Conductance of two-dimensional disordered Voronoi networks

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Resistor networks constructed from Voronoi polygons are models for transport by diffusive motion across local interfaces where both the interface strength and the local coordination number can be distributed. Computer simulations were performed on a series of two-dimensional networks with increasing degree of disorder, starting from a regular lattice. We find nonmonotonic behavior of the overall network conductance as a function of disorder. The observed increase of network conductance G as the random lattice is approached shows the importance of taking local topology variations into account in the description of disordered media. We discuss a general and simple way to estimate G from a particular, network-specific percentile of the distribution of local conductances.

Over the last few years much interest has developed in the properties of random resistor networks because they can be used to model a wide variety of transport problems in disordered media. This includes electron transport in disordered metals or semiconductors,^{1,2} fluid transport through randomly distributed bottlenecks in porous media,^{3,4} and gas transport through networks of thin membranes in rigid foams.⁵ In all these cases a complex local microstructure determines the global transport properties. In the simplest cases the main contribution to the local transport resistance is due to crossing a barrier or interface between individual grains, sites, or cells. The mapping to a resistor network then occurs by assigning effective conductance values to all interfaces between neighboring cells. This connects each cell to its nearest neighbors by a set of local conductances, each cell becoming a vertex in the associated network. The original distribution of coupling strengths across the interfaces in this way translates into a distribution of conductances. In general, both the local conductances and the local coordination numbers will be distributed around some average values reflecting the details of the microstructure.

A central problem concerns the relation between global quantities, measured across the network as a whole such as the overall conductance G , and the distribution of local quantities. In the past, work on random resistor networks has been mainly confined to regular lattices or

effective medium treatments.^{6,7} By construction, these approaches represent only an approximate description of any actual system because no direct connection between local topology, conductance values, and coordination numbers is retained.

The topology of Voronoi networks closely resembles that found in grain or domain growth from random nucleation sites.^{8,9} It also emerges from random arrangements of closely packed disks or spheres.³ In this way Voronoi networks in a natural manner lend themselves to the study of transport through disordered structures such as porous media, foams, or polycrystalline metal films. Besides providing a natural description on how to relate local conductances directly to the local geometry⁹ the Voronoi construction also allows one to cross the whole range from regular lattice to completely random network. We address the question of how disorder in the local conductances and in the local connectivity affects the global conductance across the network.

The cellular structure underlying the resistor network used in this study was constructed in the following way: Starting from an arbitrary distribution of seed points in a two-dimensional (2D) square of sidelength L , Voronoi polygons were formed by the intersecting perpendicular bisectors of lines connecting neighboring seeds. This construction, the Voronoi tessellation, follows the same rules as, e.g., the construction of Wigner-Seitz cells. Physically, it can be interpreted as a two-dimensional growth pro-

cess starting simultaneously at all nucleation sites and proceeding in the plane at constant, uniform rate until it is terminated wherever two approaching growth fronts reach each other. This process results in a space-filling cellular network and percolation effects do not play any role. The local structure of this network is uniquely determined by the starting configuration of seed points. Changing this configuration from, e.g., triangular lattice to a completely random arrangement therefore allows one to systematically move from a hexagonal cell structure to a random one (Fig. 1).

We model transport across such a cell structure by assuming that all conduction occurs by diffusive motion between neighboring Voronoi polygons. The resulting resistor network then corresponds to the dual of the network of Voronoi polygons. Neglecting any intracell resistance the local conductances g_i are taken to be a function of the edge length l_i shared by neighboring cells. We have investigated functional relationships of the form $g_i = l_i^n$ with $n = 1, 2$, and 4 . A linear relation $g_i = l_i$ corresponds to a constant conductivity per unit length across each interface, a reasonable assumption, e.g., for transport across grain boundaries or membranes of uniform height and thickness. A quadratic relationship $g_i = l_i^2$ simulates a dependence on interface area as might be appropriate for the case of intersecting spherical cavities in a porous medium. Hagen-Poiseuille fluid flow through tubes connecting individual cell centers is an example for a quartic dependence $g_i = l_i^4$.

The random resistor network in our model corresponds to a situation where all transport currents flow perpendicular to the edges of the Voronoi polygons. Different models, in which all transport occurs along the edges, have been used to simulate electromigration in random grain boundary networks¹⁰ and fluid flow through two-dimensional random packings of disks.³ We note that in these cases the coordination number, by virtue of the

Voronoi construction, is precisely 3 at all vertices and disorder enters only through variations in the edge length.

