Short-time dynamics and critical behavior of three-dimensional site-diluted Ising model

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Monte Carlo simulations of the short-time dynamic behavior are reported for three-dimensional weakly site-diluted Ising model with spin concentrations \( p = 0.95 \) and 0.8 at criticality. In contrast to studies of the critical behavior of the pure systems by the short-time dynamics method, our investigations of site-diluted Ising model have revealed three stages of the dynamic evolution characterizing a crossover phenomenon from the critical behavior typical for the pure systems to behavior determined by the influence of disorder. The static and dynamic critical exponents are determined with the use of the corrections to scaling for systems starting separately from ordered and disordered initial states. The obtained values of the exponents demonstrate a universal behavior of weakly site-diluted Ising model in the critical region. The values of the exponents are compared to results of numerical simulations which have been obtained in various works and, also, with results of the renormalization-group description of this model.

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I. 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 \( \alpha \), 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 Refs. \(^2,3,10,11\)). 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 \(^2,15\).

For critical dynamic systems, traditionally it is believed that universal scaling behavior is realized in the long-time regime of dynamic evolution. However, at first in the paper \(^10\), it was shown that systems, starting from macroscopic non-equilibrium initial states, demonstrate a universal scaling behavior on the macroscopic short-time stages of their dynamic process which is characterized by initial slip exponents \( \theta \) and \( \theta' \) for the response functions \( G(r, t, t') \) and the order parameter \( m(t) \) (magnetization for ferromagnetic systems)

\[
G(r, t, t') \sim (t/t')^\theta, \quad m(t) \sim t'^\theta. \tag{1}
\]

A remarkable property of this relaxation process is the increase of magnetization \( m(t) \) from a non-zero initial magnetization \( m_0 \ll 1 \) at short times \( t < t_{\text{cr}} \sim m_0^{-1/(\theta'+\beta/z\nu)} \). The initial rise of magnetization is changed to the well known decay \( m(t) \sim t^{-\beta/z\nu} \) for \( t > t_{\text{cr}} \). The critical exponents \( \theta \) and \( \theta' \) depend on the dynamic universality class \(^17\) and have been calculated by the RG method for a number of dynamic models \(^18\) such as the model with a non-conserved order parameter \(^16,19\) (model A), the model with an order parameter coupled to a conserved density \(^20\) (model C), and the models with reversible mode coupling \(^21\) (models E, F, G, and J). The universal scaling behavior of the initial stage of the critical relaxation for pure systems has been verified by extensive numerical simulations \(^22–26\). The developed method in these papers of short-time
critical dynamics gives the possibility to determine both the static critical exponents $\nu$, $\beta$, and dynamic critical exponents $\zeta$ and $\theta'$ in the macroscopic short-time regime of the critical relaxation. However, a number of publications devoted to the numerical study of disorder influence on non-equilibrium critical relaxation by the short-time dynamic method is surprisingly little. We know the papers [26–28] in which the non-equilibrium critical exponents $\zeta$ and $\theta'$ in the three-dimensional (3D) site-diluted Ising ferromagnets with quenched point-like defects is investigated and the values of the initial slip exponent $\theta'$ and an exponent $C_\alpha$ for autocorrelation function [28] are determined for systems with different spin concentrations. The obtained universal value $\theta' = 0.10(2)$ is in good agreement, as it is insisted in [27], with the RG estimate in Ref. [29] with the use of $\varepsilon$-expansion method, where $\varepsilon = 4 - d$, $d$ is the spatial dimension. However, some assumptions introduced during investigations in Ref. [27] and discussed below preclude from consenting to this value $\theta' = 0.10(2)$ as confirmation of the RG estimate validity. In our paper [31] the integrated Monte Carlo simulations of the short-time dynamic behavior are reported for 3D Ising and XY models with long-range correlated disorder at criticality, in the case corresponding to linear defects. Both static and dynamic critical exponents are determined for systems starting separately from ordered and disordered initial states. The obtained values of the exponents are in good agreement with results of the field-theoretic description of the critical behavior of these models in the two-loop approximation [30].

In the present paper, we numerically investigate the short-time critical dynamics with a non-conserved order parameter (model A) [17] in the 3D site-diluted Ising systems with spin concentrations $p = 0.95$ and 0.8. In the following section, we introduce the 3D Ising model with quenched point-like defects and scaling relations for the short-time critical dynamics. In Sec. III, we derive the critical short-time dynamics in Ising systems starting separately from ordered and disordered initial states. Critical exponents obtained under these two conditions with the use of the corrections to scaling are compared. The obtained universal value $\theta' = 0.10(2)$ is in good agreement with the results of other investigations and our conclusions.

II. DESCRIPTION OF THE MODEL AND METHODS

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

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

(2)

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 $\pm 1$. 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

$$P(p_i) = (1 - p)\delta(p_i) + p\delta(1 - p),$$

(3)

with $p = 1 - c$, where $c$ is the concentration of the impurity atoms.

In this paper we have investigated systems with the spin concentrations $p = 0.95$ and 0.8. We have considered the cubic lattices with linear size $L = 128$. 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 [17]. The Metropolis Monte Carlo scheme of simulation with the dynamics of a single-spin flips reflects the dynamics of model A and enables us to compare obtained critical exponents $\theta'$ and $\zeta$ to the results of RG description of the non-equilibrium relaxation of this model.

