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1985 J. Phys. A: Math. Gen. 18 L1081

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J. Phys. A: Math. Gen. **18** (1985) L1081-L1086. Printed in Great Britain

LETTER TO THE EDITOR

Is there a lower critical dimension for chemical distance?

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Received 8 July 1985

Abstract. Estimates of the fractal dimension ϕ for 'chemical distance' (shortest-path distance) between points on a percolation cluster are inferred from computations of the first-passage velocity $v(p)$ on square ($d=2$) and simple cubic ($d=3$) bond lattices with bonds randomly assigned time delay b with probability p, otherwise time delay $a \gg b$. The computations, implemented on strips in a manner analogous to the transfer matrix for conductivity, yield estimates of ϕ based on a new scaling law, $v(p_c) \sim a^{-1}(a/b)^{1/\phi}$, where p_c is the percolation threshold for b-bonds. For $d=2$, we obtain $\phi = 1.021 \pm 0.005$, which is significantly lower than previous estimates. For $d=3$, we obtain $\phi = 1.26 \pm 0.06$, in agreement with the Havlin-Nossal proposal $\phi = d-(1+\beta)/\nu$. Our results do not exclude the possibility that $\phi = 1$ for $d=2$, indicating that the chemical distance may be non-fractal below some lower critical dimension between two and three.

It has been proposed and, apparently, confirmed computationally (Grassberger 1985a, and references cited therein) that the 'chemical distance' (Havlin and Nossal 1984), or shortest path between points on a percolation cluster obeys

$$\tau \sim R^{\phi}, \tag{1}$$

where τ is the path length, $R \gg 1$ is the Euclidean distance between the points, and for spatial dimension $d \geqslant 2$, the fractal exponent ϕ obeys $\phi > 1$. In particular, a recent two-dimensional computation (Grassberger 1985a) gives $\phi = 1.132 \pm 0.003$, which excludes the proposal (Havlin and Nossal 1984) $\phi = d-(1+\beta)/\nu$, but is consistent with numerous earlier results (summarised in Grassberger 1985a) which generally fall within the range $1.1 < \phi < 1.2$.

The value $\phi = 1.021 \pm 0.005$ which we obtain for $d=2$ is significantly different from estimates obtained previously. In our computations, ϕ is estimated by a novel method, exploiting a new scaling law which we derive shortly. We remark at the outset that the key difference between our approach and previous computations is that we extrapolate a sequence of estimates of ϕ with respect to a parameter L characterising the size of the computational domain. Grassberger's result and our extrapolated result for the L value corresponding to his computational domain are in excellent agreement, indicating that our result and previous results are consistent if the latter are interpreted as finite-L estimates.

Grassberger estimates ϕ by building the 'infinite' percolation cluster at $p = p_c$ for a square bond lattice, starting from one edge of a rectangular box and adding one 'chemical layer' per time step. Actually, any such cluster must eventually terminate due to the finite span of the starting edge. One way to avoid possible statistical bias associated with cluster termination is to build clusters outward from the starting edge

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only to a distance which is short compared with the span of the edge. In fact, Grassberger's starting edge is 3840 lattice spacings wide and his clusters propagate outward by at most 600 lattice spacings, consistent with this restriction.

Our approach overcomes this restriction. We consider the problem of first-passage percolation (Wierman 1982 and references cited therein) for square ($d=2$) and simple cubic ($d=3$) bond lattices with bonds randomly assigned time delay b with probability p, otherwise assigned time delay $a \gg b$. For simplicity, we specialise the discussion to $d=2$. Starting from an edge of span L, the propagation front of 'wetted' sites can be developed indefinitely outward from this edge provided that a is finite. Denoting the furthest distance of a 'wetted' site from the starting edge as $x(t)$, then $x(t)$ converges for large t to a constant, the first passage velocity.

