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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 $p \to 0$ 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 small[1] (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 method[8] successfully used to generate self-avoiding walks ("linear polymers").[9]

METHOD

First we use the conventional cluster growth method[10] 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 $p \to 0$, 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_l).[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

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

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

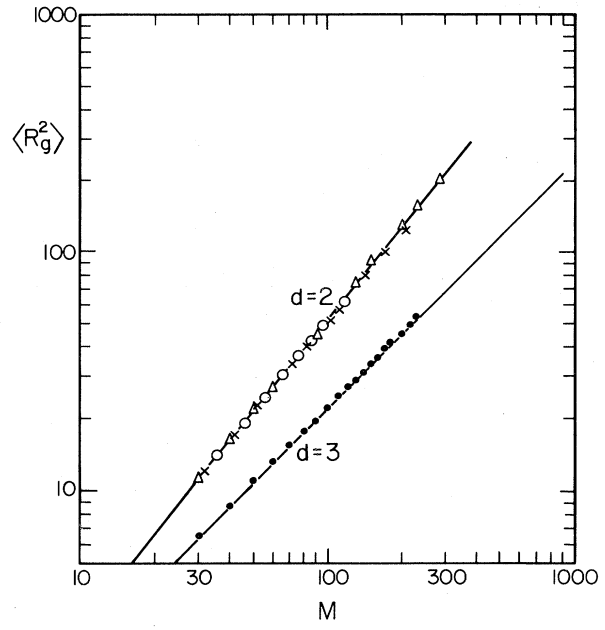

FIG. 1. Dependence on the cluster mass s of the mean-square radius of gyration $\langle R_g^2 \rangle$. Points represent averages over 1000 large branched polymers on square and simple cubic lattices. The slope of the double-logarithmic corresponds to $d_f = 1.55 \pm 0.05$ [$d=2$] and $d_f = 2.0 \pm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

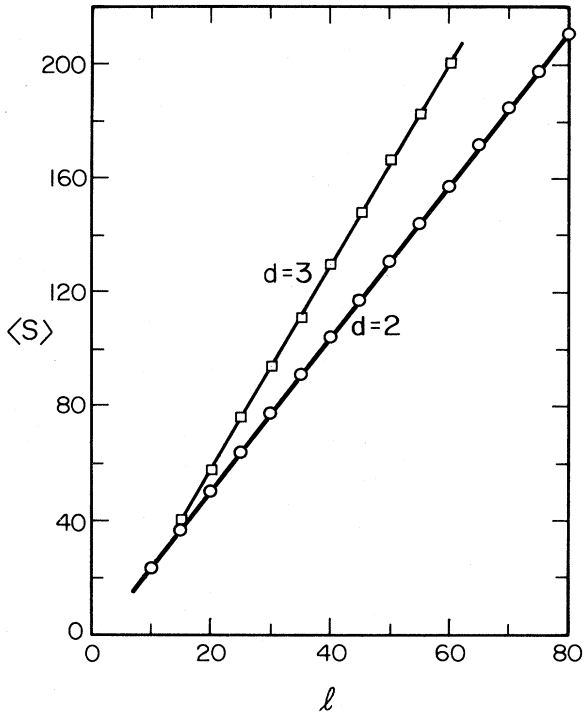

FIG. 2. Linear plot of the average of cluster mass $\langle s \rangle$ vs the chemical distance l. The fact that the data fall on straight lines suggests that $d_l = 1$ for both $d=2$ and $d=3$.

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

$$\langle s \rangle \sim l \ . \tag{2}$$

Before we proceed, we present exact results for the Cayley tree of coordination number $\sigma+1$, which describes[1] 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 $l \gg 1$ by[14]

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

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 $l \gg 1$,

$$\langle s(l) \rangle \sim (1-p)/(1-\sigma p)\, l \ . \tag{3b}$$

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 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

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

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 $p \to 0$ Eq. (4) yields

$$\langle l \rangle_s = \sum_{l,t} A_{st} l_{st} \Big/ \sum_{l,t} A_{st} \ , \tag{5a}$$

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

$$\langle s \rangle_l = \sum_{s,t} A_{st}^l s^2 p^s (1-p)^t \Big/ \sum_{s,t} A_{st}^l s p^s (1-p)^t \ . \tag{5b}$$

In this case, for $p \to 0$ 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

