Self-Avoiding Walks on Randomly Diluted Lattices

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We present new results of Monte Carlo simulations for self-avoiding walks on randomly diluted square and simple-cubic lattices performed very close to the percolation thresholds. Our results indicate the asymptotic behavior of the walk dimension to be rather similar to the undiluted lattice even at critical dilution.

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The effect of the environmental disorder on critical behavior is a long-standing problem in condensed matter physics. When the disorder is itself critical, the question is particularly delicate as two diverging lengths possibly compete. In this Letter, we address a particularly controversial case of self-avoiding walks on critically diluted lattices, relevant to linear-chain polymers in the dilute solution confined in a porous media. This question was first raised by Chakrabarti and Kertesz,[1] who applied the Harris criterion[2] to the disordered n-component spin system in the $n \to 0$ limit, and has been of much controversy for the last few years.[1,3-5]

The Harris criterion states that if the specific-heat exponent α is positive, then the fixed point for a pure system is unstable and thus the critical behavior for any amount of disorder is expected to be different from that for the normal system. Applied directly, it would imply that a crossover should occur for $d < 4$ since α for self-avoiding walks (SAW's) is positive. Derrida[5] has also studied SAW's on random strips and found an indication of a change in the critical behavior even for a weak dilution. On the other hand, Harris[3] claimed that the disorder average is very much trivial and the critical behavior of SAW's remains unchanged for any amount of disorder. This has been partially supported by field-theoretic renormalization calculations.[6]

Recently Lyklema and Kremer[4] presented an argument that the randomness is irrelevant except at the critical concentration of undiluted sites p_c above which an infinite network appears. They argued that the end-to-end distance is greater than on the full lattice and that this behavior becomes singular as $p \to p_c^+$ so that the Flory exponent p_c is expected to be greater than the full lattice value. However, a closer inspection raises a question of whether this argument rigorously rules out the possibility of an equality even for an asymptotically large number of steps N. We thus expect

$$\nu_p \geq \nu , \tag{1}$$

where ν_p is the Flory exponent on the diluted lattice of concentration p and ν is the corresponding value on the full lattice. The neglect of this possibility may have misled the conclusions of some published works.[4-7]

The only previous Monte Carlo work[8] was performed on a diamond lattice, and it indicated no change in the Flory exponent for a weak dilution, but close to p_c, a new higher value $\nu_{p_c} \cong \frac{2}{3}$ was observed. This value of ν_{p_c} agrees surprisingly well with the simply modified Flory-type formula[8] $\nu_F = 3/(D+2)$, where D is the fractal dimension of the critical percolation cluster. This has also been supported in two dimensions by simple, two-parameter cell renormalization studies,[7,9,10] where the random fixed point is found to be unstable with respect to the nonrandom fixed point.

Unfortunately, however, the agreement between Monte Carlo simulations and the modified Flory formula seems to have been accidental, being dependent on an error[11] in the data analysis in the original Monte Carlo work.[8] After correcting for this error, and otherwise using their own method of analysis, their data would yield an estimate for ν_{p_c} of about 0.62 or even less, thus making the answers to all related questions inconclusive.

In this Letter we present new results of Monte Carlo simulations for SAW's performed on the site-percolation clusters both on the square and simple-cubic lattices. We focus our study for p very close to p_c, with our values of p including $p = 0.59273$ for the square lattice and $p = 0.312$ for the simple-cubic lattice. The best currently available estimates of p_c are 0.592745 ± 0.000002 (Ref. 12) for the square and 0.3117 ± 0.0003 (Ref. 13) for the simple-cubic lattice, respectively. We will focus in our present study mainly on the exponent ν_{p_c}, leaving other aspects of the problem to a subsequent paper.

Our method is a Monte Carlo simulation using the Hoshen-Kopelman algorithm[14] developed for percolation and a simple sampling method for SAW's.[15] More efficient enrichment techniques were found to produce unacceptably biased samples in this particular problem. Site-percolating *incipient* infinite clusters are defined as a cluster spanning a lattice L^d sites along all coordinate direction. After identification of such a cluster, opposite faces are connected by the periodic boundary condition for performing SAW's on them (to reduce boundary and finite-size effects). We use $L = 100$ for the square and 50 for the simple-cubic lattice. While these values are not large, they are sufficient for our purposes as dis-

cussed below.

