Invariant Percolation Properties in Random Isotropic Systems of Conductive Discorectangles on a Plane: From Disks to Sticks

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1. Introduction

The 2D systems of randomly placed, metallic nanowires, and nanorods are being extensively studied. The interest in these systems is inspired by their combination of high electrical conductivity with excellent optical transparency that is in demand in numerous technological applications such as touch screens, transparent heaters, solar cells, electromagnetic interference shielding films, and flexible electronics.

To mimic the shape of elongated particles and, at the same time, simplify the simulations, different simple geometrical figures are used. During simulation, the shape and the aspect ratio of the particles affect the electrical and optical properties of films. However, some features of the conductive films may be insensitive both to the shape of particles and to their aspect ratio. 2D random systems of isotropically placed, overlapping, identical discorectangles (stadia) with aspect ratios ranging from 1 (disks) to $\infty$ (zero-width sticks) are studied. The particular case when only the junction resistance between conductive particles is taken into account is considered. The effect of the aspect ratio and the number density of conductive discorectangles on the behavior of the electrical conductivity, the local conductivity exponent, and the current-carrying backbone is analyzed. The computer simulations demonstrate that some of the properties of random, isotropic 2D systems of conductive discorectangles are insensitive to the aspect ratios of the particles.

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The rest of the article is constructed as follows. Section 2 describes some technical details of our simulation. In Section 3, we present our main results and discuss some open questions. Section 4 summarizes the main results and suggests possible directions for further study.

2. Experimental Section

2.1. Sampling

A discorectangle (a stadium) is a rectangle with semicircles at a pair of opposite sides (Figure 1). Its aspect ratio is

$$\varepsilon = \frac{l}{d}$$

When $\varepsilon = 1$, a discorectangle reduces in a disk. The limiting case $\varepsilon = \infty$ corresponds to a zero-width (widthless) stick.

Basically, in our study we used discorectangles with four alternative values of the aspect ratio, that is, $\varepsilon = 1, 7, 20, \infty$, while the discorectangle’s length was fixed, $l = 1$. Some additional investigations were performed for intermediate values of $\varepsilon$. Identical, permeable discorectangles with the chosen value

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To mimic the shape of elongated particles and, at the same time, simplify the simulations, different simple geometrical figures are used, for example, zero-width sticks (rods), ellipses, superellipses, and discorectangles (stadia). Comparisons of some of the properties of random isotropic systems of conductive overlapping discorectangles. Their aspect ratios ranged from 1 (disks) to $\infty$ (zero-width sticks). We analyzed the behavior of the electrical conductivity, the local conductivity exponent, and the backbone with respect to the aspect ratio and the number density of these conductive discorectangles. We have compared our results with the published results for ellipses and sticks.

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of aspect ratio were randomly placed on a substrate. Their centers were independent and identically distributed within a square domain of size \( L \times L \), while their orientations were equiprobable. To reduce the finite-size effect, periodic boundary conditions (PBCs) were applied along both mutually perpendicular directions (Figure 2).

The number density of the deposited particles is the number of particles \( N \) per unit area, that is

\[
n = \frac{N}{L^2} \tag{2}
\]

Another widely used quantity to characterize a deposit is the total area fraction of the deposited particles

\[
\eta = A_n \tag{3}
\]

where \( A \) is the area of each particle. In contrast to open boundary conditions, PBCs ensure that the relation (3) is exact. In the case of elongated particles, PBCs ensure the isotropic deposition of such particles, while the closed boundary conditions force the particles to align along the boundaries, which leads to locally anisotropic systems.

2.2. Overlapping of the Deposited Particles

Two discorctangles are considered as connected if they overlap. The overlapping occurs when the center of the second discorctangle is located within the excluded area of the first one\(^{[28]}\). The excluded area depends on the mutual orientation of the discorctangles

\[
A_{ex} = \sin \theta(l - d)^2 + 4d(l - d) + \pi d^2 \tag{4}
\]

where \( \theta \) is the angle between the two discorctangles\(^{[28,29]}\) (Figure 3).

Superposition of the excluded areas for all possible mutual angles between two discorctangles can be treated as a probability map, that is, the probability that a randomly oriented discorctangle will overlap an original discorctangle. Figure 4 presents the probability map when all orientations are equiprobable (isotropic deposition).

