ARTICLE IN PRESS

Computer Physics Communications ■ (■■■■) ■■■–■■■

Contents lists available at SciVerse ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Novel considerations about the non-equilibrium regime of the tricritical point in a metamagnetic model: Localization and tricritical exponents

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ARTICLE INFO

Article history:
Received 31 January 2013
Received in revised form
3 April 2013
Accepted 3 May 2013
Available online xxxx

Keywords:
Time-dependent Monte Carlo simulations
Tricritical point
Metamagnetic model
Refinement of critical parameters

ABSTRACT

We have investigated the time-dependent regime of a two-dimensional metamagnetic model at its tricritical point via Monte Carlo simulations. First, we obtained the temperature and magnetic field corresponding to the tricritical point of the model by using a refinement process based on optimization of the coefficient of determination in the log–log fit of magnetization decay as a function of time. With these estimates in hand, we obtained the dynamic tricritical exponents θ and z and the static tricritical exponents ν and β by using the universal power-law scaling relations for the staggered magnetization and its moments at an early stage of the dynamic evolution. Our results at the tricritical point confirm that this model belongs to the two-dimensional Blume–Capel model universality class for both static and dynamic behaviors, and they also corroborate the conjecture of Janssen and Oerding for the dynamics of tricritical points.

1. Introduction

In the study of phase transitions and critical phenomena, systems which exhibit multicritical behavior have been the subject of a great number of works. Theoretically, the tricritical phase transition of the Blume–Capel [1] model is one of the most studied. However, there are other models showing the existence of such multicritical points, for instance, the metamagnetic model [2], the Blume–Capel model with antiferromagnetic exchange interaction and external magnetic field added [3], and the random-field Ising model [4]. In order to investigate these phenomena, several techniques have been employed, including series expansions [5], linked-cluster expansion [6], mean-field theory [7], renormalization group [8–11], transfer matrix [12–15], Monte Carlo simulations [16–19], and Monte Carlo renormalization group methods [20–22]. Experimentally, the phase transitions of metamagnetic systems such as in the compound $FeBr_2$ [23,24] have also been studied in order to understand the tricritical behavior that appears as a consequence of a competition between the antiferromagnetic and ferromagnetic coupling constants present in this magnetic system.

The two-dimensional spin-$\frac{1}{2}$ metamagnetic model is defined by the Hamiltonian

$$\mathscr{H} = J_1 \sum_{nn} \sigma_i \sigma_j - J_2 \sum_{nnn} \sigma_i \sigma_k + H \sum_i \sigma_i, \tag{1}$$

where $J_1, J_2 > 0$ and $\sigma_i = \pm 1$ are the spin variables. The model considered has two sublattices: the first sum extends over all nearest-neighbor pairs (intersublattice) and the second over all next-nearest-neighbor pairs (intrasublattice), respectively. The parameters J_1 and J_2 are the antiferromagnetic and ferromagnetic coupling constants, respectively, and H is the external magnetic field.

The order parameter of the model is the staggered magnetization, conveniently defined by

$$M(t) = \frac{1}{N} \sum_{i=1}^{L} \sum_{j=1}^{L} (-1)^{i+j} \sigma_{i,j} = M_1(t) - M_2(t), \tag{2}$$

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http://dx.doi.org/10.1016/j.cpc.2013.05.005

where $N = L^2$, L being the linear size of the square lattice. Here, $M_1(t) = \frac{2}{N}\sum_{i=1}^{L}\sum_{j=1}^{L}\sigma_{i,j}\delta_{\mathrm{mod}(i+j,2),0}$ and $M_2(t) = \frac{2}{N}\sum_{i=1}^{L}\sum_{j=1}^{L}\sigma_{i,j}\delta_{\mathrm{mod}(i+j,2),1}$ denote the magnetizations of the respective sublattices. This definition shows that there is an inversion of the meaning of ordered and disordered state. In order to obtain an ordered state, it is necessary to occupy the sites of the lattice with spins $+1$ (-1) where the sum $i + j$ is odd (even), or vice versa. On the other hand, null magnetization may be obtained when all sites are occupied with spins of the same kind.