SAW's are started on this *infinite* cluster from many randomly chosen points (500 and 1000 in $d=2$ and 3, respectively); the number started from each being 200 times the number of occupied neighbors of that point. The total number of starting points with one or more SAW's surviving to twenty steps in $d=2$ is almost 700000, decreasing to about 5000 for sixty steps. In $d=3$, this number ranges from 230000 for twenty steps to 1225 for fifty steps. The average is first taken over the SAW's for a given disorder configuration C, and then the disorder average is carried out for many different C.

We concentrate on the mean-square radius of gyration $\langle\langle s_N^2\rangle_W\rangle_C$ rather than the end-to-end distance since the statistical fluctuation of the former is much smaller. The actual values of $\langle\langle s_N^2\rangle_W\rangle_C^{1/2}$ for $d=3$, for example, range from $(2.76\pm0.06)\%$ for $N=20$ to $(5.47\pm0.69)\%$ for $N=50$. We have confirmed numerically that the two measures of chain lengths show the same trend. The computing time required was about 20 min per cluster in $d=2$ and 2.5 h per cluster in $d=3$ on machines such as a VAX 11/750; some work was also done on a Control Data Corporation Cyber 205.

It should be noted that, for any given N, not every cluster can support an N-step SAW, and an average radii of gyration of N-step SAW's could only be defined over clusters that support at least one such walk. The ensemble of such clusters will be smaller for increasing N. It remains unproven that a disorder average over such successively smaller ensembles gives the same asymptotic N dependence for the radius of gyration as the average over the infinite cluster alone. However, since asymptotically long SAW's can exist only on the infinite cluster, it appears that considering only the infinite cluster is permissible.

We define an effective value ν_N for the Flory exponent ν arising from SAW's of N steps or less, by

$$\nu_N=\frac{N\langle\langle s_N^2\rangle_W\rangle_C}{\langle\langle s_1^2\rangle_W\rangle_C+\langle\langle s_N^2\rangle_W\rangle_C+2\sum_{i=2}^{N-1}\langle\langle s_i^2\rangle_W\rangle_C}-\frac{1}{2}, \quad (2)$$

and express our main results in terms of ν_N. Here, $\langle\ldots\rangle_W$ denote the average over all SAW's on a given disorder configuration and $\langle\ldots\rangle_C$ denote the average over the disorder configurations. If the correlation to scaling for this quantity is a power law, then then the asymptotic expression for ν_N should be

$$\nu_N=\nu+bN^{-\Delta}+cN^{-1}+\cdots, \quad (3)$$

where Δ is the leading correction-to-scaling exponent.

Our data for ν_N on the simple-cubic lattice for $p=0.312$ averaged over 240 percolating clusters are compared in Fig. 1 with the data on the fully occupied lattice. For small N, the value of ν_N is greater than on the full lattice, and the two are nearly parallel up to about the 25th step; however, beyond that it seems to decrease far below the previously reported value, $\frac{2}{3}$, for the diamond lattice.[8] The value of ν_N at $N=50$ is about 0.612 ± 0.01, and since the intercept with the $N=\infty$ axis represents the Flory exponent, we expect ν_{p_c} to be even smaller than this. With these data, it would require an unjustifiable bias to conclude that ν_{p_c} is greater than ν of about 0.59.[16] Our data indicate that ν_{p_c} cannot be very different (if at all) from the full lattice value.

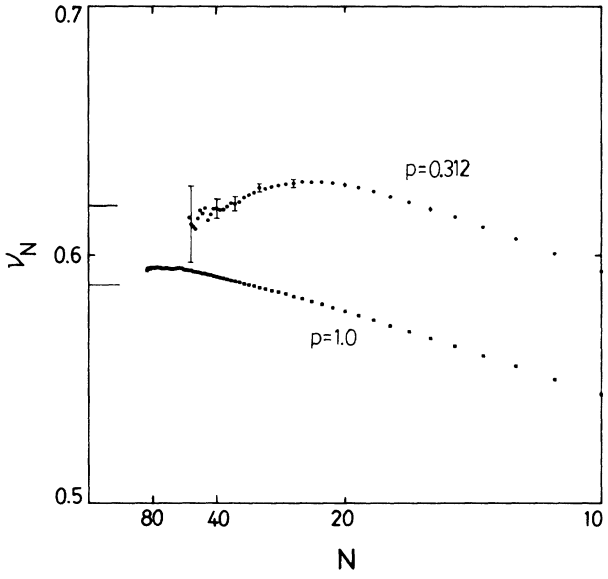

FIG. 1. ν_N vs N for the simple-cubic lattice at $p=0.312$ compared with the fully occupied lattice. Error bars indicate standard error over six batches. Indicated on the ordinate are the values (0.62) that Ref. 8 would give after correction of their error and the full lattice value (0.588).

