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The approximate invariance of the average number of connections for the continuum percolation of squares at criticality

Sameet Sreenivasan[a,*], Don R. Baker[a,b], Gerald Paul[a], H. Eugene Stanley[a]

[a] Center for Polymer Studies, Department of Physics, Boston University, Boston, MA 02215, USA
[b] Department of Earth and Planetary Sciences, McGill University 3450 rue University, Montréal, QC, Canada H3A 2A7

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Abstract

We perform Monte Carlo simulations to determine the average excluded area $\langle A_{ex}\rangle$ 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 $\langle A_{ex}\rangle$ 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 $\pi/2$.

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1. Introduction

Continuum percolation has been of significant interest in the study of porous media [1]. It offers important advantages over lattice percolation due to the fact that the

* Corresponding author.
E-mail address: sameet@buphy.bu.edu (S. Sreenivasan).

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majority of systems encountered in nature are not confined to a lattice and are therefore modeled more appropriately using continuum systems [1–4].

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 [5] demonstrated the approximate dimensional invariance of this quantity. The behavior of the analogous quantity B_c in continuum percolation systems has been previously studied [6–8]. 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 $\langle A_{ex}\rangle$ gives the critical average number of intersection per object B_c [6–8].

$$B_c = N_c\langle A_{ex}\rangle \ . \tag{1}$$

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 [9]. In the case of objects that are allowed random orientations in a specified angular interval, one defines an average excluded area $\langle A_{ex}\rangle$, that is the excluded area averaged over all possible orientational configurations of the two objects. It has been claimed [7] that B_c for percolating systems of differently shaped objects lies within a bounded range in 2-D, $3.57 \leqslant B_c \leqslant 4.48$. 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 $\langle A_{ex}\rangle$ 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 θ that specifies the orientation of the object and we constrain it to lie within $-\theta_\mu \leqslant \theta \leqslant \theta_\mu$. We determine the percolation thresholds for different values of the constraint angle θ_μ. 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 θ_μ.

2. 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 θ_μ. 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 θ_i, randomly chosen in the interval $-\theta_\mu \leqslant \theta_i \leqslant \theta_\mu$, 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 θ_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 10^9 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 $-\theta_\mu$ and θ_μ. The method used to determine the overlap of squares in 2-D is described in detail in Ref. [10].

3. 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 1×10^{-12}. Table 1 lists the Monte Carlo results for $\langle A_{ex}\rangle$ obtained for the different objects studied for the case of random isotropic orientations. Table 2 shows the variation of $\langle A_{ex}\rangle$ for squares with the constraint angle. Our values for $\langle A_{ex}\rangle$ for aligned squares are consistent with all previous results [7]. Furthermore, our $\langle A_{ex}\rangle$ values for randomly oriented widthless sticks are also consistent with earlier determinations [7]; our slightly higher value of $\langle A_{ex}\rangle$ compared to that of Ref. [7] is explained by the fact that our widthless sticks have a finite width and thus are expected

Table 1
Comparison of the average excluded area for widthless sticks and squares in 2-D

Object	$\langle A_{ex}\rangle$ 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]

The uncertainty in $\langle A_{ex}\rangle$ 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 $\langle A_{ex}\rangle$. The product of the fractional uncertainty and the estimated value of $\langle A_{ex}\rangle$ is the uncertainty in that value.

Table 2
Critical area fraction, percolation threshold, average excluded area and critical average number of connections per object for squares in 2-D

Constraint angle	ϕ_c	N_c	$\langle A_{ex}\rangle$	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

Estimation of uncertainty in ϕ_c is described in Ref. [10].

to exhibit a larger $\langle A_{ex} \rangle$ than found analytically for the zero width limit. However our $\langle A_{ex} \rangle$ for the case of randomly aligned squares is different from previous analytical results, our value being 12% above that determined by Ref. [7]. We propose a reason for this difference in the next section.

