Monte Carlo Study of Order-Disorder Layering Transitions in the Blume-Capel Model

L. Bahmad, A. Benyoussef and H. Ez-Zahraouy*

Laboratoire de Magnétisme et de la Physique des Hautes Energies
Université Mohammed V, Faculté des Sciences, Avenue Ibn Batouta,
Rabat B.P. 1014, Morocco

Abstract

The order-disorder layering transitions, of the Blume-Capel model, are studied using the Monte Carlo (MC) simulations, in the presence of a variable crystal field. For a very low temperature, the results are in good agreement with the ground state study. The first order transition line, found for low temperatures, is connected to the second order transition line, seen for higher temperatures, by a tri-critical point, for each layer. The reentrant phenomena, caused by a competition of thermal fluctuations and an inductor magnetic field created by the deeper layers, is found for the first $k_0$ layers from the surface, where $k_0$ is exactly the number of layering transitions allowed by the ground state study. The layer magnetizations $m_k$, the magnetic susceptibilities $\chi_{m,k}$ and the quadrupolar magnetic susceptibilities $\chi_{q,k}$, for each layer $k$, are also investigated.

Keywords: Blume Capel model; Monte Carlo simulations; Crystal field; Order-disorder; Layering transitions; Magnetic film.

(*) Corresponding author: ezahamid@fsr.ac.ma
1 Introduction

Since the theory of surface critical phenomena started developing, much attention has been devoted to the study of the Blume Capel (BC) model over semi-infinite lattices, with modified surface couplings. Benyoussef et al. [1] have determined the phase diagram in the mean field approximation, reporting four possible topologies at fixed bulk/surface coupling ratios. An analogous analysis have also been done using a real space renormalization group transformation [2]. Some other works referring to particular regions of the phase space are, for example, those using: the mean field approximation [3], the effective field approximation [4] and the low temperature expansion [5]. These works show that it is possible to have a phase with ordered surface and disordered bulk, which is separated from the completely ordered phase by the so-called extraordinary transition and from the completely disordered phase by the surface transition. In the absence of this phase, the transition between the completely ordered and the completely disordered phase is called ordinary. These three kinds of phase transitions have a meeting point named special and which is generally a multi-critical point. The discussion presented in Ref. [6] shows that the strong interest in these models arises partly from the unusually rich phase transition behavior they display as their interaction parameters are varied, and partly from their many possible applications. The bilinear interaction considered in most of these cases is ferromagnetic. The spin-1 Ising systems are used to describe both the order-disorder transition and the crystallisation of the binary alloy, and it was solved in the mean field approach [7]. The decomposition of a line of tri-critical points into a line of critical end points and one of double critical points is is one of the most interesting and elusive features of the mean field phase diagram for the anti-ferromagnetic spin-1 Blume-Capel model in an external magnetic field [8]. The transfer-matrix and Monte Carlo finite-size-scaling methods [9], are also applied to study this model but such decomposition does not occur in the two dimensional case. The finite cluster approximation has been applied by Benyoussef et al. [10] in order to study the spin-1 Ising model with a random crystal field.

On the other hand, the transverse field or crystal field effects of spin-1 Ising model has been studied by several authors [11-14].

The experimental measurements of layer-by-layer ordering phenomena have been established on free-standing liquid crystals films such as nmOBC (n-alkyl-4’-n-alkyloxybiphenyl-4-carboxylate) [15,16] and 54COOBC (n-pentyl-4’-n-pentanoyloxy-biphenyl-4-carboxylate) [17] for several
molecular layers. More recently, Lin et al. [18] have used the three-level Potts model to show the existence of layer-by-layer ordering of ultra thin liquid crystal films of free-standing 54COOBC films, by adjusting the interlayer and intra layer couplings between nearest- neighboring molecules.

