b) the growing of  $[n]$  as a function of the lattice size, respectively.

asymmetric distributions of  $\pm J$  bonds. The last statement indicates the presence of an infinite CSS in the thermodynamical limit, which is associated to a stable phase. These results are not shown graphically in the present paper.

#### 4. Conclusions

A new order parameter  $\Phi$  has been introduced and applied to the study of magnetic systems. It proves to be particularly essential for characterizing degenerate systems such as Ising-like models with bimodal distribution. Parameter  $\Phi$  is well behaved, having all desired properties for a drastic order parameter. This behavior is based on the properties of CSS. When this order parameter is used for systems with BD, properties similar to order parameters for non-degenerate systems are found. Then, the characterization of magnetic phases after using the scaling techniques of cumulants becomes unambiguous. In this way it was shown that the two-dimensional Edwards–Anderson model exhibits a phase transition at  $T_c = 0$ , with a critical exponent  $\nu = 2.63 \pm 0.20$ .

The identification of all CSS for each sample is the bottleneck in the present computational scheme. This procedure is very time consuming for large lattice sizes. The extra time needed for finding all CSS is well paid by the better precision achieved in the characterization of the phase, and the elimination of overlaps in the new order parameter, thus making the identification of the ergodic valley reliable.

The characteristics of this new order parameter make it also useful for other frustrated systems, where large overlaps occur due to the complex energy valley. The extension of the use of the parameter  $\Phi$  to other kind of problems is clearly foreseen. For instance, it can be the key element (i) to describe the phase diagram for the asymmetric distribution problem around the critical concentration of ferromagnetic (or antiferromagnetic) bonds of  $\approx 0.1$  and (ii) to study the critical behavior of 3D Ising spin glasses. This task requires serious

improvements in the numerical techniques used in order to get access to large lattice sizes. Work along this line is in progress.

### Acknowledgements

We thank Fondecyt (Chile) under projects 1020993 and 7020993. One author (EEV) thanks Millennium Scientific Initiative (Chile) under contract P-02-054-F for partial support. Three authors (FR, FN and AJRP) thank CONICET (Argentina) and the Universidad Nacional de San Luis (Argentina) under project 322000.

### References

- [1] S.F. Edwards, P.W. Anderson, *J. Phys. F* 5 (1975) 965; G. Toulouse, *Commun. Phys.* 2 (1977) 115.
- [2] W.L. McMillan, *Phys. Rev. B* 30 (1984) R476.
- [3] A.J. Bray, M.A. Moore, *J. Phys. C* 17 (1984) L463; A.J. Bray, M.A. Moore, in: J.L. van Hemmen, I. Morgenstern (Eds.), *Heidelberg Colloquium on Glassy Dynamics*, Springer, Heidelberg, 1987.
- [4] H. Rieger, L. Santen, U. Blasum-U, M. Diehl, M. Jünger, G. Rinaldi, *J. Phys. A* 29 (1996) 3939.
- [5] A.K. Hartmann, A.P. Young, *Phys. Rev. B* 64 (2001) 180404(R).
- [6] R.N. Bhatt, A.P. Young, *Phys. Rev. B* 37 (1988) 5606.
- [7] N. Kawashima, H. Rieger, *Europhys. Lett.* 39 (1997) 85.
- [8] J. Houdayer, *Eur. Phys. J. B* 22 (2001) 479.
- [9] A.K. Hartmann, A.J. Bray, A.C. Carter, M.A. Moore, A.P. Young, *Phys. Rev. B* 66 (2002) 224401.
- [10] C. Amoruso, E. Marinari, O.C. Martin, A. Pagnani, *Phys. Rev. Lett.* 91 (2003) 087201.
- [11] J. Lukic, A. Galluccio, E. Marinari, O.C. Martin, G. Rinaldi, *Phys. Rev. Lett.* 92 (2004) 117202.
- [12] T. Shirakura, F. Matsubara, *Phys. Rev. Lett.* 79 (1997) 2887.
- [13] M. Shiomi, F. Matsubara, T. Shirakura, *J. Phys. Soc. Jpn.* 69 (2000) 2798.
- [14] F. Matsubara, T. Shirakura, M. Shiomi, *Phys. Rev. B* 58 (1998) R11821.
- [15] K. Binder, *Rep. Prog. Phys.* 60 (1997) 488.
- [16] E.E. Vogel, S. Contreras, M.A. Osorio, J. Cartes, F. Nieto, A.J. Ramirez-Pastor, *Phys. Rev. B* 58 (1998) 8475.
- [17] E.E. Vogel, S. Contreras, F. Nieto, A.J. Ramirez-Pastor, *Physica A* 257 (1998) 256.
- [18] F. Barahona, R. Maynard, R. Rammal, J.P. Uhry, *J. Phys. A: Math. Gen.* 15 (1982) 673.
- [19] J.F. Valdes, J. Cartes, E.E. Vogel, S. Kobe, T. Klotz, *Physica A* 257 (1998) 557.
- [20] A.C.D. van Enter, J.L. van Hemmen, *Phys. Rev. A* 29 (1984) 355.
- [21] A.J. Ramirez-Pastor, F. Romá, F. Nieto, E.E. Vogel, *Physica A* 336 (2004) 454.
- [22] E. Marinari, G. Parisi, *Eurphys. Lett.* 19 (1992) 451.
- [23] W. Kerler, P. Rehberg, *Phys. Rev. E* 50 (1994) 4220.
- [24] K. Kawasaki, in: C. Domb, M. Green (Eds.), *Phase Transitions and Critical Phenomena*, vol. 2, Academic Press, London, 1972.
- [25] H.G. Katzgraber, L.W. Lee, *Phys. Rev. B* 71 (2005) 134404.
- [26] A.P. Young, *J. Phys. C* 17 (1984) L517.
- [27] H.F. Cheung, W.L. McMillan, *J. Phys. C* 16 (1983) 7027.
- [28] W.L. McMillan, *Phys. Rev. B* 28 (1983) 5216.
- [29] I. Morgenstern, K. Binder, *Phys. Rev. Lett.* 43 (1979) 1615.
- [30] I. Morgenstern, K. Binder, *Phys. Rev. B* 22 (1980) 288.