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Finite-size scaling in stick percolation

Jiantong Li[1] and Shi-Li Zhang[1,2,*]

[1]*School of Information and Communication Technology, Royal Institute of Technology (KTH), Electrum 229, SE-164 40 Kista, Sweden*

[2]*The Ångström Laboratory, Uppsala University, P.O. Box 534, SE-751 21 Uppsala, Sweden*

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This work presents the generalization of the concept of universal finite-size scaling functions to continuum percolation. A high-efficiency algorithm for Monte Carlo simulations is developed to investigate, with extensive realizations, the finite-size scaling behavior of stick percolation in large-size systems. The percolation threshold of high precision is determined for isotropic widthless stick systems as $N_c l^2 = 5.637\ 26 \pm 0.000\ 02$, with N_c as the critical density and l as the stick length. Simulation results indicate that by introducing a nonuniversal metric factor $A = 0.106\ 910 \pm 0.000\ 009$, the spanning probability of stick percolation on square systems with free boundary conditions falls on the same universal scaling function as that for lattice percolation.

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It is widely accepted that lattice percolation and continuum (or irregular lattice) percolation belong to the same universality class in the sense that the latter possesses the same critical exponents as the former as long as they have identical dimensionalities and Hamiltonian symmetry [1–3]. However, another important universality, i.e., universal finite-size-scaling functions (UFSSFs), has also attracted interest in critical phenomena [4,5]. With given dimensionality, percolating rule, boundary conditions, and aspect ratio, all percolation systems fall on the same scaling functions by introducing only a few nonuniversal system-dependent metric factors [5]. Such a UFSSF concept has been verified for many lattice percolation systems [6]. In this work, the UFSSF idea is generalized to continuum percolation. The generalization is realized through a systematic study of the finite-size scaling behavior of two-dimensional (2D) stick percolation.

Similar to disk percolation for systems consisting of randomly placed disks [1,7], stick percolation is also regarded as an important representative of continuum percolation [2,8–12]. Since the first consideration by Pike and Seager in 1974 [7], stick percolation has attracted appreciable attention. In practice, stick percolation is also of importance due to its promising applications in systems consisting of conducting fibers [8,11]. In particular, the demonstration of electronic devices based on rodlike semiconducting nanoparticles, e.g., silicon nanowires [13] and carbon nanotubes [14], as the fundamental building block for the rapidly growing field of macroelectronics [13,15], has called for extensive studies of stick percolation both theoretically [16–18] and experimentally [19]. In spite of the successful development, however, some crucial concept and knowledge are not yet well established. For example, only the original work of Pike and Seager [7] studied the percolation threshold for 2D stick systems, but no further work has provided any improvement. Moreover, a comprehensive understanding of one of the most important percolation behaviors, i.e., finite-size scaling [20] for stick systems, is still lacking. Besides its expected theoretical and experimental significances [6], finite-size scaling is especially important for stick percolation because of its promising applications in macroelectronics where device dimension scaling is technically of dominant interest [13–15].

In lattice percolation, the spanning probability $R(p,L)$, defined as the probability that the system with linear dimension L spans (i.e., percolates) at occupancy p, is best studied with respect to finite-size scaling [5,21]. It has become well understood from the finite-size scaling theory [6,20] that near the critical point p_c, the spanning probability obeys the general scaling law,

$$R(p,L) \sim F[(p-p_c)L^{1/\upsilon}] \equiv F(x), \tag{1}$$

where $x=(p-p_c)L^{1/\upsilon}$ is the scaling variable with υ being the correlation-length exponent ($\upsilon=4/3$ for 2D systems) and $F(x)$ is the scaling function. However, further studies [5] have suggested that appropriate corrections to Eq. (1) are required concerning system size L, especially for small-size systems. In general, the leading corrections include an analytical correction, of the order L^{-1}, due to the finite-size correction and a nonanalytical correction, of the order $L^{-\vartheta}$ with $\vartheta \approx 0.9$, due to irrelevant scaling variables [5,21]. For square systems with free boundary conditions, the finite-size correction is dominant near p_c [5]. Hence, in this case the leading terms in the expansion of $R(p,L)$ should actually read as