According to the argument of Janssen, et al. [16] obtained with the RG method and $\varepsilon$-expansion, one may expect a generalized scaling relation for the $k$th moment the magnetization

$$m^{(k)}(t, \tau, L, m_0) = b^{-k\beta/\nu}m^{(k)}(b^{-\delta}t, b^{1/\nu}\tau, b^{-1}L, b^{\zeta}m_0),$$

(4)

is realized after a time scale $t_{mic}$ which is large enough in a microscopic sense but still very small in a macroscopic sense. In Eq. (4), $b$ is a spatial rescaling factor, $\beta$ and $\nu$ are the well-known static critical exponents, and $\zeta$ is the dynamic exponent, while the new independent exponent $x_0$ is the scaling dimension of the initial magnetization $m_0$ and $\tau = (T - T_c)/T_c$ is the reduced temperature.

Since the system is in the early stage of the evolution the correlation length is still small and finite size problems are nearly absent. Therefore we generally consider $L$ large enough ($L = 128$) and skip this argument. We now choose the scaling factor $b = t^{1/\xi}$ so that the main $t$-dependence on the right is cancelled. Applying the scaling form (4) for $k = 1$ to the small quantity $t^{\zeta+2/\nu}m_0$, one obtains

$$m(t, \tau, m_0) \sim m_0 t^{\theta'} F(t^{1/\nu} \tau, t^{\xi+\eta}/m_0)$$

(5)

$$= m_0 t^{\theta'} (1 + a t^{1/\nu} \tau) + O(\tau^2, m_0^2),$$

where $\theta' = (x_0 - \beta/\nu)/\zeta$ has been introduced. It was shown in Ref. [16] that the critical exponents $\theta$ and $\theta'$ in Eq. (5) are related by the scaling relation $\theta' = \theta + (2 - z - \eta)/\zeta$, therefore independent exponent is one of them ($\theta$ or $\theta'$). For $\tau = 0$ and small enough $t$ and $m_0$, the scaling dependence for magnetization (5) takes the form $m(t) \sim t^{\theta'}$. The time scale of a critical initial increase of the magnetization is $t_{cr} \sim m_0^{-\xi/z_0}$. However, in the limit of $m_0 \to 0$, the time scale goes to infinity. Hence the initial condition can leave its trace even in the long-time regime. For illustration we give in Fig. 1 the time evolution of the magnetization $m(t)$ from the initial
state with magnetization $m_0 = 0.03$ at $T_c = 3.49948$ as a result of Monte Carlo simulation of samples with spin concentration $p = 0.8$ and with linear size $L = 128$.

If $\tau \neq 0$, the power law behavior is modified by the scaling function $F(t^{1/\nu})$ with corrections to the simple power law, which will be dependent on the sign of $\tau$. Therefore, simulation of the system for temperatures near the critical point allows to obtain the time-dependent magnetization behavior and the critical temperature $T_c$ can be determined by interpolation.

For the site-diluted Ising model, we measured the time evolution of the magnetization determined as follows:

$$m(t) = \left\langle \frac{1}{N_s} \sum_i N_s p_i S_i(t) \right\rangle,$$

where angle brackets denote the statistical averaging, the square brackets are for averaging over the different impurity configurations, and $N_s = pL^3$ is a number of spins in the lattice. Two other interesting observables in short-time dynamics are the second moment of magnetization $m^{(2)}(t)$,

$$m^{(2)}(t) = \left\langle \left( \frac{1}{N_s} \sum_i N_s p_i S_i(t) \right)^2 \right\rangle,$$

and the auto-correlation function

$$A(t) = \left\langle \frac{1}{N_s} \sum_i N_s p_i S_i(t) S_i(0) \right\rangle.$$

As the spatial correlation length in the beginning of the time evolution is small, for a finite system of dimension $d$ with lattice size $L$ the second moment $m^{(2)}(t, L) \sim L^d$. Combining this with the result of the scaling form in Eq. (1) for $\tau = 0$ and $b = t^{1/\nu}$, one obtains

$$m^{(2)}(t) \sim t^{-2\beta/\nu z} m^{(2)}(1, t^{-1/\nu} L) \sim t^{c_2},$$

$$c_2 = \left( d - 2\beta \right) \frac{1}{\nu z}.$$

Furthermore, careful scaling analysis shows that the auto-correlation also decays with a power law

$$A(t) \sim t^{-c_a}, \quad c_a = \frac{d}{z} - \theta'.$$

Thus, the investigation of the short-time evolution of system from a high-temperature initial state with $m_0 = 0$ allows to determine the dynamic exponent $z$, the ratio of static exponents $\beta/\nu$, and the initial slip exponent $\theta'$. Until now, a completely disordered initial state has been considered as starting point, i.e., a state of very high temperature. The question arises how a completely ordered initial state evolves, when heated up suddenly to the critical temperature. In the scaling form in Eq. (1), one can skip besides $L$, also the argument $m_0 = 1$,

$$m^{(k)}(t, \tau) = b^{-k\beta/\nu z} m^{(k)} \left( b^{-\tau/t} t^{1/\nu} \tau \right).$$

