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

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We present the results of Monte Carlo simulation for self-avoiding walks on a percolation cluster for square and simple cubic lattices performed very close to the percolation thresholds and estimate critical exponents ν and γ defined by the disorder averages of the mean-square radius of gyration and the number of self-avoiding walks, respectively. Our results for ν indicate a behavior rather similar to the self-avoiding walks on fully occupied lattice unlike the large increase in ν reported in the only previous work of this kind by Kremer given for the diamond lattice. Our results for γ suggest an increase from the full lattice value just at p_c in three dimensions, while in two dimensions the asymptotic behavior appears to be similar to that of the ordinary self-avoiding walks. We also consider the possible crossover from fractal to Euclidean behavior and discuss the reasons why no crossover scaling is observed for the mean-square radius of gyration in the present calculation.

I. INTRODUCTION

This paper deals with a particular case of the effect of a quenched disorder in the medium on critical behavior taking place in that medium. Specifically we treat the problem of self-avoiding random walks (SAW's) confined to clusters of the percolation problem on two- and three-dimensional lattices. This problem is a direct analog of the problem of a linear-chain polymer trapped in a porous medium where excluded regions can occur with the length scales of the order of the persistence length of the chain. In this work we present the full details of a previous Letter[1] by two of us on this subject as well as some additional results on the aspects of the problem not discussed there.

Some time ago Harris[2] presented an argument which states that the presence of impurities in a magnetic system can have a nontrivial effect on the critical behavior if the specific-heat exponent α is positive. The positive α in principle indicates that the fixed point for the pure system is unstable with respect to the quenched impurities, and thus, the critical behavior for any amount of impurities is expected to be different from that of a normal system. In the case of self-avoiding walks in disordered media, one might expect that the straightforward application of this argument (called Harris criterion) to the n-vector model in the $n \to 0$ limit[3,4] would apply. However, as we shall see later, there are additional complications.

The presence of impurities in a magnetic system implies that the spin interaction between nearest-neighbor sites i and j, represented by a Hamiltonian with n-vector spins,

$$H = \sum_{\langle i,j \rangle} K_{ij} \xi_{ij} \mathbf{s}_i \cdot \mathbf{s}_j \ , \tag{1}$$

is inactive if either site i or j is an impurity site. Thus for the inactive bonds, $\xi_{ij} = \xi_i \xi_j = 0$, where $\xi_i = 0$ corresponds to the site disorder or impurity site. In the $n \to 0$ limit or equivalently for SAW,[4] this implies that a walker is allowed to visit only randomly distributed nonimpurity sites, and thus, the sites of percolation clusters for a lattice model.

The specific-heat exponent α for SAW is obtained by the hyperscaling relation[4] $d\nu = 2 - \alpha$ and becomes, with the well-known Flory approximation formula[5] for ν,

$$\alpha = 2 - d\nu \cong \frac{4-d}{2+d} \ . \tag{2}$$

Thus, the critical behavior of SAW's on a randomly diluted lattice would be expected to be different from that of ordinary SAW's for any amount of disorder for $d < 4$ according to the original Harris criterion.[2] Chakrabarti and Kertesz[3] obtained the critical behavior similar to that of classical random walks ($\nu = \frac{1}{2}$, $\gamma = 1$) by applying $n \to 0$ limit to the existing work[6] on the randomly diluted ferromagnetic n-vector model. Derrida[7] has also studied SAW's on random strips and found, similarly, an indication of a change in the critical behavior even for a weak dilution. On the other hand, Harris[8] himself argued that the disorder average is very much trivial and all critical exponents remain unchanged for any $p \geq p_c$, where p represents the concentration of nonimpurity sites and p_c is the critical concentration above which an infinite network appears. Also, a modified analysis of his criterion[8] indicates that the critical behavior of SAW is not affected by lattice dilution even though α is positive. This was partially supported by field-theoretic renormalization calculations.[9]

More recently Lyklema and Kremer[10] presented an argument that the randomness is irrelevant except at the percolation threshold. They argued based on analytic calculations that for $p < 1$ the disorder average of mean-square end-to-end distance is greater than on the full lattice. In addition, they also presented an argument that as $p \to p_c^+$ this behavior becomes singular so that the Flory exponent ν is greater than the full lattice value. This singularity is claimed to come from the denominator of the disorder average of the mean-square end-to-end distance, defined by

$$\overline{\langle R_N^2(C)\rangle} = \sum_{C_N} P(C_N)\langle R_N^2(C_N)\rangle \Big/ \sum_{C_N} P(C_N) , \quad (3)$$

where $\langle \cdots \rangle$ denotes the average over all SAW's on a given disorder configuration and $\overline{\cdots}$ denotes the average over the disorder configurations, and $P(C_N)$ is the probability of having a disorder C_N which supports at least one N-step SAW on it. Since the critical behavior of SAW's is governed by asymptotically long walks and since such walks can exist only on the infinite cluster, it appears that we need to consider only the walks on the infinite cluster. (Note, however, this remains an unproven assumption and the consideration of successively larger but finite clusters may be necessary.) In this limit, thus, the denominator is proportional to the probability to start a walk on the infinite cluster;

$$\sum_{C_N} P(C_N) \to pP(p) \propto p(p-p_c)^{\beta} . \quad (4)$$

Here $P(p)$ is the probability that a given site belongs to an infinite cluster, and it approaches zero as $p \to p_c^+$; put another way, if p is fixed at p_c and $N \to \infty$, then the denominator picks up an extra singularity as a function of N which would not be present if $p \neq p_c$. However, this type of singularity would be picked up by the factor $P(C_N)$ both in the denominator and numerator. Accordingly the numerator in Eq. (3) may also acquire a similar singular form at p_c which may cancel that of the denominator. Thus it is not clear that, even in the $N \to \infty$ limit, their argument rigorously rules out the equality between the two Flory exponents. Thus we generally write

$$\nu_p \geq \nu , \quad (5)$$

where ν_p and ν are the Flory exponents on the lattice of concentration p and on the full lattice, respectively.

Kremer[11] reported the results of Monte Carlo simulations on the randomly diluted diamond lattice where he found that the Flory exponent is indeed unchanged for a weak dilution. On the other hand, as the percolation threshold is approached (to within about 29% of p_c), a crossover was found to a new higher value, $\nu_{p_c} \cong \frac{2}{3}$. An agreement with a scaling hypothesis was also reported in the same reference when this value of ν_{p_c} was used. In addition, a Flory type formula was proposed[11] which agrees well with the reported results:

$$\nu_{p_c} = \frac{3}{D+2} , \quad (6)$$

where D is the fractal dimension of the critical percolation cluster.

This has been supported in two dimensions by two-parameter, small-cell real-space renormalization studies,[12–14] where a renormalized fugacity of each step is written as a function of two different statistical weights, a probability of occupation p and a fugacity of each step K. The random fixed point at $p = p^*$ (< 1) and $K = K^*$ is found unstable with respect to the nonrandom fixed point, and thus, the renormalization flows are away from this point. This result is strictly opposite to that suggested by the original Harris criterion,[2] and in addition, the Flory exponent obtained from these renormalization studies agrees well with Eq. (6). (We do note that the instability referred to above[12–14] results from the fact that the recursion relation for p is made independent of K, and thus it is actually built into their *method* from the start.)

