Possible relations for topological and transport properties of the lattice animal model of branched polymers

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Abstract. In this paper we propose that the following relations hold exactly for the lattice animal model of branched polymers. The resistivity exponent ζ_a is exactly equal to $\bar{d}_a$, the fractal dimensionality of the *backbone* of the animals. The random walk fractal dimensionality d_w is given by, $d_w = d_a + \bar{d}_a$, where d_a is the fractal dimensionality of the animals. The spectral dimension $\bar{d}_s$ of the backbone of the animals is given by, $\bar{d}_s = 1$ *at all dimensions*, i.e. the backbone is a highly decorated but essentially chain-like object. These are in contrast with earlier suggestions that one needs *two* (*three*) topological properties to obtain $\zeta_a(d_w)$. We propose that these relations may hold for *all* clusters for which loops are irrelevant and have a finite upper critical dimensionality. The implications of these results for diffusion-limited aggregates and percolation clusters are also discussed.

1. Introduction

In the past few years random processes on fractal structures have been studied with increasing interest. The most prominent and physically appealing fractal systems are perhaps the largest percolation cluster at the percolation threshold p_c, lattice animals which are a model of dilute branched polymers in a good solvent and diffusion-limited (Witten–Sander) aggregates (DLAS). In the past two years ordinary (Pólya) random walks on these random clusters have been studied by several authors. 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 of any fractal is given by $d_s = 2d_f/d_w$ (Alexander and Orbach 1982), where d_f is the fractal dimension of the cluster and d_w is the fractal dimension of the random walks on that cluster.

Very recently considerable effort has been devoted to the study of the possible relationship between static and dynamic (transport) properties of these clusters (Alexander and Orbach 1982, Rammal and Toulouse 1983, Meakin and Stanley 1983, Sahimi and Jerauld 1984, Wilke *et al* 1984, Aharony and Stauffer 1984). However at present there is no clear picture. In this paper we present and discuss several results which we hope will help to clarify some of the presently unsettled issues. In particular we present some possibly exact results for the lattice animal model of branched polymers. The implications of these results for several hypotheses that have recently been proposed are also discussed. In particular we suggest that for the percolation conductivity problem it may be more fruitful to look for a possible relation between the conductivity exponent and the *backbone* properties.

The plan of this paper is as follows. In § 2 we summarise and discuss briefly all valid hypotheses for lattice animals. Our motivation is to give the reader an account of the state of the art and the unresolved issues concerning transport processes in lattice animals. Our own results are presented in § 3. The possible implications of these results for DLAs and percolation clusters are discussed in § 4. We summarise the paper in the last section.

2. Review of transport and topological properties of lattice animals

Wilke *et al* (1984) and Sahimi and Jerauld (1984) were the first to investigate random walks on lattice animals in order to gain insight into the transport (dynamic) properties of these fractal structures. The problem was called 'the parasite problem' by Wilke *et al* (1984), following de Genne's (1976a) 'ant problem' which is the description of random walks on percolation networks of conductors and insulators. Wilke *et al* (1984) assumed that the animals can be represented by a structure similar to the nodes and links model of the backbone of percolation clusters (Skal and Shklovskii 1974, de Gennes 1976b) and, with the aid of some heuristic arguments, attempted to establish a relation between the dynamical property d_w and the static topological properties d_a and $\bar{d}_a$, where d_w is the fractal dimensionality of random walks on the animal and d_a and $\bar{d}_a$ are the fractal dimensionalities of the animal and its backbone, respectively. Monte Carlo calculations of Wilke *et al* (1984) and the renormalisation group method (Sahimi and Jerauld 1984) yielded estimates of d_w that were in rough agreement with a generalisation of the Alexander-Orbach (AO) (1982) conjecture, $d_w = 3/2d_a$.

A more accurate study of random walks on lattice animals by Havlin *et al* (1984) showed that the AO conjecture may not hold for animals at low dimensions. In addition, Havlin *et al* (1984) proposed that the exponent ζ_a, which characterises the resistance between two widely separated points on the animal, is given by

$$\zeta_a = d_a / d_c \tag{1}$$

where d_c is 'the chemical dimension' of the animal. If M is the number of sites within path length L of a given site, then d_c is defined by, $M \sim \langle L \rangle^{d_c}$, where $\langle \dots \rangle$ denotes an average over L. Extensive computer simulations of Havlin *et al* (1984) supported equation (1). Thus a relation between dynamic (ζ_a) and static (d_a and d_c) properties was established, although at the price of introducing an additional dimensionality d_c. Djordjevic *et al* (1984) pointed out that d_c can be evaluated in two different ways. One is to take an ensemble of clusters with constant M and calculate their average L, as mentioned above. A second way is to choose clusters of the same L and make the average over M. For percolation clusters at p_c both averages give the same value d_c. However, for lattice animals Djordjevic *et al* (1984) presented numerical evidence and theoretical arguments that $d_c = 1$ at all dimensions for the constant $-L$ ensemble. They also showed that the spectal dimension d_s equals unity at all dimensions for *these particular clusters*. These results are the only hypotheses that appear to be valid for lattice animals.