$$R(p,L) \sim F(x) + b_0/L, \tag{2}$$

where b_0 is a constant. For square systems with free boundary conditions, $F(x)$ has the following polynomial form for small x:

$$F(x) = a_0 + a_1 x + a_3 x^3 + \cdots, \tag{3}$$

where a_i ($i=0,1,2,\ldots$) are constants. The system symmetry and self-duality require that $a_0=1/2$ and $a_i=0$ for other even i [5,21]. Note that when multiple systems are considered, $F(x)$ itself is not universal. But by introducing a system-dependent metric factor A and replacing x with $\hat{x}=Ax$ in Eqs. (2) and (3), the resultant scaling function $\hat{F}(\hat{x})$ becomes universal, i.e., $\hat{F}(\hat{x})$ is a UFSSF [5,6]. Because of the universality of $\hat{F}(\hat{x})$, $R_c \equiv R(p_c,\infty) = \hat{F}(0) = a_0 = 1/2$ is also universal [5,21].

In order to validate these theoretical results in continuum

*Corresponding author: shili.zhang@angstrom.uu.se

percolation, Monte Carlo simulations were performed to investigate the percolation behavior in stick percolation. Here, 2D isotropic widthless stick percolation is considered also on square systems with free boundary conditions. Each stick, of a fixed length l, is centered on a random site with a given random orientation. In this work, l is set to unity, i.e., $l=1$. The system size (or square length) is L. Two sticks lie in the same cluster if they intersect. The boundaries of the system are also regarded as extra sticks with length L and a fixed orientation. If two opposite boundary sticks lie in the same cluster, the system spans. Instead of occupancy p as in lattice percolation, the behavior of stick percolation is studied in terms of the stick density N, i.e., the number of sticks per unit area. The percolation threshold is defined by the critical density, N_c. Usually, the simulation for continuum percolation requires much more calculations than for lattice percolation. On the one hand, unlike in lattice percolation where a site or bond has fixed neighbors, the number and position of the neighbors of a site in continuum percolation are unknown so that the bonding criterion is more complicated. On the other hand, continuum percolation usually needs a higher site density to span than lattice percolation. In addition, existing algorithms for stick percolation are not sufficiently efficient. For example, if there are n sticks in the system, using algorithms directly based on the spanning rule described above to determine whether the system percolates, as applied in Refs. [2,12], needs actually to check the connectivity property between each stick and every other stick. This procedure takes time as long as $O(n^2)$ or $O(N^2L^4)$ since $N=n/L^2$. Because of these reasons, simulations of stick percolation are often performed for small amounts ($\leq 10^3$) of sticks or at small numbers ($<10^4$) of realizations [2,7–12]. In the present work, a high-efficiency algorithm is developed for Monte Carlo simulations of stick percolation. This algorithm is developed from the tree-based algorithm of Newman and Ziff [22] and the subcell algorithm [1]. The tree-based algorithm has been demonstrated to be highly efficient in lattice percolation when it comes to calculations of quantities over the entire range of occupancy in a single run [22]. The subcell algorithm has recently also proven efficient for continuum percolation [3,17]. In this work we present an algorithm based on the synergy of these two algorithms for stick systems. However, though the algorithm presented here is described for the spanning probability of stick percolation, it is generic and can be readily applied for other types of continuum percolation as well as other quantities, such as percolation probability [6,20,22], after slight modifications.

The algorithm in this work starts with a blank square system in which there are only two boundary sticks of length L on the two opposite boundaries. In order to avoid the trivial, but enormous, work of determining whether a stick is a normal one or a boundary one, each of the two boundary sticks is divided equally into L sticks with length l such that the boundary sticks are identical to the normal sticks, as shown in Fig. 1. But these L sticks are connecting and belong to the same cluster. As in Ref. [22], a tree structure is used to store these clusters. In each cluster, one stick is chosen to be the "root stick" and possesses the cluster label. All other sticks have pointers pointing either to the root stick or to another stick in the cluster, which implies that any stick in the cluster