However, the numerical agreements seem to have been accidental: In the Monte Carlo evaluation of ν_{p_c}, there was an elementary error in the data analysis[11] as was pointed out in a recent Letter.[1] Due to the failure in taking proper account of the mixing of two different logarithmic scales, the Flory exponent was significantly overestimated. A similar mistake was also made for the concentrated chains. While the Flory exponent of such chains is expected to assume the classical value ($\nu = 0.5$) for a chain concentration $c \geq 0.25$, the corrected result appears to become about 0.55. This indicates that the chains used in that simulation ($N = 50$) are probably not long enough to estimate the exponent ν by the method used there. In the case of the reported agreement with a scaling hypothesis, a critical examination of their own data suggests that their conclusion was also not fully substantiated, as will be discussed in detail below.

Unfortunately this incorrect value $\frac{2}{3}$ has been referred to as the only numerical estimate of ν_{p_c} for a number of years. Since the full lattice value of ν is about $\frac{3}{5}$, the large difference was believed to be a numerical evidence that the critical behavior of SAW at p_c is different from the full lattice. However, after correcting for this error and otherwise using the same method of analysis, their data would yield an estimate for ν_{p_c} of about 0.62 or even less, which makes the previous claim based on this particular numerical evidence essentially useless. Thus it seems very desirable to perform a high precision numerical simulation and proper analyses for this problem, which we have attempted to undertake in this work.

In this paper, we present the results of our Monte Carlo simulation for SAW's performed on the site percolation clusters both for square and simple cubic lattices. This work is the detailed and extended version of a previous study (on ν only) by two of us.[1] We study the critical behavior of SAW's placed on the *infinite* cluster. In particular, we focus on the exponent ν and γ for such walks defined by $\overline{\langle R_N^2 \rangle} \sim N^{2\nu_p}$ and $G_N \sim \mu^N N^{\gamma-1}$, respectively. To our best knowledge, our result of ν_{p_c} on the square lattice is the first numerical measurement of the Flory exponent of SAW's on a diluted lattice in two dimensions, and the estimates of γ both for square and simple cubic lattices are also the first calculations using Monte Carlo simulations for this problem.

The exponent γ for the number of SAW's averaged over *all* clusters was proved to remain unchanged by Lyklema and Kremer even at p_c.[10,15,16] In principle, this proof was given for N-step SAW's on all clusters including those that do not support any N-step SAW; this could be done for γ because the number of SAW's on such a cluster, zero, is well defined unlike the mean-square displacement of N-step SAW's. If we consider only the clusters that support at least one N-step SAW, however, the

disorder average $\overline{G_N}$ now acquires a normalization denominator just as in Eq. (3). Still, if p is fixed at some value above p_c, the denominator is not singular in N and thus γ is unchanged. However, as $p \to p_c^+$, both the denominator and the numerator of the expression $\overline{G_N}$ may acquire extra singularities in a similar way to those in Eq. (3) which may or may not cancel. In other words, γ by this definition may or may not change at p_c from the undiluted value.

This paper is organized as follows. In Sec. II we present our Monte Carlo data performed for square and simple cubic lattices. We present our raw data for the exponents ν and γ defined by the disorder averages of mean-square radius of gyration and number of SAW's, respectively. In Sec. III we describe the possible crossover of SAW's from *fractal* critical behavior to a Euclidean behavior. We first analyze our percolation cluster for p close to percolation thresholds and show that our walks are fully confined to the fractal region of clusters. We then use our present Monte Carlo data to test for the possibility of crossover scaling. In Sec. IV we discuss and summarize the results. Details of our Monte Carlo methods are presented in the Appendix.

II. MONTE CARLO RESULTS FOR THE EXPONENTS ν AND γ

We have studied SAW's on the percolation cluster by standard Monte Carlo simulations using the Hoshen-Kopelman algorithm[17] developed for percolation and a simple, unbiased sampling method[18] for SAW's.

We generate the site-percolating *incipient* infinite cluster, defined as the cluster which spans the cell of L^d lattice sites along all coordinate directions. After identifying such a cluster, any two opposite edges or faces are connected by the periodic boundary condition for the purpose of performing SAW's on them. Our cells are of a linear size L where $L=100$ for square lattice and 50 for simple cubic lattice. While these values are not large, they are sufficient for our purpose as we demonstrate in the Appendix.

We focus our study for p *very* close to p_c (within 0.1%) unlike the previous study on the diamond lattice[11] where the value of p closest to p_c was still about 29% (of p_c) off. Our values of p closest to p_c are $p=0.592\,73$ on the square lattice and 0.312 on the simple cubic lattice, where the best currently available values of p_c are $0.592\,745\pm0.000\,002$ (Ref. 19) and 0.3117 ± 0.0003 (Ref. 20) for square and simple cubic lattices, respectively. In addition we have also performed some simulations of SAW's for $p=0.4$, 0.5, and 1.0 on the simple cubic lattice and for $p=0.65$ and 1.0 on the square lattice in order to compare the convergence behavior in the asymptotic limit and to study the crossover scaling. More efficient enrichment techniques were also tried, but we found that such a method tends to produce unacceptably biased samples in this particular problem as we shall see below. Details of our method will be presented in the Appendix.

The critical exponent ν can be obtained from the Monte Carlo data for the disorder average of the mean-square radius of gyration. We concentrate on the mean-square radius of gyration rather than the more common end-to-end distance since the statistical fluctuations are much less of a problem for the former. A possible drawback of the radius of gyration is that it contains the effects of many small internal distances; however, we have confirmed that the two measures of chain lengths show the same trend. Some results for both quantities are shown in Table I. Our results for ν are expressed in terms of its *effective* value determined by SAW's of up to N steps or less, denoted by ν_N, defined by

$$\nu_N = \frac{N\overline{\langle s_N^2(C)\rangle}}{\overline{\langle s_1^2(C)\rangle}+\overline{\langle s_N^2(C)\rangle}+2\sum_{i=2}^{N-1}\overline{\langle s_i^2(C)\rangle}} - \frac{1}{2} . \quad (7)$$

If the correction to scaling for this quantity is of a power-law nature, then the asymptotic expression for ν_N should be

$$\nu_N = \nu + bN^{-\Delta} + cN^{-1} + \cdots , \quad (8)$$

where Δ is the leading correction-to-scaling exponent[21] and b and c are some nonuniversal constants.

The exponent γ can be obtained from the attrition in Monte Carlo sampling. Since each walk is not allowed to intersect with itself or to visit the randomly distributed impurity sites (vacancy), those walks which would form a closed loop or which are trapped by the impurity sites must be rejected from the ensemble of random walks. For longer walks the probability of forming loops or visiting dead ends is greater, and thus, the rate of survival decreases as N increases. In fact, the walk suffers such a high attrition rate in this particular problem that a significant number of samples were obtained only up to

TABLE I. Examples of the radii of gyration $\overline{\langle s_N^2\rangle}^{1/2}$ and end-to-end distances $\overline{\langle r_N^2\rangle}^{1/2}$ near p_c. S gives the number of starting points with one or more SAW's.

d	N	$\overline{\langle s_N^2\rangle}^{1/2}$ [a]	S	$\overline{\langle r_N^2\rangle}^{1/2}$ [a]	S
2	20	3.45±0.04%	696 266	9.41±0.05%	626 627
	40	5.77±0.09%	207 190	15.7 ±0.22%	186 916
	60	7.78±0.57%	4 854	21.1 ±1.34%	4 455
3	20	2.76±0.06%	232 430		
	40	4.24±0.15%	15 815		
	50	5.47±0.69%	1 225		

[a]The estimates are quoted with their fractional errors.

$N_{\max}=70$ and 50 for square and simple cubic lattices, respectively. While these values are relatively small, they are, however, sufficient to observe the trend for the asymptotic behavior.