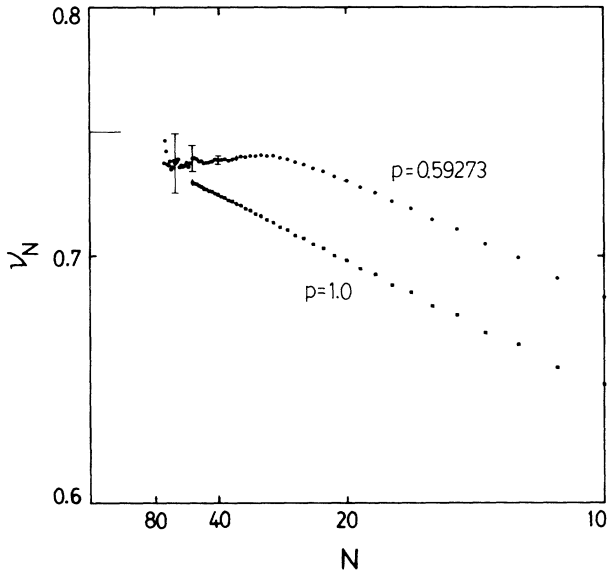

FIG. 2. ν_N vs N for the square lattice at $p=0.59273$ compared with the fully occupied lattice. Error bars indicate standard error over seven batches.

Our data on the square lattice for $p=0.59273$ averaged over 1400 clusters are plotted in Fig. 2. The behavior of ν_N is similar to that of the simple-cubic lattice, suggesting that the Flory exponent is again not very different from that on the full lattice.

Figure 3 is a log-log plot of the mean-square radii of gyration for p close to p_c divided by the data on the full lattice as a function of N, for square and simple-cubic lattices. For the square lattice, the plot 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 continuously decreases, suggesting that $N=50$ is not long enough to estimate ν in this way.

These results are consistent with the raw data of the earlier Monte Carlo work,[8] taking into account the difference of lattice type and the obvious calculational error.[11] If we neglect a decreasing trend in ν_N in Fig. 1, and compute ν_{p_c} from our data by the same method as in Ref. 8, using only the corresponding data points, we get $\nu_{p_c}\cong 0.615$. This is close to what one would get from their data after the required correction.[11]

There remains a concern that the behavior observed in Figs. 1 or 2 resembles a crossover from one universality class to another. Indeed, we would expect such a crossover to occur at the chain length $R\sim\xi$ where ξ is the coherence length for the percolation problem at the given value of p. In our case, however, ξ is of $O(10^6)$ for square and $O(10^2)$ for simple-cubic lattices and much longer than the end-to-end distance of SAW's. Therefore a full crossover is impossible. We have also confirmed this directly by plotting the number of sites on the percolating cluster as a function of distance from a *center*, then averaging over many centers and disorder configurations. No crossover was found in the slope of such a plot from the fractal dimension D to the lattice dimensionality d.

The crossover discussed above was considered by a number of previous studies[8,17,18] and a scaling form for R was postulated by the following:

$$R\propto N^{\nu_{p_c}} f(N^{\nu_{p_c}}/\xi)\,, \tag{4}$$

where $f(x)$ is supposed to behave as

$$\begin{aligned} &f(x)\to \text{const as } x\to 0\,,\\ &\sim x^{(\nu-\nu_{p_c})/\nu_{p_c}} \text{ as } x\to\infty\,. \end{aligned} \tag{5}$$

Although some numerical support for this form of scaling was claimed with use of ν_{p_c} of $\frac{2}{3}$ in three dimensions,[8] a closer inspection of those data raises some serious questions about the quality of data collapsing and the consistency with Eq. (5). We will give a reanalysis of their data in a subsequent paper.

