

## Relation between Dynamic Transport Properties and Static Topological Structure for the Lattice-Animal Model of Branched Polymers

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A direct connection is proposed between the “dynamic” transport properties and the “static” topological structure for branched polymers in any number  $d$  of spatial dimensions. Specifically, the resistivity exponent  $\tilde{\zeta}$  is given by  $\tilde{\zeta} = d_f/d_l$ , where  $d_f$  and  $d_l$  are the fractal and topological dimensions (the number of sites within path length  $l$  of a given site scales as  $M \sim l^{d_l}$ ). To confirm this new result, we carry out extensive exact and Monte Carlo calculations for  $d = 2, 3, 4$ , and  $8$ .

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How does one describe the structure of a large branched polymer in dilute solution? This question has long been of interest, both for its mathematical fascination and for its practical importance. To date, attention has been focused on the fractal dimension  $d_f$  which characterizes the dependence of the polymerization index  $M$  on the radius of gyration  $R$ ,  $M \sim R^{d_f}$ . Zimm and Stockmayer<sup>1</sup> found  $d_f = 4$  for the Cayley tree, which was later recognized to be exact for spatial dimensionalities  $d$  above  $d_c = 8$ .<sup>2</sup> Recently, the exact results  $d_f = 2$  [ $d = 3$ ]<sup>3</sup> and  $d_f = \frac{12}{5}$  [ $d = 4$ ]<sup>4</sup> were obtained.

These results concern the *geometrical* structure. Many physics questions, such as those involving transport, are thought to depend also on the *topological* structure—which does not enter into the factors determining  $d_f$ . However, the precise fashion in which a transport quantity depends on geometry and topology is not known. Very recently considerable effort has been devoted to the study of the possible relationship between geometric and transport properties for percolation<sup>5</sup> although at present there is no clear picture.<sup>6</sup> In this Letter we argue that there is a direct connection between “dynamic” transport properties and the “static” geometrical and topological structure of branched polymers through the simple relation

$$\tilde{\zeta} = d_f/d_l. \quad (1)$$

Here  $\tilde{\zeta}$  is a “dynamic” exponent:  $\rho \sim R^{\tilde{\zeta}}$ , where  $\rho$  is the electrical resistance between two points

separated by a distance  $R$ . On the other hand,  $d_f$  and  $d_l$  are “static” exponents:  $M \sim R^{d_f}$  is the cluster mass within a *direct* distance  $R$ , while  $M \sim l^{d_l}$  is the mass within the average “topological” or cluster-path distance  $l$ .<sup>7</sup> To obtain (1), we make use of the fact that for the lattice-animal model of branched polymers, we can neglect the presence of loops without affecting the statistics.<sup>2</sup> Therefore the resistance between two points separated by a distance of the order of  $R$  scales in the same fashion as the topological distance between these points:  $\rho \sim l \sim M^{1/d_l} \sim R^{d_f/d_l}$ , from which (1) follows.

In order to test (1), it is convenient to use  $d_w - d_f = \tilde{\zeta}$ , obtained by the Einstein relation.<sup>8,9</sup> Hence from (1) follows

$$d_w = d_f(1 + 1/d_l). \quad (2)$$

The quantity  $d_l$  has been calculated for percolation clusters<sup>7</sup> but not for lattice animals. Thus in the following we used Monte Carlo and exact enumeration methods to calculate  $d_l$  for  $d = 2, 3, 4$ , and  $8$ . We also calculated  $d_w$  for  $d = 2$  and  $3$  by exact enumeration of random walks<sup>9</sup> on large branched polymers.

