

# The kinetic spin-1 Blume-Capel model with competing dynamics

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**Abstract.** We have studied by means of Monte-Carlo simulation and exact finite-size analysis, the spin-1 Blume Capel model with Glauber and Kawasaki dynamics. The Kawasaki spin-exchange process transfers energy into the system from an external source. Some phase diagrams of the model are presented. For some parameter values, the system displays a kind of self-organization phenomenon within the disordered phase.

**PACS.** 75.10.Hk Classical spin models – 75.10.Nr Spin-glass and other random models – 64.60.Ht Dynamic critical phenomena

## 1 Introduction

The stochastic evolution of a spin system towards equilibrium can be studied using the Glauber single spin-flip dynamics [1] as well as multiple spin-flip processes. The latter dynamics appears natural since it can sometimes lead systems to showing the interesting phenomenon of self-organization [2]. Kinetic Ising systems may therefore be helpful in understanding, at the microscopic level, the occurrence of dissipative structures observed in physical-chemical reactions and in fluid dynamics [2,3]. An instructive case of self-organization phenomenon in a kinetic ferromagnetic Ising model has been recently reported by Tome and de Oliveira [4]. These authors studied within the dynamical pair approximation, a system which was linked to a heat bath whose dynamics is the Glauber spin-flip process and subject to an external source of energy. The flow of energy into the system is governed by a Kawasaki-type spin-exchange process [5]. The main result derived is the possible paramagnetic-antiferromagnetic phase transition beyond the usual equilibrium ferromagnetic-paramagnetic transition. Their system self-organizes in the disordered phase at high energy flux. By using Monte Carlo (MC) simulations, Grandi and Figueiredo [6] confirmed the occurrence of the phenomenon in the model but found a phase diagram which

was different from the one obtained by pair approximation. In the kinetic antiferromagnetic Ising model case, no such self-organization is found [7]. However, Ma *et al.* [8] have shown recently that a self-organization phenomenon may occur if the spin-exchange rate depends on the strength of the exchange between nearest-neighbour spins.

In this paper, we specifically consider the same problem with a different model, in particular the antiferromagnetic spin-1 Blume-Capel model [9,10] whose Hamiltonian comprises a single-ion anisotropy. The equilibrium version of this model and its generalization, the Blume-Emery-Griffiths model, [11] have been extensively studied and present a rich variety of critical and multicritical behaviour. The spin-1 Ising systems appear more interesting since they can describe order-disorder transitions and the crystallization of binary alloys. They have been solved by means of different methods: mean-field approximation [12], MC finite-size scaling methods [13], etc. In the present non-equilibrium model, the system is subject to the same competing Glauber and Kawasaki dynamics described in reference [4]. We are mainly interested in the effect of the crystal-field on the phase diagrams and the nature of the phase boundaries. The system time evolution is described by a master equation which can be solved exactly for small-size versions of the model. However, the corresponding steady-state distribution probability is not of great importance since it cannot give an indication of the large scale properties of the model. Nevertheless, using the dynamical transition matrix eigenvalue statistics, some general trends of the model can be conjectured. Larger systems are investigated by MC simulations. Our study does not show any self-organization similar to that reported in reference [4]. For some model parameters, the system tends to organize itself in the same antiferromagnetic phase within the disordered phase. This behaviour

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seems, however, to become unimportant with increasing system size. Accordingly, our phase diagrams do not include any related features, although an indication exists that in the thermodynamic limit the phenomenon may not disappear. For the zero-field splitting (anisotropy)  $D/J \leq 1$ , the antiferro-paramagnetic transition is of the second order, independent of the intensity of the external flux. For values of  $D/J > 2$ , the transition is essentially of the first order in the temperature-external flux phase diagram. Between these two limiting values, the second order transition line ends at a tricritical point.

The paper is organized as follows. In Sections 2 and 3, the model and its dynamics are specified. In Section 4, some properties of the model are fitted from the transition matrix associated with the master equation on small samples. In Section 5 the simulation algorithm is described. Section 6 is devoted to MC results.

