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Theory of Self-Avoiding Walks on Percolation Fractals

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A phenomenological approach which takes into account the basic geometry and topology of percolation fractal structures and of self-avoiding walks (SAW) is used to derive a new expression for the Flory exponent describing the average radius of gyration of SAWs on fractals. We focus on the radius of gyration and discuss the importance of the intrinsic fractal dimensions of percolation clusters in determining the lower and upper critical dimensions of SAWs. The mean-field version of our new formula corresponds to the Aharony and Harris expression, who used the standard Flory approach for its derivation.

KEY WORDS: Self-avoiding walks; percolation; fractals; random walks; shortest path.

The statistics of self-avoiding walks (SAW) on lattices with quenched random disorder, which is relevant to the behavior of chain polymers in porous media, has been investigated with keen interest during the last decade.[1-14] The principal quantity of interest in most studies is the mean square radius of gyration of a SAW of N steps, which (for asymptotically large N) scales as

$$\langle R^2 \rangle \approx N^{2\nu^{\mathrm{SAW}}} \tag{1}$$

Here ν^{SAW} is the universal critical exponent, which for the pure lattice case depends only on the Euclidean dimension d. A very good mean-field estimate for ν^{SAW} for Euclidean lattices is given by the Flory formula[15]:

$$\nu^{\mathrm{SAW}} = \frac{3}{2+d} \tag{2}$$

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The formula is exact for $d=1, 2$, and 4 ($d=4$ being the upper critical dimension) and slightly overestimates the $d=3$ case for which $\nu^{\mathrm{SAW}} = 0.592 \pm 0.003$ from the series expansion of Guttmann.[16] De'Bell and Jan[17] found $\nu^{\mathrm{SAW}} = 0.591 \pm 0.001$ from Monte Carlo calculations, which corresponds nicely with Guttmann. In a random lattice with quenched disorder a fraction p (<1) of bonds (sites) is occupied at random; below p_c, the percolation threshold,[18] no infinite cluster exists. As long as $p > p_c$, both the analytical studies[4,5,7,13] and the numerical calculations[3,10] for SAW on percolation clusters reach the same conclusion that $\nu_p^{\mathrm{SAW}} = \nu_{p=1}^{\mathrm{SAW}}$, i.e., ν_p^{SAW} stays at the pure lattice value; there is no change in the critical behavior of SAWs in random lattices for $p > p_c$. This agrees with the extended Harris' criterion[19,4] applied to the n-vector model in the $n \to 0$ limit. Unlike the $p > p_c$ case, the studies on the critical behavior of SAW on the percolation fractal, i.e., exactly at $p = p_c$, are rather controversial. An early Monte Carlo simulation[3] on the diamond lattice concluded that, at $p = p_c$, the Flory exponent of SAWs crosses over to a different value $\nu_{p_c}^{\mathrm{SAW}}$ ($> \nu_{p=1}^{\mathrm{SAW}}$), so that in $d=3$, $\nu_{p_c}^{\mathrm{SAW}} \approx 0.67$. A recent numerical simulation,[10] on the other hand, concludes that, within the error limits, $\nu_{p_c}^{\mathrm{SAW}} = \nu_{p=1}^{\mathrm{SAW}}$; moreover, this should also agree with Kremer's result[3] after reanalyzing the data.[10] Contrary to this recent suggestion, real-space renormalization-group studies[7,13] and field-theoretic treatments[13] conclude that the exponent $\nu_{p_c}^{\mathrm{SAW}}$ is determined by a new fixed point, different from that of the pure system, which leads to $\nu_{p_c}^{\mathrm{SAW}} \neq \nu_{p=1}^{\mathrm{SAW}}$. Thus, the ε expansion[13] near the percolation fixed point, where $\varepsilon = 6 - d$, leads to $\nu_{p_c}^{\mathrm{SAW}} = 1/2 + \varepsilon/42$ to first order in ε. The exact enumeration analysis[13] for $d=2$, 3, 4, and 5 percolation clusters at $p = p_c$ also supports the idea that $\nu_{p_c}^{\mathrm{SAW}} \neq \nu_{p=1}^{\mathrm{SAW}}$; the values obtained are $\nu_{p_c}^{\mathrm{SAW}} = 0.76 \pm 0.08$, 0.67 ± 0.04, 0.63 ± 0.02, and 0.54 ± 0.02 for $d=2$, 3, 4, and 5, respectively. Different analytical studies,[3,8,9,11,12] which center on calculating modified Flory formulas for $\nu_{p_c}^{\mathrm{SAW}}$ at $p = p_c$, also reach the conclusion that $\nu_{p_c}^{\mathrm{SAW}} \neq \nu_{p=1}^{\mathrm{SAW}}$ and that $\nu_{p_c}^{\mathrm{SAW}}$ is dependent on various fractal characteristics of the percolation clusters.

