Numerical test of Flory formulas for true self-avoiding walks on fractal lattices

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We review the Flory-type formulas for true self-avoiding walks (TSAW's) on fractal substrates proposed by Rammal [J. Stat. Phys. **36**, 547 (1984)] and by Bouchaud and Georges [Phys. Rev. B **39**, 2846 (1989)] and present a formula obtained by simple Flory approximation. We also present the Monte Carlo data for TSAW's on a Sierpinski gasket embedded in both two and three dimensions and on a percolation backbone at the percolation threshold in two dimensions. The previous data on an infinite percolation cluster and our present data suggest that all known formulas describe fairly well the critical behavior of TSAW's on fractals; however, that by Bouchaud and Georges and our formula show better agreement.

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In recent years, there has been considerable interest in the statistics of long-range correlated random walks on fractal lattices. Prototypical examples of such models are the self-avoiding walks (SAW's) [1] and the "true" self-avoiding walks (TSAW's) [2] on random and geometrical fractals. Physical realizations of these models were described in the statistics of linear-chain polymers in the solution confined in a porous medium (or with quenched impurities). The SAW has been widely used as a theoretical model of linear-chain polymers in dilute solution [1], while the TSAW was found to describe the statistics of linear polymers in an extremely polydispersed solution with a broad distribution of chain sizes [3].

Various methods such as field-theoretical calculations, cell renormalizations, and simple Flory approximations were employed to manifest the critical behavior of the mean end-to-end distances [4–6], and a number of Flory formulas were proposed based on various approximations [6–9], with attention being paid primarily to SAW's. For TSAW's, a relatively limited number of Flory formulas were derived in the course of studies for SAW's. Until now, however, numerical tests on these approximations have not been very successful. For SAW's, the exact results for the Flory exponent ν were found on finitely ramified fractals such as the Sierpinski gasket in two and three dimensions [8,10]. Monte Carlo simulations were also carried out on random fractal lattices, i.e., on an infinite percolation cluster at the percolation threshold, and the results have been very controversial [11–14]. For TSAW's, on the other hand, no exact results are available yet and, in addition, only a few works have attempted to estimate the exponent ν. To our knowledge, Monte Carlo simulations on a Sierpinski gasket [15] and on infinite percolation clusters [16], both in two dimensions, are the only such works reported so far. Under these circumstances, it is thus difficult to determine which approximation is the most appropriate to describe the critical behavior of such long-range correlated random walks on fractal lattices.

In this paper, we focus on the Flory formulas for TSAW's on fractals. We summarize the previously proposed Flory formulas and present a formula obtained from our own approximation. We also present the computer simulation results and, based upon our data and the previously reported ones, we closely examine these formulas.

The TSAW is a kinetic process in which the probability $p_{j\to i}$ of moving from site j to its nearest-neighbor site i depends on the number of previous visits n_i on the site i by

$$p_{j\to i}=e^{-gn_i}\Big/\sum_k e^{-gn_k}\ , \tag{1}$$

where the sum in the normalization factor runs over all nearest-neighbor sites of j and the parameter g defines the strength of self-avoidance; the extreme limit of $g=0$ corresponds to ordinary random walks (RW's). For any $g<0$, a TSAW tends to be attracted to the previously visited sites, and the mean end-to-end distances were found to yield an apparent saturation, as the number of steps N increases [17]. The most interesting case is for $g>0$, where the excluded-volume effect of a TSAW is known to be different from that of a SAW even for the case of $g=\infty$ [2].

