Percolation in a three-dimensional nonsymmetric multicolor loop model

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We conduct Monte Carlo simulations to analyze the percolation transition of a nonsymmetric loop model on a regular three-dimensional lattice. We calculate the critical exponents for the percolation transition of this model. The percolation transition occurs at a temperature that is close to, but not exactly, the thermal critical temperature. Our finite-size study on this model yields a correlation length exponent that agrees with that of the three-dimensional XY model with an error margin of 6%.

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I. INTRODUCTION

It has been observed that porous materials like charcoal, limestone, or sponge are impervious to water until a substantial fraction of the pores are filled by the water. The threshold value of these occupied pores is a measure of a kind of phase transition popularly known as percolation. This threshold value that separates the two phases is known as the percolation threshold. Perhaps, the most influential work in this field which laid the mathematical foundations of this subject was the work by Broadbent and Hammersley [1]. Following their work, there was an avalanche of activities in both physics and the field of applied sciences, which continues even today. One of the early applications of the theory was due to Anderson, who used percolation to study the localization of electrons in disordered media, a phenomenon famously known as Anderson localization [2]. Subsequently, people used it to study the conduction and transport phenomena in inhomogeneous conductors near the percolation threshold [3–5]. In statistical mechanics, Fisher and Essam studied percolation in exotic lattice systems like the Bethe lattice (infinite Cayley tree) [6]. However, it was not until the work of Fortuin and Kasteleyn [7,8] that it was shown for the first time that there exists a direct connection between the percolation problem and the Ising or Ising-like models. This connection was vital in calculating the critical exponents associated with the percolation transition [9–12]. The central idea was the concept of clustering, which was later exploited by physicists to circumvent the problem of critical slow down in the Monte Carlo simulations of spin systems [13–15]. The ideas of percolation have also been used in the study of nonphysical phenomena, e.g., forest fires [16] and interactions in social networks [17].

Compared to the conventional site and bond percolation, the phenomenon of loop percolation is a relatively less studied subject in the physics community, especially when the percolation transition is thermally driven. The statistical distribution of these loops can be thought of as clusters or connected components, whose growth has a very natural description in terms of the percolation transition [18–20]. For example, the onset of the λ transition in superfluid helium is mediated by the percolation of vortex rings [18]. Extensive studies of these condensed-matter systems have also led to our understanding of the formation of topological defects in the universe [21,22]. A statistical mechanical study of the frustrated XY model by Nguyen and Sudbo [23] showed that the temperature-driven percolation transition due to the vortices was responsible for the melting of the Abrikosov flux-line lattice in type-II superconductors. In the case where temperature was not the driving factor, a study by Pfeiffer and Rieger [24] showed that the critical exponents for the loop percolation transition belong to the same universality class as the conventional bond or site percolation. However, in the same study, the percolation transition which occurs due to minimizing the ground state ($T = 0$) energy of a loop Hamiltonian with random disorder resulted in a completely different set of critical exponents. It is worth mentioning that the work by Pfeiffer and Rieger partly serves as the motivation for the present work. An extensive study of the universal behavior of thermally driven percolating loops remains unaddressed. Therefore, we believe that there is further scope for work and our study will be a step in that direction.

In this paper we look at the finite-temperature percolation transition observed in a certain loop model, in a regular three-dimensional lattice. The model under consideration is a variant of the loop Hamiltonian used in [24]. The major differences between our loop model and the one in [24] is

