Monte Carlo Simulation of the Non-Equilibrium Critical Dynamics of Low-Dimensional Magnetics and Multilayer Structures

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Abstract—The Monte Carlo simulation of the critical behavior of low-dimensional magnets and multilayer structures based on anisotropic Heisenberg mode are presented. The aging and clustering effects are revealed in the critical relaxation of 2d XY-model from non-equilibrium initial states. The investigation of non-equilibrium critical behavior of multilayer structure which correspond to the nanoscale superlattice Co/Cr demonstrates that the aging can be observed in a wider temperature range than for bulk magnetic systems.

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1. INTRODUCTION

A significant interest has been recently focused on non-equilibrium processes in magnetic low-dimensional materials [1, 2]. The reduction of the dimension of magnets is accompanied by an increase in fluctuations of the spin density and the manifestation of the effects of critical slowing down and “memory” in the non-equilibrium behavior of low dimensional magnetic systems. Thin films and low-dimensional magnets demonstrates the slow critical evolution from a non-equilibrium initial state. Aging, coarsening and memory effects are nontrivial features in the non-equilibrium behavior of such systems with slow dynamics [3].

It is important that the peculiarities of non-equilibrium critical dynamics can be considered as basis for understanding and interpretation of the experimental data obtained for Co/Cr multilayer structures. The investigation of the magnetization relaxation in a structurally ordered magnetic Co/Cr superlattice has revealed the magnetic aging phenomena [4]. The nanoscale periodicity creates in these magnetic multilayer structures mesoscopic spatial magnetic correlations with slow relaxation dynamics when quenching of the system into a non-equilibrium state is realized. In comparison with bulk magnetic systems where the slow dynamics and aging phenomenon are displayed close to critical point, the magnetic superlattices, structured on the nanoscale, give possibility to increase relaxation time due to the increasing in the characteristic spin-spin correlation length.

Similarly to the concept of universality in equilibrium critical phenomena [5] where symmetry of the interactions and dimensionality unify otherwise microscopically different systems into classes with common critical behavior, there are some control parameters and grouping microscopically distinct model systems into classes with universal aspects of non-equilibrium critical dynamics. The universality allows one to calculate characteristic non-equilibrium properties in various statistical models [3, 6].

The paper is organized in the following manner. The Monte Carlo modeling of the non-equilibrium critical behavior and introduction to the aging effects are discussed in the Subsection 2.1. The investigation of the non-equilibrium processes of the 2D XY-model in Berezinskii–Kosterlitz–Thouless phase is presented in the Subsection 2.2. Aging effects in multilayered magnetic structure shortly discussed in the Subsection 2.3. The paper ends with concluding remarks and summary in Section 3.

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2. MODELS AND RESULTS OF MONTE CARLO SIMULATION

2.1. Non-Equilibrium Behavior of 3D Ising Model

We have considered the ferromagnetic three-dimensional Ising model. In case of presence of external magnetic field \( h \) the Hamiltonian of system is given by

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

where \( J > 0 \) is short-range exchange interaction integral between spins \( S_i = \pm 1 \) fixed at the lattice sites. We considered the cubic lattice with periodic boundary conditions. The Metropolis algorithm was used for Monte Carlo simulations.

In the studies of effects of the initial states on the non-equilibrium critical behavior, we distinguish the high-temperature initial state created at a temperature \( T_0 > T_c \) and characterized by the initial magnetization \( m_0 = 0 \) before it is quenched at \( T_c \) and the low-temperature magnetized initial state with preparation at \( T_0 < T_c \) and \( m_0 \neq 0 \). The non-equilibrium evolution starts when the system after initial preparation is placed to the thermostat with \( T = T_c \). We have begun to measure at the waiting time \( t_w \) the two-time quantities such as response and correlation functions at times \( 1 \ll t, t_w \ll t_{rel} \). Up to now, the study of the non-equilibrium critical behavior of different statistical systems are performed in the most complete form only for the case of their evolution from the initial high-temperature state (see review [3]).

