Monte Carlo renormalization group of dilute 3D Ising dynamics

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Abstract. Simulation of critical relaxation of the magnetization in a three-dimensional Ising model diluted by quenched nonmagnetic impurity atoms is carried out. The cubic systems with linear size $L = 144$ and spin concentrations $p = 0.95, 0.8, 0.6$, and 0.5 are studied. The dynamical critical exponent z is determined by the Monte Carlo method combined with the dynamical renormalization group method. The obtained results are: z(p): $z(0.95) = 2.19 \pm 0.07$, $z(0.8) = 2.29 \pm 0.06$, $z(0.6) = 2.72 \pm 0.08$, and $z(0.5) = 2.75 \pm 0.08$.

1. Introduction

The investigation of critical behavior of disordered systems remains one of the main problems in condensed-matter physics and excites a great interest because all real solids contain structural defects [1, 2]. The structural disorder breaks the translational symmetry of the crystal and thus greatly complicates the theoretical description of the material. The influence of disorder is particularly important near the critical point where behavior of a system is characterized by anomalous large response on any even weak perturbation. The description of such systems requires the development of special analytical and numerical methods. The effects produced by weak quenched disorder on critical phenomena have been studied for many years [3–8]. According to the Harris criterion [3], the disorder affects the critical behavior only if $\alpha > 0$, the specific-heat exponent of the pure system, is positive. In this case, a new universal critical behavior, with new critical exponents, is established. In contrast, when $\alpha < 0$, the disorder appears to be irrelevant for the critical behavior. Only systems whose effective Hamiltonian near the critical point is isomorphic to the Ising model satisfy this criterion.A large number of publications is devoted to the study of the critical behavior of diluted Ising-like magnets by the renormalization-group (RG) methods, the numerical Monte-Carlo methods, and experimentally (for a review, see [2, 9–11]). The ideas about replica symmetry breaking in the systems with quenched disorder were presented in Refs. [12, 13]. A refined RG analysis of the problem has shown the stability of the critical behavior of weakly disordered three dimensional systems with respect to the replica symmetry breaking effects [14]. All obtained results confirm the existence of a new universal class of the critical behavior, which is formed by diluted Ising-like systems. However, it remains unclear whether the asymptotic values of critical exponents are independent of the rate of dilution of the system, how the crossover effects change these values, and whether two or more regimes of the critical behavior exist for weakly and strongly disordered systems. These questions are the subjects of heated discussions [2, 15] and extensive Monte Carlo simulations for site-diluted [16–18] and bond-diluted [19, 20] three-dimensional Ising models.

At present paper, a computer simulations of the critical dynamics of the diluted 3D Ising model by the Monte-Carlo method are considered for samples with spin concentrations $p = 0.95, 0.8, 0.6$, and 0.5. There is reason to believe that the influence of quenched impurities on the critical dynamics will be seen more clearly than in the equilibrium state, because of the specific conservation laws.

2. DESCRIPTION OF THE MODEL AND METHODS

We have considered the following Hamiltonian for the 3D site-diluted ferromagnetic Ising model defined in a cubic lattice of linear size L with periodic boundary conditions

$$H = -J \sum_{i,j} S_i S_j p_i p_j, \tag{1}$$

where the sum is extended to the nearest neighbors, $J > 0$ is the short-range exchange interaction between spins S_i fixed at the lattice sites, and assuming values of ± 1. Nonmagnetic impurity atoms form empty sites. In this case, occupation numbers p_i assume the value 0 or 1 and are described by the distribution function

$$P(p_i) = (1 - p)\delta(p_i) + p\delta(1 - p_i) \tag{2}$$

with $p = 1 - c$, where c is the concentration of the impurity atoms. In this paper, we have investigated systems with the spin concentrations $p = 0.95, 0.8, 0.6$, and 0.5. We have considered the cubic lattices with linear size $L = 144$. The Metropolis algorithm has been used in simulations. We consider only the dynamic evolution of systems described by the model A in the classification of Hohenberg and Halperin [21]. Ising-model dynamics is customarily described by the conditional probability function $P_s(t) \equiv P(\{S\}, t)$, which satisfied the Glauber's kinetic equation

$$\frac{dP_s}{dt} = -P_s(t) \sum_{s'} W(S \rightarrow S') + \sum_{s'} W(S' \rightarrow S)P_{s'}(t), \tag{3}$$