The rate of survival is in general proportional to the number of SAW's divided by the number of unrestricted random walks (RW's). Thus, we have

$$A(N)/A(1) \propto G_N(\mathrm{SAW})/G_N(\mathrm{RW}) , \tag{9}$$

where $A(m)$ denotes the number of surviving m-step walks. Thus, using an asymptotic expression[9] for $G_N(\mathrm{SAW})$, we get

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

Here μ' denotes the connective constant on the infinite cluster and the ratio $G_N(\mathrm{RW})/G_{N-1}(\mathrm{RW})$ is simply the average number of allowed sites for a N-step RW to advance on the infinite cluster and, therefore, is independent of (or at most weakly dependent on) N. Thus, the critical exponent γ is obtained from the slope of the $\ln[A(N)/A(N-1)]$ versus $1/N$ plot.

Our data for ν_N on the simple cubic lattice for $p=0.312$ averaged over 240 clusters (grouped into six batches) are compared in Fig. 1 with the corresponding data on the fully occupied lattice. (This and the two following figures are essentially identical to those in the earlier note by two of us,[1] but they are included here for self-containedness.) For small N, ν_N near p_c is greater than the corresponding result on the full lattice; however, beyond about $N=25$ it seems to decrease far below the previously reported value of $\frac{2}{3}$ for the diamond lattice. Since the ν_N at $N=50$ is already about 0.612 ± 0.01, we expect ν_{p_c} to be even smaller than this value.

We also obtained additional data for $p=0.32$ for over 400 clusters and found the critical behavior very similar to that for $p=0.312$ (not shown). With these data, it would require an unjustifiable bias to conclude that ν_{p_c} is greater than ν. In fact our data indicate the ν_{p_c} cannot be very different (if at all) from that on the full lattice. If we accept that the leading correction term is nonanalytic as on the full lattice,[21] this conclusion is even more strongly forced on us.

Our data on the square lattice for $p=0.592\,73$ averaged over 1400 clusters (grouped into seven batches) are plotted in Fig. 2. The behavior of ν_N is similar to that on the simple cubic lattice for a wide range of N: up to about the 25th step, ν_N near p_c is monotonically increasing, and beyond that it seems to merge to the full lattice result suggesting that the Flory exponent is again not very different from that on the full lattice [with Eq. (5) in mind].

Figure 3 is a log-log plot of the mean-square radii of gyration for p close to p_c divided by the corresponding data on the full lattice as a function of the number of steps N, analogous to a figure in Ref. 11. For the square lattice, the curve becomes flat already for $N>30$, indicating that the lattice dilution simply affects the nonuniversal amplitude of the scaling ansatz with the Flory exponent remaining unchanged. In three dimensions, the result is somewhat less clear. Although we do not observe an asymptotic flat region, the slope of the plot decreases, suggesting that $N=50$ is not long enough to estimate ν in this manner. If we estimate ν_{p_c} from the slope

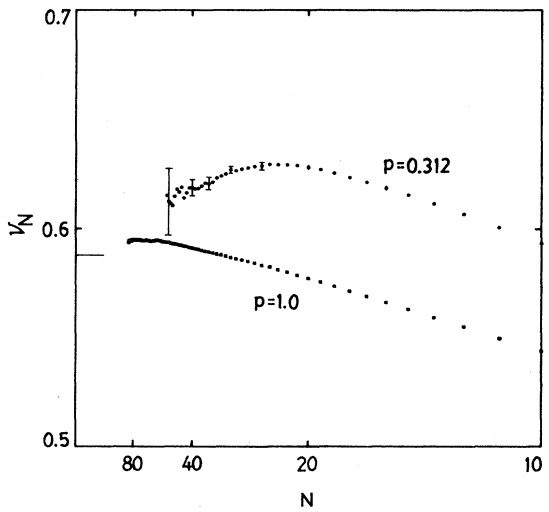

FIG. 1. The effective ν_N for $p=0.312$ on the simple cubic lattice in contrast with corresponding values on the full lattice. The error bars indicate the standard deviation among the averages from six batches of data each of which was obtained by averaging over 40 clusters.

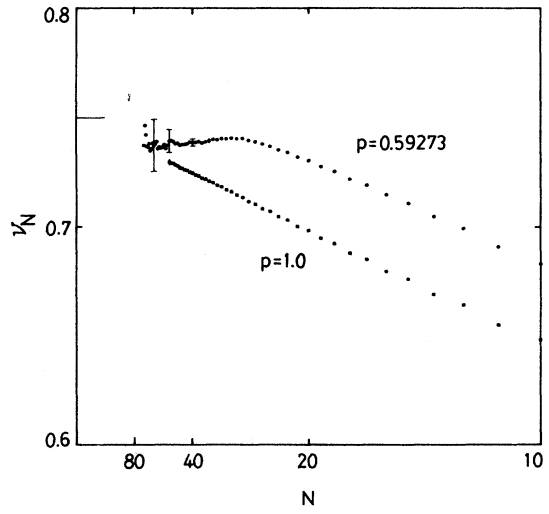

FIG. 2. The effective ν_N for $p=0.592\,73$ on the square lattice in contrast with corresponding values on the full lattice. The error bars indicate the standard deviation among the averages from seven batches of data each of which was obtained by averaging over 200 clusters.

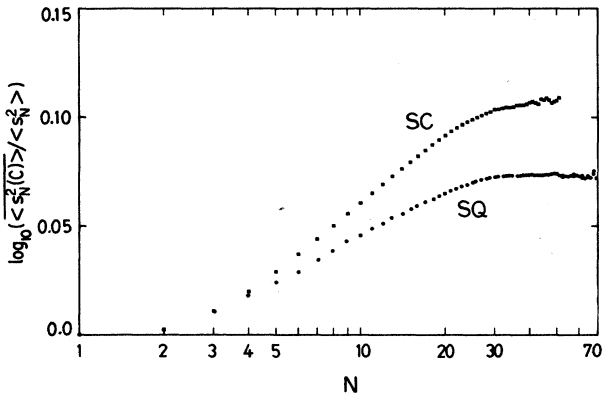

FIG. 3. Ratio of the disorder averaged mean-squared radius of gyration to the radius of gyration on the fully occupied lattice, $\langle s_N^2(C)\rangle / \langle s_N^2\rangle$, in log-log scale against N for $p=0.592\,73$ and 0.312 for square and simple cubic lattices, respectively.

near $N=50$, we will get $\nu_{p_c} \cong 0.605 \pm 0.01$, which agrees reasonably well with the linearly extrapolated vertical intercept in Fig. 1.

These results are consistent with the raw data of the earlier Monte Carlo work.[11] As is clear from Fig. 1, even the value of ν_N for the fully occupied lattice is still increasing at $N=50$ steps while it must decrease toward $\nu=0.588$ asymptotically. Since the full lattice behavior is already complicated in this three-dimensional case for a wide range of N, unlike the square lattice case where ν_N increases monotonically over a whole range, we do not know how it affects the slope in Fig. 3 for relatively small N. The decreasing trend in this kind of slope was not taken into account in the earlier work,[11] although such a trend was observable in their data. Thus our value mentioned above (about 0.605) on the simple cubic lattice should serve as an upper bound for the correct Flory exponent ν_{p_c}. It is necessary to extend considerably the length of walks in order to estimate the exponent accurately by this method.

Both for square and simple cubic lattices, the end-to-end distance itself (and equivalently the radius of gyration) for $p<1$ is in general greater than that on the full lattice, in agreement with the analytic argument referred to in the previous section.[10]

In order to observe the correct asymptotic behavior, we attempted to extend the length of walks using the standard enrichment method[22] on the square lattice. We will not discuss the details of this method here as they are well known. However, we found that this method appears to give biased samples for our particular problem at least in two respects.