The reentrant first-order layering transitions have been observed experimentally in multilayer argon films on graphite by Youn and Hess [19]. Using the mean field method we have shown recently, see Ref. [20], the existence of order-disorder layering transitions in the Blume-Capel Ising films under the effect of a variable crystal field according to the law \( \Delta_k = \Delta_s / k^\alpha \) (\( \Delta_s \) being the surface crystal field, \( k \) the layer number counted from the surface and \( \alpha \) a positive constant). Our aim in this paper is to study the model we introduced in Ref. [20], using Monte Carlo simulations in order to examine the layer-by-layer order-disorder transitions, the existence of the reentrant phenomena for each layer, in one hand, and to investigate the magnetic layer susceptibilities and the corresponding critical exponents.

This paper is organized as follows. Section 2 describes the model and the method. In section 3 we present results and discussions.

### 2 Model and method

The system we are studying here is formed with \( N \) coupled ferromagnetic square layers in the presence of a crystal field. The Hamiltonian governing this system is given by

\[
\mathcal{H} = - \sum_{i,j} J_{ij} S_i S_j + \sum_i \Delta_i (S_i)^2
\]

where, \( S_i (l = i, j) = -1, 0, +1 \) are the spin variables. The interactions between different spins are assumed to be constant so that \( J_{ij} = J \). The crystal field acting on a site \( i \) is so that \( \Delta_i = \Delta_k \) for all spins of the layer \( k \) so that: \( \Delta_1 > \Delta_2 > \ldots > \Delta_N \).

The model we are studying, in this paper, corresponds to a crystal field distributed according to the law:

\[
\Delta_k = \Delta_s / k^\alpha
\]

where \( \Delta_s = \Delta_1 \) is the crystal field acting on the surface (first layer \( k = 1 \)) and \( \alpha \) a positive constant.
The quantities computed, using the Monte Carlo simulations for each layer 'k' containing \(N_x\) spins in \(x\)–direction and \(N_y\) spins in the \(y\)–direction, are:

- The layer average magnetizations \(m_k = \langle M_k \rangle\), where the site average magnetization \(M_k\) of the layer \(k\) is given by
  \[
  M_k = \frac{\sum_{i\in k} S_i}{(N_x N_y)}
  \]  
  \(3\)

- The layer magnetic susceptibilities defined as
  \[
  \chi_{m,k} = \beta N_x N_y \langle (M_k - m_k)^2 \rangle
  \]  
  \(4\)

- The layer quadrupolar magnetic susceptibilities expressed as
  \[
  \chi_{q,k} = \beta N_x N_y \langle (q_k - \langle q_k \rangle)^2 \rangle
  \]  
  \(5\)

where
  \[
  q_k = \frac{\sum_{i\in k} S_i^2}{(N_x N_y)}
  \]  
  \(6\)

- The layer critical exponents \(\gamma_{m,k}\) related to the corresponding layer magnetic susceptibilities \(\chi_{m,k}\), for a fixed layer 'k', giving by
  \[
  \gamma_{m,k} = \frac{\partial \log(\chi_{m,k})^{-1}}{\partial \log | T_{c,k}/J - T/J |}
  \]  
  \(7\)

where \(T/J\) stands for the absolute temperature and \(T_{c,k}/J\) is the critical temperature of the layer 'k'.

In the above equations \(\beta = 1/(k_B T)\) with \(k_B\) being the Boltzmann constant.

The notation \(D^kO^{N-k}\) will be used to denote that the first \(k\) layers from the surface are disordered while the remaining \(N - k\) layers are ordered. In particular, \(O^N\) corresponds to an ordered film whereas \(D^N\) denotes a totally disordered film. The surface crystal field \(\Delta_k\), applied on each layer \(k\) is distributed according to the law given by Eq. (2).

