

# Scaling Behavior of Permeability and Conductivity Anisotropy near the Percolation Threshold

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We use the finite-size scaling method to estimate the critical exponent  $\lambda$  that characterizes the scaling behavior of conductivity and permeability anisotropy near the percolation threshold  $p_c$ . Here  $\lambda$  is defined by the scaling law  $k_{\parallel}/k_{\perp} - 1 \sim (p - p_c)^{\lambda}$ , where  $k_{\parallel}$  and  $k_{\perp}$  are the conductivity or permeability of the system in the direction of the macroscopic potential gradient and perpendicular to this direction, respectively. The results are  $\lambda(d=2) \simeq 0.819 \pm 0.011$  and  $\lambda(d=3) \simeq 0.518 \pm 0.001$ . We interpret these results in terms of the structure of percolation clusters and their chemical distance. We also compare our results with the predictions of a scaling theory for  $\lambda$  due to Straley, and propose that  $\lambda(d=2) = t - \beta_B$ , where  $t$  is the critical exponent of the conductivity or permeability of the system, and  $\beta_B$  is the critical exponent of the backbone of percolation clusters.

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**KEY WORDS:** Percolation; permeability; conductivity; anisotropy; finite-size scaling.

## 1. INTRODUCTION

Over the past two decades random percolation networks<sup>(1,2)</sup> have been an important tool for modeling transport processes in disordered systems, such as porous media,<sup>(3)</sup> branched polymers and gels,<sup>(4-7)</sup> and composite solids.<sup>(8)</sup> In particular, the effect of *disorder* on transport properties has been studied, and a better understanding has been developed by combining a variety of techniques and ideas, e.g., scaling concepts, effective-medium

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approximation,<sup>(9)</sup> renormalization-group methods, and large-scale computer simulations.<sup>(10)</sup> Considerable attention has been focused on the properties of percolation networks near their percolation threshold  $p_c$ . Consider a percolation network in which a fraction  $p$  of the bonds are conducting and the rest are insulating. As  $p_c$  is approached, the bulk conductivity  $g$  of a  $d$ -dimensional network vanishes according to the power law

$$g \sim (p - p_c)^t \quad (1)$$

where the critical exponent  $t$  is largely universal, and<sup>(10,11)</sup>  $t(d=2) \simeq 1.3$  and  $t(d=3) \simeq 2.0$ . Likewise, in a percolation network in which a fraction  $p$  of bonds represents pores of a porous medium through which a fluid flows, while the rest of the bonds are closed to fluid flow, the permeability  $k$  of the network vanishes according to the power law

$$k \sim (p - p_c)^e \quad (2)$$

where  $e$  is also largely universal. If the conductance and the permeability of the bonds are distributed according to a distribution function  $f(x)$  such that  $f(0)$  is nonsingular, then  $t=e$ . This is the case we consider in this paper.

The vast majority of the percolation systems that have been studied so far are *isotropic*, whereas transport in *anisotropic* percolation networks are relevant to many important processes and phenomena. Two important examples that are of interest to us are flow in sedimentary rocks and their fracture networks, and transport in porous catalytic systems. Sedimentary rocks and many other types of porous media are anisotropic,<sup>(3)</sup> even at very small scales. Likewise, fracture networks of rocks are anisotropic and are characterized by a permeability tensor, rather than a single value of permeability. In porous catalytic materials, transport of molecules can be restricted to a certain direction or plane such that it can be effectively considered as an anisotropic transport process, characterized by a diffusivity tensor rather than a single diffusivity. There are several other classes of disordered materials to which anisotropy is important. For example, many solid-state materials, such as  $(\text{Sn})_x$  and TCNQ salts, can be obtained only as small crystals, and their effective transport properties must be measured in compact powders where their strong anisotropic properties are averaged in a poorly-understood fashion. Carbon-black polyvinylchloride and other polymer composites are also highly anisotropic. Transport properties of such anisotropic materials have been measured.<sup>(12-16)</sup>