In this paper, we derive, considering the basic geometry and topology of percolation fractals and also SAW properties, a new formula for $\nu_{p_c}^{\mathrm{SAW}}$. Using our expression, we are able to investigate the lower and upper critical dimensions of SAWs on arbitrary fractal lattices. The mean-field approximation of our expression is the same as that of Aharony and Harris,[11] derived along the lines of the standard Flory approximation, and also the same as that of Bouchaud and Georges,[12] derived using a different statistical approach.

We start from $G_N(r)$, the number of configurations of a SAW of N steps with *radius of gyration* r (*not* end-to-end distance). We focus on

$G_N(r)$ on percolation fractals, i.e., at $p = p_c$. The value of $G_N(r)$ is severely constrained through the very basic geometry and topology of percolation fractals and of SAW statistics. Thus, $G_N(r)$ must be exceedingly low in two extreme situations:

(a) When $r < N^{1/d_B}$, where d_B is the fractal dimension of the backbone of the percolation cluster.[18] This is so because the SAW chain moves on the backbone (otherwise it would be trapped on the dangling ends) and the minimum radius of gyration corresponds to a collapsed chain.

(b) When $r > N^{1/d_{\min}}$, where $d_{\min}$ is the fractal dimension of the shortest (chemical) path on the percolation cluster.[20] Note that paths on the percolation cluster are very tortuous. The maximum radius of gyration of the SAW (i.e., the most fully-stretched configuration) corresponds to the longest achievable r distance by a SAW of a given number of steps N. This is equivalent to determining, for a given value of r, the minimal number N of SAW steps needed to reach r. The relation between N and r is represented by the exponent $d_{\min}$.

The above expressions allow us to extend to percolation clusters an argument given by Lhuillier[21]; in ref. 21 the pure lattice case was considered, for which one has $d_B = d$ and $d_{\min} = 1$. Setting G_N for the total number of configurations of a SAW of N steps, one has

$$G_N(r) = G_N P_N(r) \tag{3}$$

where $P_N(r)$ is probability distribution function of the radius of gyration. As discussed above, $P_N(r)$ must decrease strongly for $r < N^{1/d_B}$ and for $r > N^{1/d_{\min}}$. With this requirement we remark, following ref. 21, that for small r the free energy of the SAW is dominated by a term $(N/r^{d_B})^{\alpha}$, which may be thought of as being the repulsive energy between distant basic units, and for large r by a term $(r/N^{1/d_{\min}})^{\delta}$, which represents a configurational entropic term. Here α and δ are unknown positive exponents (possibly different from the pure lattice values). We thus assume for percolation fractals the following expression:

$$P_N(r) \approx \exp\left\{-N\left[C_1\left(\frac{N}{r^{d_B}}\right)^{\alpha} + C_2\left(\frac{r}{N^{1/d_{\min}}}\right)^{\delta}\right]\right\} \tag{4}$$

Now, the most probable radius of gyration of a SAW is given by the maximum of $P_N(r)$. Calculating the maximum in Eq. (4) and reexpressing r as a function of N leads to

$$\nu_{p_c}^{\mathrm{SAW}} = \frac{1 + k/d_{\min}}{d_B + k} \tag{5}$$

where k is the (positive) exponent ratio:

$$k = \delta/\alpha \tag{6}$$

Having the scaling relation[20]

$$d_{\min} = \frac{d_B}{d_L^B} \tag{7}$$

where d_L^B is the spreading or the connectivity dimension[20] of the backbone of the percolation fractal, we can write

$$\nu_{p_c}^{\mathrm{SAW}} = \frac{1}{d_B} \frac{d_B + k d_L^B}{d_B + k} \tag{8}$$

It is to be noted that apart from d_B and d_L^B, the expression for $\nu_{p_c}^{\mathrm{SAW}}$ depends on the ratio k, a typical property of the radius of gyration distribution function; but not on the individual values of δ and α. Moreover, notice that we derived Eq. (8) directly from Eq. (4) without any additional (e.g., mean-field) approximations. At this stage, to the best of our knowledge, there exists no accepted determination of the distribution of the radius of gyration for a SAW on percolation fractals or, for that matter, even for a SAW on pure lattices. We thus cannot compare Eq. (4) to literature data; this also prevents us from finding out the exact values of $\nu_{p_c}^{\mathrm{SAW}}$ for different dimensions from Eq. (8), because for this we need to know k. On the other hand, Eq. (8) allows us to extract some important information, as we proceed to show.