The main quantity of interest is the Flory exponent ν, defined by the mean-square end-to-end distances of N-step walks, $R_N^2\sim N^{2\nu}$. On a d-dimensional Euclidean lattice, ν depends only on the lattice dimensionality d. Excellent estimates for ν are given by the simple Flory formulas [3,18,19]

$$\nu_{\rm SAW}=3/(d+2) \tag{2}$$

and

$$\nu_{\rm TSAW}=2/(d+2)\ , \tag{3}$$

for SAW and TSAW, respectively. On fractal lattices, on the other hand, ν is known to depend on various fractal characteristics of the underlying structure. Rammal, Toulouse, and Vannimenus [8] argued that the quantity $\nu d_{f,B}$ for SAW's on fractals should be invariant and depend on the intrinsic properties of *backbone* because a

SAW moves only on the backbone, or else it would be trapped on a dangling end. They derived the expression

$$\nu_{\mathrm{SAW}}^{R}=\frac{d_{s,B}}{d_{f,B}}\frac{3}{d_{s,B}+2}\ , \tag{4}$$

where $d_{f,B}$ and $d_{s,B}$ are the fractal and spectral dimensions of the backbone of underlying fractals. Along the same line of thinking, Rammal [9] obtained for TSAW's,

$$\nu_{\mathrm{TSAW}}^{R}=\frac{d_s}{d_f}\frac{2}{d_s+2}\ . \tag{5}$$

It should be noted that the fractal and spectral dimensions d_f and d_s of the underlying structure of fractal (not a backbone) are used for TSAW's since TSAW's can never be trapped. A numerical test of Eq. (4) was unsatisfactory for exact fractals, and Rammal, Toulouse, and Vannimenus concluded that the properties of SAW's depend on other intrinsic aspects of the fractal [8].

On the other hand, Bouchaud and Georges derived the Flory formulas for long-range correlated-walk problems from the fully statistical grounds [6]. They obtained the leading mean end-to-end distances from the sums of correlated random variables. Applying to SAW's and TSAW's on fractal substrates, they obtained

$$\nu_{\mathrm{SAW}}^{\mathrm{BG}}=\frac{4\hat{d}_B-d_{s,B}}{d_{f,B}(2+2\hat{d}_B-d_{s,B})} \tag{6}$$

and

$$\nu_{\mathrm{TSAW}}^{\mathrm{BG}}=\frac{2\hat{d}}{d_f(2+2\hat{d}-d_s)}\ , \tag{7}$$

where $\hat{d}$ is the spreading dimension, often called the topological exponent, and is related with the fractal dimension d_f and the chemical dimension $d_{\min}$ by $\hat{d}=d_f/d_{\min}$ [20].

Recently, Eq. (6) was also obtained by different approximations. Aharony and Harris showed that the free energy of SAW's can be written as [7]

$$F=a\frac{N^2}{R^{d_f}}+b\left[\frac{R}{R_0}\right]^x\ , \tag{8}$$

where R_0 is the mean end-to-end distance of the uncorrelated RW's and scales as $R_0^{d_w}\sim N$, d_w being a fractal dimension of RW's, and $x=\alpha d_w$ with their notation of α. If one chooses $x=d_w=2d_{f,B}/d_{s,B}$ and minimizes Eq. (8) with respect to R, one would obtain Eq. (4). Aharony and Harris, however, claimed that

$$x=\frac{d_w d_{\min}}{d_w-d_{\min}} \tag{9}$$

should be used and they obtained the same result as Eq. (6). For TSAW's, the repulsive part of the free energy can be written, following Family and Daoud [3], as $F_{\mathrm{rep}}\sim N/R^{d_f}$ and one subsequently obtains Eqs. (5) and (7) by the same methods as for SAW's.

The parameter x stems from the distribution of mean end-to-end distances after N steps, $P(R,N)$, given as

$$P(R,N)\propto\exp[-b(R/R_0)^x]\ , \tag{10}$$

with x being some positive number whose values are to be determined depending on the models. It seems reasonable to assume that x depends on the step-size distribution of the walks [21]. For example, for a long-range distribution such as the Levy distribution $p(r)\propto r^{-1-\mu}$ for $1<\mu<2$, $x=\mu$ should be chosen. On the other hand, for a short-range distribution, i.e., $\mu\geq 2$, x should be 2. If we choose x in a similar way on fractal lattices as well, i.e., $x=2$, we will obtain new formulas for both SAW's and TSAW's:

$$\nu_{\mathrm{SAW}}=\frac{2d_{f,B}+d_{s,B}}{d_{f,B}(d_{f,B}+2)} \tag{11}$$

and

$$\nu_{\mathrm{TSAW}}=\frac{d_f+d_s}{d_f(d_f+2)}\ . \tag{12}$$

These simple formulas, although the derivations are trivial, were not reported previously insofar as we are aware. For $d_f=d_s=d$ on Euclidean lattices, both reduce to the usual Flory formulas, as expected. They, however, do not satisfy the requirement claimed by Rammal, Toulouse, and Vannimenus [8] that νd_f should depend upon only the intrinsic exponents, such as d_s and $\hat{d}$. In addition, the choice $x=2$ has not been proven rigorously. Despite these drawbacks, that of a TSAW shows the best agreement with the numerical data for random fractals, i.e., on percolation clusters, as we will see later.

The known exact results for SAW's on a Sierpinski gasket enable us to test the validity of the approximations. For the family of a Sierpinski gasket, the three characteristic dimensions are known exactly [8]:

$$d_{f,B}=\hat{d}_B=\ln(d+1)/\ln 2$$

and

$$d_{s,B}=2\ln(d+1)/\ln(d+3)\ .$$

Using $d_{f,B}=\hat{d}_B\simeq 1.585$ and $d_{s,B}\simeq 1.365$ for $d=2$, one obtains $\nu_{\mathrm{SAW}}^{R}\simeq 0.768$ and $\nu_{\mathrm{SAW}}^{\mathrm{BG}}\simeq 0.825$ for Eqs. (4) and (6), respectively. These values are 3–4 % deviated from the known exact result $\nu_{\mathrm{SAW}}^{\mathrm{exact}}=0.7986\ldots$ [8,10]. On the other hand, Eq. (11) gives $\nu_{\mathrm{SAW}}\simeq 0.7981$, which is amazingly close to the exact result. For TSAW's, Eqs. (5) and (7) produce, respectively, $\nu_{\mathrm{TSAW}}^{R}\simeq 0.512$ and $\nu_{\mathrm{TSAW}}^{\mathrm{BG}}\simeq 0.526$, whereas Monte Carlo data yielded $\nu_{\mathrm{TSAW}}^{\mathrm{MC}}=0.510\pm 0.005$ [15]. Equation (12), on the other hand, suggests $\nu_{\mathrm{TSAW}}\simeq 0.519$. On infinite percolation clusters in two dimensions, the best known values are $d_f=\frac{91}{48}$, $\hat{d}\simeq 1.66$, and $d_s\simeq 1.32$ [22], and thus, the previous two formulas predict $\nu_{\mathrm{TSAW}}^{R}\simeq 0.419$ and $\nu_{\mathrm{TSAW}}^{\mathrm{BG}}\simeq 0.438$, while Monte Carlo data yielded $\nu_{\mathrm{TSAW}}^{\mathrm{MC}}=0.432\pm 0.005$ [16]. Equation (12), on the other hand, predicts $\nu_{\mathrm{TSAW}}\simeq 0.435$.

Based upon these results, one can see that the Flory formulas for TSAW's seem to show reasonably good agreement with the Monte Carlo data for all approximations discussed before. For the Sierpinski gasket, the for-

mula by Rammal appears to show the best agreement, whereas for infinite percolation clusters, that by Bouchaud and Georges and Eq. (12) show better agreement. These seem to suggest that the agreement with Monte Carlo data might be fortuitous.

In order to see if the agreement is indeed accidental, we have carried out extensive Monte Carlo simulations on Sierpinski gaskets embedded in two and three dimensions and on a percolation backbone in two dimensions. Our data on the 2D gasket were found to be consistent with those of the previous work; however, the exponent ν was estimated slightly larger than the previous one. All data on the gaskets and on percolation backbone were found to be in excellent agreement with the latter two approximations, rather than with that by Rammal, as we will see below.