To detect any overlapping of the discorctangles, we used their midlines (Figure 5): 1) The discorctangles overlap, if their midlines intersect each other (Figure 5a); 2) If the two midlines do not intersect each other, but the shortest distance between these midlines is less than the width of the discorctangle, \( d \), the corresponding discorctangles overlap (Figure 5b); and 3) If the two midlines do not intersect each other and the shortest distance between these midlines is larger than the width of the discorctangle, \( d \), the corresponding discorctangles do not overlap (Figure 5c).

The limiting cases are obvious. To check whether two zero-width sticks intersect, consideration of just the first item above is enough. The two disks intersect each other when the distance between their centers is less than \( d \).

The probability that two identical particles intersect with each other can be found using the excluded area concept\(^{[28]}\)

\[
P = \frac{A_{ex}}{L^2} \tag{5}
\]

where, in the case of isotropically placed discorctangles, the angle-averaged excluded area is

\[
\langle A_{ex} \rangle = \frac{2}{\pi} (l - d)^2 + 4d(l - d) + \pi d^2 \tag{6}
\]
The mean number of intersections per deposited particle is \( \langle k \rangle = (N - 1)P \) or
\[
\langle k \rangle \approx nPL^2
\]
when \( N \gg 1 \). Hence, the total number of contacts (junctions) between particles is
\[
N_j = N \frac{nPL^2}{2} = \frac{n^2L^2 \langle A_{ex} \rangle}{2}
\]
while the number density of contacts is
\[
n_j = \frac{n^2 \langle A_{ex} \rangle}{2}
\]
Formula (12) is valid for identical particles of any shape, not only for discorectangles. Moreover, formula (12) is valid for anisotropic systems when the angle-averaged excluded area is calculated using the appropriate angle-distribution function. Thereby, there is a quadratic dependency of the number density of the contacts between the deposited particles on the number density of the deposited particles.

For all values of discorectangle aspect ratio, we used domains of a fixed size \( L = 32l \). To efficiently determine the percolation threshold (occurrence of a percolation cluster that spans the system in a given direction), the union-find algorithm\[^{30,31}\] was used. Figure 6 exhibits an example of a system under consideration exactly at the percolation threshold. The spanning cluster is highlighted. The aspect ratio of the discorectangles is 7.

\[
\langle A_{ex} \rangle = \frac{2l^2}{\pi}
\]

Figure 4. Example of the probability map when all orientations of the discorectangles are equiprobable (isotropic deposition of discorectangles) for \( \nu = 7 \). The reference discorectangle is shown. The darkest shade corresponds to the probability 1, that is, when the center of the second discorectangle is located within this area, and overlapping of these two discorectangles is ensured.

Figure 5. (a) The discorectangles overlap, since their midlines intersect each other. b) The discorectangles overlap, since the shortest distance between their midlines is less than the width of the discorectangle, \( d \). c) The corresponding discorectangles do not overlap, since the shortest distance between their midlines is larger than the width, \( d \), of a discorectangle.

(see, e.g., refs. [28,29]) or

\[
\langle A_{ex} \rangle = \frac{2}{\pi} \left( \frac{2}{\nu} (1 - \nu^{-1})^2 + 4\nu^{-2} \right)
\]

(7)

(see, e.g., ref. [16]). In the case of disks (\( l = d, \nu = 1 \))

\[
\langle A_{ex} \rangle = \pi d^2 = \pi l^2
\]

(8)

while in the case of zero-width sticks (\( d = 0, \nu = \infty \))

\[
\langle A_{ex} \rangle = \frac{2l^2}{\pi}
\]

(9)
We used the normalized number density of the deposited particles, viz., \( n/n_c - 1 \), in all our figures. Here, \( n_c \) is the percolation threshold. Notice that the normalized number density is equal to the normalized total area fraction \( \eta/n_c - 1 \).

2.3. Electrical Properties

To study the electrical properties of the deposit, we added super-conductive busses to the two opposite boundaries of the system under consideration. Only the resistance of junctions between particles was taken into account. This assumption of junction resistance dominance has previously been widely used\(^{[13,26,27]}\).

In such a way, the system under consideration can be transformed into a network, in which the edges correspond to the contacts (overlaps) between deposited particles, while the vertices of the network correspond to the deposited particles. This network is not planar. In it, each edge represents the resistance of junctions between conductive busses to the two opposite boundaries of the system.