The system is simulated numerically by starting with a completely ordered state, whose evaluation is measured at or near the critical temperature. The quantities measured are $m(t)$ and $m^{(2)}(t)$. With $b = t^{1/\nu}$, one avoids the main $t$ dependence in $m^{(k)}(t)$ and for $k = 1$ one has

$$m(t, \tau) = t^{-\beta/\nu z} m(1, t^{1/\nu} \tau)$$

$$= t^{-\beta/\nu z} \left( 1 + a t^{1/\nu} \tau + O(\tau^2) \right).$$

For $\tau = 0$, the magnetization decays by a power law $m(t) \sim t^{-\beta/\nu z}$. If $\tau \neq 0$, the power law behavior is modified by the scaling function $m(1, t^{1/\nu} \tau)$. From this fact, the critical temperature $T_c$ and the critical exponent $\beta/\nu z$ can be determined.

The scaling form of magnetization in Eq. (12) is presented as follows:

$$\ln m(t, \tau) = (-\beta/\nu z) \ln t + \ln m(1, t^{1/\nu} \tau)$$

after differentiation with respect to $\tau$ gives the power law of time dependence for the logarithmic derivative of the magnetization in the following form:

$$\partial_\tau \ln m(t, \tau) |_{\tau=0} \sim t^{1/\nu z},$$

which allows to determine the ratio $1/\nu z$. On the basis of the magnetization and its second moment, the cumulant

$$U_2(t) = \frac{m^{(2)}(t)}{(m)^2} - 1 \sim t^{d/\nu z}$$
is defined. From its slope, one can directly measure the dynamic exponent $z$. Consequently, from an investigation of the system relaxation from ordered initial state with $m_0 = 1$, the dynamic exponent $z$ and the static exponents $\beta$ and $\nu$ can be determined and their values can be compared to results of simulation of system behavior from disordered initial state with $m_0 = 0$.

### III. MEASUREMENTS OF THE CRITICAL EXPOUNENTS FOR 3D SITE-DILUTED ISING MODEL

We have performed simulations on three-dimensional cubic lattices with linear size $L = 128$, starting either from an ordered state or from a high-temperature state with zero or small initial magnetization. We would like to mention that measurements starting from a completely ordered state with the spins oriented in the same direction ($m_0 = 1$) are more favorable, since they are much less affected by fluctuations, because the quantities measured are rather big in contrast to those from a random start with $m_0 = 0$. Therefore, for careful determination of the critical exponents for 3D Ising model with spin concentrations $p = 0.95$ and 0.8, we begin to investigate the relaxation of this model from a completely ordered initial state.

#### A. Evolution from an ordered state with $m_0 = 1$

Initial configurations for systems with the spin concentrations $p = 0.95; 0.8$ and with randomly distributed quenched pointlike defects were generated numerically. Starting from those initial configurations, the system was updated with Metropolis algorithm at the critical temperatures $T_c = 4.26267(4)$ for $p = 0.95$ and $T_c = 3.49948(18)$ for $p = 0.8$, which have been determined in our paper [23] using Monte Carlo simulation of the 3D site-diluted Ising model with different spin concentrations and particularly with $p = 0.95$ and 0.8 in equilibrium state. At present investigation, simulations have been performed up to $t = 1000$ Monte Carlo steps per spin (MCS/s). We measured the time evolution of the magnetization $m(t)$ and the second moment $m^{(2)}(t)$, which also allow to calculate the time-dependent cumulant $U_2(t)$ in Eq. (15).

In Fig. 2 the magnetization $m(t)$ is plotted on a log-log scale for samples with spin concentrations $p = 0.95$ [Fig. 2, a] and $p = 0.8$ [Fig. 2, b] at $T = T_c(p)$ (curves 1) and at $T = T_s(p)$ $\mp \Delta T$ with $\Delta T = 0.005$ (curves 2 and 3). In Fig. 3, the logarithmic derivative of the magnetization $\partial_t \ln m(t, \tau)_{\tau=0}$ with respect to $\tau$ and in Fig. 4 the cumulant $U_2(t)$ are plotted on a log-log scale at $T = T_c(p)$ for samples with spin concentrations $p = 0.95$ (a) and $p = 0.8$ (b), accordingly. The $\partial_t \ln m(t, \tau)_{\tau=0}$ have been obtained from a quadratic interpolation between the three curves of time evolution of the magnetization in Fig. 2 for the temperatures $T = T_c(p)$, $T = T_s(p) \mp \Delta T$ and taken at the critical temperature $T_c = 4.26267(4)$ for samples with $p = 0.95$ and $T_c = 3.49948(18)$ for $p = 0.8$. The resulting curves in Figs. 2-4 have been obtained by averaging over 6000 and 20000 samples with different configurations of defects for systems with spin concentrations $p = 0.95$ and $p = 0.8$, accordingly.