To investigate the non-equilibrium evolution we computed such characteristics as the magnetization \( m(t) \)

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

the time-dependent autocorrelation function \( C(t, t_w) \) and the linear response \( R(t, t_w) \) to a small external field, applied at time \( t_w \), which are defined by relations

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

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

where angle brackets stands for the mean over the different realizations of initial state.

The time variable \( t_w \) characterizes the age of a sample and is called waiting time. Autocorrelation function in non-equilibrium processes depend not only on the difference \( t - t_w \) but also on each time variable individually at \( t - t_w \) and \( t_w \) much smaller than the relaxation time of the system \( t_{rel} \). The nonequilibrium evolution starts when the system after initial preparation is placed to the thermostat with \( T = T_c \). At the waiting time \( t_w \), we have begun to measure two-time correlation function within the \( 1 \ll t, t_w \ll t_{rel} \) range. The aging of a system is manifested in slowing down relaxation processes with the time passing from the preparation of a sample.

At the present time, it become established that the time dependence for magnetization, autocorrelation and response functions for systems starting from a low-temperature initial state with \( m_0 \neq 0 \) satisfies the following scaling forms [7]:

\[
m(t, t_m) = A_M t^{-\beta/z} F_M(t/t_m), \quad C(t, t_w, t_m) = A_C (t - t_w)^{\alpha + 1 - d/z}(t/t_w)^{\theta - 1} F_C(t_w/t, t/t_m),
\]

\[
R(t, t_w, t_m) = A_R (t - t_w)^{\alpha - d/z}(t/t_w)^{\theta} F_R(t_w/t, t/t_m),
\]

(2)

where \( t_m = B_m m_0^{-k} \) is a new timescale with exponent \( k = 1/(\theta + a + \beta/(\nu z)) > 0, a = (2 - \eta - z)/z, \theta = \theta' - (2 - z - \eta)/z, \theta' \) is the initial slip exponent characterizing the evolution of magnetization from high-temperature initial state [8]. The scaling functions \( F_C(t_w/t, t/t_m) \) and \( F_R(t_w/t, t/t_m) \) are finite at limits \( t_w \to 0 \) and \( t/t_m \to 0 \), \( A_C \) and \( A_R \) are non-universal amplitudes that are fixed by the condition \( F_{C,R}(0,0) = 1 \).

We presented investigation of critical relaxation of magnetization \( m(t) \) for different initial states \( m_0 \), which demonstrate an essential both qualitative and quantitative differences in relaxation from
the high-temperature initial state with $m_0 \ll 1$, from the low-temperature completely ordered initial state with $m_0 = 1$, and from the intermediate initial states with $m_0 = 0.6, 0.5, 0.4, 0.3$ and $0.2$. So, a remarkable property of the non-equilibrium critical relaxation from the high-temperature initial state with $m_0 = 0.02 \ll 1$ is the increase of magnetization $m(t) \sim t^{\eta}$. The initial rise of magnetization is changed to the well known decay $m(t) \sim t^{-\beta/z\nu}$ for $t > t_{cr} \sim m_0^{-1/(\theta^0 + \beta/z\nu)}$. The critical relaxation from the completely ordered initial state with $m_0 = 1$ is directly characterized by power-law of magnetization decay $m(t) \sim t^{-\beta/z\nu}$. The intermediate cases with $m_0 < 1.0$ are characterized by a short stage of magnetization rise under the power-law $m(t) \sim t^{\theta}$ which is changed to much long-continued stage of relaxation with $m(t) \sim t^{-\beta/z\nu}$. Thus, the critical relaxation process from the high-temperature initial state with $m_0 \ll 1$ is a most “fast” in comparison with relaxation from other magnetized initial states with $m_0 \neq 0$[6].

To check the scaling prediction for $m(t)$ as function of the initial magnetization $m_0$ given by relation (2), we plot the dependence of $t^{\beta/z\nu} m(t)$ versus $t m_0^k$. The curves $m(t)$ for different $m_0$ are collapsed into a single curve with universal scaling dependence.

