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Precise percolation thresholds of two-dimensional random systems comprising overlapping ellipses

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HIGHLIGHTS

- High-precision percolation threshold is reported for all overlapping ellipse systems.
- Vieillard-Baron's contact function is generalized to unequal ellipses.
- Intrinsic threshold symmetry is unveiled in systems of unequal ellipses/circles.

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ABSTRACT

This work explores the percolation thresholds of continuum systems consisting of randomly-oriented overlapping ellipses. High-precision percolation thresholds for various homogeneous ellipse systems with different aspect ratios are obtained from extensive Monte Carlo simulations based on the incorporation of Vieillard-Baron's contact function of two identical ellipses with our efficient algorithm for continuum percolation. In addition, we generalize Vieillard-Baron's contact function from identical ellipses to unequal ellipses, and extend the Monte Carlo algorithm to heterogeneous ellipse systems where the ellipses have different dimensions and/or aspect ratios. Based on the concept of modified excluded area, a general law is verified for precise prediction of percolation threshold for many heterogeneous ellipse systems. In particular, the study of heterogeneous ellipse systems gains insight into the apparent percolation threshold symmetry observed earlier in systems comprising unequal circles (Consiglio et al., 2004).

1. Introduction

For a long time, systems consisting of overlapping or hard ellipses have received a great deal of attention in theoretical studies [1–6]. Recently, the extensive research on percolation systems based on low-dimensional nanoparticles, such as two-dimensional (2D) layered materials (graphene, MoS_2, etc. [7–10]) and one-dimensional fiber-like nanostructure (carbon nanotubes, metal nanowires, etc. [11–13]), extends the interest in overlapping ellipse systems to many practical applications. Like ellipsoids in three-dimensional (3D) systems [14], ellipses represent the general object shape in 2D systems, ranging from extremely anisotropic fibers or rods to isotropic disks. Up to date, however, there are still some fundamental issues concerning ellipse percolation not well addressed. One the one hand, the reported percolation thresholds of homogeneous ellipse systems are still at low precision [1], not matching their counterparts, such as the systems comprising sticks [15,16], disks (circles) [17], and rectangles [18]. On the other hand, most simulation [1] and analytic [2] work employs the contact function proposed by Vieillard-Baron [5] (hereafter referred to as VB contact function) to

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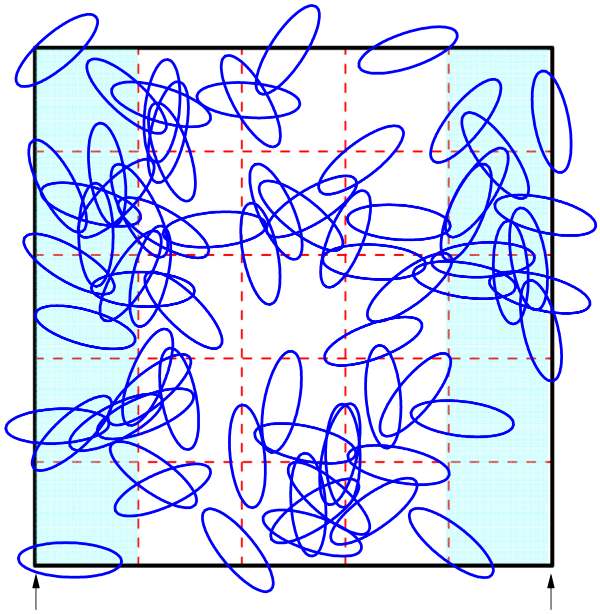

Fig. 1. Snapshot of a percolated homogeneous FBC percolation system consisting of randomly-distributed overlapping ellipses, as produced by our Monte Carlo simulation program. All the ellipses are of semi-major axis $a = 0.5$ and aspect ratio $r = 3$. The system (of size $L = 5$ in this figure) percolates when its two boundaries, labeled respectively as "LEFT" and "RIGHT" and treated as "fake" ellipses in our algorithm, are connected by intersecting ellipses (like the case in this figure).

efficiently determine the overlapping status of two identical ellipses. However, the present form of VB contact function only applies to identical ellipses, restricting relevant studies to homogeneous ellipse systems.

This work aims to advance the field and is outlined as follows. Section 2 explores the high-precision percolation thresholds for homogeneous systems with various ellipse aspect ratios. Section 3 generalizes VB contact function from identical ellipses to unequal ellipses and investigates heterogeneous systems. Relevant topics are also discussed, including excluded area [18] and apparent symmetry of percolation threshold in systems of unequal object shapes [19]. Section 4 summarizes all the conclusions.

2. Homogeneous ellipse systems

In order to obtain high-precision percolation thresholds for homogeneous ellipse systems, we conduct extensive Monte Carlo simulations (each reported percolation threshold requires 5000–40 000 core-hours of computation) through an efficient algorithm which integrates the VB contact function [5] into our prior continuum percolation algorithm [15,18]. The algorithm, based on the combination between the fast Newman–Ziff algorithm [20] and the subcell concept [21], is identical to that for stick and rectangle percolation [15,18] except that the bonding criterion is determined by the VB contact function. Briefly, we begin with a blank system (square area) and continuously add ellipses into the system until a cluster, which comprises connecting ellipses, percolates the system. An ellipse of known (fixed) major semi-axis a, minor semi-axis b and hence aspect ratio $r = a/b$, is simply stored as the combination of a random point (x, y) as its center with a random angle θ as its orientation, and can be denoted as $E : [(a, b) : (x, y), \theta]$. As shown in Fig. 1, The system of size L is divided into $L \times L$ subcells (squares), each of which has length $l = 2a$ (for simplicity, we set $l \equiv 1$ and hence $a = 1/2$). During the simulations, each ellipse is registered into a subcell where its center locates so that it is only necessary to check its connectivity with those ellipses locating in the same and eight neighboring subcells. The connectivity between any two identical ellipses, $E_1 : [(a, b) : (x_1, y_1), \theta_1]$ and $E_2 : [(a, b) : (x_2, y_2), \theta_2]$, can be determined by the VB contact function [5],

$$\Psi = 4\left(f_1^2 - 3f_2\right)\left(f_2^2 - 3f_1\right) - (9 - f_1 f_2)^2, \tag{1a}$$

where $(\beta = 1, 2)$

$$f_\beta = 3 + (a/b - b/a)^2 \sin^2 \Delta\theta - a^{-2}\left(\Delta x \cos\theta_\beta + \Delta y \sin\theta_\beta\right)^2 - b^{-2}\left(\Delta y \cos\theta_\beta - \Delta x \sin\theta_\beta\right)^2, \tag{1b}$$

with $\Delta x = x_2 - x_1$, $\Delta y = y_2 - y_1$, and $\Delta\theta = \theta_2 - \theta_1$. The two ellipses intersect (overlap) if and only if $\Psi < 0$ or all Ψ, f_1, and f_2 are positive (i.e., $\Psi > 0, f_1 > 0$, and $f_2 > 0$).

For free boundary conditions (FBC), the system percolates (spans) when a cluster connects both the two opposite boundaries, e.g., the two vertical boundary lines, $x = 0$ and $x = L$, in Fig. 1. To facilitate checking the presence of a spanning