Percolation of the Site Random-Cluster Model by Monte Carlo Method

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Herein, we propose a site random cluster model by introducing an additional cluster weight in the partition function of the traditional site percolation. To simulate the model on a square lattice, we combine the color-assignation and the Swendsen-Wang methods together to design a highly efficient cluster algorithm with a small critical slowing-down phenomenon. To verify whether or not it is consistent with the bond random cluster model, we measure several quantities such as the wrapping probability $R_e$, the percolation strength $P_\infty$, and the magnetic susceptibility per site $\chi_p$, as well as two exponents such as the thermal exponent $\gamma$ and the fractal dimension $y_c$ of the largest cluster. We find that for different exponents of cluster weight $q = 1.5, 2, 2.5, 3, 3.5$ and $4$, the numerical estimation of the exponents $\gamma$ and $y_c$ are consistent with the theoretical values. The universalities of the site random cluster model and the bond random cluster model are completely identical.

For larger values of $q$, we find obvious signatures of the first-order percolation transition by the histograms and the hysteresis loops of the percolation strength and the energy per site. Our results are helpful for the understanding of the percolation of traditional statistical models.

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I. INTRODUCTION

Broadbent and Hammersley initially presented the concept of percolation[1, 2], and then Stauffer introduced the properties of percolation in detail[3]. There have been broad applications of percolation: e.g. fluids in porous medium[4], the spread of infectious diseases on complex networks[5], the Hall effect with quantum spin[6], network vulnerability[7], forest fires[8], number of work results in the extensions of the RC model and the magnetic susceptibility per site $\chi_p$, as well as

of the site, the bond, or other microscopic details[9].

By the universalities, the phase transitions in a number of lattice statistical models can be connected with percolation transition. One important model, the random cluster (RC) model[10] created by Fortuin and Kasteleyn[11] in the 1960s, gives us a unified description of several classical statistical models, including the Ising, Potts[12], Ashkin-Teller[13] and the percolation models. This body of work results in the extensions of the RC model and many new possible critical behaviors[21–23].

An additional cluster weight factor in the partition function is the significant difference between the bond percolation model and the RC model. Inspired by this, in the present work, we propose a new model, the site RC (SRC) model which is made by combining the site percolation and the RC model, and adding a cluster weight factor in the partition function.

To investigate the critical behaviors of the new SRC model, we design a cluster-updating Monte Carlo method and simulate the new model. Many useful quantities are measured, such as the wrapping probability $R_e$, the percolation strength $P_\infty$ and the magnetic susceptibility per site $\chi_p$. By performing finite size scaling analysis of the above quantities, the very precise phase transition points are obtained. We also calculate the thermal exponent $\gamma$, and the fractal dimension $y_c$ of the largest cluster in such a way as to check that whether or not the universalities of the BRC percolation and the SRC percolation are completely consistent.

The outline of this work is as follows. Sec. II shows a brief review of the BRC model and shows how we generalize the site percolation model to the SRC model. Sec. III describes the algorithm and several sampled quantities in our Monte Carlo simulations. Numerical results are then
presented in Sec. IV. Conclusive comments are made in Sec. V.

II. MODEL

A. Potts Model and BRC model

Before the introduction of our model, this section provides a brief review of two classical models in statistical physics: the Potts model\[19\] and its generalization to the RC model\[18\]. The reduced Hamiltonian of the Potts model is:

\[\beta H = -K \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j},\]  

where \(\langle ij \rangle\) means the nearest-neighbour summation, \(K\) is the coupling interaction, \(\beta\) is the inverse temperature, \(\sigma_i\) is the state variable on the site \(i\) and can be any natural number less than or equal to \(q\). If \(q = 2\), the model is identical to the Ising model without an external field, \(s\) is the occupation number less than or equal to \(L\), in which the number of clusters \(n\) is 3 and the number of the occupied sites \(n_s\) is 17. The two circles labeled by “1” in the top and bottom of the dashed line, which means the first cluster is a wrapping cluster.