### 3 Results and discussion

Monte Carlo simulations have been made on a system with \(N\) layers and \(N_x = N_y\) spins for the \(x\) and \(y\)–directions of each layer. Runs of \(500000/N\) Monte Carlo steps (MCS) were performed with the discard of the first \(50000/N\) Monte Carlo steps.
We have found that by changing the system sizes from $N = 10$ to $N = 15, 20$ layers (and $N_x = N_y = 64$ to $N_x = N_y = 128$), the relevant measured quantities did not change appreciably. For this reason we give in all the following, numerical results for a film formed with $N = 10$ layers and $N_x = N_y = 64$ spins for the directions $x$ and $y$.

The ground state phase diagram of this model was established in Ref. [20]. It is shown that, for very small values of the surface crystal field $\Delta_s$, the system orders in the phase $O^N$. When increasing $\Delta_s$, the surface (first layer $k = 1$) disorders and the phase $DO^{N-1}$ occurs at $\Delta_s/J = 3(1)^\alpha$. Increasing $\Delta_s$ more and more, the second layer $k = 2$ becomes disordered at $\Delta_s/J = 3(2)^\alpha$, and so on. The transition from the phase $D^kO^{N-k}$ to the phase $D^{k+1}O^{N-(k+1)}$ is seen at $\Delta_s/J = 3(k + 1)^\alpha$ provided that $k + 1 \leq N$. For higher values of the surface crystal field the system is totally disordered and the phase $D^N$ occurs.

In particular, we showed the existence of a critical order layer $k_0$ corresponding to the transition $D^{k_0}O^{N-k_0} \leftrightarrow D^N$, at a reduced surface crystal field given by:

$$\Delta_s/J = (3(N - k_0) - 1)/(\sum_{k=k_0+1}^{N} (1/k^\alpha)).$$  \hspace{1cm} (8)

$k_0$ is exactly the number of layering transitions existing at $T/J = 0$. It is found that $k_0$ depends both on the parameter $\alpha$ and the film thickness $N$. The special case: $\alpha = 0$ is a situation with a constant crystal field applied on each layer and there is only a single transition $O^N \leftrightarrow D^N$, occurring at $\Delta_s/J = 3 - 1/N$ for $T/J = 0$.

In order to outline the existence of the order-disorder layering transitions we plot in Fig. 1 the temperature-crystal field phase diagram for $\alpha = 1.0$. For non null but very low temperatures, the surface crystal field values found in this phase diagram are exactly those predicted by the ground state study established in Ref. [20], namely: $\Delta_s/J = 3(k)^\alpha$ for the first $k_0$ layers. Indeed, the first layer transition is found at $\Delta_s/J = 3.0$; the second transition at $\Delta_s/J = 6.0$; the third transition at $\Delta_s/J = 9.0$ and so on. Monte Carlo simulations show that the last layers $k = 8, 9$ and 10 transit simultaneously at the numerical value of the surface crystal field: $\Delta_s/J \approx 23.84$. This is in good agreement with the predicted value ($\approx 23.80$) from the above Eq. (8) established on the basis of an analytical study.

The reentrant phenomena, shown in Fig. 1 for the first $k_0$ layers, is caused by the competition between thermal fluctuations and an inductor magnetic field created by the deeper layers. Indeed, when these thermal fluctuations become sufficiently important, the magnetization of
some spins, of deeper layers, becomes non null (+1 or -1). This leads to the appearance of an inductor magnetic field. This magnetic field is responsible of the ordered phase seen for the layer $k$. This argument can also explain the absence of the reentrant phenomena for the last layers, once the magnetization of the remaining $N - k$ layers, is not sufficient to create an inductor magnetic field. It is worth to note that the reentrant phenomena is always present for the layers $k$, $(k \leq k_0)$, and the corresponding tri-critical points $C_i$ are located at a constant temperature.