As discussed by Straley,<sup>(17)</sup> one can have at least *five* different kinds of anisotropy, especially in a percolation system. However, only one of them is of interest to us in this paper. This is a percolation network in which

bonds in each distinct direction have different conductivity or permeability. Shklovskii<sup>(18)</sup> was the first to study the conductivity anisotropy, measured as  $A = g_{||}/g_{\perp} - 1$ , where  $g_{||}$  and  $g_{\perp}$  are, respectively, the macroscopic conductivities of the network in the longitudinal direction (the direction of macroscopic potential gradient) and transverse direction (perpendicular to the direction of macroscopic potential gradient). Near  $p_c$  one has the power law

$$A \sim (p - p_c)^\lambda \quad (3)$$

where  $\lambda$  is a presumably universal critical exponent.  $A$  can also be defined in terms of the permeabilities of the system,  $A = k_{||}/k_{\perp} - 1$ . The relation between  $\lambda$  and other percolation exponents is discussed below.

Unlike the exponents  $t$  and  $e$ , and in spite of its relevance to several important and practical problems, no accurate estimate of  $\lambda$  is available. Although a few attempts have been made<sup>(19-21)</sup> for estimating  $\lambda$ , they have not yielded accurate estimates of  $\lambda$ . In this paper, we use finite-size scaling theory (FSST), perhaps the most accurate method of extracting the critical exponents, to obtain accurate estimates of  $\lambda_2 = \lambda(d=2)$  and  $\lambda_3 = \lambda(d=3)$ . Our interest in this quantity is due to our research effort for understanding flow in fractured rocks<sup>(22)</sup> and disordered solids.<sup>(23)</sup> We compare our results with the predictions of a scaling theory of conductivity anisotropy due to Straley<sup>(17)</sup> and also provide a geometrical interpretation of the results.

## 2. FINITE-SIZE SCALING THEORY

According to FSST, the variation of  $A$  for a network of linear size  $L$ , with  $L \ll \xi_p$ , where  $\xi_p$  is the correlation length of percolation, is written as

$$A \sim L^{-x} h(y) \quad (4)$$

where  $y = L^{1/\nu}(p - p_c) \sim (L/\xi_p)^{1/\nu}$ ,  $\nu$  is the critical exponent that characterizes the divergence of  $\xi_p$  as  $p_c$  is approached,  $\xi_p \sim (p - p_c)^{-\nu}$ , and  $x = \lambda/\nu$ . Here  $h(y)$  is a universal scaling function which is nonsingular at  $p = p_c$ . However, Eq. (4) is valid for very large values of  $L$ , and simulating very large networks is not straightforward. To take into account the effect of finite values of  $L$ , Eq. (4) is rewritten as

$$A \sim L^{-x} [1 + a_1 h_1(L) + a_2 h_2(L)] \quad (5)$$

where  $h_1(L)$  and  $h_2(L)$  are two *correction-to-scaling* functions which are particularly important for small and moderate values of  $L$ , and  $a$ 's are constant. There are no theoretical predictions for the general forms of  $h_1(L)$

and  $h_2(L)$ , and one usually has to try various functional forms in order to find the best fit to the numerical results. Equation (5) tells us how to estimate  $\lambda$ : Calculate  $A$  at  $p = p_c$  [where the value of  $h(0)$  is irrelevant] for various values of  $L$  and fit the results to Eq. (5) to estimate  $x$ . Since exact or accurate estimates of  $\nu$  for  $d=2$  and 3 are already available,  $\lambda$  can be estimated accurately. This is the approach that we use here, whereas earlier works measured  $A$  as a function of  $p$ .

### 3. RESULTS AND DISCUSSIONS

We carried out Monte Carlo simulations in both two and three dimensions. We imposed a potential gradient in one direction, say  $x$ , with  $k = 10$  for the bonds in this direction, and used periodic boundary condition(s) in the  $y$  and  $z$  directions with  $k = 1$  for the bonds in these directions. The governing equations for the nodal potentials were solved by the conjugate gradient method. The simulations were carried out with the square network at  $p_c = 1/2$  and with the simple-cubic network at  $p_c \simeq 0.2488$ . After calculating  $k_x$ , we imposed the macroscopic potential gradient in the  $y$  (or  $z$ ) direction and calculated  $k_y$ , from which we obtained  $A = k_x/k_y - 1$ . Table I presents the statistics of our simulations.

