Journal of Siberian Federal University. Mathematics & Physics 2018, 11(5), 622–626

УДК 538.9

# Studies of Non-Equilibrium Relaxation Heisenberg Model with Long-Range Correlations Defects

**Maria A. Medvedeva***
Omsk State University
Mira, 55A, Omsk, 644077
Institute of Engineering Physics and Radio Electronics
Siberian Federal University
Svobodny, 79, Krasnoyarsk, 660041
Russia

**Pavel V. Prudnikov**†
Omsk State University
Mira, 55A, Omsk, 644077
Russia

Received 05.12.2016, received in revised form 14.12.2017, accepted 20.06.2018

*Monte Carlo simulations of the short-time dynamic behavior are reported for three-dimensional Heisenberg model with long-range correlated disorder at criticality, in the case corresponding to linear defects. Former was carried out both from high-temperature and low-temperature initial states. The static and dynamic critical exponents are determined for systems starting from different initial state. The obtained values of the exponents demonstrated a strong influence of long-range correlated quenched defects on the critical behavior of the systems described by the many-component order parameter.*

*Keywords: Monte Carlo methods, disordered systems, short-time dynamic, Heisenberg model, disorder with long-range correlation.*
DOI: 10.17516/1997-1397-2018-11-5-622-626

Critical properties of structurally disordered magnets remain a problem of great interest in condensed matter physics, as far as real magnetic crystals are usually non-ideal. Commonly, in theoretical studies, as well as in Monte Carlo simulations, one considers point-like uncorrelated quenched non-magnetic impurities [1]. However, in real magnets one encounters non-idealities of structure, which cannot be modeled by simple point-like uncorrelated defects. Indeed, magnetic crystals often contain defects of a more complex structure: linear dislocations, planar grain boundaries, three-dimensional cavities or regions of different phases, embedded in the matrix of the original crystal, as well as various complexes (clusters) of point-like non-magnetic impurities. Therefore, a challenge is to offer a consistent description of the critical phenomena influenced by the presence of such complicated defects.

In this paper one present a numerical study of the influence of structural long-range (LR) correlated defects on the non-equilibrium critical behavior of complex systems described by the Heisenberg model. A special type of such a disorder has been considered at first by Weinrib and Halperin [2]. As a result, the existence of LR correlations in the disorder gives significant effect and wider class of disordered systems can be characterized by a new universality class of critical behavior.

*mmed@mail.ru
†prudnikp@univer.omsk.su

# 1. Model and methods

We have considered the following 3D site-diluted ferromagnetic spin model with Heisenberg Hamiltonian. Hamiltonian defined in a cubic lattice of linear size $L$ with periodic boundary conditions $H = -J\sum_{i,j} p_i p_j \vec{S}_i \vec{S}_j$, where $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$, the sum is extended to the nearest neighbors, $J > 0$ is the short-range exchange interaction between spins $\vec{S}_i$, and the $p_i$ are quenched random variables ($p_i = 1$, when the site $i$ is occupied by spin, and $p_i = 0$, when the site is empty), with long-range spatial correlation. It is believed that the effects of long-range correlations between the point like defects are implemented in the form of randomly oriented lines. We used the following method for creating impurity configurations: the lines parallel to the coordinate axes were deleted randomly from a filled three-dimensional lattice spins in order to acquire a given concentration of impurities.

According to the argument of Janssen et al. [3] obtained with the RG method and $\varepsilon$-expansion, one may anticipate a generalized scaling relation for the $k$-th moment of the magnetization

$$m^{(k)}(t,\tau,L,m_0) = b^{-k\beta/\nu} m^{(k)}(b^{-z}t, b^{1/\nu}\tau, b^{-1}L, b^{x_0}m_0). \quad (1)$$

And it is realized after a time scale $t_{\rm mic}$ which is large enough in a microscopic sense but still very small in a macroscopic sense. In (1) $b$ is a spatial re-scaling factor, $\beta$ and $\nu$ are static critical exponents, $z$ is the dynamic exponent, 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.