\[Z = \sum_{\langle ij \rangle} \prod_{\sigma} e^{K \delta_{\sigma_i, \sigma_j}}\]  

where the symbol \(u\) is the bond weight and defined as \(u = e^K - 1\)\[24\]. The above equation can be transformed into:

\[Z = \sum_{\{b\}} u^{n_b} q^{n_c}\]  

where the sum is over all bond configurations \(\{b\}\), \(n_b = \sum b_{ij}\) is the bond number in the configurations, and \(n_c\) is the number of clusters. The discrete number \(q\) now appears as a continuous variable. Thus, the BRC model can be regarded as a generalization of the Potts model. In the limit \(q \rightarrow 1\), it reduces to the bond-percolation model, whose partition function is:

\[Z = \sum_{\{b\}} (e^K - 1)^{n_b}\]  

This form can be easily transformed into:

\[Z = \sum_{\{b\}} p_b^{n_b} (1 - p_b)^{N_b - n_b}\]  

where \(p_b = \frac{u}{1 + u}\) and \(N_b\) is the total number of bonds in the lattice. The significant difference between the partition functions of the bond percolation model and the RC model is that Eq. 4 has the cluster weight \(q^{n_c}\) while Eq. 5 does not.

B. SRC model

Now, we generalize the site percolation to the SRC model\[17\]. The partition function of the site percolation is:

\[Z = \sum_{\{\sigma\}} p_s^{n_s} (1 - p_s)^{N - n_s}\]  

where \(N = L \times L\) is the total number of sites. We directly generalize it by introducing a cluster weight \(q^{n_c}\), and then derive the partition function of the SRC model as:

\[Z_{SRC} = \sum_{\{\sigma\}} p_s^{n_s} (1 - p_s)^{N - n_s} q^{n_c}\]  

where \(p_s = \frac{s}{1 + s}\), \(n_s\) is the number of occupied sites, \(N - n_s\) is the number of vacant sites, and \(p_s\) is the occupation fraction.

FIG. 1: A typical configuration of a SRC model on a two-dimensional lattice with size \(L = 7\), in which the number of clusters \(n\) is 3 and the number of the occupied sites \(n_s\) is 17.
probability for the sites in the configuration. The weight of a configuration is given by:

\[ W = p_s^{n_s} (1 - p_s)^{N - n_s} q^{n_c} \]  

(9)

As shown in Fig. 1, the weight of the typical configuration is \( p_s^{17} (1 - p_s)^{32} q^3 \).

III. ALGORITHM AND THE SAMPLED QUANTITIES

A. algorithm

There are a few efficient methods \([24, 27]\) to simulate the RC model. In the present paper, we combine the color-assignment \([24, 27]\) and the Swendsen-Wang \([28]\) methods together to design a highly efficient cluster algorithm with a small critical slowing-down phenomenon. Similar methods have been applied in several papers \([24, 30]\). The algorithm to simulate this model is as follows:

1. In a configuration, if two sites in the nearest neighborhood are occupied, then the two sites belong to a same cluster. Those vacant sites don’t belong to any cluster.

2. Assign each cluster with a green color (active), a probability of \( \frac{1}{q} \) but for a cluster with a red color (inactive), a probability of \( 1 - \frac{1}{q} \).

3. If the sites in the configuration belong to a red cluster or one of its four neighborhood sites is red, we will keep them inactive. For the remaining sites, we will let them be occupied with a probability of \( p \), and unoccupied with a probability of \( 1 - p \).

We define the percolation cluster as follows: If any cluster spans the whole lattice, the configuration is called a percolation configuration. For a finite system, it can be defined by various rules. In the present work, a percolation state means there is at least one “wrapping” cluster \([31]\) in the lattice and “wrapping” refers to a cluster that connects itself along one of the lattice directions. For example, in Fig. 1 the cluster labeled by “1” is a wrapping cluster, and the wrapping direction is the vertical direction. The wrapping cluster is only applicable to a lattice with periodic boundary conditions.

