A novel determination of the percolation exponent u in three dimensions

1987 J. Phys. A: Math. Gen. 20 L885

(http://iopscience.iop.org/0305-4470/20/13/013)

J. Phys. A: Math. Gen. 20 (1987) L885-L889. Printed in the UK

LETTER TO THE EDITOR

A novel determination of the percolation exponent u in three dimensions

J M Laugier† and J M Luck‡

† Département de Physique des Systèmes Désordonnés, Université de Provence, CNRS UA 857, St-Jérôme, 13397 Marseille Cedex 13, France
‡ Service de Physique Théorique, CEN Saclay, 91191 Gif-sur-Yvette Cedex, France

Received 12 June 1987

Abstract. We present an accurate determination of the percolation transport exponent $u = t/(s+t)$ in three dimensions, based on a transfer-matrix approach to the AC (frequency-dependent) conductivity, and a finite-size scaling analysis of the numerical data. The phase of the complex conductivity, the loss angle, assumes the universal value $\delta_c = (\pi/2)(1-u)$ at low frequency at the percolation threshold. As a test of our numerical scheme, the two-dimensional exact duality result $\delta_c = \pi/4$ (i.e. $s = t$) is recovered with a very good accuracy. In three dimensions, our data are extrapolated to $\tan\,\delta_c = 0.54 \pm 0.03$, i.e. $u = 0.69 \pm 0.02$, whereas the usually accepted values $s/\nu = 0.85 \pm 0.04$, $t/\nu = 2.2 \pm 0.1$ yield $u = 0.72 \pm 0.02$. This marginal disagreement can be attributed to ill behaved corrections to finite-size scaling.

This letter presents a novel numerical determination of the percolation transport exponent u in three dimensions. This estimation is based on a finite-size scaling analysis of transfer-matrix data concerning the AC (frequency-dependent) complex conductivity of a metal-dielectric binary random mixture at the percolation threshold of the metallic component. We employ the usual bond-percolation modelisation on a cubic lattice [1, 2], where each bond is either a conductor (resistance $R = 1$) with probability p, or an insulator (capacitance $C = 1$, i.e. impedance $(i\omega)^{-1}$ at frequency $\omega/2\pi$) with probability $q \equiv 1 - p$.

The macroscopic AC conductivity $\Sigma(p, \omega)$ of this system has a well known behaviour in two simple limiting cases. At zero frequency, the dielectric bonds are perfect insulators, and Σ vanishes for $p < p_c$, where p_c is the geometrical percolation (connectivity) threshold, and behaves as $\Sigma \sim (p - p_c)^t$ for $p \to p_c^+$. Conversely, in the limit of an infinite frequency, we have a normal-superconductor mixture, Σ is infinite for $q > p_c$, and behaves as $\Sigma \sim (p_c - q)^{-s}$ for $q \to p_c^-$. Both exponents s and t have been the subject of an intense theoretical activity.

These two kinds of critical behaviour become 'rounded' as soon as ω is not strictly zero, or infinite. In the following, we will focus our attention on the vicinity of the $(p = p_c, \omega = 0)$ fixed point. In the whole critical region, where both $(p - p_c)$ and ω are small, the AC conductivity has been shown to obey the following scaling behaviour [1-4]:

$$\Sigma(p, \omega) = |p - p_c|^t \Phi_\pm(ix) \tag{1}$$

where

$$x = \omega|p - p_c|^{-s-t} \tag{2}$$

0305-4470/87/130805+05\$02.50

and where $\Phi_\pm$ are two complex scaling functions, and $\pm$ refers to the sign of $(p-p_c)$. The conductivity $\Sigma(p, \omega)$ is a smooth function of p, even at $p=p_c$, at fixed non-zero frequency ω, as well as a real-analytic function of $\mathrm{i}\omega$, at fixed $p \neq p_c$. These regularity conditions imply that the large-x limit of both scaling functions is

$$\Phi_+(\mathrm{i}x) \sim \Phi_-(\mathrm{i}x) \sim K(\mathrm{i}x)^u \qquad x \to \infty \tag{3}$$

