Non-equilibrium critical behavior of the 3D classical Heisenberg model

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Abstract. We have investigated the non-equilibrium critical behavior of the three-dimensional classical Heisenberg model with evolution from various initial states. Initial states with magnetization $m_0 \neq 0$ lead to a new time scale $t_m \sim m_0^k$ with the exponent $k > 0$ which produces complex universal scaling forms on the temporal behavior of the magnetization, the autocorrelation function, and the response function. Aging effects have been revealed in two-time behavior of the autocorrelation function with evolution from various initial states. We show that the slowing down of the autocorrelation function during the evolution from high-temperature initial state is considerably more slow than for case of the evolution from low-temperature initial state. Using scaling forms of the magnetization and the autocorrelation function, the values of critical exponents $z = 2.035(4)$, $\theta' = 0.490(1)$, and $k = 1/(\theta' + \beta/\nu z) = 1.340(4)$ were calculated.

The 3D classical ferromagnetic Heisenberg model is the one of the traditional statistical model, which is used to describe the second order phase transition in the different spin systems, including the such materials as Fe, Co, Ni and its alloys. The static critical behavior of the systems described by this model was investigated with the use of different techniques and approximations. For example, these are the experimental methods, the summation method of the series of the high-temperature expansion, the renormalization-group methods, and the simulations by the Monte Carlo methods. The values of the critical temperature and static critical exponents obtained by these methods are in good agreement within the statistical errors in spite of the results have some differences (see the review [1]).

A much smaller attention is focused on to the study of the critical dynamics and there are less works on the non-equilibrium critical behavior of the model. At early works with the renormalization-group description of different dynamic models [2], the critical dynamics of the Heisenberg isotropic model was classified as model J with conserved order parameter (the magnetization) and non-conserved energy. The dynamic equation of the magnetization near the critical point although contains the relaxation term, but the long-wave and low-frequency dynamics of the magnetization is determined by the hydrodynamic term in the equation which describes the slow precessional rotational motion of the magnetization. The dimensional analysis of the magnetization dynamics of the Heisenberg isotropic model allows one to obtain the expression for the critical dynamic exponent $z = (d+2-\eta H)/2$, where $d$ is the spatial dimension of the system, $\eta$ is the Fisher critical exponent that determines the power-law decay of the correlation function with the distance near the critical point. The value $z \approx 5/2$ is predicted for the 3D Heisenberg model, since value of $\eta H \approx 0.021$ (with the use of two-loop approximation $\varepsilon^2$ within the $\varepsilon$-expansion method) is negligible compared to $5/2$. However, the dipole interaction
always presents in the magnetics and it is especially significant near the critical point for the isotropic magnets due to the long-range nature of the dipole interaction. The influence of the dipole interaction on the static properties of Heisenberg model was studied by the $\varepsilon$-expansion method in the work [3] and on its dynamic properties in the work [4]. The important property of the influence of the dipole interaction on the critical dynamics is noted in [4]. It leads to non-conservation of the order parameter and relaxation of the magnetization with dynamic critical exponent $z_d = 2 + c_d\eta_d \simeq 2.022$, where $c_d = (27/4) \ln(4/3) - 1 \simeq 0.942$ according to work [4], and the Fisher's exponent $\eta_d$ has the value $\eta_d \simeq 0.023$ under the influence of dipole interaction (in the two-loop approximation within $\varepsilon$-expansion method [3]). Although the numerical values of static critical exponents change slightly under influence of dipole interaction, however, the influence of the dipole interaction on the values of the dynamic critical exponent turns out to be significant due to the changes in dynamics of the magnetization.

