First Order Phase Transition in the 3-dimensional Blume-Capel Model on a Cellular Automaton

N. Seferoğlu*, A. Özkan* and B. Kutlu**

* Gazi Üniversitesi, Fen Bilimleri Enstitüsü, Fizik Anabilim Dalı, Ankara, Turkey

** Gazi Üniversitesi, Fen-Edebiyat Fakültesi, Fizik Bölümü, 06500 Teknikokullar, Ankara, Turkey
e-mail: bkutlu@gazi.edu.tr

Abstract

The first order phase transition of the three-dimensional Blume Capel are investigated using cooling algorithm which improved from Creutz Cellular Automaton for the $D/J = 2.9$ parameter value in the first order phase transition region. The analysis of the data using the finite-size effect and the histogram technique indicate that the magnetic susceptibility maxima and the specific heat maxima increase with the system volume ($L^d$) at $D/J = 2.9$.

Keywords: Blume-Capel Model; Creutz Cellular Automaton; First Order Phase Transition; Finite-Size Effect; Histogram; Simple Cubic Lattice.

1. Introduction

The Hamiltonian of the Blume-Capel model \(^{(1,2)}\) is given by,

$$H_I = -J \sum_{<ij>} S_i S_j + D \sum_i S_i^2 \quad (1)$$

where $s_i = -1, 0, 1$ and the first sum is carried out over all nearest-neighboring (nn) spin pairs on a three-dimensional simple cubic lattice. The parameters
of the $J$ and $D$ are the bilinear interaction energy and single-ion anisotropy constant, respectively.

The model is known to have a rich critical behavior and considered by both numerical and analytical methods. Recently, most of these studies mainly focused on determining the tricritical point of the model$^{(3-8)}$. In previous paper$^{(9)}$, we obtained the tricritical point value of the 3-d Blume-Capel model as $D/J = 2.82$. This results agrees with a series expansion$^{(3-4)}$, the cluster variation method$^{(5)}$, the effective field theory$^{(6)}$ and Bethe-Peierls approximation results$^{(7)}$. Although the critical behavior on the second-order phase transition region ($D/J < 2.82$) has been studied commonly, the finite-size effects in the first-order phase transition region ($D/J > 2.82$) is not investigated exactly.

Our aim of this paper is to identify the phase transition in the first order phase transition region of the Blume Capel model by the finite-size effects and the histograms of energy distribution $P(E)$ and order parameter distribution $P(M)$.

It is well known that the first order phase transitions involve the coexistence of two distinct phases and are characterized by the existence of a discontinuity in the energy and magnetization for the infinite systems. As a results of these discontinuities, the specific heat and the susceptibility show singularities of the delta function. However, the characteristic singularities and discontinuities in the first order phase transitions appears as rounded and smeared in finite systems employed in computer simulations$^{(10,11)}$. These behaviors at the first order phase transitions in finite-size systems are qualita-
tively similar to the finite-size effects at second-order phase transitions. The finite size effects at the first order phase transition have been investigated by the different methods such as the Monte Carlo\(^{12-15}\), the phenomenological renormalization group\(^{16}\), transfer matrix method\(^{17}\), renormalization-group analysis\(^{18}\). According to the results of these studies, the finite-size effects at the first order phase transition depend on the volume of the system \(L^d\). The specific heat and the susceptibility increase with \(L^d\) and the transition temperature which are locations of their extrema, approach the transition temperature in the infinite system as \(L^{-d}\). In addition, the histograms of energy distribution \(P(E)\) and the order parameter distribution \(P(M)\) are the reliable method to study first-order phase transitions\(^{10,12,13,19}\). While the probability distribution of energy shows a single peak in a second-order phase transition, it shows a double peak in a first-order phase transition. In this paper we simulate the three dimensional Blume-Capel model with the cooling algorithm which improve from the Creutz Cellular Automaton in the first order phase transition region. The finite-size scaling and the probability distribution for energy and order parameter are used to determine the nature of the phase transition. The remainder of the paper is organized as follows. The data are analyzed and the results are discussed in Section 2 and the conclusion is given in Section 3.

3. Results and discussion

The three dimensional Blume-Capel model is simulated with the cooling algorithm\(^{9}\) which improved from the Creutz Cellular Automaton. The simulations have been made at the \(D/J = 2.9\) anisotropy parameter value
in the first order phase transition region on simple cubic lattices \( L \times L \times L \) of the linear dimensions \( L = 8, 10, 12, 14, 16, 18 \) and \( 20 \) with periodic boundary conditions.

