Monte Carlo study of self-avoiding walks on a percolation cluster

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We present computer-simulation results of self-avoiding walks (SAW's) on a percolation cluster for a square lattice performed very close to the percolation threshold. We specifically consider the disorder averages of SAW's on all clusters supporting one or more N-step walks and those on a backbone of an infinite cluster and estimate the critical exponents ν and γ that characterize the disorder averages of the end-to-end distance and the number of SAW's, respectively. Our results for γ indicate a behavior rather similar to SAW's on fully occupied lattices for both cases, while for ν one of two cases shows different behavior.

I. INTRODUCTION

In recent years, there has been great interest in the statistics of self-avoiding walks (SAW's) on a randomly diluted lattice, relevant to linear-chain polymers in dilute solution confined in a porous medium. This problem was first brought to the fore by Chakrabarti and Kertesz [1], who applied the Harris criterion [2] to the disordered spin system of an n-vector model in the $n \to 0$ limit, and it has been very controversial the last few years [1,3–10]. Since the appearance of this problem, there have been a number of works that have employed field-theoretical calculations, cell renormalizations, Monte Carlo simulations, and other calculations, all of which, however, have arrived at one of the following three different conclusions: (i) the disorder is relevant for any amount of impurities for $p > p_c$ [1,3], where p is the concentration of undiluted sites and p_c the percolation threshold; (ii) the disorder is relevant for p close to p_c and irrelevant for p sufficiently far away from p_c [6,7,10]; and (iii) the disorder is irrelevant for any amount of impurities [4,5].

Kremer [11] was the first to study this problem numerically. He carried out Monte Carlo simulations on a randomly diluted diamond lattice and found that the Flory exponent is unchanged for weak dilution. On the other hand, just above p_c he found a crossover to a new higher value of this exponent, $\nu_{p_c} \simeq \frac{2}{3}$, which is significantly larger than the known full lattice value $\nu_F \simeq 0.59$ [12]. Lee and Nakanishi [9], however, pointed out that his result near p_c was in error owing to mistakes in data analysis, and should be corrected not to be greater than 0.62, which is much closer to ν_F. They also presented their own Monte Carlo data on square and simple-cubic lattices and obtained a Flory-exponent value ν, similar to the normal-lattice value even for p close to p_c, for both two and three dimensions. However, this work was claimed to be spurious by another more recent work by Lam [13] that used an enumeration technique. Nakanishi and Lee [14], in their following comment, pointed out two critical errors in Lam's work and claimed that the result should be the reverse. Considering these numerical studies, it now seems clear that the Flory exponent for p sufficiently away from p_c is unaffected by lattice dilution, while, close to p_c, the effect is still controversial.

The previous Monte Carlo studies sought to calculate the incipient infinite-cluster (IC) averages, while the ensemble, which is of theoretical interest, is comprised of the all-cluster (AC) averages in which all clusters supporting one or more N-step SAW's are included in the disorder average of the radius of gyration (and end-to-end distance). Lyklema and Kremer [6] presented a qualitative argument that the probability of starting an N-step walk at a finite cluster vanishes as $N \to \infty$, suggesting that the critical behavior is dominated by walks on an infinite cluster. Recently, Lee *et al.* [9] also argued that the two ensembles are likely to yield identical critical behavior for the following reason. Since the critical behavior of SAW's is governed by asymptotically long walks, and such walks can exist only on the infinite cluster, the contributions of finite clusters diminish as $N \to \infty$. On the other hand, Sahimi proposed the inequality of the Flory exponents for the two different ensembles

$$\nu_{\mathrm{IC}} > \nu_{\mathrm{AC}} \ (> \nu_F) \ , \tag{1}$$

where ν_{IC} and ν_{AC} are the exponents for IC and AC averages, respectively. Roy and Chakrabarti [15] suggested that, based on an analogy to the ordinary random walks (RW's), $\nu_{\mathrm{AC}} = \nu_{\mathrm{IC}}(1 - \beta_p / 2\nu_p)$, which is consistent with (1). Here, β_p and ν_p are the percolation exponents for the order parameter and correlation length, respectively. More recently, Kim [16] claimed, based on a scaling argument, that the inequality (1) is invalid and $\nu_{\mathrm{IC}} = \nu_{\mathrm{AC}}$ should hold. He also argued that the critical behavior of the IC averages is also similar to that on the backbone (BB) of an infinite cluster, suggesting

$$\nu_{\mathrm{AC}} = \nu_{\mathrm{IC}} = \nu_{\mathrm{BB}} \ . \tag{2}$$

The second equality was also assumed previously by Rammal *et al.* [17] in deriving a Flory formula for SAW's on fractal substrates. Both equalities are based on the following argument. The infinite cluster generated near p_c in general, contains many dead ends and "dan-

gling loops" that are connected to the backbone via a single path. Since the walk that visits such bonds is eventually terminated after a certain number of steps, the walks that survive in the limit $N \to \infty$ are those confined within the backbone. With Eq. (2) and the inequality

$$d_{\min} \leq 1/\nu_{\mathrm{BB}} \leq d_{Bf} \ , \tag{3}$$

where $d_{\min}$ is the chemical dimension and d_{Bf} the fractal dimension of the backbone, Kim claimed that both ν_{AC} and ν_{IC} should be larger than ν_F because otherwise the inequality (3) breaks down for $d=4$ and 5 since $d_{Bf}<2$ [18].

