Flory approximants and self-avoiding walks on critical percolation clusters

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Using the results of a recent Monte Carlo simulation and analytical studies on self-avoiding walks (SAW's) on critical percolation clusters (CPC's), the various Flory-type formulas for SAW's on fractals and disordered media are examined. The probability density formulas for a random walker on the fractals that are needed to derive the various Flory approximants are also discussed. We also try to resolve some controversial problems in the recent studies on SAW's on CPC's from a most plausible Flory approximant.

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I. INTRODUCTION

Even though many numerical and analytical studies [1–15] on self-avoiding walks (SAW's) on the randomly diluted lattice at percolation threshold ($p=p_c$) or on the lattice near p_c have recently been made the controversies surrounding this problem are still far from resolution. To be specific let us discuss numerical controversies first. The main interest in these studies is the critical exponent ν', which is defined through the relation

$$\langle R^2\rangle_N \approx N^{2\nu'} , \tag{1}$$

where $\langle R^2\rangle_N$ is the quenched average of mean-square end-to-end distances of N-step SAW's on percolation clusters at the percolation threshold ($p=p_c$) or when the correlation length of percolation $\xi_p^2 \gg \langle R^2\rangle_N$. The numerical simulation study on ν' done by Kremer [1] claimed that in three dimensions the critical index ν' of SAW's on the percolation clusters at p_c is close to $\frac{2}{3}$ and is greater than that on nonrandom lattices. But the recent Monte Carlo simulation [2] on two and three-dimensional lattices suggested that ν' of SAW's is very close to the critical index ν of SAW's on the lattice with no disorder. (From now on ν stands for the critical index for SAW's on the lattice with no disorder, whereas ν' stands for the critical index for SAW's on the percolation clusters.) In contrast Lam [3] argued from his exact enumeration study of SAW's on the two-dimensional square lattice that $\nu'\approx 0.81$, which is quite larger than $\nu=\frac{3}{4}$. But Lee and Nakanishi [2,4] recently have rebutted both Kremer's work and Lam's work on the ground that there were some mistakes in both numerical works and have also argued that $\nu'\approx\nu$ in two and three dimensions. We think the argument by Lee and Nakanishi [2,4] is quite correct and we believe that the numerical value of ν' is very close to ν. Subsequent discussions are therefore based on $\nu'\approx\nu$ is the legitimate numerical clue to understanding the critical behavior of SAW's on percolation clusters.

One traditional way to calculate numerical values for ν' is to use the Flory-type approximant for SAW's. Prior to applying the Flory formulas to SAW's on disordered structure, let us discuss some physics in the Flory formula. On the d-dimensional lattices with no disorder, the Flory formula [16] for ν for $d\le 4$ is

$$\nu=\frac{3}{d+2} , \tag{2}$$

which is an excellent estimate for ν. To derive the formula for SAW's on fractals or the disordered structure, one should write the free energy F of N-step SAW's as the sum of energetic terms and entropic terms [17] as

$$F=a\frac{N^2}{R^{d_f}}+[-\ln P(R,N)] , \tag{3}$$

where R is the distance that a SAW reaches after N steps, d_f is the fractal dimension of the fractal, and $P(R,N)$ is the probability of a random walker to reach a distance R after N steps on the fractal. The function $P(R,N)$ has been the subject of several recent publications [17–19]. In general $P(R,N)$ for large R is an exponential function as

$$P(R,N)\approx\exp[-b(R^{d_w}/N)^{\alpha}] , \tag{4}$$

where d_w is the fractal dimension of random walks (RW's) on the fractal. In recent literature [17–20], several different forms for α are suggested. Minimization of F in Eq. (3) with respect to R gives the modified Flory formula for SAW's on the fractals. Therefore, for each different α there corresponds a Flory formula. To compare recent numerical data of SAW's on the percolation-cluster fractal to the Flory formulas with various types of α is thus one way to determine which form for $P(R,N)$ is the most suitable for random walks on the percolation-cluster fractal. Even though this kind of method was attempted by Aharony and Harris [17], it was only done in comparison to the data of Kremer [1], without noticing the recent Monte Carlo data [2] and the data from the exact enumeration techniques [3,4]. It is therefore the first motivation of this paper to compare the various Flory formulas to the recent numerical data for determining which form of α is the most plausible, as suggested by Aharony and Harris in Ref. [17] with the statement that "It would be interesting to compare our new approxi-

new approximant with much more accurate Monte Carlo or exact enumeration calculations."