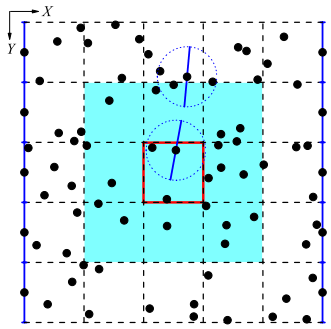

FIG. 1. (Color online) Schematic illustration of stick percolation on a square system ($L=5$). Each stick is of unity length $l=1$ and described by its center site and orientation. For clarity, most sticks are presented here only by their centers (black dots). The two interesting system boundaries (the left and right ones) are described also by L connecting sticks. The system is divided into $L\times L$ subcells (dashed lattices) with unity length l. Each stick is registered in the subcell where its center lies. It is explicitly shown that a stick in a subcell (with solid boundaries) is impossible to intersect any sticks at other subcells than the same one or its neighbors (the gray ones or light cyan ones).

points directly or indirectly (through a path comprising other sticks) to the root stick and hence has the identical root stick. The system is virtually divided into $L\times L$ subcells (or subsquares) with unity length l, as shown by the dashed lattices in Fig. 1. With these preparations, a random normal stick is generated by producing a random point (X,Y) for its center site and a random angle θ with respect to the horizontal direction for its orientation. Note that $0\leq X\leq L$, $0\leq Y\leq L$, and $0\leq\theta<\pi$. The stick is first treated as a one-stick cluster with itself as the root stick and registered into the subcell in which the point (X,Y) lies [23]. According to such a registration, a stick in a subcell (e.g., the one with solid boundaries in Fig. 1) is only possible to intersect sticks in the same or the neighboring subcells (the gray ones in Fig. 1) since the distance between its center and any stick center in other subcells is greater than l, the maximum center distance of two intersecting sticks. Then, it is only needed to check the connectivity property between the newly generated stick and those sticks belonging to the same or neighboring subcells. When two sticks intersect, if they have the same root stick, i.e., belonging to the same cluster, nothing needs to be done; if not, the two corresponding clusters should be amalgamated simply by adding a pointer from the root stick of one cluster to that of the other. In order to expedite the amalgamation, a "weighted union find with path compression" algorithm is also applied as in Ref. [22]. Following these processes, we repeat adding a random stick, registering it in a subcell, checking its connectivity with other sticks in the same and neighboring subcells, and amalgamating, if necessary, the clusters until two opposite boundary sticks, e.g., the left-top and right-top ones in Fig. 1, point to the same root stick. In this case, the system percolates for the first time and the total number of sticks is recorded as n_f. By now, the whole simulation procedure for one realization is accomplished. After performing the simulation for m realizations, the spanning probability $R_{n,L}$ for n sticks on a system of size L is readily obtained by initiating all $R_{n,L}=0$ and then for each realiza-

tion, adding $1/m$ to any $R_{n,L}$ with $n \geq n_f$. Note that simply by virtue of the relation $N=n/L^2$, one cannot obtain $R(N,L)$ from $R_{n,L}$ for any N with arbitrary precision. As n represents the number of sticks in the system, N should be a multiple of $1/L^2$. Such difficulty can be resolved in lattice percolation by convolving all the measured observables with the binomial distribution so as to generate a common "canonical ensemble" for any value of p [21,22]. However, the binomial distribution is not applicable in continuum percolation. Then the Poisson distribution is instead employed in this work for the convolution

$$R(N,L) = \sum_{n=0}^{\infty} \frac{\lambda^n e^{-\lambda}}{n!} R_{n,L}, \tag{4}$$

where $\lambda = NL^2$ for any N with arbitrary precision. Therefore, this algorithm only takes time $O(N^2L^2)$, i.e., $\sim O(n)$ [24], to produce $R(N,L)$ for all N, which is a significant improvement over previous algorithms for stick percolation and comparable to those efficient algorithms for lattice percolation [22].

Hence, the present algorithm also permits Monte Carlo studies of large-size stick systems with a large number of realizations. Figure 2 shows the simulation results of stick percolation for square systems with large sizes up to $L=256$. In Fig. 2, $R_{n,L}$ were collected on the basis of more than 10^8 independent realizations for any $L<100$ and still more than 10^7 realizations for any $L>100$. The summation in Eq. (4) did not stop until the value of a proceeding term in the series decreased below 10^{-20}.

