Peculiarities of non-equilibrium critical behavior of site-diluted 2D Ising model

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Abstract. The results of a numerical Monte Carlo study of features of nonequilibrium critical behavior in a two-dimensional pure and structurally disordered Ising models are presented with realization of evolution from different initial states within the wide range of spin concentrations \( p = 1.0, 0.95, 0.9, 0.85, 0.8, 0.75, \) and 0.7. Analysis of the two-time dependences of the autocorrelation function and dynamic susceptibility revealed a substantial influence of the initial states on the aging effects. The violation of the fluctuation-dissipation theorem is studied, and the asymptotic values of the fluctuation-dissipation ratio are calculated.

At the present time systems with slow dynamics attract considerable interest of researchers. This is associated with the aging properties and violations of the fluctuation-dissipation theorem \cite{1}. These features of the nonequilibrium behavior can be observed in systems undergoing the second order phase transition \cite{2}, because their critical dynamics is characterized by anomalously long relaxation times \( t_{\text{rel}} \).

The effect of critical slowing-down is one of the features appearing in the critical behaviour of various systems. This phenomenon is associated with an abnormal increase in the relaxation time of a system \( t_{\text{rel}} \) when the temperature tends to the critical temperature \( T_c \) of the second order phase transition: \( t_{\text{rel}} \sim \abs{T - T_c}^{-z\nu} \), where \( z \) and \( \nu \) are the dynamic critical exponent and the critical exponent for the correlation length, respectively. As a result of this, a system in the critical point turns out to be unable to come to equilibrium state during the relaxation process. The aging effects manifest themselves in the nonequilibrium behavior just at times \( t < t_{\text{rel}} \) and are characterized by the two-time dependence of the correlation and response functions on the observation time \( t \) and waiting time \( t_w \). The waiting time characterizes the time interval from the preparation of the sample until starting measurements of its characteristics. The basically important manifestation of the slow dynamics is the violation of the fluctuation-dissipation theorem \cite{1, 2}, which suggests relation between autocorrelation function \( C(t, t_w) \) and response function \( R(t, t_w) \) on some external field as

\[
R(t, t_w) = \frac{X(t, t_w)}{T} \frac{\partial C(t, t_w)}{\partial t_w}, \tag{1}
\]

where \( X(t, t_w) \) is an additional parameter referred to as the fluctuation-dissipation ratio (FDR). For times \( t > t_w \gg t_{\text{rel}} \), the fluctuation-dissipation theorem gives \( X(t, t_w) = 1 \). However, in the general case, for times \( t, t_w < t_{\text{rel}} \), we have \( X(t, t_w) \neq 1 \). The asymptotic FDR is introduced as

\[
X^\infty = \lim_{t_w \to \infty} \lim_{t \to \infty} X(t, t_w) \tag{2}
\]
and can be used as an universal quantity of nonequilibrium processes in various systems.

In this work, we report the numerical Monte Carlo study of the effects of initial states and structural defects on the aging phenomena and the asymptotic values of the FDR in the two-dimensional Ising model. The Hamiltonian for the ferromagnetic Ising model diluted by nonmagnetic impurities with external magnetic field \( h \) is given by the expression

\[
H = -J \sum_{\langle i,j \rangle} p_i p_j S_i S_j - h \sum_i p_i S_i,
\]

where \( J > 0 \) is the short-range exchange interaction between spins \( S_i = \pm 1 \) fixed at the sites of a planar square lattice. The occupation numbers \( p_i \) assume the value 0 or 1, and \( p_i \) equals 1 if site contains spin and 0 otherwise if spin is absent (a magnetic atom is replaced by a nonmagnetic impurity atom). The structural defects are distributed in the system in a canonical manner according to the distribution function \( P(p_i) = (1-p)\delta(p_i) + p\delta(p_i) \), where \( p = \langle p_i \rangle \) specifies the spin density in the system.

