The Approximate Invariance of the Average Number of Connections for the Continuum Percolation of Squares at Criticality

Sameet Sreenivasan,* Don R. Baker,*† Gerald Paul,* and H. Eugene Stanley*
*Center for Polymer Studies and Dept. of Physics, Boston University, Boston, MA 02215 USA
†Department of Earth and Planetary Sciences, McGill University
3450 rue University, Montréal, QC H3A 2A7 Canada
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We perform Monte Carlo simulations to determine the average excluded area $<A_{\text{ex}}>$ of randomly oriented squares, randomly oriented widthless sticks and aligned squares in two dimensions. We find significant differences between our results for randomly oriented squares and previous analytical results for the same. The sources of these differences are explained. Using our results for $<A_{\text{ex}}>$ and Monte Carlo simulation results for the percolation threshold, we estimate the mean number of connections per object $B_c$ at the percolation threshold for squares in 2-D. We study systems of squares that are allowed random orientations within a specified angular interval. Our simulations show that the variation in $B_c$ is within 1.6% when the angular interval is varied from 0 to $\pi/2$.

I. INTRODUCTION

Continuum percolation has been of significant interest in the study of porous media. It offers important advantages over lattice percolation due to the fact that the majority of systems encountered in nature are not confined to a lattice and are therefore modeled more appropriately using continuum systems.

When studying the transport properties in porous media, the connectivity properties of the spanning cluster at percolation threshold are important. One measure of the connectivity is the mean number of connections per site. In the case of lattice percolation, Scher and Zallen demonstrated the approximate dimensional invariance of this quantity. The behavior of the analogous quantity $B_c$ in continuum percolation systems has been previously studied. In the case of continuum percolation, the product of the critical concentration $N_c$ of objects at the percolation threshold and the average excluded area $<A_{\text{ex}}>$ gives the critical average number of intersections per object $B_c$.

$$B_c = N_c <A_{\text{ex}}>.$$ (1)

The excluded area of an object is defined as the area around an object into which the center of another similar object is not allowed to enter if intersection of the two objects is to be avoided. In the case of objects that are allowed random orientations in a specified angular interval, one defines an average excluded area $<A_{\text{ex}}>$, that is the excluded area averaged over all possible orientational configurations of the two objects. It has been claimed that $B_c$ for percolating systems of differently shaped objects lies within a bounded range: in 2-D, $3.57 \leq B_c \leq 4.48$. $B_c$ represents the connectivity in the spanning cluster and is of interest as the invariance of $B_c$ would enable us to estimate the percolation threshold $N_c$ using Eq. (1), once $<A_{\text{ex}}>$ has been calculated.

In the present work we focus on continuum percolation systems of squares in 2-D, in which the objects are allowed random orientations within a specified angular interval. The motivation for the study of such orientationally constrained systems comes from the geological observation that fractures in rocks do not have random isotropic orientations but are oriented within a more or less fixed angular interval. For our system of squares there is one angle $\theta$ that specifies the orientation of the object and we constrain it to lie within $-\theta_{\mu} \leq \theta \leq \theta_{\mu}$. We determine the percolation thresholds for different values of the constraint angle $\theta_{\mu}$. Simulations are also performed to find the excluded area for each case. Our results show that for a given object shape $B_c$ is constant to within 1.6% for squares independent of the value of the constraint angle $\theta_{\mu}$.

II. SIMULATION METHOD FOR FINDING EXCLUDED AREA

Here we describe the method used to determine the excluded area for a pair of objects that are allowed random orientations within the angular interval $-\theta_{\mu}$ to $\theta_{\mu}$. For rectangles (squares being a particular case) $\theta_{\mu} = 0$ corresponds to the case where the objects are aligned parallel to each other and $\theta_{\mu} = \pi/2$ corresponds to the random isotropic case. We describe the algorithm for finding the excluded area of squares in 2-D.

A square of unit side is placed with its center coinciding with the center of a lattice of edge length $L = 5$. The lattice size is chosen to be larger than the excluded area, but small enough to sufficiently minimise the number of wasted trials and yield good statistics. The square is given an orientation $\theta_i$, randomly chosen in the interval $-\theta_{\mu} \leq \theta_i \leq \theta_{\mu}$, with the reference axis. A second square is then introduced into the lattice with its center randomly positioned in the lattice. This square is given an orientation $\theta_j$ chosen randomly from the same interval as for the first object. We then determine if the two squares overlap. We repeat this procedure for $10^5$ trials.
and record the number of times the two squares overlap. This number divided by the number of trials is the probability that the two objects overlap. The probability of overlap times the area, \( L^2 \), of the lattice yields the average excluded area for a pair of squares oriented randomly between \(-\theta_\mu\) to \(\theta_\mu\). The method used to determine the overlap of squares in 2-D is described in detail in Ref. [1].