In absence of the surface crystal field, $\Delta_s/J \to 0$, each layer of the film disorders at a fixed temperature $T_c/J = 3.15$. In order to compare this critical temperature value obtained for $N = 10$ layers, with the three-dimensional spin-1 critical temperature, we performed Monte Carlo simulations on films with a fixed surface $(N_x, N_y) = (128, 128)$ and increasing thicknesses: $N = 16; 32; 64$ and 128. It is found that the corresponding critical temperature increases very slowly with the number of layers once $N \geq 32$. For $N = 128$, the critical temperature we computed did not exceed the value $T_c/J = 3.19(5)$. This value is smaller than that one computed by the mean field approach for a three-dimensional cubic lattice spin-1 Ising model, which is exactly $T_c/J = 4.0$.

On the other hand, as it is shown in Fig. 1, the first $k_0$ tri-critical temperature values, established by MC simulations are approximately: $T_{ci}/J \approx 0.50$. These temperature values are smaller than those established in Ref. [20] when using the mean field method: $T_{ci}/J \approx 0.78$

A detailed study is done for a very low temperature, as it is shown in Figure 2 for $T/J = 0.2$

Indeed, Fig. 2a shows that the individual layering transition temperatures undergo a first order transition at the crystal field values predicted by the analytical study, namely: $\Delta_s/J = 3.0$ for the first layer $k = 1$, $\Delta_s/J = 6.0$ for the second layer $k = 2$, $\Delta_s/J = 9.0$ for the third layer $k = 3$, and so on. The last layers $k = 8$, $k = 9$ and $k = 10$ transit simultaneously at $\Delta_s/J \approx 23.84$. On the other hand the layer quadrupolar magnetic susceptibilities $\chi_{q,k}$ defined by Eq. (5), for each layer $k$, present a strong peak at the surface crystal field values corresponding to each layer transition; as it is illustrated by Fig. 2b. For a higher temperature, Fig. 3 corresponding to $T/J = 1.0$, the layering transitions are second order type. Indeed, this is shown in Fig. 3a for the individual layering temperature behaviors, as a function of the surface crystal field. The corresponding magnetic susceptibilities $\chi_{m,k}$, defined by Eq. (4) for each layer $k$, present a strong peak at the corresponding surface crystal field. It is worth to
note that Figs. 2b and 3b are plotted for reduced numerical values of the layer magnetic and the layer quadrupolar magnetic susceptibilities: $\chi_{q,k}$ and $\chi_{m,k}$ respectively.

To show the increasing temperature effect, for a fixed surface crystal field, on the order-disorder transitions; we illustrate in Fig. 4 the corresponding layering transitions for $\Delta_s/J = 2.0$ for each layer. It is found that these transitions are second order type and are located at $T/J \approx 2.95$, see Fig. 4a for the layer magnetization behavior and Fig. 4b for the layer magnetic susceptibilities $\chi_{m,k}$. On the other hand the reentrant phenomenon, seen for the first $k_0$ layers is well illustrated in Fig. 5 for the layer $k = 7$ at a fixed surface crystal field value $\Delta/J = 22.0$. Indeed, the two transitions: from disorder to order and from order to disorder of the layer $k = 7$ are well seen in Fig. 5 for the layer magnetization $m_7$. The corresponding layer magnetic susceptibility $\chi_{m,7}$ exhibits two strong peaks at these transitions. In order to complete this study, we have investigated the layer critical exponents $\gamma_{m,k}$ for $N = 10$ layers and several system sizes $N_x \times N_y = 16 \times 16$, $N_x \times N_y = 32 \times 32$, $N_x \times N_y = 64 \times 64$, and $N_x \times N_y = 128 \times 128$; see Fig. 6. It is found that $\gamma_{m,k}$ decreases, for a fixed order 'k', with the system size $N_x \times N_y$ and stabilizes at certain value; and due to the free boundary conditions the critical exponents of the layers $k = 1$ and $k = N$ are found to be greater than those of the internal layers $2 \leq k \leq N - 1$.