However, the validity of either (1) or (2) has not yet been tested numerically. Although reliable arguments for the first equality in Eq. (2) exist, we believe that it is still important to test it by simulation since it lends validity to the interpretations of theoretical predictions made with existing Monte Carlo data. The second equality is also important to examine numerically since it resolves, if correct, the problem concerning the universality of SAW's on diluted lattices. While the argument given previously appears to be correct, doubt still remains since the infinite percolation cluster and its backbone have totally different characteristics, such as different fractal and spectral dimensions. It is therefore interesting to study the critical behaviors of SAW's confined to clusters of all sizes and those on the backbone.

In this paper we study—via Monte Carlo simulations—the critical behaviors of the AC and BB averages of SAW's on two-dimensional site percolations for a square lattice, performed at percolation threshold. We specifically consider the critical exponents ν and γ for each disorder average of the SAW's. In Sec. II we describe our Monte Carlo procedure. Our simulation results shall be presented in Sec. III. The critical exponents ν and γ are estimated from the Monte Carlo data of the mean-square radii of gyration (and end-to-end distances) and the number of surviving N-step walks. The connective constants for various ensembles are also calculated. In Sec. IV we summarize the results.

II. MONTE CARLO PROCEDURE

Applying a Monte Carlo method to SAW's on a percolation cluster consists mainly of two steps. First, one must generate percolation clusters and second, one generates SAW's on it. We describe our methods in the following.

A. Generation of percolation clusters

Our primary purpose is to study the SAW's on clusters of all sizes (AC averages), namely, those clusters that support at least one N-step walk, and the SAW's on the backbone (BB averages). For SAW's on all clusters, since walks start from any undiluted site, one does not have to identify an infinite cluster for each realization, and, thus, generation of percolation clusters is simple. We pick a random number between 0 and 1 for each site of the cell containing L^2 lattice sites and, if the number lies between 0 and p_c, a given site is filled (undiluted), and empty otherwise (diluted). (We used the best currently available value, $p_c=0.592\,745$ [19]). In order to identify various clusters in a cell, we employ the well-known Hoshen-Kopelman algorithm [20].

For SAW's on a backbone, one must first identify an infinite cluster, and then extract the backbone from it. In order to obtain an infinite cluster, we follow Lee *et al.* [9]. We generate the site-percolated *incipient* infinite clusters, defined as clusters that span the cell along all coordinate directions, and after identifying such clusters,

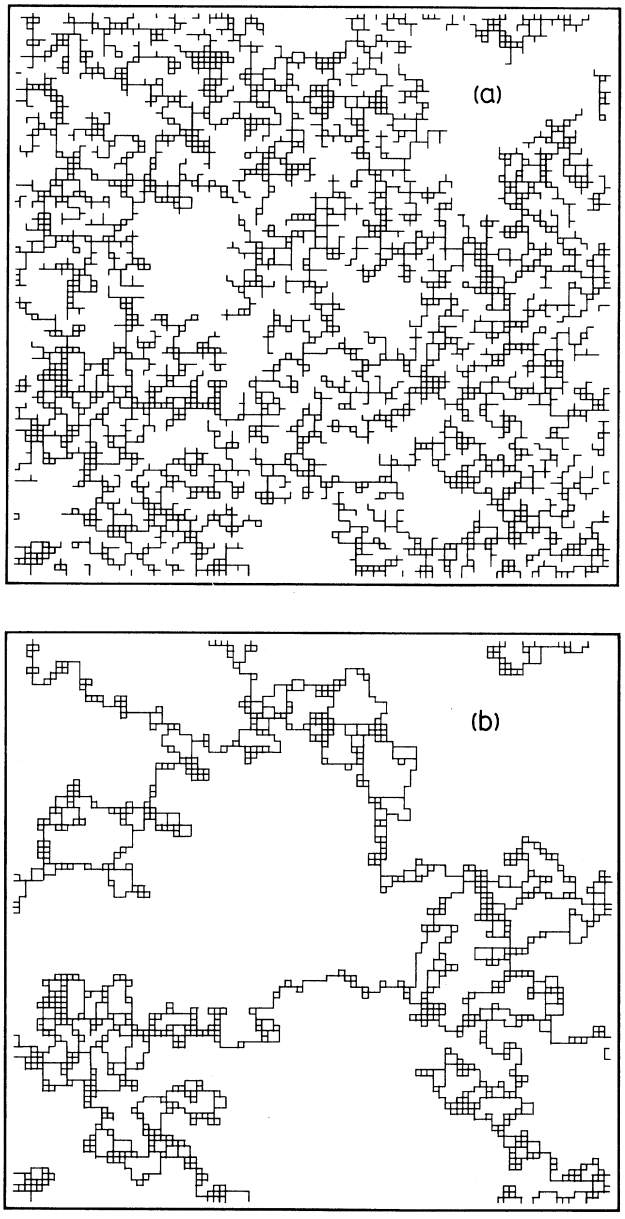

FIG. 1. Computer-generated (a) incipient infinite cluster and (b) corresponding backbone for a 100×100 square lattice for $p=0.592\,745$. The number of occupied sites is 4828 and 2216 for the infinite cluster and the backbone, respectively.

