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LETTER TO THE EDITOR

Self-avoiding walks on percolation clusters

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Abstract. We study self-avoiding walks (SAWs) on percolation clusters. A scaling function representation for R, the mean end-to-end distance, is proposed which describes a crossover from ordinary SAWs to SAWs on fractals. We distinguish between SAWs on a single cluster for which $R \sim N^{\nu_1}$ and SAWs on all clusters for which $R \sim N^{\nu_2}$, where N is the number of monomers in the walk. We estimate $\nu_1(d=2) \simeq 1.285$ and the correction-to-scaling exponent $\Omega(d=2) \simeq 1.3$, and $\nu_1(d=3) \simeq 1.38$. Two plausible generalisations of the Flory approximation for ν_1 are investigated and it is argued that none of them provides a satisfactory approximation for ν_1 at all dimensions.

In the past few years random processes on fractal structures have been studied with increasing interest. The most prominent and physically appealing fractal system is the largest percolation cluster at the percolation threshold p_{c_1} which also possesses a fractal structure above p_c on any length scale smaller than the percolation correlation length ξ_{p} . Experimental work of several authors (Voss *et al* 1982, Kapitulnik and Deutscher 1982) has shown the importance of fractal structure of the percolation clusters in representing disordered systems. In the past two years ordinary (Pólya) random walks on percolation clusters have been studied by several authors (Alexander and Orbach 1982, Gefen et al 1983, Rammal and Toulouse 1983, Ben-Avraham and Havlin 1982, 1983, Pandey and Stauffer 1983, Sahimi and Jerauld 1983). These random walks provide a simple way of measuring the spectral dimension d_s which describes the power-law behaviour of harmonic excitations $N(\omega)$ at low frequency ω : $N(\omega) \sim \omega^{d_s-1}$. The spectral dimension for any fractal structure is defined (Alexander and Orbach 1982) as twice the ratio of the fractal dimension $d_{\rm f}$ of the cluster and the fractal dimension d_w of the random walk on the cluster: $d_s = 2d_f/d_w$. The spectral dimension appears to be an intrinsic property of the fractal structure.

In this letter we study self-avoiding walks (sAws) on percolation clusters. This problem was first studied by Chakrabarti and Kertész (1981) who were interested in the effect of the lattice disorder on the critical properties of sAws. According to Harris's criterion (Harris 1974) if the specific heat exponent α of a pure system is positive, the introduction of impurities should introduce new critical properties for the system. Since for sAws on fully connected lattices α is positive for all dimensionalities $1 \le d < 4 = d_c$, where d_c is the upper critical dimensionality, Chakrabarti and Kertész (1981) concluded that sAws on percolation clusters at any $p > p_c$, the fraction of occupied bonds or sites, should belong to a different universality class from the ordinary sAws. This was disputed by Kremer (1981) who presented Monte Carlo simulation results for sAws on the diamond lattice which indicate that above p_c the critical properties

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of saws remain unchanged. Dhar (1978) solved saw problems exactly on several pseudo lattices. The saws on percolation clusters may have relevance to the backbone of the clusters. This matter will be discussed elsewhere.

The main quantity of interest is the mean end-to-end distance R which varies with the number of visited sites N as

$$R \sim N^{\nu}, \tag{1}$$

where ν is a universal critical exponent. For sAWs on fully connected lattices $\nu(d=1) =$ 1, while for $d \ge 4$ the self-avoiding effect becomes negligible and R grows in the same way as in ordinary (Pólya) random walks; thus $\nu(d \ge 4) = \frac{1}{2}$ with a logarithmic correction at d=4. The value of ν at d=2 was conjectured by Nienhuis (1982) to be $\frac{3}{4}$. This conjecture is supported strongly by the works of Guttmann (1983) and Majid et al (1983a). The exact value of ν at d = 3 is also not known; the most accurate estimate is $\nu \simeq 0.588$ (Le Guillou and Zinn-Justin 1980, Majid et al 1983b), while Sahimi (1984) has suggested $\nu(d=3) = 113/192$. For saws on percolation networks one has to distinguish several cases. Above p_c and for $R \gg \xi_p$, we expect to have ordinary saws, i.e., ν remains unchanged. Slightly above p_c and for $R \ll \xi_p$, we do not expect to recover the percolation saws critical behaviour; this situation is similar to saws on percolation clusters at p_c . At p_c the correlation length ξ_p is infinite and thus R is characterised by a new critical exponent. However, depending on whether the saw is performed only on the largest percolation cluster at p_c or on all clusters, we expect to have two different critical exponents, just as in the case of ordinary random walks (Gefen et al 1983). If the saw is performed on a single cluster, we expect to have

$$R \sim N^{\nu_1},\tag{2}$$

whereas if the SAW takes place on *all* clusters and the results are averaged over *all* clusters, we anticipate that

$$R \sim N^{\nu_2},\tag{3}$$

where $\nu_1 \neq \nu_2$ and these exponents are universal. Moreover, we should have

$$\nu_1 > \nu_2 > \nu, \qquad d \le 4 \tag{4}$$

since the fractal structure of the clusters should enhance the self-avoiding effect. We propose the following scaling function representation for R:

$$R \sim N^{\nu} \xi_{\rm p}^{-x} f(N/\xi_{\rm p}^{1/\nu}).$$
 (5)