## 2 The model Hamiltonian

The model Hamiltonian is:

$$H = J \sum_{\langle i,j \rangle} S_i S_j + D \sum_i S_i^2. \quad (1)$$

Here, the local spin variables are restricted to taking the values  $\pm 1, 0$ . The first term describes the antiferromagnetic coupling ( $J > 0$ ) between neighbouring spins  $i$  and  $j$ . The second term describes the single-ion anisotropy. This model Hamiltonian has been well-studied in the literature by means of different methods [10,11]. In the temperature-anisotropy phase diagram, the ordered phase is separated from the disordered paramagnetic phase by a phase boundary which changes nature at a tricritical point. Analysis of the ground states and mean-field calculations show that the first order transition line ends at zero at  $D/J = 2$  for a two-dimensional system [10].

In the present work, the system is driven out of equilibrium by an external source of energy and is subject to two competing dynamics: the Glauber spin-flip process [1] which simulates the contact of the system with a heat bath at a given absolute temperature and the Kawasaki spin-exchange [5] which simulates the flow of external energy into the system.

## 3 Kinetic equation of the model

At equilibrium as in dynamics, a statistical time-dependent weight  $P(\sigma, t)$  is associated with each lattice configuration  $\sigma$  at time  $t$ . The dynamics of the model become specified when one fixes the transition rate  $W(\sigma, \sigma')$  through a kinetic equation:

$$\frac{dP(\sigma, t)}{dt} = \sum_{\sigma'} (-W(\sigma, \sigma')P(\sigma, t) + W(\sigma', \sigma)P(\sigma', t)). \quad (2)$$

This relation expresses that the rate of change of  $P(\sigma, t)$  is given by the difference between the flux into  $\sigma$  from other configurations  $\sigma'$  and the flux out of  $\sigma$  to other configurations. These transitions occur in the model by the two competing Glauber and Kawasaki dynamics.

The Glauber move on a single spin  $i$  has the transition probability per unit time and per site:

$$w_i(\sigma, \sigma') = \frac{p}{2} \min(1, \exp(-\Delta E_i/kT)), \quad (3)$$

where  $\Delta E_i$  denotes the change of the system energy associated with the spin-flip process. The prefactor  $1/2$  arises from the fact that two final states are possible in the spin-flip move. The Kawasaki spin-exchange process on neighbouring sites  $(i, j)$ , only occurs when energy can flow into the system. It has the transition rate:

$$w_{ij}(\sigma, \sigma') = 1 - p. \quad (4)$$

The global transition rate  $W(\sigma, \sigma')$  can be rewritten in the form:

$$W(\sigma, \sigma') = W_G(\sigma, \sigma') + W_K(\sigma, \sigma'), \quad (5)$$

where

$$W_G(\sigma, \sigma') = \sum_i w_i(\sigma, \sigma') \quad (6)$$

is the sum of the rates of transitions by spin-flip on sites  $i$ , leading  $\sigma$  to  $\sigma'$  and

$$W_K(\sigma, \sigma') = \sum_{\langle i,j \rangle} w_{ij}(\sigma, \sigma'). \quad (7)$$

Denoting the set of lattice configuration probabilities  $P(\sigma, t)$  at time  $t$  by  $P(t)$ , then the system time evolution is given by the equation:

$$\frac{d}{dt}P(t) = M P(t) \quad (8)$$

where  $M$  denotes the Glauber-Kawasaki (GK) non-equilibrium transition matrix for the model.