*Static topological structure: Calculations of  $d_l$ .*—One first needs a method of obtaining large statistical samples. If one generates percolation clusters at a constant value of the site occupancy  $p$  ( $p < p_c$ ), then those clusters with characteristic linear dimension  $R \ll \xi(p)$  will be self-similar with fractal

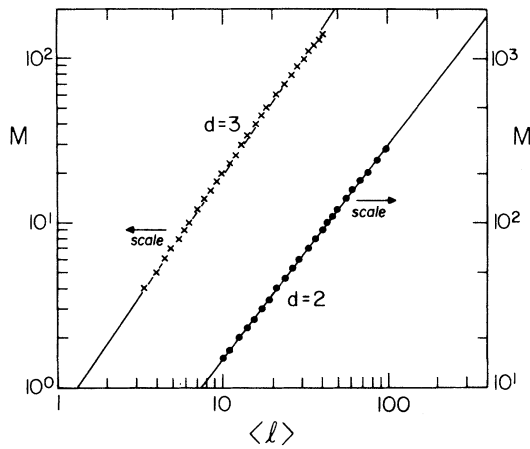


FIG. 1. The mass  $M$  as a function of the average chemical distance  $\langle l \rangle$ . The slope yields  $d_l = 1.33 \pm 0.05$  ( $d=2$ ) and  $d_l = 1.45 \pm 0.05$  ( $d=3$ ). The results were obtained from analyzing 1000 clusters of size up to 300.

dimension  $d_f$  given by percolation theory, while those with  $R \gg \xi(p)$  will have fractal dimension given by the branched polymer or "lattice-animal" model. The problem is that the probability of finding an  $M$ -site cluster with  $R > \xi(p)$  decreases exponentially with  $M$ ,<sup>10</sup> so that it has not been possible in the past to generate branched polymers directly.<sup>11</sup>

Here we use a new "direct" method which is for branched polymers what the enrichment model is for linear polymers. First we use the conventional cluster-growth method<sup>12</sup> to generate a percolation cluster of  $M_0$  sites, say  $M_0 = 20$ , using a value of  $p$  so small that the probability of obtaining a twenty-site cluster,  $\Pi$ , is typically about 0.01 (i.e., 100 trials may be necessary to succeed in growing the twenty-site cluster). After finally obtaining a cluster of size  $M_0$ , we make a fixed number  $A$  of attempts to increase it to size  $2M_0$ , where  $A$  is chosen to satisfy  $A \ll 1/\Pi$ .<sup>13</sup> If we fail, then we discard the entire cluster and return to the beginning. If we succeed, then we make  $A$  attempts to increase our cluster from size  $2M_0$  to size  $3M_0$  and so on.

Using this procedure, we typically generated lattice animals of size 300. In order to confirm that they had the structure of lattice animals, we measured the mean square radius of gyration  $R_g^2$  as a function of the number of sites; from the slope we find  $d_f = 1.55 \pm 0.05$  for  $d=2$  and  $d_f = 2.0 \pm 0.05$  for  $d=3$ , consistent with independent estimates of the fractal dimension.<sup>14</sup>

To analyze for the topological properties of the lattice animals, we choose randomly a site to call the origin. The occupied neighbors of that site

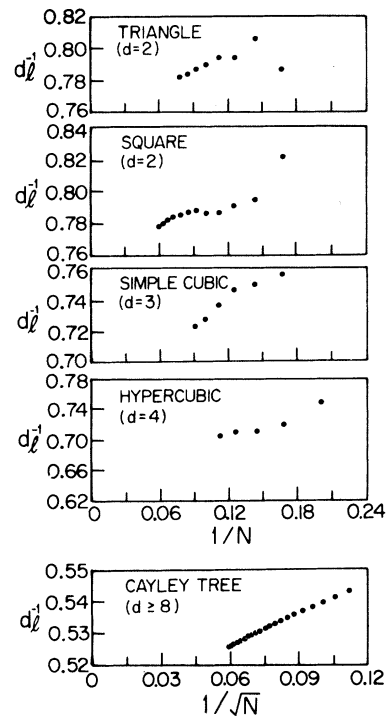


FIG. 2. Successive estimates of  $d_l$  for  $d=2, 3, 4$ , and 8 obtained from exact enumeration methods. Extrapolations of these sequences to  $M \rightarrow \infty$  yield our final estimates  $d_l = 1.33 \pm 0.02$  ( $d=2$ ),  $1.47 \pm 0.04$  ( $d=3$ ),  $1.61 \pm 0.06$  ( $d=4$ ), and  $2.00 \pm 0.01$  ( $d=8$ ).