The scaling function f(y) has the following properties. If $N \gg \xi_p^{1/\nu}$, i.e. $p \gg p_c$, then

$$f(y) \sim y^0, \qquad y \gg 1 \tag{6}$$

whereas if $N \ll \xi_p^{1/\nu}$, i.e. $p = p_c$ or $p > p_c$ but $R \ll \xi_p$, the function f(y) obeys

$$f(y) \sim y^{\nu_1 - \nu}, \qquad y \ll 1.$$
 (7)

It is easily shown that $x = (\nu - \nu_1)/\nu$. For equation (5) to be valid below p_c we should have $f(y) \sim y^{-\nu}$, so that R becomes independent of N and approaches a (p-dependent) quantity ξ_{∞} which should diverge as p_c is approached from below. Our scaling function representation of R suggests that $\xi_{\infty} \sim (p_c - p)^{-z}$, where $z = \nu_p \nu_1 / \nu$, where ν_p is the critical exponent of percolation correlation length ξ_p .

If the saws are performed on *all* clusters then the statistics of interest should be averaged over all clusters. However, for saws, the singly connected (dead-end) bonds

do not play any role and thus one can remove them from the clusters. Therefore the statistics of interest must be averaged over the distribution of the backbone of the clusters which is given by $n_s \sim s^{-\tau'}$ where τ' is a universal critical exponent which is related to other backbone exponents through scaling laws (Stauffer 1979), and s is the number of sites in the backbone. This establishes a connection between the statistics of sAWs on percolation clusters and those of the backbone of the clusters, a matter to be discussed elsewhere.

Rammal and Toulouse (1983) presented an argument which indicates that as long as the spectral dimension d_s of a fractal is less than 4, the self-avoiding effect would never become negligible, and thus $\nu_1 \neq \nu_2 \neq \frac{1}{2}$. This argument should hold for the largest percolation cluster at p_c , the spectral dimension of which is approximately $\frac{4}{3}$ at all dimensions. Since for ordinary random walks at p_c we have (Gefen *et al* 1983) $\nu_1(d \ge 6) = \frac{1}{6}$ and $\nu_2(d \ge 6) = 0$, we conclude that for sAWS one must have $\nu_1(d \ge 6) > \frac{1}{6}$ and $\nu_2(d \ge 6) > 0$, since a sAW should always grow faster with N than an ordinary random walk does.

We now present a position-space renormalisation group (PSRG) approach to estimate ν_1 in two and three dimensions. The exponent ν_2 can probably be estimated only by Monte Carlo simulations. We choose site-disordered lattices because it enables us to use large cells without using much computer time. Each site is occupied with probability p and empty with probability (1-p). We consider a cell as percolating if a set of connected occupied sites of the cell spans the cell in a given direction. For the sAWs we use the PSRG method of Family (1980) and de Queiroz and Chaves (1980). With each step of the sAW we associate a fugacity W and consider all vertical (or horizontal, which is equivalent) spanning sAWs which start at the lower-left corner of the cell; we use standard renormalisation cells, see e.g. Sahimi and Jerauld (1983). Because the sAW can take place along a bond if and only if the two end sites of the bond are occupied, the RG transformation W' is written as

$$p'^{2}W' = \sum_{i}^{n} p'(1-p)^{n-i} \left(\sum_{m} C_{m}W^{m}\right),$$
(8)

where *n* is the total number of sites in the cell $(n = b^2)$, where *b* is the linear dimension of the cell) and C_m is the total number of sAWs of *m* steps that span the cell in the vertical (horizontal) direction if *i* sites of the cell are occupied. The two RG transformations *W'* and *p'* (the probability that a site is occupied in the renormalised cell) have unstable fixed points at $W = W^*$ and $p = p^*$. The exponent ν_1 is given by $\nu_1 = \ln \lambda / \ln b$, where $\lambda = \partial W' / \partial W$ is the eigenvalue of the linearised RG transformation (8) evaluated at p^* and W^* . A fractal dimension *D* for the sAW is defined by $D = 1/\nu_1$. A similar two-parameter PSRG method was recently used to study random walks on percolation clusters (Sahimi and Jerauld 1983) and on lattice animals (Sahimi and Jerauld 1984).