any two opposite edges are connected by periodic boundaries. In order to extract the backbone from the infinite cluster, one must eliminate all bonds that are connected singly to the backbone. For this, we employ the "modified" Roux-Hansen algorithm [21], which is very efficient and is specific only in two dimensions. We obtain a site-percolated infinite cluster on a square lattice (prime lattice) and then construct the network of bonds by connecting all neighboring occupied sites. We then consider the connectivity among the sites in a dual lattice, assuming that the bonds in the dual lattice cannot cross the bonds in the prime lattice. (Note that the square lattice is self-dual.) If a bond in a prime lattice is occupied, it corresponds to the fact that the bond between two neighboring sites in a dual lattice is missing, or vice versa. If a bond in a prime lattice is a dangling bond, then the two neighboring sites in a dual lattice are connected to each other via other bonds. We thus sweep through the prime lattice and remove all bonds that are in between two neighboring sites connected to each other in the dual lattice. This algorithm extracts the backbone from an infinite cluster with free boundaries. In order to obtain the backbone with periodic boundaries, we construct eight nearest-neighbor replicated cells surrounding the original cell and employ the above procedure over the original cell and replicas of it. Figure 1 shows the computer-generated incipient infinite cluster and the backbone of it for 100×100 square lattice.

B. Disorder averages of SAW's

The disorder averages of the end-to-end distance (or radius of gyration) for N-step SAW's is, in principle, defined as

$$\langle\langle R_N^2\rangle\rangle_C=\sum_C P(C)\langle R_N^2(C)\rangle \Big/ \sum_C P(C)\ , \tag{4}$$

where $P(C)$ is the probability of having a disorder C that supports at least one SAW, and $\langle\ \rangle$ denotes the average over all SAW's in a given disorder C and $\langle\ \rangle_C$ the average over the disorder configurations. For the BB averages, $\langle R_N^2(C)\rangle$ is simply the configurational average of N-step walks on a given disorder C. For the AC averages, on the other hand, one must consider the probability that walks start on the clusters of size s, $p(s)\sim s^{1-\tau}$. Therefore, $\langle R_N^2(C)\rangle$ should be written as

$$\langle R_N^2(C)\rangle=\sum_s\sum_r s^{1-\tau}G_N(r,C,s)r^2 \Big/ \sum_s\sum_r s^{1-\tau}G_N(r,C,s)\ , \tag{5}$$

where $G_N(r,C,s)$ is the number of N-step walks with the end-to-end distance r confined to a cluster of size s in a given disorder C, and τ is the critical index characterizing the mean number of clusters of size s per site, defined by $n_s\sim s^{-\tau}$ at p_c. From a simulation standpoint, these two averages should be carried out distinguishably.

The disorder average in Eq. (4) for BB ensembles is, in principle, obtained as follows. One must first carry out the configurational average over all possible N-step walks starting from *every* undiluted site on the backbone. One then repeats this over many disorders and, from the results, the disorder average is obtained straightforwardly. In the Monte Carlo procedure, on the other hand, one is assumed to sample a certain number of probable configurations in each disorder, rather than generating all possible walks. We discuss here, among the many possible, two distinct ways for finding walk averages. In the first, one can sample a certain number of walks for a given disorder, each of which starts from the randomly selected site on the backbone. In the second, one chooses a *single* starting point (near center) and generates a predetermined number of walks from it. The average over the sampled walks weighted equally gives the walk average for a given disorder for both cases, and the disorder average can be carried out, repeating over many disorders.

In our simulations, we employ, following Lee *et al.* [9], the latter method with some modifications. Since the walks growing from the central site are able to probe only relatively small portions of the backbone around the center, the latter method is too uneconomical. In order to utilize fully the backbone, we choose the starting point randomly. We then effectively translate this point to the geometric center of the cell and form a new configuration by moving the pieces on the edges using periodic boundaries. After completing this procedure, the new backbone will look different from the original one. It is thus clear that the effective disorder for SAW's depends on the starting points. Thus, instead of using only one starting point per cluster, we choose many different starting points in each backbone and generate a predetermined number of SAW's from each starting point. Since a different starting point corresponds to a different backbone configuration, the disorder average must be carried out first over the starting points, and then over the replaced backbones. For the sake of consistency, we tested our method for RW's and found that the results were consistent with the previous data ($\nu_{\rm RW}\simeq0.38$) [18].

