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Convexity and Exponent Inequalities for Conduction near Percolation

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The bulk conductivity $\sigma^*(p)$ of the bond lattice in $\mathbb{Z}^d$ with a fraction p of conducting bonds is analyzed. Assuming a hierarchical node-link-blob (NLB) model of the conducting backbone, it is shown that $\sigma^*(p)$ (for this model) is convex in p near the percolation threshold p_c, and that its critical exponent t obeys the inequalities $1 \le t \le 2$ for $d=2,3$ while $2 \le t \le 3$ for $d \ge 4$. The upper bound $t=2$ in $d=3$, which is realizable in the NLB class, virtually coincides with two very recent numerical estimates obtained from simulation and series expansion.

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The random-resistor network[1-5] is the simplest model of a disordered conductor which exhibits complex macroscopic behavior in the form of a conducting phase transition. In particular, consider the bulk conductivity $\sigma^*(p)$ of the bond lattice in $\mathbb{Z}^d$, where the conductivity of the bonds is either 1 with probability p, or $\epsilon \ge 0$ with probability $1-p$. When $\epsilon=0$, $\sigma^*(p)=0$ for $p \le p_c$, the percolation threshold, and it is believed[6] that $\sigma^*(p) \sim (p-p_c)^t$ as $p \to p_c^+$. In this Letter we introduce a new approach to studying $\sigma^*(p)$ when $\epsilon=0$, motivated by the simple observation that in numerical simulations[6-10] the graph of $\sigma^*(p)$ for bond or site models in $d \ge 2$ is always convex near p_c. Our approach is to analyze $d^2\sigma^*/dp^2$ and investigate the consequences for the critical exponent t, assuming a self-similar, hierarchical structure for the conducting backbone near p_c, and certain technical conditions.

The principal results of our investigation and the assumptions under which they are obtained are as follows. First, the most serious assumption is that the conducting backbone near p_c has a hierarchical node-link-blob (NLB) structure.[11,12] This model contains both singly and multiply connected bonds, has "loops" on arbitrarily many length scales in a self-similar fashion, and incorporates the few rigorously known features[5,12] about the backbone on a macroscopic scale. We further make some technical assumptions about $\sigma^*(p)$: It obeys the above scaling law near p_c, has at least three derivatives for all $p > p_c$, and obeys $d^2\sigma^*/dp^2 + d\sigma^*/dp > 0$ at $p=1$, which we have verified numerically. Under these assumptions, we prove exact asymptotics for $d^2\sigma^*/dp^2$ as $p \to p_c^+$. The proof employs a novel technique whereby $d^2\sigma^*/dp^2$ for the NLB model with $\epsilon=0$ and p near p_c is computed using perturbation theory for $\sigma^*(p)$ (for two- and three-component resistor lattices) around $p=1$, with a sequence of ϵ's converging to 1 as one goes deeper in the hierarchy. Our asymptotics yield not only convexity near p_c, which implies $t \ge 1$, but delineate in which dimensions $d^2\sigma^*/dp^2 \to 0, +\infty$, or a positive constant as $p \to p_c^+$. Combining this information with the scaling law $d^2\sigma^*/dp^2 \sim (p-p_c)^{t-2}$ yields the inequalities $1 \le t \le 2$ for $d=2,3$ and $2 \le t \le 3$ for $d \ge 4$. The inequality $t \le 3$ for $d \ge 4$ is obtained by applying a similar analysis to $d^3\sigma^*/dp^3$ for the simpler node-link model, and can be viewed as a mean-field bound, since it is believed that $t=3$ for $d \ge 6$. We stress that the convexity and inequalities are not rigorous for the actual backbone near p_c for the original lattice, but *are* rigorous for the NLB model of the backbone, under the above technical assumptions.