When system evolving from high-temperature state ($m_0 \ll 1$) we can choose the scaling factor $b = t^{1/z}$ and applying the scaling form (1) for $k = 1$ to the small quantity $t^{x_0/z}m_0$, one obtains

$$m(t,\tau,m_0) = m_0 t^{\theta'} m(t^{1/\nu z}\tau, t^{x_0/z}m_0) = m_0 t^{\theta'}\left(1 + a t^{1/\nu z}\tau\right) + O(\tau^2, m_0^2), \quad (2)$$

where $\theta' = (x_0 - \beta/\nu)/z$ has been introduced. For $\tau = 0$ and small enough $t$ and $m_0$, the scaling dependence for magnetization (2) takes the form $m(t) \sim m_0 t^{\theta'}$. For almost all statistical systems studied so far, the exponent $\theta'$ is positive. Time scale for this initial increase of magnetization is $t_0 \sim m_0^{-z/x_0}$.

Other interesting observable in short-time dynamics is the second moment of magnetization $m^{(2)}(t)$ and autocorrelation function $A(t)$. 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 (2) for $\tau = 0$ and $b = t^{1/z}$, one obtains

$$m^{(2)}(t) \sim t^{-2\beta/\nu z} m^{(2)}(1, t^{-1/z}L) \sim t^{c_2}, \quad A(t) \sim t^{-c_a}, \quad (3)$$

where $c_2 = (d - 2\frac{\beta}{\nu})/z$ and $c_a = d/z - \theta'$.

For ferromagnetic films the order parameter can be defined as magnetization. For disordered system $k$-th moment of magnetization and autocorrelation function can be determined like

$$m^{(k)}(t) = \left[\left\langle \frac{1}{N_s^k}\left|\sum_i^{N_s} p_i \vec{S}_i(t)\right|^k \right\rangle\right], \quad A(t) = \left[\left\langle \frac{1}{N_s}\sum_i p_i \vec{S}_i(t)\vec{S}_i(0)\right\rangle\right], \quad (4)$$

where angle brackets denote the statistical averaging, the square brackets are for averaging over the different impurity configurations, $N_s = pL^3$ is a number of spins in the lattice, and $p$ is a spin concentration. 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 (2), one can skip besides $L$, also the argument $m_0 = 1$ with $b = t^{1/z}$ and for $k = 1$ one has

$$m(t,\tau) = t^{-\beta/\nu z} m(1, t^{1/\nu z}\tau) = t^{-\beta/\nu z}\left(1 + a t^{1/\nu z} + O(\tau^2)\right). \quad (5)$$

In order to calculate the critical exponent $z$ we have used the ratio [4]

$$F_2(t) = m^{(2)}(t)|_{m_0=0}/m^2(t)|_{m_0=1} \sim t^{d/z}.$$

## 2. Results of Monte Carlo modeling and analysis of results

Most of the work is devoted to the study of weakly disordered systems with spin concentration $p = 0.80$ and above. Strong-diluted systems with spin concentration $p < 0.69$ down to the spin percolation threshold $p_c = 0.31$ are less studied. Initial configurations for systems with the spin concentration $p = 0.60$ and randomly distributed quenched linear defects were generated numerically. Starting from initial configurations, the system was updated with Metropolis algorithm at the critical temperatures $T_c(p = 0.60) = 0.888(2)\ J/k_b$[5]. Simulation have been performed up to $t = 2000$ Monte Carlo steps per spin (MCS/s).

For calculating the critical exponents $z$ and $\theta'$ of ferromagnetic we considered systems with linear size $L = 64$. We have studied evolution both from high-temperature ($m_0 \ll 1$): $m_0 = 0.03$, 0.02, 0.01, 0.003, 0.002, 0.001, 0.0001 (Fig. 1a) and from low-temperature ($m_0 = 1$) (Fig. 1b) initial states.

