Finite-size effects in two-dimensional continuum percolation

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(Received 17 June 1988)

We have investigated the finite-size effects of anisotropic continuum percolation in two dimensions. The elements that percolate are widthless sticks. We have developed a simple theory to explain the dependence of longitudinal and transverse critical lengths on anisotropy and the finite number of sticks in the sample. By comparing the theory to simulations, we find good agreement.

I. INTRODUCTION

In recent years there has been interest in the electrical properties of composite materials consisting of conducting fibers or sticks, embedded in an insulating polymer matrix. Typically, the composites are prepared by mixing the fibers and polymer in a liquid state and letting the result cool while being poured. This leads to an angular distribution of the fibers in the solid state, about the flow direction. Experimentally, such composites are found to have a threshold dependence of the electrical conductivity on the fiber length.[1] Various models have been tried to explain such behavior. These include the effective medium theory.[2] This has not been very successful as there is a large difference between the conductivities of the fibers and the insulating polymer.[3]

More promising are percolation simulations. The first was done by Pike and Seager.[4] They considered widthless (one-dimensional) sticks of constant length, in a two-dimensional medium, isotropic on a macroscopic scale. Their work was considerably extended by Balberg and Binenbaum[5] to the case of anisotropic systems where, as mentioned above, the fibers have an average preferred orientation. They also considered various distributions of stick length. From their simulations, the critical stick lengths for percolation along the average stick orientation and transverse to this were found as functions of anisotropy (defined in Sec. II) and the number of sticks in the sample. However, due to computing constraints, they only considered a few random configurations of sticks. They showed that in the limit of an infinite ensemble of sticks, the longitudinal and transverse percolation thresholds converge to a common function. In this paper we wish to extend their work by considering more thoroughly the finite-size effects on the percolation thresholds of ensembles with small numbers of sticks. In Ref. 5 and other papers[6,7] on continuum percolation this appears to have been a neglected point of interest. We will derive a simple model for the dependences of the thresholds on anisotropy and numbers of sticks and compare this to the results of extensive simulations.

Our paper is arranged as follows. Section II describes the simulations. Section III contains the model of the percolation thresholds. Section IV compares the model with the simulations. Finally, we give a conclusion in Sec. V.

II. SIMULATIONS

In this section we outline a method of performing simulations to find the critical lengths. (This is based on the procedure by Balberg and Binenbaum.[5]) First, we define the basic terms. Then, we give the procedure for obtaining the critical lengths.

To start, let us define some quantities. Consider a set of N widthless sticks. We place the centers of the sticks uniformly in the unit square, $[0,1]\times[0,1]$. The sticks have some angular probability distribution $f(\theta)$ about the y axis, where θ is the angle between a stick and the y direction. The angular distributions we consider all have the feature that

$$f(\theta)=f(-\theta), \quad \theta\in(0,\pi/2) \tag{1}$$

and that the average angle is $E[\theta]=0$. The sticks' lengths are given by another probability distribution, $g(L)$. We assume θ and L to be independent. Given a random configuration of N sticks with lengths and angles $\{(L_i,\theta_i)\}$, the following quantities may be defined:

$$P_l\equiv\frac{1}{N}\sum_{i=1}^{N}L_i|\cos\theta_i| \tag{2a}$$

and

$$P_t\equiv\frac{1}{N}\sum_{i=1}^{N}L_i|\sin\theta_i| \ . \tag{2b}$$

These are the average longitudinal and transverse stick components with respect to the y direction, respectively. From these we define the macroscopic anisotropy as

$$P\equiv\frac{P_l}{P_t} \ . \tag{2c}$$

For an isotropic sample, we have $P=1$. The larger P is, the more oriented the sticks are along the y direction. A given sample of sticks is considered to be percolating along the y direction if a continuous path can be traced between intersecting sticks from $y=0$ to $y=1$. Similarly for the x direction. The longitudinal critical length, L_{cl} is the lowest average length that gives the onset of y percolation. The transverse critical length, L_{ct} is likewise defined for x percolation.