For the AC averages, one must calculate the configurational average of the walks according to Eq. (5). In order to incorporate the probability that walks start on the clusters of size s, we choose a starting point ran-

domly on any undiluted site and generate only one walk from it, and then repeat it over many starting points in a given disorder. In this way, it is clear that the number of walks starting from the clusters of size s is proportional to $sn_x \sim s^{1-\tau}$. Thus, the average of the surviving N-step walks, each of which is weighted equally, gives the approximate walk average for a given disorder C. The disorder average is carried out over many disorder configurations.

III. RESULTS AND DISCUSSIONS

We have calculated the mean-square end-to-end distances and radii of gyration for two types of disorder averages of SAW's on a percolation cluster for a system of size $L=100$. In order to obtain unbiased samples, we employed a standard, simple sampling method since it was found previously that the standard enrichment method [22] may possibly cause biased samples [9].

Data were analyzed using a common method [23]. We define an effective exponent ν_N as a function of N and find the asymptotic value in the limit $N\to\infty$. The two frequently employed definitions in this particular problem are

$$\nu_N^{(1)}=N\langle\langle R_N^2\rangle\rangle_C \Big/ \left[2\int_0^N \langle\langle R_n^2\rangle\rangle_C dn\right]-\tfrac{1}{2} \tag{6}$$

and

$$\nu_N^{(2)}=\frac{1}{2(N-M)}\left[N\ln\langle\langle R_N^2\rangle\rangle_C - M\ln\langle\langle R_M^2\rangle\rangle_C - \int_M^N \ln\langle\langle R_n^2\rangle\rangle_C dn\right] . \tag{7}$$

The former was employed by Lee and Nakanishi [9], while the latter was used more recently by Lam [13]. If $\langle\langle R_N^2\rangle\rangle_C$ is of a form similar to an ordinary SAW ansatz, the asymptotic expression of ν_N should be

$$\nu_N=\nu+aN^{-\Delta}+bN^{-1}+\cdots \tag{8}$$

for both Eqs. (6) and (7). Thus, the intercept on the ordinate in the plot of ν_N versus N^{-1} gives the Flory exponent ν. It seems, in general, that the latter definition yields smaller fluctuations for each N, and, therefore, we employ it in the present work.

The integral in Eq. (7) is to be calculated using the Simpson rule. Since $N-M$ is required to be an even integer larger than 4 for Simpson-rule quadrature, one must choose M to equal either 1 or 2, depending on N. These two choices, however, result in severe oscillations in the plot of ν_N, which make an accurate determination of ν rather difficult. If we use trapezoidal rule instead, the ν_N would always be overestimated. To overcome these difficulties, we pick 100 points equally spaced between any two consecutive data of N and calculate $\ln\langle\langle R_N^2\rangle\rangle_C$ on such points using the cubic-spline interpolation. Then we employ either the Simpson (with M=1) or the trapezoidal rule. We found that both rules yielded consistent results.

The critical exponent γ defined by the number of N-step SAW's,

$$G_N \propto \mu^N N^{\gamma-1} , \tag{9}$$

was analyzed by a method similar to that of Lee *et al.* [9] from attrition of surviving walks in the Monte Carlo sampling. Suppose that $A(N)$ is the number of surviving SAW's for N-step walks. Then the rate of survival is, in general, proportional to the number of SAW's divided by the number of RW's with *no* immediate backstep, i.e.,

$$A(N)/A(1) \propto G_N(\mathrm{SAW})/G_N(\mathrm{RW}) ,$$

where $G_N(\mathrm{RW})$ is the number of N-step RW's with immediate backstep prohibited. Thus the exponent γ can be determined from the relation

$$\ln\left[\frac{A(N)}{A(N-1)}\right]=\ln\mu-\ln\left[\frac{G_N(RW)}{G_{N-1}(\mathrm{RW})}\right] +(\gamma-1)\frac{1}{N}+\cdots , \tag{10}$$

where μ denotes the connective constant. Since $G_N(\mathrm{RW})/G_{N-1}(\mathrm{RW})$ does not depend on the number of steps N, the exponent γ is determined from the plot of $\ln[A(N)/A(N-1)]$ versus N^{-1}. We now present our simulation results.

1. All cluster averages

We have generated, for the configurational average of N-step walks, 10^6 walks from the randomly chosen starting points for each disorder configuration, and the disorder average was carried out over 600 clusters. Since the walks starting from the points on finite clusters terminate after only few steps, the significant number of samples was obtained only up to 50 steps.