The nonequilibrium process is characterized by the magnetization

\[
M(t) = \frac{1}{V} \int d^d x \langle S(x, t) \rangle = \left[ \frac{1}{N_s} \sum_{i=1}^{N_s} p_i S_i(t) \right], \tag{4}
\]

two-time correlation function \( C(t, t_w) \), and linear response function \( R(t, t_w) \) to a weak field applied at time \( t_w \). The functions \( C(t, t_w) \) and \( R(t, t_w) \) can be defined as

\[
C(t, t_w) = \frac{1}{V} \int d^d x \left[ \langle S(x, t) S(x, t_w) \rangle - \langle S(x, t) \rangle \langle S(x, t_w) \rangle \right], \tag{5}
\]

\[
R(t, t_w) = \frac{1}{V} \int d^d x \left. \frac{\delta \langle S(x, t) \rangle}{\delta h(x, t_w)} \right|_{h=0}, \tag{6}
\]

where the angle brackets stand for averaging over the different realizations of initial state and the square brackets are for averaging over the different impurity configurations. \( N_s = pL^2 \) in (4) characterizes the number of spins in the lattice with the linear size \( L \).

In this work, we use by analogy with [3,4] the technique allowing us to calculate the response function at zero applied magnetic field by calculating the generalized susceptibility in the form of the integral response function (thermostatic susceptibility):

\[
\chi(t, t_w) = \int_0^{t_w} dt' R(t, t') = \frac{1}{T_c N} \sum_i [(p_i S_i(t) \Delta S_i(t_w))], \tag{7}
\]

with the response function specified by (6) and \( \Delta S_i(t_w) = \sum_{s=0}^{t_w} [S_i(s) - S_i^W(s)] \) calculated in the simulation process from initial state at \( t = 0 \) until the time \( t_w \), where \( S_i^W(s) = \tanh(J \sum_{j \neq i} p_j S_j/T) \).

We have simulated systems with different spin concentrations \( p \) for the square lattice with the linear size \( L = 1024 \) at the corresponding critical temperatures shown in Table 1. We used for simulation the thermal bath algorithm with single-spin overturns. At the early stage of the evolution of the system, the correlation length is still sufficiently small and the finiteness of the system used in the simulations is insignificant. Therefore, the use of the lattice with the large enough linear size \( L = 1024 \) allows us to neglect the finite size effects in comparison to their manifestations in the simulations of the equilibrium critical phenomena. We prepared initial states of the system with values of the magnetization \( m_0 = 0.01 \ll 1 \) and \( m_0 = 1 \). The behavior
of autocorrelation function and dynamic susceptibility was studied for different values of waiting time. The positions of defects are fixed for a specified impurity configuration. The behavior of the system was studied at times up to 10000 Monte Carlo steps. At the simulations of the pure system with \( p = 1 \), we performed the statistical averaging over 15000 runs. At the simulations of the structurally disordered Ising model, the averaging of the calculated parameters was performed over 2000 impurity configurations and over 15 runs for each impurity configuration.

For the high-temperature initial states with \( m_0 \ll 1 \), the stage of nonequilibrium evolution exhibits the characteristic growth of magnetization described by a power law \( m(t) \sim t^{\theta'} \), where \( \theta' \) is the independent dynamic critical exponent [2] with calculated values presented in Table 1. This magnetization growth is of purely fluctuation nature. Indeed, if the fluctuations are not taken into account, we have \( \theta' = 0 \). At times \( t > t_m \), \( m(t) \sim m_0^k \) with \( k = 1/(\theta' + \beta/\nu z) \), this stage of evolution is changed by the regime characterized by the relation \( m(t) \sim t^{-\beta/\nu z} \). At the evolution from the initial state with \( m_0 = 1 \), the relaxation of magnetization is determined from the very beginning by the power law dependence \( m(t) \sim t^{-\beta/\nu z} \) [7].