For a cell of linear dimension b = 2, we obtain

$$p' = p^4 + 4p^3q + 2p^2q^2, (9)$$

and

$$W' = (p^4 W^4 + 2p^3 W^3 + p^2 W^2) / p'^2, (10)$$

where q = 1 - p. The fixed points are $p^* = 0.61804$ and $W^* = 0.5546$, thus the fractal dimension D is found to be $D \approx 1.3279$. The global flow diagram for the coupled recursion relations (9) and (10) is shown in figure 1. Note that the flow on the critical surface is from sAW at p_c to sAW at p = 1 (denoted by pure sAW). Hence we conclude



Figure 1. Global diagram of flow vectors from (9) and (10). Arrows indicate the direction of flow, and the important fixed points are labelled.

that sAWs above p_c and on length scales much larger than ξ_p have the same critical properties as those of sAWs at p = 1. Larger cells yield the same qualitative result.

We determined the RG transformation p' and W' for cells of sizes b = 2-4 on a square lattice in closed form and for b = 5, 8 and 10 by Monte Carlo method. The results for the fractal dimension D are displayed in table 1. As in the case of sAws on fully connected lattices (de Queiroz and Chaves 1980, Family 1980, Redner and Reynolds 1981) the convergence of D to its asymptotic value $(b \rightarrow \infty)$ is slow. The results of Stauffer (1981) and Tsallis (1982) indicate that in PSRG studies the finite b results may be extrapolated to $b \rightarrow \infty$ by the following equation:

$$D(b) = D + (a_1 + a_2 b^{-\Omega D})(\ln b)^{-1},$$
(11)

where a_1 and a_2 are some constants. Here Ω is a correction-to-scaling exponent which is believed to be universal. For saws on fully connected lattices Djordjevic *et al* (1983) estimated that $\Omega \approx 0.66 \pm 0.07$ in two dimensions, but for the present problem Ω is not known. If we fit our finite cell results to equation (11), we find that $D \approx 1.281$ and $\Omega \approx 1.3$. In many previous PSRG studies (see e.g. Eschbach *et al* 1981) the finite *b* results were extrapolated to $b \rightarrow \infty$ by the following equation:

$$D(b) = D + c_1 (\ln b)^{-1} + c_2 (\ln b)^{-2},$$
(12)

Table 1. The fractal dimension D for self-avoiding walks at the site percolation threshold of a square lattice. b denotes the linear dimension of the renormalisation cell.

b	D	
2	1.3279	
3	1.3258	
4	1.3212	
5	1.3179	
8	1.3128	
10	1.3107	

where c_1 and c_2 are again some constants. From this equation we obtain $D \approx 1.285$, which is comparable to the above estimate. This fractal dimension implies that $\nu_1(d = 2) \approx 0.788$, in agreement with the inequality (4). By using this value of ν and the hyperscaling law $\alpha = 2 - \nu_1 d$, we obtain $\alpha(d = 2) \approx 1.475$, where we have used $d_t = \frac{91}{48}$ in place of d.

In three dimensions the RG transformation can be calculated in closed form only for a b = 2 cell. The results for a simple cubic lattice are $p^* \simeq 0.282$, $W^* \simeq 0.556$ and $D \simeq 1.382$. No calculations for larger cells were attempted since previous PSRG studies of sAWs on the simple cubic lattice (for p = 1) showed (Family 1981) that the convergence to asymptotic results is not monotonic. However, our estimate $D \simeq 1.382$ is only 7.8% smaller than $D \simeq 1.5$ which was estimated by Kremer (1981) by Monte Carlo simulations.

We now discuss a plausible generalisation of the Flory theory for the exponent ν_1 . Pietronero (1983) has developed a self-consistent method by which one can derive the Flory-Fisher formula (Flory 1953, Fisher 1969) for the exponent ν which is given by $\nu = 3/(2+d)$ where d is the dimensionality of the system. It is straightforward to generalise this method to fractals. The result is

$$\nu_1 = 3/(2+d_{\rm f}),\tag{13}$$

where d_f is the fractal dimension of the cluster. For the largest percolation cluster at p_c we have $d_f(d=2) = \frac{91}{48} \approx 1.896$, which then results in $\nu_1(d=2) = \frac{144}{187} \approx 0.770$. This is in excellent agreement with our estimate, $\nu_1(d=2) \approx 0.778$. In three dimensions with $d_f(d=3) \approx 2.53$ (Margolina *et al* 1982) we obtain $\nu_1(d=3) \approx 0.662$, in good agreement with Kremer's estimate and about 9.3% smaller than our b=2 cell estimate. However, since $d_f(d \ge 6) = 4$, equation (13) yields $\nu_1(d \ge 6) = \frac{1}{2}$ which is not possible because this value of ν_1 implies a diffusive random walk. Thus while equation (13) works well in low-dimensional systems, it gives poor (and unphysical) values for ν_1 at high dimensions.