### 2.2. Aging and Coarsening Effects in Non-Equilibrium Behavior of 2D XY-Model

A two-dimensional XY-model is a lattice model of the low-dimensional magnets with continuous symmetry, and the Hamiltonian is $H = -J \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j$, where $J > 0$ is the exchange integral, $\mathbf{S}_i$ is the classical planar spin associated with the $i$th site of the two dimensional lattice. In the two-dimensional XY-model occurs of topological phase transition at a temperature $T_{BKT} = 0$, associated with the dissociation of vortex pairs. Below this temperature vortices are bound in pairs, and the correlation length is infinite. Presence of vortices in non-equilibrium configurations (even below $T_{BKT}$) may change essentially the dynamical properties of the system [9]. The presence of vortices lead to the time dependence of the correlation length $\xi(t) = (t/\ln t)^{1/2}$, which acquires logarithmic correction. The resulting two time dependence for the autocorrelation function $C(t, t_w)$ clearly demonstrate the slowing down of relaxation processes with increasing $t_w$. These aging effects are manifested at times $t - t_w \approx t_w$.

The autocorrelation function in the non-equilibrium critical state for the two dimensional system has the scaling form $C(t, t_w) = t_w^{-\eta(T)/2} \Phi [\xi(t - t_w)/\xi(t_w)]$, where $\eta$ is the Fisher critical exponent. The curves of $t_w^{\eta/2} C(t, t_w)$ versus $\xi(t - t_w)/\xi(t_w)$ are collapsed at the long time stage of evolution with $t - t_w \gg t_w \gg 1$ for various $t_w$ on universal curve.

The relaxation of the two-dimensional XY-model from the initial high-temperature state is accompanied by a process of critical cluster coarsening (Fig. 1), which characterized by an anomalous slowdown effects. The inertial effects are revealed in the process of coarsening. The size of large clusters first rises above the equilibrium size, and after that reduced to equilibrium at sufficiently large times.

![Fig. 1. Visualization of the non-equilibrium process of cluster coarsening for relaxation from the initial high-temperature state. The growth of quasi long-range order regions is shown at times: 50 000, 200 000, 500 000 MCS/s.](image)
2.3. Aging and the Influence of Non-Equilibrium Initial States on Critical Behavior of the Co/Cr Multilayered Magnetic Structure

The magnetic properties of Co, Fe, and Ni films on non-magnetic substrate are described by anisotropic Heisenberg model [10, 11], with Hamiltonian

\[ H = - \sum_{\langle i,j \rangle} J_{ij} [S_i S_j - \Delta(N)S_i^z S_j^z] - h \sum_i S_i^z, \]

where \( S_i = (S_i^x, S_i^y, S_i^z) \) is a three-dimensional spin in the lattice site \( i \); \( h \) is applied magnetic field. Anisotropy parameter \( \Delta \) characterizes the amount of anisotropy: \( \Delta = 0 \) corresponds to the isotropic Heisenberg case, \( \Delta = 1 \) — the case of XY-model. The value of \( \Delta = 0.7 \) is chosen for describing multilayer structure Co(0.6 nm)/Cr. The Co thin films in such structures demonstrates a magnetization \( m \), which lies in XY plane below \( T_c \) [11]. The estimated value of \( J_1 = 4.4 \times 10^{-14} \text{erg} \) corresponds to Co.

The two-times dependencies of the autocorrelation function \( C(t, t_w) \) for different non-equilibrium initial states demonstrate the presence of aging effects not only in vicinity of \( T_c = 249.6 \text{K} \), but for \( T = 160 \text{K} < T_c \) and \( T = 96 \text{K} < T_c \). The relaxation of the thermoremanent “staggered” magnetization \( m^{\text{stg}}(t, t_w) \) from low-temperature initial non-equilibrium state \( m_0^{\text{stg}} = 1 \) demonstrates scaling “collapse”, which corresponds to form (2).

3. CONCLUSIONS

The Monte Carlo simulation of the aging in different magnetic systems with slow dynamics shows that these “spin–glass” effects brightly appear in non-equilibrium relaxation from different initial states. The dynamical “collapse” confirms the validity of the two-time scaling forms in the critical region and give the possibility to estimates the values of critical exponents. The study of the 2D XY magnets and multilayer structures revealed that the aging can be observed in a wider temperature range than for bulk magnetic systems. The presence of such non-equilibrium effects would be taken into account in application of magnetic multilayers structures.

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