In contrast to the Blume–Capel model, the phase diagram of the metamagnetic model is not yet completely understood. This is due to the controversial results between the experimental and theoretical works concerning the phase transitions of the system. If, on the one hand, this model exhibits a rich phase diagram in the temperature–field plane with a line of second-order phase transitions, a line of first-order phase transitions, and a tricritical point which is located at the point where the first-order and second-order transition lines join each other with the same slope, on the other hand, mean-field theory [25] predicts that such a tricritical point depends on the value of the ratio between the coupling constants. The theory only predicted the existence of a tricritical point for $R = J_2/J_1 > 3/5$, while for $R < 3/5$ in the mean-field approximation the model exhibits two Ising-like critical points: a critical endpoint corresponding to a point that ends at the first-order line coming from the second-order line and a double critical endpoint (bicritical) that corresponds to the terminal point of the first-order transition line. Although for the three-dimensional metamagnetic model Herrmann et al. [26] showed via Monte Carlo (MC) renormalization group theory that such critical endpoints exist, experimental works have not found those points in any real metamagnetic system, and also there is no evidence of such points for the two-dimensional metamagnetic systems as verified in different works (see, for example, [13,27]). Similarly, Santos and Figueiredo [28] by using a master equation formalism in the context of dynamical pair approximation, also in two dimensions, did not find any evidence for the decomposition of the tricritical point into the critical and bicritical endpoints as predicted by mean-field theory. More recently, other authors exclude the possibility of existence of these two critical endpoints even for three dimensions: Geng et al. [29], by using effective-field theory, showed that there is no fourth-order critical point or reentrant phenomenon in the phase diagram. Finally, other authors [30], by performing MC simulations, showed that there is no evidence of such a decomposition in a critical endpoint and a bicritical endpoint, and such simulations produce a tricritical behavior even for a coupling ratio as small as $R = 0.01$.

Although previous estimates of the critical exponents for this model support the assertion that it belongs to the same universality class as the Blume–Capel model, the non-equilibrium critical behavior of this system has not been completely investigated to date. Santos and Figueiredo [31] studied a similar layered metamagnetic model far from equilibrium by using short-time Monte Carlo simulations. They estimated the static critical exponents β and ν and the dynamic critical exponent z on the continuous transition line, but the tricritical exponents were not obtained. They also showed that, although the critical exponent ν remains the same along the continuous transition line, the exponent β departs from the expected value as we approach the tricritical point of the model.

Our goal in this work was to study the non-equilibrium critical dynamics of a metamagnetic model through short-time Monte Carlo simulations. In the next section, we estimate the tricritical parameters of the model (temperature and magnetic field) by using a refinement process based on optimization of the coefficient of determination in the log–log fit of magnetization decay as a function of time. With these estimates in hand, we also obtain the dynamic tricritical exponents θ and z and the static tricritical exponents ν and β by using the universal power-law scaling relations for the staggered magnetization and its moments at an early stage of the dynamic evolution. Our conclusions are presented in Section 3.

2. Short-time critical dynamics and results

The study of the dynamic critical properties of statistical systems has been a subject of considerable interest in non-equilibrium physics; see the works by Janssen, Schaub, and Schmittmann [32], and Huse [33]. By using, respectively, renormalization group techniques and numerical calculations, these authors showed that universality and scaling behavior are already present in systems since their early stages of time evolution after quenching from high temperatures to the critical one. As a result, the study of the critical properties of statistical systems became in some sense simpler, because they allow one to circumvent the well-known problem of critical slowing down, characteristic of the long-time regime.

The dynamic scaling relation obtained by Janssen et al. for the kth moment of the magnetization M, extended to systems of finite size [34,35], is written as

$$\langle M^k\rangle(t,\tau,L,m_0) = b^{-k\beta/\nu}\langle M^k\rangle(b^{-z}t, b^{1/\nu}\tau, b^{-1}L, b^{x_0}m_0), \qquad (3)$$

where t is the time, b is an arbitrary spatial rescaling factor, $\tau = (T - T_c)/T_c$ is the reduced temperature, and L is the linear size of the lattice. Here, the operator $\langle\cdots\rangle$ denotes averages over different configurations due to different possible time evolution from each initial configuration compatible with a given initial magnetization m_0. The exponents β and ν are the equilibrium critical exponents associated to the order parameter and the correlation length, respectively, and z is the dynamic exponent characterizing time correlations at equilibrium.