We have analyzed the time dependence of the cumulant $U_2(t)$ for samples with spin concentrations $p = 0.8$ and clarified that in the time interval $t \in [10, 500]$ MCS/s the $U_2(t)$ is best fitted by power law with the dynamic exponent $z = 2.068(24)$, corresponding to the pure Ising model [24, 34] and the influence of defects is developed for $t > 400$ MCS/s only. An analysis of the $U_2(t)$ slope measured in the interval $t \in [500, 950]$ MCS/s shows that the exponent $\delta / z = 1.268(15)$ which gives $z = 2.366(28)$. We have taken into account these dynamic crossover effects for the analysis of the time dependence of magnetization and its derivative. So, the slope of magnetization measured in the interval $t \in [400, 950]$ MCS/s and its derivative over the interval $t \in [500, 950]$ MCS/s provides the exponents $\beta / \nu z = 0.213(2)$ and $1 / \nu z = 0.600(8)$ which give $\nu = 0.704(18)$ and $\beta = 0.365(8)$. The same analysis of the observable variables for samples with spin concentrations $p = 0.95$ leads to the value of exponent $\delta / z = 1.475(12)$, with $z = 2.034(16)$, in the time interval $t \in [10, 200]$ MCS/s and its derivative over the interval $t \in [500, 950]$ MCS/s provides the exponents $\beta / \nu z = 1.369(13)$, $\beta / \nu z = 0.213(2)$, and $1 / \nu z = 0.600(8)$ in the time interval $t \in [365, 500]$ MCS/s, which give $z = 2.191(21)$, $\nu = 0.704(18)$, and $\beta = 0.365(8)$.

For demonstration of crossover effects between the pure and the dilute regimes, we inserted in Fig. 2(a) and 2(b) results of the magnetization measurements for pure Ising model at the critical temperature $T_c = 4.51142(35)$. Comparison of obtained curves in the insets confirms our conclusion that the influence of disorder on the non-equilibrium critical relaxation is developed for $t > 550$ MCS/s for samples with $p = 0.95$ and for $t > 400$ MCS/s for samples with $p = 0.8$.

In the next stage, we have considered the corrections to the scaling in order to obtain accurate values of the critical exponents. We have applied the following expression for the observable $X(t)$:

$$X(t) = A_x t^\delta (1 + B_x t^{-\omega / z}),$$

where $\omega$ is a well-known exponent of corrections to scaling, $A_x$ and $B_x$ are fitting parameters, and an exponent $\delta = -\beta / \nu z$ when $X \equiv m(t)$, $\delta = d / z$ when $X \equiv U_2(t)$, and $\delta = 1 / \nu z$ when $X \equiv \partial_t \ln m(t, \tau)_{\tau=0}$. This expression reflects the scaling transformation in the critical range of time-dependent corrections to scaling in the form of $t^{-\omega / z}$ to the usual form of corrections to scaling $\tau^{\omega / z}$ in equilibrium state for time $t$ comparable to the order parameter relaxation time $\tau_r \sim \xi^z \Omega(k \xi)$ [17]. Field-theoretic estimate of the $\omega$ value gives $\omega \approx 0.25(10)$ in the six-loop approximation [36]. Monte Carlo studies show that $\omega \approx 0.370(63)$ from Ref. [55] and $\omega \approx 0.26(13)$ from Ref. [36].
FIG. 2: Time evolution of the magnetization $m(t)$ is plotted on a log-log scale for samples with spin concentrations $p = 0.95$ (a) and $p = 0.8$ (b) at $T = T_c(p)$ (curves 1) and at $T = T_c(p) \pm \Delta T$ with $\Delta T = 0.005$ (curves 2 and 3). In insets curves 4 correspond to pure Ising model.

FIG. 3: Time evolution of the logarithmic derivative of the magnetization $\partial_\tau \ln m(t, \tau)$ with respect to $\tau$ is plotted on a log-log scale for samples with spin concentrations $p = 0.95$ (a) and $p = 0.8$ (b).

FIG. 4: Time evolution of the cumulant $U_2(t)$ is plotted on a log-log scale at $T = T_c(p)$ for samples with spin concentrations $p = 0.95$ (a) and $p = 0.8$ (b).
spin concentrations corresponding minimal values of the mean-square errors for a function of the exponent \(\beta/\nu z\) as a function of this fitting procedure determines the exponents \(\delta\) and the cumulant \(c\) as a function of the exponents \(\beta/\nu, 1/\nu z, \) and \(d/z\) for \(p = 0.8\).

We have used the least-squares method for the best approximation of the simulation data \(X(t)\) by the expression in Eq. (16). Minimum of the mean square errors \(\sigma\) of this fitting procedure determines the exponents \(\delta\) and \(\omega/z\). As example, for samples with spin concentrations \(p = 0.8\), we plot in Fig. 5 the \(\sigma\) for the magnetization (a) as a function of the exponent \(\beta/vz\) for \(\omega/z = 0.275\), logarithmic derivative of the magnetization (b) as a function of the exponent \(1/\nu z\) for \(\omega/z = 0.142\), and the cumulant (c) as a function of the exponent \(d/z\) for \(\omega/z = 0.132\). In Table I we present the computed values of the exponents \(\beta/vz, d/z, 1/\nu z, \) and \(\omega/z,\) corresponding minimal values of the mean square errors \(\sigma\) in these fits. The statistical errors for exponents are estimated by dividing all data into five data sets. On the base of these values of exponents and average value of \(\omega/z\), we determine the final values of the critical exponents \(z = 2.185(25), \beta/\nu = 0.533(13), \nu = 0.668(14), \beta = 0.356(6),\) and \(\omega = 0.369(96)\) for \(p = 0.95,\) and \(z = 2.208(32), \beta/\nu = 0.508(17), \nu = 0.685(21), \beta = 0.348(11),\) and \(\omega = 0.404(110)\) for \(p = 0.8\).