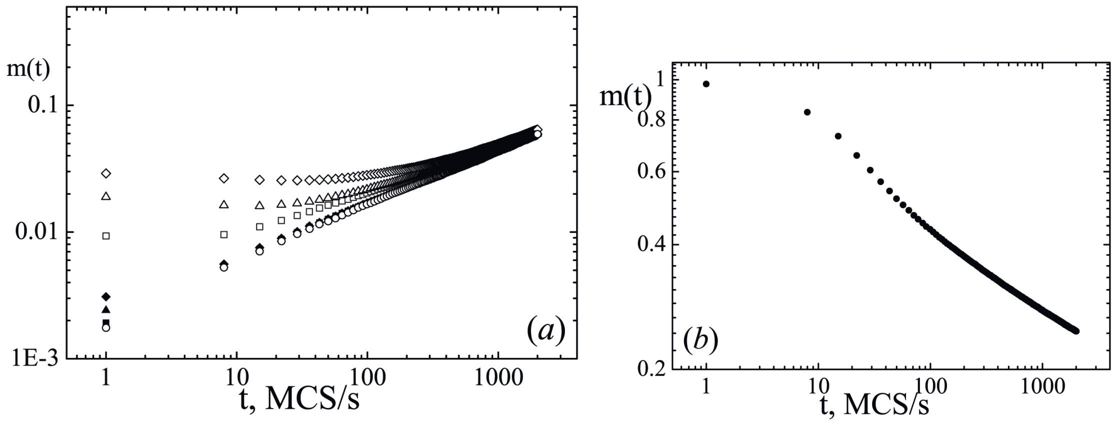


Fig. 1. Time dependencies of magnetization for different initial state $m_0 \ll 1$ ($a$): 0.03 (◇), 0.02 (△), 0.01 (□), 0.003 (♦), 0.002 (▲), 0.001 (■), 0.0001 (○) and $m_0 = 1$ ($b$)

In this work we investigated the time dependencies of the magnetization $m(t)$, second moment of magnetization $m^{(2)}(t)$, cumulant $F_2(t)$ and autocorrelation function $A(t)$. From the slope of this curve we can estimate the value of critical exponents $\theta'$, $c_2$, $d/z$ and $c_a$ for different initial state, correspondingly. Final values of exponents obtained by linear interpolation of the initial magnetization to zero. From this ratios we calculate values of $z$, $\beta/\nu$ and $\theta'$.

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 LR-correlated disorder and is the alternative to traditional Monte Carlo methods. The dynamic and static critical exponents were computed with the use of the leading corrections to scaling for the 3D Heisenberg model with linear defects and their values $z = 2.497(2)$, $\beta/\nu = 0.473(4)$, $\theta' = 0.425(3)$ can be considered as final.

The obtained results confirm the strong influence of LR-correlated quenched defects on the critical behavior of the systems described by the many-component order parameter. It was shown that weakly and strongly diluted Heisenberg model with long-range correlation disorder defects belong to different universality classes. We have found that increasing of the concentration structural defects with long-range correlations lead to significant slowdown in the critical processes of relaxation compared with order and weakly disordered systems. This is indicated by the values of the critical exponents for weakly disordered Heisenberg model $z = 2.257(61)$, $\beta = 0.393(77)$, $\nu = 0.770(74)$ (MC simulation [6]), $z = 2.264$, $\beta/\nu = 0.481$ (RG [7]) and the values of the critical exponents for pure Heisenberg model $\beta/\nu = 0.516(10)$, $\nu = 0.705(3)$, $\beta = 0.364(5)$ [8] and $z = 2.049(31)$, $\beta/\nu = 0.510(10)$ [6].