Angles d'Auriac and Rammal [15] have carried out Monte Carlo simulations for TSAW's on a 2D Sierpinski gasket. They have estimated the Flory exponent from the double logarithmic plot of the mean-square end-to-end distances R_N^2 against the number of steps N. Recently, however, Lee and Lee [16] pointed out that a TSAW exhibits relatively large corrections depending on the excluded-volume parameter g. For $g \gg 1$, since the walk tends to avoid the previously visited sites, a TSAW behaves like a SAW for the first several steps. For $g \ll 1$, on the other hand, the strength of self-avoidance is negligible unless n_i is very large, and thus, a TSAW is similar to a RW for small N. Since the TSAW for any $g > 0$ is expected to exhibit the same critical behavior according to the universality, both extreme cases of g ($g \gg 1$ and $g \ll 1$) should cross over to the same critical behavior as $N \to \infty$. Apparently, this kind of saturation results in the slow convergence behavior for large and small g values, and therefore, it would be difficult to estimate ν accurately from the plot of R_N^2 against N. This is our motivation to repeat the same simulation on a 2D gasket in the present work.

In order to estimate accurately the critical exponent ν, we have calculated the "effective" exponent ν_N measured up to N steps, defined as usual [12,13], by

$$\nu_N = NR_N^2 \Big/ \left[2\int_0^N R_n^2 dn \right] - \frac{1}{2} \tag{13}$$

and

$$\nu_N = \frac{1}{2(N-M)} \left[N \ln R_N^2 - M \ln R_M^2 - \int_M^N \ln R_n^2 dn \right] . \tag{14}$$

Since $R_N^2 \propto N^{2\nu}$, both definitions must yield the same value of ν as $N \to \infty$. For any finite N, however, the two appear to exhibit slightly different values for each N. In general, the former shows larger fluctuations which might be due to the integral in the denominator, and we therefore present the results for the latter. Our estimates for ν, however, were obtained considering both results.

Our Monte Carlo method for a TSAW on a Sierpinski gasket is basically similar to that by Angles d'Auriac and Rammal [15]. The gasket was generated up to the ninth order of iteration, a total of 29 526 sites (seventh order of iteration, 32 770 sites for 3D), and the periodic boundaries were employed as shown in Fig. 1. Walks are started from the randomly selected sites in the triangle ABC and, when the walk exits the cell through either the site B or C, then it has been assumed to reenter through the site A. When the walk exits via the site A, it has always been assumed to reenter through the site C. This type of periodic boundary condition requires additional attention if the spanning length of the walk is larger than the edge of the cell, for the same boundary condition is no longer valid for further stages of the gasket. In order to avoid such a complexity, we have measured the spanning distance of each walk along edge of the gasket and found that no such walks were sampled in our simulation for N up to 5000 steps.

We have carried out Monte Carlo simulations for a TSAW on a 2D gasket, for various values of g, $g = 0$, 0.01, 0.1, 0.2, 0.3, 0.5, and 1.0. Plotted in Fig. 2 are the effective exponent ν_N against $1/N$, averaged over 5×10^4 walks to some 10^5 walks. (Note that we have plotted some selected data to avoid congestion in the large N region). The open circles are the mean-square radii of gyration and the closed circles the mean-square end-to-end distances. For $g = 0$, i.e., for ordinary RW's, data converge on the exactly known value of

$$\nu_{\mathrm{RW}}^{\mathrm{exact}} = d_{s,B}/2d_{f,B} \simeq 0.431 .$$

For any $g > 0$, although plots show bumps presumably caused by lattice anisotropy, all data appear to converge on the same point on the ordinate, indicating that the TSAW for any $g > 0$ exhibits the same critical behavior. Estimated from the plot is

$$\nu_{\mathrm{TSAW}}^{\mathrm{MC}} = 0.531 \pm 0.005 ,$$

which is about 4% larger than the previous estimate [15]. This new result of ν is rather close to the prediction by Eq. (7) and also to that of Eq. (12), in contrast to the earlier result. We note that our data are of much higher statistics than the previous work. One possible source of