3. Possible relations for topological and transport properties of lattice animals

To derive our results for lattice animals, we make use of the fact that for the lattice animal model of branched polymers, one can usually neglect the presence of loops

without affecting the statistics (Lubensky and Isaacson 1978). Therefore a lattice animal on a large scale can be viewed as a branched fractal without loops. Thus the resistivity exponent ζ_a, should be equal to $\bar{d}_a$, the fractal dimension of the backbone of lattice animals

$$\zeta_a = \bar{d}_a \tag{2}$$

because when loops are not important all paths between two widely separated points have the same fractal dimension. Although this result may seem obvious at first, to our knowledge it has not been published before, but it is the key to our results discussed below. This is perhaps because the concept of the backbone has not been investigated extensively for animals (Sahimi 1985). The notion of chemical or topological dimension was instead introduced to relate ζ_a to other quantities, as discussed above. We now present numerical evidence in support of (2). Equation (2) is trivially satisfied at $d = 1$, where $\zeta_a = \bar{d}_a = 1$. Also at and above $d = 8$, the upper critical dimensionality of lattice animals (Lubensky and Isaacson 1978), one has $\zeta_a = \bar{d}_a = 2$. Further numerical evidence is provided by the work of Havlin *et al* (1984) and Sahimi (1985). If we combine equations (1) and (2) we obtain

$$d_c = d_a / \bar{d}_a. \tag{3}$$

One has (Derrida and De Seze 1982) $d_a(d = 2) \simeq 1.56$ and (Parisi and Sourlas 1981) $d_a(d = 3) = 2$. On the other hand (Sahimi 1985), $\bar{d}_a(d = 2) \simeq 1.14$ and $\bar{d}_a(d = 3) \simeq 1.39$. These together with equation (2), mean that $d_c(d = 2) \simeq 1.37$ and $d_c(d = 3) \simeq 1.44$, in good agreement with the estimates of Havlin *et al* (1984), $d_c(d = 2) \simeq 1.33 \pm 0.05$ and $d_c(d = 3) \simeq 1.45 \pm 0.05$. We also note that the percolation conductivity exponent $\hat{t}(\hat{t} = t/\nu_p$, where ν_p is the correlation length exponent) can be written as $\hat{t} = d - 2 + \hat{\zeta}_p$, where $\hat{\zeta}_p$ is the analogue of ζ_a for percolation. At and above $d = 6$, the upper critical dimensionality of percolation, loops become irrelevant for the conductivity problem and $\hat{\zeta}_p$ takes its meanfield value, i.e. $\hat{\zeta}_p(d \geq 6) = 2$. This means that as soon as loops become irrelevant for percolation, $\hat{\zeta}_p = \bar{d}_p$, where $\bar{d}_p$ is the fractal dimension of the backbone of the largest percolation cluster at p_c. However, below $d = 6$ loops are relevant and an equation similar to (2) does not hold for the percolation conductivity problem. With the aid of equation (3) and the estimates of Havlin *et al* (1984) for d_c, one can calculate $\bar{d}_a$ for $1 \leq d \leq 8$. The results are presented in table 1. It can be seen that $\bar{d}_a$ and thus ζ_a rise smoothly from their value at $d = 1$ to their mean-field value of 2 for $d \geq 8$. This monotonic dependence of $\bar{d}_a$ on d not only supports equation (3)

Table 1. Values of the fractal dimension d_u and $\bar{d}_a$ of lattice animals and their backbone, respectively, at dimension d.

d	d_a	$\bar{d}_a$
1	1	1
2	1.56	1.14
3	2	1.39
4	2.4	1.49
5	2.78	1.61
6	3.17	1.76
7	3.57	1.88
8	4	2

(since for a loopless fractal one expects ζ_a to be monotonically dependent upon d), but also is in contrast with $\bar{d}_p$, which has non-monotonic dependence on d (Harris and Lubensky 1983).