Our data for ν_N for the radius of gyration are compared, in Fig. 2, with the corresponding data for the ordinary square lattice. Results for the AC averages are larger than those on the full square lattice for each N, indicating that the lattice dilution enhances the end-to-end distance. As N grows, the difference becomes smaller and, in the limit of $N\to\infty$, it seems eventually to disap-

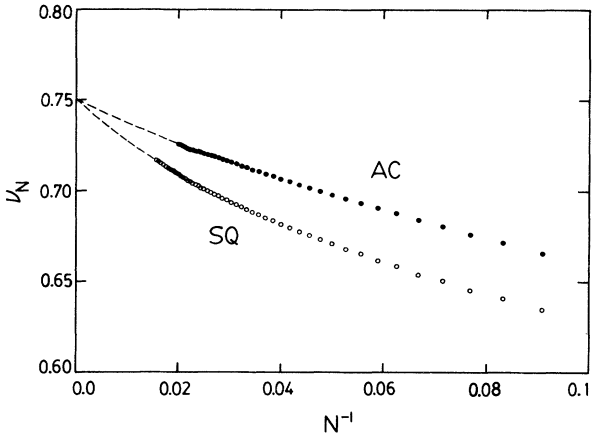

FIG. 2. Effective exponent ν_N, defined in Eq. (7), vs N^{-1} for the radius of gyration for AC averages, in comparison to the corresponding data for a full lattice. The errors were estimated from six batches, each of which was averaged over 100 clusters, and they were found to be nearly the same size as the size of the symbols for all N.

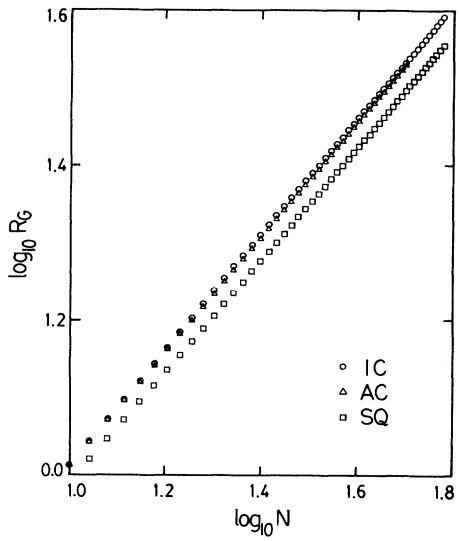

FIG. 3. Double-logarithmic plot of the mean-square radii of gyration. The circles denote the IC averages, the triangles the AC averages, and the squares the full square lattice results.

pear. A simple linear fit of our data for the AC averages for $N \geq 30$ already yields the intercept with an ordinate of about 0.745; however, considering the curvature of the plots, one can easily expect that ν_{AC} is close to the full lattice value, $\nu_F = 0.75$, indicating that the critical behavior of the radii of gyration for the AC averages is similar to that of the ordinary SAW's, even for p close to p_c. (Note that ν_{AC} cannot be smaller than the full lattice value [24]). The dashed lines in the plot are guides for the eye.

We have also similarly analyzed the mean-square end-to-end distances of SAW's for AC averages, and the results yielded a very similar picture and are thus not presented here.

Our data are compared to the IC averages of Lee and Nakanishi [9]. Figure 3 exhibits the double-logarithmic plot of the mean-square radius of gyration (R_G) versus N for the AC and IC averages, in comparison to the corresponding data on the full square lattice. Data for disorder averages are, in general, larger than those on the full lattice over the whole range of N, in agreement with the recent analytic prediction [6]. As can be seen from the plot, all three cases become nearly parallel for large N, suggesting that the exponent ν remains unchanged under lattice dilution for both types of disorder average, and also that $\nu_{AC} = \nu_{IC}$ indeed holds. (Note that the asymptotic slope in the limit $N \to \infty$ gives the Flory exponent ν.) The raw AC and IC averages are very close to each other for each N. We believe that this is because the finite clusters in two-dimensional percolations are of relatively small size and, thus, the effect of such small clusters is negligible, suggesting that the critical behavior of SAW's on all clusters is dominated by the walks on the infinite cluster. This is supported by numerical observations as well. Our simulation data indicate that the number of occupied sites on nonspanning finite clusters is only about 20% of all occupied sites, and most of the finite clusters are comprised of, at most, a few sites. Thus, for relatively large N, most walks starting from the finite clusters are terminated after only a few steps, and most surviving walks are on the infinite cluster.

2. *Backbone averages*

The backbone was extracted from an infinite cluster, eliminating all singly connected bonds, and SAW's were generated from the randomly chosen starting points. For each starting point, 1000 walks along each undiluted neighboring site were generated for the walk average, and 100 starting points were selected in each cluster.

