Simulation of non-equilibrium critical behavior of the 3D isotropic and anisotropic Heisenberg models

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Abstract. Monte Carlo study of non-equilibrium critical behavior of three-dimensional Heisenberg model in isotropic case and with anisotropy of easy axis type is carried out. Relaxational Glauber-like dynamics of these models with evolution from high-temperature initial state is investigated. Realization of aging is demonstrated for two-time dependence of the autocorrelation function and dynamical susceptibility. Asymptotic fluctuation-dissipation ratios are determined for isotropic $X^\infty = 0.383(6)$ and anisotropic $X^\infty = 0.392(7)$ Heisenberg models. Significant influence of easy-axis anisotropy on non-equilibrium critical behavior of the 3D Heisenberg model leading to characteristics typical for the 3D Ising model is revealed.

Three-dimensional ferromagnetic Heisenberg spin systems are traditional models for the study of critical phenomena. One of the features arisen in describing the critical behavior is the critical slowing down effect. It is associated with an anomalous increase of relaxation time $t_{rel}$ in the system close to the critical temperature $T_c$. As a result, a statistical system at the critical point cannot achieve the equilibrium state during the whole relaxation process. The non-equilibrium evolution in this case displays some of the peculiarities, such as aging phenomena, memory about the initial states and violation of the fluctuation-dissipation theorem (FDT) [1, 2, 3].

The non-equilibrium behavior of a system is realized via its transition at the starting instant $t_0$ from the initial state at temperature $T_0$ to the state with temperature $T_s$ differing from $T_0$. The accompanying equilibration process is characterized by relaxation time $t_{rel}(T_s)$, and equilibrium corresponding to temperature $T_s$ is reached in times $t \gg t_{rel}(T_s)$. However, in times $t \ll t_{rel}(T_s)$, the evolution of the system depends on its initial state. In this connection, the non-equilibrium behavior of the system depends on whether it evolves from a high-temperature $T_0 > T_s$ or a low temperature $T_0 < T_s$ initial state.

In this paper, we study by Monte Carlo methods the non-equilibrium critical behavior of the three-dimensional Heisenberg model in isotropic case and with easy-axis anisotropy. We consider the evolution of these systems from high-temperature initial state and its influence on two-time properties of the autocorrelation function and dynamical susceptibility with revealing the aging effects. At first time, we present calculations of the asymptotical fluctuation-dissipation ratio for isotropic and anisotropic Heisenberg models.

The Hamiltonian of the ferromagnetic Heisenberg model with the easy-axis anisotropy is given by the expression

$$H = -J \sum_i \left[(1 - \Delta)(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z\right],$$

where $J > 0$ is the short-range exchange interaction between spins $S_i$ fixed at the sites of the simple cubic lattice. Spin $S_i = (S_i^x, S_i^y, S_i^z)$ is determined as the classical unit vector. Summation
over \( j \) affects only nearest neighbors of the \( i \)-th spin. \( \Delta \) is the anisotropy parameter. For \( \Delta = 0 \), the isotropic Heisenberg model is realized when the anisotropic Heisenberg model is characterized by \( \Delta \neq 0 \). In this work, we take the value \( \Delta = 0.63 \) for the anisotropy parameter [4]. The value of critical temperature \( T_c = 1.44292(8) \) is used for the 3D isotropic Heisenberg model taken from [5], when for the 3D anisotropic Heisenberg model with \( \Delta = 0.63 \), we calculated the critical temperature \( T_c = 1.64497(45) \) with use of the Binder’s cumulant method.

To investigate the non-equilibrium evolution, we consider such characteristics as the magnetization \( M(t) \), the two-time dependent autocorrelation function \( C(t, t_w) \) and the dynamical susceptibility \( \chi(t, t_w) \) as integrated response function, which are defined by the relations

\[
\hat{M}(t) = \frac{1}{V} \int d^d x \left\langle \vec{S}(x, t) \right\rangle = \left\langle \frac{1}{L^d} \sum_{i=1}^{L^d} \vec{S}_i(t) \right\rangle, \quad (2)
\]

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

\[
\chi(t, t_w) = \int_0^{t_w} dt' R(t, t'), \quad R(t, t_w) = \frac{1}{V} \int d^d x \frac{\delta \left\langle \vec{S}(x, t) \right\rangle}{\delta h(x, t_w)} \bigg|_{h=0}, \quad (4)
\]

where the angle brackets characterize the statistical averaging over different realizations of initial spin configurations. In relation (4), \( R(t, t_w) \) is the linear response to a small external field \( h(x, t_w) \), applied at waiting time \( t_w \).