B. the sampled quantities

In order to obtain the critical phase transition points, we define the wrapping probability as:

\[ R_e = (R_x + R_y) / 2, \]  

(10)

where the subscript \( e \) represents a cluster forming along the \( x \) or \( y \) direction, and \((...)\) denotes ensemble averaging. If a wrapping cluster exists in the \( x \) direction, then \( R_x = 1 \), otherwise, \( R_x = 0 \). The rule is the same for the \( y \) direction.

The SRC model can be explored in view of site percolation. Therefore, we can define the order parameter of the percolation strength and magnetic susceptibility per site:

\[ P_\infty = \langle P \rangle = L^{-d} \langle S_{max} \rangle \]  

(11)

\[ \chi_p = L^{-2d} \langle \sum_{i=1}^{n_c} n_i^2 \rangle \]  

(12)

where \( S_{max} \) is the size (the number of sites) of the biggest cluster.

According to the finite-size scaling theory \([32, 33]\), the above parameters provide us the scaling behavior of them as a function of the system size \( L \) and the site occupation probability \( p \):

\[ R_e = R_e^{(0)} + a_1 (p - p_c) L^{y_1} + a_2 (p - p_c)^2 L^{2y_1} + \cdots \]  

(13)

\[ P_\infty = L^{y_h-d} (a_0 + a_1 (p - p_c) L^{y_1} + a_2 (p - p_c)^2 L^{2y_1} + \cdots ) \]  

(14)

\[ \chi_p = L^{2y_h-2d} (a_0 + a_1 (p - p_c) L^{y_1} + a_2 (p - p_c)^2 L^{2y_1} + \cdots ) \]  

(15)

It should be noted that the occupation probability is for the site occupation, instead of the bond occupation probability \([34]\), where \( p_c \) is the percolation threshold, \( y_1 \) is the thermal exponent, \( y_h \) is the fractal dimension of the largest cluster, \( d \) is the space dimension, and \( y_1, y_2, \cdots \) are negative correction-to-scaling exponents. The unknown parameters \( a_1, a_2, b_1, b_2 \) are to be determined later by a least squares fit of Eqs. (13)-(15). At the percolation point \( p_c \), Eqs. (14) and (15) reduce to:

\[ P_\infty = L^{y_h-d} (a_0 + b_1 L^{y_1} + b_2 L^{y_2} + \cdots ) \]  

(16)

and

\[ \chi_p = L^{2y_h-2d} (a_0 + b_1 L^{y_1} + b_2 L^{y_2} + \cdots ) \]  

(17)

which will be used to determine the exponent \( y_h \). The parameters \( b_1, b_2, \cdots \), in Eq. (17) are not necessarily equal to those in Eq. (17). If they were the same or negligible, that would automatically imply a power law obtained from the ratio of Eqs. (16) to (17) i.e. \( P_\infty / \chi_p \propto L^{d-y_h} \).
The theoretical values of the exponents \( y_t \) and \( y_h \) can be obtained by the Coulomb gas method \[35\] or conformal invariance \[36\], and they are given by:

\[
\begin{align}
\sqrt{q} &= -2 \cos(\pi g), \quad (18a) \\
y_t &= 3 - \frac{3}{2g}, \quad (18b) \\
y_h &= 1 + \frac{g}{2} + \frac{3}{8g}. \quad (18c)
\end{align}
\]

where the coupling constant \( g \) of the Coulomb gas is in the range \( 1/2 \leq g \leq 1 \). According to the above equations, the theoretical values of the both exponents will be shown in the following section.

### IV. Results

Firstly, we do a Monte Carlo simulation of the SRC model on the square lattice with the above algorithm. We find the algorithm has a small critical slowing-down phenomena with \( q \leq 4 \) and consequently we sample between every two Monte-Carlo steps. As the system enters into equilibrium states, we take \( 10^8 \) samples to calculate each quantity for the system sizes \( 8 \leq L \leq 64 \), and we take \( 10^6 \) samples for the system sizes \( 128 \leq L \leq 256 \)[37].

