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CONDENSED MATTER

Short-Time Dynamics of the Three-Dimensional Ising Model with Competing Interactions

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The critical relaxation from the low-temperature ordered state of the three-dimensional Ising model with competing interactions on a simple cubic lattice has been studied for the first time using the short-time dynamics method. Competition between exchange interactions is due to the ferromagnetic interaction between the nearest neighbors and the antiferromagnetic interaction between the next nearest neighbors. Particles containing 262144 spins with periodic boundary conditions have been studied. Calculations have been performed by the standard Metropolis Monte Carlo algorithm. The static critical exponents of the magnetization and correlation radius have been calculated. The dynamic critical exponent of the model under study has been calculated for the first time.

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Competing interactions in magnetic materials lead to the appearance of a large variety of magnetic ordered states and phase transitions between them. In this connection, a three-dimensional Ising model including the spin exchange interaction not only between the nearest neighbors but also between the next nearest neighbors is of certain interest. The Hamiltonian of such a model can be represented in the form

$$H = -\frac{1}{2}J_1\sum_{\langle i,k\rangle}S_iS_k - \frac{1}{2}J_2\sum_{\langle l,m\rangle}S_lS_m, \quad S_i = \pm 1, \tag{1}$$

where S_i is the Ising spin at the lattice site i, the first sum describes the ferromagnetic exchange interaction between the nearest neighbors ($J_1 > 0$), and the second sum describes the antiferromagnetic exchange interaction between the next nearest neighbors ($J_2 < 0$). The type of magnetic ordering at low temperatures depends on the frustration parameter $\alpha = |J_2/J_1|$. This model was studied both theoretically using the effective field theory [1] and by computational physics methods (the Wang–Landau method and the classical Metropolis algorithm) [2]. The authors of these studies showed that the low-temperature ferromagnetic ordering takes place at $0.0 < \alpha < 0.25$, and collinear ordering, which is also called superantiferromagnetic (alternating ferromagnetic layers with oppositely directed spins), occurs at $0.25 < \alpha < 1.0$. At high temperatures, the model is in the paramagnetic state for all frustration parameter values. The interface between the ferromagnetic and paramagnetic phases is a line of second-order phase transitions, whereas the interface between the collinear and paramagnetic phases is a line of first-order phase transitions [1, 2].

Using the short-time dynamics method, we studied the critical relaxation of the three-dimensional Ising model with competing interactions from the low-temperature ordered state in the interval of the frustration parameters of $0.001 \le \alpha \le 0.24$. Recently, this method has been successfully applied to study the critical dynamics of models of magnetic materials [3–8], in which the critical relaxation of the magnetic model from the nonequilibrium state to the equilibrium one is studied within the model A (the Halperin–Hohenberg classification of universality classes of the dynamic critical behavior [9]).

When relaxation starts from the completely ordered low-temperature state, the kth moment of the magnetization after a microscopically small time interval has the scaling form [3, 10]

$$M^{(k)}(t, \tau, L) = b^{-k\beta/\nu}M^{(k)}(b^{-z}t, b^{1/\nu}\tau, b^{-1}L). \tag{2}$$

Here, $M^{(k)}$ is the kth moment of the magnetization; t is the time; $\tau = (T - T_c)/T_c$ is the reduced temperature; b is the scaling factor; β and ν are the static critical exponents of the magnetization and correlation radius, respectively; z is the dynamic critical exponent; and L is the linear dimension of the system. Assuming $b = t^{1/z}$ [3], we obtain the following expression for the magnetization of systems with large linear dimensions L:

$$M(t,\tau) \sim t^{-\beta/\nu z} M(1, t^{1/\nu z}\tau). \quad (3)$$

At the phase transition point ($\tau = 0$), the magnetization depends only on time according to the power law

$$M(t) \sim t^{-c_1}, \quad c_1 = \frac{\beta}{\nu z}. \quad (4)$$

By taking the logarithmic derivatives of both sides of Eq. (3) with respect to τ at $\tau = 0$, we obtain a power law for the logarithmic derivative at the phase transition point

$$\partial_\tau \ln M(t,\tau)|_{\tau=0} \sim t^{-c_{l1}}, \quad c_{l1} = \frac{1}{\nu z}. \quad (5)$$

For the Binder cumulant $U_L(t)$ calculated from the first and second moments of the magnetization, the finite-size scaling theory gives the following dependence at $\tau = 0$:

$$U_L(t) = \frac{M^{(2)}}{(M)^2} - 1 \sim t^{c_U}, \quad c_U = \frac{d}{z}, \quad (6)$$

where d is the dimensionality of the system.