where K is a real constant and the universal exponents s, t, u are related by

$$u = t/(s+t). \tag{4}$$

The conductivity at $p=p_c$, and at low frequency, is therefore

$$\Sigma(p_c, \omega) = K \exp(\mathrm{i}\pi u/2)\omega^u. \tag{5}$$

In more physical words, the loss angle δ, usually defined through

$$\tan\delta = \mathrm{Re}\,\Sigma/\mathrm{Im}\,\Sigma \tag{6}$$

assumes the universal value

$$\delta_c = \frac{\pi}{2}\frac{s}{s+t} = \frac{\pi}{2}(1-u) \tag{7}$$

for $p=p_c$ and $\omega \ll 1$.

The remarkable consequence (7) of the scaling law (1) of the AC conductivity, which seems to have been noticed only recently [5-7], is the key observation which has motivated the present work; the critical exponent u can be directly measured through the finite quantity δ, at p_c but for $\omega \neq 0$, and hence off criticality, without extraction of a slope or any other fit except the extrapolation to the $\omega \to 0$ limit, and of course subject to the finite size of the samples that transfer matrices can handle.

The transfer-matrix method (TMM) for electrical problems in percolation has been introduced by Derrida and co-workers [8, 9] for the conductor-insulator problem (exponent t). It consists in computing with a very high accuracy, through the recursive construction of an impedance matrix, the transverse conductivity of a strip of width N, or a bar of cross-sectional area $N \times N$, for the two- and three-dimensional problems, respectively, and of length $L \gg N$. An extrapolation of the conductivities Σ_N yields a determination of the exponent t, since a finite-size scaling [10] argument shows that $\Sigma_N(p_c) \sim N^{t/\nu}$. We will come back to this point in a more precise way later on, since finite-size scaling is also the cornerstone of the present work. The TMM has provided one of the most accurate determinations of the exponent t: $t/\nu = 0.973 \bullet 0.005$ [11], and $t/\nu = 2.2 \pm 0.1$ [12], in two and three dimensions, respectively.

The TMM was then extended by Herrmann *et al* [13] to the normal-superconductor problem (exponent s). In this case, the transfer matrix is used to compute the longitudinal conductivities of strips or bars. This geometry permits the use of periodic transverse boundary conditions which are known to minimise the systematic finite-size corrections. The main limitation of the TMM lies in the statistical errors: since Σ_N are self-averaging, the error bars are proportional to $L^{-1/2}$, $L \gg N$ being the system length, and hence can only be reduced by increasing L. The results of [13] $s/\nu = 0.977 \pm 0.01$ in two dimensions and $s/\nu = 0.85 \pm 0.04$ in three dimensions are the most accurate estimates of the exponent s in the literature.

In a previous publication [14], in collaboration with Clerc and Giraud, we have used the TMM to study various properties of the AC conductivity $\Sigma(p, \omega)$ of the two-dimensional metal-dielectric mixture mentioned above, with emphasis on a finite-size scaling analysis of the critical region around $(p=p_c,\ \omega=0)$. The very same extension of the TMM is used in the present work to compute the three-dimensional exponent u through (7); we therefore refer the reader to [14] for a description of the method.

We restrict ourselves to the longitudinal conductivities of bars at the three-dimensional percolation threshold: $p_c=0.2492\pm0.0002$ [15]. We have argued in [14] that these quantities obey the following finite-size scaling behaviour, for $\omega\ll1$ and $N\gg1$:

$$\Sigma_N(p_c,\omega)=N^{-t/\nu}F(\mathrm{i}X). \tag{8}$$

The real scaling variable

$$X=\omega N^{(s+t)/\nu} \tag{9}$$

plays an analogous role to x, defined in (2): the distance $|p-p_c|$ to the threshold is replaced by the appropriate power of the system size. We are mainly concerned with the loss angles, defined through (6). Their scaling behaviour is

$$\delta_N(p_c,\omega)=f(X) \tag{10}$$

and the scaling function f goes to δ_c, defined in (7), as its argument X becomes large. The way in which this limit is reached follows from finite-size scaling theory [16]; the corrections to the thermodynamical limit are exponentially small in N as soon as one of the relevant variables (here ω) is non-zero. We have therefore

$$f(X)=\delta_c+\mathrm{O}\{\exp(-AX^{\nu/(s+t)})\}\qquad X\to\infty \tag{11}$$

where A is some positive constant.