From the computational viewpoint, propagation along a strip of width L offers advantages analogous to those of the transfer-matrix (Vannimenus and Nadal 1984) method for computation of conductivity in this geometry. In fact, we can exploit the analogy to the conductivity problem in order to obtain scaling laws relating v to a, b, and p. We adopt the homogeneous function representation developed by Straley (1976) for the conductivity problem. The propagation analogue of his equation (2) is

$$v = \mu S(\varepsilon\lambda^{-1}, a^{-1}\mu^{-1}\lambda^{-\psi}, \mu b\lambda^{-\theta}), \tag{2}$$

where the macroscopic effective conductivity is replaced by v and the dielectric-bond and metallic-bond conductances are replaced by a^{-1} and b^{-1} respectively. As in Straley's analysis, $\varepsilon = p - p_c$, μ can be chosen arbitrarily due to invariance under scale transformation, λ is the scaling parameter representing proximity to the critical point, and ψ and θ are critical exponents whose significance is demonstrated shortly. Equation (2) is presumed to be valid in the limit of small λ.

Particular cases of equation (2) yield known scaling laws and an additional scaling law which we will exploit. The substitutions $a=\infty$, $\lambda = \varepsilon > 0$, and $\mu = b^{-1}\lambda^{\theta}$ give

$$v = \varepsilon^{\theta} b^{-1} S(1, 0, 1). \tag{3}$$

This is the scaling law for the 'chemical propagation' regime (Kerstein 1985b) of first-passage percolation, where θ obeys (Grassberger 1983, Ritzenberg and Cohen 1984)

$$\theta = \nu(\phi - 1). \tag{4}$$

The substitutions $b=0$, $\lambda = -\varepsilon > 0$ and $\mu = a^{-1}\lambda^{-\psi}$ give

$$v = |\varepsilon|^{-\psi} a^{-1} S(-1, 1, 0). \tag{5}$$

This is the scaling law for a particular case of the 'contact propagation' regime of first-passage percolation, where for this case, $\psi = \nu$ (Kerstein 1985b). Finally, the substitutions $\varepsilon = 0$, $\lambda^{\theta+\psi} = b/a$, and $\mu = b^{-1}\lambda^{\theta}$ give

$$v = (b/a)^{\theta/(\theta+\psi)} b^{-1} S(0, 1, 1). \tag{6}$$

This is a new result, giving the dependence of v on the ratio a/b at $p = p_c$. Substituting equation (4) and $\psi = \nu$ into equation (6) gives

$$v \sim a^{-1}(a/b)^{1/\phi}. \tag{7}$$

Elsewhere (Kerstein and Edwards 1985), we present a derivation of equation (6) which does not depend on the homogeneous function representation. Straley (1983) has similarly presented an alternative derivation of the conductivity analogue of equation (6). The conductivity analogue has recently been verified computationally

for $d=2$ (Bunde *et al* 1985). The computational results discussed here, in addition to providing estimates of ϕ, serve to verify the new scaling law for $d=2$ and $d=3$.

Equation (7), while providing us with a means of overcoming the cluster-termination problem mentioned earlier, does not entirely circumvent finite-size effects. In particular, equation (7) predicts that for fixed a, v diverges as b approaches zero. However, on a strip of finite width L, the effective correlation length at $p=p_c$ is of order L, so any b-cluster through which the front is propagating will terminate in a distance of this order. To get to the next b-cluster, the front must cross at least one a-bond. From this we conclude that v cannot exceed order L/a, therefore there must be a crossover from the scaling predicted by equation (7) to

$$v \sim L/a \tag{8}$$

when $L/a \approx a^{-1}(a/b)^{1/\phi}$.

Our calculation employs periodic transverse boundary conditions, which avoid surface effects associated with fixed boundary conditions (Herrmann *et al* 1984, Rapaport 1985). Although a finite longitudinal span of $3L$ is used for the computations, periodic longitudinal boundary conditions are applied so that the computational domain is traversed repeatedly, simulating propagation along an infinite strip. New bonds are randomly generated just ahead of the furthest longitudinal advance $x(t)$ of the 'wetted' front as the front propagates. Test cases with longitudinal span larger than $3L$ confirm that our algorithm is equivalent to propagation on an infinite strip.

