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MAGNETISM

Critical Relaxation of a Three-Dimensional Fully Frustrated Ising Model

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Abstract—Critical relaxation from the low-temperature ordered state of the three-dimensional fully frustrated Ising model on a simple cubic lattice is studied by the short-time dynamics method. Cubic systems with periodic boundary conditions and linear sizes of $L = 32$, 64, 96, and 128 in each crystallographic direction are studied. Calculations were carried out by the Monte Carlo method using the standard Metropolis algorithm. The static critical exponents for the magnetization and correlation radius and the dynamic critical exponents are calculated.

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1. INTRODUCTION

The investigation of dynamic critical properties of spin systems is one of the topical problems of modern statistical physics and physics of phase transitions. To date, significant progress has been made in this area, mainly due to theoretical and experimental research. Nevertheless, the development of a rigorous and consistent theory of dynamic critical phenomena based on microscopic Hamiltonians is one of the central problems of the modern theory of phase transitions and critical phenomena, which is still far from being solved.

Recently, the method of short-time dynamics [1–5] has been successfully used to study the critical dynamics of the models of magnetic materials [1–5], in which the critical relaxation of a magnetic model from a nonequilibrium state to equilibrium is studied within the A model (the Halperin and Hohenberg classification of universality classes of the dynamic critical behavior [6]). Traditionally, it is believed that universal scaling behavior exists only in thermodynamic equilibrium. However, it was shown that the universal scaling behavior for some dynamic systems can be realized at the early stages of their evolution from a high-temperature disordered state to a state corresponding to the phase transition temperature [7]. This behavior is realized after a certain time, which is sufficiently large in the microscopic sense but remains small in the macroscopic sense. A similar picture is observed in the case of the evolution of a system from the low-temperature ordered state [1, 2].

Earlier, we studied the critical relaxation from the low-temperature ordered state of a three-dimensional fully frustrated Ising model on a simple cubic lattice for a linear dimension of $L = 64$ [8]. In this paper, we estimate the critical relaxation of this model for the linear dimensions of $L = 32$, 64, 96, and 128 in order to estimate the influence of system sizes on the result obtained. In addition, we improved the statistics of calculations and modified the method for determining the critical temperature. This allowed us to increase the accuracy of determining the critical temperatures and critical exponents.

2. METHOD OF STUDY

Using the renormalization group method, the authors of [7] showed that, far from the equilibrium point, after a microscopically small time, for the kth moment of magnetization, the scaling form

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

is realized, where $M^{(k)}$ is the kth moment of magnetization, t is the time, τ is the reduced temperature, L is the linear size of the system, b is the scale factor, β and ν are the static critical exponents for the magnetization and correlation radius, z is the dynamic critical exponent, and x_0 is a new independent critical exponent that determines the scaling dimension of the initial magnetization m_0.

For systems with sufficiently large linear sizes L, starting from the low-temperature ordered state ($m_0 = 1$) at the critical point ($\tau = 0$), the theory predicts (setting $b = t^{1/z}$ in Eq. (1)) a power-law behavior of the magnetization in the short-time mode:

$$M(t) \sim t^{-c_1}, \quad c_1 = \frac{\beta}{\nu z}. \tag{2}$$

Logarithmizing both sides of Eq. (2) and taking the derivatives with respect to τ at $\tau = 0$, we obtain a power law for the logarithmic derivative:

$$\partial_\tau \ln M(t,\tau)|_{\tau=0} \sim t^{-c_{l_1}}, \quad c_{l_1} = \frac{1}{\nu z}. \tag{3}$$

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

$$U_L(t) = \frac{M^{(2)}}{(M)^2} - 1 \sim t^{c_U}, \quad c_U = \frac{d}{z}, \tag{4}$$

where d is the dimension of the system.

Thus, in one numerical experiment, the short-time dynamics method allows one, using relationships (2)–(4), to determine the three critical exponents β, ν, and z. In addition, dependences (2) constructed for different temperatures allow one to determine the value of T_c from their deviation from a straight line in the log–log scale.

3. THE MODEL

Using the given method, we studied the critical relaxation from the low-temperature ordered state of a three-dimensional fully frustrated Ising model on a simple cubic lattice. This model was first proposed by Villain [9] in the two-dimensional case on a square lattice for describing spin glasses. Later it was generalized by Blankschtein [10] to the three-dimensional case. The model is shown schematically in Fig. 1.