The comparison of the obtained values of critical exponents shows their belonging to the same class of universal critical behavior of the diluted Ising model which can be characterized by the averaged critical exponents \(z = 2.196(17), \nu = 0.677(11), \beta = 0.352(5),\) and \(\omega = 0.387(60)\).

### TABLE I: Values of the exponents \(\beta/vz, d/z, 1/\nu z, \) and \(\omega/z\), corresponding minimal values of the mean-square errors for spin concentrations \(p = 0.95\) and \(p = 0.80\).

| \(p\) | Exponent | Mean value | Approximation errors | Statistical errors | \(\omega/z\) |
|---|---|---|---|---|---|
| 0.95 | \(\beta/vz\) | 0.244 | 0.00011 | 0.00131 | 0.234 |
| | \(d/z\) | 1.373 | 0.00938 | 0.00642 | 0.092 |
| | \(1/\nu z\) | 0.685 | 0.00117 | 0.00583 | 0.181 |
| | \(\omega/z\) | 0.230 | 0.00081 | 0.00393 | 0.275 |
| | \(d/z\) | 1.359 | 0.01209 | 0.00785 | 0.132 |
| | \(1/\nu z\) | 0.661 | 0.00418 | 0.00700 | 0.142 |

### B. Evolution from a disordered state with \(m_0 \ll 1\)

In this part of the paper, we present the numerical investigations of the short-time critical dynamics of the 3D site-diluted Ising model on the lattice with linear size \(L = 128,\) starting from a disordered state with small initial magnetizations \(m_0 = 0.01, 0.02,\) and \(0.03\) for samples with spin concentration \(p = 0.8\) only. For independent determination of the dynamic critical exponent \(z\) and the ratio of static exponents \(\beta/\nu\) we investigate also a time dependence of the second moment of magnetization \(m^{(2)}(t)\) and the auto-correlation function \(A(t)\) for system, starting from a high-temperature initial state with \(m_0 = 0\) (in fact, with \(m_0 = 10^{-4}\)). In accordance with Sec. II, a generalized dynamic scaling predicts in this case a power law evolution for the magnetization \(m(t)\), the second moment \(m^{(2)}(t)\) and the auto-correlation function \(A(t)\) in the short-dynamic regime.

Initial configurations for systems with the initial magnetization \(m_0\) were generated numerically. The initial magnetization has been prepared by flipping in an ordered state a definite number of spins at randomly chosen sites in order to get the desired small value of \(m_0\). Starting from those initial configurations, the system was updated with Metropolis algorithm at the critical temperature \(T_c = 3.49948(18)\), which has been determined in our paper [33] using Monte Carlo simulation of the 3D site-diluted Ising model with \(p = 0.8\) in equilibrium state.

We measured the time evolution of the magnetization \(m(t)\) with values of the initial magnetization \(m_0 = 0.01, 0.02,\) and \(0.03,\) the second moment \(m^{(2)}(t)\) and the auto-correlation function \(A(t)\) with \(m_0 = 0.0001\) up to \(t = 1000\) MCS/s. We show the obtained curves for \(m(t)\) in Fig. 6, for \(m^{(2)}(t)\) in Fig. 7a, and for \(A(t)\) in Fig. 7b, which are plotted on a log-log scale. These curves were obtained by averaging over 4000 different samples with 25 runs for each sample. We can see an initial increase of the magnetization, which is a very prominent phenomenon in the short-time critical dynamics. But in contrast to dynamics of the pure systems [24], we can observe the crossover from dynamics of the pure system on early times of the magnetization evolution from \(t \simeq 15\)
up to \( t \simeq 60 \text{ MCS/s} \) to dynamics of the disordered system with the influence of point-like defects in the time interval \( t \in [300, 800] \) MCS/s. The same crossover phenomena were observed in evolution of the second moment of magnetization \( m^2(t) \) and the autocorrelation function \( A(t) \). In the result of linear approximation of these curves in both the time intervals we obtained the values of the exponent \( \theta'(m_0) \) for initial states with \( m_0 = 0.01, 0.02, \) and \( 0.03 \) and the exponents \( c_2 \) and \( c_a \) in accordance with relations in Eqs. (5), (9), and (10) (Table II). The final value of \( \theta' \) is determined by extrapolation to \( m_0 = 0 \).

Note that the similar crossover phenomena in the non-equilibrium critical relaxation of systems with quenched disorder have been revealed earlier in Ref. [31] by means of numerical simulations of the critical behavior of the 3D Ising and XY models with linear defects.

In the next stage, we have applied the procedure of corrections to the scaling determining by the expression (10) for analysis of the observable \( m(t), m^2(t), \) and \( A(t) \). We have used the least-squares method for the best approximation of the simulation data by the expression (10). Minimum of the mean-square errors \( \sigma \) of this fitting procedure determines the exponents \( \theta'(m_0), c_2, \) and \( c_a \) with their respective \( \omega/z \).

