

New method for growing branched polymers and large percolation clusters below p_c

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We propose a new Monte Carlo method for generating large branched polymers; it is based on enrichment of percolation clusters below p_c . We find that one must take care to distinguish two different ensemble averages: one at constant mass s and the other at constant chemical distance l . For constant s , we obtain clusters belonging to the universality class of lattice animals, while for constant l we get topologically one-dimensional structures for all d .

The structural properties of percolation clusters and lattice animals are currently a subject of intensive study.¹⁻¹³ Whereas percolation clusters are used to model gels,¹ lattice animals represent the principal model for branched polymers in dilute solutions.² For all concentrations p below the percolation threshold p_c the large clusters seem to have the critical exponents of lattice animals, i.e., of the $p \rightarrow 0$ limit. Thus we denote here as "animals" all clusters with radius much greater than correlation length ξ .¹ Since the probability of generating such a cluster using Monte Carlo methods is very small¹ (decays exponentially with size) there has not been much study of their structure compared to percolation.^{3-7,10}

Here, we propose a new method for generating statistical ensembles of large lattice animals ("branched polymers").³ The method is analogous to the enrichment method⁸ successfully used to generate self-avoiding walks ("linear polymers").⁹

METHOD

First we use the conventional cluster growth method¹⁰ to generate a percolation cluster of s_0 sites, say $s_0 = 20$, using a value of p so small that the probability of obtaining a 20-site cluster π is typically about 0.01 (i.e., 100 trials may be necessary to succeed in growing the 20-site cluster). After finally obtaining a cluster of size s_0 , we make a fixed number A of attempts to increase it to size $2s_0$, where A is chosen to satisfy $A \ll 1/\pi$.^{8,9} If we "fail" (i.e., the cluster terminates for all A attempts), then we discard the *entire* cluster and return to the beginning. If we succeed, then we make A new attempts to increase our cluster from size $2s_0$ to size $3s_0$ and so on. Being interested in "universal" quantities only we did not make the difficult extrapolation $p \rightarrow 0$, since already at finite p animal exponents are expected.

RESULTS

Using this procedure, we typically generated lattice animals of size 300 on a square lattice with $p = 0.4$ and $p = 0.22$ for a cubic lattice. In order to confirm that they had the critical exponents of lattice animals, we measured the mean-square radius of gyration R_g^2 as a function of the number of sites (Fig. 1); 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.¹¹ We found that different values of s_0 and p give the same values of d_f if we maintain the condition $A\pi \ll 1$.

In general, a cluster is characterized not only by its geometric structure (parametrized by the fractal dimension d_f) but also by its topological structure (parametrized, for example, by the chemical dimension d_t).¹² First we define the chemical distance l as follows.¹² We choose a site to call the origin. The occupied neighbors of this site form the first "shell"; its chemical distance l from the origin is one. The next-nearest neighbors of the origin form the second shell with $l = 2$ and so on. The total number of sites or "mass" at a chemical distance less than or equal to l scales as

$$s(l) \sim l^{d_t} . \quad (1)$$

There are two possible ways to form the ensemble averages in order to calculate d_t . One is to take an ensemble of clusters with constant s and calculate their average l : $s(l) \sim \langle l \rangle_s^{d_t}$. A second way to choose clusters of the same l and make the average over s : $\langle s \rangle_l \sim l^{d_t}$. For percolation clusters at p_c , both averages give the same value for d_t .¹² However, for $p < p_c$ and large clusters, the two averages yield completely different results. For the constant s en-

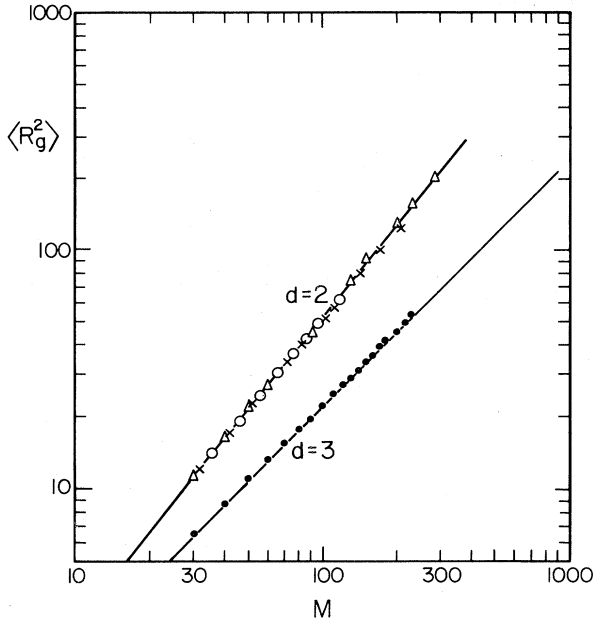


FIG. 1. Dependence on the cluster mass s of the mean-square radius of gyration $\langle R_g^2 \rangle$. Points represent averages over 1000 large branched polymers on square and simple cubic lattices. The slope of the double-logarithmic corresponds to $d_f = 1.55 \pm 0.05$ [$d=2$] and $d_f = 2.0 \pm 0.05$ [$d=3$]. Three different values of s_0 were used for $d=2$ in order to test that the fractals were independent of s_0 , $s_0 = 15(\Delta)$, $20(O)$, and $30(\times)$.