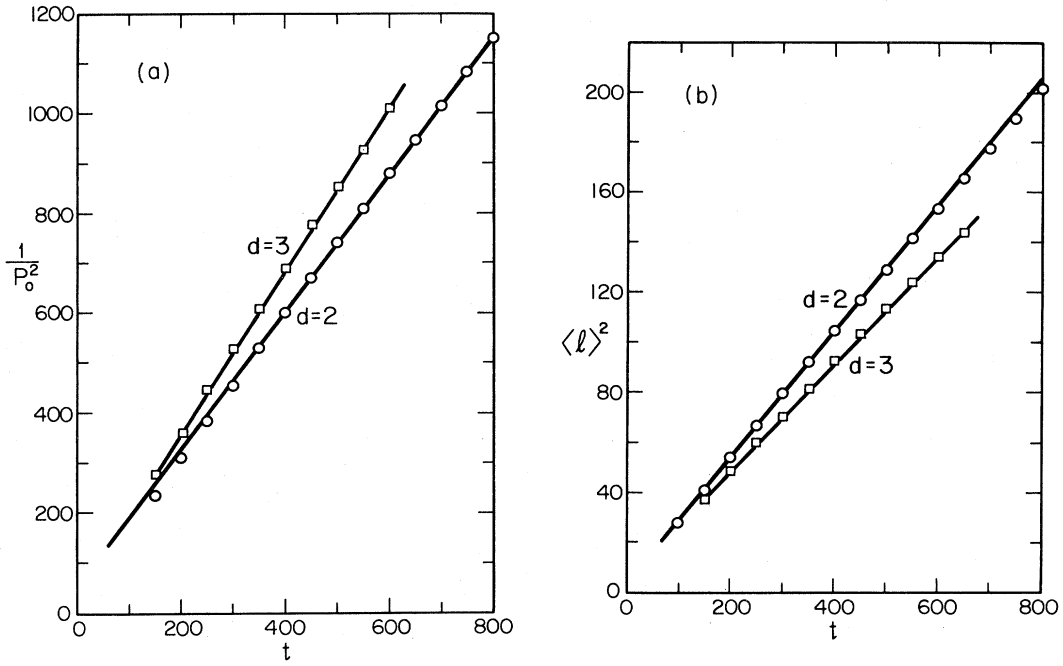

FIG. 3. Results of exact enumeration of random walks on lattice animals using $s_0 = 20$; similar results were found for other values of s_0. (a) Linear plot of P_0^{-2} vs t, where P_0 is the probability of returning to the origin at time t; (b) linear plot of $\langle l \rangle^2$ vs t, where $\langle l \rangle$ 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 calculated 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 by[17] $\tilde{\mu} = (d_w - d_f) + (d-2)$. 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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[1] D. Stauffer, Phys. Rep. **54**, 1 (1979); J. W. Essam, Rep. Prog. Phys. **43**, 733 (1980); D. Stauffer, A. Coniglio, and M. Adam, Adv. Poly. Sci. **44**, 103 (1982); H. E. Stanley and A. Coniglio, in *Percolation Clusters and Structures,* edited by J. Adler, G. Deutscher, and R. Zallen [Ann. Israel Phys. Soc. **5**, 181 (1983)].

[2] B. H. Zimm and W. H. Stockmayer, J. Chem. Phys. **17**, 1301 (1949); T. C. Lubensky and J. Isaacson, Phys. Rev. Lett. **41**, 829 (1978).

[3]D. Stauffer has proposed an "indirect" method of simulating large branched polymers [see, e.g., H. P. Peters, D. Stauffer, H. P. Hölters, and K. Loewenich, Z. Phys. B **34**, 399 (1979)].

[4]S. Wilke, Y. Gefen, V. Ilkovic, A. Aharony, and D. Stauffer, J. Phys. A **17**, 647 (1984); M. Sahimi and G. R. Jerauld, *ibid.* **17**, L165 (1984).

[5]D. Stauffer, Phys. Rev. Lett. **41**, 1333 (1978); H. J. Herrmann, Z. Phys. B **32**, 335 (1979).

[6]C. Domb, J. Phys. A **9**, L141 (1976); J. A. M. S. Duarte, Z. Phys. B **33**, 97 (1979).

[7]H. Gould and K. Holl, J. Phys. A **14**, L443 (1981).

[8]F. T. Wall, S. Windwer, and P. J. Gans, Methods Comput. Phys. **1**, 217 (1963).

[9]See, e.g., S. Havlin and D. Ben-Avraham, Phys. Rev. A **27**, 2759 (1983); C. Brender, D. Ben-Avraham, and S. Havlin, J. Stat. Phys. **31**, 661 (1983).

[10]P. L. Leath, Phys. Rev. Lett. **37**, 940 (1976).

[11]G. Parisi and G. Sourlas, Phys. Rev. Lett. **46**, 871 (1981); A. Margolina, F. Family, and V. Privman, Z. Phys. (to be published); I. Majid and H. E. Stanley (unpublished).

[12]S. Havlin and R. Nossal, J. Phys. A **17**, L427 (1984); see also the early work of R. Pike and H. E. Stanley, *ibid.* **14**, L169 (1981) for $d=2$ only (where d_l is denoted ψ_{13}); D. C. Hong and H. E. Stanley, *ibid.* **16**, L475 (1983); **16**, L525 (1983) for all d (where d_l is denoted $d_f/d_{\min}$); and see the recent calculations of J. Vannimenus, J-P. Nadal, and C. Martin, *ibid.* (to be published); and H. J. Herrmann (unpublished) (where d_l is denoted $\hat{d}$).

[13]S. Havlin, Z. Djordjevic, I. Majid, H. E. Stanley, and G. H. Weiss, Phys. Rev. Lett. (to be published).

[14]G. Pakes, Adv. Appl. Prob. **3**, 176 (1971).

[15]D. Ben-Avraham and S. Havlin, J. Phys. A **15**, L691 (1982); I. Majid, D. Ben-Avraham, S. Havlin, and H. E. Stanley, Phys. Rev. B (to be published); D. C. Hong, S. Havlin, H. J. Herrmann, and H. E. Stanley (unpublished).

[16]Clusters used had typically 300 sites, which is a smaller size than used for many percolation studies. The reason such relatively small clusters are sufficient is that we work in a constant-l ensemble, with $l_{\max}=150$ typically. We found that changing $l_{\max}$ from 100 to 170 had *no effect* on the quantities calculated.

[17]S. Alexander and R. Orbach, J. Phys. (Paris) Lett. **43**, L625 (1982).