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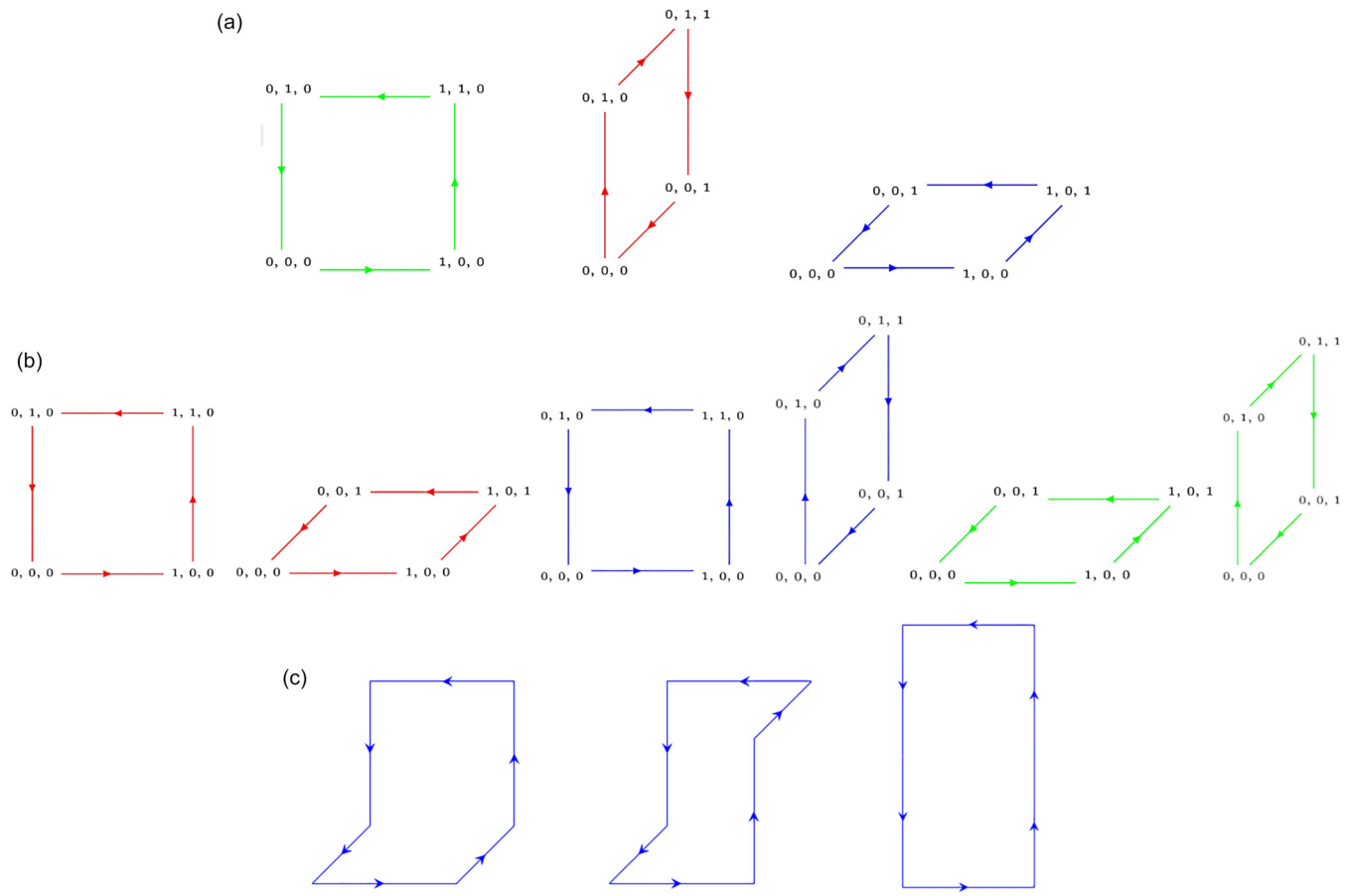

FIG. 1. Elementary excitations in NS loops: (a) the first excited state with 1 unit of energy (k_BT units) and degeneracy 6, (b) the second excited state with 1.5 units of energy and degeneracy 6, and (c) the third excited state (left and middle) with 2 units of energy and the fourth excited state (right) with 2.5 units of energy.

that our loop model Hamiltonian is devoid of any random disorders and it has multiple loop components where each component is termed a color. We refer to our model as the nonsymmetric (NS) loop model, for reasons that have been discussed in the preceding paper [25]. That paper contains the thermodynamic properties of the NS loop model, including its thermal (specific-heat) critical exponent α and the correlation length exponent ν. In the present work we calculate the critical exponents for percolation transition seen in the NS loop model. We observe that the percolation transition happens at a temperature close but not equal to the thermal critical temperature. Our finite-size scaling analysis suggests that the correlation length exponent for the NS loops is that of the XY model in three dimensions. Since the loop percolation transition in NS loops is a thermally driven transition, its percolation properties are intertwined with its thermal properties. Therefore, it is important to discuss the finite-temperature properties of the NS loop model before we discuss its percolation properties.