## 4 Analysis of the GK transition matrix

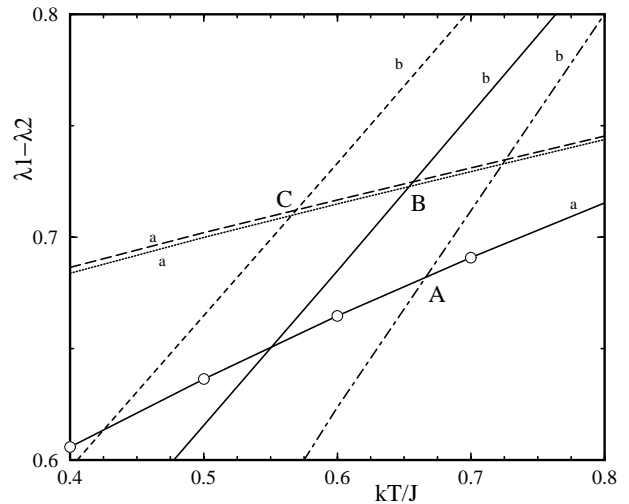
### 4.1 Subgroup classification of system configurations

We could only study very small systems of about 8 sites. The procedure we use is that of subgroup classification of system configurations. The reader should refer to references [14,15] for more details on the method. In general, the configurations of a table  $L \times L'$  are classified into groups subdivided into subgroups where configurations only differ by translation. Here we have only one group and  $L$  and  $L'$  are chosen even due to the antiferromagnetic coupling. Periodic boundary conditions are imposed on the systems. By means of this procedure, we find 855 subgroups for the system  $2 \times 4$  and 27 subgroups

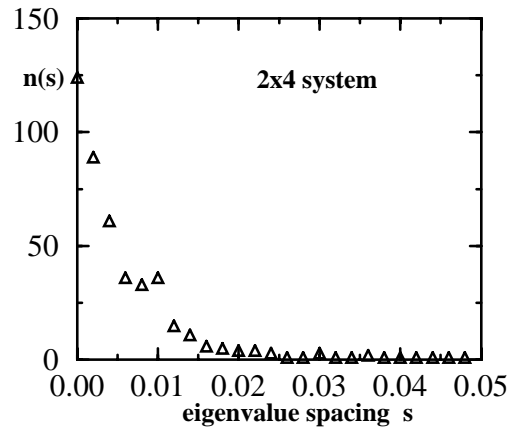
for the system  $2 \times 2$ . One can remark that the number of subgroups rapidly increases with system size. During the table evolution, the system configurations run from one subgroup to another in the group due to the model ergodicity within the group. Such behaviour enables one to define a transition matrix between subgroups. For the  $2 \times 4$  system, the matrix is  $855 \times 855$ . The eigenstates associated to the eigenvalue  $\lambda = 0$  correspond to the steady state distribution which might be used to compute physical quantities. The other eigenvectors are not probability distributions. The present finite size study is far from the thermodynamic limit and cannot help reasonably to fit the large scale properties. Nonetheless, some insight into the general behaviour of the model is expected from the eigenvalue statistics.