After choosing the scaling $b^{-1}L = 1$ at $T = T_c$ $(\tau = 0)$, and $k = 1$, we obtain $\langle M\rangle(t, L, m_0) = L^{-\beta/\nu}\langle M\rangle(L^{-z}t, L^{x_0}m_0)$. Denoting $u = tL^{-z}$ and $w = L^{x_0}m_0$, one has $\langle M\rangle(u,w) = \langle M\rangle(L^{-z}t, L^{x_0}m_0)$. The derivative with respect to L is

$$\frac{\partial\langle M\rangle}{\partial L} = (-\beta/\nu)L^{-\beta/\nu-1}\langle M\rangle(u,w) + L^{-\beta/\nu}\left[\frac{\partial\langle M\rangle}{\partial u}\frac{\partial u}{\partial L} + \frac{\partial\langle M\rangle}{\partial w}\frac{\partial w}{\partial L}\right],$$

where $\partial u/\partial L = -ztL^{-z-1}$ and $\partial w/\partial L = x_0 m_0 L^{x_0-1}$. In the limit $L \to \infty$, $\partial_L\langle M\rangle \to 0$, one has $x_0 w\frac{\partial\langle M\rangle}{\partial w} - zu\frac{\partial\langle M\rangle}{\partial u} - \beta/\nu\langle M\rangle = 0$. The separability of the variables u and w in $\langle M\rangle(u,w) = M_1(u)\,M_2(w)$ leads to $x_0 w M_2'/M_2 = \beta/\nu + zuM_1'/M_2$, where the prime means the derivative with respect to the argument. Since the left-hand side of this equation depends only on w and the right-hand side depends only on u, they must be equal to a constant c. Thus, $M_1(u) = u^{(c/z)-\beta/(\nu z)}$ and $M_2(w) = w^{c/x_0}$, resulting in $\langle M\rangle(u,w) = m_0^{c/x_0}L^{\beta/\nu}t^{(c-\beta/\nu)/z}$. Returning to the original variables, one has $\langle M\rangle(t,L,m_0) = m_0^{c/x_0}t^{(c-\beta/\nu)/z}$.

On the one hand, choosing $c = x_0$ and denoting $\theta = (x_0 - \beta/\nu)/z$, at criticality $(\tau = 0)$, we obtain the algebraically behavior of the magnetization:

$$\langle M\rangle(t) \sim m_0 t^{\theta}. \qquad (4)$$

This can be observed by a finite time scaling $b = t^{1/z}$, Eq. (3), at critical temperature $(\tau = 0)$, which leads to $\langle M\rangle(t,m_0) = t^{-\beta/(\nu z)}\langle M\rangle(1, t^{x_0/z}m_0)$. Defining $x = t^{x_0/z}m_0$, an expansion of the averaged magnetization around $x = 0$ results in $\langle M\rangle(1,x) = \langle M\rangle(1,0) + \partial_x\langle M\rangle|_{x=0}x + \mathcal{O}(x^2)$. By construction, $\langle M\rangle(1,0) = 0$, since $x = t^{x_0/z}m_0 \ll 1$ and $\partial_x\langle M\rangle|_{x=0}$ is a constant. Discarding the quadratic terms, we obtain the expected power-law behavior $\langle M\rangle_{m_0} \sim m_0 t^{\theta}$, which is valid only for a characteristic time scale $t < t_{\max} \sim m_0^{-z/x_0}$.

Please cite this article in press as: R. da Silva, et al., Novel considerations about the non-equilibrium regime of the tricritical point in a metamagnetic model: Localization and tricritical exponents, Computer Physics Communications (2013), http://dx.doi.org/10.1016/j.cpc.2013.05.005