In [8,9], it was shown that the existence of uncorrelated structural defects is insignificant for the statical critical behavior of the two-dimensional Ising model. Indeed, the critical exponents retain the same values as those for the pure model, namely, \( \beta = 0.125 \) and \( \nu = 1 \), and the defects lead only to logarithmic corrections to the thermodynamic and correlation characteristics. This prediction was confirmed numerically in a number of papers [5,10,11]. At the same time, the studies of the critical dynamics of the model reported in [12,13] demonstrated that, near the spin percolation threshold (for the systems with the spin concentrations \( p \leq 0.85 \)), the dynamic critical exponent \( z \), determining the temperature dependence of the relaxation time, exhibits the dependence on the concentration of defects with the violation of the standard form of dynamic scaling and takes the form

\[
z = A |\ln(p - p_c)| + B.
\]

Taking into consideration the logarithmic corrections, we assume the time dependence of the magnetization for low-temperature initial state in the form:

\[
m(t) \sim t^{-\beta/\nu z} \left( 1 + \left( \frac{g}{z} \right) \ln t \right)^{-\beta/(2\nu)},
\]

where \( g = \frac{4}{\pi} g_0 = \frac{4}{\pi} \frac{1}{(1 + \sqrt{2})^2} \frac{1 - p}{p} \approx 4.843 \frac{1 - p}{p} [5,8] \). For the pure system it corresponds to the conventional power-law time dependence of the magnetization \( m(t) \sim t^{-\beta/\nu z} \). To check (8), we calculated the values of the exponents \( \beta/\nu z \) and \( z \) according to (9) and considered logarithmic dependence of the exponents on the spin concentrations (Fig.1). The relation (8) is confirmed in

| \( p \) | \( T_c \) | \( \theta' \) | \( \beta/\nu z \) | \( z \) | \( X_{LT}^{(t-t_w=t_w)} \) | \( X_{LT}^\infty \) | \( X_{HT}^\infty \) |
|---|---|---|---|---|---|---|---|
| 1.0 | 2.2692 | 0.192(4) | 0.05784(30) | 2.161(11) | 0.751(24) | 0.375(24) |
| 0.95 | 2.08989(8) | 0.191(3) | 0.05794(32) | 2.157(12) | 0.750(25) | 0.329(20) |
| 0.9 | 1.9032(5) | 0.190(3) | 0.05798(33) | 2.172(13) | 0.748(25) | 0.317(21) |
| 0.85 | 1.7098(4) | 0.180(2) | 0.05352(33) | 2.336(15) | 0.726(26) | 0.265(21) |
| 0.8 | 1.5103(4) | 0.166(1) | 0.05034(34) | 2.483(17) | 0.714(26) | 0.256(23) |
| 0.75 | 1.2980(10) | 0.155(1) | 0.04522(35) | 2.764(21) | 0.682(28) | 0.215(24) |
| 0.7 | 1.0729(10) | 0.128(1) | 0.03906(33) | 3.197(25) | 0.669(31) | 0.178(24) |

Table 1. Values of the critical temperature \( T_c \), critical exponents \( \theta', \beta/\nu z, \) and the fluctuation-dissipation ratio for a low-temperature \( X_{LT} \) and a high-temperature \( X_{HT} \) initial states at different spin concentrations \( p \). Values of \( T_c \) were taken from [5,6].
The aging effects increase in the structurally disordered systems in comparison to those in the pure system. Analysis of the scaling functions presented in Fig. 3 revealed that the canonical exponent \( z \) for different spin concentrations \( p \). The right graph illustrates the logarithmic dependence of the exponent \( z \) on the spin concentration.