Another motivation for considering the numerical approximants to SAW's on disordered structure is how one can interpret physically and analytically the coincidence of $\nu' \approx \nu$ as in our previous discussion of numerical studies about ν'. The direct interpretation, which we think is rather naive, is that SAW's on the percolation clusters at $p = p_c$ belong to the same universality class as that of SAW's on nonrandom lattices. Another possibility is that the universality class of SAW's at $p = p_c$ is different from that of SAW's on nonrandom lattices and thus $\nu' \neq \nu$, even though $\nu' \approx \nu$. In terms of renormalization-group (RG) language, the fixed point on the parameter plane of p and the fugacity K of SAW's that governs the critical property of SAW's at $p = p_c$ is different from that of SAW's at $p = 1$, as in the several RG studies [8–11], but an eigenvalue of the linearized RG transforms around the former fixed point and is quite close to the corresponding eigenvalue around the latter fixed point. If this picture is correct, there should be a crossover scaling [14,15] in SAW's that arises as the number of the steps of SAW's increases near the percolation threshold. SAW's on the percolation clusters at $p = p_c$ or where $\xi_p^2 \gg \langle R^2 \rangle_N$ is in the fractal regime [14,15], in which the behavior of SAW's should be the same as that on the deterministic fractal [20,21]. One of our motivations in this paper is to show numerically that the second picture is more possible than the first one. Since the percolation clusters (PC's) in the fractal regime are the fractals [14,15] in the statistical sense, the exact analytic calculations of the properties of SAW's on PC's in the fractal regime is nearly impossible in two and three dimensions. Thus we want to calculate the critical index ν' in the dimensionality between 2 and 6 by the modified Flory approximants. As we shall see, the suitable choice of a modified Flory formula with the numerical data for several kinds of the fractal dimensions of the percolation clusters reasonably reproduces the numerical data [2] and this fact, we believe, is the numerical evidence for the second interpretation. In this sense this work is a detailed but concise addendum to our previous studies [14,15].

We believe that to find a most plausible Flory formula for SAW's on the percolation fractal by comparing the formula to the recent numerical data is not only to give us the most plausible form for $P(R,N)$ for RW's on the percolation clusters but to give us a clue to resolving a recent controversy for SAW's on the critical percolation clusters.

II. FLORY APPROXIMANTS

The first but rather crude Flory formula for ν' for SAW's on the fractal was suggested by Kremer [1] as

$$\nu' = \frac{3}{d_f + 2} , \tag{5}$$

which is from the simple replacement of d in Eq. (2) by d_f. More sophisticated Flory formulas have been obtained from the minimization of Eq. (3) to R with Eq. (4), which yields

$$\nu' = \frac{2+\alpha}{d_f + \alpha d_w} . \tag{6}$$

In Eq. (6) the choice of α is related to the probability of $P(N,R)$ of the random walks on the fractal. So far there are several suggestions for α. Rammal, Toulouse, and Vannimenus [20], as well as O'Shaughnessy and Procaccia [18], guessed that

$$\alpha = 1 . \tag{7}$$

Havlin and co-workers [19] suggested that

$$\alpha = 1/(d_w - 1) . \tag{8}$$

Aharony and Harris [17] proposed that

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

where $d_{\min}$ is the fractal dimension of the minimum path on a fractal. If one uses three forms for α in Eqs. (7), (8), and (9), we get three corresponding Flory-type formulas for ν'.