We have first tested the scheme explained above on the two-dimensional case, where the duality of planar graphs yields the property

$$s=t\qquad u=\tfrac{1}{2}\qquad \delta_c=\pi/4\qquad (D=2). \tag{12}$$

Our data, obtained on strips on a square lattice, are shown in figure 1, which presents a plot of $\tan\delta$ against the inverse scaled frequency $1/X$ defined in (9), for strip widths $5\leq N\leq20$. We have used the numerical value $(s+t)/\nu=1.95$ [11, 13]. A clear data collapse can be seen: the systematic finite-size corrections to the scaling form (10) become smaller than the unavoidable statistical data scatter for widths $N\sim5$. The extrapolated $X\to\infty$ value cannot be distinguished from the exact result $\tan\delta_c=1$, implied by (12). The quality of the data does not allow for a reliable fit of the leading large-X behaviour with (11). The straight line on the figure is a least-squares fit, meant as a guide for the eye.

We have performed the same analysis in the three-dimensional case (bars on a cubic lattice). Our data, corresponding to bar widths $4\leq N\leq10$, are shown in figure 2. The systematic corrections to the scaling result (10) are more important than in the two-dimensional case. Fortunately, the $X\to\infty$ limit seems to be rather insensitive to these corrections. The data collapse in a better way for smaller values of $1/X$, and the limit $\tan\delta_c\approx0.54$ appears clearly. Putting an error bar to this number is a more delicate task, since both statistical errors and corrections to (10) are involved. In order to observe an appreciable improvement in the data scatter, the amount of computer time we have used, 30 h of the array processor 3090 VF of CNUSC at Montpellier, would have to be increased roughly by a factor of ten! The rather small range of sizes

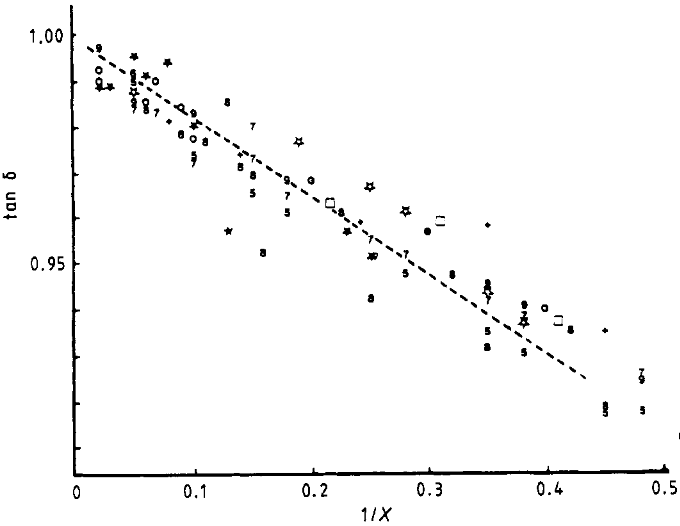

Figure 1. The tangent of the loss angles $\delta_N(p_c, \omega)$, of strips of width N at the two-dimensional percolation threshold $p_c = \frac{1}{2}$, plotted against the reciprocal of the scaled frequency X defined in (9). The digits stand for strip widths $N \leqslant 9$; larger widths are denoted by symbols for $N = 10$ (○), 11 (☆), 12 (★), 16 (□) and 20 (+). The $X \to \infty$ limit of the scaling function agrees with the exact result $\tan \delta_c = 1$.