According to general concepts about non-equilibrium processes, it is expected that for times \( t > t_w \gg t_{\text{rel}}(T_s) \), \( C(t, t_w) = C^\text{eq}(t - t_w) \) and \( R(t, t_w) = R^\text{eq}(t - t_w) \), where \( C^\text{eq} \) and \( R^\text{eq} \) are equilibrium values related by the FDT \( R^\text{eq}(t-t_w) = \frac{1}{T_s} \int dC dC' \frac{\partial C(t, t_w)}{\partial t}, \) in the case of non-equilibrium behavior of systems for \( t, t_w < t_{\text{rel}}(T_s) \), the generalized FDT assumes the form [6]

\[
R(t, t_w) = \frac{X(t, t_w)}{T_s} \frac{\partial C(t, t_w)}{\partial t_w}, \quad (5)
\]

with introduction of the quantity \( X(t, t_w) \) which is called as the fluctuation-dissipation ratio (FDR). For times with \( t > t_w \gg t_{\text{rel}} \), the FDT establishes that \( X(t, t_w) = 1 \). However, at the critical temperature with \( T_s = T_c \), \( X(t, t_w) \neq 1 \) such as \( t, t_w \ll t_{\text{rel}} \rightarrow \infty \) for \( T_s \rightarrow T_c \). The asymptotic FDR introduced as

\[
X^\infty = \lim_{t_w \rightarrow \infty} \lim_{t \rightarrow \infty} X(t, t_w), \quad (6)
\]

is an important universal characteristic of non-equilibrium processes in the various systems.

The relation (4) using (5) for the response function can be written as

\[
T_c \chi(t, t_w) = \int_0^{t_w} X(t, t') \frac{\partial C(t, t')}{\partial t'} dt' = \int_0^{C(t, t_w)} X(C) dC, \quad (7)
\]

which leads to definition of the FDR in the form:

\[
X(t_w) = \lim_{C \rightarrow 0} T_c \frac{\partial \chi(t, t_w)}{\partial C(t, t_w)}, \quad (8)
\]

that can be used to determine an asymptotic value of the FDR in compliance with relation (6).

The simulations were carried out on cubic lattice with linear size \( L = 100 \) and with applied periodic boundary conditions. We have used a standard Metropolis dynamics for the numerical
analysis of non-equilibrium critical behavior of the magnetization and the autocorrelation function. However, application of Glauber-like dynamics enables to calculate directly the response function and the susceptibility without the application of a magnetic field. Glauber-like dynamics is determined by the transition probabilities of single-spin flips from configuration with a spin $S_i$ to a new value $S'_i$ given by

$$W(S_i \rightarrow S'_i) = \frac{\exp[-\beta H_i(S'_i)]}{\exp[-\beta H_i(S_i)] + \exp[-\beta H_i(S'_i)]}$$

with $\beta = 1/T$. Both dynamics have the same dynamical exponents and one expect no significant changes for thermodynamical quantities.

We have realized the following procedure of spin flips from $S_i$ to $S'_i$ defined as

$$S'_i = S_i - 2(S_i \cdot r_i) r_i,$$

where $\parallel_i$ is a parallel projection of $S_i$ to $r_i$, this spin transformation consists in flip of parallel projection of spin $\parallel_i \rightarrow -\parallel_i$ with conservation of perpendicular projection $\perp_i$ to $r_i$.

In accordance with methodology [7, 8, 9], relation for the susceptibility $\chi(t,t_w)$ can be presented for case of the Heisenberg model in following form:

$$\chi(t,t_w) = \frac{\beta}{N} \sum_{i=1}^{N} \langle S_i(t) \cdot \Delta S_i(t_w) \rangle,$$

with $\Delta S_i(t_w) = \sum_{s=1}^{t_w} (S_i(t) - S_i^{(W)}(t))$, where $S_i^{(W)} = S_i \tanh(\frac{\beta}{2} \Delta H_i)$ is the Weiss field.