where $W(S \rightarrow S')$ is the transition rate from a microscopic state given by the spin configuration $\{S\}$ to a state with the configuration $\{S'\}$. In order that the Markov process described by Eq. (2) converge to the equilibrium state of a Gibbs ensemble with $P_s = \exp(-E_s/kT)$, the detailed-balancing condition $W(S \rightarrow S')P_s = W(S' \rightarrow S)P_s$ is sufficient but not necessary. This freedom of choice gives $W(S-> S')$ which is not determined uniquely. The function W is usually chosen in the form of the Metropolis's function

$$W(S \rightarrow S') = \begin{cases} \exp(-\triangle E_{ss'}/kT), & \triangle E_{ss'} > 0 \\ 1, & \triangle E_{ss'} \leq 0 \end{cases} \tag{4}$$

or the Glauber's function

$$W(S \rightarrow S') = \exp(-\triangle E_{ss'}/kT)/[1 + \exp(-\triangle E_{ss'}/kT], \tag{5}$$

where $E_{ss'} = E_{s'} - E_s$.

The relation $< A(t) >= \sum_s A_s P_s(t)$ determines the dynamical evolution of the quantity A_s, by means of the function $P_s(t)$ which is the solution of Eq.(3). Metropolis's algorithm, which consists of choosing randomly the spin S_i, and flipping the spin with probability determined by the function W in Eq.(4), makes is possible to implement directly the Ising-model dynamics with relaxation of the magnetization $m_b(t) = \sum_i^N S_i/N$ to the equilibrium value determined by the thermostat temperature T. The time scale t can be associated with the scale $\{S\}$ of successive configurations, assuming that N system sites are chosen randomly per unit time. One time unit

corresponds to one Monte Carlo step per spin. In simulation of the critical dynamics the initial state of the system is chosen when all spins are parallel ($m_b = 1$) and the temperature of the system is equal to the critical temperature. The critical temperature T_c for dilute magnetic materials is a function of the impurity concentration c_{imp} decreasing with increasing c_{imp} and vanishing at the threshold concentration $c_{imp} = 1 - p_c$. For a cubic lattice of Ising spins $p_c \simeq 0.31$ and $T_c(p)$ are equal to: $T_c(0.95) \simeq 4.26267$, $T_c(0.8) \simeq 3.49948$, $T_c(0.6) \simeq 2.42413$, and $T_c(0.5) \simeq 1.84509$ [17] in the units J/k. We have used here the Monte Carlo method combined with the dynamical renormalization group method [22], to determine the dynamic exponent z characterizing the critical increase in the relaxation time of the system $t_{rel} \sim |T - T_c|^{-z\nu}$. For this, the system was partitioned into blocks, where a block b^d of neighboring spins was replaced by a single spin whose direction is determined by the direction of most spins in the block. The redefined spin system forms a new lattice with magnetization m_b. Let the magnetization of the initial lattice relax to some m_1 over a time t_1, and let the redefined system reach the same value m_1 over the time t_b. Then by using two systems with block size b and b' and determining the relaxation times t_b and $t_{b'}$ of the block magnetizations m_b and $m_{b'}$ to the same value m_1, the dynamic exponent z can be determined from the relation

$$t_b/t_{b'} = (b/b')^z \qquad (6)$$

or

$$z = \ln(t_b/t_{b'})/\ln(b/b') \qquad (7)$$

in the limit of sufficiently large b and $b' \to \infty$.

3. MEASUREMENTS OF THE DYNAMICAL CRITICAL EXPONENT z FOR 3D SITE-DILUTED ISING MODEL

We applied this algorithm to dilute systems with linear size $L = 144$ and spin concentrations presented above. The size of the system made it possible to partition it into blocks with sizes $b = 2, 3, 4, 6, 8, 9, 12, 16, 18, 24, 36, 48$, and 72. The procedure of block partitioning of the initial spin and impurity configurations was implemented on the basis of the criterion of spin connectivity. Thus a b^d-dimensional block was considered to be a spin block and replaced by an effective spin oriented in a direction determined by the direction of most spins in the block if the block contained a spin cluster connecting both opposite faces of the block. Otherwise, the block was considered to be an impurity block and replaced by an empty site in the renormalized lattice. A relaxation simulating procedure consisting of 10000 Monte Carlo steps per spin was performed for each system with 1000 runs with different impurity configurations over which the function $m_b(t)$ was averaged.