Taking into account influence of dipole interaction, the Heisenberg model dynamics expressed by the relaxation dynamic of the model A in Hohenberg-Halperin classification (see review [2]), in which both the order parameter and the energy are not conserved. The model has dynamic critical exponent $z = 2 + c\eta$ with $c = 6\ln(4/3) - 1 \simeq 0.726$ and one could find the value $z_H = 2 + c_H\eta \simeq 2.015$ for the Heisenberg model using the value $\eta \simeq 0.021$, which also is close enough to $z_d$ for the Heisenberg model with influence of the dipole interaction. In the paper [5, 6] the dynamic critical exponents $z = 1.975(10)$ and $z = 1.976(9)$ were found by the short-time dynamics method of simulations. The values are consistent within statistical errors with the value $z = 1.96(6)$ that is earlier calculated in the work [7] using the equilibrium technique simulation of the autocorrelation function. However, the values of $z$ obtained in [5, 6] are less than 2 and it provokes an alertness by reason of these values should lead to the divergence of the kinetic coefficients. It is conflicted with fundamentals of the renormalization-group theory for the relaxation model A and never observed in the experiments.

The behavior of the systems characterized by the anomalously slow dynamics is of the great current interest. This is related to the aging properties of non-equilibrium characteristics and the violations of the fluctuation-dissipation theorem predicted and observed at the slow evolution of the systems from the non-equilibrium initial state [8]. Such features of the non-equilibrium behavior are also characteristic of the systems exhibiting the second order phase transitions [9], because the critical dynamics of such systems is characterized by anomalously large relaxation times.

Near the second order phase transition critical temperature $T_c$ the relaxation time of the system is divergent value $t_{rel} \sim |T - T_c|^{-\nu z}$, where $z$, $\nu$ are critical exponents. Thus, the systems at the critical point never reach equilibrium during the whole relaxation process. The aging in the non-equilibrium behavior of systems appears at times $t \ll t_{rel}$. It is expressed in the existence of the two-time dependencies for the correlation and response functions and in dependence of its evolution on the initial states. It is distinguished a high-temperature initial state created at the temperatures $T \gg T_c$ and a low-temperature initial state created at $T < T_c$. The high-temperature state is characterized by the initial magnetization $m_0 \ll 1$, when the low-temperature one is characterized by the initial magnetization $m_0 = 1$ (this state also called as completely ordered initial state). In the paper we have investigated the influence of various initial states with magnetization in the range $0 < m_0 \leq 1$ on critical relaxation of the magnetization and the autocorrelation function for the 3D Heisenberg model.

The Hamiltonian of the ferromagnetic isotropic Heisenberg model is given by the expression

$$ H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, $$

(1)

where $J > 0$ is the short-range exchange interaction between spins $\vec{S}_i$ fixed at the sites of the simple cubic lattice. Spin $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$ is determined as the classical unit vector. Summation
over \( j \) affects only nearest neighbors of the \( i \)-th spin. The simulations were carried out on lattice with sizes \( L \times L \times L \) and with applied periodic boundary conditions. To calculate characteristics of the non-equilibrium critical behavior, the dynamic process of one-spin flips was numerically simulated within the Monte Carlo statistical method. The dynamic process of one-spin flips was implemented using the Metropolis algorithm. Simulations were carried out at the critical temperature \( T_c = 1.44292(8) \) calculated in work [10].

To investigate the non-equilibrium evolution, we computed such characteristics as the magnetization \( \langle \vec{M}(t) \rangle \) and the two-time dependent autocorrelation function \( C(t, t_w) \), which are defined by relations

\[
\vec{M}(t) = \frac{1}{V} \int d^d x \langle \vec{S}(x, t) \rangle = \left\langle \frac{1}{L^3} \sum_{i=1}^{L^3} \vec{S}_i(t) \right\rangle,
\]

\[
C(t, t_w) = \frac{1}{V} \int d^d x \langle \left( \vec{S}(x, t) \vec{S}(x, t_w) \right) - \vec{M}(t) \vec{M}(t_w) \rangle = \left\langle \frac{1}{L^3} \sum_{i=1}^{L^3} \vec{S}_i(t) \vec{S}_i(t_w) \right\rangle - \vec{M}(t) \vec{M}(t_w),
\]

where the angle brackets stand for averaging over the different realizations of initial state.

