Numerical investigation of the critical behavior of the three-dimensional Ising model near the percolation threshold

M A Shlyakhtich¹,⁴, P V Prudnikov²,⁴, A S Papushin²

¹ Department of Theoretical Physics and Wave Phenomena, Siberian Federal University, 79 Svobodny Av., Krasnoyarsk, 660041, Russia
² Department of Theoretical Physics, Omsk State University, Mira prospekt 55-A, Omsk, 644077, Russia

E-mail: ¹mmed@mail.ru, ²prudnikp@univer.omsk.su

Abstract. In this work we investigate the critical behavior of the disordered three-dimensional Ising model with an impurity concentration close to the threshold of impurity percolation on high-performance computing systems. Starting from initial configurations, the system was updated with Metropolis algorithm and invaded cluster algorithm. The values of dynamic critical exponent $z$ and static critical exponent $\beta/\nu$ were obtained in this paper for both algorithm.

1. Introduction

The question of how structure defects modifies a phase transition is not fully solved. Many issues is still open, even in the case of the ferromagnetic transition in the the system with quenched disorder, from the qualitative nature of the ordered phase near criticality [1, 2].

The description of phase transitions is considered to be one of the most urgent and complex problems of statistical physics. The anomalously long-lived and large fluctuations of some thermodynamic quantities observed as the phase transition point approaches are characterized by strong interactions, which creates considerable difficulties in the experimental and analytical investigation of critical behavior. Computer simulation is an independent tool for investigating the abnormal behavior of a second-order phase transition [3, 4], as evidenced by the progress in the development of various methods of computer simulation. Therefore, one of the important tasks is the development of computer simulation methods that depend weakly on the effects of critical slowdown.

In recent years, the study of various disordered models near the threshold of impurity percolation has become an interesting and actual problem [5, 6, 7]. In this paper we have investigated the critical properties of the Ising model near the percolation threshold. At a concentration close to critical, a cluster appears that connects the opposite sides of the lattice. The largest cluster has a fractal dimension at the critical concentration $p = p_c$. In the theoretical description of the behavior of such systems, the concentration of defects by a small quantity can no longer be considered. That makes their theoretical description very difficult or even impossible. A Invaded cluster algorithm was proposed in [8], which is much more effective than all previous methods near the impurity percolation threshold.
2. Algorithms and Methods
Anomalous properties of system in second order phase transitions is a critical slowing down of the relaxation process. Which manifests itself in a slow change over time, the characteristic thermodynamic quantity - of the order parameter (magnetization for ferromagnetic systems) tends to equilibrium:

$$\tau_{rel} \sim |T_c - T|^{-z\nu} \quad (1)$$

where $\tau_{rel}$ – the relaxation time diverges on approaching the critical temperature.

In the theoretical description of the behavior of systems with critical spin concentration $p = p_c$, the concentration of defects by a small quantity can no longer be considered. That makes their theoretical description very difficult. The algorithm proposed in [8] is much more effective than all previous methods near the impurity percolation threshold. The new algorithm called Invaded cluster algorithm. The primary goal is to reduce the effective autocorrelation time and, therefore, to improve the statistical sampling of generated configurations.

The Invaded cluster algorithm works as follows. The bonds of the lattice are given a random order starting with an Ising spin configuration $S$. Correlated invasion percolation clusters are grown until one of clusters spans the system. After the growth process is terminated, cluster is flipped with probability $P_n$ yielding a new spin configuration $S'$. $P_n = \exp(-\Delta E/kT)$, \quad (2)

where $\Delta E$ is the change in the energy of the system caused by the test configuration change.

According to Janssen’s arguments [9] obtained using the $\varepsilon$-expansion and renormalization group method, one may anticipate a generalized scaling relation for the $k$-th moment of the magnetization

$$m^{(k)}(t, \tau, L, m_0) = b^{-k\nu} m^{(k)}(t/b^z, b^{1/\nu}\tau, L/b, b^{x_0}m_0). \quad (3)$$

This relation realized after a very small time $t_{mic}$ in macroscopic sense but this time is large enough. In (3) $b$ is a spatial rescaling 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.

Problem of finite size is almost absent while the correlation length is small. This happens in the early stage of system evolution. Therefore, we consider $L = 128$ large enough and solve this problem.

We can skip the argument $m_0 = 1$ in (3) like a large enough linear size $L$,

$$m^{(k)}(t, \tau) = b^{-k\nu} m^{(k)}(b^{-z}t, b^{1/\nu}\tau). \quad (4)$$

In this work computer simulation was carried out. It began from a completely ordered initial state. The system is simulated at critical temperature. We measured the magnetization $m(t)$ and second order moment of magnetization $m^{(2)}(t)$. One can steer clear of the main dependence from time in (4) when $b = t^{1/z}$ and $k = 1$. And we have

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

For critical point $\tau = 0$

$$m(t) \sim t^{-\beta/\nu}. \quad (6)$$

In order to calculate the critical exponent $\nu$ we have used the second order Binder cumulant

$$U_2(t) = \frac{\langle (m^{(2)}) \rangle}{\langle (m) \rangle^2} - 1 \sim t^{\beta/\nu}. \quad (7)$$
3. Results of Monte Carlo modeling

For calculating the critical exponents of disordered Ising model we considered simple cubic lattices with linear size $L = 128$.