Near the critical point, the correlation function and susceptibility are the generalized homogeneous functions with respect to its parameters.

$$C(t,t_w) = t^{-2\beta/\nu z} F_C(t/t_w), \quad \chi(t,t_w) = t^{-2\beta/\nu z} F_\chi(t/t_w),$$

where $F_C$ and $F_\chi$ are the generalized homogeneous functions with respect to its parameters.

**Figure 1.** Time dependence of total magnetization $M(t)$, $M_z(t)$ and $M_{xy}(t)$ components of magnetization for anisotropic model (a), and relaxation of magnetization $M(t,m_0)$ with initial magnetization $m_0 = 1.0$ (b) for various spin models: (1) the anisotropic and (2) isotropic 3D Heisenberg models and (3) the 3D Ising model.

We determined (Fig. 1 a) that only $M_z$-component of the magnetization is characterized by slow dynamics at the critical temperature for the 3D anisotropic Heisenberg model. Therefore,
the characteristics of the non-equilibrium critical behavior should display themselves in the autocorrelation function only for $S_z$-components of the spins:

$$C_{zz}(t, t_w) = \sum_{i=1}^{L^3} \left( \frac{1}{L^3} \sum_{i} S_{zi}^2(t) S_{zi}^2(t_w) \right) - M_z(t) M_z(t_w). \quad (12)$$

The values of critical exponent $\beta/\nu z$ were determined by analyzing time dependence $M(t) \sim t^{-\beta/\nu z}$ for isotropic and $M_z(t) \sim t^{-\beta/\nu z}$ for anisotropic models with evolution from $m_0 = 1$ (Fig. 1 a,b). The exponent $\beta/\nu z = 0.25599(5)$ for isotropic and $\beta/\nu z = 0.25654(4)$ for anisotropic models were obtained as a result of the linear approximation of the data on $M(t)$ in the time interval $\Delta t = 5002000$ MCs/s and $M_z(t)$-component in the time interval $\Delta t = 1502000$ MCs/s.

To find the exponent $z$ for isotropic model, the ratio $\beta/\nu = 0.521(1)$ from [11] was used. The determined value of the dynamic critical exponent $z = 2.035(4)$ is in good agreement with results of the RG $\epsilon$-expansion calculations [12].

Both equilibrium and dynamic critical characteristics of the Heisenberg model with the easy-axis anisotropy must be similar to the Ising model characteristics, since, in both models, preferential direction of the magnetization is given along axis $z$ (Fig. 1 b). The Ising model can be considered as the limiting case of the anisotropic Heisenberg model with anisotropy parameter $\Delta = 1$. Thus, to find the exponent $z$, we calculated time-dependence of cumulant $U_2(t) = M(t)^2/(M(t))^2 - 1 \sim t^{d/z}$ for 3D anisotropic Heisenberg model with evolution from completely ordered initial state ($m_0 = 1$). The obtained value of exponent $d/z = 1.483(5)$ leads to $z = 2.023(7)$ which is in good agreement with results of the theoretical field calculations [13] for exponent $z$ in the 3D Ising model. This value of $z$ gives possibility to determine of exponent ratio $\beta/\nu = 0.519(5)$ from $\beta/\nu z = 0.25654(4)$ for anisotropic model, which agrees very well with $\beta/\nu = 0.518(7)$ calculated in [14] for the 3D Ising model by Monte Carlo methods.

Also, we have considered the systems with the initial states $m_0 = 0.001, 0.003$ and $0.005$ in order to compute the exponent $\theta'$ for initial evolution of the magnetization $M(t) = m_0 t^{\theta'}$ [15, 16]. 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 $\theta'(m_0 \rightarrow 0) = 0.490(1)$ for isotropic model and $\theta' = 0.529(1)$ for anisotropic model.