### 4.2 Eigenvalue statistics

Both positive and negative eigenvalues are found. The three largest eigenvalues are always positive and non-degenerate. The eigenvalues increase for increasing model parameters. This may indicate an increase of disorder in the system. With decreasing temperature, the density of eigenvalues close to zero increases. Of particular importance is the separation  $\Delta = \lambda_1 - \lambda_2$  between the two largest eigenvalues of the GK matrix. We find that  $\Delta(T)$  is non-exponential for given parameters  $D$  and  $q = 1 - p$ . By following Melin's work [16] on the Ising model with Glauber dynamics, one can conclude that we are in fact in the presence of a system with broken symmetry. Order-disorder transition is then possible in the model. In the same framework,  $\Delta(T)$  may decrease with system size and reach the value zero in the thermodynamic limit if  $T$  is less than the critical temperature  $T_c$ . Above  $T_c$ , it must be finite. In the present mixed dynamics, we find that the decrease of  $\Delta$  with system size is only possible below some temperature  $T_c^0$  (see points A, B, C in Fig. 1 where curves  $\Delta$  of two samples of different sizes meet). The temperature  $T_c^0$  is the finite-size analog of the real critical temperature  $T_c$ . Numerical simulations show (see Sect. 6) that  $T_c^0$  is in fact somewhat close to  $T_c$  for very small external flux  $q$  and relatively large value of  $D/J$ . The behaviour of  $T_c$  is reflected in that of  $T_c^0$ . Accordingly, from Figure 1, we believe that  $T_c$  must decrease with increasing model parameters. These features of the model also appear when one uses the Nightingale condition often considered in the transfer matrix finite-size scaling method [17–19] by taking the correlation length of the system as related to the ratio  $\lambda_1/\lambda_2$ . The quantity  $\Delta'(T) = \lambda_1 - \lambda_3$  where  $\lambda_3$  is the third largest eigenvalue, is very sensitive to the existence of a second order transition. In fact in the neighbourhood of the “transitions” shown in Figure 1, the profile of  $\Delta'(T)$  somewhat changes for the  $2 \times 4$  system. Such a feature has also been found in Melin's work [16]. Another interesting behaviour is that of the separation  $s$  of consecutive eigenvalues. We give an example in Figure 2 at  $T/J = 0.1$  for the  $2 \times 4$  system.  $n(s)$  gives the number of eigenvalue spacing  $s$  in consecutive intervals of width  $\Delta_s = 0.002$ . Our calculations show that there is no normalization of



**Fig. 1.** Curves  $\Delta(T) = \lambda_1 - \lambda_2$  for two systems:  $2 \times 2$  (a) and  $2 \times 4$  (b) and for different model parameters. Curves which cross at A, B, C correspond respectively to the parameters  $D/J = 1.7, q = 0.01$ ;  $D/J = 1.9, q = 0.01$ ;  $D/J = 1.9, q = 0.02$ .



**Fig. 2.** Number of eigenvalue spacing in consecutive intervals of width  $\Delta_s = 0.002$ . The parameters are:  $D/J = 1.9, T/J = 0.1, q = 0.02$ .

the eigenvalue spacing  $s$  and  $n(s)$  which may give an exponential form to the whole curve (Poisson distribution). We therefore think that the eigenvalue spacing statistics of the GK matrix are not universal since the profile of the curve just changes slightly with other parameter values. The latter feature of the curve is due to the fact that spins in the  $2 \times 4$  system, do not experience all the possible environments which exist in large systems.

### 5 Monte Carlo simulation

The method appears simpler than the difficult problem of subgroup classification. We use the Monte Carlo simulation procedure of reference [7]. Systems with different

sizes, with periodic boundary conditions, are considered. We often start from different initial configurations to ensure that the final state (steady state) obtained is correct. The simulation is propagated using the following procedure. A lattice with even size is considered. For given parameters of the model, a lattice site  $i$  is first randomly chosen. Then one chooses a random number  $r_1$  between 0 and 1. If  $p \geq r_1$ , a spin-flip process is attempted and another random number  $r_2$  (compared to 0.5) is chosen to decide which state the spin may take among the two others. The move is realized with probability  $w_i$ . If  $p < r_1$ , spin-exchange of site  $i$  is attempted with a randomly selected neighbouring site  $j$  of  $i$  with probability  $1 - p$ . The latter move is only accepted when  $\Delta E_{ij} > 0$ . The number of Monte Carlo steps (MCS) needed to reach the steady state depends on the model parameters and the system size considered. Typically, we use from  $10^4$  to  $10^5$  MCS for size  $L$  ranging from 16 to 40. The physical quantity of interest used to locate the phase boundary is the staggered magnetization (order parameter) and its variance. The order parameter is estimated by a time-averaging procedure [17]:

$$|M| = \langle |M_s| \rangle = \frac{1}{NS} \sum_c \sum_i \delta_i S_i(c), \quad (9)$$

where  $i$  runs over the lattice sites and  $\delta_i = +1$  ( $\delta_i = -1$ ) for sites of even (odd) sublattice, respectively. The variable  $c$  runs over the configurations obtained to update the lattice over one sweep of the entire  $N$  spins of the lattice (one Monte Carlo Step, MCS), counted after the system reaches thermal equilibrium.  $S$  is the number of MCS. For  $L = 40$ , about  $10^4$  sweeps of the lattice are always initially discarded to set this thermal equilibrium. The fluctuations in  $M_s$  are given by the reduced staggered magnetic susceptibility:

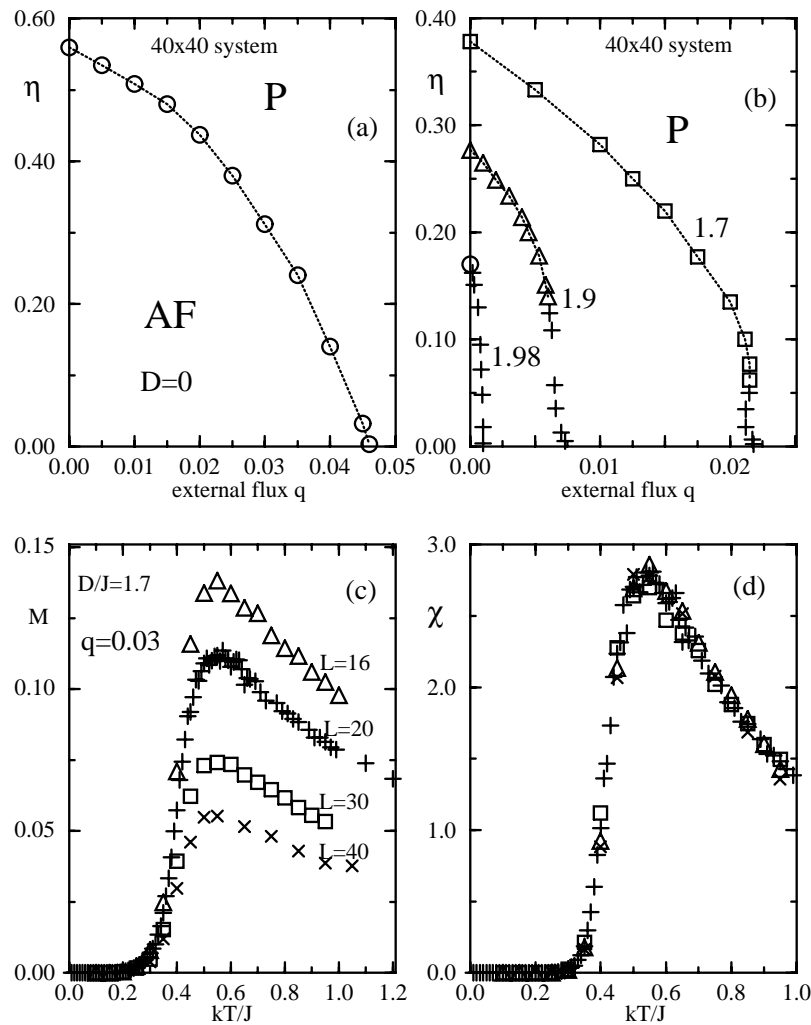
$$\chi_M = N(\langle M_s^2 \rangle - \langle |M_s| \rangle^2). \quad (10)$$

Other quantities that we control are the fourth-order cumulant associated with the order parameter and the reduced specific heat.