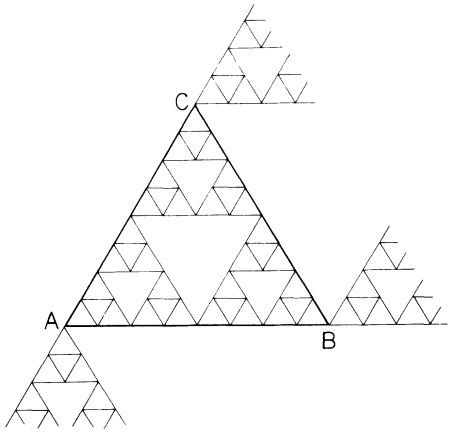

FIG. 1. The periodic boundaries of Sierpinski gasket used in the simulation. If the TSAW exits through either site B or C, it has been assumed to reenter through site A along the same direction as it exits.

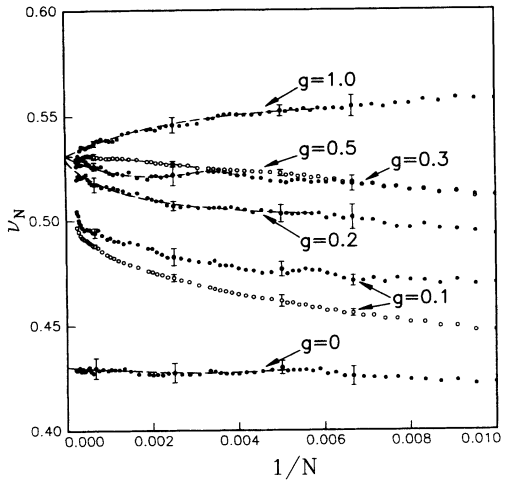

FIG. 2. The effective exponent ν_N against $1/N$ for a TSAW on a 2D Sierpinski gasket. The closed circles are for the mean-square end-to-end distance and the open circles for the radius of gyration. The errors were calculated from 4–6 batches, each of which was averaged over 10^4 walks.

underestimation we can conceive of is the apparent neglect of all corrections in the R_N^2 in the earlier work.

Shown in Fig. 3 are the data on a 3D gasket, averaged over 10^5 walks. For $g=0$, simple extrapolation of the plot yields $\nu_{\mathrm{RW}}^{\mathrm{MC}}=0.386\pm0.003$, which is consistent with

$$\nu_{\mathrm{RW}}^{\mathrm{exact}}=d_{s,B}/2d_{f,B}=0.3868\ldots .$$

For other values of g, $g=0.2$, 0.3, 0.5, and 1.0, all data appear to converge on the same value on the ordinate, as expected. Estimated from the plot is

$$\nu_{\mathrm{TSAW}}^{\mathrm{MC}}=0.450\pm0.005 .$$

This value is amazingly close to the prediction by Eq. (7) and is also close to that of Eq. (12), but appears to be slightly larger than Eq. (5) predicts. In all cases, however, the deviations are within 4%.

We have also carried out Monte Carlo simulations for TSAW's on a percolation backbone in two dimensions. Our method of obtaining backbone is similar to that described recently by Woo and Lee [23] developed for SAW's, while that of sampling for TSAW's is similar to that by Lee and Lee [16] employed for TSAW's on infinite percolation clusters. The percolation backbone was generated on a 400×400 square lattice at p_c, $p_c=0.592\,745$ [24].

Plotted in Fig. 4 are the ν_N for various values of g. For $g=0$, ν_N appears to approach $\nu_{\mathrm{RW}}\simeq0.381$ as $N\to\infty$. Since $d_{f,B}$ and $d_{s,B}$ are known to vary depending on method of measurement [20], the theoretically predicted value of $\nu_{\mathrm{RW}}=d_{s,B}/2d_{f,B}$ is in the range 0.37–0.39. Although our present estimate is slightly larger than the previously reported value [25] it is still within this range.