Data for ν_N averaged over 400 clusters are plotted in Fig. 4 as a function of N^{-1}. The solid circles show the mean-square radii of gyration (R_G) and the open circles, the mean-square end-to-end distances (R_E). Since both the radius of gyration and the end-to-end distance are expected to show the same critical behavior according to the universality, the ν_N for both cases should approach asymptotically the same value as $N \to \infty$. If we do not accept the unusually strong correction terms for large N, the estimate from the plot would be $\nu_{BB} = 0.77 \pm 0.01$, which is about 3% larger than the full lattice value. Since ν_{IC} and ν_{AC} were found to be close to the full lattice value, our data appear to indicate that the asymptotic behavior of SAW's on a backbone is different from the other two cases, and that $\nu_{BB} > \nu_{IC}$ holds. This is in disagreement with the recent argument of Kim, but appears to agree with the suggestion of Sahimi. It should be noted that if similar results hold for higher dimensions, such as

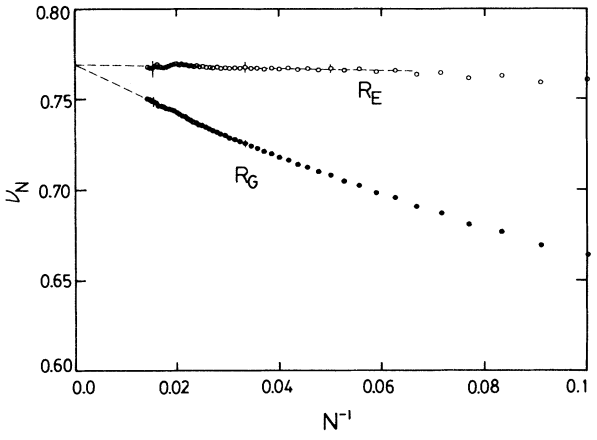

FIG. 4. Effective exponent ν_N, defined in Eq. (7), vs N^{-1} for the mean-square radius of gyration (R_G) and the end-to-end distance (R_E) for BB averages. The errors were estimated from five batches, each of which was averaged over 80 clusters.

$d=4$ and 5, as well, the inequality (3) would not be sufficient to clarify the universality of SAW's on diluted lattices.

Removal of the dead ends and "dangling loops" from the backbone seems to affect the end-to-end distances of SAW's in such a way that elimination of them significantly enhances the characteristic lengths of SAW's, even for large N. One may argue that such an effect diminishes as $N\rightarrow\infty$, as discussed earlier. We, however, claim that such an argument would be valid only if all dead ends and dangling loops are of relatively small size. Since the infinite percolation cluster is known to possess a fractal nature, the dangling bonds would be self-similar, implying that (infinitely) large sizes of dead ends and dangling loops may possibly exist. From a simulation standpoint, all dead ends and dangling loops are finite for any finite-sized system. However, in order to generate (infinitely) long walks, one must increase the size of system sufficiently that the linear size of the cell is always larger than the largest end-to-end distance, in order to avoid walks moving over the repeated cells by periodic boundaries. As the size of system increases, we believe that the mean sizes of dead ends and dangling loops also increase, and that they can still modify the asymptotic behavior of SAW's to be different from the BB averages. This was observed numerically in our simulations. Whereas nearly 80% of the occupied sites belong to the infinite cluster, only about 48% of the sites on the infinite cluster are on the backbone for our 100×100 system. As the size of system increases, these numbers decrease, implying that larger dead ends and dangling loops exist for larger systems. For example, for 400×400 square lattices, only about 36% of the sites on the infinite cluster belong to the backbone. Thus, walks that visit or start from such large loops may possibly grow infinitely long and, hence, contribute to the critical behavior even for very large N. We also note that the fractal dimension of a backbone is different from that of an infinite cluster, and thus the two are different types of substrates (see below).

3. *Critical exponent* γ

The critical exponent γ was also studied using the number of surviving N-step walks. Plotted in Fig. 5 is $\ln[A(N)/A(N-1)]$ as a function of N^{-1}: the slope of the plot gives $\gamma-1$. (The plot for the IC averages was taken from Ref. [9] for purposes of comparison.) As can be seen from the figure, the data show reasonably good straight lines for all cases, indicating that γ is sharply defined under lattice dilution. The estimated values are $\gamma_{AC}=1.32\pm0.02$ for AC averages and $\gamma_{BB}=1.31\pm0.03$ for BB averages. These values are consistent within statistical errors, and are reasonably close to the full lattice value of about $\frac{4}{3}$ and also to that for IC averages obtained by Lee *et al.*, $\gamma_{IC}=1.33\pm0.02$, indicating that the exponent γ remains unchanged under lattice dilution in two dimensions.

However, one might raise the natural question of whether or not the connective constant μ defined in Eq. (9) is larger than 1 [25]. The connective constant is, in principle, the mean number of neighboring sites on which walks can take a next step without violating self-avoidance. For a percolation cluster, since the SAW's have the additional constraint that walks cannot visit the diluted sites, μ might be less than 1. If this is indeed the case, then G_N in Eq. (7) approaches zero as $N\rightarrow\infty$, implying that the exponent γ might not be defined. The