Another kind of Flory-type formula is suggested by Alexandrowicz [22] as

$$\nu' = \frac{4 + d_f}{4 d_f} , \tag{10}$$

which is from the argument of a dimer formation of two SAW's. Before applying these formulas to SAW's on the critical percolation clusters (CPC's), there is a point to clarify. If one believes that the SAW's can only move on the backbone of CPCs (otherwise they would be trapped at the dangling ends of CPC's [14,15,17,20], d_w and d_f for CPC's should be replaced by the corresponding d_{Bw} and d_{Bf} for the backbone of CPC's. In contrast, if one believes that there can statistically exist very long dangling ends so that they can carry reasonably long SAW's, one should use the formulas with the dimensions of CPC's, not those of backbones. In this paper for a given formula we have used both the formula with fractal dimensions of CPC itself and the formula with fractal dimensions of backbone of CPC to calculate ν' between two and six dimensions, because we know that the upper critical dimension of percolation is 6. For example, to calculate exponent ν' by Eq. (6), with Eq. (9) as the form for α, we have used both formulas with the fractal dimensions of CPC itself as

$$\nu' = \frac{2+\alpha}{d_f + \alpha d_w} \left[\alpha = \frac{d_{\min}}{d_w - d_{\min}} \right] , \tag{11}$$

and one with the fractal dimensions of the backbone of CPC as

$$\nu' = \frac{2+\alpha_B}{d_{Bf} + \alpha_B d_{Bw}} \left[\alpha_B = \frac{d_{\min}}{d_{Bw} - d_{\min}} \right] . \tag{12}$$

A more general version of Eq. (12) was recently derived by Roy and Blumen [23] based on the geometrical structure of the percolation-cluster fractal and the property of

SAW's. The mean-field version of Roy and Blumen's formula [23] is exactly the same as Eq. (12), which is also derived by Bouchaud and Georges [24] by a different method.

Since there are not enough data directly for d_{Bw}, we have also used the relation

$$d_{Bw}=d_{Bf}+\zeta \ , \tag{13}$$

or

$$d_{Bw}=d_{Bf}+2+\mu-d \ , \tag{14}$$

where ζ_R is the critical index for the resistance of the random- resistor network (RRN) on CPC's and μ is the conductivity exponent of the RRN. As you can see from Table I, the existing data for d_f, d_w, $d_{\min}$, d_{Bf}, and d_{Bw} in the dimensions between $2 \le d \le 6$ are relatively scattered.

The results for ν' calculated by the various Flory-type formulas are displayed in Table II. when one considers SAW's on the diluted Cayley tree $\nu'=\frac{1}{2}$, because on the Cayley tree there is no loop [14,17]. The upper critical dimension of percolation is 6 and the results on the Cayley tree should be the same as that of mean-field theory, $\nu'=\frac{1}{2}$ for $d \ge 6$. Among the possible five Flory-type formulas considered in this paper, those that cannot predict $\nu'=\frac{1}{2}$ for $d=6$ have been excluded in Table II. The formulas displayed in Table II and their results for ν' are only those that predict $\nu'=\frac{1}{2}$ for $d=6$.

III. DISCUSSION AND CONCLUSION

In Table II, we have not displayed the results that use Eq. (8) for α and by its corresponding backbone formula

$$\nu'=\frac{2+\alpha_B^{(1)}}{d_{Bf}+\alpha_B^{(1)}d_{Bw}} \quad [\alpha_B^{(1)}=1/(d_{Bw}-1)] \ , \tag{15}$$

not only because they cannot reproduce the result that $\nu'=\frac{1}{2}$ for $d=6$, but because they predict quite larger values for ν' for $d=2$ and 3 than the simulation results [2]. As one can see in Table II, it is quite surprising that in $d=2$ a few Flory-type formulas that use several kinds of fractal dimensions of CPC's in complex ways predict that ν' is in the range between 0.75–0.77, which is very close to 0.75, the value of ν for SAW's on two-dimensional nonrandom lattices. In contrast, for $3 \le d \le 5$, ν's are larger than corresponding values of ν on the nonrandom lattices. In the simulation by Lee and Nakanishi [2], the data for ν' in $d=3$ with the step number N around 80 are about 0.62, which is larger than 0.59, i.e., the value of ν for SAW's on a nonrandom medium, and the data for ν' are still decreasing. There is still a possibility that $\nu' > \nu$. Moreover, for $d=4$ and 5, the reasonable Flory-type formulas do predict $\nu' > \frac{1}{2}$. Therefore, if numerically ν' is very close to ν in $d=2$ and 3, we believe that this is not because the universality class of SAW's on the percolation clusters at $p=p_c$ is the same as that of SAW's on the nonrandom lattices, but because it is coincidental, as explained in the Introduction. There should therefore be the same crossover behavior as suggested in Ref. [15]. So we suggest the numerical tests on SAW's on CPC's in $d=4$ and 5, because whether ν' in $d=4$ and 5 is equal to $\frac{1}{2}$ or not is the true test of whether SAW's on CPC's belong to the same universality class as that of SAW's on nonrandom lattices.