We wish to investigate the dependences of L_{cl} and L_{ct}

on the anisotropy, P, and on the number of sticks in the system, N. First, consider systems with a given N. To vary the anisotropy, we change the variance of $f(\theta)$. For example, for a normal distribution of angles f is $N(0,\theta_d)$, where θ_d is the standard deviation. By progressively reducing θ_d from some initial value, we can correspondingly increase the anisotropy. Consider now that we have selected a variance of $f(\theta)$. We start with some small average value of L, $E[L]$. With the parameters of f and g chosen, 20 random configurations of sticks are generated, each with N sticks. We look for any percolation. Twenty random configurations at each value of anisotropy and $E[L]$ were made to increase the statistical reliability of finding accurate critical lengths. This is an improvement over Balberg and Binenbaum who presented critical lengths found from three to five configurations per value of anisotropy. Note that for sufficiently small $E[L]$, few of the sticks will overlap. Systematically, $E[L]$ is incremented until percolation is found. Often this is longitudinal percolation. This should be expected, as it is easier to percolate along a preferred direction than normal to it. (Occasionally, at low anisotropy, $P \le 1.4$, we may first encounter transverse percolation.) By further incrementing $E[L]$, we eventually come upon transverse percolation. During the varying of $E[L]$ we record P for each random configuration. It is found that to good approximation, P is independent of $E[L]$. Our results and a comparison with the theory of Sec. III will be presented in Sec. IV.

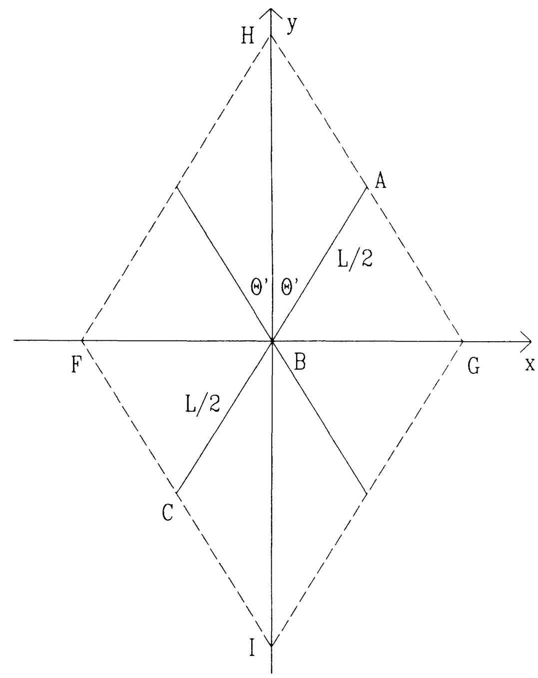

FIG. 1. A stick $\overline{AC}$ of length L is at an angle θ' with respect to the y axis, where θ' is defined in Eq. (3). Sticks at an angle $-\theta'$, with centers inside the parallelogram $HFIG$ will intersect $\overline{AC}$.

III. THEORY

Here we present a simple model that attempts to explain the dependence of the longitudinal and transverse critical lengths on the anisotropy and the number of sticks in the ensemble. As before, let there be N sticks in the ensemble, with an angular distribution $f(\theta)$ and a stick length distribution $g(L)$. Our first approximation is to replace all the stick lengths L_i with the average length $L_0 \equiv \sum_i L_i / N$. Next, let us replace the angular distribution $f(\theta)$ by one in which half the sticks are oriented at θ' and the other half at $-\theta'$ with respect to the y axis, where θ' is defined by

$$\tan\theta' \equiv \frac{\langle |\sin\theta| \rangle}{\langle |\cos\theta| \rangle} = \frac{P_t}{P_l} . \tag{3}$$

For definitiveness, we now look at longitudinal percolation. That is, we wish to find a set of overlapping sticks that goes from $y=0$ to $y=1$. Consider a stick at an angle θ', labeled $\overline{AC}$ in Fig. 1, where B is the center of the stick. The only sticks which can intersect $\overline{AC}$ with nonzero probability are oriented at $-\theta'$. Furthermore, the centers of these sticks must lie in the parallelogram shown in Fig. 1. (Balberg *et al.*[8] define this as the excluded area of the two sticks.) Suppose, in tracing out a possible cluster, that we started at $y=0$ and that $\overline{AC}$ is the highest stick in the cluster, thus far. Let $\overline{AC}$ be the jth stick in the cluster. To make progress towards $y=1$ we ask for the probability that a stick has a center in ΔHFG and is oriented at $-\theta'$. Remembering that the sticks are distributed uniformly, the probability is given by the product of the probability of one stick intersecting $\overline{AC}$ with a higher y center times the number of such sticks. Thus we have