We have analyzed realization of aging in two-time dependence of the dynamic susceptibility $\chi(t, t_w)$ and the correlation functions $C(t, t_w)$ and $C_{zz}(t, t_w)$ for isotropic and anisotropic models. We used the waiting times $t_w = 20, 40, 80$ and $160$ MCS/s for simulation of evolution from the high-temperature state with $m_0 = 0.001$. Curves in Fig.2 well display the aging in two-time dependence of $C(t, t_w)$, $C_{zz}(t, t_w)$ and $\chi(t, t_w)$ which are characterized by more slow decreasing with increasing waiting time $t_w$. At the same time, the $C(t, t_w)$ and $\chi(t, t_w)$ are decreased more slowly for isotropic model than $C_{zz}(t, t_w)$ and $\chi(t, t_w)$ for anisotropic model.
At aging regime with $t - t_w \gg t_w$, one expects the following scaling forms for the correlation function and the dynamic susceptibility $C(t,t_w) \sim t_w^{-\beta/\nu z} F_C(t/t_w)$ and $\chi(t,t_w) \sim t_w^{-\beta/\nu z} F_{\chi}(t/t_w)$ with the scaling functions $F_C(t/t_w)$ and $F_{\chi}(t/t_w)$ characterized by power-law dependence at times $t - t_w \gg t_w$: $F_C(t/t_w) \sim (t/t_w)^{-\epsilon_C}$, $F_{\chi}(t/t_w) \sim (t/t_w)^{-\epsilon_{\chi}}$.

The scaling properties of the autocorrelation function and the susceptibility (11) are confirmed by constructed dependences $t_w^{\beta/\nu z} C(t,t_w)$ and $t_w^{\beta/\nu z} \chi(t,t_w)$ on $(t - t_w)/t_w$ in Fig.3 using the obtained values of exponent $\beta/\nu z = 0.25599(5)$ for isotropic model and $\beta/\nu z = 0.2565(4)$ for anisotropic model. The results demonstrate the collapse of the data obtained for various $t_w$ in the universal curves corresponding to scaling functions $F_{C,\chi}(t/t_w)$. At time stage $t/t_w \gg 1$, we have determined the values of exponents $c_a^{(is)} = 0.979(6)$ and $c_{\chi}^{(is)} = 0.984(2)$ for isotropic model and $c_a^{(anis)} = 0.956(2)$ and $c_{\chi}^{(anis)} = 0.954(3)$ for anisotropic model.

The theory predicts [1] that exponents $c_a = c_{\chi}$ and $c_a = d/\nu - \theta'$ for case of evolution from the high-temperature initial state. The calculated values $c_a$ and $c_{\chi}$ have good match with theory predictions giving $c_a^{(is)} = \frac{3}{2} - \theta' \approx 0.984$ for isotropic and $c_a^{(anis)} \approx 0.956$ for anisotropic models.

In later investigations, we computed the fluctuation-dissipation ratios for our Heisenberg models in compliance with relation (8) from parametric dependence of $T_{C,\chi}(t,t_w)$ versus $C(t,t_w)$ in limit $C \to 0$ that corresponds to long-time limit. The obtained data are plotted in Fig.4 for different values of waiting time $t_w$. The values of the asymptotic FDRs $X^\infty = 0.383(6)$ for isotropic and $X^\infty = 0.392(7)$ for anisotropic models were determined as a realization of relation (6) for various $t_w$, giving values $X(t_w)$ in Fig.5, with subsequent application of linear approximation and extrapolation $X(t_w \to \infty)$. 

Figure 3. Scaling collapse of autocorrelation function (a) and dynamic susceptibility (b) for isotropic and anisotropic models.

Figure 4. Dependence of susceptibility on autocorrelation function determining the FDRs for isotropic (a) and anisotropic (b) models.
Figure 5. Calculation of the asymptotic FDRs in the limit $1/t_w \to 0$ for isotropic (a) and anisotropic (b) models.

The value of asymptotic FDR $X^\infty = 0.383(6)$ for isotropic model is in excellent agreement with the theoretical field value $X^\infty = 0.386(23)$ obtained in paper [17] in the two-loop approximation at the fixed space dimension $d = 3$ using Padé-Borel summation for asymptotic series and in sufficiently good agreement with RG calculations of the FDR $X^\infty = 0.405(10)$ obtained in paper [18] with the use of $\varepsilon$-expansion method for description of the non-equilibrium critical dynamics of the dissipative model A. The value of asymptotic FDR $X^\infty = 0.392(7)$ for anisotropic model is in very good agreement with value $X^\infty = 0.391(12)$ for the 3D Ising model determined in [19] by the same simulation method as in present paper.

In conclusion, we note that the results of current Monte Carlo investigations demonstrate a significant influence of easy axis anisotropy on non-equilibrium critical behavior of the 3D ferromagnetic Heisenberg model leading to characteristics typical for the 3D Ising model.

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