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Universality of self-avoiding walks on critical percolation clusters

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By comparing some of the problems of self-avoiding walks (SAW's) on critical percolation clusters (CPC's) to those of random walks, specific issues that need classification in order to understand the critical behavior of SAW's on CPC's are considered. From these issues and the node-link-blob picture of CPC's we discuss crossover scaling theory and the universality of SAW's on CPC's. Recent simulation results are also considered.

Even though many studies have been done on self-avoiding walks (SAW's) on diluted lattices[1-15] during the last decade, there is still much to do to understand the critical properties of SAW's on the lattices at or near the percolation threshold.[16] The main quantity of interest is the quenched average of mean-square end-to-end distance (or radius of gyration) of N-step SAW's $\langle R^2\rangle_s$, where $\langle\rangle$ denotes averages over configurations in which each bond (site) is occupied with probability p. The results of the recent studies[2,6-15] on the exponent ν' are quite contradictory, where ν' is defined through the relation

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

at the percolation threshold (T_p, $p=p_c$) or when the correlation length of percolation $\xi_p^2 \ll \langle R^2\rangle_s$ near T_p. The earlier real-space renormalization-group (RSRG) studies[6-8] and the most recent RG study[10] have predicted a new fixed point at T_p that governs the critical properties of SAW's near T_p and is different from the pure fixed point at $p=1$, while the RSRG study of Markovic, Milosevic, and Stanley[9] concluded something different. The earlier Monte Carlo study[2] concluded that ν' near T_p should be larger than the ν of SAW's on nonrandom lattices, while a recent simulation study[14] concluded that ν' is much closer to ν, which might suggest $\nu'=\nu$. At present the big question on the critical properties of SAW's near T_p is whether the equality $\nu'=\nu$ is exact or not. That is, whether the universality of SAW's at T_p is the same as that on the nonrandom lattices. But by comparing with the case of successful crossover scaling theory for random walks[17-20] (RW's) on the diluted lattices near T_p or at T_p, the more exact forms of the questions on SAW's near T_p and the answers to them are necessary for understanding the universality-related problem. The objectives of this paper are (i) to suggest what kind of questions and answers are needed to understand the above-mentioned problem, (ii) from those questions and answers to discuss the crossover properties of SAW's near T_p as well as to answer the universality-related questions, and (iii) to reinterpret a recent simulation result.[14]

We first want to explain motivations and suggestions of this paper clearly by a comparison with problems of SAW's to corresponding ones of RW's.[17-20] In studying physical phenomena on percolating clusters near T_p, one should remember that there are two different averages (ensembles).[17,18] Studies on RW's (Refs. 17-19) clearly distinguish the averages over RW's on clusters of all sizes (AC averages) from averages over only those on the largest clusters (LC averages) at given concentration p. To be specific, we consider the mean-square end-to-end distance $\langle R^2\rangle_r$ of RW's on the percolation clusters. At T_p, or when $\langle R^2\rangle \ll \xi_p^2$ near T_p, the geometry of critical clusters is a *fractal* geometry[17] and

$$\langle R^2\rangle_r \approx N^{2y}, \tag{2}$$

with $y < \frac{1}{2}$. There are two different exponents[17,18] for y, y_1 for AC averages and y_2 for LC averages. The exact relation[17,18] between the two exponents is also known as

$$y_1 = y_2(1-\beta_p/2\nu_p)\ (y_1 < y_2), \tag{3}$$

where β_p and ν_p are the critical exponents of the percolation transition. The relation in Eq. (3) has been explained by using a scaling argument[17,18] and has been confirmed by simulations.[18,19] In contrast, among the papers on SAW's, only Sahimi,[7] Roy and Chakrabarti,[11] and Markovic *et al.*[9] distinguish AC averages from LC averages. Both simulations[1,14] on SAW's do not specify which averages were taken. At $p=p_c$ there should be two different exponents for ν' in Eq. (1), ν_1' for AC averages and ν_2' for LC averages. The *first suggestion* of this paper for both numerical and analytical studies that relate to the universality of SAW's is as follows. There should be a clear distinction between LC averages and AC averages when one calculates ν'. Without this distinction the comparison of one result to another is hardly meaningful.