We demonstrate in fig.1 a)-d) the plots of the initial and renormalized magnetizations $m(t)$, as functions of time, for systems with spin concentrations $p = 0.95, 0.8, 0.6$, and 0.5 averaged over different impurity configurations. The relation (7) can be employed in order to determine the values of the exponent z independently. However, the power-law character found for the relaxation of the magnetization at the critical temperature enabled us to employ, in contrast to [22] and [23], a different and, we believe, better-founded procedure for processing the curves for the renormalized magnetizations $m_b(t)$, as in our paper [24]. Thus the $m_b(t)$ curves plotted in a double logarithmic scale were approximated by the straight lines $\lg m_b = k_b \lg t + n_b$, by the least squares method in intervals $\triangle m_b$, corresponding best to a power-law variation of $m_b(t)$. Then, the coefficients k_b were averaged and the average value k_{av} gives possibility to determine the parameters n_b of the straight lines $\lg m_b = k_{av} \lg t + n_b$ by extending the lines through the point of intersection with $\lg m_b = k_b \lg t + n_b$ at the center of the intervals $\triangle m_b$. As a result, the formula (7) for z becomes as

$$z = (\bar{n}_{b'} - \bar{n}_b)/[k_{av} \lg(b/b')] \qquad (8)$$
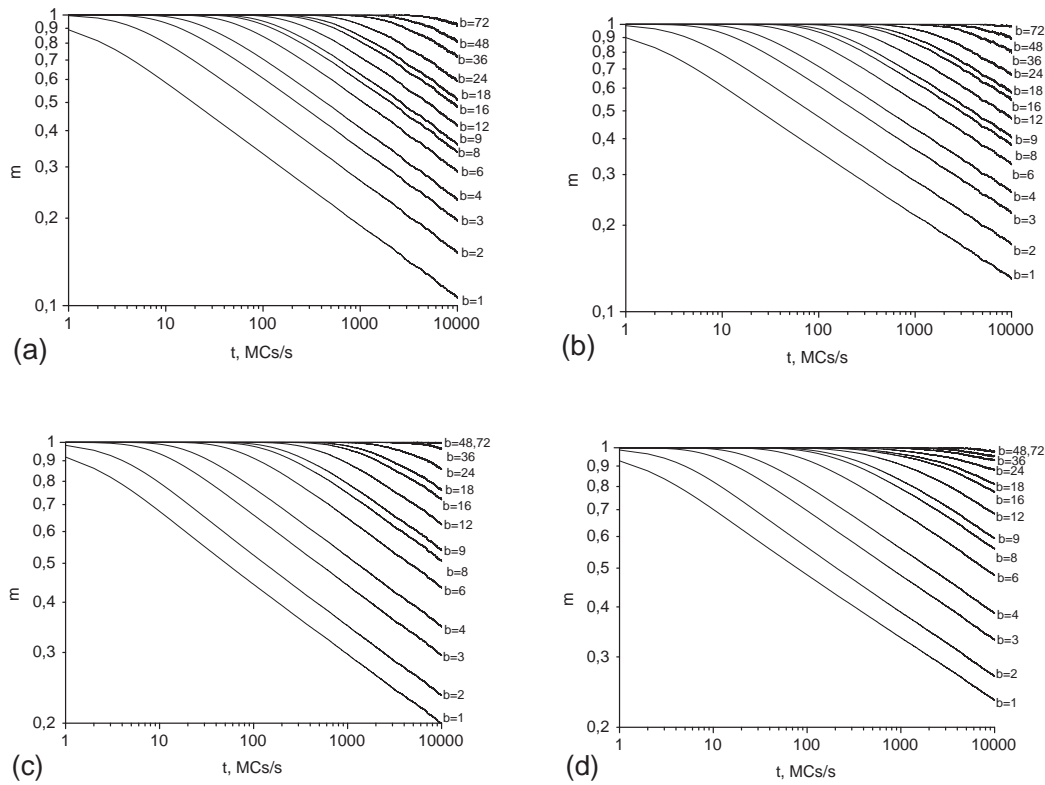
Figure 1. Initial m_1 and renormalized m_b magnetizations as functions of time for the dilute Ising model with spin concentrations $p = 0.95$ (a), 0.8 (b), 0.6 (c), 0.5 (d)