The dynamic critical exponent $z = 3.529(125)$ and static critical exponent $\beta/\nu = 0.946(48)$, $\nu = 0.821(14)$ were obtained in work [5] in the investigation of defects influence on the characteristics of the non-equilibrium critical behavior of the three-dimensional Heisenberg model in its evolution from low temperature initial state ($m_0 = 1$). We suppose that there is carried out the non-equilibrium domain structure changes during the transition from the single-domain state at $T_0 = 0$ to multi domain fluctuation structure arising at the critical temperature of $T_c$. This results due to the pinning of domain walls on the structural defects to significant changes in the characteristics of the non-equilibrium behavior of structurally disordered Heisenberg model compared to the simulation case from the high temperature state.

*The work was performed within the grants no. MD-6024.2016.2 and MD-6868.2018.2 of Council on grants of the President of the Russian Federation and within the projects of Russian Foundation of Basic Research no. 16-32-00581, 17-02-00279, 18-42-550003. The calculations were performed using the resources provided by the Shared Facility Center "Data Center of FEB RAS" (Khabarovsk), the Supercomputing Center of Lomonosov Moscow State University, Moscow Joint Supercomputer Center and St. Petersburg Supercomputer Center of the Russian Academy of Sciences.*

# References

[1] R.Folk, Yu.Holovatch, T.Yavors'kii, Critical exponents of a three-dimensional weakly diluted quenched Ising model, *Phys. Usp.*, **46**(2003), no. 6, 169–191.

[2] A. Weinrib, B. I Halperin, Critical phenomena in systems with long-range-correlated quenched disorder, *Phys. Rev. B.*, **27**(1983), 413–428.

[3] H.K.Janssen, B.Schaub, B.Schmittmann, New universal short-time scaling behaviour of critical relaxation processes, *Z. Phys. B.*, **73**(1989), 539–549.

[4] R. da Silva, N.A.Alves, J.R.Drugowich de Felécio, Mixed initial conditions to estimate the dynamic critical exponent in short-time Monte Carlo simulation, *Phys. Lett. A*, **298**(2002), 325–329.

[5] P.V.Prudnikov, M.A.Medvedeva, Nonequilibrium critical behavior of highly disordered magnets with long-range defect correlation, *Low Temp. Phys.*, **40**(2014), 443–452.

[6] P.V.Prudnikov, M.A.Medvedeva, Non-equilibrium critical relaxation of the 3D Heisenberg magnets with long-range correlated disorder, *Progr. Theor. Phys.*, **127**(2012), 369–382.

[7] V.V.Prudnikov, P.V.Prudnikov, A.A.Fedorenko, Field-theory approach to critical behavior of systems with long-range correlated defects, *Phys. Rev. B.*, **62**(2000), 8777–8786.

[8] K.Chen, A.M.Ferrenberg, D.P.Landau, Static critical behavior of three-dimensional classical Heisenberg models: A high-resolution Monte Carlo study, *Phys. Rev. B.*, **48**(1993), 3249–3256.

# Исследование неравновесной релаксации модели Гейзенберга с дальнодействующей корреляцией дефектов

**Мария А. Медведева**
Омский государственный университет
Мира, 55а, Омск, 644077
Институт инженерной физики и радиоэлектроники
Сибирский федеральный университет
Свободный, 79, Красноярск, 660041
Россия

**Павел В. Прудников**
Омский государственный университет
Мира, 55а, Омск, 644077
Россия

*Было проведено компьютерное моделирование методами Монте-Карло для трехмерной модели Гейзенберга с дальнодействующей корреляцией дефектов вблизи критической точки в случае, соответствующем линейным дефектам. Моделирование проводилось как из высокотемпературного так и из низкотемпературного начального состояния. Статические и динамические критические индексы были рассчитаны для систем из различных начальных состояний. Полученные значения показателей демонстрируют сильное влияние дальнодействующей корреляции вмороженных дефектов структуры на критическое поведение систем с многокомпонентным параметром порядка.*

*Ключевые слова: методы Монте-Карло, неупорядоченные системы, коротко-временная динамика, модель Гейзенберга, дефекты с дальнодействующей корреляцией.*