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Transfer matrix calculation of conductivity in three-dimensional random resistor networks at percolation threshold

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Résumé. — Pour des barreaux de taille $n \times n \times L$, avec $L \geqslant n$ et $n \leqslant 18$, nous calculons la conductivité d'un réseau aléatoire de conducteurs et d'isolants. Au seuil de percolation sur un réseau cubique simple, nos résultats Monte Carlo donnent une conductivité qui décroît comme $n^{-2,1}$ quand la largeur n du barreau augmente pour la percolation de sites et celle de liens. Quand on tient compte des corrections au scaling avec un exposant de correction ω d'ordre 1, notre meilleure estimation pour l'exposant t de la conductivité est $t/\nu = 2,2 \pm 0,1$ à la fois pour le cas des liens et celui des sites. Ces résultats sont en accord avec la conjecture de Alexander-Orbach $t/\nu \simeq 2,26$ pour l'exposant de la conductivité en dimension 3.

Abstract. — For very long bars of size $n \times n \times L$, with $L \geqslant n$, and n up to 18, we calculate the conductivity of a random network of resistors and insulators. At the percolation threshold in a simple cubic lattice our Monte Carlo data give a conductivity decreasing with bar diameter n as $n^{-2.1}$ for site and bond percolation. Taking into account corrections to scaling with a correction exponent ω near unity, our best estimate for the conductivity exponent t is $t/\nu = 2.2 \pm 0.1$ in both the bond and the site cases. These results strongly support the Alexander-Orbach [8] conjecture $t/\nu \simeq 2.26$ for the conductivity exponent in three dimensions.

The transfer matrix approach introduced by Nightingale [1] is one of the most accurate methods for the numerical determination of critical exponents near second order phase transitions of pure systems. It consists in exactly calculating the physical quantities on strips of finite width and in using finite size scaling to extract critical exponents from these data. For almost all disordered systems, it is not possible to calculate exactly physical quantities on strips. However, by constructing a very large strip with a Monte Carlo procedure, one can obtain the physical quantities with sufficient accuracy to use finite size scaling. For the evaluation of the conductivity in random resistor networks [2] at the percolation threshold this has been done recently in two dimensions [3].

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Up to now, transfer matrix techniques, exact or by Monte Carlo simulation, were mostly restricted to two dimensions ; see [4-6] for three-dimensional work using this method. The present paper generalizes the method of reference 3 to three dimensions, where contradictory values by different Monte Carlo simulations were obtained in the past [2, 7]. A clarification is desirable in order to check the conjecture of Alexander and Orbach [8] for the conductivity exponent ; this scaling law relates the conductivity exponent to other, better known, critical exponents of percolation.

Our method is a straightforward generalization to the three-dimensional case of the technique of Derrida and Vannimenus [3]. We calculate the electrical current in a bond percolation problem, with minor modifications for site percolation, on a simple cubic lattice of height m, depth n, and length $L \gg n, m$. Periodic boundary conditions are used in y-direction, see figure 1. Each bond between nearest neighbours is randomly conducting with probability p ; otherwise it is insulating. A unit voltage is applied between the top and the bottom planes, and the total current is calculated. A very large L automatically averages over many configurations and leaves no ambiguity over whether one should average the conductivity, the resistivity, or functions of them. This effect is an advantage over the method to average over many disjointed cubes [7].
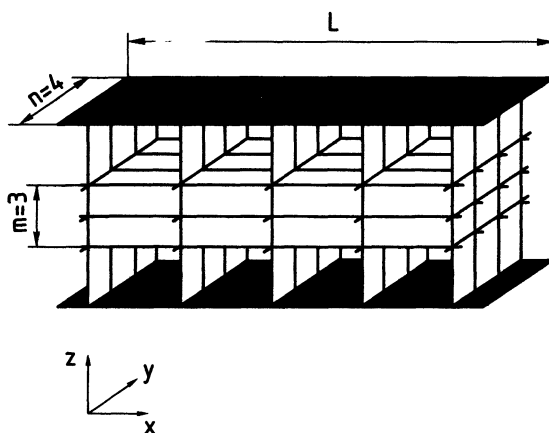

Fig. 1. — A bar of length L, height m and depth n. We calculate the conductivity between the two black planes.

