Monte Carlo simulation of the critical behavior near the percolation threshold with invaded cluster algorithm

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Abstract. We investigated the critical behavior of the disordered three-dimensional Ising model with an impurity concentration close to the threshold of impurity percolation \( p = p_c = 0.688313500 \) on high-performance computing systems. The system was updated using Metropolis algorithm and invaded cluster algorithm from initial configurations. The values of dynamic critical exponent \( z \) and static critical exponents \( \beta \) and \( \nu \) were obtained in this paper.

1. Introduction

Percolation exhibits a continuous crossover between a macroscopically disconnected state and a connected state [1, 2]. It is a classical model in statistical physics. The elements of a lattice (sites or bonds) are absent with probability \( 1 - p \) and present with probability \( p \). The cluster is composed of sites connected by bonds. There is at least one cluster connecting two sides of a lattice with free boundary conditions above a critical value \( p > p_c \). The scale-free behavior is observed at the critical point \( p = p_c \). Amplitude ratios, critical exponents and correction-to-scaling exponents are important characteristics of the percolation transition. Its are universal and so are independent of the microscopic lattice details such as system shape (square, triangular, honeycomb), lattice type (simple cubic lattice, body-centered cubic lattice, face-centered cubic lattice) and type of boundaries (rectangle, rhombus, square) [3, 4, 5, 6, 7]. While others properties depends on the considered lattice [1, 8].

In the last years, the investigation of different disordered models near the threshold of impurity percolation has become an actual and interesting problem [9, 10, 11, 12]. We investigated the critical properties of the Ising model near the percolation threshold in this paper. A cluster appears when concentration of spin close to critical. It connects the opposite sides of the cubic lattice. The largest cluster has a fractal dimension at the critical concentration \( p = p_c \). Theoretical description of such disordered system is very complex or even impossible. Because the concentration of defects cannot be used like a small quantity. A invaded cluster algorithm was proposed in [13]. This algorithm is much more effective than all early methods near the impurity percolation threshold.
2. Methods and Algorithms

Critical slow-down of the relaxation process is anomalous property of system in second order phase transitions. This is manifested in the slow change in time of the order parameter when approaching equilibrium:

\[ \tau_{\text{rel}} \sim |T_c - T|^{-\nu} \]  

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

When the spin concentration is equal to critical \( p = p_c \) then we cannot considered the concentration of defects as a small quantity in the theoretical description of the behavior of systems. This makes their theoretical description so hard or even impossible. A Invaded cluster algorithm is much more effective than all early methods near the impurity percolation threshold. It was proposed in [10]. The main aim of this algorithm is to make less the effective autocorrelation time and, therefore, to make better the statistical sampling of generated configurations.

The new method called 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-up until one of the clusters extend from side to side of the system. Process is terminated after the growth, the cluster is flipped with probability \( P_n \) yielding a new spin configuration \( S' \).

\[ P_n = \exp \left( -\frac{\Delta E}{kT} \right), \]  

where \( \Delta E \) is the change in the energy of the system result in the test configuration change.

It is known that the asymptotic critical mode becomes difficult to achieve when introducing quenched disorder as non-magnetic impurities into a pure system. Moreover, here is observed a bad averaging of \( R_x \rightarrow \text{const} \neq 0 \) where \( X \) stands for any thermodynamic parameter, \( R_x \) is the mean-square deviation of the thermodynamic parameter \( X \). Values of \( R_x \) demonstrate the achievement of the asymptotic mode in the dependence on a number of disordered configurations [14, 15].

The short-time dynamics method (STD) was developed in paper [16] to describe the effect of non-equilibrium initial conditions on the critical dynamics. This method allows us to calculate values dynamic critical exponents. However, it can be used to calculate static critical exponents. A feature of the STD is that information on universal critical behavior can be obtained until the asymptotic mode.

Based on the \( \varepsilon \)-expansion and renormalization group analysis [16], we can expect that the main scaling dependence for the \( k \)-th moment of magnetization

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

This dependence is work out after a time \( t_{\text{mic}} \) which is very small in a macroscopic sense but still large enough. In (3) \( z \) is the dynamic exponent, \( \beta \) and \( \nu \) are static critical exponents, \( b \) is a spatial rescaling factor and \( \tau = (T - T_c)/T_c \) is the reduced temperature. New independent exponent \( x_0 \) is the scaling dimension of the start magnetization \( m_0 \).