semble one gets the lattice animal statistics with d_l varying from $d_l = 1.33$ for $d=2$ to $d_l = 2$ for $d=8$.¹³ However, for the constant- l ensemble, one obtains a new universality class: *chemically one-dimensional* branched polymer ensembles with $d_l = 1$ for all d . Numerical evidence will be given in the following as well as a theoretical interpretation. In Fig. 2 we plot the average mass s as a function of the chemical distance l for $d=2$ and $d=3$. The linearity of these plots suggests strongly that

$$\langle s \rangle \sim l . \quad (2)$$

Before we proceed, we present exact results for the Cayley tree of coordination number $\sigma + 1$, which describes¹ the critical exponents above $d_c = 8$. The distribution of $s(l)$ conditioned on the number of sites in shell l positive (so that the tree does not terminate at an earlier generation) is given for $p < p_c = 1/\sigma$ and $l \gg 1$ by¹⁴

$$\begin{aligned} Pr[s(l) = l(1-p)/(1-\sigma p)] &\leq v(Hl)^{1/2} \\ &= (2\pi)^{-1} \int_{-\infty}^v \exp(-u^2/2) du , \quad (3a) \end{aligned}$$

where $H = (\sigma - 1)p(1 + p - 2\sigma p^2)/(1 - \sigma p)^3$. Hence, the conditional expectation value of $s(l)$ is, for $l \gg 1$,

$$\langle s(l) \rangle \sim (1-p)/(1-\sigma p) l . \quad (3b)$$

Thus the percolation clusters with $l \gg 1$ shells at $p < p_c$ are chemically one dimensional in contrast to the result $d_l = 2$ for percolation clusters for $p = p_c$ on the same Cayley tree lattice and the same type of average.¹²

Fractal dimensions used thus far in statistical physics have been found to be nondecreasing functions of d ; indeed, it is

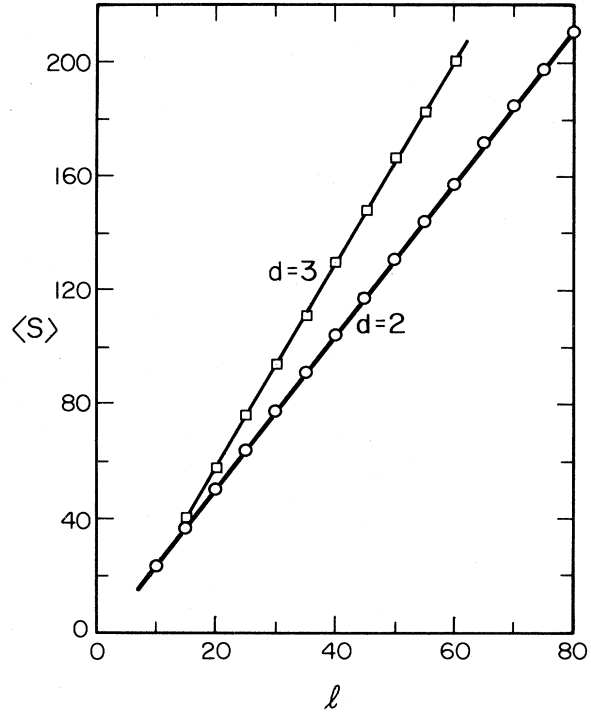


FIG. 2. Linear plot of the average of cluster mass $\langle s \rangle$ vs the chemical distance l . The fact that the data fall on straight lines suggests that $d_l = 1$ for both $d=2$ and $d=3$.

hard to imagine how increasing d could serve to decrease a fractal dimension. Thus, from the results $d_l = 1$ for $d = 1, 2, 3$ and for $d \geq 8$, we can argue that $d_l = 1$ for all d and all p below p_c .

DISCUSSION

In order to understand the difference between the constant- l ensemble and the constant- s ensemble, we study the two different averages carefully. For the constant s ensemble, the average chemical distance is given by

$$\langle l \rangle_s = \frac{\sum_{l,t} A_{st} l_{st} s p^s (1-p)^t}{\sum_{l,t} A_{st} s p^s (1-p)^t} , \quad (4)$$

where A_{st} and l_{st} are the number of configurations and the chemical distance of a cluster with s cluster sites and t perimeter sites. For $p \rightarrow 0$ Eq. (4) yields

$$\langle l \rangle_s = \frac{\sum_{l,t} A_{st} l_{st}}{\sum_{l,t} A_{st}} , \quad (5a)$$

which represents the animal average.¹ For the constant- l ensemble, the average mass s is given by

$$\langle s \rangle_l = \frac{\sum_{s,t} A_{st} s^2 p^s (1-p)^t}{\sum_{s,t} A_{st} s p^s (1-p)^t} . \quad (5b)$$

In this case, for $p \rightarrow 0$ because of the factor p^s , the dominant configurations will be those with the minimum s . The minimum s for a given l is simply $s \sim l$, so we obtain $\langle s \rangle \sim l$ for all dimensions.