As in reference 3 we use a step-wise procedure to calculate the electrical current at every moment of the simulation. If the bar has been constructed up to length L, the conductive properties of this bar are represented by a matrix A_L, see equation 1 of [3]. Then we add new bonds, conducting or insulating, to construct the bar up to length $L + 1$. The matrix A_{L+1} can be calculated from the matrix A_L and from the knowledge of the new bonds ; see equation 12 of reference 3.

In comparison to other techniques [2, 7, 9] we think that our method has two advantages in addition to the averaging problem mentioned above : first, in contrast to the usual Monte Carlo evaluation of conductivities, no relaxation iteration is needed to find the solution of Kirchhoff's equations ; instead these are solved exactly. Second, in contrast to Fogelholm's and similar methods [9], our method can be applied rather easily to dimensions d higher than two. The only limitation besides computer time is that the number of elements in the matrix A_L increases like the square of n^{d-1}, where n measures the linear extent in the transverse direction of the bar. Our method can also be applied to cases where the probability distribution of resistors is more complicated than the present two delta functions distribution. We performed our calculations on a Cray 1 Computer for bond percolation and on a CDC Cyber 76 for site percolation.

For bond percolation, one can choose between two possible geometries : geometry I with $m = n - 1$ or geometry II with $m = n$ (see Fig. 1). In geometry I, there are $n - 1$ sites and n bonds in the z-direction whereas in geometry II, there are n sites and $n + 1$ bonds in the z-direction. Both geometries can be physically justified. Our first calculations on short bars gave a smaller curvature of the results for geometry I and therefore we decided to restrict ourselves to that case. On a Cray 1 Computer we needed all together about 2 1/2 hours of execution time for the bond case.

For site percolation we chose the geometry $n \times n$ only. On a CDC Cyber 76 we needed less than 0.04 seconds to add one plane for $n = 15$. (For both bond and site case the computer time increased roughly as n^4). For larger n, an auxiliary large core memory had to be used, increasing appreciably the time to about 0.15 seconds per slice for $n = 18$.

A comparison of vector computers (Cray 1 for bond, CDC Cyber 205 for site) with a normal « scalar » computer (Cyber 76) showed the vector computer to need about 30 % less execution time if no major changes are made in the program. However we hope (J. G. Zabolitzky, private communication) that the speed could be increased on vector computers by utilizing their special features more efficiently.

All our calculations were made at or near the percolation threshold p_c which was taken as 0.249 2 from Wilke [13] for bond and as 0.311 7 from Heermann and Stauffer [11] for site percolation, with error bars of the order of 0.000 2.

Our results for the conductivity Σ_n (normalized to unity at $p = 1$) as a function of the linear transverse dimension n (at $p = 0.249\ 2$ for bond percolation and at $p = 0.311\ 7$ for site percolation) are summarized in table I and figure 2. A direct determination on figure 2 gives a slope

Table I. — *Conductivity Σ_n (in units of 10^{-5}) as a function of transverse size n for bond (at $p = 0.249\ 2$) and site (at $p = 0.311\ 7$) percolation. The length L of the bar is indicated in parenthesis. We estimate the errors to be of order of several units of the last decimal.*