The chemical dimension d_c has been studied by Vannimenus *et al* (1984) for directed lattice animals and percolation. For directed lattice animals they have argued that $d_c = 1/\nu_{11}$, where ν_{11} is the longitudinal correlation length of the animal. If one uses the correlation length exponent of animals, $\nu_a = 1/d_a$ and the backbone of animals, $\bar{\nu}_a = 1/\bar{d}_a$ one can rewrite (2) as $d_c = \bar{\nu}_a/\nu_a$, which is similar to the result of Vannimenus *et al* (1984). (Note that unlike percolation $\nu_a \neq \bar{\nu}_a$.)

Since one can use the Einstein relation to write ζ_a as $\zeta_a = d_w - d_a$, then in view of (2) one obtains

$$d_w = d_a + \bar{d}_a. \tag{4}$$

Aharony and Stauffer (1984) presented an argument according to which, $d_w = d_a + 1$ for $d_a \leq 2$. This, together with (4), means that $\bar{d}_a = 1$, for $1 \leq d \leq 3$. This not only contradicts the data of table 1, but also means that the fractal dimension of the backbone of lattice animals remains constant in the range $1 \leq d \leq 3$, which is not possible. Thus we believe that the Aharony–Stauffer relation does not hold for lattice animals, although in view of (1) it does hold if d_a is replaced by d_c. On the other hand, one can write ζ_a as $\zeta_a = \bar{d}_w - \bar{d}_a$ (Stanley and Coniglio 1984), where $\bar{d}_w$ is the fractal dimension of the random walks on the backbone of lattice animals. Therefore, in view of equations (3) and (4), the spectral dimension $\bar{d}_s = 2\bar{d}_a/\bar{d}_w$ of the backbone of lattice animals is given by

$$\bar{d}_s = 1 \qquad \text{for all } d. \tag{5}$$

Thus, *the spectral dimension of the backbone of lattice animals is superuniversal and equals one.* This is in contrast with the spectral dimension of the backbone of percolation clusters which varies continuously (Stanley and Coniglio 1984) between $\bar{d}_s(d = 2) \simeq 1.25$ and $\bar{d}_s(d \geq 6) = 1$. Equation (4) also shows that the AO conjecture, $d_w = 3/2d_a$, does not hold for lattice animals for all $d < 8$, since this conjecture, together with (4), yields $\bar{d}_a = 1/2d_a$, which contradicts the data of table 1. Family and Coniglio (1984) pointed out that the AO conjecture cannot hold for lattice animals at $d = 2$, while Havlin *et al* (1984) presented numerical evidence against the AO conjecture for animals at low dimensions. We find the present argument somewhat more transparent and convincing since it relies on analytic results that may hold at all dimensions. The recent numerical calculations of Rammal *et al* (1984) indicate that the AO conjecture may also be an excellent approximation for percolation clusters for all $d < 6$, but not an exact result.

We point out that our result $\bar{d}_s = 1$ for the backbone of animals is not the same as that of Djordjevic *et al* (1984) mentioned above. Indeed, the fractal dimension of the *L*-constant clusters described above is not the same as $\bar{d}_a$. Here, we are presenting a result (equation (5)) without any reference to the type of ensemble or averaging process. The backbone of lattice animals arises naturally in their structure in the same way that the backbone of percolation clusters does. In this sense the backbone of lattice animals may be one of the very few fractals that have a superuniversal property.

4. Possible implications for percolation clusters and diffusion-limited aggregates

For percolation clusters one can similarly define a 'chemical distance' as follows. Suppose one arbitrarily chooses an occupied site in a percolation cluster as the reference

site. The occupied nearest neighbours of this site represent a 'shell' lying at a chemical distance $L = 1$ from the reference site. The next-nearest-neighbour sites constitute a shell at chemical distance $L = 2$, and so forth. Suppose $S(L)$ is the average of the total number of occupied sites included in a sub-cluster bounded by the Lth shell. Then (Havlin and Nossal 1984), $S(L) \sim L^{\hat{v}d_{\rm p}}$, where $d_{\rm p}$ is the fractal dimension of the largest percolation cluster at $p_{\rm c}$ and $\hat{v}$ is a universal exponent. Thus one may observe that since $\hat{v}$ is similar to $1/d_{\rm c}$ investigated above for the animals one may write