The *second suggestion* deals with the relation between ν_1' and ν_2', which is very important to the universality-related question. The suggestion by Sahimi[7] was

$$\nu_2' > \nu_1' > \nu, \tag{4}$$

and that by Roy and Chakrabarti[11] was

$$\nu_1' = \nu_2'(1-\beta_p/2\nu_p), \tag{5}$$

which were based on a simple analogy to the RW case [Eq. (3)]. However, the self-avoiding property on disordered lattices[13] is quite different from that of RW's, thus both Eqs. (4) and (5) must be wrong. In this paper I show, from a qualitative argument,

$$\nu_2' = \nu_1', \tag{6}$$

which is the *second suggestion*. To show Eq. (6) qualitatively, we review[17,18] how one can show Eq. (3) for RW's. For RW's on the cluster with s sites (s cluster) we expect

from Eq. (2) and from the definition of y_2 that

$$\langle R^2\rangle_r^s \approx \begin{cases} N^{2y_2} & (N^{2y_2} < R_s^2)\,, \\ R_s^2 & (N_s^{2y_2} > R_s^2)\,, \end{cases} \tag{7}$$

where R_s^2 is the square of the average radius of the s cluster at $p=p_c$ and

$$R_s^2 \approx s^{2/d_f}\,. \tag{8}$$

Here d_f is the fractal dimension of the large clusters at T_p and $d_f = d - \beta_p/\nu_p$.[17,18] For the AC average at T_p, $\langle R^2\rangle_r$ satisfies

$$\langle R^2\rangle_r \approx N^{2y_1} = \sum_s^{\infty} \langle R^2\rangle_r^s n_s s \propto \left[\sum_s^{s_c} R_s^2 s^{1-\tau}\right] + \sum_{s=s_c}^{\infty} N^{2y_2} s^{1-\tau}\,, \tag{9}$$

where $n_s s = s^{1-\tau}$ is the probability[17,18] that a RW starts on an s cluster at T_p and s_c is the cluster mass for which the crossover occurs in Eq. (7) with $s_c^{2/d_f} \approx N^{2y_2}$. From $\tau = 2+\beta_p/(\beta_p+\gamma_p)$ (Refs. 17 and 18) and Eq. (9) we can see that Eq. (3) holds. But as far as SAW's are concerned, there cannot be a corresponding term to the term in large parentheses of Eq. (9) because an N-step SAW cannot finish its walk on an s cluster with $N < s$.[13] So, for SAW's on an s cluster

$$\langle R^2\rangle_s^s \approx \begin{cases} N^{2\nu_2'} & (s > N) \\ \text{no possible SAW's} & (s < N)\,. \end{cases} \tag{10}$$

For AC averages at T_p, $\langle R^2\rangle_s$ satisfies

$$\langle R^2\rangle_s \approx N^{2\nu_1'} = \sum_{s>N} \langle R^2\rangle_s^s n_s s \propto \sum_s N^{2\nu'} s^{1-\tau} = \mathscr{f} N^{2\nu_2'}\,, \tag{11}$$

where $\mathscr{f}$ is a finite number, because $\sum_s n_s = 1$ (Refs. 17 and 18) at $p=p_c$. From this we see that Eq. (6) holds. The result of this argument for RW's has been confirmed by simulations.[17–19] The same level of qualitative argument for SAW's should also demonstrate validity, because we think that at T_p, ν_2' is not dependent on cluster size s if s is reasonably large.

The *third suggestion* is related to the crossover properties of SAW's near T_p. The crossover properties of RW's are as follows.[17–20] There are three regimes.[17–19] The first one, which we will call the *fractal* regime,[17–19] is the regime at $p=p_c$ or when $\langle R^2\rangle_r \ll \xi_p^2$ near T_p, in which the end-to-end distance of RW $\langle R^2\rangle_r$ behaves as Eq. (2). The second regime is the regime at $p<p_c$ and in $N\to\infty$ which we call the saturation regime. In this regime,[17–19] on a cluster with s sites,

$$\langle R^2\rangle_r \approx R_s^2 \quad (\text{LC average})\,. \tag{12a}$$

For AC averages[17–19] in this regime,

$$\langle R^2\rangle_r \approx \sum_s n_s s R_s^2 \approx (p_c - p)^{-k} \quad (k>0)\,. \tag{12b}$$

The final regime is the *Eucledian* regime at $p>p_c$ and $\langle R^2\rangle_r \gg \xi_p^2$, where there is the infinite cluster. RW in this regime should have the normal Eucledian property[17–20] as

$$\langle R^2\rangle_r \approx \begin{cases} D(p)N & (\text{AC averages}),\ D(p) \approx (p-p_c)^{\mu}\,, \\ D(p)N & (\text{LC averages}),\ D(p) \approx (p-p_c)^{\mu+\beta_p}\,, \end{cases} \tag{13}$$

where $D(p)$ is the diffusion constant[17,18] on any cluster, $D(p)$ is the constant[17,18] on the infinite cluster, and μ is the conductivity exponent of the random-resistor network[17,18] on percolation clusters. The crossover scaling function[17–20] for $\langle R^2\rangle_r$ near T_p which satisfies Eqs. (2), (12b), and (13) is known as