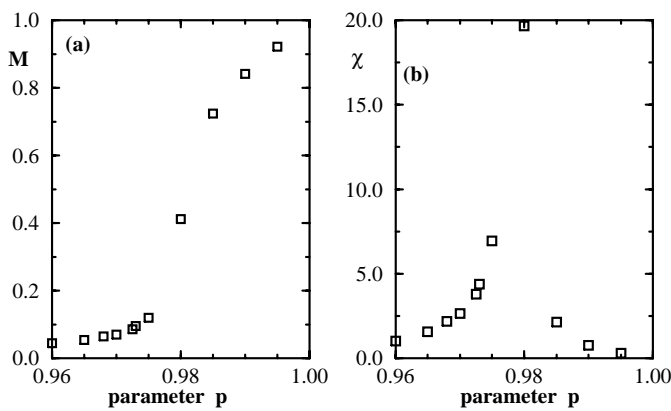
## 6 Results and discussion

We study the steady states of the system as a function of the model parameters. These states are characterized by the constancy of the relevant thermodynamic quantities outlined above. Typically three types of stationary states are expected: the paramagnetic (P), the ferromagnetic (F) and the antiferromagnetic (AF) phases. In the disordered P-phase, it is possible to get phase segregation or self-organization. In the small flux  $q$  region, Glauber dynamics dominates the whole dynamics. One expects the system to show an order similar to that of equilibrium: AF phase at low  $q$  and P-phase otherwise. At large  $q$ , the Kawasaki process dominates and the system is in a high energy state

(disordered phase). Between these two states, there is a phase transition which can be of first or second order. In our calculations, the first order transition occurs when the single-ion anisotropy is non-zero and takes large values. It appears at relatively low temperature. To determine it, we first increase the number of MC steps to locate typical hysteresis in the phase diagrams. For size  $L = 40$ , this number is typically set to  $10^5$ . Then, we use the mixed start technique in which the upper half of the lattice is initialized to the  $T = 0$  configuration expected on one side of the first order boundary (e.g.,  $m_1 = 1$ ,  $m_2 = -1$ ) and the lower half of the lattice initialized to the configuration expected on the other side of the lattice (e.g.,  $m_1 = 1$ ,  $m_2 = 1$ ). The order parameters  $m_1$  and  $m_2$  denote the average magnetization of the two sublattices. For  $D/J = 0$ , the system goes continuously from the antiferromagnetic phase to the disordered phase when the external flux  $q$  increases (Fig. 3a) and no hysteresis behaviour is seen in the order parameter. The whole transition line is of second order. The full dynamics in this case respects the nature of the phase boundary found in equilibrium at zero anisotropy. When  $D/J$  is large, but less than 2, the second order transition line and the first order line meet at a tricritical point (see Fig. 3b). For the  $40 \times 40$  system analyzed, this point has the coordinates  $T_c/J \simeq 0.56$ ,  $q_c \simeq 0$  for  $D/J = 1.98$ ;  $T_c/J \simeq 0.49$ ,  $q_c \simeq 0.006$  for  $D/J = 1.9$  and  $T_c/J \simeq 0.345$ ,  $q_c \simeq 0.0214$  for  $D/J = 1.7$ . Concerning the case  $D/J = 1.98$ , the phase boundary is almost of first order (see Fig. 3b, where the circle is the unique second order transition point). Our results show that there exists a line which passes by these tricritical points (tricritical line). Below the transition lines, the Neel order prevails. Above, we have the P-phase. However, we find some anomalous behaviours of the AF order parameter in the disordered phase and this seems to be the exciting result of the present work. In fact, from Figure 3c, it emerges that although the order parameter is almost zero, it shows a maximum at fixed parameters  $q$  and  $D$  for varying temperature. In that region we think that the competition between the two dynamics is giving rise to some instability which seems to indicate the presence of an AF-phase inside the disordered phase. This is in fact a sort of local self-organization which has not been seen in the AF spin-1/2 Ising model studied with the same dynamics [7]. Also the specific heat and the susceptibility (see Fig. 3d) show a peak in the region, peak which does not disappear or diverge with increasing system size. At fixed  $T$ ,  $D$  and varying  $q = 1 - p$ , no anomalous behaviour is however found for the order parameter (Fig. 4a) and its variance (Fig. 4b) around the maximum in Figure 3c. A direct investigation of the lattice morphology in that region shows sparse AF-phase clusters on the lattice. Around the maximum in Figure 3c, these clusters coalesce and percolate across the lattice. Through the phase diagram, we find that in the disordered P-phase, the F-order parameter becomes larger than the AF order parameter at very high temperature although both are almost zero. At fixed  $q$  and  $D/J$ , this parameter increases from  $T/J \simeq 0$ , reaches a maximum and then decreases when  $T/J \rightarrow \infty$ .