First, enrichment does not seem to give the correct exponent γ. While the simple sampling method produces a sharp straight line in the plot of $\ln[A(N)/A(N-1)]$ versus $1/N$ as we will see later, the result of the enrichment method seems to be rather dependent on the number of trials in each stage, unlike on the full lattice.[23] (Note that the number of surviving walks of this method does not decrease monotonically; however, the ratio from two consecutive steps must provide a consistent behavior.)

Second, the distribution of the radius of gyration appears to be significantly shifted from that obtained by simple sampling. We obtained distribution functions of the radius of gyration $P(s^2)$ by Monte Carlo simulation using both simple sampling and enrichment methods for $N=25$, 45, 65. For the enrichment method, we chose the length of each stage to be ten steps and the number of trials to be seven in each stage. Our data for $N=25$ and 45 are shown in Fig. 4. For $N=25$, two curves overlap nearly completely showing that the two methods are consistent for the first few stages, while for $N=45$ a significant shift is already apparent. We found for $N=65$ the discrepancy to be even greater than this (not shown). It is obvious that both methods produce similar results for the first few stages where the two methods are not very different anyway.

These observations appear to emphasize the relative importance of an unbiased sampling and thus, restrict further extensions of this type of numerical calculations for this problem due to the requirement of prohibitively long computing times, even with today's fast computer systems.

Our data for a simple cubic lattice of the function defined in Eq. (10) versus $1/N$ are shown in Fig. 5. For p above p_c, e.g., $p=0.4$ and 0.5, data show parallel lines with a slope 0.166 ± 0.01, indicating that the critical exponent γ is well defined and is unchanged for weak dilutions in agreement with theoretical expectations.[8,10,15] For $p=0.312$ our data indicate a nontrivial slope over a wide range of N obtained in our simulation. [For $p=0.32$ we also obtained a similar result (not shown).] If we calculate the exponent γ from this slope, we will obtain

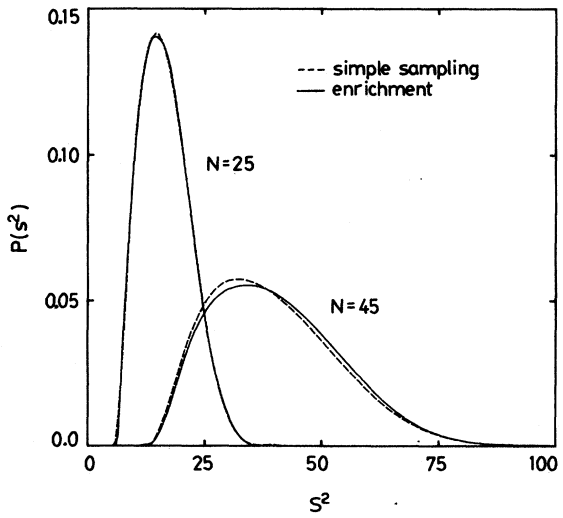

FIG. 4. The distributions of the radius of gyration for $N=25$ and 45 using simple sampling and enrichment technique. The distribution function was obtained for each starting point and averaged over all starting points with equal weighting.

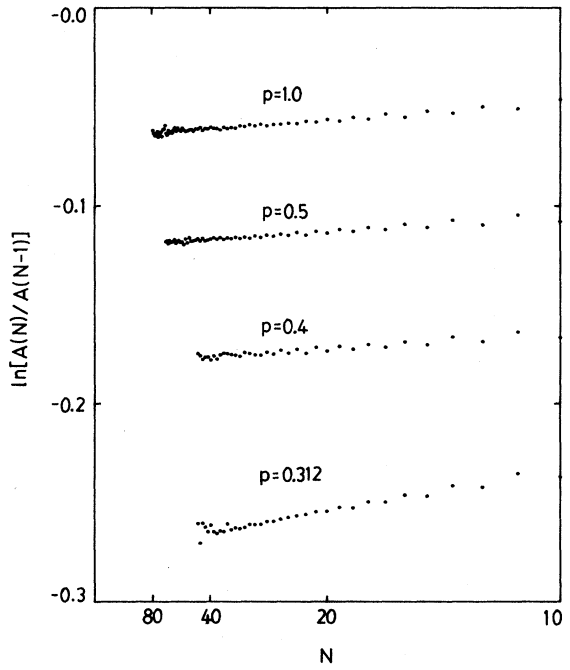

FIG. 5. Function $\ln[A(N)/A(N-1)]$ in Eq. (10) plotted against $1/N$ for various values of p for the simple cubic lattice. An asymptotic slope of each plot gives $\gamma-1$ for a given p.

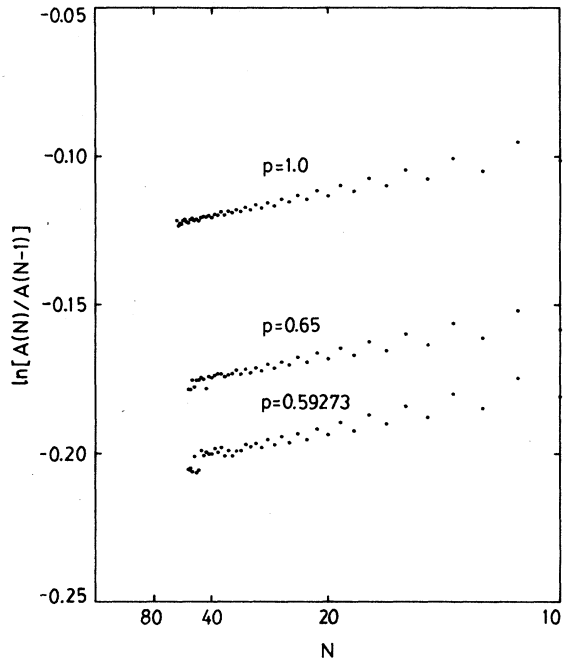

FIG. 6. Function $\ln[A(N)/A(N-1)]$ in Eq. (10) plotted against $1/N$ for various values of p for the square lattice. An asymptotic slope of each plot gives $\gamma-1$ for a given p.

$$\gamma_{p_c}=1.40\pm0.02 \quad \text{(3D)},$$

which is significantly greater than the full lattice value[3] ($\cong\frac{7}{6}$).

Corresponding data for the square lattice are shown in Fig. 6. Unlike the case of a simple cubic lattice, the plots for $p=0.592\,73$, 0.65, and 1.0 in this figure are all parallel indicating no change in γ even at p_c. Our estimated value of γ near p_c is

$$\gamma_{p_c}=1.33\pm0.02 \quad \text{(2D)},$$

which is very close to the full lattice value[4] ($\cong\frac{4}{3}$).

Our result for γ on the simple cubic lattice is rather surprising in view of the theorem proven by Lyklema and Kremer[10] that, if γ is defined using averages over all clusters, then it remains unchanged at any dilution.[10,15,16] However, this definition is somewhat unnatural since even the clusters which do not support a N-step SAW are included for that N, as we discussed earlier. With our present definition of γ using the averages only over those clusters supporting at least one N-step SAW, the exponent γ should not change for $p>p_c$, but what happens at p_c remains unclear. Still, in view of our conclusion on the exponent ν, we would normally expect γ to remain unchanged even there. This could actually be the case even though we seem to obtain a different value of γ at p_c for two possible reasons.

