Journal of Statistical Physics, Vol. 54, Nos. 3/4, 1989

Flory Approximant for Self-Avoiding Walks on Fractals

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Received September 2, 1988

A Flory approximant for the exponent describing the end-to-end distance of a self-avoiding walk (SAW) on fractals is derived. The approximant involves the fractal dimensionalities of the backbone and of the minimal path, and the exponent describing the resistance of the fractal. The approximant yields values which are very close to those available from exact and numerical calculations.

KEY WORDS: Flory approximant; self-avoiding walks; fractals; percolation; random walks; lattice animals.

The statistics of self-avoiding walks (SAWs) has been the subject of much interest for a long time.[1,2] These are relevant to the behavior of single polymer chains in good solvents. The mean square end-to-end distance of a chain of N monomers scales (for large N) as $\langle R^2 \rangle \sim N^{2\nu}$, and the universal exponent ν depends only on a few characteristics of the space on which the walk is embedded.

On Eucledean d-dimensional spaces, ν depends only on d. An excellent (although not exact) estimate for ν, in $d \leqslant 4$, is given by the Flory formula,[1,2]

$$\nu = 3/(2+d) \tag{1}$$

In the present paper we present a new Flory formula, to describe SAWs on fractal structures. It has been known since 1980 that critical phenomena depend crucially on various fractal characteristics of the underlying structure.[3] It has since become clear that in addition to the

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0022-4715/89/0200-1091$06.00/0

fractal dimensionality D,[4] physics on fractals depends on many other dimensionalities,[5] including the fractal dimensionality of the backbone D_B, that of the minimal (or chemical) path $d_{\min}$,[6] etc. It has also become clear that regular random walks on fractals have an anomalous fractal dimensionality d_w,[7] and that the spectrum of vibrational excitations on fractals is characterized by the fracton dimensionality $\bar{d} = 2D/d_w$.[8,9]

In view of this plenitude of dimensionalities, it became a challenge to find a modified Flory formula for SAWs on fractals. It was already noted by Dhar[10] that the fractal dimensionality D may not be sufficient to characterize ν. However, Kremer[11] found that if one replaces d by D in Eq. (1), then the expression

$$\nu = 3/(2+D) \tag{2}$$

is in good agreement with Monte Carlo simulations of walks on percolation clusters at the threshold. Equation (2) also agreed with real space renormalization group results.[12]

The expression (2) was criticized by Rammal *et al.*,[13] who argued that since the SAW moves only on the backbone (or else it would be trapped on a dangling end), ν should depend only on properties of the *backbone* (and not on D). Rammal *et al.* derived the modified expression

$$\nu = \frac{1}{D_B} \frac{2+\alpha}{1+(2\alpha/\bar{d}_B)} = \frac{2+\alpha}{D_B + d_{w,B}\alpha} \tag{3}$$

where $d_{w,B}$ is the fractal dimensionality of random walks on the backbone, $\bar{d}_B = 2D_B/d_{w,B}$, and α is a random walk exponent discussed below. Arbitrarily ("for simplicity") they chose to use $\alpha = 1$ (in their notation, $z = 2/\bar{d}_B$) and found

$$\nu = \frac{1}{D_B} \frac{3\bar{d}_B}{\bar{d}_B + 2} = \frac{3}{d_{w,B} + D_B} \tag{4}$$

Equation (4) gave unsatisfactory agreement with exact fractals, and Rammal *et al.* concluded with doubts on the existence of a general Flory approximation which retains both simplicity and accuracy.

Recently Havlin and Ben Avraham (HBA)[14] gave an alternate discussion leading to Eq. (3) and made a suggestion which amounted to setting

$$\alpha = \frac{1}{d_{w,B}^{\min} - 1} \tag{5}$$

where $d_{w,B}^{\min} = d_{w,B}/d_{\min}$ is the fractal dimension of random walks on the

backbone measured in a chemical, or minimum, distance metric. HBA showed that the choice (5) gave satisfactory results for ν in several cases. However, as explained below, their arguments involved several arbitrary steps whose justification was not clear. The purpose of this paper is to present a complete physical justification for (3) and (5). In particular, our discussion explains the difference between the Pythagorean and the chemical metrics, in terms of "annealed" and "quenched" averages.