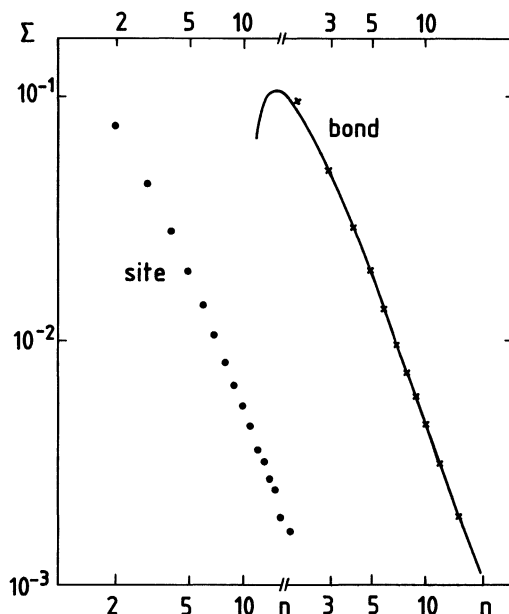| n	Bond $m = n - 1$		Site $m = n$	
	$10^5 \Sigma_n$	L	$10^5 \Sigma_n$	L
2	9570	(10^5)	7588	(10^7)
3	4943	(10^5)	4390	(10^6)
4	2879	(10^5)	2813	(10^6)
5	1918	(10^5)	1933	(10^6)
6	1331	(10^5)	1387	(10^6)
7	953	(10^5)	1047	(10^6)
8	743	(10^5)	819	(10^6)
9	580	(10^5)	651	(5×10^5)
10	458	(10^5)	538	$3 \times (1.25 \times 10^5)$
11			445	(1.3×10^5)
12	320	(2×10^4)	360	(1×10^5)
13			318	(8×10^4)
14			271	$3 \times (1.3 \times 10^5)$
15	188	(2×10^4)	245	(3×10^4)
16			187	(4×10^4)
18			165	$2 \times (4 \times 10^4)$
20			128	(10^4)
21			126	(10^4)

Fig. 2. — The log-log plot of the conductivity Σ_n *versus* transverse size n of a bar, at the percolation threshold. The dots refer to site, the crosses to bond percolation. The data of bond percolation are fitted by a curve with $x = 2.23$ and taking the amplitudes and ω of order unity (see Eq. 3).

$x \simeq 2.1$ for both site and bond problems. The slope x is the asymptotic critical exponent, for the conductivity at the percolation threshold

$$\Sigma_n \sim n^{-x} \,. \tag{1}$$

According to finite size scaling, x is related to the exponent t of the conductivity $(\Sigma_\infty(p) \sim (p - p_c)^t)$ and to the exponent v of the correlation length $(\xi(p) \sim |p - p_c|^{-v})$ by

$$x = \frac{t}{v} \,. \tag{2}$$

We used a more sophisticated analysis to fit our data taking into account corrections to scaling. We assumed a correction factor $(1 + \text{const } n^{-\omega})$ with ω between 0.5 and 2.0, a range of values which seems possible for ω. So we have for the conductivity

$$\Sigma_n \sim an^{-x}(1 + bn^{-\omega}) \,. \tag{3}$$

Theoretical arguments can be given that this corresponds to an irrelevant operator in the renormalization sense. $\omega = 1.5$ is the value predicted by Reeve [12]; see Adler [10] for a review of corrections to scaling in percolation. As an example, we show in figure 2 our bond percolation data with a fit for $\omega = 1$. It is satisfactory that the amplitudes a and b of equation 3 are both of order unity. For this choice of ω, we find good fits for $x = 2.23 \pm 0.1$.