In this study the network consisted of 5016 cells. An external potential difference was applied across opposite edges of the network. We define all conductances as dimensionless quantities normalized to the conductance across one of the cell interfaces in the regular triangular lattice Fig. 1(a). Comparing the numerical results for the regular triangular network with the exact value $G = \sqrt{3}$ we find that finite size effects introduced a systematic error on G of 5% or less. In all cases G was obtained from the Kirchhoff equations for the network in an iterative manner using the Lanczos algorithm.¹¹ The results for G shown in the figures are averages for the conductance across both network directions.

Starting from a regular triangular lattice of seed points corresponding to a cell structure as in Fig. 1(a) disorder was introduced by displacing individual seeds within a disk of radius d around their original regular lattice position. The total number of cells was kept constant. We chose a procedure by which both the magnitude and the angle of the displacement vector were assigned randomly within the intervals $[0, d]$ and $[0, 2\pi]$, respectively. For small disorder, $d \ll 1$ [in units of the distance between the centers of neighboring cells in the regular lattice in Fig. 1(a)], this merely leads to a stretching or compression of individual cells. For larger d the Voronoi construction in addition gives rise to local changes of the number of cell edges (and therefore the number of nearest neighbors z). The first vanishing of edges can occur above $d^* = (\sqrt{3} - 1)/4 = 0.183$. On average, however, z remains at its original value of 6, regardless of disorder.^{9,15} The distribution in the number of nearest neighbors around this average value nevertheless leads to a fraction of shorter paths with fewer cell boundaries involved for traversing the network. As a consequence, topological disorder tends to result in an increase in overall conductance G . That this is indeed the case is shown in Fig. 2(a), where all g_i were chosen equal and independent of l_i . Choosing the g_i from a random distribution leads to a qualitatively similar result. The initial flat section in Fig. 2(a) corresponds to the small d regime in which the topology stays untouched. Deformation of individual cell edges here does not produce any effect as edge length and local conductance are not correlated.

When the local conductances are assigned as a function of the edge length between neighboring cells, disorder in the cell structure leads to a broadening of their distribution $P(g_i)$. Above $d^* = 0.18$ an increasing fraction of very short edges appears and the distribution becomes highly asymmetric. In topologically regular networks broadening of the conductance distribution leads to a decrease in conductance.⁶ In Voronoi networks, on the other hand, we find nonmonotonic behavior as a function of disorder d [Fig. 2(a)]. The overall change in G is less than 5% for $g_i = l_i$ but the quadratic and quartic dependencies there is a pronounced increase for sufficiently large d [Fig. 2(b)]. As the fully random configuration is approached, further increase in d has little effect and the curves flatten off for $d \gg 1$.

FIG. 1 Voronoi cell structure as a function of disorder (details of larger networks). At each stage the maximum displacement of the seed points with respect to their regular, triangular lattice positions in (a) is given by the parameter d (see text). Transport occurs perpendicular to the cell edges. (a) $d = 0$; (b) $d = 0.4$; (c) $d = 0.8$; (d) fully random distribution of seed points.

This peculiar result is a consequence of a competition between effects on G stemming from changes in coordination number and broadening of the conductance distribution. In the small d limit Fig. 2(a) reveals an initial decrease of G . Plotted against the variance δ^2 of the conductance distribution for a given degree of disorder, this decrease closely follows the linear relation $G/\langle g \rangle = \sqrt{3}(1 - 2\delta^2/z)$ for $d^2 \ll 1$ known^{6,12} from first-order perturbation expansions for regular lattices and from effective-medium approximations (Fig. 3). Both approaches break down once the network becomes topologically disordered.¹³ Here $\langle g \rangle$ is the average conductance computed from the distribution of local g_i for a given value of d .