Let \( y_i \) be the admittance (i.e., the reciprocal impedance) associated with the \( i \)-th branch, while \( y_{1} \) is the admittance seen from the endpoints of the \( i \)-th branch when \( y_{i} \) is disconnected. For an irregular network with identical branch admittances \( y_i = y_m \)

\[
\frac{y_m}{y_m + y_{1}} = \frac{2}{\langle \text{deg } V \rangle}
\]  

(13)

where \( \langle \text{deg } V \rangle \) is the average degree of the network nodes\(^{[34]}\). In our case, admittance is simply conductance, since the current is direct. Accounting for Equation (10) and (5),

\[
\langle \text{deg } V \rangle = \langle k \rangle \approx n(A_n)
\]

\[
\frac{\sigma_i}{\sigma_j + y_{1}} = \frac{2}{n(A_n)}
\]  

(14)

To identify a current-carrying part (the backbone) of the percolation cluster, we used the algorithm as follows (for the sake of clarity some irrelevant details have been omitted).

Let \( G \) be the percolation cluster of the network \( G \). The vertices of \( G \) belonging to one bus are considered as inputs, while the vertices belonging to the other bus are considered as outputs. Initially, all vertices and all edges of the network \( G \) are marked as “unremoved”: 1) Add vertices \( V_1 \) and \( V_2 \) to the network \( G \) in such a way that \( V_1 \) is connected to all the inputs, while \( V_2 \) is connected to all the outputs; 2) Find all articulation points; and 3) Check each articulation point. If the current articulation point (vertex \( X \)) is marked as “unremoved”, then a) Find all vertices adjacent to \( X \); b) Mark \( X \) and all its incident edges as “removed”; c) Check each vertex, \( Y \), that is adjacent to \( X \); i) Check the presence of paths from vertex \( Y \) to vertices \( V_1 \) and \( V_2 \) in the subgraph \( H \), which consists of “unremoved” vertices and edges of the network \( G \); ii) If there is a path leading from vertex \( Y \) to neither \( V_1 \) nor \( V_2 \), then we mark as “removed” all vertices and edges of the connected component of network \( H \) containing vertex \( Y \); d) Mark the vertex \( X \) as “unremoved”; and e) Mark as “unremoved” all edges between the vertex \( X \) and the vertices marked as “unremoved”.

In fact, we are looking for a geometrical backbone, that is, a biconnected component of the network. A geometrical backbone can contain perfectly balanced bonds (Wheatstone bridges). Since the potential difference between the ends of a perfectly balanced bond is equal to zero, electrical current through this bond is absent\(^{[35]}\). However, it is intuitively clear that the fraction of perfectly balanced bonds has to be negligible, if there are any at all. In contrast, direct identification of the current-carrying part of the percolation cluster is hardly reliable, since some apparent, but actually nonexistent, currents may arise both in dead ends and in perfectly balanced bonds due to rounding-off errors. These currents may be of the same order of magnitude as the real currents in some parts of the network.

A definition for the local transport exponent\(^{[13,18,16,37]}\) is

\[
t = \frac{\frac{d \ln \sigma}{d \ln(\eta - \eta_c)}}{\frac{\eta - \eta_c}{\sigma}} = \frac{n - n_c}{\sigma/c} \frac{d \sigma}{d n}
\]

(15)

Using an analytical formula for the electrical conductivity of 2D system of randomly placed conductive sticks that was obtained within a mean-field approach\(^{[21]}\)

\[
\sigma = \frac{n^{2} h^{4}}{12 \pi R_{f}}
\]

(16)

the local transport exponent may be derived as

\[
t = 2 \frac{n - n_c}{n}
\]

(17)

This local transport exponent tends to \( 2 \), when \( n \gg n_c \).

The error bars in the figures correspond to the standard deviation of the mean. When not shown explicitly, they are of the order of the marker size.

3. Results

Figure 7 demonstrates the strength of the percolation cluster (filled markers) and its backbone (open markers) against the normalized number density, \( n/n_c - 1 \), for discorctangles possessing different aspect ratios, that is, from disks to sticks. First of all, the results seem to be independent or almost independent of the aspect ratio. However, a small deviation for disks can be noticed. This deviation requires an additional detailed study. Moreover, three different regimes can be observed, that is, 1) a percolation regime (\( n \leq 1.1 n_c \)); 2) a transient regime (\( 1.1 n_c \leq n \leq 1.7 n_c \)); and 3) a bulk regime (\( n \geq 1.7 n_c \)). In the bulk regime, all, or almost all, the particles belong to the percolation cluster. It is noteworthy that universal (aspect ratio invariant) behavior is observed in all three regimes. Naturally, in the thermodynamic limit (\( L \to \infty \)), both quantities under consideration have to tend to zero as the number density approaches the percolation threshold. In Figure 7, both quantities differ from zero at the percolation threshold due to finite-size effect.