In Table III, we present the computed values of these exponents and the final value of \( \theta' = 0.127(16) \) obtained by extrapolation of \( \theta'(m_0) \) for different values of the initial magnetization \( m_0 \) to \( m_0 = 0 \). In Table III, we also give the values of critical exponents \( z, \beta/\nu, \) and the average value of \( \omega \) and compare the values of these exponents to values of corresponding exponents for the pure Ising model [24]. The obtained values agree quite well with results of simulation from an ordered state with \( m_0 = 1 \).

Comparison of the value \( \theta' = 0.127(16) \) to \( \theta' = 0.10(2) \) from Ref. [27] also measured by simulation of the 3D site-diluted Ising model shows their not bad agreement within the limits of statistical errors of simulation and numerical approximations. In Ref. [27] the non-equilibrium relaxation of the magnetization \( m(t) \) has been investigated from the initial random spin configurations with mean magnetization \( m_0 = 0.01 \) only for samples with different spin concentrations \( p = 0.499, 0.6, 0.65, \) and 0.8 and with linear sizes \( L = 8, 16, 32 \) and 64. However, in accordance with Ref. [24], the initial slip exponent \( \theta' \) must be determined in the asymptotical limit with \( m_0 \to 0 \) on the basis of results of \( m(t) \) computing for a few small values of the initial magnetization \( m_0 \). Furthermore, as it follows from Eq. (5), the magnetization undergoes a powerlaw initial increase characterized by \( \theta' \) for sufficiently small \( t^{\omega/z}m_0 \). For \( m_0 \) and \( t \) not too small, the powerlaw behavior will be modified. For strongly diluted systems which are also considered in Ref. [27], the influence of disorder is observed for longer times than for weakly diluted systems. Therefore, the use of the same value of the initial magnetization for determination of the initial slip exponent \( \theta' \) for both weakly and strongly diluted systems is unjustified. It should be noted that in Ref. [27] the data analysis of \( m(t) \) for samples with different spin concentrations \( p \) was carried out with the use of the corrections

\[
\begin{array}{cccccc}
\text{Exponent} & \text{Value} & \omega/z \\
\theta'(m_0 = 0.03) & 0.104(12) & 0.074 \\
\theta'(m_0 = 0.02) & 0.117(10) & 0.068 \\
\theta'(m_0 = 0.01) & 0.118(10) & 0.096 \\
\theta'(m_0 \to 0) & 0.127(16) & 0.079 \\
c_2(m_0 = 0) & 0.909(4) & 0.112 \\
c_a(m_0 = 0) & 1.242(10) & 0.160 \\
z & 2.191(21) & \\
\beta/\nu & 0.504(14) & \\
(\omega/z)_w & 0.117(24) & \\
(\omega)_{aw} & 0.256(55) & 
\end{array}
\]

\[
\begin{array}{cccccccc}
\hline
m_0 & \theta' & c_2 & c_a & z & \beta/\nu \\
\hline
0.03 & 0.1016(9) & t & [5, 30] & \\
0.02 & 0.1031(10) & t & [5, 30] & \\
0.01 & 0.1043(12) & t & [5, 30] & \\
0 & 0.1057(17) & 0.936(4) & 1.347(8) & 2.065(14) & 0.534(6) & \\
\hline
0.03 & 0.083(3) & t & [300, 800] & \\
0.02 & 0.099(5) & t & [300, 800] & \\
0.01 & 0.105(9) & t & [300, 800] & \\
0 & 0.122(11) & 0.859(5) & 1.135(10) & 2.387(20) & 0.475(14) & \\
\hline
\end{array}
\]

TABLE III: Values of the exponents for the 3D site-diluted Ising model to \( p = 0.80 \) obtained with the use of corrections to the scaling.
to scaling procedure during realization of which the universal value of the dynamic critical exponent \( z = 2.62(7) \) obtained in Ref. 38 was applied. But this value \( z \) is inconsistent with values calculated both in the present paper and in Ref. 39 in the three-loop approximation of the field-theoretic RG description, and with experimentally measured value \( z = 2.18(10) \) for weakly diluted Ising-like systems which is larger than the value of exponent \( \theta \) for directly three-dimensional diluted Ising model and \( \theta \) in 2D systems [19, 24] rather than smaller as predicted by the revealed tendency that \( \theta(m_0 = 0.90) < \theta(m_0 = 0.01) \) from Ref. 27. It is explained by the revealed tendency that \( \theta'(m_0^{(2)}) > \theta'(m_0^{(1)}) \) for the initial magnetization which are in the following correspondence with each other as \( m_0^{(2)} < m_0^{(1)} \). Therefore, the distinguished good agreement in Ref. 27 of the obtained value \( \theta' = 0.10(2) \) with \( \theta' \approx 0.0867 \) from Ref. 29 is unjustified. The results of investigations carried out in this paper give reasons to consider that the value of the initial slip exponent \( \theta' = 0.127(16) \) is more realistic for description of non-equilibrium critical relaxation of the 3D weakly diluted Ising-like systems which is larger than the value of exponent \( \theta' = 0.108(2) \) for the pure 3D Ising systems 13, 24 rather than smaller as predicted by results from Refs. 27 and 29.