Near the critical point the magnetization and the correlation function are the generalized homogeneous functions with respect to the observation time \( t \), the waiting time \( t_w \) and the new time scale \( t_m \sim m_0^{-k} \). The \( m_0 = |\langle \vec{M}(0) \rangle| \) is the initial magnetization. The exponent \( k = 1/(\theta' + \beta/z \nu) > 0 \) is expressed on static critical exponents \( \beta \) and \( \nu \) and dynamic ones \( \theta' \) and \( z \). At the present time, it become established that the time dependence for the magnetization and the autocorrelation function for systems starting from an initial state with \( m_0 \neq 0 \) satisfies the following scaling forms [11]:

\[
M(t, t_m) \sim t^{-\beta/\nu z} F_m(t/t_m)
\]

\[
C(t, t_w, t_m) \sim t^{-2\beta/\nu z} F_C(t/t_w, t/t_m),
\]

where \( F_m \) and \( F_C \) are the generalized homogeneous functions with respect to its parameters.

\[\text{Figure 1. Relaxation of the magnetization } M(t) \text{ for various values of the initial magnetization } m_0.\]

To check the scaling form (6) for the 3D Heisenberg model, the magnetization was computed for various initial states with magnetization \( m_0 \leq 1 \). The obtained data are plotted in Fig.1.
As shown in Fig. 1, the relaxation curves for the initial magnetization $m_0 \neq 1$ clearly tend to the curve characterized by the completely ordered initial state with $m_0 = 1$. The non-equilibrium power-law time dependence of the magnetization $M(t) \sim m_0 t^{\theta}$ is well displayed for the systems with initial states $m_0 < 1$ with the exponent $\theta' > 0$ [12, 13]. The increasing magnetization of such configurations is changed to power-law decay of the magnetization $M(t) \sim t^{-\beta/\nu z}$ at times $t > t_{cr} \sim m_0^{-k}$. The critical relaxation from the completely ordered initial state with $m_0 = 1$ is immediately characterized by power-law decay of the magnetization $M(t) \sim t^{-\beta/\nu z}$.

We have considered the systems with the initial states $m_0 = 0.001, 0.003$ and $0.005$ in order to compute the exponent $\theta'$. We have used about 1000 realizations for each initial system state with given. Using the critical exponents $\theta'(m_0)$, we obtained the approximated value $\theta(m_0 \to 0) = 0.490(1)$. The exponent computing data are presented in Fig. 2 a). By analyzing the magnetization curve for the system with evolution from $m_0 = 1$, the exponent $\beta/\nu z$ was computed with final value $\beta/\nu = 0.521(1)$ from work [14], we found the dynamic critical exponent $z = 2.035(4)$.

We have checked the scaling form for magnetization (5). To do that we plotted $t^{\beta/\nu z} M(t, t_m)$ versus $t/t_m$ with $t_m = m_0^{-k}$. It is shown in Fig. 2 b. The curves for various initial states are well collapsed at one universal curve that defines the scaling function $F_m(x = t/t_m)$. It has a power-law dependence $F_m(x) \sim x^{1/k}$ at initial evolution stage. Using obtained data, we have found the value of exponent $k = 1.340(4)$.

In addition to the magnetization, we have analyzed realization of aging for the two-time connected correlation function $C(t, t_w)$. We used the waiting times $t_w = 20, 40, 80,$ and $160$ MCS/s for simulations of evolution from the low-temperature initial state with $m_0 = 1$ and the high-temperature state with $m_0 = 0.001$. The correlation functions versus the observation time are plotted in Fig. 3. The both systems well display the aging in the its time dependencies. Comparing the plots one could see more ”strong” aging for evolution from the low-temperature initial state opposite to the high-temperature one. At the same time, the $C(t, t_w)$ is decreased more slowly for the $m_0 \ll 1$ than for case with $m_0 = 1$.