Our results for $d=3$ are particularly intriguing. First, the inequality $t \le 2$ excludes roughly one-third of published numerical estimates of t in $d=3$, which have ranged from 1.5 to 2.36. Furthermore, this inequality is based on an exact calculation of $t=2$ for one particular NLB model which provides an upper bound on t for the full class. In view of this result, it is quite striking that very recently Gingold and Lobb[13] have obtained for

$d=3$ the estimate $t=2.003\pm0.047$ from simulation on lattices up to 80^3, and Adler *et al.*[14] have obtained $t=2.02\pm0.05$ from a thirteenth-order series expansion. In addition, our inequality is compatible with the results of an $\epsilon=6-d$ expansion,[15] and the general view that "roughly $t=2$".[2] (We should also mention the recent work of Roman[16] on the ant-in-the-labyrinth problem, who indirectly obtains a value of $t\approx2.16$. However, he acknowledges the inconsistency with other results, which is discussed further in Ref. 13.) The recent numerical results in Refs. 13 and 14, in conjunction with our work on the NLB model, suggest the possibility that $t=2$ is an *exact* result for $d=3$. To our knowledge, the present work is the first to relate t in a direct and natural way to the number 2, rather than to other (unknown) critical exponents of percolation theory.

Before we begin, we refer the reader to Ref. 17. In addition to containing the mathematical details of the results discussed here, we obtain there numerical and rigorous results concerning the regimes in ϵ and p of convexity of $\sigma^*(p)$ for bond and site models, the principal rigorous results being that for the $d=2$ bond problem, while $\sigma^*(p)$ cannot be convex for all p when $\epsilon=0$, it is convex for every $\epsilon>0$ near $p_c=\frac{1}{2}$.

We now formulate the bond conductivity problem for $\mathbb{Z}^d$, where, for simplicity, we begin with $d=2$. Take an $L\times L$ sample G_L of the bond lattice with M $(\sim dL^d)$ bonds. Assigned to G_L are M independent random variables c_i, $1\leq i\leq M$, the bond conductivities, which take the values 1 with probability p and $\epsilon\geq0$ with probability $1-p$. We attach perfectly conducting bus bars to two opposite edges, and let $\sigma_L(p)$ be the effective conductivity of this network, averaged over realizations of the bond conductivities. For $d\geq1$, the bulk conductivity of the lattice is defined as

$$\sigma^*(p)=\lim_{L\to\infty}L^{2-d}\sigma_L(p)\,. \tag{1}$$

For $\epsilon>0$, the infinite-volume limit in (1) has been shown to exist,[18-21] and for $\epsilon=0$ the existence of σ^* has recently been proven in the continuum.[22]

The calculation of $d^2\sigma^*/dp^2$ will require the following definition. For any graph B with bonds b_i of unit conductivity, define

$$\delta^2\sigma(B)=\sum_{\substack{b_i,b_j\in B\\ b_i\neq b_j}}[\sigma_{ij}(1,1)+\sigma_{ij}(0,0)-\sigma_{ij}(1,0)-\sigma_{ij}(0,1)]\,, \tag{2}$$

where in (2) $\sigma_{ij}(1,1)=\sigma(B)$ the conductivity of B measured between two vertices, $\sigma_{ij}(0,0)$ is the conductivity of B with b_i and b_j removed, and so on. The expression in (2) represents the discrete second derivative of σ with respect to p, as follows. Let G be the lattice in $d\geq2$ with bond conductivities 1 and 0 and bulk conductivity function $\sigma^*(p)$. If $B=B(p)$ is a realization of occupied bonds of G at probability p, then[17]

$$p^2\frac{d^2\sigma^*}{dp^2}=\delta^2\sigma^*(B(p))\,, \tag{3}$$

where $\delta^2\sigma^*$ is the scaled infinite-volume limit of (2) and the right-hand side in (3) is appropriately averaged. [We are assuming in (3) that $\sigma^*(p)$ is twice differentiable for $p>p_c$ when $\epsilon=0$.] In (2) note that dangling bonds do not contribute, so that one may think of $B(p)$ as a realization of the backbone at bond fraction p. For clarity, note that at $p=1$, $B(p)=G$. We remark that analysis of simple graphs shows that, typically, positive contributions to (2) arise from series pairs, while negative contributions arise from pairs in parallel.