Problem of finite size is almost absent while the correlation length is small. This takes place in the early stage of system evolution. That is why, we regarded \( L = 128 \) large enough to solve this problem.

Also in the scaling form (3), we passed the argument \( m_0 = 1 \),

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

In this work, computer simulation was began from a completely ordered initial state. The system was simulated at or near critical temperature. We measured the cumulant \( U_4 \) in
equilibrium in order to check up the value of critical temperature. It is defined as

\[ U_4 = \frac{1}{2} \left( 3 - \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} \right). \]  

(5)

The cumulant \( U_4(L, T) \) is characterized a scaling form

\[ U_4(L, T) = u \left( L^{1/\nu} (T - T_c) \right). \]  

(6)

In this study the critical temperature \( T_c \) was determined using the scaling relation of the cumulant 6. This \( T_c \) was measured from the coordinate of the intersection points of the temperature dependence of \( U_4(L, T) \) for different \( L \). The scaling relation of the cumulant was used to calculate critical exponents \( \nu \). The effective exponent \( 1/\nu \) was defined from the derivative of the cumulant \( U_4 \) with respect to \( T \) at \( T = T_c \)

\[ \frac{dU_4}{dT} \sim L^{1/\nu}. \]  

(7)

The \( m(t) \) and \( m^{(2)}(t) \) are measured quantities. One avoids the main \( t \) dependence in \( m^{(k)}(t) \) with \( b = t^{1/z} \). One has (8) for \( k = 1 \)

\[ m(t, \tau) = t^{-\beta/\nu z} m(1, t^{1/\nu z} \tau) = t^{-\beta/\nu z} (1 + a t^{1/\nu z} + O(\tau^2)). \]  

(8)

For \( \tau = 0 \) (\( T = T_c \))

\[ m(t) \sim t^{-\beta/\nu z}. \]  

(9)

We have used the second order Binder cumulant \( U_2(t) \) in order to estimate the critical exponent \( z \)

\[ U_2(t) = \frac{\langle m^{(2)} \rangle}{\langle m \rangle^2} - 1 \sim t^{d/z}. \]  

(10)

**Figure 1.** Temperature dependencies of cumulant \( U_4(L, T) \) for different \( L \).
3. Results and Conclusions

Here we investigated the critical behavior of bulk system such as the disordered three-dimensional Ising model with an impurity concentration close to the threshold of impurity percolation $p_c = 0.688313500$ on high-performance computing systems. The system was updated using the Metropolis algorithm and the invaded cluster algorithm starting from initial configurations. The $m(t)$ and $m^{(2)}(t)$ are measured quantities. Simulations have been performed up to $t = 10000$ MCS/s. The resulting curves have been obtained by averaging over 600 samples.

Because computer simulations must necessarily be done on finite systems. That is why the main part of work is to determine the nature of the finite-size corrections. The use of periodic boundary conditions reduces those corrections to subsurface terms.

Firstly temperature dependencies of $U_4(L, T)$ were obtained. These quantities were calculated in equilibrium state. In order to bring the system into equilibrium we used invaded cluster algorithm. This curves are presented in figure 1 for different size of lattice $L = 128 \div 256$. We considered simple cubic lattices with periodic boundary conditions. The critical temperature $T_c$ was determined from the coordinate of the intersection points of the temperature dependence of $U_4(L, T)$ for different $L$.

In the next part of our work the values of dynamic critical exponent $z$ and static critical exponent $\nu$ were obtained using both algorithm Metropolis and invaded cluster algorithm. These exponents were obtained in the early stage of system evolution before equilibrium using short-time dynamics method. This method proposed by Janssen et al. [16].

Problem of finite size is almost absent while the correlation length is small. This takes place in the early stage of system evolution. That is why, we regarded simple cubic lattices with linear size $L = 128$ large enough to solve this problem. The system was simulated numerically from a completely ordered state $m_0 = 1$. Further, the evolution of the system was studied at the critical temperature $T_c = 3.091266(20)$.