One may argue that the ratio d_t/D must be an intrinsic property and thus it should depend only on the spectral dimension d_s of the fractal. Then a plausible generalisation of the Flory-Fisher formula would be

$$\nu_1 = \frac{3}{d_{\rm f}} \frac{d_{\rm s}}{2+d_{\rm s}},\tag{14}$$

which reduces to $\nu = 3/(2+d)$ for Euclidean spaces. If we take $d_s \approx \frac{4}{3}$ for $2 \le d \le 6$, equation (14) would then yield $\nu_1(d=2) \approx 0.633$ and $\nu_1(d=3) \approx 0.473$. These estimates violate the inequalities (4) and are not in good agreement with our estimate of ν_1 in two dimensions and with Kremer's estimate in three dimensions. However, for $d \ge 6$, equation (14) yields $\nu_1 = \frac{3}{10}$, a value which seems to be reasonable. In fact, we conjecture that this is an exact result. More work is necessary to assess the validity of equations (13) and (14). In table 2 we compare the predictions of equation (13) and (14).

In summary, we have studied self-avoiding walks on percolation clusters. We have proposed a scaling function representation for the mean end-to-end distance R which describes a crossover from ordinary sAWs (above the percolation threshold p_c) to sAWs on percolation clusters at or below p_c . By using a two-parameter position-space renormalisation group method we have estimated the exponent ν_1 in two and three dimensions and showed that sAWs at any p larger than p_c have the same critical

d	d_{f}	ds	D (equation (13))	D (equation (14))
2	91 48	1.321	0.778	0.633
3	2.53	1.330	0.662	0.473
4	3.06	1.316	0.593	0.389
5	3.52	1.327	0.543	0.340
6	4	4 3	$\frac{1}{2}$	$\frac{3}{10}$

Table 2. Comparison of the predictions of equations (13) and (14) for the fractal dimension D of sAWs at dimension d. d_t denotes the fractal dimension of the largest percolation cluster at the percolation threshold, and d_s is the spectral dimension of the largest percolation cluster.

properties as those of sAWs at p = 1. We have discussed two plausible generalisations of the Flory-Fisher formula for ν_1 and showed that none of them yields satisfactory results at all dimensions.

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References

Alexander S and Orbach R 1982 J. Physique Lett. 43 L625 Ben-Avraham D and Havlin S 1982 J. Phys. A: Math. Gen. 15 L691 - 1983 J. Phys. A: Math. Gen. 16 L483 Chakrabarti B K and Kertész J 1981 Z. Phys. B 44 221 Dhar D 1978 J. Math. Phys. 19 5 Djordjevic Z V, Majid I, Stanley H E and dos Santos R J 1983 J. Phys. A: Math. Gen. 16 L519 Eschbach P D, Stauffer D and Herrmann H J 1981 Phys. Rev. B 23 422 Family F 1980 J. Phys. A: Math. Gen. 13 L325 — 1981 J. Physique 42 189 Fisher M E 1969 J. Phys. Soc. Japan 26 Suppl 44 Flory P J 1953 Principles of Polymer Chemistry (Ithaca, New York: Cornell University Press) Gefen Y, Aharony A and Alexander S 1983 Phys. Rev. Lett. 50 77 Guttmann A J 1983 Preprint Harris A B 1974 J. Phys. C: Solid State Phys. 7 1671 Kapitulnik A and Deutscher G 1982 Phys. Rev. Lett. 49 1444 Kremer K 1981 Z. Phys. B 45 149 Le Guillou J C and Zinn-Justin J 1980 Phys. Rev. B 21 3976 Majid I, Djordjevic Z V and Stanley H E 1983a Phys. Rev. Lett. 51 143 - 1983b Phys. Rev. Lett. 51 1282 Margolina A, Herrmann H J and Stauffer D 1982 Phys. Lett. 93A 73 Nienhuis B 1982 Phys. Rev. Lett. 49 1062 Pandey R B and Stauffer D 1983 Phys. Rev. Lett. 51 527 Pietronero L 1983 Phys. Rev. B 27 5887 de Queiroz S L A and Chaves C M 1980 Z. Phys. B 40 99 Rammal R and Toulouse G 1983 J. Physique Lett. 44 L13 Redner S and Reynolds P J 1981 J. Phys. A: Math. Gen. 14 2679 Sahimi M 1984 Preprint Sahimi M and Jerauld G R 1983 J. Phys. C: Solid State Phys. 16 L1043 - 1984 J. Phys. A: Math. Gen. 17 L165 Stauffer D 1979 Phys. Rep. 54 1 — 1981 Phys. Lett. 83A 404 Tsallis C 1982 J. Physique Lett. 43 L471 Voss R F, Laibowitz R B and Allessandrini E I 1982 Phys. Rev. Lett. 49 1441