First, as stated before, since the length of walks for which enough samples were obtained in our simulation is not very large, our data do not rule out the possibility of a slow crossover to the full lattice result for N much larger than $N_{\max}$ obtained in our simulation. Second, our data are obtained from just the *infinite* or percolating cluster. If this average is different from that over all clusters (including the *finite* or nonpercolating clusters as long as they support at least one N-step SAW), then this could also explain the discrepancies.

In general, the contributions from nonpercolating clusters are expected to diminish more slowly in three dimensions than in two as $N\rightarrow\infty$ because the mean size of the clusters is more slowly decreasing in three dimensions when p is away from the percolation threshold.[24] This result is also expected from numerical observations: for the square lattice, the number of occupied sites on the spanning cluster is over 78% of all occupied sites, while for the simple cubic lattice less than 36% are on the infinite cluster indicating that there are more small clusters in three dimensions. Thus, in order to observe a correct asymptotic behavior explicitly, we again need to extend the length of walks considerably. We believe this part of the problem deserves much further study.

III. FRACTAL TO EUCLIDEAN CROSSOVER

Recently we have seen some studies[11,25,26] which propose generalized homogeneity for functions such as the mean-square end-to-end distance of the SAW's on randomly diluted lattices and study the crossover scaling from *fractal* to *Euclidean* behavior. Since the percolation cluster can be represented as a fractal[27] up to the coherence length ξ, where

$$\xi=\xi_{0+}\left|\frac{p-p_c}{p_c}\right|^{-\nu_{\rm perc}}, \tag{11}$$

with $\nu_{\rm perc}$ being the percolation coherence length exponent, one normally expects that for $\langle R_N\rangle \ll \xi$, a walk feels a fractal substrate structure and at $\langle R_N\rangle \sim \xi$ it crosses over to a Euclidean lattice behavior. Therefore the crossover region is defined by

$$\langle R_N\rangle \sim \xi \propto |p-p_c|^{-\nu_{\rm perc}} \tag{12}$$

or equivalently

$$N|p-p_c|^{\nu_{\rm perc}/\nu_{p_c}} \sim 1 . \tag{13}$$

In particular, a natural crossover scaling ansatz for the end-to-end distance in this case would be

$$\overline{\langle R_N^2\rangle}=N^{2\nu_{p_c}} f(N|p-p_c|^{\nu_{\rm perc}/\nu_{p_c}}) , \tag{14}$$

where

$$f(x)=\begin{cases}\text{const}, & \text{as } x\to 0 ,\\ x^{2(\nu-\nu_{p_c})}, & \text{as } x\to\infty .\end{cases} \tag{15}$$

This type of scaling function was first proposed by Kremer,[11] and more recently, by Roy and Chakrabarti[25] and by Kim[26] from the nodes-links model[27–29] of a percolation cluster. All these works assumed that the critical behavior right at p_c is different from that on the full lattice. Reference 11 in particular made a numerical study of this ansatz and reported good agreement with their Monte Carlo data. In this section, we analyze this problem in detail. First, we will show that our own Monte Carlo data obtained close to p_c fall well within the fractal regime and thus do not show such a crossover behavior. Next, we consider additional data away from p_c to study the possibility of scaling as in Eq. (14). Third, we reanalyze the data of Ref. 11 in the same way to show the apparent absence of the proposed scaling form, and finally, we discuss some alternate forms of crossover scaling.

A. Absence of crossover in our data near p_c

Our data observed in Figs. 1 and 2 appear somewhat similar to a crossover from one universality class to another as occurs in some problems in critical phenomena. Thus the basic question we can ask is, did such a crossover distort our conclusions on the asymptotic value of the exponent ν? In order to answer this, we will first see if the walks generated in our simulation indeed reached the crossover region where we expect $\langle R_N\rangle \sim \xi$.

If our observed behavior in Figs. 1 and 2 is indeed such a crossover, we would expect at least $R_{\rm max} > \xi$ where $R_{\rm max}$ is the longest end-to-end distance ($<N_{\rm max}$) obtained in our simulation. On the other hand, if $R_{\rm max} \ll \xi$, then the walk would be fully confined to a fractal region of the cluster and, thus, would be expected to show a fully *disordered* critical behavior. We believe that the coherence length of the clusters generated in our simulation is considerably longer than the end-to-end distance of SAW's we obtained in our simulation. Rough estimation gives, using the best known values[30] of $\nu_{\rm perc}$, $\nu_{\rm perc}(d=2)=\frac{4}{3}$ (exact) and $\nu_{\rm perc}(d=3)\cong 0.88$, $\xi/\xi_{0+}\cong 2\times 10^6$ and 5×10^2 for square and simple cubic lattices, respectively. Thus, assuming that the amplitude ξ_{0+} is of order unity, we have a coherence length $\approx 1-4$ orders of magnitude greater than the contour length of walks.

To confirm this in another way we measure the extent where a percolation cluster shows its fractal features. We have plotted on the log-log scale the number of occupied sites $M(r)$ on the infinite cluster in the circle (sphere for $d=3$) of radius r whose center is set on every starting point of SAW's. We expect at $r\sim\xi$ the slope of such a plot to increase from a fractal dimension D to a spatial dimension d. This break point should appear at $r\sim\xi<R_{\rm max}$ if our observation is indeed a crossover. Using the method described in the Appendix, we obtained the results as shown in Fig. 7. This figure clearly indicates that no such crossover occurs over the range of $r<L/2$. Here L is the linear dimension of the cluster we have chosen in the simulation and is 100 and 50 for square and simple cubic lattices, respectively.

We believe that a slight decrease in the slope near the edge in each plot is due to the underlying finite-size effect associated with the free boundaries. In fact such a finite-size effect exists at every point in the figure and results in our measured fractal dimensions near p_c, $D=1.88\pm0.005$ for $d=2$ and 2.50 ± 0.005 for $d=3$, to be very slightly smaller than the theoretically expected values.[31] For $p=0.32$ on the simple cubic lattice, data also show a straight line for a wide range of r, however with the slope ($\cong 2.75\pm0.005$) significantly greater than the expected fractal dimensionality $D\cong 2.52$.[31] This seems to indicate that the cluster for $p=0.32$ resembles a fractal of somewhat different fractal dimension for a certain extent of length scale, and presumably, this might be a reason that the critical behavior for this value of p was

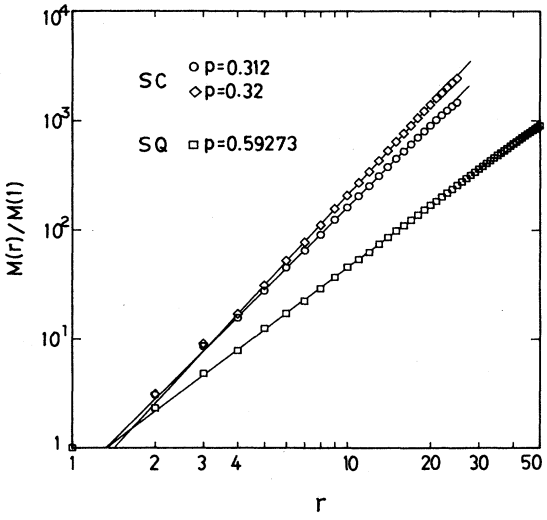

FIG. 7. The number of occupied sites $M(r)$ on the infinite cluster within the circle (sphere for 3D) of radius r plotted against r.

not very different from that for $p=0.312$ as we discussed before.