4. Discrepancy with previous analytical determination of excluded area

We investigated the cause of the difference between our value of $\langle A_{ex} \rangle$ for squares in 2-D and the previous analytical result in Ref. [7] and found it to be the following: In arriving at the expression for $\langle A_{ex} \rangle$ Ref. [7] finds the excluded area for a pair of rectangles (Eq. (18)) with a given relative orientation θ (see Fig. 1). For squares, using equation (Eq. (18)) in Ref. [7],

$$A_{ex} = (\sin\theta + \cos\theta + 1)^2 - 2\sin\theta\cos\theta \; , \tag{2}$$

where

$$\theta \equiv |\theta_i - \theta_j| \; , \tag{3}$$

θ_i and θ_j being the individual orientations of the two squares. Ref. [7] then obtains the average excluded area by averaging the right-hand side of Eq. (2) over all possible orientations of both objects, $-\theta_\mu \leqslant \theta_i \leqslant \theta_\mu$ and $-\theta_\mu \leqslant \theta_j \leqslant \theta_\mu$, using a uniform probability distribution

$$P(\theta_i) = P(\theta_j) = 1/2\theta_\mu \; . \tag{4}$$

However, it appears Ref. [7] overlooked the fact that Eq. (2) holds only for $0 \leqslant \theta \leqslant \pi/2$ (hence $0 \leqslant \theta_\mu \leqslant \pi/4$), since for $\pi/2 \leqslant \theta \leqslant \pi$, the expression gives a value of A_{ex} less

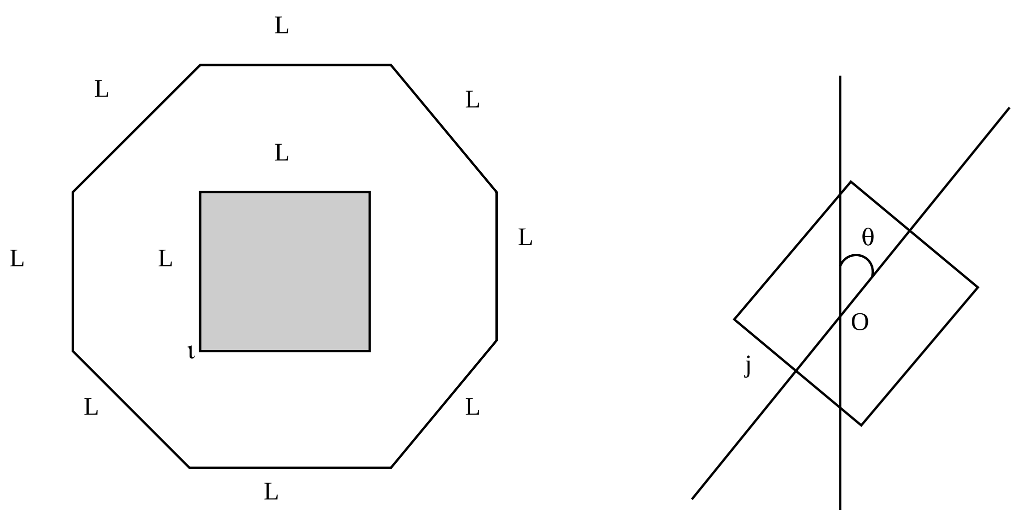

Fig. 1. Procedure for determining the excluded area of two squares of side L: the first square i (shaded), is kept fixed while the second square j having orientation θ with respect to i, is moved around i always keeping contact, and the locus of the center of j is found. The area within the locus gives the excluded area for a given relative orientation of the two squares.

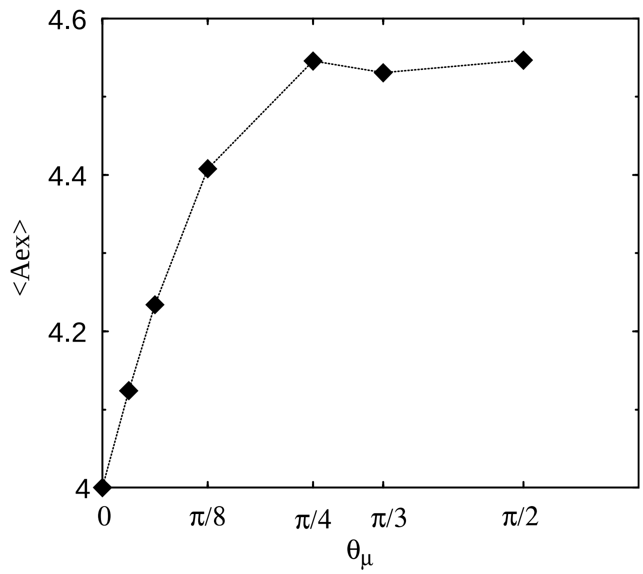

Fig. 2. Plot of the excluded area $\langle A_{ex} \rangle$ for squares in 2-D versus the constraint angle θ_μ. The uncertainties are smaller than the symbols.