For our more accurate site conductivities, we made in addition a graphical analysis in figure 3, giving results consistent with a numerical analysis as in the bond case. From consecutive values of n we determine the effective exponent $x = - \mathrm{d}(\log \Sigma_n)/\mathrm{d} \log n$ and plot this slope of the log-log plot *versus* the reciprocal average value of n. The data follow well a straight line within
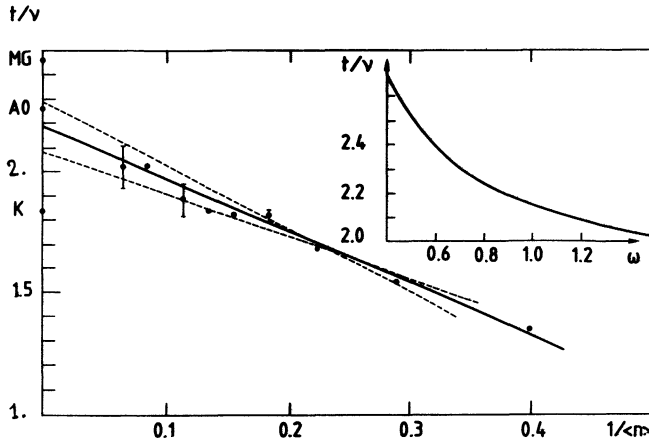
Fig. 3. — Effective exponent t/v *versus* reciprocal dimension $1/n$ for site percolation at $p = 0.311\ 7$. This exponent is the negative slope of the curve shown by dots in figure 2. Three representative error bars are shown. The intercept gives the asymptotic exponent if the correction exponent omega equals unity. The solid line gives the best fit, the dashed lines plausible upper and lower limits. The letters K, AO and MG refer to the previous estimates of Kirkpatrick [17], Alexander and Orbach [6], and Mitescu and Greene [7]. The inset shows the variation of the asymptotic exponent with an assumed omega value.

the statistical error, which means that one cannot see reliably from the data whether ω is smaller or larger than unity. We conclude from figure 3 :

$$x = \frac{t}{v} = 2.2 \pm 0.1 \tag{4}$$

is a realistic estimate. This estimate is entirely consistent with our bond analysis, as it should be according to the universality hypothesis.

But errors larger than the one estimated in equation 4 may arise from the unknown value of ω. If we increase ω from 0.5 to 1.5, the exponent x found as an intercept of a plot of effective exponents *versus* $n^{-\omega}$ is found to decrease from 2.5 to 2.05, as shown in the inset of figure 3. We obtain the best fit at $\omega \simeq 0.9$ but the correlation is not significantly worse in the whole interval considered for ω. Our table allows the reader to make his own analysis. Should later research fix ω sufficiently precisely (see for example reference 12), one can read off from our graph the revised estimate of t/v.

Another source for systematic errors is the inaccuracy in p_c. From less complete simulations at $p = 0.310\ 7$ and $p = 0.312\ 7$, we estimate t/v to decrease by about 0.04 if p_c is increased by 0.001 in the site case, a shift appreciably larger than the estimated errors in p_c. A shift in the same direction and of the same order of magnitude was obtained in the bond case. This error is negligible compared with our statistical error.

Equation 4 means

$$\Sigma_\infty(p) \sim (p - p_c)^t \sim (p - p_c)^{1.94 \pm 0.1} \tag{5}$$

(again assuming ω near unity) for the conductivity itself when we take $v = 0.88 \pm 0.01$ from Heermann and Stauffer [11]. Again the error for v is negligible compared with our own statistical errors and the inaccuracies in ω.

Our results should be compared with presumably less accurate estimate $t \simeq 1.65$ from references 2,17 and with $t/v \simeq 2.5$ from reference 7. The scaling law [8, 16] $t/v = 3\ d/2 - 2 - \beta/2\ v =$

$2.5 - \beta/2\,v$ together with $\beta/v = 0.47$ from reference 14 and $\beta/v = 0.515$ from reference 15 predicts $t/v = 2.265$ and $t = 2.24$ respectively, or $t = 1.99$ with an error of about 0.02 much smaller than ours. Thus our result is in good agreement with the prediction of Alexander-Orbach. It is also in good agreement with the series prediction $t = 1.95$ [18]. It agrees also with the recent work of Sahimi *et al.* [19] who used finite size scaling and obtained $t = 1.87 \pm 0.04$.

In this letter we presented results for periodic boundary conditions in three dimensions. It would be interesting to apply the same method to free boundaries. Also one could use it in four dimensions in order to test further the validity of the Alexander-Orbach scaling relationship.

Acknowledgments.

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