We also note that no walks starting from the center of cluster reach the boundary of the cluster for $N \leq N_{\max}$ both for simple cubic and square lattices and thus, $R_{\max} < L/2 \ll \xi$. Thus we confirm for our values of $N_{\max}$ the walk is fully confined to the fractal region and no crossover from a *disordered* critical behavior to a *pure* full lattice behavior can possibly exist in our data near p_c.

B. Test of crossover scaling from our extended data

We have also studied the proposed scaling form of Eq. (14) with our present Monte Carlo data for the simple cubic lattice. Since an asymptotic behavior of the end-to-end distance is in general similar to that of the radius of gyration, the same scaling form should also be valid for the radius of gyration as well. We thus studied the scaling function of the mean-square radius of gyration in large and small limits of the scaling variable $x \equiv N|p-p_c|^{\nu_{\text{perc}}/\nu_{p_c}}$.

Our data for the simple cubic lattice plotted on the log-log scale are shown in Fig. 8. Figure 8(a) is for the trial value of $\nu_{p_c}=0.59$ assuming that the Flory exponent remains unchanged for any p (in agreement with our observation). Since $\langle s_N^2 \rangle \propto N^{2\nu}$ for $N \gg 1$, this graph is in principle similar to Fig. 4 in the asymptotically large N limit except that the horizontal scale is changed; $N \to N|p-p_c|^{\nu_{\text{perc}}/\nu}$. Thus, as was discussed in Sec. II, since $N=50$ is not long enough to observe an asymptotic limit, our data for $p=0.312$ and 0.32 in this figure do not show the correct limit of scaling in the $x \ll 1$ region. Since the observed value of effective ν_N is 0.612 ± 0.01 up to $N_{\max}=50$, the asymptotic value of ν_{p_c} ($=0.59$) would be too small to observe the correct $x \ll 1$ behavior up to our values of $N_{\max}$ even for p considerably greater than p_c; however, we expect our data for each p to eventually show a flat curve if we extend the length of walks sufficiently. In practice, however, it would be difficult to observe a correct asymptotic behavior in this kind of figure even for a relatively large N by Monte Carlo simulation. Recent work[32] indicates that, for N over 2000 steps on the full lattice, the observed effective Flory exponent is just about 0.593, while theoretically the best known value is 0.588.

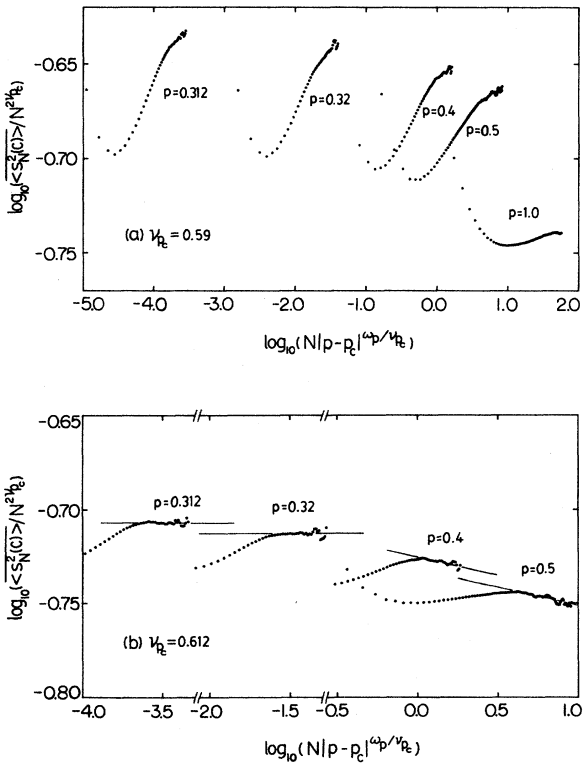

FIG. 8. Function $f(x)$ in Eq. (14) plotted against the proposed scaling variable using our Monte Carlo data. (a) is for the choice of $\nu_{p_c}=0.59$ and (b) is for $\nu_{p_c}=0.612$. Solid lines are intended for visual aids.

Figure 8(b) is for the trial choice of $\nu_{p_c}=0.612$ which is identical to our observed value of effective ν_N at $N=50$. Assuming that the length of walks is sufficient to observe an asymptotic behavior (despite our earlier observation), we try to examine the possibility of data collapsing. Since some of our values of p are extremely close to the best known p_c, and since the contour length of the walk is relatively short, data are far apart for each given p, and thus, it is rather difficult to visualize the degree of data collapsing in our case. (Notice that the horizontal scale is broken in two places.) An asymptotic straight line drawn for each given p is for a visual aid. For this value of ν_{p_c}, data seem to show correct $x \to 0$ limit, i.e., $f(x)=$const for $x \ll 1$; however, the prefactor seems to depend upon p. Thus, the data do not seem to scale in this limit. (Note that we only need to consider $N \gg 1$ since an asymptotic behavior of SAW's for each p is expected only in this limit.)

For $x \gg 1$, since walks are not long enough for p close to p_c, our data for $p=0.312$ and 0.32 do not reach this region. We, instead, use the Monte Carlo data for $p=0.4$ averaged over 130 clusters and for $p=0.5$ over 80 clusters to observe this limit. The data for these values of p show parallel straight lines with nonzero slope for $N \gg 1$ but do not seem to collapse onto a single line even in this limit. The absolute slope of these lines is less than the expected value of $2(\nu_{p_c}-\nu) \cong 0.048$ (with the present choice of the trial value of ν_{p_c}), which indicates that our $N_{\max}$, even for p relatively larger than p_c ($N_{\max}=100$ for $p=0.5$), is still not long enough to reach the asymptotic limit. This has been already observable in Fig. 8(a), where the plots for $p=0.4$ and 0.5 were not flat for large N when scaled with $\nu_{p_c}=0.59$.

Thus, in both limits, the scaling function shows the correct limit with the choice of $\nu_{p_c}=0.612$; however, the data do not seem to collapse onto a single curve. Although a proper asymptotic limit has not been reached yet, our data in Fig. 8(b) seems to be suggestive of the absence of such a crossover scaling. We have in addition studied the possible scaling form with the previously re-

ported value[11] of $\nu_{p_c}=\frac{2}{3}$, but we were not able to obtain the correct $x\to 0$ limit where the data should become flat.

C. Reanalysis of Kremer's data for crossover scaling

We have also reviewed the same scaling ansatz with Kremer's Monte Carlo data[11] and plotted them in Fig. 9. Figure 9(a) is for Kremer's original choice of $\nu_{p_c}(=\frac{2}{3})$. Although these data have previously been claimed to scale with this value of ν_{p_c}, our plot indicates that this choice is too large to observe a correct $x\to 0$ limit, in agreement with our observation from our own data. Figure 9(b) is plotted for a test value of $\nu_{p_c}=0.635$ which shows the correct $x\to 0$ limit, but data do not seem to scale. Also this value of ν_{p_c} does not seem to give a correct slope in the $x\gg 1$ region. While an asymptotic slope $2|\nu-\nu_{p_c}|\cong 0.16$ for this choice of ν_{p_c} is expected, a measured value is less than 0.14, indicating that the length of walks used in his simulation is also not long enough. (Note that he used $N_{\max}=70$ for $p=0.75$ and 0.85.)

Thus even Kremer's own data do not exclude the possibility that the slope for the $x\ll 1$ region goes further down in the asymptotic limit of $N\to\infty$. In fact, this is already seen in Fig. 9: for $p=0.55$ indicated as circles in both (a) and (b), the slope calculated between the last two points ($N=30$ and 50) is less than that of the first two points ($N=20$ and 30), and thus, in the large N limit, even $\nu_{p_c}=0.635$ may not seem to result in the correct $x\to 0$ limit of scaling function if the length of chain is further extended. Thus, the data collapsing for his measured value of ν_{p_c} seem also accidental.