form the first "shell"—its topological or chemical distance from the origin is 1. The next-nearest neighbors of the origin form the second shell, and  $l=2$ . The total number of sites or "mass" at a chemical distance less than or equal to  $l$  scales as  $M(l) \sim \langle l \rangle^{d_l}$  or, equivalently, the mass in shell at distance  $l$ ,  $B(l) = dM/dl \sim l^{d_l-1}$ . From Fig. 1 we see that for lattice animals the simulations yield  $d_l = 1.33 \pm 0.05$  for  $d=2$  and  $d_l = 1.45 \pm 0.05$  for  $d=3$ .<sup>15</sup>

The exponent  $d_l$  was calculated by exact

TABLE I. Summary of the values for the different exponents discussed in the text.

$d$	$d_f$	$d_l$	$d_w$	$\tilde{\zeta} = d_f/d_l$	$d_s/2 = d_f/d_w$
1	1	1	2	1	$\frac{1}{2}$
2	1.56	1.33	2.78	1.17	0.57
3	2	1.47	3.37	1.36	0.60
4	2.4	1.61	3.89	1.49	0.62
8	4	2	6	2	$\frac{2}{3}$

enumeration ("series expansions").<sup>16</sup> Here we exhaustively study each configuration of lattice animal of mass  $M$ , and for each configuration we calculate the topological distance  $l$  of each site from the "origin" in the cluster-counting algorithm. The maximum topological distances for each cluster are averaged over all configurations with the same mass. We found that successive estimates of  $d_l$  behave smoothly with increasing values of  $M$ , just as we found earlier for successive estimates of  $d_f$  obtained from calculations of the radius of gyration.<sup>14</sup> Hence we used analogous extrapolation pro-

cedures (Fig. 2) to obtain the limiting exponents, with the results  $d_l = 1.33 \pm 0.02$  ( $d = 2$ ),  $1.47 \pm 0.04$  ( $d = 3$ ), and  $1.61 \pm 0.06$  ( $d = 4$ ). These estimates, based on exact enumerations up to 18, 12, and 11 terms for  $d = 2, 3$ , and 4, agree with the Monte Carlo work for  $d = 2$  and 3. Also, for lattice animals on the Cayley tree we calculated exact results up to 300 terms and our extrapolation methods give  $d_l = 2.00 \pm 0.01$ . The Cayley tree is solved exactly by use of a recursion relation for  $T(l, M)$ , the number of lattice-animal configurations with  $l$  shells ("generations") and mass  $M$ . We find

$$T(l+1, M+1) = 2 \sum_{M'=0}^M T(l, M') T'(l, M-M') - \sum_{M'=0}^M T(l, M') T(l, M-M') + 2T(l, M), \quad (3)$$

where  $T'(l, M) = \sum_{l'=0}^l T(l', M)$ . This result stems from the fact that the trees with  $l+1$  generations and  $M+1$  sites are constructed from all possible combinations of two trees with  $l$  generations.

Table I gives our values of  $d_l$ , together with predictions of Eqs. (1) and (2) that follow from them.