The idea now is to replace an actual backbone graph $B(p)$ for p near p_c by a node-link-blob graph A, which is based on the work of Stanley[11] and Coniglio.[12] This graph is a "superlattice" constructed by replacing the bonds of the hypercubic lattice G in $d\geq2$ by first-order necklaces composed of strings (links) and first-order beads (blobs), and separating the nodes of G by a correlation length ξ, as in Fig. 1(a). The beads themselves have a hierarchical structure, as shown in Fig. 1(b), consisting of two second-order necklaces in parallel, and so on, in a self-similar fashion to order N for an arbitrary large integer N. We assume that any kth-order necklace has $\beta-1$ beads on it for an arbitrary large integer β, and that each pair of beads is joined by a string of n_k bonds, so that there are a total of βn_k string bonds on each necklace. The βn_1 string bonds on any first-order necklace are called singly connected because removal of one of them breaks the connection between nodes separated by ξ. All the rest of the bonds in the NLB graph are multiply connected, and among these it is useful to iden-

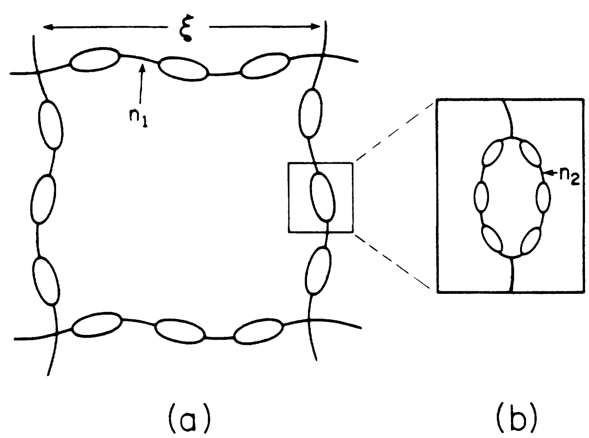

FIG. 1. Node-link-blob model of the conducting backbone near p_c. In (a), the nodes are a correlation length ξ apart, and are connected by necklaces of beads (blobs) and strings (links) with n_1 bonds connecting two beads. The beads have a self-similar structure, as shown in (b), with n_2 bonds connecting two beads.

tify the βn_2 string bonds on a second-order necklace as doubly connected, since it is possible to remove two of them (in parallel) and break a connection between nodes. Based on a result of Coniglio's,[12] implying in our context that the number of singly and doubly connected bonds between the nodes both diverge with exponent 1 as $p \to p_c^+$, we assume that $n_1 = 2\beta n_2$. Because of self-similarity, we assume that

$$n_{j-1} = 2\beta n_j, \quad j = 2, \ldots, N. \tag{4}$$

Relation (4) can be used to solve for the n_j, $j > 1$ in terms of n_1 with $n_2 = n_1/2\beta$, $n_3 = n_1/4\beta^2$, and so on, and we refer to the NLB graph as $A(n_1)$. In this model the percolation limit $p \to p_c^+$ is characterized by the limits $n_1, \beta, N, \xi \to \infty$, so that the lengths of all orders of necklaces, and the numbers and sizes of all orders of blobs, diverge as $p \to p_c^+$.

Before we give the asymptotics of $\delta^2\sigma^*(A(n_1))$, we must discuss the conditions under which they are proven. Consider $\sigma^*(q_1,q_2)$ for the bond lattice in $\mathbb{Z}^d$ with three conductivities 1, ϵ_1, and ϵ_2 in proportions p, q_1, and q_2, in addition to our standard two-component conductivity $\sigma^*(p)$. We require that $\sigma^*(q_1,q_2)$ has second-order partials at $q_1 = q_2 = 1$ for all $\epsilon_1, \epsilon_2 \geq 0$, and that $\sigma^*(p)$ has two derivatives at $p = 1$ for all $\epsilon \geq 0$. For ϵ, ϵ_1, and $\epsilon_2 > 0$, these conditions are satisfied by our general results[17] that $\sigma^*(p)$ is analytic for all $p \in [0,1]$ and $\sigma^*(q_1,q_2)$ is analytic for all $(q_1,q_2) \in [0,1] \times [0,1]$. The $\epsilon = \epsilon_1 = 0$ requirements will be assumed, although Kozlov[23] has proven the existence of $d\sigma^*/dp|_{p=1}$ for a class of continuum analogs.