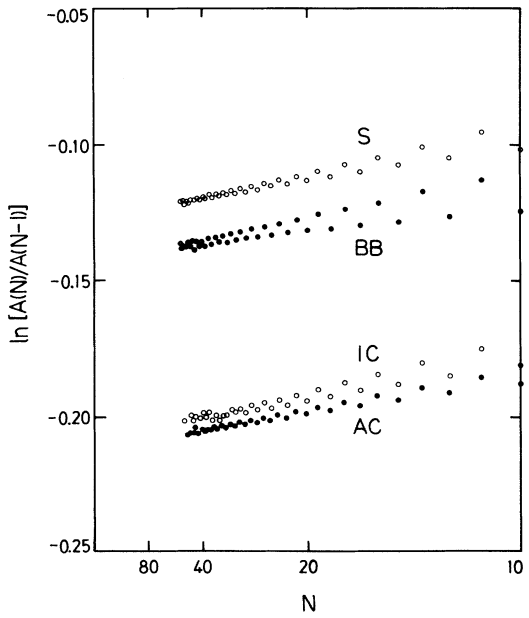

FIG. 5. The function $\ln[A(N)/A(N-1)]$ in Eq. (10) vs N^{-1} for various disorder averages: S labels the data for ordinary square lattices; other acronyms are defined in the text.

TABLE I. Summary of Monte Carlo estimates of the critical exponent γ and the connective constants μ. b and k are defined in the text before and after Eq. (11).

	γ	b	k	μ
AC averages	1.32±0.02	−0.214±0.001	1.4374	1.160±0.002
BB averages	1.31±0.03	−0.145±0.002	1.6870	1.459±0.003
IC averages	1.33±0.02	−0.206±0.001	1.5184	1.236±0.002
Ordinary SAW's	1.33±0.02	−0.129±0.001	3	2.637±0.003

earlier work, however, indicated that this is not the case for at least one type of disorder average that we consider in the present work. Chakrabarti *et al.* [26] enumerated all walks starting from the central site of a 100×100 square lattice, up to the preset number of steps, $N_{\max}$, ranging from 16 to 20, and obtained $\mu=1.21\pm0.15$. Although they did not explicitly describe which averages they pursued, we believe that their disorder averages are similar to our IC averages, or some sort between the AC and IC averages. For SAW's on a backbone, μ is not yet known; however, we can plausibly expect that μ for the BB averages is larger than that for the IC averages because all dead ends and dangling loops were eliminated for each site on a backbone. (Note that the attrition rate in Monte Carlo sampling is much lower on the backbone, as is clear from Fig. 5.) The μ for the AC averages, on the other hand, is expected to be smaller than that for the IC averages. Since μ for an infinite cluster is already close to 1, one may possibly expect that μ for the AC averages might be even less than 1.

To resolve this possible concern, we have estimated μ for various disorder averages of SAW's. The connective constant μ can be obtained from the intercept with the ordinate b in the plot in Fig. 5,

$$\mu \simeq k e^{b} , \tag{11}$$

where $k=G_N(\mathrm{RW})/G_{N-1}(\mathrm{RW})$. Since k is the number of nearest-neighbor sites to which RW's (of no immediate return) can take an Nth step, it can be obtained by subtracting 1 from the mean number of neighboring sites of every occupied site, for a given disorder configuration.

We first calculated μ for a regular square lattice to validate our method. For a square lattice, the value of k is exactly 3. Using $b=0.129\pm0.001$ from Fig. 5, μ was found to be 2.637±0.003. This is in excellent agreement with the previous estimate, $1/\mu=0.379\,003\pm0.000\,015$ [27], and therefore we believe this to be sufficient to validate our method. The value of μ for other cases can be similarly obtained. Our estimates of k, b, and μ are summarized in Table I. As can be seen from the table, the values of μ for all cases are larger than 1, thus indicating that γ is defined as given in Eq. (9). We note here that our estimate of μ for the IC averages is close to the aforementioned estimate [26].

One interesting point we should mention is that our estimates of μ for all cases (except for a regular square lattice) are considerable smaller than the theoretical prediction, which is considered to be valid for the AC averages. Since the probability of survival for each N-step SAW on a percolation cluster is p^{N+1}, the disorder average of the number of SAW's would be $p^{N+1}G_N \sim p(p\mu)^N N^{\gamma-1}$, implying that the connective constant μ is modified simply as $\mu \to p\mu$ ($\simeq 1.56$), with the exponent γ remaining unchanged. Our data, however, appear to suggest that such a simple argument may not solve the problem, as long as our simulations are carried out. We believe that this deserves future work.

4. Cluster-size distribution and the fractal nature of clusters

In order to show that the percolation clusters we have sampled in our simulations are unbiased and satisfy the general percolation theory, we have studied the cluster-size distribution of clusters of all sizes, as well as the fractal nature of the backbone.

The mean number of clusters, n_s, of size s is known to scale, for p right at p_c, as $n_s \sim s^{-\tau}$, with $\tau \simeq 2.05$ in two

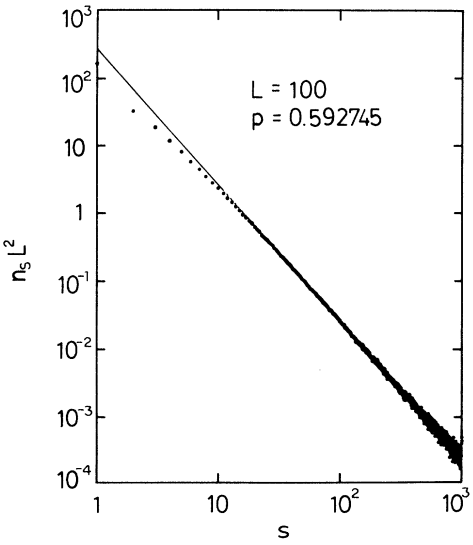

FIG. 6. Cluster-size distribution n_s vs s in a double-logarithmic plot. The linear fit through the centers of scatters gives $\tau \simeq 2.03$.