Each estimate of the first-passage velocity v is based on five independent replicate simulations, from which the mean value and the standard deviation of v are computed. For each replicate, propagation along a longitudinal distance of order 10^3 lattice spacings is dedicated to elimination of initial transients, and the first-passage velocity is taken to be the remaining propagation distance (of order 10^4 lattice spacings) divided by the corresponding passage time. The computations are discussed in greater detail elsewhere (Kerstein and Edwards 1985).

Figure 1 shows first-passage velocities as a function of the ratio a/b of time delays at the percolation threshold $p=p_c$, which is exactly 0.5 for a square bond lattice (Wierman 1982). To vary a/b, we take $a=1$ and vary b. Computations were performed

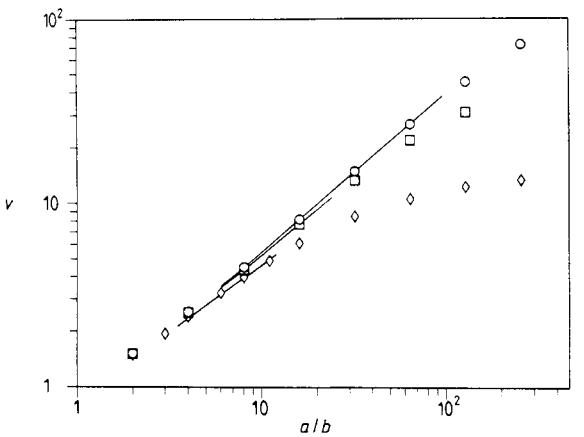

Figure 1. Estimated first-passage velocity v at $p=p_c$ against bond time-delay ratio a/b for the square bond lattice ($d=2$) for strip width $L=8$ (◇), 32 (□) and 128 (○). Fitted line segments indicate the respective finite a/b scaling regimes.

for L values ranging from 6 to 256 for $d=2$. For clarity, only representative L values ($L=8$, 32 and 128) are shown. Fitted line segments indicate the regimes of finite a/b scaling according to equation (7). (Additional data confirming equation (7) for $d=2$ and $d=3$ are presented in Kerstein and Edwards (1985).) The slopes of these weighted linear least-squares fits give estimates of $1/\phi(L)$, where $\phi(L)$ is the fractal exponent at finite L. Departures from scaling at higher values of a/b signal the crossover to finite-size scaling. The finite-size scaling regime (equation (8)) was verified previously in the context of a stirred percolation problem (Kerstein 1985a).

To ensure reliable estimates of $\phi(L)$, we use a statistical procedure to select the points included in the linear fits. Starting with a range of points wider than the scaling regime, points are removed from either end until the weighted sum of squared deviations, χ^2, attains a reasonable value based on the χ^2 distribution for the number of fitted points. The line segments in figure 1 include only the points used in the fits.

Figure 2 shows our estimates of $\phi(L)$ for $d=2$ (circles) as a function of $1/\ln L$. The usual (Adler *et al* 1983, Binder and Stauffer 1984, Kerstein and Edwards 1985) correction-to-scaling analysis predicts a dependence on L of the form $\phi(L)=\phi+(c_1/\ln L)(1+c_2L^{-\omega})$. The high degree of linearity of $\phi(L)$, when plotted with respect to $1/\ln L$, indicates that c_2 and/or the correction-to-scaling exponent ω is close to zero. Therefore we extrapolate to the intercept at $L=\infty$ based on a weighted linear least-squares fit (full line) to our data, obtaining the estimate $\phi=1.021\pm0.005$. For comparison, Grassberger's estimate (□) is plotted at $L=600$, which is an upper bound on the $x(t)$ values reached in his simulations. The actual L value corresponding to his simulations may be smaller, but nonetheless, it is clear that our extrapolated line is in excellent agreement with Grassberger's estimate, provided that the latter is interpreted as a finite-L approximation. The precision of this agreement is fortuitous because, as we show elsewhere (Kerstein and Edwards 1985), different methods for computing $\phi(L)$ can yield different estimates for given finite L, with convergence of the different methods occurring only in the large-L limit. This observation may account for the