At the algorithm, the cooling rate is equal to \( 0.01 H_k \) per site for \( D/J = 29/10 \) value and the kinetic energy of the system reduced by the different cooling amounts per site because the kinetic energy, \( H_k \), is an integer variable in the interval \((0, 24J)\). The computed values of the quantities are averages over the lattice and over the number of time steps \((1.000.000)\) with discard of the first 100.000 time steps during which the cellular automaton develops.

The simulations were done about 10 times with different initial configurations at each lattice size. Measurements shown that the variation of thermodynamic quantities and the histogram of \( P(E) \) and \( P(M) \) for each different initial configuration are different from each other around the transition temperature. At the same time, some of the simulations do not exhibit the double peak in the histogram of the \( P(E) \) and the three peaks in the histogram of the \( P(M) \) which characterize the first order phase transition. Therefore, we choose the simulations which exhibit the characteristic double peak in the histogram of \( P(E) \) and the three peaks in the histogram of the \( P(M) \) to study finite-size effects at \( D/J = 2.9 \).

In Fig.1, the temperature variation of the order parameter \( M = \frac{1}{L^3} \sum_{<ij>} S_i \) and \( Q = \frac{1}{L^3} \sum_{<ij>} S_i^2 \), the energy \( E = -J \sum_{<ij>} S_i S_j / E_0 \) where \( E_0 \) is the ground state Ising energy at \( kT/J=0 \), and histograms of \( P(M) \) and \( P(E) \) are shown for a chosen simulation result on \( L = 18 \) as an example. There are discontinuities which characterize a first order phase transition in tempera-
ture dependence of the order parameter and energy in Fig.1 (a) and (c). On the other hand, another evidence for the first order transition is seen in the histograms of $P(M)$ and $P(E)$ in Fig.1 (b) and (d). The shape of distribution $P(E)$ shows a double peak around the transition temperature corresponding to the coexistence of the ordered and disordered phases. In the distribution of the magnetization $P(M)$, the middle peak indicate to the value of disordered phase while the other peaks indicate the order phase. The histograms of $P(M)$ and $P(E)$ around the transition temperature is given in Fig.2(a) and (b) for a chosen simulation, respectively. Histograms of $P(M)$ and $P(E)$ have a single peak above the transition temperature. As the temperature is close to the transition value the histogram of $P(E)$ has a double peak while $P(M)$ has three peaks indicate the coexistence region. With the decreasing temperature, the histogram of $P(E)$ converges to a single peak and the middle peak in the histogram of $P(M)$ is depressed while other peaks are enhanced corresponding to order region. The behavior of $P(M)$ and $P(E)$ around the transition region are in good agreement with the characteristic behavior of the first order phase transition $^{(10,12,13,19)}$.

In Fig.3 (a) and (b) the temperature dependence of the order parameter, the magnetic susceptibility, the energy and the specific heat are shown at different lattice sizes for a selected simulation which shows a double peak in the histogram of $P(E)$ and three peaks in the $P(M)$. The results are seen in Fig.3 show that the energy and the order parameter have discontinuity at transition region and the peaks of the susceptibility and the specific heat increase with lattice size as expected in the first order phase transition.
The finite-size effects of the specific heat and the susceptibility at the transition temperature are given by

\[ C_{\text{max}} \propto L^d \]  
(2)

\[ \chi_{\text{max}} \propto L^d \]  
(3)

The magnetic susceptibility maxima \( \chi_{\text{max}}(L) \), the specific heat maxima \( C_{\text{max}}(L) \) are obtained from the average over the maximum of magnetic susceptibility and specific heat at each lattice size for chosen simulations. However, the transition temperature \( T_t(L) \) for each lattice is estimated from the location of the magnetic susceptibility and the specific heat maxima for chosen simulations. The infinite lattice transition temperature are estimated from the extrapolation of susceptibility \( T_t^\chi(L) \) and specific heat maxima \( T_t^C(L) \) for various lattice sizes. The estimated infinite lattice transition temperature values are \( T_t^\chi(\infty) = 1.29\pm0.02 \), \( T_t^C(\infty) = 1.28\pm0.03 \) from \( \chi_{\text{max}} \) and \( C_{\text{max}} \), respectively. The logarithm of the specific heat and the susceptibility maxima as a function of the logarithm \( L \) is shown in Fig.4(a) and (b). The data lies on a single curve and the slope gives 3.01 and 3.07 from the specific heat maxima \( C_{\text{max}}(L) \) and the susceptibility maxima \( \chi_{\text{max}}(L) \), respectively. These estimated values are in good agreement with the system dimension \( (d = 3) \). This result show that, the magnetic susceptibility and the specific heat maxima increase with the system volume \( (L^d) \) as a characteristic property of the first order phase transition\(^{(12-18)}\).