The rest of the paper is organized as follows. In Sec. II we introduce the NS loop model and briefly discuss its finite-temperature properties. In Sec. III we discuss the percolation transition in the NS loop model using finite-size scaling. In Sec. IV we present and discuss our results. We briefly summarize in Sec. V.

II. MULTICOLORED LOOP MODEL

The order-disorder transitions in a regular three-dimensional lattice system can occur due to topological defects. Their topological nature protects them and prevents their removal by any smooth deformation of the lattice. They obey a continuity condition [see Eq. (1)], for which their lattice realizations assume the form of closed loops (Fig. 1). In solids, these topological defects are called dislocations and disclinations. The former is responsible for the breakdown of the broken translational symmetry, while the latter destroys the broken rotational symmetry [26–28]. The topological defects in solids are second-rank symmetric tensors, which can cause melting. In three-dimensional solids, the melting transition is a first-order transition. In the preceding paper [25] we argue the theoretical possibility of tensor loop defects which can be nonsymmetric, hence the name NS loops. The NS loops undergo a second-order phase transition, but we have shown that strong interactions among the various colors can alter the nature of the transition in these loop systems. In this section we briefly discuss the NS loop model and refer the reader to [25] for more details.

Let $\eta_{ij}(\mathbf{x})$ represent the integer-value NS tensors at each point $\mathbf{x}$ in the lattice. The tensor has nine independent elements, with each column denoted by index j, which corresponds to the color of the loop, e.g., $j \in \{1, 2, 3\} =$

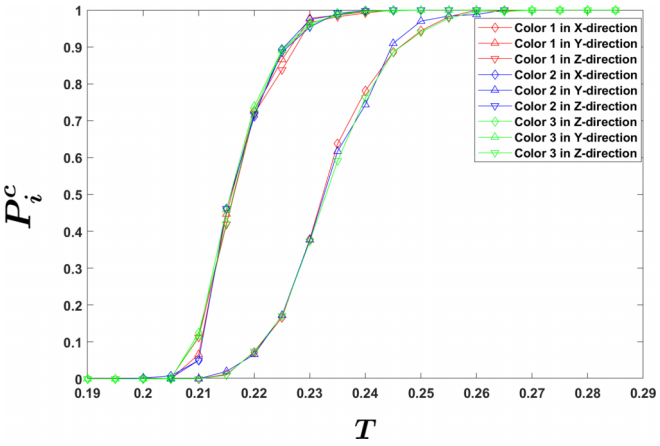

FIG. 2. Percolation probability among different colors c in different directions i with size $L = 16$.

{red, blue, green}. For each color, we have the lattice continuity equation

$$\Delta_i \eta_{ij}(\mathbf{x}) = 0, \quad j \in \{1, 2, 3\}. \tag{1}$$

The Hamiltonian, which is a function of η_{ij}, is given by

$$\begin{aligned} H(\eta_{ij})_{\text{loop}} = \sum_{\mathbf{x}} & A\left[\eta_{11}^2(\mathbf{x}) + \eta_{22}^2(\mathbf{x}) + \eta_{33}^2(\mathbf{x})\right] \\ & + B\left[\eta_{12}^2(\mathbf{x}) + \eta_{21}^2(\mathbf{x}) + \eta_{23}^2(\mathbf{x})\right. \\ & \left. + \eta_{32}^2(\mathbf{x}) + \eta_{13}^2(\mathbf{x}) + \eta_{31}^2(\mathbf{x})\right] \\ & + D[\eta_{11}(\mathbf{x})\eta_{22}(\mathbf{x}) + \eta_{22}(\mathbf{x})\eta_{33}(\mathbf{x}) \\ & + \eta_{33}(\mathbf{x})\eta_{11}(\mathbf{x})], \end{aligned} \tag{2}$$

where $A = 0.5$, $B = 0.25$, and $D = 0.1$, in units of $k_B T$. If $E^{(\text{color})}_{(\text{plane})}$ denotes the energy of an elementary excitation of color c along a given plane, then the excitations in Figs. 1(a) and 1(b) will have energies given by