We also study, from our own 3D data for various values of p, the proposed scaling function of the mean radius of gyration in terms of the scaling variable $x\equiv N|p-p_c|^{\nu_{\rm perc}/\nu_{p_c}}$ where ν_{p_c} is left as a parameter. If $\nu_{p_c}=0.59$ is used assuming that the Flory exponent remains unchanged for any p, then the plot is similar to Fig. 3 except for a change in the horizontal scale. Such a plot (not shown) produces neither the correct $x\to 0$ behavior nor data collapsing. The former result is expected because the length of the SAW's for the simple-cubic lattice is not sufficient to give the asymptotic exponent. Since the observed value of ν_N is 0.612 ± 0.01 at $N=50$, we may try to test scaling with this value for ν_{p_c}. The result is displayed in Fig. 4. Unfortunately our data for different p are far apart; note the two breaks in the abscissa of Fig. 4. However, they do seem to give the correct $x\to 0$ behavior, while the case for data collapsing is weak at best: The $x\to 0$ limit seems to depend on p, and for $x\gg 1$ the data seem to give parallel lines without collapsing into a single line.

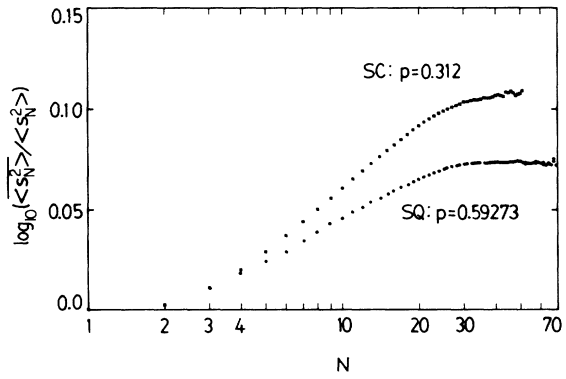

FIG. 3. Log-log plot of $\langle\langle s^2\rangle_W\rangle_C$ close to p_c divided by $\langle s^2\rangle$ on the full lattice, vs N, for square and simple-cubic lattices.

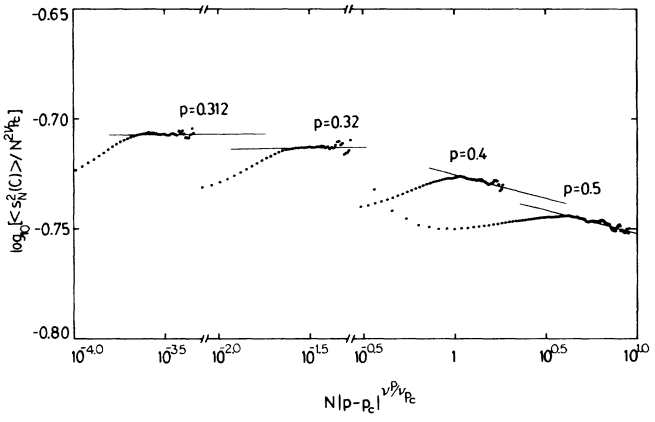

FIG. 4. Test of crossover scaling [Eq. (4)] from our data on the simple-cubic lattice, for the trial choice of $\nu_{p_c}=0.612$. The maximum lengths of the SAW's range from 50 for $p=0.312$ to 100 for $p=0.5$, and the lines drawn are for visual aid only.

Beyond numerical difficulties, we may note that there exist several other equally plausible crossover scaling *Ansatz* with the same N dependences as (4) in both the *fractal* and *Euclidean* limits but with different p dependences if $\nu_{p_c} \neq \nu$. This observation again leads us to suspect that the only reasonable, simple scaling form would require $\nu = \nu_{p_c}$.

Thus, based on our Monte Carlo data, we have demonstrated that the critical behavior of SAW's even at p_c is similar to that of ordinary SAW's, rather than very different as was widely believed. In addition, simple scaling in terms of the ratio of two diverging lengths does not appear to be consistent with our data. Our result is different from the case of some regular fractals where ν does change.[19-21] This reinforces the idea of Rammal, Toulouse, and Vannimenus[19] that the Flory exponent of SAW's depends on many aspects of the fractal substrate. Such effects of percolation clusters evidently conspire so that the disorder average leaves the critical behavior associated with ν unchanged.

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