Thus, the short-time dynamics method allows determining three critical exponents β, ν, and z in a single numerical experiment using Eqs. (4)–(6). In addition, the dependences (4) plotted for different temperatures make it possible to determine the T_c value from their deviation from a straight line on a log–log scale. Another advantage of the method is the absence of the critical slowing down because the spatial correlation radius remains small in the short-time segment even near the critical point [10].

We studied a cubic particle containing $L \times L \times L$ unit cells in each crystallographic direction with periodic boundary conditions. We considered a system with the linear size $L = 64$ containing $N = L^3 = 262144$ spins. This L value is chosen as the minimally necessary one in order to exclude the effect of the finite sizes on the result [3].

The calculations were carried out by the standard Metropolis Monte Carlo algorithm. The relaxation of the system occurred from the completely ordered low-temperature initial state with the starting magnetization $m_0 = 1$ during the time $t_{\max} = 10^3$, where one Monte Carlo step per spin was taken as the “time” unit. The relaxation dependences were calculated $n = 10^4$ times, and the resulting data were averaged.

The simulation was carried out for five temperatures near the phase transition point for each α value. These temperatures in units of the exchange integral k_bT/J_1 are given in Table 1. The T_3 value was chosen as close as possible to the T_c value. Thus, the simulation gave five time dependences of the magnetization (4)

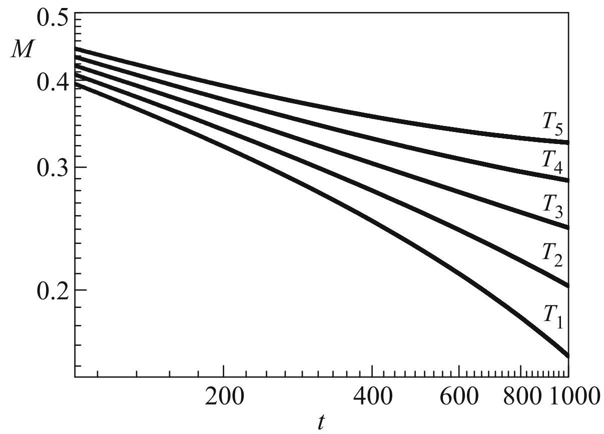

Fig. 1. Time dependence of the magnetization at five temperature values for the frustration parameter $\alpha = 0.15$. The temperature values are given in Table 1.

for each α value. Then, these dependences were interpolated for the entire temperature range from T_1 to T_5 with the step $\Delta T = 10^{-4}$ by the least squares method. The analysis of all curves (obtained by the direct calculation and interpolation) allowed us to determine the critical temperature with a high accuracy, since dependence (4) should be a straight line on a log–log scale at the phase transition point. The deviation from the straight line was determined by the least squares method. The temperature at which this deviation was minimal was taken as the critical value. Figure 1 shows a typical time dependence of the magnetization at different temperatures for the frustration parameter $\alpha = 0.15$ (hereinafter, all values are given in arbitrary units).

Similarly, the time dependence of the Binder cumulant (6) was calculated by interpolation for the found T_c value. The logarithmic derivative at the phase transition point was calculated by the least squares approximation over the five time dependences of the magnetization plotted for the temperatures indicated in Table 1.