$$P_{j/2} \equiv A(\Delta HFG)\left[\frac{N}{2}-\frac{j}{2}\right] = P_t P_l \left[\frac{N}{2}-\frac{j}{2}\right] , \tag{4}$$

where A is the area. [Since $P_{j/2}$ is a probability, if the right-hand side of Eq. (4) is greater than 1, we set $P_{j/2}=1$.] Furthermore, if such an intersection occurs we see that the average y coordinate of the intersecting stick will be at a distance $P_l/3$ higher than the y coordinate of $\overline{AC}$'s center. Thus, the average number of intersections for y percolation is

$$n \equiv \frac{3}{P_l} . \tag{5}$$

The probability of finding one percolating cluster in the y direction is given by the product of n terms of the form of Eq. (4), which we can write as

$$P^l_{\text{cluster}} = \prod_{j=1}^{n/2} P_j^2 , \tag{6}$$

where from Eq. (4), P_j is defined as

$$P_j \equiv \begin{cases} a_j, & a_j \le 1 \\ 1, & a_j > 1 \end{cases} \tag{7}$$

and

$$a_j \equiv P_t P_l \left| \frac{N}{2} - j \right| . \tag{8}$$

Note that in Eq. (6) we have assumed that n is even. If n is odd, Eq. (6) is multiplied by $P_{n/2+1}$.

Equation (6) gives the probability of forming one cluster. However, it may be possible for several clusters to form, especially for longitudinal percolation in highly anisotropic samples. As mentioned above, the y coordinate of the intersecting stick in the cluster is at an average distance of $P_l/3$ higher. For the x coordinate of the intersecting stick, averaging over ΔHFG gives 0. This comes from

$$\mathcal{P}(x < x_B) = \mathcal{P}(x > x_B) = \tfrac{1}{2} ,$$

where $\mathcal{P}$ is the probability function. But, we see that the average x coordinate of the interesting stick is $P_t/3$, assuming that $x > x_B$, and it is $-P_t/3$ if $x < x_B$. Hence, for longitudinal percolation we have a random walk in the x direction, of average step size $P_t/3$ and equal probability of stepping positive or negative. From Eq. (5), it takes n steps to percolate in the y direction. During these steps, the cluster will span an approximate distance[9] in the x direction of

$$v_0 \equiv \sqrt{n} \frac{P_t}{3} . \tag{9}$$

Since we are bounded by 0 and 1 in the x direction, let

$$v = \begin{cases} v_0, & v_0 \le 1 \\ 1, & v_0 > 1 \end{cases} . \tag{10}$$

Then v is the fractional transverse distance covered when we are looking at longitudinal percolation. Therefore, the total probability for a longitudinal percolating cluster is given by dividing Eq. (6) by v to give

$$P_{\text{tot}} = \frac{1}{v} P^{l}_{\text{cluster}} . \tag{11}$$

To find transverse percolation, we merely interchange P_l and P_t in the above equations. Given values for $\langle |\sin\theta| \rangle$ and $\langle |\cos\theta| \rangle$, we can use the above equations to find the critical lengths and the anisotropy.

One further matter needs to be addressed. Given a $\langle |\cos\theta| \rangle$, which is defined by a particular $f(\theta)$ and a choice of variance of f, there corresponds a unique $\langle |\sin\theta| \rangle$. But for the set of arbitrary probability distributions f, subject to the constraints of Eq. (1), there will be no unique relation between $\langle |\cos\theta| \rangle$ and $\langle |\sin\theta| \rangle$. How can we find an anisotropy that is in some sense independent of a particular f? To answer this, note that we have the following inequalities:

$$0 \le \langle |\cos\theta| \rangle, \quad \langle |\sin\theta| \rangle \le 1 \tag{12a}$$

and

$$1 \le d \le 2 , \tag{12b}$$

where

$$d \equiv \langle |\cos\theta| \rangle + \langle |\sin\theta| \rangle , \tag{12c}$$

and the triangle inequality was used to get the lower bound of Eq. (12b). We do the following. A value of d is chosen to satisfy Eq. (12b). We then vary $\langle |\sin\theta| \rangle$ in steps, starting from $d/2$ and decrementing to 0 (though not going all the way). Then $\langle |\cos\theta| \rangle$ is given by

$$\langle |\sin\theta| \rangle = \begin{cases} d - \langle |\sin\theta| \rangle, & d - \langle |\sin\theta| \rangle \le 1 \\ 1, & d - \langle |\sin\theta| \rangle > 1. \end{cases} \tag{13}$$

With these values, we can find the anisotropy and use Eq. (11) to obtain the critical lengths. We choose 1.5, the midpoint of Eq. (12b), as the most reasonable value of d. It should be realized that the procedure of using Eqs. (12c) and (13) is an approximation. In general, a given f will not yield $\langle |\cos\theta| \rangle$ and $\langle |\sin\theta| \rangle$ satisfying the linear relationship of Eq. (12c) over a range of values of the variance.