![Figure 2. a) Extrapolation of exponent values $\theta'(m_0 \to 0)$ computed for $m_0 = 0.001; 0.003; 0.005$. b) Dependence of the magnetization scaling function $F_m(t_m^{k}) = t^{\beta/\nu z} M(t, m_0)$ on $x = t/m_0^{k}$.](image)
Figure 3. Time dependence of the autocorrelation function $C(t, t_w)$ for various waiting times $t_w$ with evolution from a) the completely initial state with $m_0 = 1$ and b) the low-temperature initial state with $m_0 = 0.001$.

The exponent $c_a$ is equal to $c_a^{LT} = 1 + \frac{\beta(4 + 2)}{z\nu}$ for the completely ordered initial state $m_0 = 1$ [11, 16, 17] and $c_a^{HT} = \frac{d}{z} - \theta'$ for the high-temperature initial state $m_0 \ll 1$ [18, 19]. In order to check the scaling form (5) we have plotted $t_w^{2/\nu z} C(t, t_w)$ versus $t/t_w$ using our result $\beta/\nu z = 0.256(1)$. The data are shown in Fig. 4 for the both initial states.

Figure 4. Dependence of the autocorrelation scaling function $t_w^{2/\nu z} C(t, t_w)$ on $t/t_w$ for evolution from a) the low-temperature initial state and b) the high-temperature initial state.

The plots show well collapse for the different waiting times $t_w$. The universal curve defines the scaling function $F_C(t/t_w)$. We have found the value of exponent $c_a^{LT} = 2.734(7)$ for the completely ordered initial state with $m_0 = 1$ and $c_a^{HT} = 0.979(6)$ for the high-temperature initial state with $m_0 = 0.001$ at time stage $t/t_w > 1$. The values have good match with the theory predictions giving $c_a^{LT} \approx 2.730$ (for the Heisenberg model $\delta = 4.758(11)$) and $c_a^{HT} = \frac{d}{z} - \theta' = 0.984$.

We have investigated the non-equilibrium behavior of the 3D ferromagnetic Heisenberg models for the wide range of the initial states. We have revealed the ageing in the behavior of the
two-time connected correlation function. The scaling forms are confirmed for the magnetization and the correlation function.

We have obtained the dynamical critical exponents $\theta' = 0.490(1)$ and $z = 2.035(4)$. The exponent $\theta'$ is well matched with the one $\theta' = 0.482(3)$ that was found at [5, 6] using short-time dynamics method. Additionally we note that we used the lattice with more large linear sizes ($L = 60, 100$ compared to $L = 40$) than in works [5, 6] and more small values of the initial magnetization $m_0 \ll 1$. It allows us to state the value $\theta' = 0.490(1)$ more precise.

As for the exponent $z$, our result with the value $z = 2.035(4)$ has good agreement with $z_H = 2 + \epsilon_H \simeq 2.015$ obtained in two-loop approximation within $\epsilon$-expansion method for the model A [2]. Moreover using the value $\eta_H = 0.0413(16)$ [14] and the value $c = 6 \ln(4/3) - 1 \approx 0.726$, one could find $z = 2.0315(11)$. The method of short-time dynamics gives $z = 1.976(9)$ [5, 6], but this result has strong disagreement with the expected value of $z > 2$ for the relaxation model A with non-conserved order parameter and was never confirmed experimentally.

We have analyzed the magnetization relaxation for wide range of the initial states. It is shown the power-law $M(t) \sim t^{-\beta/\nu z}$ for the perfect ordered initial state. The data for the $m_0 \neq 1$ are clearly displayed the asymptotic tends to that law at some stage of the relaxation. For the initial states $m_0 \ll 1$ and the regime $t < t_c \sim m_0^{-k}$ the curves are shown another power-law $M(t) \sim m_0 t^{\theta'}$.

For the two-time correlation function, the aging and the scaling are checked and proved. The dependence of the correlation function on the waiting times is more strong for the case of evolution from the low-temperature initial state with $m_0 = 1$ than from the high-temperature initial state with $m_0 = 0.001$.

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