$$\begin{aligned} & E^1_{YZ} = E^2_{XZ} = E^3_{XY} = 4B, \\ & E^1_{XY} = E^1_{XZ} = E^2_{XY} = E^2_{YZ} = E^3_{YZ} = E^3_{XZ} = 2(A + B), \end{aligned} \tag{3}$$

where $4B < 2(A + B)$. From the calculations above, it is evident that the excitations carrying $4B$ units of energy have greater chances of acceptance than the ones carrying $2(A + B)$ units of energy. As a result, color 1 in the Y and Z directions, color 2 in the X and Z directions, and color 3 in the X and Y directions have their corresponding percolation probabilities shooting up close to the criticality as shown in Fig. 2. We must emphasize that despite such directional preferences, the critical behaviors of this model and of the model with complete isotropy are the same.

III. PERCOLATION TRANSITION IN NS LOOPS

In the preceding section we saw that the basic excitations in the NS loop system are elementary loops (plaquettes). They can be oriented along any arbitrary plane and can have both clockwise and counterclockwise chiralities. Every site associated with such a loop will have an incoming and an outgoing arrow whose number is always conserved. Near the critical point, when the system is proliferated by such loopy networks, the system is said to be disordered and there will exist a path or multiple paths connecting the opposite sides of the system running through the bulk. The analogy between site percolation and percolation due to loops stems from the following fact. A single loop [Fig. 1(a)], which is the most basic excitation in the system, is a connected component of size 4, that is, it connects four sites in the lattice. As the number of loops increases in the system, they will join one another to form bigger loops or clusters [Fig. 1(c)]. Near the percolation transition, the typical size of the connected components will grow until we end up having a percolating cluster. This implies that we can always find a path or a set of paths within the cluster that run through the bulk of the system connecting its opposite faces (boundaries). In other words, we will have loops whose diameter will scale as the size of the system when the system is driven near the critical region. Unlike conventional phase transitions, this kind of transition is a thermally driven geometrical transition. It is a continuous transition which involves occupation of the sites (site percolation) or bonds (bond percolation) in a lattice and therefore will have its own critical exponents.

With increasing temperature these loops interact with one another to form clusters or connected components of varying sizes. If two points within the system are connected by a path, then they belong to the same cluster. If these two points happen to be at the two opposite boundaries or faces of the system, then we say that we have a percolating path and the cluster is a percolating cluster. We will see that near the critical point, the number of such paths and the size of the percolating cluster have a scaling behavior. Our knowledge of the statistics of the connected components (loop statistics) provides information about the geometry of these networks and enables us to calculate the critical exponents. Contrary to ordinary percolation, where bonds or sites are randomly and independently occupied (or emptied) with some probability, the thermal problem will have them filled or emptied based on the Metropolis algorithm. The algorithm's conditional addition or removal of bonds or sites puts it in a special category of problems in statistical mechanics known as correlated percolation. They are correlated because the loops are generated by a first-order Markov chain of events.

Method

Our goal is to investigate the percolation transition in NS loops within a regular three-dimensional lattice with periodic boundary conditions using computer simulations. As previously stated, the loop variables are integer-value quantities that obey a continuity condition. Therefore, the update equations must satisfy this constraint [25]. Since the percolation transition is thermally driven, we employ the Metropolis algorithm [29,30] to simulate the Hamiltonian in Eq. (2) at a finite temperature T. According to the algorithm, the evolution of the system of loops is a Markov process. If ΔE represents the change in the energy of the system when transitioning from state a to state b, then the transition probability $W(a \to b)$ is given by

$$W(a \to b) = \begin{cases} \exp(-\Delta E/k_B T) & \text{for} \quad \Delta E > 0 \\ 1 & \text{otherwise.} \end{cases} \tag{4}$$