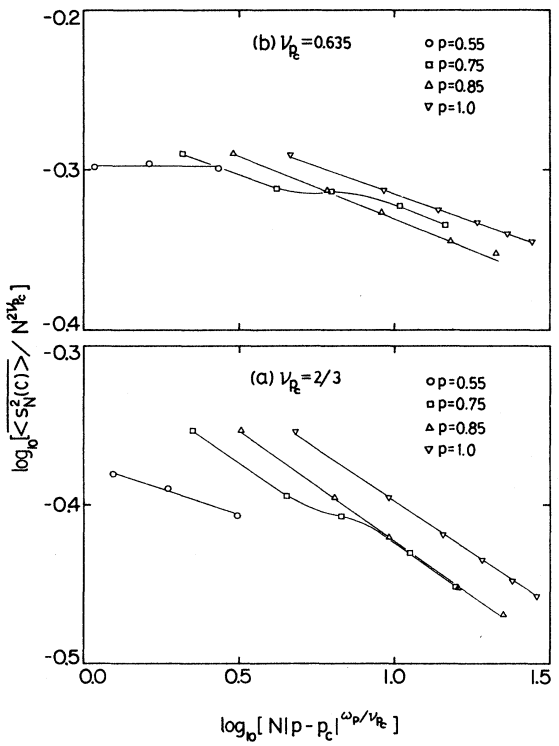

FIG. 9. Function $f(x)$ in Eq. (14) plotted against the proposed scaling variable using the data in Ref. 11 for (a) $\nu_{p_c}=\frac{2}{3}$ and (b) $\nu_{p_c}=0.635$. Solid lines are intended for visual aids.

One important point we should mention here is that if we choose a higher ν_{p_c}, then the slope in the $x\gg 1$ region will generally become (negatively) greater up to a certain extent, and thus, the gap between any two asymptotic parallel lines will become smaller [see Fig. 9(b)]. For an appropriate choice of ν_{p_c}, we can artificially make any two sets of data fall on a single line; however, this does not indicate a scaling of data since this value of ν_{p_c} does not necessarily produce a correct $x\to 0$ limit and since this does not guarantee the third set of data for different p to fall on the same curve. For our data for $p=0.4$ and 0.5, this seems to occur for $\nu_{p_c}\cong 0.62$.

D. Alternative crossover scaling possibilities

Beyond these numerical difficulties, we may note that there can exist at least several other equally plausible crossover scaling ansatz if the crossover scaling indeed exists: e.g., we can replace ν_{p_c} in Eq. (19) by ν and write

$$\overline{\langle R_N^2\rangle}=N^{2\nu}g(N|p-p_c|^{\nu_{\rm perc}/\nu}) , \tag{16}$$

where $g(x)$ should behave as

$$g(x)=\begin{cases} x^{2(\nu_{p_c}-\nu)}, & \text{as } x\to 0 , \\ \text{const}, & \text{as } x\to\infty . \end{cases} \tag{17}$$

This scaling form would produce the same N dependence in the *disordered* and *pure* limits as those of Eq. (14), but they are distinct as the p dependence is clearly different if $\nu_{p_c}\neq\nu$.

This observation again leads us to suspect that the only reasonable scaling form (if scaling holds at all), would require $\nu=\nu_{p_c}$. In this case, we may suppose, say, the form in Eq. (17) with

$$g(x)=\begin{cases} a, & \text{as } x\to 0 , \\ b, & \text{as } x\to\infty . \end{cases} \tag{18}$$

where a and b are some constants with $a>b$. This kind of saturation of a scaling function is not new and can be seen, e.g., in the problem of surface magnetism with surface magnetic fields. Our observation for the Flory exponent is not inconsistent with such a scaling form although neither our present data nor Kremer's data[11] appear to probe a sufficiently asymptotic region, and thus it has not been confirmed numerically yet.

IV. SUMMARY AND DISCUSSIONS

Based on extensive Monte Carlo simulations performed much closer to p_c than the only previous work of this type,[11] we have estimated the critical exponents ν and γ for SAW's on randomly diluted square and simple cubic lattices. Our observation for ν for the simple cubic lat-

tice is very different from that previously reported in Ref. 11 from Monte Carlo results on the diamond lattice and also, ν for the square lattice is very different from those for SAW's on some two-dimensional geometrical fractals where exact Flory exponents are known. While new higher values of ν were obtained for various fractal lattices[33–35] and also higher ν was reported previously for the randomly diluted diamond lattice,[11] our results are rather similar to that on the full lattice, or, if different at all, the difference seems to be much smaller than previously suggested.[11] These results are also different from those of free random walks and from those of so-called true self-avoiding walks (TSAW's) on the critical percolation cluster, where sharp changes in ν to the new lower values ($\nu_{p_c} \cong 0.35$ in 2D and $\nu_{p_c} \cong 0.27$ in 3D) were observed.[36,37]

A crude argument that explains why the critical behavior of SAW's may be different from that of TSAW's (or RW's) may be as follows. In general the lattice dilution seems to affect the random walks mainly in two different ways. Since the percolation cluster generated near p_c contains many singly connected (red) bonds,[38] the walk is, in many cases, allowed to grow locally along only the particular direction of the bond if the particular site lies on such a bond. On the other hand, in some cases, the dilution effectively traps the walk and induces the self-intersections or immediate returns (backscattering). The overall disorder average of the former effect seems to favor larger end-to-end distances than on the fully occupied lattice, while the latter effect favors shorter end-to-end distances.

For the TSAW's and RW's where both effects exist, the disorder average of the end-to-end distance is in general shorter than that on the full lattice, and thus, the latter effect seems to dominate the end-to-end distance. For the SAW, on the other hand, if the walk is trapped by its previous path or by the diluted sites, it must stop and the whole sample must be discarded. Thus only the former effect seems to remain, which results in longer end-to-end distances than on the full lattice. However, since the particular elongated walks that pass through many singly connected bonds may more easily visit the dead ends and stop growing, the probability of survival of such walks should be relatively small. Thus the average occurrence of such effective elongations does not seem to increase sufficiently rapidly as the walk grows. We surmise that this may be the cause of the value of the Flory exponent being similar to the full lattice one.

We have also estimated the critical exponent γ on the square and simple cubic lattices. While a similar result to that on the full lattice is observed for all $p \geq p_c$ in two dimensions, a new considerably higher value was indicated at p_c for the simple cubic lattice. This observation may suggest that a clear distinction should be made in the statistics of SAW's between the average only over the clusters which support at least one SAW of a given length and the average over all clusters, where in the latter case the exponent γ is known to remain unchanged even at p_c. (The possible distinction[25] between using only the infinite cluster even for finite N and using the average over all clusters supporting N-step SAW's is yet another matter.) We do caution, however, that the maximum number of steps for which enough samples were obtained in our simulation is not sufficiently large to observe an asymptotic behavior accurately, and thus, we do not exclude the possibility of a slow crossover to the full lattice result for N much larger than that we obtained in our simulation.

In regard to the question of fractal-to-Euclidean crossover possibly creeping into our data near p_c, we have performed extensive analysis of the size of the fractal region in our simulation. Through this analysis, we have concluded that the walks generated in our simulation are fully confined to the fractal region of the percolation clusters both for square and simple cubic lattices. This can also be confirmed by considering a recently observed behavior[37] of TSAW for the same value of p as the one used in our simulation for the square lattice. The effective ν_N defined in Eq. (12) for such walks shows a sharp decrease far below the full lattice value ($=\frac{1}{2}$) at the same p, and thus, the fractal region seems relatively wide at least for the square lattice case.