The time dependences of the magnetization, its logarithmic derivative, and the Binder cumulant

Table 1. Temperature values for which the calculations were performed

α	T_1	T_2	T_3	T_4	T_5
0.001	4.490	4.495	4.500	4.505	4.510
0.05	3.895	3.900	3.905	3.910	3.915
0.10	3.276	3.281	3.286	3.291	3.296
0.15	2.630	2.635	2.640	2.645	2.650
0.20	1.945	1.950	1.955	1.960	1.965
0.24	1.329	1.334	1.339	1.344	1.349

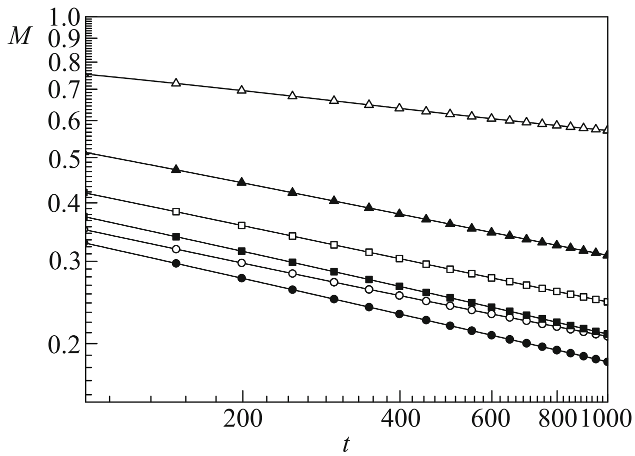

Fig. 2. Time dependence of the magnetization at the phase transition point for the frustration parameters α = (●) 0.001, (○) 0.05, (■) 0.10, (□) 0.15, (▲) 0.20, and (△) 0.24.

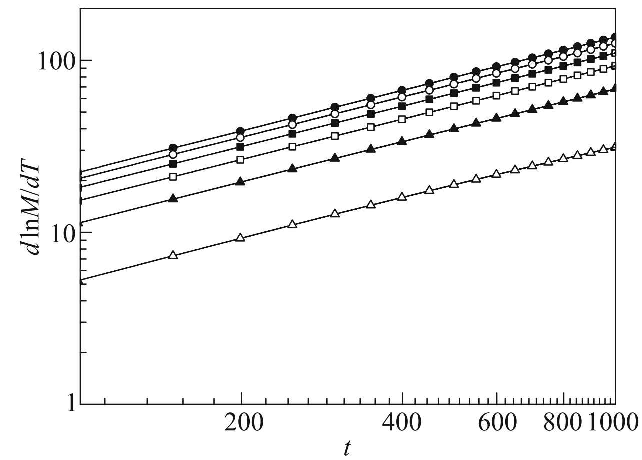

Fig. 3. Time dependence of the logarithmic derivative of the magnetization at the phase transition point for the frustration parameters α = (●) 0.001, (○) 0.05, (■) 0.10, (□) 0.15, (▲) 0.20, and (△) 0.24.

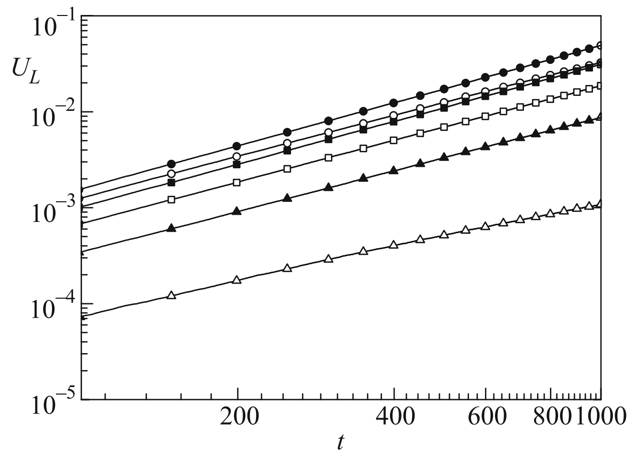

Fig. 4. Time dependence of the Binder cumulant at the phase transition point for the frustration parameters α = (●) 0.001, (○) 0.05, (■) 0.10, (□) 0.15, (▲) 0.20, and (△) 0.24.