III. EXCLUDED AREA SIMULATION RESULTS

We determine the average excluded area for a unit square for different constraint angles. We also determine the excluded area of widthless sticks for the case of random isotropic orientations. In our simulations the widthless stick is represented by a rectangle of edge lengths 1 and \(1 \times 10^{-12}\). Table 1 lists the Monte Carlo results for \(< A_{ex} >\) obtained for the different objects studied for the case of random isotropic orientations. Table 2 shows the variation of \(< A_{ex} >\) for squares with the constraint angle. Our values for \(< A_{ex} >\) for aligned squares are consistent with all previous results [3]. Furthermore, our \(< A_{ex} >\) values for randomly oriented widthless sticks are also consistent with earlier determinations [7]: our slightly higher value of \(< A_{ex} >\) compared to that of Ref. [3] is explained by the fact that our widthless sticks have a finite width and thus are expected to exhibit a larger \(< A_{ex} >\) than found analytically for the zero width limit. However our \(< A_{ex} >\) for the case of randomly aligned squares is different from previous analytical results, our value being 12% above that determined by Ref. [3]. We propose a reason for this difference in the next section.

IV. DISCREPANCY WITH PREVIOUS ANALYTICAL DETERMINATION OF EXCLUDED AREA

We investigated the cause of the difference between our value of \(< A_{ex} >\) for squares in 2-D and the previous analytical result in [3] and found it to be the following: In arriving at the expression for \(< A_{ex} >\) Ref. [3] finds the excluded area for a pair of rectangles (Eq. 18) with a given relative orientation \(\theta\) (see Figure 1). For squares, using equation (Eq. 18) in Ref. [3],

\[
A_{ex} = (\sin \theta + \cos \theta + 1)^2 - 2 \sin \theta \cos \theta,
\]  

where

\[
\theta \equiv |\theta_i - \theta_j|,
\]

\(\theta_i\) and \(\theta_j\) being the individual orientations of the two squares. Ref. [3] then obtains the average excluded area by averaging the right hand side of Eq.(3) over all possible orientations of both objects, \(-\theta_\mu \leq \theta_i \leq \theta_\mu\) and \(-\theta_\mu \leq \theta_j \leq \theta_\mu\), using a uniform probability distribution

\[
P(\theta_i) = P(\theta_j) = 1/2\theta_\mu.
\]

However, it appears Ref. [3] overlooked the fact that Eq.(3) holds only for \(0 \leq \theta \leq \pi/2\) (hence \(0 \leq \theta_\mu \leq \pi/4\)), since \(\pi/2 \leq \theta \leq \pi\), the expression gives a value of \(A_{ex}\) less than the minimum possible value of 4 [3]. Thus the procedure of Ref. [3] does not work when the constraint angle \(\theta_\mu\) is greater than \(\pi/4\). The correct result can be obtained by replacing \(\theta\) in Eq.(3) by

\[
\theta' = \theta \mod (\pi/2),
\]

so that Eq.(3) holds for all values of \(\theta_\mu\). For the random isotropic case \(\theta_\mu = \pi/2\), using the modified Eq.(4) and integrating numerically we obtain \(< A_{ex} > = 4.54647\) which is in close agreement with our Monte-Carlo simulation result.

We also calculate the values of \(< A_{ex} >\) for squares with other values of \(\theta_\mu\) between 0 and \(\pi/2\) (Table 2). We notice that the values of \(< A_{ex} >\) are the same for \(\theta_\mu = \pi/4\) and \(\theta_\mu = \pi/2\), which is true since the rotation of a square in a particular configuration through an additional angle of \(\pi/4\) yields the same configuration.

Note that the value of \(< A_{ex} >\) appears to decrease for \(\theta_\mu > \pi/4\), reaches a local minimum near \(\theta_\mu = \pi/3\) and then increases again till it reaches a maximum at \(\theta_\mu = \pi/2\) (see Fig. 1). This can be explained as follows. The case \(\theta_\mu = \pi/4\) is equivalent to the case of random isotropic orientation. Here the angle \(\theta = |\theta_i - \theta_j|\) can range from 0 to \(\pi/2\). When \(\theta_\mu\) is greater than \(\pi/4\), \(\theta\) can take values greater than \(\pi/2\) which means that in addition to the configurations obtained for \(\theta_\mu = \pi/2\), there are other configurations for which the relative orientation \(\pi/2 \leq \theta \leq 2\theta_\mu\). However the latter configurations are, in fact, the same as those for \(\theta = (2\theta_\mu - \pi/2) < \pi/2\) due to the symmetry of squares. Thus, the decrease in the \(< A_{ex} >\) between \(\theta_\mu = \pi/4\) and \(\theta_\mu = \pi/2\) can be attributed to the increased probability of achieving configurations with smaller excluded areas.