Interest in this model is due to the fact that the study of frustrated systems focuses on models on triangular and hexagonal lattices, while the properties of models on a cubic lattice have been studied little. In particular, the dynamic critical behavior of these systems has not been studied at all.

The Hamiltonian of the frustrated Ising model can be represented in the form

$$H = -\frac{1}{2}\sum_{\langle i,k\rangle} J_{ik} S_i S_k, \quad S_i = \pm 1, \tag{5}$$

where S_i is the Ising spin at the ith lattice site, J_{ik} is the exchange interaction between spins for ferromagnetic ($J > 0$) and antiferromagnetic ($J < 0$) coupling. Frustrations in this model are caused by the competition of exchange interactions [9].

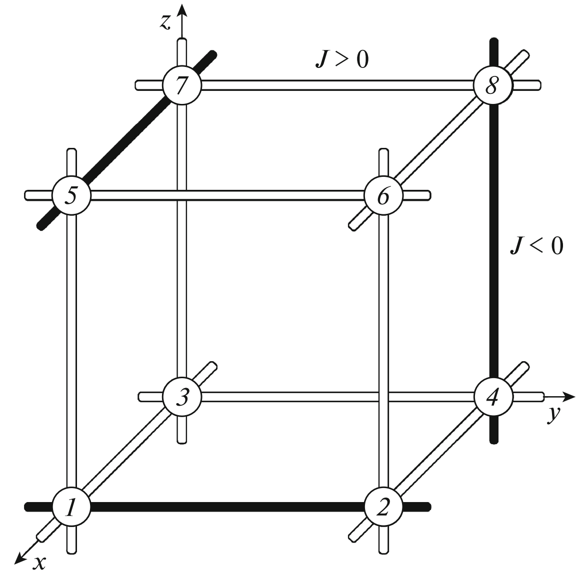

Fig. 1. Fully frustrated Ising model on a simple cubic lattice. White color indicates ferromagnetic coupling ($J > 0$), and black color, antiferromagnetic ($J < 0$).

4. RESULTS

We studied cubic systems with periodic boundary conditions containing $L \times L \times L$ unit cells. The calculations were performed for systems with linear sizes $L = 32$, 64, 96, and 128, respectively, containing $N =$ 32768, 262144, 884736, and 20977152 spins by the Monte Carlo method using the standard Metropolis algorithm. The relaxation of the system started from the initial low-temperature fully ordered state with the initial magnetization $m_0 = 1$ and lasted for a time $t_{\max} =$ 1000, where the unit of "time" is one step of the Monte Carlo method per spin. The relaxation dependences for each temperature were calculated n times, and the obtained data were averaged. The number n depended on the size of the system and was taken equal to $n = 10^5$ for $L = 32$ and 64, $n = 8 \times 10^4$ for $L =$ 96, and $n = 7 \times 10^4$ for $L = 128$. It should be noted that, in [8], we used $n = 5 \times 10^4$ for a linear size $L = 64$.

For each linear size, the calculations were carried out at five values of temperature in the vicinity of the phase transition point. These values in units of the exchange integral $k_bT/|J|$ are given in Table 1. The

Table 1. Temperatures at which the calculations were performed

L	T_1	T_2	T_3	T_4	T_5
32	1.3387	1.3437	1.3487	1.3537	1.3587
64	1.3387	1.3437	1.3487	1.3537	1.3587
96	1.3389	1.3439	1.3489	1.3539	1.3589
128	1.3387	1.3437	1.3487	1.3537	1.3587

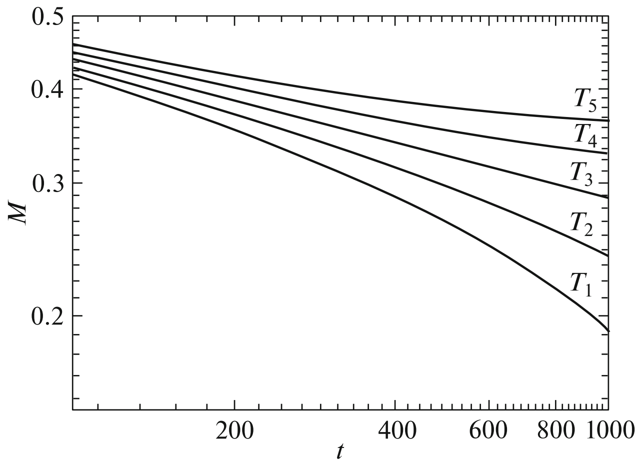

Fig. 2. Time dependence of magnetization at five temperatures for a linear sizes of L = 64. The temperatures are given in Table 1.