At least in the large disorder limit a simple, quantitative estimate of the total conductance G can be obtained from an approximation scheme which relies on a conjecture originally due to Ambegaokar, Halperin, and Langer (AHL).¹ It requires knowledge about a particular percentile of the distribution of local conductances $P(g_i)$ and is based on the following procedure: Imagine removing all conductances g_i from the network and then putting them back in their old places one by one in order of descending conductance starting with the highest value within distribution. Clearly, G stays zero until enough

FIG. 2 Total network conductance G as a function of disorder parameter d . (a) Circles: local conductances fixed at $g_i = 1$ independent of local cell edge lengths l_i or disorder. Squares: local conductances assigned as $g_i = l_i$. (b) Local conductances assigned as $g_i = l_i$ (squares), $g_i = l_i^2$ (diamonds), and $g_i = l_i^4$ (triangles). The data at $d = 60$ correspond to a fully random Voronoi network.

FIG. 3 Total network conductance G normalized by the average conductance $\langle g \rangle$ as a function of the variance δ^2 of the distribution of local conductances. The dashed line indicates the linear behavior expected, to lowest order in δ^2 , for regular triangular lattices. The slope is -0.45 .

conductors are inserted such that the percolation threshold p_c is reached. This happens at the $(1 - p_c)$ th percentile of the distribution, counted from $g_i = 0$, at a particular conductance value g_c . Formally, g_c is defined by

$$\int_{g_c}^{\infty} P(g) dg / \int_0^{\infty} P(g) dg = p_c.$$

At p_c the total conductance G clearly is smaller than g_c because of the series combination with other, previously placed conductances $g_i > g_c$. However, the remaining conductances $g_i < g_c$, when filled in to restore the complete network, will form paths parallel to the path which includes g_c and thus increase G . AHL conjectured that, for a sufficiently broad distribution $P(g_i)$, $G = g_c / \eta$ with $\eta \approx 1$. This approximation was first proposed by AHL within the context of hopping conduction in disordered metals in the strongly localized regime near the metal-insulator transition. It later was shown¹⁴ to be accurate within 10–15% on regular square lattices for a variety of distributions $P(g_i)$. On the square lattice $p_c = \frac{1}{2}$ for bond percolation and G corresponds to the median of the distribution of local conductances. Note that this approximation neither depends on the detailed shape of $P(g_i)$ nor explicitly on the network topology.

For the random resistor network dual to the Voronoi tessellation the bond percolation threshold is the same for the triangular lattice, i.e., $p_c \approx 0.347$.¹⁵ Thus if the AHL conjecture holds we expect that G can be approximated by the conductance of the 0.65th percentile of the distribution. Figure 4 shows that, for large disorder, this indeed holds to within 10% for $\eta \approx 0.8$, independent of functional dependence $g_i(l_i)$. Note that, e.g., in the quartic case G has increase by over 100% for large d . Once $d \rightarrow 0$ and the triangular lattice is approached, the AHL conjecture is seen to underestimate G . This can be traced back to the fact that the requirement of a broad distribution of local conductances becomes violated. Of course, if the local conductances are uncorrelated with the local topology, as in the case of a uniform random distribution, the AHL conjecture stays valid throughout (triangles in Fig. 4).

These results have implications for the estimation of

FIG. 4 Test of the AHL conjecture (see text). The ratio $\eta = g_c/G$ of the conductance at the $(1-p_c)$ th percentile of the distribution to the total network conductance is seen to approach a common value close to $h=0.8$ for large disorder d . Local conductances assigned as $g_i = l_i$ (squares), $g_i = l_i^2$ (diamonds), and from a uniform random distribution (triangles). The data at $d=60$ corresponds to a fully random Voronoi network.

sheet resistances in two-dimensional granular metal films. In these films the local resistances are dominated by grain boundaries, weak links, or tunnel barriers between individual grains. For uniform film thickness a dependence $g_i \propto l_i$ is reasonable, even though, particularly in the case of tunnel junctions, considerable further broadening of

the conductance distribution might arise from the dependence of the g_i on variations in grain separation. Experimentally, the onset of global superconductivity in such films was found¹⁶⁻¹⁸ to depend on their normal-state resistance falling below a threshold value R_q close to $h/(2e)^2$. Ferrell¹² recently addressed the question of universality of this threshold in the presence of disorder. Assuming a regular lattice with fixed coordination number z he found the threshold R_q to shift to higher values with disorder by a factor $(1+2\delta^2/z)$. Such increase is in accordance with the effective-medium approximations mentioned above and our simulation results for very small parameter d . If, on the other hand, the actual film topology more closely resembles a Voronoi network than a regular lattice our results indicate that any increase in $R_q (= 1/G_q)$ stays below a few percent and is compensated by topological disorder.

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