The case of the spin concentrations \( p \leq 0.85 \). However, the values of the exponents \( \beta/(\nu\zeta) \) and \( z \) for systems with \( p = 0.95 \) and \( p = 0.9 \) coincide within the statistical errors with the values for the pure system \( \beta/(\nu\zeta) = 0.05784(30) \) and \( z = 2.161(11) \). This result confirms that the values of the dynamic critical exponent \( z \) for weakly disordered systems with \( p \geq 0.9 \) remain constant and the critical dynamics of the structurally disordered Ising model belongs to the universality class of the pure model [13, 14]. The value of \( z \) for the pure system is in a good agreement with the value \( z = 2.1667(5) \) from the work [15]. The exponent \( z'(p) \) calculated for structurally disordered systems as \( m(t) \sim t^{-\beta/(\nu\zeta')} \) is characterized by the values \( z'(0.9) = 2.646(13), z'(0.8) = 3.085(19), z'(0.7) = 4.004(35) \), which are much more in comparison to values of \( z(p) \) computed subject to the logarithmic corrections (Table 1). Therefore, logarithmic corrections provide a marked contribution to the values of \( z \). As for the values of the exponent \( \theta' \), they coincide for systems with \( p = 0.95 \) and \( p = 0.9 \) within the error bars with the value \( \theta' = 0.192(4) \) for the pure system.

We also calculated the two-time dependence of the autocorrelation function \( C(t, t_w) \) and the susceptibility \( \chi(t, t_w) \) (Fig. 2). The aging effects clearly manifest themselves at the observation times \( t \sim t_w \) and are characterized by the slowing down of these functions with increase of the waiting time \( t_w \) in compliance with the generalized scaling forms [2]

\[
C(t, t_w) \sim t_w^{-2\beta/\nu_z} F_C(t/t_w^\mu),
\]

\[
\chi(t, t_w) \sim t_w^{-2\beta/\nu_z} F_\chi(t/t_w^\mu).
\]

The aging effects increase in the structurally disordered systems in comparison to those in the pure system. Analysis of the scaling functions presented in Fig. 3 revealed that the canonical aging with exponent \( \mu = 1 \) is observed for evolution from the high-temperature initial state with \( m_0 \ll 1 \). The scaling function \( F_C(t/t_w^\mu) \) is characterized for case of evolution from

Figure 1. Time dependence of the magnetization \( m(t) \) for \( m_0 = 1 \) (left) and \( m(t)(1 + (g/z)\ln t)^{-\beta/2\nu} \) (center), determining the dynamical critical exponent \( z \) for different spin concentrations \( p \). The right graph illustrates the logarithmic dependence of the exponent \( z \) on the spin concentration.

Figure 2. Nonequilibrium dependence of the autocorrelation function \( C(t, t_w) \) for \( m_0 = 0.01 \ll 1 \) (left) and \( m_0 = 1 \) (center) and the dynamic susceptibility \( \chi(t, t_w) \) for \( m_0 = 1 \) (right) on the observation time \( t - t_w \) at different spin concentrations \( p \) and waiting times \( t_w \).
the low-temperature initial state by \( \mu = 1 \) only for the pure system, whereas in structurally disordered systems the correlation effects are strongly slowed down in comparison to the pure system. It leads to superaging effects with values of the exponent \( \mu(p) > 1 \): \( \mu(0.9) = 6.15(5), \mu(0.85) = 6.50(5), \mu(0.8) = 6.75, \mu(0.75) = 7.00(5), \) and \( \mu(0.7) = 7.50(5) \). For \( F_X(t/t_w) \), the canonical aging is observed for both pure and structurally disordered systems.