4 Conclusion

The order-disorder layering transitions of the Blume-Capel Ising model have been studied under the effect of a variable crystal field according to the law Eq. (2) and using Monte Carlo simulations. The reentrant phenomena, caused by a competition of thermal fluctuations and an inductor magnetic field created by the deeper layers, is found for the first $k_0$ layers counted from the surface; where $k_0$ is exactly the number of layering transitions allowed by the ground state study. We established the temperature-crystal field phase diagrams and found that the last $N - k_0$ layer tri-critical points are located at higher temperature values for a fixed exponent $\alpha$ and film thickness $N$. For very low temperatures, the results are in good agreement with those predicted by the ground state study. The first order and the second order transition lines are connected by a tri-critical point, for each layer. On the other hand, the layer magnetizations $m_k$, the magnetic susceptibilities $\chi_{m,k}$, the quadrupolar magnetic susceptibilities $\chi_{q,k}$, and the critical exponents $\gamma_{m,k}$ for each layer $k$, have been computed.
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Figure Captions

Figure 1.: The critical temperature behavior as a function of the surface crystal field $\Delta_s/J$ for $\alpha = 1.0$ and a film thickness $N = 10$ layers. For each layer '$k'$ ($k = 1, 2, ..., N$), the first-order transition line (vertical dashed line) is connected to the second-order transition line (up-triangular points) by a tri-critical point $C_k$ (open circle). The notations $D^kO^{N-k}$ are defined in the body text.

Figure 2.: The behavior of the reduced layer magnetizations $m_k$ (Fig. a), and the layer quadrupolar magnetic susceptibilities $\chi_{q,k}$ (Fig. b), showing a first-order transition, as a function of the surface crystal field $\Delta_s/J$, for a very low temperature: $T/J = 0.2$. The number accompanying each curve denotes the layer order from the surface to deeper layers.

Figure 3.: For a higher temperature $T/J = 1.0$, the dependency of the layer magnetizations $m_k$ (Fig. a), and the reduced layer magnetic susceptibilities $\chi_{m,k}$ (Fig. b), undergoes a second-order transition, as a function of the surface crystal field $\Delta_s/J$.

Figure 4.: For a fixed surface crystal field value $\Delta_s/J = 2.0$, the layer magnetizations $m_k$ (Fig. a) and the reduced layer magnetic susceptibilities $\chi_{m,k}$ (Fig. b) show a second-order transition as a function of increasing temperature. For each layer '$k'$ ($k = 1, 2, ..., N$), the transition is located at $T/J = 2.95$.

Figure 5.: Thermal behavior of the layer magnetization $m_7$ (line with solid circles) and the reduced layer magnetic susceptibility $\chi_{m,7}$ (line with open circles) for a deeper layer $k = 7$. The reentrant phenomena as well as the second order transition are both outlined by the layer magnetization transition from $D^7O^3$ to $D^6O^4$ and from $D^6O^4$ to $D^{10}$ corresponding to two peaks of the reduced layer magnetic susceptibility $\chi_{m,7}$ for $\Delta_s/J = 22.0$.

Figure 6.: Layer critical exponents $\gamma_{m,k}$ for $\Delta_s/J = 2.0$ as a function of the position '$k$' for a film thickness $N = 10$ layers, and several sizes: $N_x \times N_y = 16 \times 16$ (fill squares);
$N_x \times N_y = 32 \times 32$ (fill circles); $N_x \times N_y = 64 \times 64$ (open circles); and $N_x \times N_y = 128 \times 128$ (filled up-triangulars).
Fig. 1

\[ \alpha = 1.0 \]

\[ T_c / J \]

\[ \Delta_s / J \]
Fig. 2a

α = 1.0
T/J = 0.2
Fig. 3a

\[ \alpha = 1.0 \]

\[ T/J = 1.0 \]
Fig. 4a

$\alpha = 1.0$

$\Delta s/J = 2.0$
Fig. 4b

\[ \chi_{m,k} \]

\[ T/J \]

\[ \alpha = 1.0 \]

\[ \Delta_s/J = 2.0 \]
Fig. 5

\[ \alpha = 1.0 \]
\[ k = 7 \]
\[ \Delta_s / J = 22.0 \]