The result $d_l = 1$ has implications for transport, for which topological concepts are physically relevant. We shall see that in the constant- l ensemble the fracton or spectral

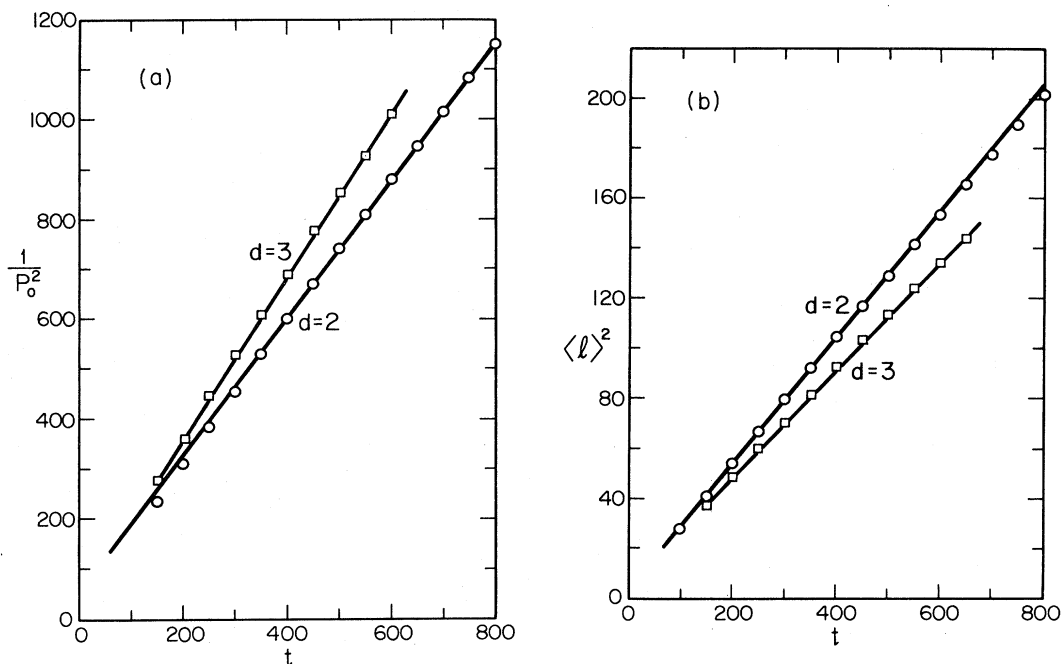


FIG. 3. Results of exact enumeration of random walks on lattice animals using $s_0=20$; similar results were found for other values of s_0 . (a) Linear plot of P_0^{-2} vs t , where P_0 is the probability of returning to the origin at time t ; (b) linear plot of $\langle l \rangle^2$ vs t , where $\langle l \rangle$ is the average chemical distance. The linearity supports the result of (6) that $d_s=1$ and $d_w=2$.

dimension $d_s = 2d_f/d_w = 1$ for all $d \geq 1$. We begin by noting that the chemical diffusion exponent d_w^l , defined through $t \sim l^{d_w^l}$, must satisfy the inequality $d_w^l \geq 2$, since $d_w^l = 2$ for a Euclidean lattice. Thus, the number of distinct sites visited by the random walk $s(t)$ scales as $s(t) \sim t^{1/d_w^l}$. But $s(t) \sim t^{d_s/2}$, and $d_s \geq 1$ for any connected fractal. Hence the only way that we can simultaneously satisfy $d_w^l \geq 2$ and $d_s \geq 1$ is to have

$$d_w^l = 2, \tag{6a}$$

and

$$d_s = 2d_f/d_w = 1. \tag{6b}$$

To test (6) by direct simulation, we have used the method of exact enumeration of random walks on fractal structures.¹⁵ In this fashion we have obtained the exact statistics for 1000 different clusters each containing at least $l=150$ shells.¹⁶ Results for the probability of a random walk being at the origin at time t are shown in Fig. 3(a), and results for the average chemical distance $\langle l \rangle$ are shown in Fig. 3(b). For the high degree of linearity of both plots we conclude that the corresponding values of d_s and d_w^l agree with the predictions of Eqs. (6b) and (6a). We also calcu-

lated the mean-square displacement $\langle R^2 \rangle$ for $d=2,3$ and the corresponding values of d_w agree with the prediction of (6b) that $d_w = 2d_f$. For an arbitrary fractal, the conductivity exponent $\tilde{\mu}$ can be related to d_f and d_w by¹⁷ $\tilde{\mu} = (d_w - d_f) + (d - 2)$. From Eq. (6b) follows a direct relation between the conductivity and the fractal dimensionality for these topologically one-dimensional clusters, $\tilde{\mu} = d_f + (d - 2)$.

In summary, we have developed a new Monte Carlo method for generating large percolation clusters below p_c . The method produces clusters in the universality class of lattice animals for the constant- s ensemble. For the constant- l ensemble, we find clusters that are topologically linear. We argue that the fracton dimension $d_s = 1$ for these topologically one-dimensional cluster and confirm this result numerically.

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