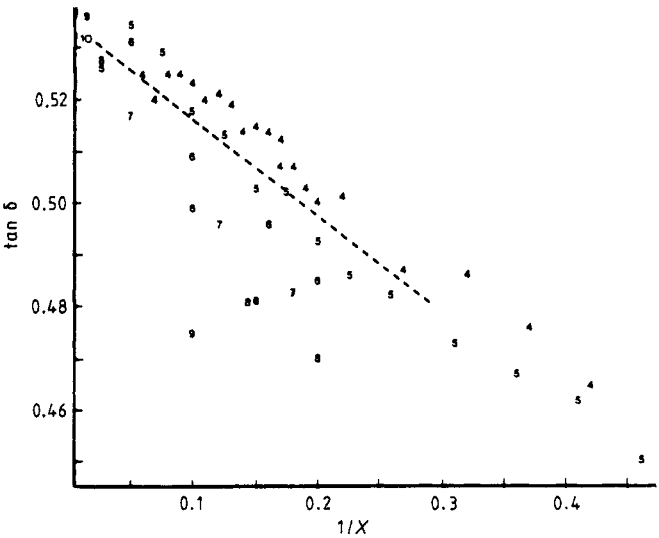

Figure 2. Same as figure 1 for bars of section $N \times N$ at the three-dimensional threshold $p_c \approx 0.2492$. The $X \to \infty$ limit is estimated to be $\tan \delta_c = 0.54 \pm 0.03$.

we have explored makes any correction analysis difficult and hardly credible. We have therefore chosen to present only a least-squares linear fit, just as we did in the two-dimensional case, and to estimate the following error bar, in a global, and hence subjective, way:

$$\tan \delta_c = 0.54 \pm 0.03 \qquad u = 0.69 \pm 0.02. \tag{13}$$

The above-mentioned values of s and t [12, 13] yield tan $\delta_c = 0.47 \pm 0.04$; $u = 0.72 \pm 0.02$. We think that the marginal disagreement between both estimates can easily be explained by an effect of ill behaved corrections to finite-size scaling, either in the present work or in one of the quoted works, like, e.g., a slowly disappearing transient regime, which cannot be noticed except by going to much larger systems.

It is a pleasure to thank J P Clerc, B Derrida, G Giraud, and H Herrmann for useful discussions.

References

[1] Webman I, Jortner J and Cohen M H 1975 *Phys. Rev.* B **11** 2885
[2] Efros A L and Shklovskii B I 1976 *Phys. Status Solidi* b **76** 475
[3] Straley J P 1976 *J. Phys. C: Solid State Phys.* **9** 783; 1977 *Phys. Rev.* B **15** 5733
[4] Stephen M J 1978 *Phys. Rev.* B **17** 4444
[5] Clerc J P, Tremblay A M S, Albinet G and Mitescu C D 1984 *J. Physique Lett.* **45** L913
[6] Clerc J P, Giraud G, Laugier J M and Luck J M 1985 *J. Phys. A: Math. Gen.* **18** 2665
[7] Luck J M 1985 *J. Phys. A: Math. Gen.* **18** 2061
[8] Derrida B and Vannimenus J 1982 *J. Phys. A: Math. Gen.* **15** L557
[9] Derrida B, Zabolitzky J G, Vannimenus J and Stauffer D 1984 *J. Stat. Phys.* **36** 31
[10] Fisher M E 1972 *Critical Phenomena, Proc. 51st Enrico Fermi Summer School, Varenna* ed M S Green (New York: Academic)
[11] Zabolitzky J G 1984 *Phys. Rev.* B **30** 4077
[12] Derrida B, Stauffer D, Herrmann H J and Vannimenus J 1983 *J. Physique Lett.* **44** L701
[13] Herrmann H J, Derrida B and Vannimenus J 1984 *Phys. Rev.* B **30** 4080
[14] Laugier J M, Clerc J P, Giraud G and Luck J M 1986 *J. Phys. A: Math. Gen.* **19** 3153
[15] Wilke S 1983 *Phys. Lett.* **96A** 344
[16] Lüscher M 1986 *Commun. Math. Phys.* **104** 177
Brézin E and Zinn-Justin J 1985 *Nucl. Phys.* B [FS14] **257** 867