than the minimum possible value of 4 [7]. Thus the procedure of Ref. [7] does not work when the constraint angle θ_μ is greater than $\pi/4$. The correct result can be obtained by replacing θ in Eq. (2) by

$$\theta' = \theta \bmod(\pi/2) , \tag{5}$$

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

We also calculate the values of $\langle A_{ex} \rangle$ for squares with other values of θ_μ between 0 and $\pi/2$ (Table 2). We notice that the values of $\langle A_{ex} \rangle$ are the same for $\theta_\mu = \pi/4$ and $\pi/2$, 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 $\langle A_{ex} \rangle$ 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. 2). 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 θ_μ is greater than $\pi/4$, θ can take values greater than $\pi/2$ which means that in addition to the configurations obtained for $\theta_\mu = \pi/4$, there are other configurations for which the relative orientation $\pi/2 \leqslant \theta \leqslant 2\theta_\mu$. 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 $\langle A_{ex} \rangle$ between $\theta_\mu = \pi/4$ and $\pi/2$ can be attributed to the increased probability of achieving configurations with smaller excluded areas.

5. Percolation thresholds

Using the procedure of Ref. [10], we perform Monte Carlo simulations for the determination of the percolation threshold based upon the Leath method [11] 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 θ_μ. We determine the percolation thresholds of squares in 2-D for different values of the constraint angle θ_μ. These results are shown in Table 2. We also show the values of critical area fraction ϕ_c. Fig. 3 shows a plot of the percolation threshold N_c for squares in 2-D versus the constraint angle θ_μ. 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.

6. Approximate invariance of B_c

Using the percolation thresholds and excluded area obtained from our Monte Carlo simulations, we find the average number [7] 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 θ_μ. The change in B_c in going from a constraint angle of $\theta_\mu = 0$ to $\pi/2$ is less than 1.6%. Using the old values of $\langle A_{ex} \rangle$ [7], the variation in B_c is seen to be $\approx$ 9.5%. We see that the slight decrease in $\langle A_{ex} \rangle$ between $\theta_\mu = \pi/4$ and $\pi/2$ (see Fig. 2) 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

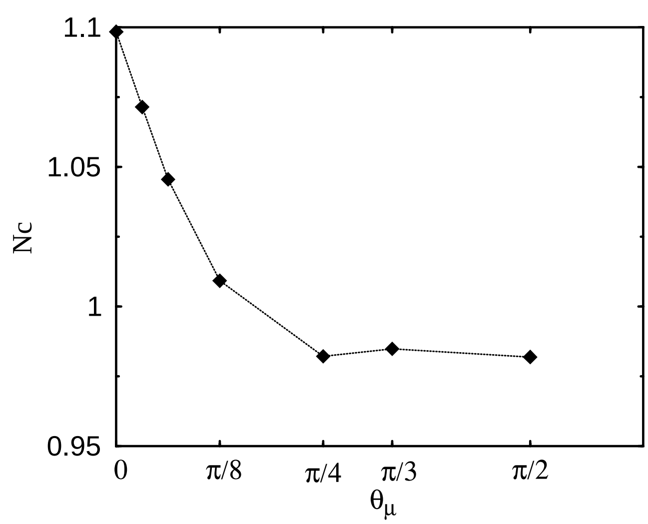

Fig. 3. Plot of the percolation threshold N_c for squares in 2-D versus the constraint angle θ_μ. The uncertainties are smaller than the symbols.

the hypothesis that B_c is approximately invariant for continuum percolating systems of a particular shape.

7. 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 $\langle A_{ex} \rangle = 4$ [7], 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 [6–8].

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