For a coarse observation, the four curves in Fig. 2(a) intersect at $R=0.5$ [the dashed horizontal line in Fig. 2(a)], implying that $R_c \equiv R(N_c,\infty)=0.5$. This result, which will be justified below, supports the conclusion that R_c is universal [5,21] and extends it into continuum percolation.

However, for studies of the finite-size scaling behavior, a high-precision value of the critical density N_c is yet to be found. So far only a rough value has been reported by Pike and Seager [7] as $N_c l^2 = 5.71 \pm 0.24$ [25]. The current simulation results are of great potential for extraction of a high-precision N_c. A good estimate for the critical density, $N_{Rc}(L)$, can be given by the solution of $R[N_{Rc}(L),L]=R_c$ [21]. In this study, $R_c=0.5$ so that $N_{Rc}(L)$ can be denoted as $N_{0.5}(L)$. From Eq. (2), $N_{0.5}(L)$ is expected to converge to the true N_c as

$$N_{0.5}(L) - N_c = -\frac{b_0}{a_1} L^{-1-1/\nu} + \cdots. \tag{5}$$

Figure 2(b) plots the calculated $N_{0.5}(L)$ versus $L^{-1-1/\nu}$ for several large systems ($L \geq 32$) and nearly a perfect linearity appears, consistent with Eq. (5). The best fit to these data gives an estimate of $N_c = 5.637\ 26 \pm 0.000\ 02$. For a general stick length l, the percolation threshold should therefore be

$$N_c l^2 = 5.637\ 26 \pm 0.000\ 02. \tag{6}$$

This value is consistent with, but significantly more precise than, the result of Pike and Seager [7]. It is about 4 (3.924 79 to be exact) times that of the corresponding disk percolation [26] with the disk diameter equal to l. It is also in agreement with the result of Pike and Seager that the critical bonding

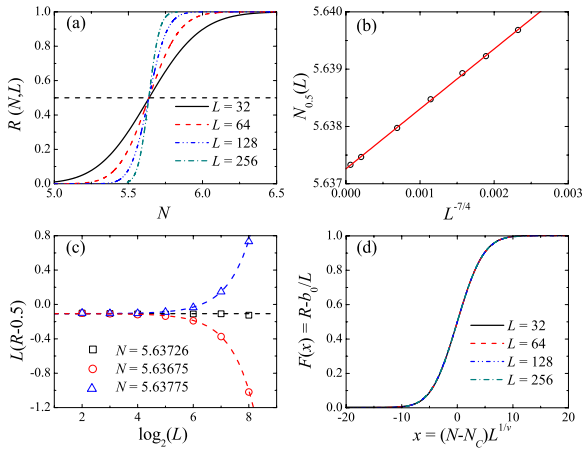

FIG. 2. (Color online) Monte Carlo simulation results for stick percolation on square systems with free boundary conditions. (a) The spanning probability R as a function of stick density N for different system sizes L. The horizontal dashed line represents $R=0.5$. (b) The estimated critical density $N_{0.5}(L)$, for $L=32$, 36, 40, 48, 64, 128, and 256, as a function of $L^{-1-1/\nu}$. (c) Plot of $L(R-0.5)$ against $\log_2(L)$ for N near N_c, with $L=4$, 8, 16, 32, 64, 128, and 256. The dashed curves represent $R(N,L)$ given by Eq. (2), neglecting higher orders than x, with $b_0=-0.107$ and $a_1=0.107$. (d) Finite-size scaling plot of R after finite-size corrections. $N_c=5.637\ 26$.

radius in stick percolation is approximately twice as large as that in disk percolation [7].