We have realized a field-theoretic renormalization-group description of non-equilibrium critical relaxation for directly three-dimensional diluted Ising model and calculated the initial slip exponent \( \theta' \) in two-loop approximation without using the \( \varepsilon \)-expansion method. As a result, we have obtained

\[
\theta' = \frac{1}{6} g^* + 0.125v^* - 0.123968(g^*)^2 + 0.14680608g^*v^* - 0.0156245(v^*)^2,
\]

where \( g^* \) and \( v^* \) are values of the vertices describing interaction of the order parameter fluctuations in the fixed-point of the renormalization-group equations 41, 42. For further calculations, we use the FP with \( g^* = 2.2514(42), v^* = -0.7049(13) \) which determines the critical behavior of the 3D dilute Ising model. The coordinate of this FP has been obtained in our paper 39 as average of numerical values \( g^* \), \( v^* \) which were calculated with the use of different methods of resummation technique. It is well known that the series expansions for the critical exponents exhibit factorial divergence, but they can be considered in an asymptotic context. In order to obtain physically reasonable values of the critical exponents for 3D systems, special methods for the summation of asymptotic series have been developed 39, 43–47, the most effective being the Padé-Borel, Padé-Borel-Leroy (PBL), and conformal mapping techniques. We employ the PBL resummation method extended to the two-parameter case. The PBL method is a generalization of the Padé-Borel method with the integral Borel transformation

\[
f(g) = \sum_{n=0}^{\infty} c_n g^n = \int_0^{\infty} dt e^{-t} B(g^t),
\]

where the value of parameter \( b = 2.221426 \) was chosen in Ref. 39 from convergence analysis of the test series for exactly solvable problem of calculating the anharmonic oscillator energy with the asymptotic convergence of the series, which is similar to the series for the RG \( \beta \) and \( \gamma \) functions in the theory of critical phenomena. As a result, the following value \( \theta' = 0.1203 \) has been calculated which very well agrees with our results of simulation.

IV. ANALYSIS OF RESULTS AND CONCLUSIONS

In a summary Table IV, we present the values of critical exponents \( z, \theta', \beta/\nu, \nu, \beta, \) and \( \omega \) obtained in this
paper by comprehensive Monte Carlo simulations of the short-time critical evolution of the 3D site-diluted Ising model both from an ordered initial state with \(m_0 = 1\) for samples with spin concentrations \(p = 0.95\) and \(0.8\) and from a disordered initial states with \(m_0 \ll 1\) for samples with spin concentration \(p = 0.8\). For comparison, we give in Table IV the results of calculation of these exponents by the field-theoretical method with fixed-dimension \(d = 3\) expansion \([36, 39]\), the results of experimental investigations of the Ising-like magnets \([40, 54, 56]\), and the results of numerical studies \([27, 33, 35, 38, 48, 53, 55]\). As shown in Table IV, our values of exponents are in good agreement within the limits of statistical errors of simulation and numerical approximations with results of the field-theoretical description of the statics in six-loop approximation \([36]\) and critical dynamics in three-loop approximation \([31]\) and with the results of experimental investigations of the static \([54, 56]\) and dynamic \([40]\) critical behaviors of weakly diluted Ising-like magnets.

Comparison to results of Monte Carlo simulations shows that our static exponents \(\beta/\nu\), \(\nu\), and \(\beta\) agree well with those exponents measured in equilibrium for weakly diluted systems in the most cited papers and for systems with wide dilution range in Ref. \([54]\) where the critical exponents were obtained for \(p \leq 0.8\) as dilution-independent after a proper infinite volume extrapolation with taking into account the leading corrections-to-scaling terms. However, it was found that the case with \(p = 0.9\) falls out from this dilution-independent scheme of fits with common exponent \(\omega = 0.37\) for samples with different spin concentrations. Authors draw a conclusion that the \(p = 0.9\) data seem to be still crossing over from the pure Ising fixed point to the diluted one. Most of the computations have been carried out at \(p = 0.8\) as in this case the scaling corrections are very small and the results even in small lattices are stable. So, in Ref. \([49]\), it was shown that for case with \(p = 0.8\), the observed corrections to scaling could be the next-to-leading with \(\omega_2 \approx 0.80\). However, our present investigation and the results of computations in equilibrium \([36]\) show that the systems with \(p = 0.95\) and \(p = 0.8\) are characterized by close agreement of the critical exponent values and they belong to the same class of universal critical behavior of the site-diluted Ising model with the averaged critical exponents \(\nu = 0.677(11)\), \(\beta = 0.352(5)\), and \(\omega = 0.387(60)\).

