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Conduction through a damaged honeycomb lattice

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ABSTRACT

The temperature distribution and rate of heat transfer across an infinite periodic strip of a honeycomb lattice consisting of conductive segments or links joined at nodes or junctions is discussed. A pristine honeycomb behaves like an isotropic medium whose effective conductivity is independent of the orientation of an applied macroscopic temperature gradient. Monte Carlo simulations are performed to determine the effect of link damage or disruption and lattice deformation due to junction displacement. In the simulations, a specified percentage of randomly distributed links are assigned a conductivity that is lower than that of the undamaged links. The balance equations governing the nodal temperatures at the junctions are solved by iteration subject to a periodicity condition along the strip and the Dirichlet condition along the two infinite edges of the strip. The results illustrate the effect of imperfections on the temperature distribution over the network and document the dependence of the effective conductivity on the percentage and conductivity of the defective links. In the case of nonconductive damaged links, the effective conductivity becomes nearly zero when a critical percentage of links are clipped, in agreement with bond percolation theory. However, the functional form of the number density of possible pathways connecting the lower to the upper edge of the strip predicted by percolation theory differs from that of the effective conductivity. Lattice deformation due to random node displacement has a small effect on the effective conductivity of the network.

1. Introduction

Assessing the rate of transport of heat, mass, electricity, or another appropriate scaled field across a pristine or randomized network of conducting segments or links is a problem of long-standing interest in the physical, engineering, and mathematical sciences. In biomechanics, networks of tubes carrying blood are useful models of capillary flow in healthy and neoplastic tumor tissue. Tree networks originating from a point of entry and bifurcating into multiple exit points have been employed in studies of steady and unsteady blood flow (e.g., [1,2]). Periodic networks with simple geometries and more general networks produced by Voronoi tessellation have been employed in recent computational studies (e.g., [3]). The conductive properties of networks of elongated nanoparticles and nanotubes are of interest in the materials science of composite media (e.g., [4]).

The effect of link disruption on the number of pathways connecting an entrance to an exit of a particulate or perforated medium has been studied under the auspices of bond percolation theory. A key parameter is the probability, p, that a conductive link exists next to another conductive link in a network with a prescribed geometry. The probability, p, can also be interpreted as the fraction of undisrupted links in a network: $p = 1$ corresponds to a pristine network, and $p = 0$ corresponds to a completely disrupted network. The probability, q, of disrupted links in a network can likewise be defined as $q = 1 - p$. Series expansion, other analytical methods, and Monte Carlo simulations have provided us with critical thresholds for the percentage of undisrupted links, p_c, below which transport is not possible in an idealized network extending to infinity in all directions, or is negligible in a realistic network with finite dimensions due to the absence of conductive pathways (e.g., [5,6]). For example, Monte Carlo simulations of the percolation properties of a hexagonal lattice consisting of a bidisperse mixture of regular and attenuated bonds were recently carried out [7].

The predictions of percolation theory regarding the number of possible pathways connecting an entrance to an exit, regarded as a function of p and expressed by the percolation probability $\mathcal{P}(p)$ for $p > p_c$, do not describe the effective conductivity of the network, $k_{\mathrm{eff}}(p)$ [8]. However, both $k_{\mathrm{eff}}(p)$ and $\mathcal{P}(p)$ vanish at the same critical threshold, p_c. Last and Thouless [9] conducted experiments and presented data on the effective electrical conductivity of a sheet of colloidal graphite paper perforated randomly with holes. Similar experiments were performed by Watson and Leath [10] with a steel-wire, square-mesh screen. Kirkpatrick [11,12] studied by numerical simulation the effective conductivity of a cubic or square lattice where defective links are assigned the same low

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Nomenclature

a	outer radius of hexagonal cell	q	percentage of defective links
A	link cross-sectional area	q_c	critical percentage of clipped links
$\mathbf{a}_1, \mathbf{a}_2$	lattice base vectors	q_m	maximum percentage of clipped links
b	inner radius of hexagonal cell	Q	rate of heat transport
D	inner width of test strip	Q_0	rate of heat transport across a pristine lattice
k	thermal conductivity	Q_1	rate of heat transport across a composite slab
$k_{\rm eff}$	effective thermal conductivity	Q_l	rate of heat transport through a link
ℓ	link length	r	equivalent radius of link cross-section
L	period length	T	node temperature
m, n	numerical exponents	$\mathcal{T}$	continuous temperature field
M	number of cells in the y direction	W	outer width of test strip
N	number of cells in the x direction	β	thermal conductivity ratio
N_l	number of links	γ	effective temperature gradient
p	percentage of intact links	ϵ_x, ϵ_y	node displacement coefficients in the x and y directions
p_c	critical percentage of intact links	ζ	scaled rate of heat transport
$p_{\rm hor}$	percentage of intact horizontal links	λ	conductivity, k, integrated over the cross-section of a link
$p_{\rm incl}$	percentage of intact inclined links	μ	network mobility transfer function
$p_{\rm vert}$	percentage of intact vertical links	ϱ	number of nearest neighbors
$\mathcal{P}$	percolation probability		

conductivity. Experimental and theoretical studies have indicated that $k_{\rm eff}(p)$ decreases slowly as p approaches p_c according to a power law with a lattice-dependent exponent.