**Fig. 3.** Phase diagrams of the model corresponding to different values of  $D/J$  given on the curves (a) and (b). Continuous lines indicate second order transition whereas + signs give first order transition points.  $\eta = \exp(-J/kT)$ . Antiferromagnetic order parameter (c) of four systems as a function of temperature at  $D/J = 1.7$  and  $q = 0.03$  for different system sizes given on the curves. Magnetic susceptibility (d) at  $D/J = 1.7$  and  $q = 0.03$  for four system sizes  $L = 16$  ( $\Delta$ ),  $L = 20$  (+),  $L = 30$  ( $\square$ ),  $L = 40$  ( $\times$ ).



**Fig. 4.** Behaviour of the order parameter (a) and its variance (b) for a  $30 \times 30$  system at fixed  $T/J = 0.5$ ,  $D/J = 1.7$  and varying  $p$ .

## 7 Conclusion

In this paper, we report results on the spin-1 Blume-Capel model studied with competing Glauber and Kawasaki dynamics. A local self-organization phenomenon is found within the disordered phase for some model parameters. One open question is how the AF-phase clusters found in the P phase coarsen during the simulation. Another problem which is under investigation is the Ising model spin 3/2 in the antiferromagnetic coupling case. This model is prolific at equilibrium and we expect it to display, when studied with competing dynamics, interesting self-organization phenomena.

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## References

1. R.J. Glauber, *J. Phys.* **4**, 294 (1963).
2. G. Nicolis, I. Prigogine, *Self-Organization in Non-Equilibrium Systems* (Wiley, New York, 1977).
3. H. Haken, *Synergetics*, 3rd ed. (Springer-Verlag, Berlin, 1983).
4. T. Tomé, M.J. de Oliveira, *Phys. Rev. A* **40**, 6643 (1989).
5. K. Kawasaki, in *Phase Transitions and Critical Phenomena*, edited by C. Domb, M.S. Green (Academic Press, London 1972), vol. 2.
6. B.C.S. Grandi, W. Figueiredo, *Phys. Rev. E* **53**, 5484 (1996).
7. B.C.S. Grandi, W. Figueiredo, *Phys. Rev. E* **56**, 5240 (1997).
8. Y. Ma, J. Liu, W. Figueiredo, *Phys. Rev. E* **57**, 3625 (1998).
9. M. Blume, *Phys. Rev.* **141**, 517 (1966).
10. H.W. Capel, *Physica (Amsterdam)* **32**, 966 (1966); **33**, 295 (1967).
11. M. Blume, V.J. Emery, R.G. Griffiths, *Phys. Rev. B* **4**, 1071 (1971).
12. Y. Saito, *J. Chem. Phys.* **74**, 713 (1981).
13. J.D. Kinel, P.-A. Rikvold, Y.L. Wang, *Phys. Rev. B* **45**, 7237 (1992).
14. F. Hontinfinde, J. Krug, M. Touzani, *Physica A* **237**, 363 (1997).
15. F. Hontinfinde, *J. Phys. I France* **7**, 767 (1997).
16. R. Melin, *J. Phys. I France* **6**, 469 (1996).
17. S. Bekhechi, A. Benyoussef, *Phys. Rev. B* **56**, 13954 (1997).
18. M.P. Nightingale, *Physica A* **83**, 561 (1996); *Phys. Lett. A* **59** 486 (1977); *J. Appl. Phys.* **53**, 7927 (1982).
19. S. Bekhechi, A. Benyoussef, N. Moussa, *Phys. Rev. B* **61**, 3362 (2000).