Figure 8 presents a close look at the behavior of the percolation cluster strength. The strength of the percolation cluster is normalized by the strength of the percolation cluster of the sticks.
For any studied value of the number density, this normalized strength of the percolation cluster approaches unity as the aspect ratio increases. However, this approach may be nonmonotonic (Figure 9).

Figure 10 shows the density of particles belonging to the backbone of the percolation cluster, normalized by the density of particles at the percolation threshold, \( n_c \). The filled markers correspond to our results, while the open markers correspond to data extracted from the literature (PRB2021) and ref. [13]. Inset: Dependence of the normalized density of the particles belonging to the backbone of the percolation cluster on the aspect ratio of the discocotangle for the fixed value of the number density of the particles of \( n = 2n_c \). Our results are averaged over 100 independent runs.

Figure 11 demonstrates the density of the junctions or bonds in the backbone normalized by the density of the junctions at the percolation threshold, \( n_c \). The filled markers correspond to our results, while the open markers correspond to data extracted from the literature (PRB2021) and ref. [13]. The inset shows that, for the
fixed value of the number density \( n = 2n_c \), the normalized density of the junctions belonging to the backbone of the percolation cluster decreases as the aspect ratio of the discorectangles is increased from 1 to 5 and remains constant within the error bars with further increase. Our results are averaged over 100 independent runs. Since our results obtained using both geometrical and conductive backbones are consistent within the marker size, only one dataset is presented in Figure 11. All our data collapse to one curve, confirming the proposition of an aspect-ratio-invariant behavior.\(^{[13]}\) For \( n/n_c - 1 \geq 0.2 \), our results for sticks agree with the results presented in ref. \([18]\). Again, a noticeable divergence when \( n/n_c - 1 \lesssim 0.2 \) may arise due to both a finite-size effect and a strong dependency on the accuracy of the percolation threshold estimate. However, our results are located significantly above the data for ellipses.\(^{[13]}\) The more natural assumption about differences in methods was not confirmed in our discussion with one of the authors of ref. \([13]\).

**Figure 12** compares the behavior of the electrical conductivity for ellipses (open markers)\(^{[13]}\) and discorectangles (filled markers). Again, the dependence of the electrical conductivity on the normalized number density seems to be independent of the aspect ratio. Moreover, the dependencies for both the ellipses\(^{[13]}\) and the discorectangles collapse to a single curve except for a region slightly above the percolation threshold.

**Figure 13** presents the behavior of the local transport exponent for ellipses (open markers)\(^{[13]}\) and discorectangles (filled markers). Again, the dependence of the electrical conductivity on the normalized number density seems to be independent of the aspect ratio. Moreover, the dependencies for both ellipses\(^{[13]}\) and discorectangles collapse to a single curve. The exponent tends to the analytical prediction (17) when the number density increases.

### 4. Conclusion

Recently, the dynamics of 2D disordered systems of ellipses has been simulated.\(^{[13]}\) Using a particular definition of the normalized proximity to the percolation threshold, the authors found an eccentricity-invariant dynamic behavior. The authors suggested that this invariance might also arise in systems with other particle geometries having zero-width sticks as the limiting case. To check this suggestion, we performed a study using discorectangles including their limiting cases, that is, disks and zero-width sticks. Our computer simulations demonstrate that some properties of random isotropic 2D systems of conductive discorectangles are insensitive to the aspect ratio of the particles. Our study presents some arguments that the suggestion may be correct.
At least, the behavior of 2D systems of randomly placed, conductive, permeable discorectangles is fairly close to that reported for ellipses.\textsuperscript{[1,3]} The only exception was the density of the junctions in the backbone. Although our results differ from the results reported in ref.\textsuperscript{[13]}, in the limit case of sticks, they do coincide with the results reported in ref.\textsuperscript{[18]}. We suggest this deviation is due to differences in the definitions or algorithms. Unfortunately, our conversation with one of the authors of ref.\textsuperscript{[13]} did not elucidate any possible source of this deviation. In order to assist readers, we have presented a detailed description of our own algorithm.

Although, slightly above the percolation threshold, the finite-size effect may presumably be significant, as the wide range of the number densities, when the invariant behavior can be observed, implies that the invariant behavior is insensitive to the domain size. Moreover, we suppose that the reported “eccentricity-invariant dynamic behavior” may be observed for a wide range of particles, not only for particles having zero-width sticks as their limiting case.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

electrical conductivity, percolation, simulations

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