In order to determine coefficient b_0 for the finite-size correction, $L[R(N,L)-0.5]$ is plotted against L in Fig. 2(c) for different N near N_c. They almost converge to the same intercept confirming the aforementioned $R_c=0.5$ in this stick percolation and yielding $b_0 \approx -0.107$. Finally, the simulation data are plotted in Fig. 2(d) as $F(x)=R(N,L)-b_0/L$ versus $x=(N-N_c)L^{1/\nu}$, which exhibits a remarkable scaling behavior since all the data within the interval $-5<x<5$ give nearly a perfect fit (adjusted $R^2=0.999\ 993$) to Eq. (3) with i up to 5. This observation implies that the system symmetry and self-duality also hold for stick percolation on square systems with free boundary conditions. The fitting results are $a_1=0.106\ 910 \pm 0.000\ 009$, $a_3=-0.001\ 289 \pm 0.000\ 002$, and $a_5=0.000\ 010\ 93 \pm 0.000\ 000\ 05$. Defining the metric factor [5] $A=\partial F(0)/\partial x = a_1 = 0.106\ 910 \pm 0.000\ 009$ and replacing x with $\hat{x}=Ax$, we finally obtain the UFSSF as $\hat{F}(\hat{x}) = \frac{1}{2} + \hat{x} + K_3\hat{x}^3 + K_5\hat{x}^5 + \cdots$ with $K_3=-1.055 \pm 0.002$ and $K_5=0.783 \pm 0.004$. It agrees excellently with the UFSSF for lattice percolation, where $K_3=-1.02 \pm 0.02$ [5] and $K_5 \approx 1$ [6]. This agreement confirms that stick percolation shares the same UFSSF as lattice percolation.

Finally, it is worth mentioning that when the stick number is very large, interpolation is also an effective method in addition to convolution with the Poisson distribution. As a matter of fact, using the "cubic spline" interpolation method [27], we have also obtained results that agree well with all the parameters above except b_0. The value of b_0 is more sensitive in small-size systems so that the difference between the two methods is relatively large ($b_0 \approx -0.097$ from the interpolation method).

In summary, a high-efficiency algorithm has been devel-

oped for Monte Carlo simulations of stick percolation. This algorithm allows for study of continuum percolation problems in large-size systems with extensive realizations and high-precision results. This algorithm has been used to investigate the finite-size scaling behavior of isotropic widthless stick percolation on square systems with free boundary conditions. In addition, the percolation threshold with significantly improved accuracy has been determined for stick percolation. Simulation results show that similar to lattice percolation, stick percolation is also subjected to finite-size corrections. After such corrections, the spanning probability exhibits an excellent finite-size scaling behavior. With the introduction of a nonuniversal metric factor, the scaling function coincides with that for lattice percolation. These results generalize the concept of universal finite-size scaling function and make it applicable for continuum percolation. The present work is of both practical and theoretical significances. In practice, the knowledge of finite-size scaling of stick percolation is helpful in expediting the development of the newly emerging macroelectronics based on rodlike nanoparticles. In theory, this work confirms that continuum percolation belongs to the same universality class as lattice percolation, not only because they share the same critical exponents but also because they fall on the same universal scaling functions.

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[23] The registration can be very simple. For example, in this work we index a subcell as (i,j) with $i+1$ being its row number and $j+1$ being its column number and register a stick centered on (X,Y) into the subcell (i,j) if floor $(X)=i$ and floor $(Y)=j$ where the function floor (x) returns the largest integer no greater than x. According to this rule, a stick even centered exactly on a subcell boundary or corner can also be registered into a specific subcell. In addition, we add a row of auxiliary subcells to the bottom and a column of auxiliary subcells to the right-hand side of the system. Then actually there are totally $(L+1)\times(L+1)$ subcells so that sticks centered on the bottom or right boundary or the bottom-right corner of the system can also be registered into available subcells.
[24] The time is estimated as follows. For a system of size L and stick density N, there are in total $n=NL^2$ sticks and on average each subcell contains N sticks. Each stick may meet $9N-1$ sticks at the worst case; these sticks come from the same subcell and the eight neighboring subcells. So, the whole process should check the connectivity between sticks for $(9N-1)NL^2/2$ times, i.e., it takes time $O(N^2L^2)$. Since in large-size stick systems, N of interest is usually less than 10. Hence, the time can be approximated as $O(NL^2)=O(n)$. Note that it might be possible to improve the efficiency a little, at the expense of increased complexity, by using smaller subcells and considering more surrounding subcells as the neighbors. A similar algorithm is discussed by R. L. C. Vink and T. Schilling, Phys. Rev. E **71**, 051716 (2005).
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