To obtain the critical point \( p_c \), and the exponent \( y_t \), we perform a finite-size scaling analysis of the wrapping probability \( P_e \) for various system sizes near the critical occupation probability \( p_c \). At the critical point \( p_c \), we calculate the percolation strength \( P_\infty \) and the magnetic susceptibility per site \( \chi_p \) to obtain the exponent \( y_h \) by a power-law fitting. We also study the cases for larger values of \( q \), such as \( q = 10 \).

#### A. \( q = 1.5 - 4 \)

\( R_e \) versus site-occupation probability \( p \) at \( q = 1.5 \) in the ranges (a) \( 0.2 < p < 1 \) and (b) \( 0.7260 < p < 0.7272 \), with different sizes \( L = 4, 8, 16, 32, 64, 128, \) and 256. The critical point is \( p_c = 0.726525(2) \) and \( R_e = 0.5822(3) \). The error bars are smaller than the symbols. The lines in the right figure are plotted to guide the reader.

As shown in Fig. 2(a), we calculate the wrapping probability \( R_e \) as a function of site occupation probability \( p \) at \( q = 1.5 \) for lattices with different sizes \( L = 4, 8, 16, 32, 64, 128, \) and 256. In the limit \( p \rightarrow 0 \), no sites are occupied and hence no clusters exist and \( R_e = 0 \). In the limit \( p \rightarrow 1 \), all sites are occupied and a wrapping cluster forms and \( R_e = 1 \).

In the region of critical points, i.e., \( 0.7260 < p < 0.7272 \), there is no jump as shown in Fig. 2(b) and consequently it is a continuous phase transition. By the Levenberg-Marquardt least-squares method \[40\] and Eq. (13), we find that the critical percolation probability is at \( p_c = 0.726525(2) \). Correspondingly, the thermal exponent is \( y_t = 0.884(4) \), which is very consistent with the theoretical result \( y_t = 0.887 \).

By the fitting method based on Eqs. (14) and (15), the quantities \( P_\infty \) and \( \chi_p \) depend on the coefficients \( a_i \). So it is necessary to deduce the value of \( P_\infty \) and \( \chi_p \) at the percolation threshold \( p_c \) according to Eqs. (10) and (17).

FIG. 2: Wrapping probability \( R_e \) versus site-occupation probability \( p \) at \( q = 1.5 \) in the ranges (a) \( 0.2 < p < 1 \) and (b) \( 0.7260 < p < 0.7272 \), with different sizes \( L = 4, 8, 16, 32, 64, 128, \) and 256. The critical point is \( p_c = 0.726525(2) \) and \( R_e = 0.5822(3) \). The error bars are smaller than the symbols. The lines in the right figure are plotted to guide the reader.

Figure 3 displays the log-log plot of \( P_\infty \) and \( \chi_p \) versus system size \( L \) for \( q = 1.5 \) of the SRC model on the square lattice, \( P_\infty \propto L^{-0.1168(3)} \) and \( \chi_p \propto L^{-0.2332(4)} \). The two lines represent fits to the data points according to Eqs. (13) and (17).

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We take the logarithm on both sides of the equation and then we fit the numerical data for \( P_\infty \) to get the frac-
tal dimension of the percolation cluster $y_h = 1.8832(3)$ which is consistent with the theoretical value 1.8832, at the critical point $p_c = 0.726525(2)$ as labeled in Fig. 2.

For small systems with sizes $L = 4$ and 8, the data of $P_\infty$ deviate from the fitted line. This is different from the models studied before [44]. We also plot $\chi_p$ and find that, there is no obvious phenomena of deviation for small systems and the fitted exponent $y_h = 1.8832(2)$ from $\chi_p$ has the same precision with the result from $P_\infty$, as shown in Fig. 3.