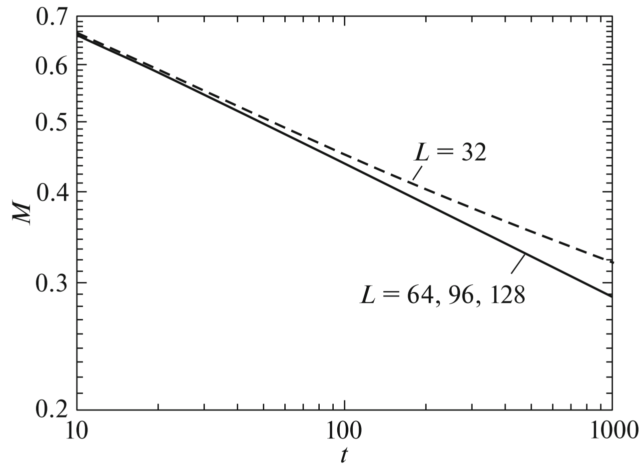

Fig. 3. Time dependence of magnetization at the phase transition point for all linear sizes L.

value of T_3 was chosen as close as possible to T_c. From the results obtained, dependences (2), (3), and (4) were approximated by least squares in the temperature interval from T_1 to T_5 with a step $\Delta T = 10^{-5}$.

The critical temperature was determined from the time dependence of the magnetization (2), which, at the phase transition point, must be a straight line in the log–log scale. The deviation from the straight line was determined by the method of least squares. The critical temperature was the temperature at which this deviation was minimal. Figure 2 shows a typical time dependence of the magnetization at different temperatures (hereinafter, all values are given in arbitrary units). The critical temperatures found in this way for all linear sizes are given in Table 2.

In [8], we analyzed the temperature curves of the magnetization with a step $\Delta T = 10^{-4}$ near the phase transition point, after which we performed direct calculations at the critical temperature found. The modification in the procedure of determining the critical temperature in this work made it possible to increase the accuracy of our calculations.

The obtained time dependences of the magnetization, its logarithmic derivative, and the Binder cumulant at the critical point in the time interval t = [10; 1000] are presented in the log–log scale in Figs. 3, 4, and 5, respectively. The solid lines represent the results for the linear sizes L = 64, 96, and 128. The dashed lines represent the results for the linear size L = 32.

As can be seen from Figs. 3 and 4, the graphs for L = 64, 96, and 128 practically coincide with each other. In particular, the difference in the values of M at each instant of time t for each of these sizes L is on the order of 10^{-3}. However, the dependences for L = 32 are significantly different and their behavior significantly deviates from the scaling behavior for the times $t \ll 1000$. As a result, the graphs for L = 32 in the log–log scale are not straight lines even at the phase transition point.

The situation with the time dependence of the Binder cumulant is slightly different. Since the value of the cumulant is small, the difference in the dependences for different linear sizes is manifested rather well. The approximation lines plotted by formula (4) for L = 64, 96, and 128 do not coincide but have almost the same slope angle. For L = 32, as in the case of Figs. 3 and 4, the scaling behavior is not realized and its graph is not a straight line in the log–log scale.

Analysis of the graphs showed that the power scaling behavior of the system with the linear sizes of L = 64, 96, and 128 is realized starting from the time about t = 150. Therefore, all the curves were approximated in the time interval t = [200; 1000]. The logarithmic derivative at the phase transition point was calculated by the least squares approximation over the five time

Table 2. Critical exponents and critical temperatures

L	T_c	c_1	c_{l1}	c_U	β	ν	z
32	1.34362(2)	0.142(3)	0.702(3)	1.186(7)	0.202(4)	0.563(4)	2.530(7)
64	1.34872(3)	0.184(3)	0.839(3)	1.343(7)	0.220(4)	0.534(4)	2.234(7)
96	1.34870(3)	0.183(3)	0.839(3)	1.345(7)	0.218(4)	0.534(4)	2.230(7)
128	1.34873(3)	0.183(3)	0.839(3)	1.344(7)	0.218(4)	0.534(4)	2.232(7)