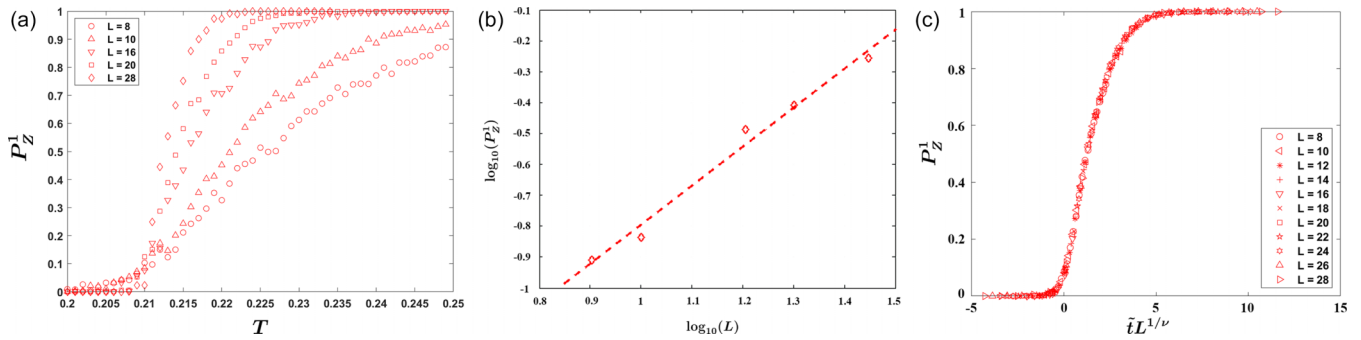

FIG. 3. Percolation probability P_i^c in NS loops: (a) the raw data for P_Z^1 vs temperature (T), (b) the log - log plot for P_Z^1 vs $L^{1/\nu}$ for the correlation length exponent ν, and (c) the finite-size scaling results for P_Z^1 (for other colors, see Table I).

After the system has equilibrated at temperature T, we will have a canonical ensemble of loops with a certain configuration. We use the depth-first search [31,32] algorithm to calculate all the connected components in the system. For example, in two-dimensional magnetic systems, the islands of magnetization are connected components of various sizes. The order-disorder transition in such systems is determined by the value of the magnetization order parameter. Unlike magnetic systems, the NS loops have no such order parameter. However, one can draw a close analogy with the idea of magnetization and the average number of loops of various sizes as a measure of disorder in such loop systems. With a slight abuse of terminology, one may choose to call it a disorder parameter.

The quantities that will be important for the present study are the percolation probability P^c and the percolating cluster P_∞. In the preceding section we looked at the concept of a percolating path. If N_i^c represents the number of times a percolating path of a given color c occurs in a given direction i, out of N_M trials, then

$$P_i^c = \frac{N_i^c}{N_M} \tag{5}$$

is simply the percolation probability of color c in the ith direction. A percolating path is a connected component of a certain size which is determined by the number of lattice sites belonging to the percolating path. If N_∞^c represents the size of such a cluster of a specific color c, then we can define our second quantity of interest, the percolating cluster, as

$$P_\infty^c = \frac{N_\infty^c}{L^3}, \tag{6}$$

where L^3 is the total number of lattice sites. It indicates the size of the largest cluster that spans the opposite boundaries of the system. This can be interpreted as the probability of a randomly chosen site being part of this cluster. Furthermore, it is an indicator of the random geometric networks created by the loops.

In the next section we will observe that close to the critical region, these quantities exhibit scaling behavior. By using finite-size scaling analysis, we will determine the critical exponents associated with these quantities.

IV. RESULTS

A. Finite-size scaling of the percolation probability

As the system approaches criticality $T \to T_c$, the loops grow in size and the system reaches the percolation threshold. Near this threshold point, the correlation length of an infinitely large system goes to infinity, but the correlation length is upper bound by the size of the finite-size system L. We find that with increasing system size, the P_i^c vs T curves become steeper near the percolation threshold as shown in Fig. 3(a). A crude estimate of the critical temperature $T \approx 0.21$ may be obtained from the intersection point of these curves. However, to get a more quantitative and accurate result, we have performed finite-size scaling analysis of these loops of different colors using AUTOSCALE.PY by Melchert [33] and our own numerical methods. Close to the critical point, P_i^c has the scaling form