The second main condition is that given the hypercubic base lattice G for $A(n_1)$,

$$\kappa(G) = \frac{d\sigma^*}{dp}\bigg|_{p=1} + \frac{d^2\sigma^*}{dp^2}\bigg|_{p=1} > 0. \tag{5}$$

In any $d \geq 2$, $d\sigma^*/dp|_{p=1} = d/(d-1)$,[1] while $d^2\sigma^*/dp^2|_{p=1}$, if negative, is quite small, e.g., ≈ -0.21 in $d = 2$,[9,17] indicating that $\sigma^*(p)$ is quite straight near $p = 1$, so that (5) is satisfied. Condition (5) amounts to a consequence of the long-held view that effective-medium theory (giving a straight-line solution) provides an accurate description of $\sigma^*(p)$ near $p = 1$, which also holds for general lattices. In fact, the asymptotics below can be proven for a variety of periodic base lattices G which satisfy (5), and presumably hold even for random lattices.

We may now state our principal result.

Under the above assumptions, for fixed, large n_1, β, and N,

$$\delta^2\sigma(A(n_1)) = \alpha_N \kappa(G) \beta n_1 + \sum_{i=0}^{\infty} \frac{a_i n_1 + b_i}{\beta^i}, \tag{6}$$

where $(\alpha_N)^{-1} = \sum_{i=0}^{N} (\frac{1}{4})^i$ and the series in (6) converges, so that

$$\delta^2\sigma^*(A(n_1)) \sim \frac{\alpha_N \kappa(G) \beta n_1}{\xi^{d-2}} > 0, \quad n_1, \beta, N, \xi \to \infty. \tag{7}$$

The idea of the proof[17] of (6) is first to write

$$\delta^2\sigma(A(n_1)) = \sum_{\substack{j,k=1 \\ k \geq j}} \delta_{jk}, \tag{8}$$

where δ_{jk} is the sum of all contributions to $\delta^2\sigma(A(n_1))$ in (2) arising from pairs with one bond in a jth-order string and the other in a kth-order string, which is in either the same or a different first-order necklace. Now let z_k be the conductivity of a single first-order necklace with one bond removed from a kth-order string, with $z_0 = \alpha_N/\beta n_1$ for no bond removed, $z_1 = 0$, and

$$z_k = z_0 (1 + \gamma_k/\beta^{k-1})^{-1}, \quad k \geq 2, \tag{9}$$

where $\gamma_k \to 0$ as $k \to \infty$ geometrically fast. There are analogous formulas for the various forms of z_{jk} with two bonds removed, say, in series or in parallel. Then through representations like (2) and (3), we obtain formulas for the δ_{jk} in terms of derivatives of $\sigma^*(p)$ and $\sigma^*(q_1,q_2)$ at $p = 1$, such as

$$\delta_{11} = z_0 \left[\beta n_1 (\beta n_1 - 1) \frac{d\sigma^*}{dp}(p=1,h_1) + (\beta n_1)^2 \frac{d^2\sigma^*}{dp^2}(p=1,h_1) \right], \tag{10}$$

$$\delta_{12} = z_0 \left[(\beta n_1)^2 \frac{d\sigma^*}{dp}(p=1,h_1) + (\beta n_1)^2 \frac{\partial^2\sigma^*}{\partial q_1 \partial q_2}(p=1,h_1,h_2) \right], \tag{11}$$

where $(d\sigma^*/dp)(p=1,h_1)$, e.g., is for G with bond conductivities 1 and $h_1 = 0$, with $h_k = z_k/z_0$. As $k \to \infty$, $h_k \to 1$, and as $\beta \to \infty$, $h_k \to 1$ for all $k \geq 2$, and similarly for $h_{jk} = z_{jk}/z_0$. The necessary control of the δ_{jk} is then obtained either from (5), or from perturbation theory around a homogeneous medium ($\epsilon = 1$ or $\epsilon_1 = \epsilon_2 = 1$), which establishes (6). All the details appear in Ref. 17.