We apply the same procedure described above to the cases $q = 2, 2.5, 3, 3.5$ and 4. The percolation threshold $p_c$, the wrapping probability $R_c$, the thermal exponent $y_t$, and the fractal dimension of the percolation cluster $y_h$ are obtained in the same way. The results are listed in Table 1. We find that for the range $q = 1.5 - 3.5$, the numerical results $y_h$ and $y_t$ are very consistent with the theoretical values. For $q = 4$, the precision of the critical point and the exponents are lower than the case with other values of $q$, due to the logarithmic correction [41–43].

| $q$ | $p_c$ | $R_c$ | $y_t$ | $y_h$ | $\chi_p$ |
|-----|-------|-------|-------|-------|----------|
| 1.5 | N     | 0.726525(2) | 0.5822(3) | 0.884(4) | 1.8832(2) |
|     | T     |       |       | 0.887 | 1.8832 |
| 2   | N     | 0.805000(1) | 0.6270(1) | 1.000(5) | 1.8750(1) |
|     | T     |       |       | 1.000 | 1.8750 |
| 2.5 | N     | 0.854411(2) | 0.6270(1) | 1.000(5) | 1.8750(1) |
|     | T     |       |       | 1.000 | 1.8750 |
| 3   | N     | 0.887435(1) | 0.6270(1) | 1.000(5) | 1.8750(1) |
|     | T     |       |       | 1.000 | 1.8750 |
| 3.5 | N     | 0.910600(2) | 0.750(1) | 1.44(7) | 1.874(2) |
|     | T     |       |       | 1.50  | 1.875  |

TABLE I: Numerical results (N) for the percolation threshold $p_c$, the wrapping probability $R_c$, the thermal exponent $y_t$, and the fractal dimension $y_h$ from $\chi_p$. Theoretical predictions (T) are included where available by the Coulomb gas method [35] or conformal invariance [36]. The estimated errors in the last decimal place are shown between parentheses.

B. $q = 10$, a first-order phase transition

Figure 4 (a) shows a histogram of the energy per site $E$ at the critical point $p_c = 0.987$, in which the double distribution is a typical signature of the first-order phase transition from the non-percolation phase to the percolation. We obtain the histogram in such a way. Firstly, we initialize a configuration by assigning each site with an occupied or an empty state, a probability of 1/2. After the system enters into an equilibrium state, we measure the energy per site $E$. We repeat the above steps until the shape of the histogram converges.

To confirm the first-order of the percolation transition, Fig. 4 (b) shows the hysteresis loop around the critical point region, i.e., 0.975 < $p$ < 1. The hysteresis loops have been observed both in classical [44] and quantum systems [46–47]. To form a closed hysteresis loop, we start at $p = 0.975$. Then we increase the occupation probability $p$ and sample the energy per site $E$. In the simulation, we use the configuration of the previously completed simulation for a given value of "$p$", as the (new) initial configuration of the simulation of another value of "$p$". The energy per site $E$ of the system does not jump to a higher value immediately until $p$ exceeds over a short distance of the transition point $p_c$. After $p$ reaches 1, we decrease $p$ in the same way with regards to the initialization of configurations. A closed hysteresis loop forms when $p$ becomes smaller than $p_c$. We repeat similar steps for the percolation strength and the results are shown in Figs. 4 (c) and (d).

V. CONCLUSION

In conclusion, we have proposed a new statistical model, which can be considered as a SRC model with an additional cluster weight in the partition function with respect to the traditional site percolation model.

We have also designed a color-assigned cluster updating Monte Carlo simulation algorithm suffering little from the boring critical slowing-down phenomena.

Both of the BRC and SRC percolation models have the same universality by simulations of the SRC model on the square lattice and behaviors of the quantities $R_c$, $\chi_p$, $y_t$ and $y_h$.

At the critical phase transition point the case of $q = 1.5$, the correction-to-scaling of $P_\infty$ is relatively stronger than that of $\chi_p$, which is different from the models studied before. For $q = 4$, the estimation of exponents $y_t$ and $y_h$ is less precise due to the log-correction. For $q = 10$, FIG. 4: The signature of the first-order phase transition for the SRC model at $q = 10$ on a 16 × 16 square lattice. Histogram of energy per site $E$ (a) and the percolation strength $P_\infty$ (c) at the critical point $p_c = 0.987$. Hysteresis loop of the both quantities $E$ (b) and $P_\infty$ (d) around the critical point $p_c$.
the obvious first-order transition is observed.

Our results can be considered as a first study of the counterpart for the BRC percolation model and are helpful for the understanding of the percolation of traditional statistical models.

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