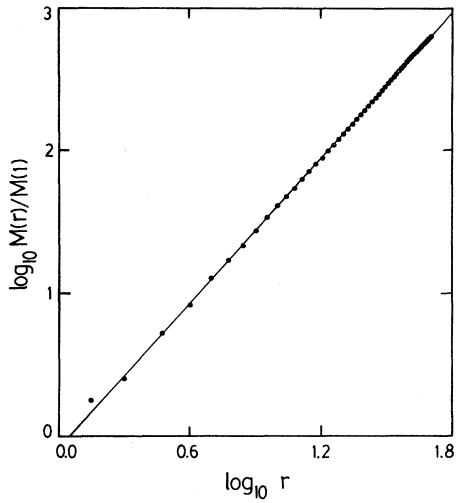

FIG. 7. Double-logarithmic plot of the number of occupied sites $M(r)$ on the backbone within the circle of radius r vs r. The fractal dimension estimated from the slope is $d_{Bf} \simeq 1.71$.

dimensions [28]. The backbone, on the other hand, is expected to show a fractal nature with fractal dimension $d_{Bf} < 2$. The fractal dimension is defined in many different ways from a theoretical point of view [29]. The simplest definition is for the mass distribution in the range of the distance r. The mass $M(r)$, corresponding to the number of occupied sites, in a circle of radius r, increases as $M(r) \sim r^{d_{Bf}}$, as r increases. The fractal dimension is known to be $d_{Bf} \simeq 1.68$ [30].

We first calculated n_s for the 100×100 systems. Plotted in Fig. 6 are the results averaged over 10^5 clusters generated by the same method as for the AC averages. Although data are scattered significantly for $s \geq 100$, the linear fit through the centers of scatters appears to satisfy the power law with the critical index $\tau = 2.03 \pm 0.01$, which is reasonably close to the known value. This confirms that our AC averages of SAW's were carried out on unbiased percolation clusters.

In Fig. 7 the mass $M(r)$ is plotted against the radius of circle r measured on the backbone at p_c. The number of occupied sites $M(r)$ was counted for 100 centers of circles selected randomly on a backbone, and the results were averaged over 100 clusters. The estimated slope from the plot is $d_{Bf} = 1.71 \pm 0.01$, which is also close to the previous estimate. The slight deviation can probably be attributed to the finite-size effect, which always appears in the percolation problem and makes numerical estimates difficult.

IV. SUMMARY AND CONCLUSIONS

Based on Monte Carlo simulations, we have studied the two types of disorder averages (AC and BB averages) of SAW's on site-percolated square lattices obtained at the percolation threshold. Our observation for ν for the AC averages is similar to that for the fully occupied lattice and also to that for the IC averages. On the other hand, for the BB averages, we obtained a ν value slightly (but clearly) larger than the full lattice value. From these, we conclude that the critical behaviors of SAW's for the AC and IC averages are similar, while the BB averages exhibit different behavior. As a consequence, we claim that the inequality (3) does not resolve the universality of SAW's on diluted lattices because the second equality in Eq. (2) appears to be incorrect, as long as our simulations are carried out.

On the contrary, our result for the AC averages might appear to suggest the universality between SAW's on a percolation cluster and the ordinary SAW's. However, we emphasize that one should be extremely careful when one draws conclusions on universality from Monte Carlo simulations. In general, since the Monte Carlo data include relatively large statistical errors, it is not sufficient to clarify universality using Monte Carlo data alone for many delicate problems like this, and, thus, our present work should not be dealt with as constituting numerical evidence of the universality of SAW's on dilute lattices. We simply claim that the exponent ν is close to the full lattice value and, if any, the difference would be very small and virtually unobservable using Monte Carlo simulations. In order to clarify universality, one must carry out further investigations using more accurate methods, such as field-theoretical calculations. Monte Carlo simulation in higher dimensions might also be critical, and such works are in progress by one of us (S.B.L.). (We note here that there exist several small-cell-renormalization studies of this problem, and all but one [8] suggest a new universality for diluted lattices.)

Our estimate of ν_{BB} appears to be close to the recent small-cell-renormalization prediction [7] and also close to the enumeration result of Meir and Harris [10]; however, we believe this closeness to be accidental, since they considered different ensembles in their works.

We have also estimated the exponent γ from the attrition rates in Monte Carlo sampling, and the exponent value was found to be similar to the full lattice value for both cases. The connective constants for AC and BB averages were also presented.

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