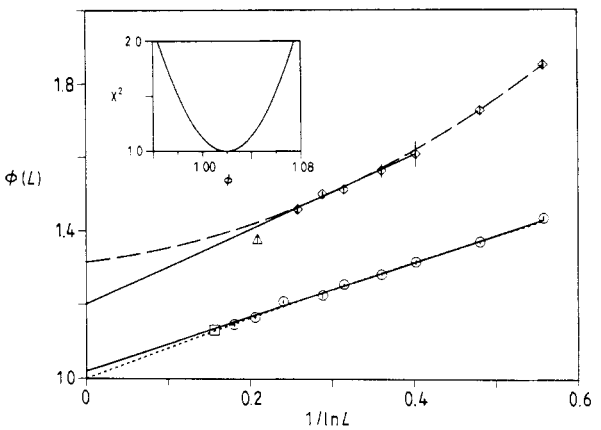

Figure 2. Estimated chemical distance exponent $\phi(L)$ against $1/\ln L$ for $d=2$ based on present computations (○) and a previous (Grassberger 1985a) computation (□), and for $d=3$ based on present computations (◇) and a previous (Grassberger 1985b) computation (△). Also shown are weighted linear fits (full), a weighted parabolic fit for $d=2$ constrained to intercept $\phi=1$ at $L=\infty$ (broken), and a weighted parabolic fit with unconstrained intercept for $d=3$ (chain). Inset: Weighted sum of squared deviations χ^2 (in relative units) against constrained intercept ϕ based on weighted parabolic fits for $d=2$.

discrepancies noted by Grassberger (1985a) among the various estimates quoted in the literature.

Our estimate is so close to unity that it warrants an assessment of the possibility that ϕ is exactly unity for $d=2$, especially since the exact functional dependence of $\phi(L)$ on L is not known. Accordingly, we perform weighted parabolic fits to our data with predetermined values of the intercept. The inset to figure 2 shows χ^2 from these fits (in relative units) as a function of the intercept. The minimum at $\phi=1.019$ is in agreement with the linear estimate $\phi=1.021\pm0.005$, indicating that the quadratic correction predicted by the data is insignificant. Even so, χ^2 from z parabolic fit with intercept at $\phi=1$ (broken curve) exceeds the minimum χ^2 by only 13%. Hence we cannot exclude the possibility that $\phi=1$ for $d=2$.

Also shown in figure 2 are the computed estimates ($\diamond$) of $\phi(L)$ for the simple cubic bond lattice, for which we take $p_c=0.2492$ (Wilke 1983). For $d=3$, the computations employ a finite span L in the two transverse directions which ranges from 6 to 48. Due to the apparent curvature of the data, we extrapolate to $L=\infty$ using two different procedures, a weighted linear fit to estimates for the five highest L values, and a weighted parabolic fit to all the data, both with unconstrained intercept. We take the average of the indicated intercepts to be our best estimate of ϕ for $d=3$, and half the difference of the intercepts to be the uncertainty, giving $\phi=1.26\pm0.06$. This result is in agreement with the proposed scaling law of Havlin and Nossal (1984), which predicts $\phi=1.35$ for $d=3$. For comparison, Grassberger's (1985b) estimate ($\triangle$) is plotted at $L=120$, which is an upper bound on the $x(t)$ values reached in his three-dimensional simulations.

Finally, we speculate on the implications of the result that ϕ may be exactly unity for $d=2$. This result is in strong disagreement with the Havlin-Nossal proposal which, however, appears to be in agreement with computed results, including ours, for $d\geqslant 3$. An interpretation consistent with these observations is that the Havlin-Nossal proposal is valid only above a lower critical dimension d_l, where $2\leqslant d_l<3$, rather than the trivial value $d_l=1$. (Below d_l, the chemical distance is non-fractal, so $\phi=1$.) The theoretical significance of this interpretation is an open question.

The authors would like to thank Amy Bug and Muhammad Sahivni for helpful discussions. This research was supported by the Office of Basic Energy Sciences, US Department of Energy.

Note added in proof. Our numerical results are in good agreement with the Flory calculation by Roux (1985). Cardy and Grassberger (1985) have recently shown that the Havlin-Nossal proposal cannot be exact for any d because it disagrees with the ϵ expansion

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