A program was written to find the lowest lengths that set $P_{\text{tot}} \ge$ in Eq. (11) as a function of anisotropy, for both longitudinal and transverse percolation. These are the critical lengths. The number of sticks in the sample was a parameter in this calculation.

IV. RESULTS

Here we present and compare the results of Sec. II and III. First, let us consider the predictions of the model of the preceding section. The values of critical lengths from Eq. (11) are displayed in Figs. 2 and 3 for 100 and 500 sticks, respectively. In each figure, the solid line is for longitudinal percolation while the dashed line is for transverse percolation. Following Balberg and Binenbaum,[5] we have normalized the critical lengths in units of the average interstick separation, r, where

$$r \equiv \frac{1}{\sqrt{\pi N}} . \tag{14}$$

From the simulations we have found the critical lengths L_{cl}, L_{ct} as functions of anisotropy, for ensembles of 100 and 500 sticks. These are displayed in Figs. 2 and 3, respectively. For Fig. 2, we have found the critical lengths for three types of ensembles: Those with normal distributions for f and g; with a uniform f and a normal g; and with constant absolute angle and a δ function for g (i.e., all the sticks in an ensemble are the same length). This last pair of distributions corresponds to the simplified choices of distributions made in Sec. III. Similar remarks hold for Fig. 3. The solid objects in the figures are the critical longitudinal lengths. The hollow objects are the critical transverse lengths.

We see from Figs. 2 and 3 that for both the simulations and the theory the transverse critical lengths lie distinctly above the longitudinal critical lengths. Considering separately the transverse and longitudinal results, we see that the simulations with constant length and absolute angle tend to yield larger critical lengths than the other simulations. This is expected,[5] as a distribution of lengths will cause the sticks with lengths greater than the mean length to contribute preferentially to the percolation. Hence percolation will start sooner than if all the lengths in a sample are constant. Nonetheless, the simulation re-

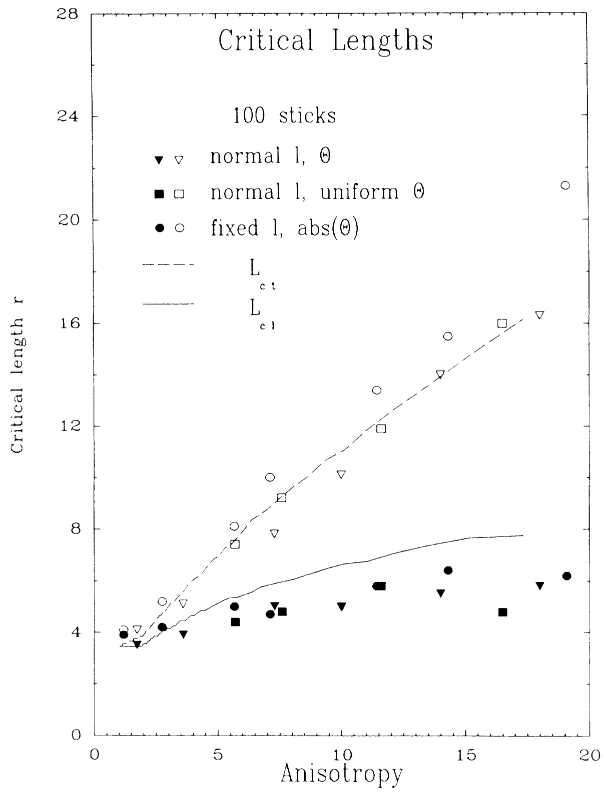

FIG. 2. The critical lengths as a function of anisotropy for samples of 100 sticks. The anisotropy is defined in Eq. (2). The solid and open symbols are from simulations for longitudinal and transverse percolation, respectively. The lines are from Eq. (11).