For relatively large values of g, such as $g=\infty$ and 1.0, the ν_N decrease for both end-to-end distance and radius of gyration. A simple eyeball fit indicates that the exponent ν is slightly smaller than the full lattice value, 0.5. For $g=0.2$ and 0.3, plots for ν_N are nearly linear for sufficiently large N and appear to converge on the slightly different values on the ordinate. This might be due to the slow convergence behavior of TSAW's on the backbone, compared to other cases. The TSAW on the backbone is less likely to exhibit its characteristic features of making loops and immediate backsteps for relatively small N because all dangling ends are eliminated. We thus believe that ν_N would eventually converge on the same value as $N\to\infty$ for all $g>0$. Such a signal is indeed seen for smaller g values. For $g=0.1$, the plot for ν_N shows a marked deviation from that of RW's and appears to exhibit a clear upturn for large N. Considering the data for $g=0.2$ and 0.3, we estimate

$$\nu=0.490\pm0.005 .$$

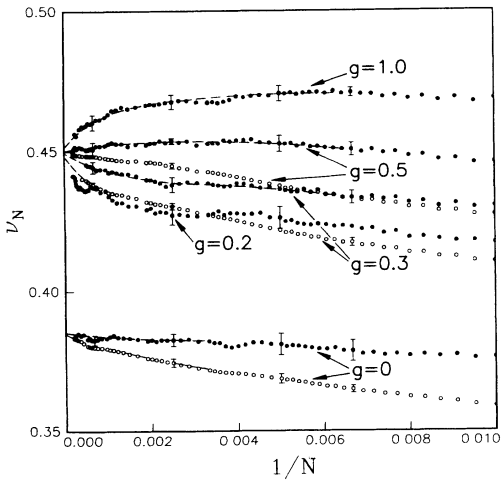

FIG. 3. The effective exponent ν_N against $1/N$ for a TSAW on a 3D Sierpinski gasket. The closed circles are for the mean-square end-to-end distance and the open circles for the radius of gyration. The errors were calculated from 5–6 batches, each of which was averaged over 2×10^4 walks.

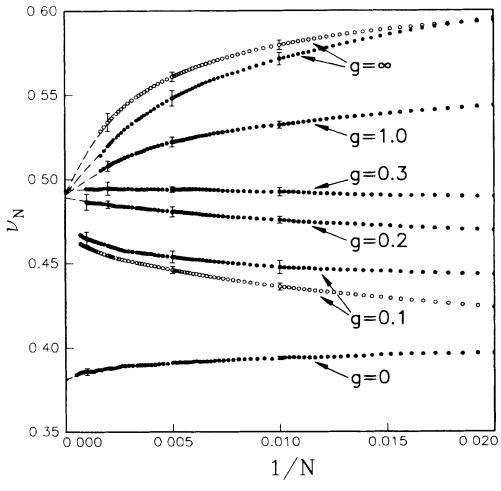

FIG. 4. The effective exponent ν_N against $1/N$ for a TSAW on percolation backbone for $p=0.592\,745$. The closed circles are for the mean-square end-to-end distance and the open circles for the radius of gyration. The errors were calculated from five batches, each of which was averaged over four clusters.

TABLE I. Summary of predictions from various Flory formulas for SAW's and TSAW's in comparison with the known numerical data.