Now we compare the values of the dynamic critical exponent \(\nu\) obtained in this paper by the short-time dynamics method to the results of Monte Carlo simulations of the critical dynamics in equilibrium, realized in Refs. \([51]\) and \([55]\), to the results of non-equilibrium studies of the

| \(p, m_0\) | \(z\) | \(\nu\) | \(\beta\) | \(\omega\) |
|----------------|-----------------|-----------------|-----------------|-----------------|
| \(0.95, 1\) | \(2.18(25)\) | \(0.53(13)\) | \(0.66(14)\) | \(0.36(6)\) | \(0.36(96)\) |
| \(0.80, 1\) | \(2.20(32)\) | \(0.50(17)\) | \(0.68(21)\) | \(0.34(11)\) | \(0.40(110)\) |
| \(0.80, \ll 1\) | \(2.19(21)\) | \(0.12(17)\) | \(0.50(14)\) | \(0.25(55)\) |
susceptibility in Refs. \[38\] and \[54\], and to the results of Monte Carlo renormalization group application to description of the site-diluted Ising model relaxation from the ordered initial state with $m_0 = 1$ in Ref. \[52\]. Values of $z$ from paper \[51\] agree rather well with our results only for weakly diluted systems with $p \geq 0.9$, while a noticeable difference between 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 degree of dilution, the author in Ref. \[51\] obtained the asymptotic value $z = 2.4(1)$ using the effective values of the exponent listed in Table IV. The off-equilibrium critical dynamics of the 3D Ising model with the spin concentration varying in a wide range was analyzed in Ref. \[38\]. Also assuming that the critical behavior of diluted Ising systems is universal under dilution, 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 Ref. \[38\] is strongly inconsistent with $\omega = 0.25(10)$ from the field theory calculations \[39\] and not so well agreement with $\omega = 0.37(6)$ from Monte Carlo results in Ref. \[54\]. In the approximations realized in Ref. \[58\], the results for weakly diluted systems were characterized by the largest errors. In Ref. \[58\], it was carried out the Metropolis dynamics in equilibrium for site-diluted Ising model with $p = 0.8, 0.85,$ and $0.65$. For case with $p = 0.8$, authors investigated in detail the scaling corrections which were the next-to-leading with $\omega_2 = 0.82(8)$ and gave the exponent $z = 2.35(2)$. Investigations for other values of $p$ did not permit to determine $z$ in these systems accurately. Also, in Ref. \[58\], investigated was the off-equilibrium relaxational critical dynamics in the site-diluted Ising model at $p = 0.8$. The results show that equilibrium estimate $z = 2.35(2)$ is perfectly consistent with the off-equilibrium MC data. Authors did not observe a large-time scaling corrections proportional to $t^{-\omega_2/z}$; instead, their data show corrections that are proportional to $t^{-\omega_2/z}$ with the static correction-to-scaling exponents $\omega = 0.29(2)$ and $\omega_2 = 0.82(8)$. We have some doubts in validity of $z = 2.35(2)$. As it was shown in \[32\], the realization of correction to scaling procedure demands the six simulation data points at least for their approximation by four-parameter function such as in Eq. (110) for lattices with $L > L_{\text{min}}$. Whereas in paper \[58\], the asymptotical value $z = 2.35(2)$ was obtained with the use of four or five data points as it was demonstrated in Figs. 1-4 in \[58\]. It is necessary to use additional data points for lattices with $L > 64$.

The early results of our numerical investigations of the critical dynamics for diluted Ising systems in Ref. \[52\] by Monte Carlo renormalization-group method show very good agreement with our present results for weakly diluted systems, while a noticeable difference between the results is observed for strongly diluted systems. We are planning to continue the Monte Carlo study of critical behavior of the site-diluted Ising model by short-time dynamics method with $p = 0.6$ and $0.5$ focusing on the problem of dilution independence of asymptotic characteristics.

The present results of Monte Carlo investigations allow us to recognize that the short-time dynamics method is reliable for the study of the critical behavior of the systems with quenched disorder and is the alternative to traditional Monte Carlo methods. But in contrast to studies of the critical behavior of the pure systems by the short-time dynamics method \[23\] \[24\], in case of the systems with quenched point-like disorder after the microscopic time $t_{\text{mic}} \approx 5 / 10$ MCS/s, there exist three stages of dynamic evolution. For systems starting from the ordered initial states $(m_0 = 1)$ in the time interval of 10-50 MCS/s, the power-law dependence is observed at the critical point for Binder cumulant $U_2(t)$, which is similar to that in the pure system. In the time interval [400,950], the power-law dependences are observed in the critical point for the magnetization $m(t)$, the logarithmic derivative of the magnetization, and cumulant $U_2(t)$ which are determined by the influence of disorder. However, careful analysis of the slopes for $m(t)$ and $U_2(t)$ reveals that a correction to scaling should be considered in order to obtain accurate results. The dynamic and static critical exponents were computed with the use of the corrections to scaling, which demonstrate their good agreement with results of the field-theoretic description of the critical behavior of these models with disorder. In the intermediate time interval of 100-400 MCS/s, the dynamic crossover behavior is observed from the critical behavior typical for the pure systems to behavior determined by the influence of disorder.

The investigation of the critical behavior of the Ising model with defects starting from the disordered initial states with $m_0 \ll 1$ also has revealed three stages of the dynamic evolution. It was shown that the power-law dependences for the magnetization $m(t)$, the second moment $m^{(2)}(t)$, and the autocorrelation $A(t)$ are observed in the critical point, which are typical for the pure system in the common interval [5,60] for observable quantities and for the disordered system in the common interval [150,800]. In the intermediate time interval the crossover behavior is observed in the dynamic evolution of the system. The obtained values of exponents demonstrate good agreement within the limits of statistical errors of simulation and numerical approximations with results of simulation of the pure Ising model by the short-time dynamics method for the first time interval and with our results of simulation of the critical relaxation of this model from the ordered initial state.

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