V. PERCOLATION THRESHOLDS

Using the procedure of Ref. [4], we perform Monte Carlo simulations for the determination of the percolation threshold based upon the Leath method [1] and the methods Lorenz and Ziff [12] used in their study of continuum percolation of spheres. The only difference in our present simulations is that the random numbers generated to fix the orientation of an object lie within a specified angular range from \(-\theta_\mu\) and \(\theta_\mu\). We determine the percolation thresholds of squares in 2-D for different values of the constraint angle \(\theta_\mu\). These results are shown in Table 2. We also show the values of critical area fraction \(\phi_c\). Fig. 2 shows a plot of the percolation threshold \(N_c\) for squares in 2-D versus the constraint angle \(\theta_\mu\). An interesting feature of the 2-D plot is that as we increase the orientational freedom beginning from \(\theta_\mu = 0\),
$N_c$ drops until it reaches the value for $\theta_\mu = \pi/4$, then begins increasing until it reaches a maximum and then falls again. This behavior is expected if $B_c$ is to remain approximately invariant, as we shall explain below.

VI. APPROXIMATE INVARiance OF $B_c$

Using the percolation thresholds and excluded area obtained from our Monte Carlo simulations, we find the average number of connections per object at threshold $B_c$. Table 2 shows the values of $B_c$ for squares for various values of the constraint angle $\theta_\mu$. The change in $B_c$ in going from a constraint angle of $\theta_\mu = 0$ to $\theta_\mu = \pi/2$ is less than 1.6%. Using the old values of $<A_{ex}>$ [7], the variation in $B_c$ is seen to be $\approx 9.5\%$. We see that the slight decrease in $<A_{ex}>$ between $\theta_\mu = \pi/4$ and $\theta_\mu = \pi/2$ (see Fig. 3) is compensated by an increase in the corresponding $N_c$ (see Fig. 3) to give an approximately invariant $B_c$. The closeness of $B_c$ values for a given system is striking and is consistent with the hypothesis that $B_c$ is approximately invariant for continuum percolating systems of a particular shape.

VII. SUMMARY

Our results show that the value of $B_c$ is approximately independent of orientational constraints. The $B_c$ value of a shape is indicative of the efficiency of the object in forming a percolating cluster. Not only the magnitude of the excluded area plays a part in the formation of connections, but also the distribution of the average excluded area in space. This is easily seen from the fact that both unit area discs and aligned unit area squares have $<A_{ex}> = 4 [3]$, but the percolation threshold of aligned squares $\phi_c = 0.6666 [10]$ is lower than that of discs $\phi_c = 0.676339 [13]$. Our results suggest that the value $B_c$ can be considered as a unique quantitative characteristic of a shape and can therefore be useful in the prediction of the percolation threshold as has been previously pointed out [6].

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TABLE I. Comparison of the average excluded area for widthless sticks and squares in 2-D. The uncertainty in \( < A_{ex} > \) is estimated as follows. The reciprocal of the square root of the number of Monte Carlo trials yielding intersection of the two objects is the fractional uncertainty in the determination of \( < A_{ex} > \). The product of the fractional uncertainty and the estimated value of \( < A_{ex} > \) is the uncertainty in that value.

| Object          | \( < A_{ex} > \) for unit area object | Previous Result |
|-----------------|---------------------------------------|-----------------|
| Widthless sticks| 0.6367 ± 0.0001                       | 0.6366 \[7\]    |
| Aligned squares | 3.9998 ± 0.0003                       | 4 \[8\]         |
| Random Squares  | 4.5466 ± 0.0004                       | 4.084 \[7\]     |
TABLE II. Critical area fraction, percolation threshold, average excluded area and critical average number of connections per object for squares in 2-D. Estimation of uncertainty in $\phi_c$ is described in [10].

| Constraint Angle | $\phi_c$      | $N_c$     | $<A_{ex}>$     | $B_c$  |
|------------------|---------------|-----------|----------------|--------|
| $\pi/2$          | 0.6254 ± 0.0002 | 0.981896 | 4.5466 ± 0.0004 | 4.464  |
| $\pi/3$          | 0.6265 ± 0.0005 | 0.984837 | 4.5309 ± 0.0004 | 4.462  |
| $\pi/4$          | 0.6255 ± 0.0001 | 0.982163 | 4.5459 ± 0.0004 | 4.465  |
| $\pi/8$          | 0.6355 ± 0.0005 | 1.009229 | 4.4076 ± 0.0004 | 4.448  |
| $\pi/16$         | 0.6485 ± 0.0005 | 1.045546 | 4.234 ± 0.0004  | 4.443  |
| $\pi/32$         | 0.6575 ± 0.0005 | 1.071484 | 4.1240 ± 0.0004 | 4.419  |
| 0                | 0.6666 ± 0.0004 | 1.098412 | 3.9998 ± 0.0003 | 4.394  |
FIG. 1. Procedure for determining the excluded area of two squares of side $L$: the first square $i$ (shaded), is kept fixed while the second square $j$ having orientation $\theta$ with respect to $i$, is moved around $i$ always keeping contact, and the locus of the center of $j$ is found. The area within the locus gives the excluded area for a given relative orientation of the two squares.

FIG. 2. Plot of the excluded area $\langle A_{ex} \rangle$ for squares in 2-D versus the constraint angle $\theta_\mu$. The uncertainties are smaller than the symbols.

FIG. 3. Plot of the percolation threshold $N_c$ for squares in 2-D versus the constraint angle $\theta_\mu$. The uncertainties are smaller than the symbols.