$$\langle R^2\rangle_r^{1/2} = N^{y_1} F[N^x(p-p_c)]\,, \tag{14}$$

where $x = 2y_1/(2\nu_p - \beta_p)$. To establish the similar crossover scaling function for SAW's near T_p we should know the critical behavior of SAW's in each of three regimes. Until now the studies of SAW's near T_p are only on SAW's in the *Eucledian* regime and in the *fractal* regime. But it is also important for answering the universality-related questions on SAW's to know the critical behavior of SAW's for the regime in which $N\to\infty$ and $p<p_c$. In the *fractal* regime SAW's behave as Eq. (1). In the *Eucledian* regime, $\langle R^2\rangle_s$ behaves as

$$\langle R^2\rangle_s (p \gg p_c \text{ and } N\to\infty) = A(p) N^{2\nu}\,, \tag{15}$$

where $A(p)$ depends only on p. In the regime $p<p_c$ and $N\to\infty$, we expect quite a different critical behavior of SAW's from that of RW's. $\langle R^2\rangle_r$ in this regime does not depend upon the step number N [see Eqs. (12a) and (12b)]. In contrast to a normal kind of SAW kinetics,[13] $\langle R^2\rangle_s$ ($p<p_c$ and $N\to\infty$) must have N dependences,[21] as was shown exactly for a Cayley tree and qualitatively for hypercubic lattices in a previous paper.[13] $\langle R^2\rangle_s$ within normal SAW's must satisfy

$$\langle R^2\rangle_s (p < p_c \text{ and } N\to\infty) \approx N^{2\nu''} \tag{16}$$

and the exponent ν'' must be different from ν' in Eq. (1). In the regime $p<p_c$ and $N\to\infty$, $\langle R^2\rangle_s \gg \xi_p^2$ and the clusters which can carry N-step SAW's cannot have the memory of the percolation correlation.[17] In this regime SAW's on such clusters are similar to that of SAW's on lattice animals,[17] because the clusters whose linear size is larger than ξ_p are similar to lattice animals[17] and SAW's on such clusters are analogous to the RW's problem studied by Wike *et al.*[22] The third suggestion is that the exponent ν'' in Eq. (11) is equal to the exponent of SAW's on the lattice animals,[17] and we call this regime the *animal* regime of SAW's instead of the *saturation* regime. (Approximate numerical values[16] for ν'' are given in Table I.) With the information of ν', ν'', and $A(p)$ we can establish the crossover scaling form for $\langle R^2\rangle_s$ similar to Eq. (9), and from that scaling form we can answer the universality-related problem completely and clearly. Such a scaling form is far from completion, because at present we have no information on ν'' and $A(p)$ and there is only restrictive information on ν'.

From these suggestions we now want to discuss the

TABLE I. Fractal dimensions of percolation clusters and critical exponents of SAW's on percolation clusters.

	$d=2$	$d=3$	$d=4$	$d=5$	$d\geq 6$
d_{Bf}	1.62 ± 0.02 [a]	1.83 [b]	1.94 [b]	1.93 ± 0.02 [a]	2
		1.74 ± 0.04 [a]	1.9 ± 0.2 [a]		
$d_{\min}$	1.15 ± 0.03 [a]	1.38 ± 0.02 [a]	1.47 [b]	1.69 ± 0.02 [a]	2
	1.13 [a]	1.333 [b]	1.61 ± 0.05 [a]		
d_{Bw}	2.62 ± 0.04 [c]	3.14 [d]	3.53 [c]	3.78 ± 0.16 [c]	4
	2.57 ± 0.03 [c]	2.84 ± 0.24 [c]	3.44 ± 0.20 [c]		
ν' [e]	0.76	0.65	0.58		$\frac{1}{2}$
ν' [f]	0.75–0.76	0.64–0.66	0.57–0.59	0.55–0.57	$\frac{1}{2}$
ν'' [e]	0.84	0.75	0.68		$\frac{1}{2}$ $(d\geq 8)$

[a]Dat from Ref. 18 and references therein.
[b]Data from Ref. 16 and references therein.
[c]From $d_{Bw}=d_{Bf}+\zeta(=\mu-d+2)$, and numerical data from Ref. 18.
[d]From $d_{Bw}=d_{Bf}+\zeta$ and numerical data from Ref. 16.
[e]From Ref. 16.
[f]The range of values for ν' is from Eq. (18) [see the text below Eq. (18)].