At the next stage of our studies, we calculated the fluctuation-dissipation ratio according to the relation [16, 17]:

\[
X(t, t_w) = \lim_{C \to 0} T_C \frac{\partial \chi(t, t_w)}{\partial C(t, t_w)}
\]  

(12)

Dependences \( T_\chi \) on \( C \) are presented in Fig. 4 for the evolution of system from initial states with \( m_0 = 0.01 \) and \( m_0 = 1 \). We calculated the FDR for each value of the waiting time \( t_w \), and then the asymptotic value of the FDR \( X^\infty \) was determined by extrapolation \( X(t_w \to \infty) \). The sought asymptotic values of the FDR are presented in Table 1. The value \( X^\infty_{HT} = 0.339(19) \) for the pure system relaxing from the high-temperature initial state is in very good agreement with the value \( X^\infty_{HT} = 0.33(1) \) determined in [3] by the MC simulation method. The asymptotic values of the FDR determined for a weakly disordered systems with \( p = 0.95 \) and \( p = 0.9 \) coincide within the statistical errors with the value for the pure system. Therefore, these systems belong to the universality class of the pure system. The asymptotic values of the FDR for a strongly disordered systems are appreciably dependent on the concentration of defects owing to the crossover effects in the percolation behavior [12].

For the pure system relaxing from a low-temperature initial state with \( m_0 = 1 \), the plot of \( T_\chi \) versus \( C \) is linear for the time range \( t - t_w \geq t_w \) of variation of the autocorrelation function and characterized by the asymptotic value of the FDR \( X^\infty_{HT} = 0.75(24) \). This value is in very good agreement with the field-theoretical value \( X^\infty_{HT} = 0.75 \) determined in [3]. However, the dependences of \( T_\chi \) versus \( C \) for the structurally disordered systems relaxing from the initial state

\[
\frac{\partial \chi(t, t_w)}{\partial C(t, t_w)}
\]
ordered state with $m_0 = 1$ exhibit two linear segments because of the found slowing down of the correlation effects at times $t - t_w \geq t_w$ owing to the pinning of domain walls by the defects. The first segment corresponds to the changes in the autocorrelation function $C(t, t_w)$ at times $t - t_w \sim t_w$, whereas the second segment corresponds to the long-term stage of the evolution with $t - t_w \gg t_w$ (Fig. 4). Second segments lead to the asymptotic FDR values $X_{LT}^{\infty} = 0$ for all spin concentrations $p < 1$ under study. At the same time, the analysis of the dependences of $T_X$ versus $C$ in the first segments using (12) without considering the limit $C \to 0$ demonstrates that the extrapolation $X_{LT}(t_w \to \infty)$ applied to certain $X_{LT}(t_w)$ gives the values $X_{LT}^{(t-t_w\sim t_w)}$ presented in the Table 1. These values of the FDR for systems with $p = 0.95$ and $p = 0.9$ are close to the asymptotic FDR value for the pure Ising model.

To conclude, we note that our numerical studies have revealed an appreciable role of defects in the nonequilibrium critical dynamics of the two-dimensional Ising model. It was shown that for disordered systems logarithmic corrections provide a significant contribution to values of the dynamic critical exponent $z$. The realization of two types of universal behavior corresponding to influence of high-temperature and low-temperature initial states is revealed. It has been shown that the weakly disordered systems with $p \geq 0.9$ belong to the universality class of the pure system and are described by the same characteristics of critical behavior. In the case of structurally disordered systems relaxing from the low-temperature initial state, the significant slowing down of the correlation is revealed due to the pinning of domain walls on defects.

As a result, superaging effects occur in time behavior of the autocorrelation function and the asymptotic FDR values determined by the domain dynamics in the long-term become equal to zero. For the high-temperature initial state, the asymptotic values of the FDR weakly disordered systems with $p \geq 0.9$ are coincide within the statistical errors with the value for the pure two-dimensional Ising model $X^{\infty} = 0.339(19)$, whereas for strongly disordered systems with $p \leq 0.85$ the asymptotic values of FDR demonstrate a significant decrease. This indicates that nonequilibrium critical behavior of systems with $p \geq 0.9$ belongs to the universality class of the pure system, and the nonequilibrium critical behavior of systems with $p \leq 0.85$ depends on the concentration of defects with the violation of the standard form of dynamic scaling due to the influence of crossover effects of percolation behavior [12, 13].

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