$$P_i^c(L) = P_i^c(\tilde{t}L^{1/\nu}). \tag{7}$$

The right-hand side of Eq. (7) is a homogeneous function of the scaled temperature $\tilde{t}L^{1/\nu}$, where $\tilde{t} = (T - T_c)/T_c$. The exponent ν is associated with the correlation length [25]. Note that $P_i^c(L)$ becomes independent of the system size only at $\tilde{t} = 0$, i.e., $T = T_c$. The correct choice of the exponent and the critical temperature T_c will compel all the curves of different system sizes to collapse onto one another [Fig. 3(c)]. The critical temperature shown in Table I is close to $T_c = 0.21(0003)$. The correlation length exponent is approximately $\nu = 0.74(0024)$. The exponent ν calculated from the three-dimensional XY model gives $1/\nu = 1.48(0091)$ [34].

TABLE I. Comparison of the critical temperature T_c and correlation length exponent ν for different colors in different directions.

Percolation probability	T_c	$1/\nu$
P_Y^1	0.20(00971)	1.36(005)
P_Z^1	0.20(00971)	1.36(002)
P_X^2	0.20(00962)	1.36(002)
P_Z^2	0.20(00973)	1.36(002)
P_X^3	0.20(00978)	1.36(002)
P_Y^3	0.20(00978)	1.36(002)

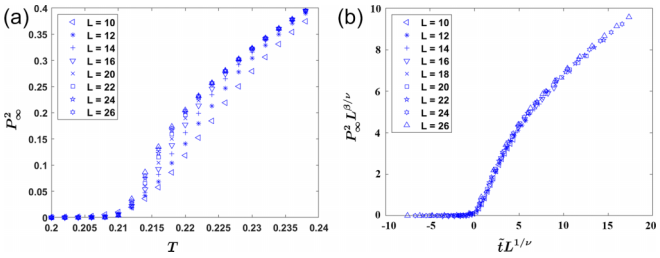

FIG. 4. Percolating cluster P_∞^c in NS loops. Raw data and finite-size scaling results are plotted for (a) P_∞^2 vs T (color 2) and (b) $P_\infty^2 L^{\beta/\nu}$ vs $\tilde{t}L^{1/\nu}$ (for other colors, see Table II).

B. Finite-size scaling of the percolating cluster

Similar to the percolation probability, P_∞^c also has a scaling form given by

$$P_\infty^c(L) = L^{-\beta/\nu}\bar{P}_\infty^c(\tilde{t}L^{1/\nu}), \tag{8}$$

where $\bar{P}_\infty^c$ is a homogeneous function of $\tilde{t}L^{1/\nu}$. For varying system sizes, P_∞^c has the behavior shown in Fig. 4(a). Finite-size scaling analysis gives us the values of the exponents for various colors. The critical temperature obtained from Table II is close to $T_c = 0.21(0003)$ and the exponent $\beta = 0.61(007)$.

V. CONCLUSION

Using Monte Carlo simulations, we have studied percolation in the nonsymmetric loop model (2). The exponents are tabulated in Tables I and II. The effects of anisotropy (directional preference) are seen while the system transits from an ordered to a disordered state. The scaling exponent for the percolation probability [$\nu = 0.74(0024)$] and percolation cluster [$\beta = 0.61(007)$] for NS loops have been calculated. The percolation transition occurs at a temperature $T \approx 0.20(0098)$, which is close but not exactly equal to the thermal critical temperature $T_c = 0.212$ [25]. A numerical study of the stochastic Gross-Pitaevskii equation by Kobayashi and Cugliandolo showed that the percolation temperature of the vortices differed from the thermal critical temperature by only 2% [35]. Similarly, finite-size scaling calculations of the correlation length exponent of the three-dimensional XY model by Schultka and Manousakis [36] and Campostrini *et al.* [34] agree with our model within a 6% deviation.

TABLE II. Comparison of the critical temperature T_c, correlation exponent ν, and the exponent β for different colors.

Percolation cluster	T_c	$1/\nu$	β/ν	β
P_∞^1	0.21(0003)	1.31(0057)	0.80(0056)	0.61(002)
P_∞^2	0.21(0003)	1.31(0057)	0.82(0049)	0.62(007)
P_∞^3	0.21(0001)	1.31(0057)	0.80(0056)	0.61(002)

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