4. Conclusion
The three dimensional Blume-Capel model is simulated using cooling algorithms on a cellular automaton. The simulations are done about 10 times with different initial configurations at each lattice size and some of this simulations having double and three peaks in the histograms of P(E) and P(M) are chosen. To identify the phase transition of the model, the analysis of the first order phase transition effects and the histogram technique are used. The temperature variations of the order parameter and the energy show the discontinuity at the transition temperature while the histogram of P(E) and P(M) have a double and three peak structures. Furthermore, the magnetic susceptibility and the specific heat maxima increase with the system volume \((L^d)\) as expected in the first order phase transition.

Acknowledgements

This work is supported by a grant from Gazi University (BAP:05/2003-07).

References

[1] M.B. Blume, Phys. Rev. B 141 (1966) 517.
[2] H.W. Capel, Physica(Utrecht) 32 (1966) 966.
[3] D.M. Saul, M. Wortis and D.Stauffer, Phys. Rev. B 9 (1974) 4964.
[4] J.G. Brankov, J. Przystawa and E. Pravecki, J. Phys. C 5 (1972) 3384.
[5] W.M. Ng and J.H.Barry, Phys. Rev. B 17 (1978) 3675.
[6] A.F. Siqueira and I.P. Fittipaldi, Physica A 138 (1986) 592.
[7] A. Du, Y.Q. Yü and H.J. Liu, Physica A 320 (2003) 387.
[8] J.W. Tucker, J.Phys.:Condens. Matter I, (1989) 485.
[9] B. Kutlu, A. Özkan, N. Seferoğlu, A. Solak and B. Binal, Int. J. Mod.
Phys.C 16 (2005) (in press).

[10] O.G. Mouritsen, ”Computer Studies of Phase Transitions and Critical Phenomena”, New York Tokyo, 1984.

[11] V.Privman, ”Finite Size Scaling and Numerical Simulation of Statistical Systems”, Singapore, 1990.

[12] M.S.S.Challa, D.P.Landau and K.Binder, Phys. Rev. B 34 (1986) 1841.

[13] K.Binder and D.P.Landau, Phys. Rev. B 30 (1984) 1477.

[14] S.Chen, A.M.Ferrenberg and D.P.Landau, Phys. Rev. Lett. 69 (1992) 1213.

[15] J. Lee and M.Kosterlitz, Phys. Rev. B 43 (1991) 3265.

[16] M.E. Fisher and A.N.Berker, Phys. Rev. B 26 (1982) 2507.

[17] V. Privman and M.E.Fisher, J. of Stat. Phys. 33 (1983) 385.

[18] J.L. Cardy and M.P. Nightingale, Phys. Rev. B 27 (1983) 4256.

[19] I. Puha and H.T. Diep, J. Magn. Magn. Mater. 224 (2001) 85.

**Figure Captions**

Fig.1. The temperature dependence of (a) the order parameters M and Q, (b) the histogram of P(M), (c) the energy, (d) the histogram of P(E) for a chosen simulation on L=18.

Fig.2. The histogram (a) P(M) and (b) P(E) for several temperatures around the transition temperature for chosen simulations on L =10 and L =18.

Fig.3. The temperature dependence of (a) the order parameters, (b) magnetic susceptibility, (c) the energy and (d) the specific heat on L =
8,10,12,14,16,18 and 20.

Fig.4. Log-log plot of (a) the specific heat maxima and (b) the magnetic susceptibility maxima against linear dimension L.
Figure 1:
Figure 2:
Figure 3: 12
\begin{align*}
\textbf{L=8} & \quad (a) \\
\text{P}(M) & \quad \bullet \ T=1.414 \\
 & \quad + \ T=1.335 \\
 & \quad \times \ T=1.290 \\
 & \quad * \ T=1.296 \\
\textbf{L=10} & \quad (b) \\
\text{P}(E) & \quad \bullet \ T=1.342 \\
 & \quad + \ T=1.283 \\
 & \quad \times \ T=1.251 \\
 & \quad * \ T=1.267
\end{align*}
(a) \[ \text{Log}(C_{\text{max}}) \]

slope = 3.01

(b) \[ \text{Log}(\chi_{\text{max}}) \]

slope = 3.07