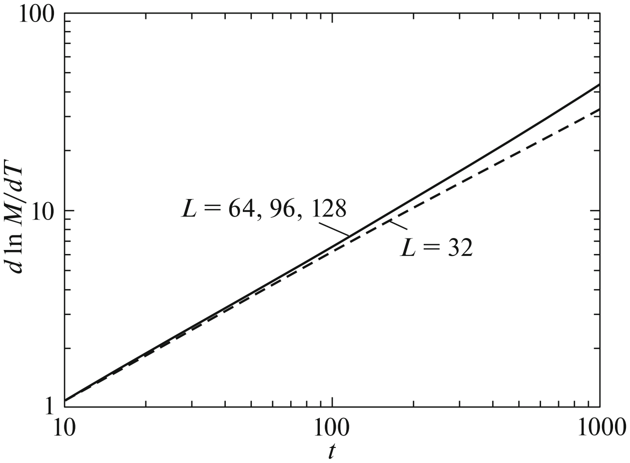

Fig. 4. Time dependence of the derivative of the logarithm of magnetization at the phase transition point for all linear sizes L.

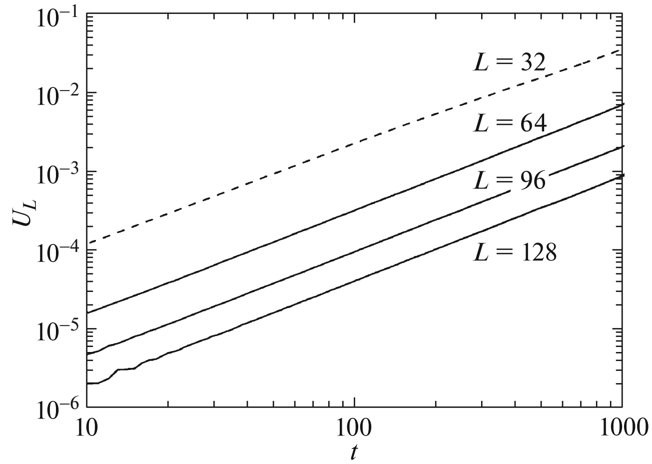

Fig. 5. Time dependence of Binder cumulant at the phase transition point for all linear sizes L.

dependences of the magnetization constructed for the temperatures presented in Table 1. We note that, in [8], the logarithmic derivative was calculated using three dependences of the magnetization on time.

As a result of the least squares approximation of the obtained data in the time interval t = [200; 1000], the exponents c_1, c_{l1}, and c_U were calculated by formulas (2)–(4). This made it possible to calculate the static critical exponents for β, the static critical exponents for the correlation radius ν, and the dynamic critical exponents for z. All our results are presented in Table 2.

As can be seen from Table 2, the values of critical exponents and critical temperatures for the linear sizes $L = 64$, 96, and 128 are equal within the error and the values for $L = 32$ are significantly different from them. Strictly speaking, it is not entirely correct to speak about critical exponents for $L = 32$, since the scaling behavior is not fully realized for this size.

Due to the strong influence of the size effects, it is impossible to accurately determine the critical temperature and critical exponents for $L = 32$. Therefore, the results for this system should be excluded from consideration. In this case, for the systems with the linear sizes of $L = 64$, 96, and 128, no appreciable influence of the size effects on the result is observed.

Table 3 presents the literature data on the static critical properties of the model under consideration [11–13]. Comparison of Tables 2 and 3 shows that our results for the linear dimensions $L = 64$, 96, and 128 are in a good agreement with the results of these works. The dynamic critical exponent for the fully frustrated Ising model was obtained in this work for the first time and is close to the theoretically predicted value for anisotropic magnets ($z = 2$, model A [6]). The difference from $z = 2$ can be explained by the influence of frustrations, but a definitive answer to this question requires further studies of the critical dynamics of frustrated systems.

Table 3. Literature data

Parameter	[11]	[12]	[13]
T_c	1.344(2)	1.355(2)	1.347(1)
β	0.21(2)	–	0.25(2)
ν	0.55(2)	0.55(2)	0.56(2)

5. CONCLUSIONS

The results of the work demonstrate the efficiency of applying the short-time dynamics method to the study of the critical properties of three-dimensional models with frustration. The advantage of this method is that it allows one to obtain in one numerical experiment not only the dynamic critical exponent but also the static critical exponents and the critical temperature. In addition, this approach does not exhibit critical slowing down, since the spatial correlation radius remains small in the short-time interval even near the critical point [7]. It has been shown that, for a fully frustrated Ising model with a linear size of $L = 64$ and more, there is no influence of finite sizes on the result obtained.

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