In this work computer simulation was carried out. It began from a completely ordered initial state. The system is simulated at critical temperature $T_c = 3.091266(20)$. We measured the magnetization $m(t)$ and second order moment of magnetization $m^{(2)}(t)$. Simulations have been performed up to $t = 10000$ MCS/s. The final lines were obtained after averaging more than 600 samples. Starting from initial configurations, the system was updated with Metropolis algorithm and Invaded cluster algorithm.

For ferromagnetic films the order parameter can be defined as magnetization and calculate by equation

$$m^{(k)}(t) = \left[ \langle \left( \frac{1}{N_s} \sum_{i=1}^{N_s} p_i S_i(t) \right)^k \rangle \right].$$

In (8), the angular and square brackets designate statistical averaging and averaging over the different impurity configurations, respectively, $N_s = pL^3$ is a number of spins in the simple cubic lattice, and $p = p_c = 0.688313500$ is a spin concentration.

Time dependencies of magnetization are presented on figure 1 both for Metropolis algorithm and Invaded cluster algorithm. We can estimate the value of critical non-equilibrium exponent $\beta/\nu z$ from slope of magnetization at low-temperature initial state on $t \in [1000; t_{\text{right}}]$. The minimum error of determining the critical exponent $\beta/\nu z$ is reached on time interval $[1000; t_{\text{right}}]$ with $t_{\text{right}} = 5400$ for Metropolis algorithm and $t_{\text{right}} = 3100$ for invaded cluster algorithm. We got the values of critical exponent $\beta/\nu z = 0.7225$ for Metropolis algorithm and $\beta/\nu z = 2.1792$ for invaded cluster algorithm.

From the slope of time dependence of the second order Binder cumulant $U_2(t)$ (figure 2) we can estimate the value of critical exponent $d/z$. The time interval $[t_{\text{left}}; 9800]$ for $t_{\text{left}} = 3700$ gives the minimum of errors for exponent $d/z$ for Metropolis algorithm. The time interval $[t_{\text{left}}; 2900]$ for $t_{\text{left}} = 1300$ gives the minimum of errors for exponent $d/z$ for invaded cluster algorithm. We got the values of critical exponent $d/z = 1.3835$ for Metropolis algorithm and $d/z = 4.1528$ for invaded cluster algorithm.

We have regarded the influence of a principal corrections to the scaling on asymptotic values of exponents [4] in order to get exact values of the critical exponents. We have used the next
Figure 3. Dependencies of global mean-square error \( \Delta_{d/z} \) for all time intervals as a function of the exponent \( \omega/z \): (a) Metropolis algorithm, (b) Invaded cluster algorithm.

relation for the observable \( X(t) \):

\[
X(t) = A_x t^\delta (1 + B_x t^{-\omega/z}),
\]

where \( \omega \) is an exponent of the principal corrections to scaling, \( A_x \) and \( B_x \) are fitting parameters. In (9) \( \delta = \beta/\nu z \) when \( X \equiv m(t) \), \( \delta = d/z \) when \( X \equiv U_2(t) \). We can determine the exponents \( \delta \) and \( \omega/z \) from minimum of the mean square errors \( \sigma_\delta \) of this fitting procedure. after that all minimal values of \( \delta \) are averaged by all intervals of time. The global mean-square error \( \Delta_\delta \) (Figure 3) is determined from averaged values of \( \delta \) [4].

4. Conclusion

The value of exponent \( \beta/\nu z = 0.6518(609) \) was calculated using \( \omega/z = 0.0860 \), value of \( d/z = 1.1838(109) \) was calculated using \( \omega/z = 0.3275 \) for Metropolis algorithm. The value of \( \beta/\nu z = 2.254(327) \) was calculated using \( \omega/z = 0.2700 \), value of \( d/z = 4.0994(881) \) was calculated using \( \omega/z = 0.0975 \) for invaded cluster algorithm. We defined the final values of \( z \) and \( \beta/\nu \) using the values given above. The calculated values of \( z \) and \( \beta/\nu \) are presented in table 1.

| Algorithm       | \( z \)       | \( \beta/\nu \) |
|-----------------|---------------|-----------------|
| Metropolis      | 2.534(234)    | 1.652(37)       |
| Invaded cluster | 0.732(16)     | 1.650(60)       |

The value of dynamic critical exponent \( z \) obtained by the invaded cluster algorithm three times smaller than the value for the Metropolis algorithm. That’s why the invaded cluster algorithm can be successfully applied to introduce a disordered system into an equilibrium state.

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References

[1] Tarjus G and Dotsenko V 2002 J. Phys. A 35 1627
[2] Krzakala F, Ricci-Tersenghi F, Sherrington D, and Zdeborova L 2011 J. Phys. A 44 042003
[3] Prudnikov V V, Prudnikov P V, Krinitsyn A S, et. al. 2010 Phys. Rev. E 81 011130
[4] Prudnikov P V, Medvedeva M A 2012 Progr. Theor. Phys. 127 369
[5] Balog I, Uzelac K 2007 Phys. Rev. E 76 011103
[6] Faraggi E 2008 Phys. Rev. B 78 134416
[7] Dixon K, Venus D 2017 Phys. Rev. B 95 245438
[8] Machta J, Choi Y S, Lucke A, Schweizer T 1995 Phys. Rev. Lett. 15 2792
[9] Janssen H K, Schaub B, Schmittmann B 1989 Z. Phys. B 73 539