	Sierpinski gasket		2D infinite	2D	3D infinite	3D
	2D	3D	Cluster	Backbone	Cluster	Backbone
$d_f, d_{f,B}$	1.585	2	1.896[a]	1.61[b]	2.51[a]	1.74[b]
$\hat{d}, \hat{d}_B$	1.585	2	1.66[c]	1.44[d]	1.83[c]	1.26[b]
$d_s, d_{s,B}$	1.365	1.547	1.32[c]	1.25[c]	1.33[b]	1.23[e]
ν_{SAW}^{R}	0.768	0.654		0.72		0.66
ν_{TSAW}^{R}	0.512	0.436	0.419	0.478	0.318	0.438
ν_{SAW}^{BG}	0.825	0.725		0.77		0.67
ν_{TSAW}^{BG}	0.526	0.449	0.438	0.493	0.337	0.44
Eq. (11)	0.7981	0.693		0.77		0.72
Eq. (12)	0.519	0.443	0.435	0.492	0.339	0.456
Exact or MC						
ν_{SAW}	0.7986	0.674		0.77		
ν_{TSAW}	0.531	0.450	0.432	0.490	0.34(?)	

[a]Data from Ref. [26].
[b]Data from Ref. [20].
[c]Data from Ref. [22].
[d]Data from Ref. [25].
[e]From $d_s = 2d_f/d_w$ and numerical data from Ref. [20].

Our method of estimating ν appears to be somewhat crude in the sense that we obtained it by taking an average of linear fits for $g = 0.2$ and 0.3, rather than finding a true asymptotic value for all g values. However, taking a close look at the data, one can see that the rate of increase in ν_N for $g = 0.3$ decreases slowly, while that for $g = 0.2$ increases. Thus the true value of ν is expected to lie between these two sets of data, and we believe that our estimate is accurate within the error quoted. The value of ν agrees fairly with all three Flory formulas within statistical errors, but appears to show the best agreement with the prediction by Eq. (12). The results are summarized in Table I, together with the predictions for SAW's.

In summary, we have reviewed the Flory-type formulas for TSAW's on fractals obtained from various approximations and presented a formula from our own Flory approximation. We have also presented simulation data for TSAW's on a Sierpinski gasket in both two and three dimensions and on a percolation backbone in two dimensions. The previous data on an infinite percolation cluster at p_c and our present data suggested that all existing formulas describe fairly well the critical behavior of TSAW's on fractals; however, Eq. (12) and that by Bouchaud and Georges show much better agreement. For geometrical fractals, the formula by Bouchaud and Georges yielded the best agreement and, for random fractals, i.e., for percolation clusters at p_c, Eq. (12) was just as good as that of Bouchaud and Georges. Our preliminary calculation on a simple cubic lattice supports similar results. Monte Carlo data obtained for $p = 0.312$ ($p_c \simeq 0.3117$; cf. Ref. [27]) and $g = 0.1$ appear to show the asymptotic value of ν_N about 0.34, which is again close to the prediction by Eq. (12). (For three dimensions, since the fractal dimension of infinite cluster is larger than the upper marginal dimension of a TSAW, there might be additional complexities, however. The full results shall be published elsewhere).

For SAW's, we have seen that our formula predicted ν amazingly close to the exact results for a 2D Sierpinski gasket, while those from the other two approximations deviated appreciably. For an infinite percolation cluster in two dimensions at p_c, the formula by Rammal, Toulouse, and Vannimenus [8] predicts ν smaller than the full-lattice value, strictly disagreeing with the recent analytical argument by Lyklema and Kremer [28]. On the other hand, that by Bouchaud and Georges and Eq. (11) predict ν about 0.77. This value is close to the cell renormalization result with finite-size effects taken into account [4] and is also close to the recent Monte Carlo data for SAW's on a percolation backbone [23]. For higher dimensions, such as three and four dimensions, the situation become less satisfactory. Equation (11) predicts the exponent ν much larger than that by Bouchaud and Georges. While the latter suggests $\nu = 0.67$ and 0.58 for $d = 3$ and 4, respectively, Eq. (11) yields 0.72 and 0.66, which are just too large to be accepted. On the other hand, recent estimates are about 0.65 (Ref. [29]) and 0.57 (Ref. [30]) for two and three dimensions, respectively. These suggest that the agreements of Eq. (11) with the known results in low dimensions might be accidental.

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