$$\hat{v} \simeq \bar{d}_{\rm p}/d_{\rm p} \tag{6}$$

which appears to be very accurate. For example at $d = 2$ one has $\bar{d}_{\rm p} \simeq 1.65$ and $d_{\rm p} = \frac{91}{48}$, and therefore (6) predicts that $\hat{v} \simeq 0.87$, in complete agreement with the numerical estimate (Havlin and Nossal 1984, Hong *et al* 1984), $\hat{v} \simeq 0.87 \pm 0.02$. One also has (Sahimi 1984b) $\bar{d}_{\rm p}(d = 3) \simeq 1.92$ and $\bar{d}_{\rm p}(d = 4) \simeq 2.10$, which together with $d_{\rm p}(d = 3) \simeq 2.53$ and $d_{\rm p}(d = 4) \simeq 3.06$, yield, $\hat{v}(d = 3) \simeq 0.76$ and $\hat{v}(d = 4) \simeq 0.68$. These are in good agreement with the estimates (Alexandrowicz 1980), $\hat{v}(d = 3) \simeq 0.74 \pm 0.02$ and $\hat{v}(d = 4) \simeq 0.64 \pm 0.04$. Equation (6) is also exact at $d = 1$ and for $d \geq 6$.

We remark that one usually writes $\hat{v}$ as $\hat{v} = d_{\rm c}/d_{\rm p}$, where here $d_{\rm c}$ is the chemical dimension of percolation clusters. In view of (6) and its accuracy one should have $d_{\rm c} \simeq \bar{d}_{\rm p}$. Indeed, recent extensive Monte Carlo calculations of Grassberger (1985a) yielded $d_{\rm c}(d = 2) \simeq 1.675$, which is close to the currently accepted value of $\bar{d}_{\rm p}(d = 2)$ mentioned above. However, $d_{\rm c}$ and $\bar{d}_{\rm p}$ cannot be equal for general dimensionality d. Recent field-theoretic calculations of Cardy and Grassberger (1985) and Janssen (1985) show that

$$\hat{v} = \tfrac{1}{2} + \tfrac{1}{24}\varepsilon + {\rm O}(\varepsilon^2) \tag{7}$$

where $\varepsilon = 6 - d$. This yields $d_{\rm c} = 2 - \frac{1}{14}\varepsilon + {\rm O}(\varepsilon^2)$, in contrast with $\bar{d}_{\rm p} = 2 + \frac{1}{21}\varepsilon + {\rm O}(\varepsilon^2)$ (Harris and Lubensky 1983). One should note that $\hat{v}$ is essentially a dynamical property and it was first used by Alexandrowicz (1980) in the definition of 'time' in his cluster growth model of percolation clusters. Equation (7) also shows that the conjecture of Havlin and Nossal (1984), $d_{\rm p} = v_{\rm p}^{-1} + \hat{v}^{-1}$, cannot be correct for general d. The fact that $\hat{v}$ does not seem to be related to the static properties of percolation clusters is another indication that the static and dynamical properties of percolation clusters (or more generally, all clusters for which loops are relevant) may not be related in a simple manner. Very recently, Margolina (1985) proposed a derivation of the Havlin–Nossal, based on the radom walk of the 'butterfly' which visits only the perimeter sites of the cluster generated by the walk.

It is widely believed that for DLAs loops are not relevant (although we are not aware of any published proof of this). Since DLAs do not have an upper critical dimensionality (Witten and Sander 1983) their fractal dimensionality $d_{\rm ws}$ diverges as $d \to \infty$. This can be understood by considering DLAs on the Cayley tree (i.e. $d = \infty$). All of the sites of the tree are occupied by the incoming particles and the screening effect is absent. Consequently, the aggregate fills the tree completely and $d_{\rm ws} = \infty$. Since there is a unique path between any two points on the tree which is also the minimum path, one has $d_{\rm c} = d_{\rm ws}$ for a Cayley tree. Therefore, (1) predicts that $\zeta_{\rm ws} = 1$ on the tree, whereas it is easily seen that $\zeta_{\rm ws} = 2$ in this limit (Family and Coniglio 1984). In fact recent computer simulations of Meakin *et al* (1984) and Sahimi *et al* (1985) suggest that $d_{\rm c} = d_{\rm ws}$ for *all* dimensionalities and thus (1) is not valid at any d because it predicts $\zeta_{\rm ws} = 1$ for all d. Since (1) was hypothesised based on the assumption that loops are irrelevant in the structure of the cluster, its breakdown for DLAs may

indicate that loops *are* relevant for these clusters. On the other hand, the breakdown of (1) for DLAS might be caused only by the fact that these clusters do not have an upper critical dimensionality. We thus propose that the results of this paper may hold for all clusters for which loops are irrelevant and *have a finite upper critical dimensionality*.