In order to obtain accurate estimates of  $\lambda$ , we tried various forms for the functions  $h_1(L)$  and  $h_2(L)$ . The most accurate fit of our results was provided by  $h_1(L) = (\ln L)^{-1}$  and  $h_2(L) = 1/L$ , as previously suggested by us.<sup>(24)</sup> The functional forms of  $h_1(L)$  and  $h_2(L)$  proposed by Duering and Roman<sup>(25)</sup> did not provide fits of our results with a comparable accuracy. Thus, we believe that our estimates of  $\lambda$  are very accurate. Figures 1 and 2 show the results, from which we estimate that

$$\lambda_2 \simeq 0.819 \pm 0.011 \quad (6)$$

$$\lambda_3 \simeq 0.518 \pm 0.001 \quad (7)$$

The estimated errors are purely statistical. Our estimates should be compared with the results of Sarychev and Vinogradoff,<sup>(20)</sup>  $\lambda_2 \simeq 0.9 \pm 0.1$  and

Table I. Number of Realizations  $N$  for Each Network Size  $L$

$L(d=2)$	8	16	32	64		128
$N(d=2)$	2000	2000	1250	550		250
$L(d=3)$	4	8	16	32	48	64
$N(d=3)$	1000	400	200	60	35	25

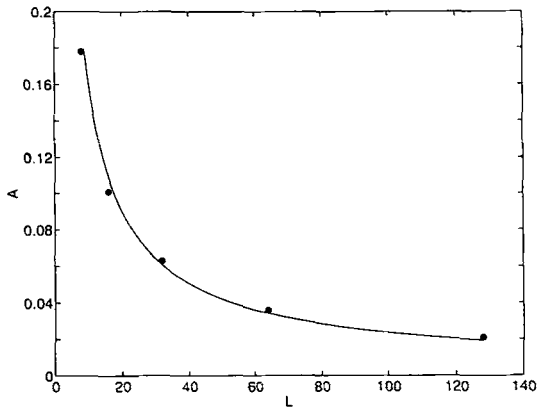


Fig. 1. Permeability anisotropy  $A$  versus the linear size  $L$  of the square network at the percolation threshold  $p_c = 1/2$ .

$\lambda_3 \approx 0.3 \pm 0.1$ , and with the results of Lobb *et al.*,<sup>(19)</sup>  $\lambda_2 \approx 0.86 \pm 0.1$ . Our  $\lambda_2$  is consistent with their estimates, but with much smaller estimated errors.

The result  $\lambda_2 > \lambda_3$  is surprising, since one expects that on a three-dimensional network, which contains a much larger number of current-carrying transport paths than a two-dimensional network, the anisotropy vanish faster, i.e.,  $\lambda_3 > \lambda_2$ . Sarychev and Vinogradoff have argued that in order to understand why  $\lambda_2 > \lambda_3$  one must consider the structure of the backbone, i.e., the current-carrying part of the sample-spanning percolation cluster. The backbone consists of<sup>(26)</sup> of links and blobs. A link is a bond

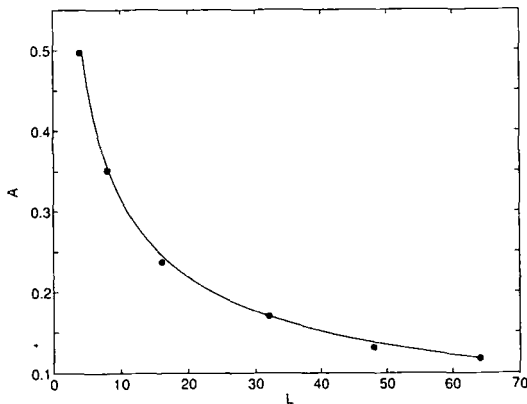


Fig. 2. Permeability anisotropy  $A$  versus the linear size  $L$  of the simple-cubic network at the percolation threshold  $p_c \approx 0.2488$ .

that connects two blobs such that if it is cut, the backbone is split into two pieces, and the blobs are the multiply-connected aggregates of current-carrying bonds. Sarychev and Vinogradoff have argued that since the blobs are less dense in three dimensions than in two dimensions, one must have  $\lambda_2 > \lambda_3$ . However, since we do not know how to relate  $\lambda$  to the exponents that characterize the structure of the blobs, it is difficult to check the rigor of their argument.