The order parameter can be defined as magnetization for ferromagnetic films and can be calculated by equation

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

where angle brackets designate the statistical averaging, the square brackets designate the
averaging over the different impurity configurations, \( N_s = p \cdot L^3 \) is a number of spins in the lattice, and \( p = p_c = 0.688313500 \) is a spin concentration.

One may expect a common scaling relation for the \( k \)-th moment of magnetization with \( b = t^{1/z} \), \( k = 1 \) and \( \tau = 0 \):

\[
m(t) \sim t^{-\beta/\nu z}.
\]

This relation was obtained by Janssen et al. [16] using the RG method and \( \varepsilon \)-expansion.

In order to determine the critical exponent \( z \) we have applied next form for calculating the second order Binder cumulant

\[
U_2(t) = [(m^{(2)})^2]/\langle m \rangle^2 - 1 \sim t^{d/z}.
\]

Time dependencies of magnetization and second order Binder cumulant are shown in figure 2 and figure 3, respectively, both for Metropolis algorithm and invaded cluster algorithm. The value of exponent \( d/z \) and \( \beta/\nu z \) was computed from the slope of these dependencies.

These values were obtained taking into account the leading correction to the scaling. We have applied the next expression for the observable quantities \( X(t) \):

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

where \( \omega \) is an exponent of the leading corrections to scaling, \( A_x \) and \( B_x \) are approximation parameters, and an exponent \( \delta = \beta/\nu z \) for \( X \equiv m(t) \), \( \delta = d/z \) for \( X \equiv U_2(t) \). The exponents \( \delta \) and \( \omega/z \) were obtained from the minimum of the mean square errors \( \sigma_\delta \) of this approximation procedure. All this values of \( \delta \) are averaged by all time intervals. The global mean-square error \( \Delta_\delta \) is determined based on averaged values of \( \delta \) [17].

We calculated value of exponent \( d/z = 1.184(11) \) with \( \omega/z = 0.328 \), value \( \beta/\nu z = 0.652(61) \) with \( \omega/z = 0.086 \) for Metropolis algorithm. Also we computed value of exponent \( d/z = 4.099(88) \) with \( \omega/z = 0.098 \), value \( \beta/\nu z = 2.255(33) \) with \( \omega/z = 0.270 \) for invaded cluster algorithm. We obtained the end values of the critical exponents \( z = 2.534(234) \) and \( \beta/\nu = 1.652(37) \) for Metropolis algorithm and \( z = 0.732(16) \) and \( \beta/\nu = 1.650(60) \) for invaded cluster algorithm based on the previous values of exponents.

Finally the scaling relation of the cumulant was used to calculate critical exponents \( \nu \). The effective exponent \( 1/\nu \) was defined from the derivative of the cumulant \( U_4 \) with respect to \( T \) at \( T = T_c \) (7). We obtained the critical exponent \( \nu \) for different temperatures above
Table 1. The values of critical exponents for Ising disordered system

| Algorithm          | Metropolis | Invaded cluster |
|--------------------|------------|-----------------|
| $z$                | 2.534(234) | 0.732(16)       |
| $\beta/\nu$       | 1.652(37)  | 1.650(60)       |
| $\nu$              | 0.958(40)  |                 |
| $\beta$            | 1.582(96)  | 1.581(118)      |

$T_c$ and for different linear sizes of lattice $L = 128, 192, 256, \infty$ (figure 4). The effective value of $\nu = 0.958(40)$ can be defined only in the thermodynamic limit. These values were calculated using the linear approximation of linear size $L$ to infinity (blue curve). In addition we approximated the temperature to $T = T_c$ [17]. The cumulant $U_4$ as a function of the scaling variable $(T - T_c)L^{1/\nu}$ is shown in figure 5. It is obtained using the calculated values $\nu$.

The calculated values of $z$ and $\beta/\nu$ are presented in table 1. The value of dynamic critical exponent $z$ for invaded cluster algorithm is smaller than the value for Metropolis algorithm. That’s why the invaded cluster algorithm may be successfully used to introduce a disordered system into an equilibrium state.

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