In the "standard" derivation of the Flory formula, one writes the free energy as the sum of energetic and entropic terms, both depending on R and on N,[13]

$$F = a(N^2/R^{D_B}) + b(R^{d_{w,B}}/N)^{\alpha} \tag{6}$$

Minimization with respect to R yields Eq. (3). In the potential energy part, R^{D_B} represents the number of sites on the backbone, within radius R, in which the SAW might self-interact. The entropic part arises from the probability of a regular random walker to reach a distance R after N steps on the backbone, $P(R, N)$. The function $P(R, N)$ has been the subject of several recent publications. Since the dependence on R is expected to arise via the scaled variable $(R^{d_{w,B}}/N)$, and since for large R one expects an exponential decay, it is reasonable to expect that

$$P(R, N) \sim \exp[-b(R^{d_{w,B}}/N)^{\alpha}] \tag{7}$$

which indeed yields the form (6). The exponent α is in fact defined via Eq. (7). The value of α has been the subject of some confusion: O'Shaughnessy and Procaccia[15] guessed that $\alpha = 1$, and Havlin *et al.*[14,16] proposed (based on some exact fractals) that $\alpha = 1/(d_{w,B} - 1)$.[17] Although the value $\alpha = 1$ chosen by Rammal *et al.*[13] agrees with that of ref. 15, we have recently shown[18] that it is wrong. In fact, the value of α depends on the type of *averaging* used. If one considers only *typical* walks, which is equivalent to averaging of $\ln P(R, N)$, then[18]

$$\alpha = d_{\min}/(d_{w,B} - d_{\min}) \tag{8}$$

On the other hand, averaging of $P(R, N)$ over all possible starting points and local geometries, including very rare ones, yields[18]

$$\alpha = 1/(d_{w,B} - 1) \tag{9}$$

It was argued in ref. 18 that for averages over finite few samples, α may turn out to be between these two limits.

In the present case, the free energy (6) contains the entropy, i.e., $-\ln P(R, N)$. Simulations over different samples yield different values of

the free energy, or of the sizes of the SAWs, and these are then averaged. This is similar to the "quenched" average appropriate for thermodynamic properties of random systems, in which the free energy is to be averaged, and distinct from the "annealed" case, when the random variables move on the time scale of the experiment and must be included in the distribution (or partition) function itself, i.e., $P(R, N)$. It therefore follows from ref. 18 that we should use Eq. (8) for α. Using also $d_{w,B} = D_B + \tilde{\zeta}_R$,[5,7] where $\tilde{\zeta}_R$ describes the scaling of the resistance between two points on the fractal, Eq. (3) yields

$$\nu = \frac{2D_B + 2\tilde{\zeta}_R - d_{\min}}{d_{\min}\tilde{\zeta}_R + D_B{}^2 + D_B\tilde{\zeta}_R} \tag{10}$$

It is interesting to note that Eq. (8) is equivalent to Eq. (5), proposed by HBA, in view of the relation $d_{w,B}^{\min} = d_{w,B}/d_{\min}$. However, their discussion seemed to require measuring distances in a chemical distance metric. In their formulation (in our notation) one uses the relation $l \sim R^{d_{\min}}$ to write (6) in terms of l:

$$F \sim a(N/l^{D_B/d_{\min}}) + b(l^{d_{w,B}^{\min}}/N)^{\alpha_{\min}} \tag{11}$$

where $\alpha_{\min}$ is the corresponding exponent when $P(R, N)$ is likewise expressed in terms of l:

$$P(l, N) \sim \exp[-a(l^{d_{w,B}^{\min}}/N)^{\alpha_{\min}}] \tag{12}$$

It might seem, then, that here one has the equivalent question, i.e., what is the correct value of $\alpha_{\min}$? However, HBA argue that $\alpha_{\min} \sim (d_{w,B}^{\min} - 1)^{-1}$, a result which is rigorously derived in ref. 18. Their argument thus seems to sidestep the question of what value of α one should use. However, in the HBA argument the role of the chemical distance metric is unclear. As they say, one can use either normal or chemical metrics. "The chemical space is used [to agree with the] exact results of percolation in $d = 1$ and $d = 6$. The Flory approximation, using normal Pythagorean space, fails in these cases." We disagree with the statement concerning Pythagorean space. We believe one can work in *any* metric, providing the proper value of α is used. In particular, in Pythagorean space, α should be set by Eq. (8), according to our argument concerning quenched averages. The reason the HBA formulation works in chemical space is that only in chemical space do the quenched and annealed averages become identical. Using Eq. (8) yields Eq. (10) in *all* metrics.

We now discuss the implications of Eq. (10). Whenever loops are irrelevant, the backbone, the minimal path, and the resistance all scale the

same way, i.e., $D_B = \zeta_R = d_{\min}$. In this case, Eq. (10) yields $\nu = 1/D_B$, as expected (since there is practically only one SAW, which also scales like the minimal path). In this case, we have $\alpha = 1$ and our result coincides with that of Rammal *et al.*, Eq. (4). One case to which this applies is percolation for $d > 6$, where we recover $\nu = 1/2$, as expected. Another case of interest concerns lattice animals.[12] Using measured values of ζ_R from ref. 19, we find $\nu = 1$, 0.85, 0.74, 0.67, and 0.5 for lattice animals in $d = 1$, 2, 3, 4, and 8 dimensions. The value at $d = 2$ is not far from that of real space renormalization group estimate,[12] $\nu \simeq 0.80$. It is interesting to note that Kremer's formula, Eq. (2), yields $\nu = 1$, 0.84, 0.75, 0.68, and 0.5, very close to our values of $1/D_B$. This suggests the new approximate relation $D_B \simeq (D+2)/3$ between the fractal dimensionalities of the full cluster and its backbone for lattice animals. This approximation agrees with the data for $\zeta_R = D_B$ and D of ref. 19 to within their error bars. For animals the Flory formula[20] $D = (2d+4)/5$ gives exact results for $d = 3$, 4, and 8. We therefore suggest the Flory-like approximant for $2 \leqslant d \leqslant 8$:

$$D_B = (2d+14)/15 \tag{13}$$

The situation becomes more complicated for fractals with loops. In his pioneering work, Dhar[10] solved exactly the SAW problem on the Sierpinski gaskets in 2 and 3 dimensions. The two-dimensional results were then extended, by Elezović *et al.*,[21] to a family of generalized gaskets, containing $b(b+1)/2$ triangles in a large triangle of linear size b. For $b = 2$, 3,..., 8 they found $\nu = 0.7986$, 0.7936, 0.7884, 0.7840, 0.7803, 0.7772, and 0.7744. Our Eq. (10) yields $\nu = 0.8249$, 0.8137, 0.8065, 0.8014, 0.7976, 0.7946, and 0.7921, all within 3% from the exact values. This is to be contrasted with Rammal *et al.*'s[13] approximant, Eq. (4), which yields $\nu = 0.7679$, 0.7584, 0.7525, 0.7485, 0.7455, 0.7432, and 0.7413, whose deviations from the exact results are about twice those of our Eq. (10). Kremer's approximant, Eq. (2), typically overestimates the exact results by about 4%. Similar comparisons apply to the branching Koch curve.[13] In contrast, Rammal *et al.*'s value, $\nu = 0.654$, is closer to the exact result for the three-dimensional gasket, $\nu = 0.674$,[10] than our approximant, $\nu = 0.725$.

Finally, we consider SAWs on the infinite percolation cluster at the percolation threshold. Table I lists values of D, as collected in ref. 22, of D_B, as collected in ref. 23, and of ζ_R and $d_{\min}$, based on series evaluations from ref. 24. Typical errors in these numbers are a few percent. The resulting estimates of Eq. (10) are practically indistinguishable from available literature values. They are also in excellent agreement with new series values for SAWs on percolation clusters.[26] The value $\nu = 0.66$ in

Table I. Estimates for the Flory Approximant for the SAW Exponent ν on Percolation Clusters[a]

					ν			
d	D	D_B	ζ_R	$d_{\min}$	Eq. (2)	Eq. (4)	Eq. (10)	Other
2	91/48	1.62	0.99	1.13	0.77	0.71	0.76	0.77,[12] 0.66[25]
3	2.5	1.83	1.31	1.36	0.67	0.60	0.65	0.67[11]
4	3.2	1.94	1.59	1.62	0.58	0.55	0.58	—
$\geqslant 6$	4	2	2	2	1/2	1/2	1/2	—

[a] Equations (2), (4), and (10) represent the approximants of Kremer,[11] Rammal *et al.*,[13] and the present work, respectively.

$d=2$, from ref. 25, is probably too low because the algorithm used only walks which connect two fixed terminals, at a fixed end-to-end distance. Again, Eq. (10) gives a much more satisfactory approximant than Rammal *et al.*'s approximant, Eq. (4). We note again the closeness of the values from Eqs. (2) and (10), which may imply a useful approximate numerical relation between D, D_B, ζ_R, and $d_{\min}$. Specifically, this approximate relation implies that

$$\frac{3}{2+D}=\frac{2D_B+2\zeta_R-d_{\min}}{d_{\min}\zeta_R+D_B{}^2+D_B\zeta_R} \tag{14}$$

In conclusion, we have shown that the correct theory for regular random walks also yields a good Flory approximant for SAW on fractals. As anticipated by Rammal *et al.*[13], this Flory approximant is not very simple, and it involves three geometrical dimensionalities, D_B, ζ_R, and $d_{\min}$. It would be interesting to compare our new approximant with much more accurate Monte Carlo or exact enumeration calculations.

After concluding this work, we received a preprint by J. P. Bouchaud and A. Georges (ENS, Paris), who obtain the same approximant as our Eq. (10) using a different statistical approach.

ACKNOWLEDGMENTS

This work started during the visit of A. A. at the University of Oslo, where discussions with J. Feder are gratefully acknowledged. Work at Tel Aviv was supported by grants from the U.S.–Israel Binational Science Foundation and from the Israel Academy of Sciences and Humanities. Work at the University of Pennsylvania was supported by the National Science Foundation under grant DMR 85-20272.

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Communicated by D. Stauffer.