Table 1. Values of the dynamic exponent z for systems with different spin concentrations p

b	$p = 0.5$	$p = 0.6$	$p = 0.8$	$p = 0.95$
8	2.638(50)	2.554(45)	2.283(35)	2.246(25)
9	2.659(50)	2.571(50)	2.285(35)	2.240(30)
12	2.689(60)	2.604(60)	2.287(40)	2.226(30)
16	2.699(60)	2.636(60)	2.288(40)	2.213(35)
18	2.690(65)	2.655(65)	2.290(45)	2.210(35)

Sets of values of the exponent z corresponding to different values of b with $b' = 1$ were obtained using the relation (8) (Table 1). For impurity systems the renormalization-group-transformation procedure reaches the proven asymptote of m_b, as a function of the block-partition parameter b, at larger values of b than in the case of a pure system. So, for blocks with small values b the presence of defects leeds both to loss of some initial paths of spin connectivity and appearance of a new paths of spin connectivity which are absent in the original lattice. This effect becomes less likely with increasing b. On the other hand, the changes of the renormalized magnetization m_b are decreased with time for large values of b and an errors for m_b and therefore for the determination of z are increased. For this reason, we selected for the analysis the values of the exponent z corresponding to $b = 8, 9, 12, 16$, and 18.
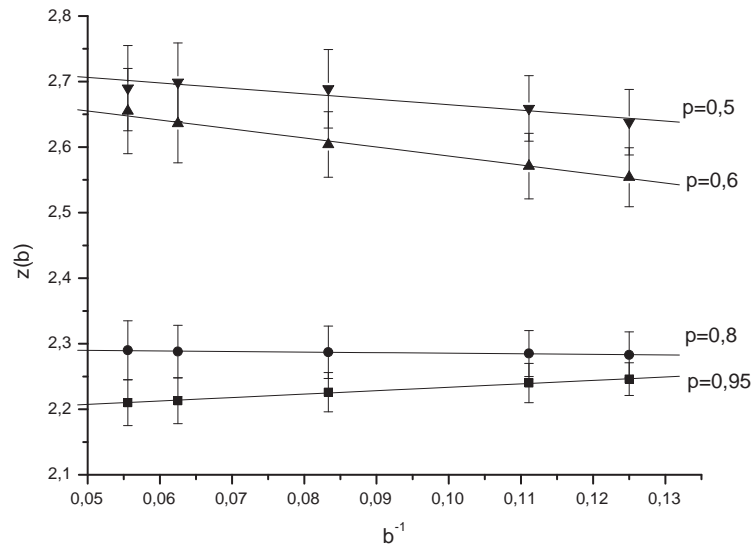
Figure 2. Dependence of dynamic exponent z on b for different spin concentrations p

The obtained dependence of z on b (fig. 2) made possible to realize the typical extrapolation for renormalization-group transformation to the case $b \to \infty$, assuming in concordance with [23] that

$$z_b = z_{b=\infty} + const \cdot b^{-1}. \tag{9}$$

The following results were obtained for considered impurity systems: $z(0.95) = 2.19 \pm 0.05, z(0.8) = 2.29 \pm 0.06, z(0.6) = 2.72 \pm 0.08$, and $z(0.5) = 2.75 \pm 0.08$. Hence it is clear that the value of the dynamical exponent z for $p = 0.6$ is virtually identical to the value for $p = 0.5$, while for $p = 0.95$ and 0.8 they are in agreement with each other only to within the statistical uncertainties in their values.

4. ANALYSIS OF RESULTS AND CONCLUSIONS

We now compare the simulation results with other results of Monte Carlo simulations (MC), application of field-theoretical method with fixed-dimension $d = 3$ expansion (FTM), and experimental (EXP) investigations (Table 2). Values of z from paper [27] with EXP results agree rather well with our results only for weakly diluted systems with $p = 0.95$, while a noticeable difference of the results is observed for strongly disordered systems. Starting from the universality concept for critical behavior of diluted Ising systems and that the asymptotic value of z is independent of the dilution degree, the author in [28] obtained the asymptotic value $z = 2.41$ using the effective values of the exponent listed in Table II. The off-equilibrium critical dynamics of the 3D Ising model with the spin concentration varying in a wide range was analyzed in [29]. Assuming that $\gamma/(\nu z)$ and ω/z exponents are dilution independent, the authors obtained the asymptotic value of $z = 2.62(7)$ taking into account the leading corrections to the scaling dependence for the dynamical susceptibility. In this case, the value of the exponent $\omega = 0.50(13)$ obtained in [29] is strongly inconsistent with $\omega = 0.25(10)$ from the field theory calculations [31] and not so well agreement with $\omega = 0.37(6)$ from Monte Carlo results computed in [16]. In addition, so small errors for the dynamical critical exponent $z = 2.62(7)$ couldn't explain given by authors so large errors for non-universal parameters $A(p)$ and $B(p)$ for strongly diluted samples