To reconcile the percolation probability with the effective conductivity, we write $k_{\rm eff}(p) = \mu(p)\mathcal{P}(p)$, where $\mu(p)$ is a transfer function describing the effective network mobility. The functional form of $\mu(p)$ was discussed by Stinchcombe [13] for branching networks with arbitrary coordination number, known as Bethe lattices or Cayley trees. A comprehensive discussion of the relation between percolation and conductivity was presented by Pike and Seager [14,15]. A number of authors performed simulations of planar and three-dimensional conductive networks and random networks produced by Voronoi tessellation (e.g., [16,17]). In recent work, the effect of junction resistance on the effective conductivity was considered [18]. Although scaling laws for particular networks have been proposed near the percolation threshold (e.g., [11,18,19]), a general theoretical framework is not available.

In this paper, we study by analytical and numerical methods heat transport across a test section of a pristine and perturbed honeycomb lattice consisting of conductive links. The honeycomb lattice is made of two hexagonal Bravais lattices separated by an inner displacement. Previous authors have considered ordered square or triangular networks parametrized by two indices, or completely disordered random networks described by connectivity tables. The honeycomb lattice is of particular interest due to its significance in the engineering design of honeycomb plates, panels, sheets and cages, and its relevance to the atomic structure of carbon atoms in graphene and other crystals. Our results will demonstrate that the honeycomb lattice is able to capture the response of more general surface tilling produced, for example, by Voronoi tessellation.

Our main goal in this work is to document the effect of geometrical irregularities and link weakening or disruption on the temperature distribution and effective conductivity of a honeycomb lattice. Defective links with reduced conductivity and damaged links with zero conductivity will be considered. The computational model consists of an infinite periodic strip of a honeycomb structure resembling chicken wire, as described in Section 2. We will show that the pristine lattice behaves like an isotropic conductive medium at length scales that are larger than the cell size; we will develop an expression for the effective conductivity; and we will point out that the balance equations at the nodes, or junctions, of the pristine lattice are finite-difference approximations of the Laplacian of an underlying continuous function of position, with an error that scales with the square of the cell radius. The effect of random perturbations will be assessed by the Monte Carlo simulations presented in Section 3 and discussed with reference to the predictions of percolation theory. The main findings, their significance, and possible generalizations are discussed in Section 4.

2. Honeycomb lattice

We consider heat conduction through a periodic test section of an imperfect honeycomb lattice. In the absence of imperfections, the test section is an infinite horizontal strip of a pristine honeycomb, as shown in Fig. 1, where one period of the strip is confined between vertical dashed lines. The cell sides can be generated by the Voronoi tessellation of a companion hexagonal (equilateral triangular) lattice with base vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. The nodes of the companion hexagonal lattice are located at the centers of the hexagonal cells of the honeycomb lattice, as shown in Fig. 1. In a different construction, the honeycomb lattice arises by selectively removing rows or columns of nodes from a triangular lattice, indicated by the dotted lines in Fig. 1, so that the surviving nodes are located at the vertices of two displaced hexagonal lattices.

2.1. Armchair and zigzag orientations

Due to the anisotropy of the hexagonal geometry, two orientations must be considered. The first orientation yields the armchair lattice shown in Fig. 1(a), and the second orientation yields the zigzag lattice shown in Fig. 1(b). This terminology is consistent with standard convention in the theory of carbon nanotubes where one period of a graphene test section is rolled around the y axis to produce an armchair or zigzag nanotube. A length scale is provided by the radius of a circle circumscribing a hexagonal cell, a. The radius of an inscribed circle is given by $b = \frac{\sqrt{3}}{2}a$.

The test section of the armchair lattice shown in Fig. 1(a) consists of N whole cells in the x direction and M whole cells in the y direction, where N is an even integer and $M > 1$ is an arbitrary integer. For the configuration shown in Fig. 1(a), $N = 6$ and $M = 5$. The length of each period of the test section is $L = \frac{3}{2}Na$, the outer width of the strip is $W = 2Mb$, and the inner width of the strip is $D = 2(M-1)b$. The test section of the zigzag lattice shown in