As one can see from Table II, the best Flory-type formula for SAW's on CPC's is the formula (12) with Eq. (9) as the form for α that uses the backbone fractal dimensions, and we can say that the best formula for α in Eq. (4) for $P(R,N)$ of RW's on the disordered fractal is

$$\alpha=\frac{d_{\min}}{d_w-d_{\min}} \ . \tag{16}$$

TABLE I: Fractal dimensions and critical exponents of percolation clusters.

	$d=2$	$d=3$	$d=4$	$d=5$	$d \ge 6$[a]
d_f	91/49[b]	2.51±0.02[c]	3.05±0.05[c]	3.69±0.02[c]	4
			3.21±0.07[b]	3.54[d]	
d_{Bf}	1.62±0.02[e]	1.74±0.04[e]	1.9±0.2[b]	1.93±0.02[b]	2
		1.83[d]	1.94[d]		
ζ	0.99[d]	1.31[d]	1.59[d]		2
μ	0.98±0.11[b]	2.3±0.2[b]	3.56[b]	4.85[b]	2
	0.95±0.05[b]		3.52[b]	4.77[b]	6
$d_{\min}$	1.15±0.03[b]	1.38±0.2[b]	1.61±0.05[b]	1.69±0.02[b]	2
	1.13[d]	1.333[b]	1.47±0.11[b]		
d_{Bw}	2.62±0.03[g]	3.14[g]	3.53[g]	3.8±0.2[h]	4
	2.57±0.03[h]	2.84±0.24[h]	3.4±0.2[h]	3.7±0.2[h]	

[a]Cayley tree results (see Ref. [17]).
[b]Reference [25].
[c]Reference [26].
[d]Reference [17].
[e]Reference [27].
[f]Reference [28].
[g]From Eq. (13) and numerical data for ζ in this table.
[h]From Eq. (14) and numerical data for μ in this table.

TABLE II: The SAW exponent ν' on percolation clusters by various Flory-type formulas. Reference numbers (within table) refer to the reference in which the formula has been derived. Reference numbers in footnotes refer to the work in which the data have been obtained by the random simulation or by the exact enumeration.

	$d=2$	$d=3$	$d=4$	$d=5$	$d\geq 6$
$\nu'=\frac{3}{d_f+2}$ [Ref. 1]	0.77	0.66	0.57–0.59	0.53–0.54	$\frac{1}{2}$
$\nu'=\frac{3}{d_{Bf}+d_{Bw}}$ [Ref. 20] $(\alpha=1)$	0.71–0.72	0.61–0.65	0.55–0.56	0.53–0.54	$\frac{1}{2}$
$\nu'=\frac{2+\alpha_B}{d_{Bf}+\alpha_B d_{Bw}}$ [Eq. (12)] $\left[\alpha_B=\frac{d_{\min}}{d_{Bw}-d_{\min}}\right]$	0.75–0.77	0.64–0.66	0.57–0.59	0.52–0.58	$\frac{1}{2}$
$\nu'=\frac{4+d_f}{4d_f}$ [Ref. 22]	0.77–0.78	0.64–0.66	0.56–0.58	0.52–0.53	$\frac{1}{2}$
ν'	0.75–0.76[a] 0.81±0.03[b]	0.61–0.62[a] 0.65[c]			

[a]Reference [2].
[b]Reference [3].
[c]Reference [1].