universality-related questions. The recent simulation of Lee and Nakanishi[14] has shown that ν' is very close to $\frac{3}{4}$, the value of ν on two-dimensional (2D) nonrandom lattices, and ν' for $d=3$ is 0.61, which is close to 0.59, the value of ν on 3D nonrandom lattices. Lee and coworkers[14] also reanalyzed the Kremer's simulation[2] in 3D to deduce $\nu'\simeq 0.62$, which is much closer to 0.59 than Kremer's original value of $\frac{2}{3}$. These analyses[14] suggest that $\nu'=\nu$ and SAW's on the diluted lattices even at $p=p_c$ (SAW's at T_p) belong to the same universality class of those on the nonrandom lattice (normal SAW's). Since in both 2D and 3D ν' is numerically close to ν in 2D and 3D, one should analyze the situation rigorously before jumping to conclusions. What we want to show is that even though the numerical data may lead one to conclude that $\nu'=\nu$, the universality class of SAW's at T_p cannot belong to that of the normal SAW's. If one believes $\nu'=\nu$, $\nu'=\frac{1}{2}$ for the dimensions with $d\geq 4$, because $\nu(d\geq 4)=\frac{1}{2}$. When $N\rightarrow\infty$ SAW's move only on the backbone of the percolation clusters,[13,15,16,23] because otherwise they would eventually be trapped on a dangling end, even though these ends would be quite long. We then know, from the node-link-blob picture[23] of that incipient infinite cluster (IIC), at $p=p_c$ the inequality[23]

$$d_{\min}\leq d'_{\mathrm{SAW}}=1/\nu'\leq d_{Bf} \tag{17}$$

always holds, where $d_{\min}$ is the chemical dimension[18] of the cluster, d_{Bf} is the fractal dimension of the backbone, and $d_{\mathrm{SAW}}=1/\nu'$ is the fractal dimension of SAW's on IIC. The equality in Eq. (17) holds for $d\geq 6$, where $d=6$ is the upper critical dimension of percolation.[13,23] $\nu'=\frac{1}{2}$ for $d=4$ and 5 breaks down the inequality (17), because d_{Bf} for $d=4$ and 5 is less than two. SAW's at T_p therefore cannot belong to the same universality class of normal SAW's. Furthermore, we want to emphasize that one need not only the results for $d=2$ and 3, but those on $d=4$, 5, and 6 to resolve the universality-related problems, because the upper critical dimension of percolation is 6.

I now want to show numerically that the closeness of ν' to ν in 2D and 3D is coincidental. Until now the best Flory approximant on nonrandom media is the formula by Aharony and Harris[16] (AH formula). The AH formula[16] for ν' is

$$\nu'=\frac{2+\alpha}{d_{Bf}+\alpha d_{Bw}}, \tag{18}$$

where

$$\alpha=d_{\min}/(d_{Bw}-d_{\min}) \tag{19}$$

and d_{Bw} is the fractal dimension of RW's on the backbone of IIC.[18] Original values[16] for the AH formula are given in Table I. The published data[16–18] for d_{Bw}, d_{Bf}, and $d_{\min}$, however, are spread over a range (see Table I). We, therefore, calculate the range of values of ν' from the range of data of d_{Bw}, d_{Bf}, and $d_{\min}$. From the AH formula the calculated range for ν' in 2D is $\sim$0.75–0.77, which is very close to the results of the simulation.[14] For ν' in 3D the range is $\sim$0.64–0.66 and has a deviation of only 3% from 0.62. Considering the fact that the AH formula predicts 3% larger values to the exact known results[24] for SAW's on the family of gaskets, the AH formula's results are in quite good agreement with the simulation results. Therefore, the numerical evidence that $\nu'\approx\nu$ in 2D and

3D is coincidental and it should not be interpreted as proof that $\nu' = \nu$. This means, from the viewpoint of RG theory, that the fixed point governing the SAW's near PT should be different from that for SAW's on nonrandom lattices, but an eigenvalue of the linearized RG transformation around the former is different, but close to, an eigenvalue around the latter. The exponent for SAW's with lattice animals has also been calculated from Eq. (17) by Aharony and Harris,[16] and this is thought to be the same value as that of ν'' in Eq. (16). These numerical values for ν'' have also been redisplayed in Table I.

When one checks the suggestions in this paper by simulations or other means, the important point concerns the number of steps of SAW's, N. Both simulations[2,14] have studied SAW's up to 80 steps or so, which we think are too small to confirm the theoretical results. For these small SAW's it might seem that $\nu_2' > \nu_1'$. But for physically meaningful steps[25] ($\approx 10^5$) we believe the proof for Eq. (6) should hold. For the small step numbers it might also seem that the end-to-end distance exponent of SAW's on the backbone of IIC is larger than that on IIC, which includes quite long dangling ends. However, I think these two exponents also coincide when the number of steps is on the order of 10^5.

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