In defining the backbone of DLAS on a Cayley tree an ambiguity may arise. If the backbone is defined as the set of sites on *all* paths connecting the origin to the perimeter of the tree, then all of the sites of the tree are part of the backbone and $\bar{d}_{ws} = d_{ws} = \infty$. This means that (2) cannot hold for DLAS, consistent with our assertion that an infinite upper critical dimensionality may cause the breakdown of (2) for DLAS. This definition of the backbone is also consistent with the usual definition for the percolation clusters, since with this definition all of the sites of the network will be part of the current-carrying part of it. However, if the backbone is defined as the set of sites that connect two points on the tree by a random walk, then $\bar{d}_{ws} = d_w = 2$, which means that (2) is valid for DLAS in this limit. We believe that the first definition is the relevant one, since with this definition (1) and (2), which are hypothesised on the assumption that loops are irrelevant, do not contradict each other (they both do not hold) in the limit of the Cayley tree. The results of Sahimi *et al* (1985) also suggest that the Aharony-Stauffer relation, $d_w = 1 + d_{ws}$ may not hold for DLAS at $d = 2$, although it may be a very good approximation.

The results presented in this paper indicate that for percolation conductivity it may be more fruitful to look for a relation between the exponent t and the *backbone exponents*. Indeed, it was recently observed (Sahimi 1984a) that the relation $t \simeq 1 + \beta_B$, where β_B is the backbone exponent, is very accurate for $d_p \geqslant 2$. However, an equation similar to (4) holds for percolation clusters only for $d \geqslant 6$ and therefore the relation between t and other exponents (if it indeed exists) is probably more complicated than the results presented here.

5. Summary

In summary, we presented and discussed several relations between dynamical and static properties of lattice animal model of branched polymers. We also proposed that these relations may hold for all clusters for which loops are irrelevant and have a finite upper critical dimensionality. Our results indicate that the AO conjecture does not hold for animals at all $d < 8$, and that the Aharony-Stauffer relation also does not hold for lattice animals. We also discussed the implications of our results for diffusion-limited aggregates and percolation clusters.

Very recently, Havlin *et al* (1985) proposed that the general relation between the random walk fractal dimensionality d_w and the topological properties of clusters for which loops are irrelevant is given by

$$d_w = (d_f / d_c)(2 + d_c - d_c^s) \tag{8}$$

where d_f is the fractal dimensionality of the cluster and d_c^s is the chemical dimension of its skeleton. The skeleton of a cluster whose chemical radius is L is defined as the subcluster which contains only sites belonging to the shortest paths from a chosen site to its Lth chemical shell. This definition implies that all dead-ends, except those terminating at the Lth shell, do not belong to the skeleton. Therefore, according to equations (1) and (8) one needs two topological properties to obtain the resistivity

exponent and three properties to obtain d_w. The results presented in this paper indicate that this may not be the case and one may need only two(one) topological properties to obtain d_w (resistivity exponent), at least for the class of loopless fractals considered in this paper.

Acknowledgments

Note added in proof. Very recently Grassberger (1985b) and Edwards and Kerstein (1985) have obtained new estimates for the chemical dimension d_c of the percolation clusters. Grassberger (1985b) has obtained $d_c(d=3) \simeq 1.82 \pm 0.02$ and $d_c(d=4) \simeq 1.98 \pm 0.05$ Edwards and Kerstein (1985) have used the concept of the first-passage velocity and have obtained $d_c(d=2) \simeq 1.857 \pm 0.009$ and $d_c(d=3) \simeq 2.0 \pm 0.1$. Their estimate of $d_c(d=2)$ is very close to $d_p = \frac{91}{48} \simeq 1.896$ for the percolation clusters. This may mean that there may be a lower critical dimensionality d_l below which $d_c = d_p$ (i.e., $\hat{\nu} = 1$). A Flory approximation (Roux 1985) also predicts $d_l = 2$, in contrast with the traditional value $d_l = 1$. The numerical results of these authors also show that for $d > d_l$, the fractal dimensionalities d_c and $\bar{d}_p$ are indeed close to each other. The existence of d_l for d_c (i.e., for $\hat{\nu}$ which is essentially a dynamical property) is consistent with the hypothesis (see, e.g., Aharony and Stauffer 1984, Sahimi 1984) that there may be a lower critical dimensionality for the dynamical properties of percolation clusters. I thank Peter Grassberger and Alan Kerstein for sending me the preprints of their work prior to publication.

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