Harris and Aharony [17] have argued that α in Eq. (9) is equal to the upper bound of true α, which is from averages over typical configurations; while α in Eq. (8) is equal to the lower bound when one averages over all possible configurations, including very rare ones. In contrast, simulation data [2] for ν' lie between ν' by Eq. (12) and ν' by the Flory-type formula [20]

$$\nu'=\frac{3}{d_{Bf}+d_{Bw}}(\alpha=1)\ . \tag{17}$$

From these results we can conclude that as far as SAW's on CPC's are concerned, α satisfies

$$\frac{d_{\min}}{d_w-d_{\min}}\leq\alpha\leq 1\ . \tag{18}$$

The exact results of ν' of SAW's on the generalized $2d$ gaskets [21] are in between ν' by Eq. (12) and ν' by Eq. (17) and the SAW's on $2d$ gaskets also support the inequality (18). As far as SAW's on the fractal are concerned, we believe that the true α should satisfy the inequality (18).

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[1] K. Kremer, Z. Phys. B **45**, 149 (1981).
[2] S. B. Lee and H. Nakanishi, Phys. Rev. Lett, **61**, 2022 (1988); S. B. Lee, H. Nakanishi and Y. Kim, Phys. Rev. B **39**, 9561 (1989).
[3] P. M. Lam, J. Phys. A **23**, L831 (1990).
[4] S. B. Lee and H. Nakanishi, J. Phys. A **24**, 1355 (1991).
[5] A. B. Harris, Z. Phys. B **49**, 347 (1983).
[6] Yup Kim, J. Phys. C **16**, 1345 (1983).
[7] A. K. Roy and B. K. Chakrabarti, Phys. Lett. **91A**, 393 (1982).
[8] P. M. Lam and Z. Q. Chang, Z. Phys. B **56**, 155 (1984).
[9] M. Sahimi, J. Phys. A **17**, L379 (1984).
[10] D. Markovic, S. Milosevic, and H. E. Stanley, Physica **144A**, 1 (1987).
[11] Y. Meir and A. B. Harris, Phys. Rev. Lett **63**, 2819 (1989).
[12] A. K. Roy and B. K. Chakrabarti, J. Phys. A **20**, 215 (1987).
[13] Yup Kim, J. Phys. A **20**, 1293 (1987).
[14] Yup Kim, Phys. Rev A **39**, 4923 (1989).
[15] Yup Kim, Phys. Rev. A **41**, 4554 (1990.
[16] P. G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, 1979).
[17] A. Aharony and A. B. Harris, J. Stat. Phys. **54**, 1091 (1989); Euro. Phys. Lett. **4**, 1355 (1987).
[18] B. O'Shaughnessy and I. Procaccia, Phys. Rev. A **32**, 3073 (1985).
[19] S. Havlin and D. Ben Abraham, Adv. Phys. **36**, 155 (1987); S. Havlin, D. Movshovitz, B. L. Trus, and G. H. Weiss, J. Phys. A **18**, L179 (1984); R. A. Guyer, Phys. Rev. A **32**, 2324 (1985).
[20] R. Rammal, G. Toulouse, and J. Vannimenus, J. Phys. (Paris) **45**, 389 (1984).
[21] S. Elezevic, M. Knezevic, and S. Milosevic, J. Phys. A **20**, 1215 (1987).
[22] Z. Alexandrowicz, Phys. Rev. Lett. **53**, 1088 (1984).
[23] A. K. Roy and A. Blumen, J. Stat. Phys. **59**, 1581 (1990).
[24] J. P. Bouchaud and A. Georges, Phys. Rev. B **39**, 2846 (1989).
[25] S. Havlin and D. Ben Abraham, Adv. Phys. **36**, 155 (1987).
[26] S. Grassberger and R. I. Cohen, J. Phys. A **19**, 1681 (1986).
[27] T. A. Larsson, J. Phys. A **20**, L291 (1987).
[28] D. C. Hong and H. E. Stanley, J. Phys. A **16**, 1475 (1983); **16**, L525 (1983).