Let us first calculate the upper critical dimension d_c of a SAW on a fractal lattice. d_c is defined as that dimension for which the SAW statistics will behave in a mean-field-like way, i.e., $\nu_{p_c}^{\mathrm{SAW}} = 1/d_{W,B}$, where $d_{W,B}$ is the fractal dimension of random walks on the backbone of the percolation fractal.[9,18] The other way to express this fact is that the repulsive energy part in the total free energy of a SAW chain becomes independent of N. The term $N^{1+\alpha}/r^{\alpha d_B}$ in Eq. (4) can be thought of as being proportional to the number of contacts between distant basic units, i.e., as giving the repulsive energy.[21] We now use the Alexander–Orbach relation[22] that $d_{W,B} = 2d_B/d_S^B$, where d_S^B is the fracton (or spectral) dimension[22] of the backbone of the percolation fractal. At d_c the mean-field value of α is 1,[21] so that, with $r \sim N^{1/d_{W,B}}$, the repulsive energy part will be proportional to $N^{2-d_S^B/2}$. Therefore, the SAW statistics on fractal lattices will behave in a mean-field-like way if and only if $d_S^B \geqslant 4$, in accordance with the conclusion of Rammal *et al.*[8] (for pure lattices $d_S^B = d$ and thus $d_c = 4$).

Consider now the lower critical dimensionality $\tilde{d}_c$ of a SAW on fractal clusters; $\tilde{d}_c$ is defined as being the dimensionality at which the SAW fractal dimension equals the fractal dimension of the embedding lattice. Thus, for percolation clusters at $\tilde{d}_c$ one has $\nu_{p_c}^{\mathrm{SAW}} = 1/d_B$. If we take up our formula (8) for $\nu_{p_c}^{\mathrm{SAW}}$ and use it to find $\tilde{d}_c$, we see that a SAW chain on a fractal lattice is on its lower critical dimension if d_L^B (not d_B) of the lattice is equal to 1. For pure lattices $d_L^B = d$ and thus we have $\tilde{d}_c = 1$. Thus, we see that the upper and lower critical dimensions of SAW on fractal lattices depend solely on the intrinsic topological fractal dimensions (d_S^B and d_L^B, respectively), and not on the extrinsic geometric fractal dimensions.

We are now in the position to analyse the result of Lee *et al.*[10] that $\nu_{p_c}^{\mathrm{SAW}} = \nu_{p=1}^{\mathrm{SAW}}$. Then in dimensions 4 and 5 for percolation fractals one would have $\nu_{p_c}^{\mathrm{SAW}} = 1/2$ since $\nu_{p=1}^{\mathrm{SAW}} = 1/2$ for $d = 4$ and 5. On the other hand, for percolation clusters in $d = 4$ and 5 the value of d_B is less than 2.[23] This, together with $\nu_{p_c}^{\mathrm{SAW}} = 1/2$, leads to the conclusion that in $d = 4$ and 5 the SAW fractal dimension would be greater than d_B, the dimension of the embedding fractal, which is clearly impossible. Our analysis thus supports the conclusion of Meir and Harris[13] that $\nu_{p_c}^{\mathrm{SAW}}$ is in general different from $\nu_{p=1}^{\mathrm{SAW}}$; from our phenomenological formula (8) we read off that $\nu_{p_c}^{\mathrm{SAW}}$ should lie midway between the bounds of $1/d_B$ and d_L^B/d_B.

Next, we come to the percolation cluster in $d = 6$, for which $d_B = 2$ and $d_L^B = 1$.[20] From our expression (8) we find for this fractal $\nu_{p_c}^{\mathrm{SAW}} = 1/2$, which reconfirms ref. 13. We like to stress here that on $d = 6$, $\nu_{p_c}^{\mathrm{SAW}}$ is exactly equal to $1/2$ ($= 1/d_B$) because SAWs on $d = 6$ here are at the lower critical dimension $\tilde{d}_c$, since $d_L^B = 1$ in $d = 6$. This means that the SAW radius of gyration (as well as the end-to-end distance) on $d = 6$ percolation clusters will be Dirac-delta distributed. From this finding we also conjecture that there will be no collapse transition of SAW chains on $d = 6$ percolation fractals, a fact which is due to the topology of the fractal lattice structure itself.