The fact that  $A$  vanishes as  $p_c$  is approached is due to the tortuous nature of the transport paths. Near  $p_c$  the transport paths are so tortuous that it becomes impossible to distinguish between different directions, and as a result  $A$  vanishes at  $p_c$ . Thus, to understand why  $\lambda_2 > \lambda_3$ , we must have a measure of the tortuosity of percolation clusters and their backbone. One measure may be the length  $l_{\min}$  of the minimum path or *chemical distance* between two points of the cluster.<sup>(27-29)</sup> In general  $l_{\min}$  is greater than  $r$ , the Pythagorean distance between the two points. For  $r < \xi_p$  one has

$$l_{\min} \sim r^{d_{\min}} \quad (8)$$

where  $d_{\min}$  is the fractal dimension of the shortest path, and is a universal quantity. Equation (8) implies that near  $p_c$  one has

$$l_{\min} \sim (p - p_c)^{-v_{d_{\min}}} \quad (9)$$

Since<sup>(30)</sup>  $d_{\min}(d=2) \simeq 1.13$  and  $d_{\min}(d=3) \simeq 1.34$ , we obtain  $l_{\min} \sim (p - p_c)^{-1.5}$  for two-dimensional systems and  $l_{\min} \sim (p - p_c)^{-1.18}$  for three-dimensional systems. That is, as  $p_c$  is approached,  $l_{\min}$  increases less strongly in three dimensions than in two dimensions. This may be interpreted as meaning that near  $p_c$  the tortuosity of the three-dimensional transport paths increases less strongly than that of the two-dimensional ones. As a result, at a fixed distance from  $p_c$ , the tortuosity of two-dimensional transport paths is *larger* than that of three-dimensional ones. Since  $A$  vanishes at  $p_c$  because the tortuosity is infinite, the implication is that the anisotropy should vanish faster in two dimensions than in three dimensions, consistent with our results.

Straley<sup>(17)</sup> has proposed a scaling relation between  $t$ ,  $v$ , and  $\lambda$ , which is given by

$$\lambda = 2t - 2(d-1)v \quad (10)$$

Since  $v(d=2) = 4/3$  and  $v(d=3) \simeq 0.88$ , Eq. (10) predicts that  $\lambda_2 \simeq -0.06$  and  $\lambda_3 \simeq 0.48$ . The two-dimensional prediction is clearly wrong, as it predicts that the anisotropy *diverges* at  $p_c$ . However, Straley's prediction

for  $\lambda_3$  is close to our estimate. Moreover, Eq. (10) predicts that at  $d=6$ , the mean-field limit of percolation,  $\lambda=1$ , which, according to Straley,<sup>(17)</sup> is an exact result. Thus, Straley's scaling equation provides a reasonable estimate of  $\lambda$  for high-dimensional systems, but not for low-dimensional ones. Therefore, there may be a lower critical dimension  $d_l > 2$  such that for  $d > d_l$  a scaling relation such as (10) is very accurate, whereas the same scaling relation may break down completely for  $d < d_l$ . If this is the case, we should clearly have  $2 < d_l < 3$ . The existence of such a lower critical dimension for the critical exponents of transport properties of percolation networks was already suggested several years ago.<sup>(31,32)</sup>

Finally, we observe that in two dimensions, where Straley's relation breaks down, we have  $\lambda_2 \simeq t - \beta_B$ , where  $\beta_B$  is the critical exponent of the backbone fraction, i.e., the fraction of conducting bonds in the backbone. Since<sup>(33)</sup>  $\beta_B(d=2) \simeq 0.48$ , our scaling relation predicts that  $\lambda_2 \simeq 0.82$ , in excellent agreement with our estimate. In future papers<sup>(22,23)</sup> we will discuss the anisotropy of the permeability and conductivity of percolation networks in which the distributions of the bond conductance or permeability may be singular or contain long-range correlations, situations that are frequently encountered in natural porous media such as rocks.

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