We wish to make the following remarks concerning the above result. First, a result similar to (7) holds if we replace (4) by $n_{j-1} = \eta_j \beta_j n_j$, where the blobs of order $j-1$ are made of η_j necklaces in parallel, with reasonable assumptions about η_j and β_j. Even if the blobs have a more complicated superlattice structure themselves, an analog of (7) presumably holds. Also, as noted above, (7) can be proven for a variety of base lattices G. Finally, while the principal assumption of the NLB graph replacing the actual backbone is quite serious, our proof of (6) shows that the dominant contribution to (7) comes from δ_{11}, which comes from macroscopic contributions in the NLB graph, where the model reflects well the actual structure. A similar result will hold for any reasonable assumption about microscopic backbone structure.

We now proceed to the implications of (7). First, its positivity establishes convexity of $\sigma^*(p)$ for the NLB model, which implies [under our assumptions, including scaling and the existence of three derivatives of $\sigma^*(p)$ for all $p > p_c$ when $\epsilon = 0$] that $t \geq 1$, for any $d \geq 2$ (the inequality $t \geq 1$ has been previously established in a different manner in Refs. 24 and 25). Now let $\lambda(n_1)$ be the length of a first-order necklace, so that $\lambda(n_1) \approx \beta n_1 + \beta^2 n_2 + \cdots + \beta^N n_N = \theta_N \beta n_1$, $\theta_N = \sum_{i=0}^{N} 2^{-i}$. By (7), we then have

$$\delta^2 \sigma^*(A(n_1)) \sim \frac{\rho_N \lambda(n_1)}{\xi^{d-2}}, \quad n_1, \beta, N, \xi \to \infty, \tag{12}$$

where $\rho_N = a_N \kappa(G)/\theta_N$, so that $\rho_N \approx \frac{2}{3}$ for large N in $d=2$. Since all the parameters n_1, β, N and ξ are diverging as $p \to p_c^+$, we can define a whole class of NLB models by how fast $\lambda(n_1)$ scales to ∞ relative to ξ. By the structure of the model, clearly $\lambda(n_1) \geq \xi$, and typically, $\lambda/\xi \to \infty$. Thus as a consequence of (12) we have in $d=2$ and 3

$$\delta^2 \sigma^*(A(n_1)) \to +\infty, \quad n_1, \beta, N, \xi \to \infty, \tag{13}$$

except in $d=3$ when $\lambda(n_1) = C\xi$, $C \geq 1$, in which case

$$\delta^2 \sigma^*(A(n_1)) \to \rho C > 0, \tag{14}$$

where $\rho = \lim_{N \to \infty} \rho_N$. In $d \geq 4$, if λ and ξ are scaled so that $\lambda(n_1)/\xi^{d-2} \to 0^+$, then

$$\delta^2 \sigma^*(A(n_1)) \to 0^+. \tag{15}$$

Under our assumptions, in particular, that $d^2\sigma^*/dp^2 \sim (p-p_c)^{t-2}$, we then have, collecting our results

$$1 \leq t \leq 2, \quad d=2,3; \quad 2 \leq t \leq 3, \quad d \geq 4. \tag{16}$$

In (16) the last inequality $t \leq 3$ for $d \geq 4$ is obtained by a result that $\delta^3 \sigma^*(A'(n_1)) \sim C' \lambda^2(n_1)/\xi^{d-2}$ for a simpler node-link graph $A'(n_1)$, which is believed to be adequate in higher dimensions.[26] For models in $d=4,5$ which satisfy $\lambda^2(n_1)/\xi^{d-2} \to \infty$, we have $\delta^3 \sigma^*(A(n_1)) \to \infty$, so that $d^3\sigma^*/dp^3 \sim (p-p_c)^{t-3} \to \infty$, which gives the inequality.

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