Now we present a mean-field version of our phenomenological expression (8) for $\nu_{p_c}^{\mathrm{SAW}}$. For this, we have to calculate the "ideal" (i.e., mean-field) value of k ($= \delta/\alpha$) in Eq. (8). The term $N(r/N^{1/d_{\min}})^{\delta}$ in Eq. (4) can be thought of as being the elastic energy part,[21] which arises from the configurational entropic term. In the mean-field approximation one can write this elastic energy term as

$$N\left(\frac{r}{N^{1/d_{\min}}}\right)^{\delta} \approx -\ln \Phi_N(r) \tag{9}$$

where $\Phi_N(r)$ is the probability distribution of random walks on the backbone of the percolation fractal.

According to Havlin and Ben-Avraham,[9] $\Phi_N(r)$ is not Gaussian, but follows rather

$$\Phi_N(r) \approx \exp\left[-C\left(\frac{r}{N^{1/d_{W,B}}}\right)^u \right] \tag{10}$$

where u ($\neq 2$) is an unknown exponent. Putting Eq. (10) into Eq. (9) and comparing the r terms and the N terms, we get

$$\delta = u \qquad \text{and} \qquad 1 - \delta/d_{\min} = u/d_{W,B}$$

i.e., we obtain

$$\delta = u = \frac{d_{W,B} d_{\min}}{d_{W,B} - d_{\min}} \tag{11}$$

Very recently Harris and Aharony[24] derived in a completely different manner (in the context of superlocalization of impurity quantum states for a tight-binding model on random fractal structures) the same expression for u as in Eq. (11) for the quenched average case. But here we see that the correct expression for u follows easily from Eq. (8), derived considering the gyration radius and the basic geometry and the topology of the fractal structure. With this value of δ, Eq. (11), and the mean-field value of α ($=1$),[21] we get for $k = \delta/\alpha$ the mean-field result

$$k = \frac{d_{W,B} d_{\min}}{d_{W,B} - d_{\min}} \tag{12}$$

(Note that for pure lattices in all dimensions $d_{W,B} = 2$ and $d_{\min} = 1$ and thus one has as mean-field value $k = 2$ for all dimensions; this result is exact for $d = 1$, 2, and 4 and is slightly off in $d = 3$.)

Putting Eq. (12) in Eq. (8) and with $d_{\min} = d_B/d_L^B$, we get the mean-field expression for $\nu_{p_c}^{\text{SAW}}$ as

$$\nu_{p_c}^{\text{SAW}} = \frac{1}{d_B} \frac{4d_L^B - d_S^B}{2d_L^B - d_S^B + 2} \tag{13}$$

The same expression was found recently by Aharony and Harris,[11] using a standard derivation of Flory formula. Comparisons with numerical results are summarized in Table I for percolation fractals in different dimensions as well as for some nonrandom fractals such as Sierpinski gaskets and Koch curves. The agreement is quite good within the error limits of the numerical data. Thus, the mean-field value of k ($=\delta/\alpha$) gives good agreement of $\nu_{p_c}^{\text{SAW}}$ with its numerically determined values. We note

Table I. Exponent $\nu_{p_c}^{SAW}$ for SAWs on Different Fractal Lattices and Comparison between Numerical (or Exact) Values and Equation (13)

				$\nu_{p_c}^{SAW}$	
d	d_B	d_L^B	d_S^B	Eq. (13)	Other
Percolation fractal					
2	1.61 ± 0.01[25]	1.43[26]	1.25 ± 0.01[8]	0.77	0.767[7]
3	1.75 ± 0.01[27]	1.26 ± 0.03[27]	1.23 ± 0.03[8]	0.66	0.67 ± 0.04[13]
4	1.9 ± 0.2[23]	1.18[9]	1.18 ± 0.05[8]	0.62	0.63 ± 0.02[13]
5	1.93 ± 0.16[23]	1.14[23]	1.18[8]	0.56	0.54 ± 0.02[13]
6	2	1	1	1/2	1/2[13]
Sierpinski gasket					
2	$\ln 3/\ln 2$[8]	$\ln 3/\ln 2$[8]	$2 \ln 3/\ln 5$[8]	0.825...	0.798...[8]
3	2[8]	2[8]	$2 \ln 4/\ln 6$[8]	0.724...	0.718...[8]
Koch curve					
2	$\ln 5/\ln 3$[8]	$\ln 5/\ln 3$[8]	1.2427[8]	0.855...	0.891...[8]

that it would be really interesting to have a good Monte Carlo simulation for $P_N(r)$ of SAWs on percolation fractals to estimate k and thus to determine whether k really takes the mean-field value or not for all dimensions.

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