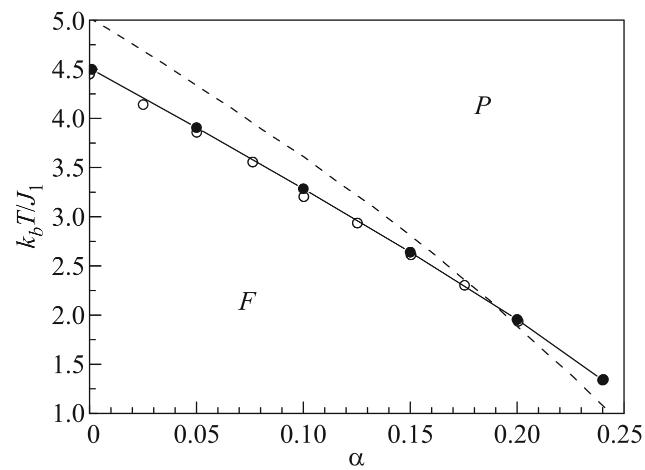

Fig. 5. Phase diagram of the Ising model with competing interactions including the (*F*) ferromagnetic and (*P*) paramagnetic phases according to (dashed line) [1], (○) [2], and (●) this work.

obtained at the critical point for different frustration parameters α are presented on a log–log scale in Figs. 2–4, respectively. We note that the numerical experiment was performed with the time step $\Delta t = 1$, but for clarity, the results in Figs. 2–4 are given with the time step $\Delta t = 50$.

The analysis of the final dependences (4)–(6) showed that the power-law scaling behavior of the studied system begins with a time of about $t = 100$. For this reason, the approximation of all curves was performed in the time interval $t = [100, 1000]$. As a result of the approximation, the critical exponents c_1, c_{l1}, and c_u were obtained for each α value, which, in turn, made it possible to calculate the critical exponents β, ν, and z. The critical exponents β, ν, and z found in this way, as well as the critical temperatures T_c, are given in Table 2.

It can be seen in Table 2 that the critical exponents are almost independent of the frustration parameter α in the range of $0.001 \le \alpha \le 0.15$. The exponents β and ν are close to the values for the classical three-dimensional Ising model [11], and the exponent z is close to that predicted theoretically for anisotropic magnets ($z = 2$, model *A* [6]). Further, the picture changes: the deviation of the critical exponents from the values characteristic of the range $0.001 \le \alpha \le 0.15$ increases with the frustration parameter α. Correspondingly, the exponents β, ν, and z near the frustration point no

Table 2. Critical exponents and critical temperatures

α	T_c	c_1	c_{l1}	c_u	β	ν	z
0.001	4.4990 (3)	0.244 (3)	0.779 (3)	1.43 (2)	0.313 (4)	0.61 (2)	2.10 (2)
0.05	3.9063 (3)	0.241 (3)	0.782 (3)	1.47 (2)	0.308 (4)	0.63 (2)	2.05 (2)
0.10	3.2849 (3)	0.238 (3)	0.777 (3)	1.41 (2)	0.306 (4)	0.60 (2)	2.13 (2)
0.15	2.6400 (3)	0.234 (3)	0.779 (3)	1.43 (2)	0.300 (4)	0.61 (2)	2.11 (2)
0.20	1.9548 (3)	0.219 (3)	0.771 (3)	1.37 (2)	0.284 (4)	0.59 (2)	2.20 (2)
0.24	1.3395 (3)	0.127 (3)	0.750 (3)	1.13 (2)	0.170 (4)	0.50 (2)	2.66 (2)

longer correspond to the classical three-dimensional Ising model.

In our opinion, this kind of critical behavior occurs because local fluctuations in the system near the frustration point $\alpha = 0.25$ increase with the competing interactions and begin to significantly affect the critical behavior of the model under study. This result somewhat contradicts the conclusions made in [2] that the static critical exponents along the entire line of second-order phase transitions between the ferromagnetic and paramagnetic phases correspond to the universality class of the three-dimensional classical Ising model.

Figure 5 shows the phase diagram of the Ising model with competing interactions in the range of $0.001 \leq \alpha \leq 0.24$. It can be seen that the values obtained in this work agree qualitatively well with the theoretical results obtained using the effective field theory [1] and quantitatively coincide with the results obtained by computational physics methods [2].

The results of our work demonstrate good agreement with the results of other authors, which indicates the efficiency of the application of the short-time dynamics method to the study of the critical properties of models with competing interactions. At the same time, the effect of frustrations on the character of the critical behavior along the line of phase transitions remains questionable, especially near the frustration point. Note that the dynamic critical exponents for this model are calculated for the first time.

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