Table 2. Values of the obtained critical exponent z and comparison to other results of Monte Carlo simulations (MC), field-theoretical method with fixed-dimension $d = 3$ expansion (FTM), and experimental (EXP) investigations

	0.5	0.6	0.8	0.95
Rosov et al., 1992 [27] EXP			2.18(10)	
Prudnikov et al.., 1992 [24] MC	2.65(12)	2.58(9)	2.20(7)	2.19(7)
Heuer, 1993 [28] MC		2.93(3)	2.38(1)	2.16(1)
Parisi et. al., 1999 [29] MC	2.62(7)	2.62(7)	2.62(7)	2.62(7)
Hasenbusch et. al., 2007 [30] MC		2.35(2)	2.35(2)	
Prudnikov et al., 1992 [25] FTM			2.237(34)	
Prudnikov et al., 2006 [26] FTM			2.1792(13)	
Prudnikov et al., 2010 [18] MC			2.208(22)	2.185(17)
present paper	2.75(8)	2.72(8)	2.29(6)	2.19(5)

in comparison with lightly diluted samples. It must be inversely from physics of phenomenon. In [30] the purely relaxational dynamics (model A) at criticality in three-dimensional disordered Ising systems whose static critical behaviour belongs to the randomly diluted Ising universality class was studied. Authors considered the site-diluted and bond-diluted Ising models, and the $\pm$J Ising model along the paramagnetic-ferromagnetic transition line. They performed Monte Carlo simulations at the critical point using the Metropolis algorithm and studied the dynamic behaviour in equilibrium at various values of the disorder parameter. The results provide an evidence of the existence of a unique model-A dynamic universality class which describes the relaxational critical dynamics in all considered models. In particular, the analysis of the size dependence of suitably defined autocorrelation times at the critical point provides the estimate $z = 2.35(2)$ for the universal dynamic critical exponent. Authors also study in [30] the off-equilibrium relaxational dynamics following a quench from $T = \infty$ to T_c. In agreement with the field-theory scenario, the analysis of the off-equilibrium dynamic critical behaviour gave an estimate of z that is consistent with the equilibrium estimate $z = 2.35(2)$.

In [25] we gave a field-theoretical description of the critical dynamics of dilute magnetic materials directly for the three-dimensional case. In the two-loop approximation, using the Pade-Borel summation technique, we obtained the critical exponent $z(p) = 2.237$, valid for impurity concentrations much less than the spin-percolation threshold. A similar calculation performed in the three-loop approximation for diluted Ising system [26] with the use of different methods of summation gave the value $z = 2.1792(13)$. The comparison of these FTM results with our present MC results and results in [18,24] shows that they are in good agreement for weakly diluted systems with $p = 0.95$ and 0.8 and with experimental value of $z = 2.18(10)$ obtained in [27] under investigations of the dynamic critical behavior of weakly diluted Ising-like magnet $Fe_pZn_{1-p}F_2$ with $p = 0.9$. The simulation results give a much higher values of the dynamic exponent z for spin concentrations $p = 0.6$ and 0.5. We attribute this to the fact that for a cubic lattice of Ising spins with $p \leq p_c^{(imp)} \simeq 0.69$ the impurities form a connecting cluster, which for $T < T_c$, coexists with a connecting spin cluster right up to the spin percolation $p_c = 1 - p_c^{(imp)}$. As a result, the spin correlation length in the region $p_c \leq p \leq p_c^{(imp)}$ is not the only scale determining the behavior of the system near the critical temperature $T_c(p)$). The character of impurity scattering of long-wavelength fluctuations of the magnetization also changes. By analogy with [32,33] and the works of one of us, [34,35], where the influence of the correlation of the impurities and extended structural defects on the critical properties of disordered systems

was investigated, there are grounds for believing that in the region $p_c \leq p \leq p_c^{(imp)}$ the existence of an extended impurity structure results in a change in the Harris criterion for the effect of quenched point defects. For this reason, the change in sign of the heat-capacity exponent α (from positive to negative) at a transition from pure to impurity critical behavior in Ising-like magnetic materials does not limit the new type of critical behavior determined by extended impurity structure.

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