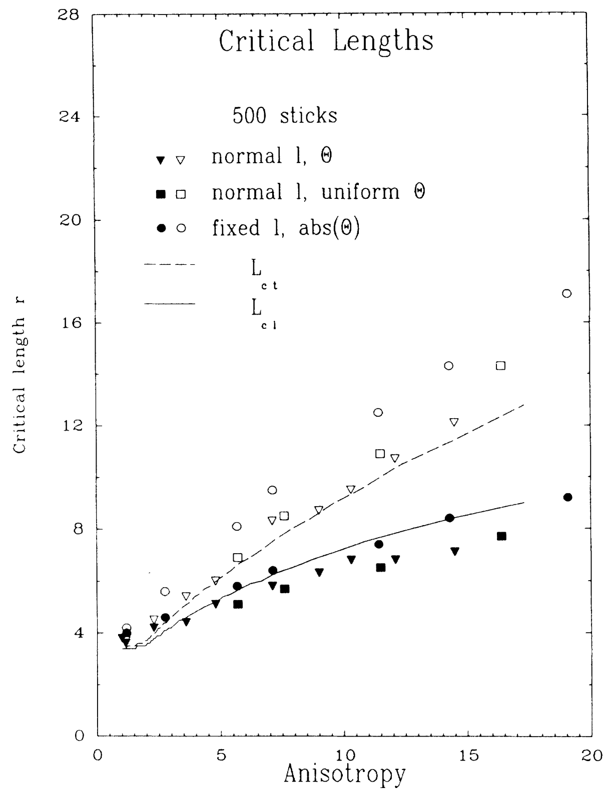

FIG. 3. The critical lengths as a function of anisotropy for samples of 500 sticks. The anisotropy is defined in Eq. (2). The solid and open symbols are from simulations for longitudinal and transverse percolation, respectively. The lines are from Eq. (11).

sults for transverse percolation are clustered close enough, and likewise for longitudinal percolation, that we find a universal behavior of the critical lengths on the anisotropy that is largely independent of the choice of distributions. Comparing the theory with the simulations, we see good agreement for both 100 and 500 sticks. The largest disagreement is for the longitudinal percolation of 100 sticks, with the theory lying above the simulations. But even here, the theoretical curve exhibits the same trends as the simulations and the disagreement is only semiquantitative.

Note that in comparing Figs. 2 and 3, the longitudinal and transverse results tend to converge together as we go from 100 sticks to 500 sticks. This is in accordance with Balberg and Binenbaum[5] who showed by a topological argument that in the limit of infinite N, the two types of critical lengths coincide.

Let us add a comment about the midrange choice of $d=1.5$ made in Eqs. (12) and (13) in the preceding section. This was done to give a definite prescription for the anisotropy. If we set d equal to the lower limit, 1, we get curves that start at a critical length around 5 at isotropy, and remain above the displayed curves as we increase the anisotropy. This was found for both longitudinal and transverse percolation. The agreement between the (undisplayed) $d=1$ curves and the simulations is not as good as for the $d=1.5$ curves shown here in Figs. 2 and 3. Alternatively, choosing d equal to the upper limit of 2 gives curves that start and remain slightly lower than the displayed curves. Hence, we believe our choice of $d=1.5$ to be a reasonable one.

Therefore, we suggest that our theory of Sec. III gives good predictions of critical length. The theory also has the computational advantage of being much faster to run. The curves in Figs. 2 and 3 took less than a minute of CPU (central-processing-unit) time each to find, on a VAX 11/785. By contrast, the CPU time for the simulations is measured in hours. This is especially true for the simulations of 500 sticks. The CPU time required scales roughly as the square of the number of sticks, as the most intensive task is to find the possible intersections amongst N sticks.

V. CONCLUSION

We have investigated the finite-size effects of anisotropic continuum percolation in two dimensions. The elements that percolate are widthless sticks. We have developed a simple theory to explain the dependence of longitudinal and transverse critical lengths on anisotropy and the finite number of sticks in the sample. By comparing the theory to simulations, we find good agreement. It also affords significant computational advantages over performing simulations. We believe that our theory is the first to explain the finite-size simulation results for anisotropic continuum percolation in two dimensions. Thus, we suggest that the theory offers a useful complement to the running of simulations.

ACKNOWLEDGMENTS

We would like to gratefully acknowledge the support of the Office of Naval Research under Contract No. N00014-84-K-0501. One of us (W.J.B) is the recipient of support from the IBM Corporation.

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