We have also studied the possibility of crossover scaling in the radius of gyration based on our Monte Carlo data from a broad region around p_c. We, however, did not observe any evidence of data collapsing for a given scaling form in Eq. (14) in disagreement with a previous study.[11] One possibility that would be suggested is that the percolation threshold is not a special point for SAW's. For example, if the lattice dilution simply changes the connective constant ($\mu \rightarrow p\mu$) for SAW's for all p including p_c, we would expect the disorder to be irrelevant. If this were indeed the case, our observation for the Flory exponent would be in disagreement with the real-space renormalization-group studies and apparently also with our observation for γ for the simple cubic lattice (assuming no slow transient effects). One possible way we can reconcile these discrepancies would be that the difference of the Flory exponent between *disordered* and *pure* cases is just too small, and it would be virtually unobservable by Monte Carlo simulation, or otherwise, the two different fixed points give the same Flory exponent although the critical behavior may be different. In the latter case, however, we would normally expect the crossover scaling to hold in a way similar to Eq. (18) near the percolation threshold and in the asymptotically large N limit. Our data do not seem sufficient to observe this kind of scaling, and we leave this part of the problem to a future study.

ACKNOWLEDGMENTS

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APPENDIX: MONTE CARLO METHOD

In this appendix we discuss some details of our Monte Carlo method whose data are displayed in Fig. 1–9. Our simulation method consists of two parts: (i) generation of

a percolation cluster and (ii) generation of SAW's on a percolation cluster.

Our method for the generation of a percolation cluster is a simple extension of the Hoshen-Kopelman algorithm.[17] We will not discuss the details of this algorithm as they are now well known. We generate the *site-percolating* clusters on the square and simple cubic lattices. The choice of the lattice in a given dimensional space is for programming simplicity, and we believe that the lattice type has no effect on universal quantities such as the critical exponents.

We follow a usual algorithm for percolation: pick a random number between 0 and 1 for each site of the cell that contains L^d lattice sites, and if this number lies between 0 and p, a given site is filled (undiluted), and otherwise empty (diluted). We generate the site-percolated *incipient* infinite clusters defined as clusters which span the cell along all coordinate directions, and after identifying such clusters, any two opposite edges or faces are connected by the *periodic* boundaries for the purpose of performing SAW's on them. One complete procedure of generating clusters for a square cell of 10^4 lattice sites takes, when there is no failed attempt, less than 2.5 sec of CPU time on the Digital Equipment Vax 11/750 computer system.

Since the cluster is not isotropic, and since the center point of the cell may not be on the *infinite* (or spanning) cluster, a walk cannot generally start from the center, and, thus, we choose the starting point randomly on the infinite cluster. 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 performing this procedure, the new disorder configuration may look different from the original one; however, the connectivity is unchanged. Thus, for any chosen starting point, the effective disorder configuration for SAW's depends upon the starting points, and thus, instead of using only one starting point per cluster, we choose many different points in each cluster and generate a predetermined number of SAW's from each starting point. The number of starting points chosen on each cluster is 500 and 1000 for square and simple cubic lattice, respectively.

In general, however, since the number of SAW's is different for different disorder, it is necessary to weight each disorder. Assuming that, for a given disorder (also for a given starting point), the number of SAW's is *roughly* proportional to the number of occupied nearest-neighbor sites to the starting point, say z' (number of one-step walk is proportional to this), we attempt $z'w$ walks for each given point, where we used $w=200$ both for square and simple cubic lattices. The SAW's are averaged first for each starting point and then for all starting points with equal weighting for each cluster. To carry out a sufficient disorder average, we repeat the same procedure over many entirely new clusters, the number of which being 240 for the simple cubic and 1400 for the square lattice. The final disorder average for each given N is carried out for many different clusters with the weighting proportional to the number of starting points for which at least one N-step walk is obtained.

The generation of the SAW's follow the usual simple sampling method. We assign an equal probability for each nearest-neighbor occupied site where a walk could advance when the next step is taken (if the site is empty, a probability 0 is assigned). We pick a random number between 0 and 1 and choose the next step as usual. If the walk makes a closed loop or if it visits the dead end, it will stop immediately and a new walk will be attempted from the given starting point. In practice, these were carried out with great efficiency by relabeling every site on the infinite cluster specifying the number of nearest-neighbor occupied sites and their positions for each given point, e.g., for the square lattice, using the integer arithmetic with the first four digits specifying the positions of nearest-neighbor undiluted sites and the fifth digit the total number of undiluted nearest-neighbor sites.

In practice, since we are not able to generate a true infinite cluster, we will always be faced with the finite-size effect. To minimize such an effect, we would like to have as large a cluster as possible; however, the generation of large clusters is quite time consuming and thus we must choose the optimal size of the cluster. In principle, the finite-size effect on the percolation problem is mainly caused by many small clusters near the edges (faces for 3D) which are artificially connected to the infinite cluster because of the periodic boundaries, but which would not be connected if free boundaries were used. In our problem, however, since the walk effectively starts from the center of the cluster, such small clusters do not affect the SAW's as long as the cluster size is larger than twice the longest end-to-end distance of the walks we obtain, $R_{\max}(<N_{\max})$. Thus, we generated many small batches of data to estimate the length of walks for which we were able to obtain enough samples in a reasonable amount of computer time. Unfortunately because of the extremely high attrition rates, we were able to obtain only up to 70 and 50 steps for square and simple cubic lattices, respectively. For these lengths of walks, we found that walks never reached the edges of the cluster of size L, where $L=100$ and 50 for square and simple cubic lattices, respectively.

We have chosen in each cluster 500 starting points for the square lattice and 1000 starting points for the simple cubic lattice. For the square lattice at $p=0.592\,73$, each cluster takes about one minute to generate and to perform the above number of SAW's on it on the Cyber205 computer system (without vectorization). On Vax 11/750 and Masscomp 5500 (which were used for the bulk of the data), the corresponding time was about 20 min. For $p=0.312$ on the simple cubic lattice, it takes about 2.5 h to construct and perform SAW's on an infinite cluster on the Vax 11/750 computer system; most of the time is spent in searching for a spanning cluster. For p far above p_c, e.g., $p=0.4$, and 0.5 for the simple cubic lattice, and $p=0.65$ for the square lattice, the computing time for the percolation step would be reduced. However, the time for the SAW step would be increased since the longer walks can easily be obtainable because of fewer singly connected bonds and fewer dead ends on the cluster. If all computer times were simply added, it would amount to over 1000 h; of course much of this was

performed on relatively small computers such as Vax 11/750 and Masscomp 5500.

We have also measured the extent of the region in which the cluster shows fractal features. We counted the number of occupied sites on the infinite cluster inside the circle (sphere for $d=3$) of radius r to search for a break point where a cluster may begin to show a Euclidean dimensionality. The number of occupied sites $M(r)$ was measured as follows. We first randomly choose the center for the cluster and translate the cell boundaries using a periodic boundary condition so that it does become the geometric center. After this has been done, we apply a free boundary condition at the edges and remove parts of the cluster which becomes disconnected in this operation. The number of occupied sites are counted inside the circle (sphere) of radius r, given as $r=(\sum_{i=1}^{d} n_i^2)^{1/2}$ for any combinations of integers $n_i=0,1,2,\ldots$ up to $r=L/2$. The final results are then averaged over many choices for the center and over many disorder configurations. (Note that in Fig. 5 we displayed the results only for integer values of r.)

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