*Dynamical transport properties: Calculations of  $d_w$ .*—To test (1), we now need to calculate the diffusion exponent  $d_w = d_f + \zeta$ . To this end, we have used the method of exact enumeration of random walks on clusters.<sup>9</sup> We obtained exact results for the probability  $P(r, t)$  that a random walk starting from the origin at time  $t = 0$  will be at site  $r$  at time  $t$ . We calculated this function exactly for  $t \leq 1500$ , using 1000 different lattice-animal configurations, each configuration containing at least 330 sites. From  $P(r, t)$  we can calculate any diffusion-related quantity, e.g., the mean square displacement

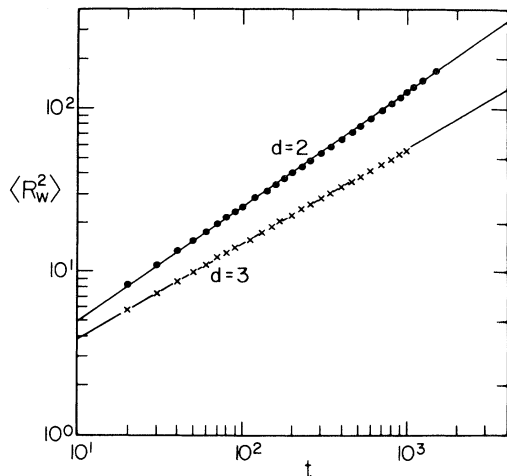


FIG. 3. The dependence on  $t$  of the mean square displacement  $\langle r^2 \rangle$ . The slopes yield  $d_w = 2.78 \pm 0.08$  ( $d = 2$ ) and  $3.37 \pm 0.10$  ( $d = 3$ ).

$\langle r^2 \rangle \sim t^{2/d_w}$ . Figure 3 shows the dependence on  $t$  of  $\langle r^2 \rangle$ , from which we find  $d_w = 2.78 \pm 0.08$  ( $d = 2$ ) and  $3.37 \pm 0.10$  ( $d = 3$ ). Both estimates agree with the prediction of Eq. (1) (cf. Table I).<sup>17</sup> From the knowledge of  $d_w$  and  $d_f$ , we can also calculate the fracton dimension  $d_s = 2d_f/d_w$  [which also equals  $2d_l/(d_l+1)$  independent of  $d_f$ ]. The results (Table I) clearly show that the Alexander-Orbach conjecture that  $d_s = \frac{4}{3}$  cannot be extended to lattice animals.<sup>18</sup>

In summary, we have found a relation, Eq. (1), between "dynamic" and "static" properties. This relation holds for any fractal structure for which loops are not relevant: branched polymers for all  $d$ , percolation clusters for  $d > 6$ , and Witten-Sander clusters (if loops are indeed irrelevant as widely believed). Our new results, Eqs. (1) and (2), are borne out by detailed numerical calculations using Monte Carlo simulations and exact enumeration methods. It is of interest to compare our results for the topological dimension of branched polymers

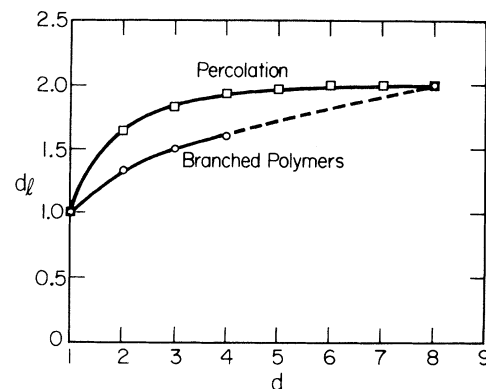


FIG. 4. Comparison of our results for  $d_l$  with results for percolation clusters taken from Ref. 7.

(BP) with other recent results for percolation clusters (Fig. 4).<sup>7</sup> For  $d \geq 8$ , both exponents are the same but the amplitudes differ, with  $A_{\text{perc}} = \frac{1}{8}$  and  $A_{\text{BP}} = \frac{1}{12}$ , where  $M \sim A l^{d_l}$ . For  $1 < d < 8$ , it appears that  $d_l^{\text{BP}} < d_l^{\text{perc}}$ , just as  $d_f^{\text{BP}} < d_f^{\text{perc}}$ .

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