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Critical behavior of self-avoiding walks on percolation clusters

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We study the critical properties of a self-avoiding walk on percolation clusters using exact enumerations, in both $d=2$ and $d=3$. Calculations of the exponent χ, which measures free-energy fluctuations, clearly show the existence of two distinct phases, one for strong disorder (at the percolation threshold), the other for weak disorder (above the percolation threshold). The ν exponent is, within numerical accuracy, the same in the two phases. However in $d=3$, its value, $\nu=0.64\pm0.015$ is significantly larger than on a pure lattice.

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The effect of quenched randomness on the properties of a polymer in a good solvent is a problem which has attracted much interest in the last ten years [1–14]. Despite extensive theoretical work, there is not yet any definite answer to the question whether or not critical properties of the polymer are modified by the randomness. In such theoretical studies the polymer is often modeled as a self-avoiding walk (SAW) on a lattice. Most attention has focused on the behavior of the average squared end-to-end distance $\overline{\langle R_N^2\rangle}$ of an N-step SAW (here $\langle\rangle$ indicates an average over all SAW configurations, while the overbar denotes the quenched average over randomness). For N sufficiently large, one expects

$$\overline{\langle R_N^2\rangle}\sim N^{2\nu}. \tag{1}$$

In the absence of randomness, one has in $d=2$, $\nu=\frac{3}{4}$ [15] and in $d=3$, $\nu=0.592\ldots$ [16].

Extensive Monte Carlo simulations [6] seemed to indicate that critical properties, such as the exponent ν, of the SAW are not affected by quenched randomness, neither in two nor in three dimensions. In these calculations the randomness was modeled by performing the SAW on the clusters of a site percolation problem where sites are present (absent) with probability p $(1-p)$.

In contrast, renormalization-group calculations [7], both of real-space and of field-theoretic type indicated that the critical properties of a SAW are modified at the percolation threshold $p=p_c$ (but not for $p>p_c$) for $d\geq 2$.

Parallel to, and independent of, these developments a considerable understanding was achieved of the (simpler) problem of a directed polymer (DP) in a random environment [17], a model which is of importance for such diverse issues as fractal growth and flux lines in high-T_c superconductors [18]. The results found for the DP have more recently been applied also to the study of a SAW in a random environment.

Exploiting some similarities with the DP problem led Obukhov [10] to conjecture that in $d=3$ ν would be changed to $\frac{2}{3}$, independently of the strength of the randomness, while in $d=2$ excluded volume effects dominate and ν would stay unchanged at $\frac{3}{4}$. A similar conclusion (at least for $d=3$) was reached on the basis of a Flory-like theory [9].

Most recently, Le Doussal and Machta [13] found numerical support for the ideas of Obukhov from exact renormalization-group calculations on hierarchical lattices. However, they find within their calculations a different behavior for the cases $p=p_c$ and $p>p_c$. To be more specific, consider first a slightly more general problem of a SAW which can step on all sites of a regular lattice. To each site i of the lattice a random energy E_i is given according to the following distribution (independently for all lattice sites)

$$E_i=\begin{cases}0 & \text{with probability } p\\ 1 & \text{with probability } 1-p\end{cases}.$$

A particular SAW α is then given an energy E_α which is the sum of the energies E_i of the sites visited by the SAW. We can then define a partition function,

$$Z_N=\sum_\alpha \exp(-\beta E_\alpha), \tag{2}$$

where the sum is over all N-step SAW's.

As usual in systems with quenched randomness we are interested in $\overline{\ln Z_N}$. When $\beta=0$, we recover from (2) the well-known case of a SAW without randomness. For $\beta\to\infty$, only configurations of minimal energy (i.e., where the SAW at each step visits a site with energy 0) contribute. In this limit, we thus recover the statistics of a SAW on site percolation clusters.

In Ref. [10] it was argued that for any finite β the model would, under renormalization, flow to a zero-temperature (or disorder) fixed point. Indeed, the work of Le Doussal and Machta [13] shows that this is the case on hierarchical lattices, but they find that there are two disorder fixed points, one for $p=p_c$, the other one for $p>p_c$.

At such a fixed point, sample-to-sample fluctuations in the free energy become relevant and define a new exponent χ:

$$[\mathrm{var}(\ln Z_N)]^2\equiv[\overline{(\ln Z_N)^2}-\overline{(\ln Z_N)}^2]\sim N^{2\chi}. \tag{3}$$

In the present work we present results for the exponents ν and χ. As we will see, especially the latter exponent is very helpful to understand the problem. Our results were obtained from extensive numerical calculations. The

technique which we used was an exact enumeration, up to $N=30$ steps of all SAW's (for the smallest values of p considered, we went up to $N=35$) on a great number of percolation configurations, both in $d=2$ and $d=3$ (the number of configurations depended on p, and varied from a few hundred for high p values to $\approx 10^5$ for the smallest p values).

This same exact enumeration method was already used successfully by us to investigate the behavior of $\overline{\ln Z_N}$ [12]. In that work we found

$$\overline{\ln Z_N} \sim |\ln p|^{1/\nu_p d} N , \tag{4}$$

where ν_p is the ν exponent in absence of randomness.

Figure 1(a) shows our results for $\overline{\ln\langle R_N^2\rangle}$ vs $\ln N$ for several different p values in $d=2$. The estimates for the exponent 2ν which we get from these data are, within numerical accuracy, the same for all values of p and equal to $2\nu_p = \frac{3}{2}$. Our best estimate is $2\nu = 1.49 \pm 0.02$ [19].

The situation is far more interesting in $d=3$ [Fig. 1(b)]. Again all estimates of ν are the same (within the accuracy of the data, of course) independently of p. However, the value which we obtain is significantly different from the value at $p=1$. Our estimate is $2\nu = 1.28 \pm 0.03$, to be compared with $2\nu_p = 1.184\ldots$. Our result is only slightly lower than that obtained from Flory-like arguments [9,10] $2\nu = \frac{4}{3}$.

We would like to point out that our results thus contradict the conclusion from Monte Carlo calculations that ν does not change in $d=3$. However, it should be pointed out that the exact enumeration method gives more accurate results for the range of N values to which it can be applied.

Before closing the discussion of the ν exponent it may be interesting to remark that when we restrict our SAW to the "infinite" (or lattice spanning) cluster at p_c we find in $d=2$ a higher value of ν; we estimate $2\nu = 1.54 \pm 0.02$, in agreement with recent Monte Carlo results [14]. We have no results for the infinite cluster at p_c in $d=3$. In this paper our results always are obtained by allowing the SAW on all possible clusters.

We now turn to the exponent χ. When $\beta \to \infty$ in (2), Z_N becomes equal to the number of self-avoiding walks of minimal energy (i.e., walking on the percolation clusters). We would like to point out that a successful calculation of $\overline{\ln Z_N}$ [or $\overline{(\ln Z_N)^2}$] crucially depends on the use of the exact enumeration technique. We have also performed some calculations using standard Monte Carlo techniques for SAW's (with the purpose of extending our results to larger N values) but noticed that already after a few steps the value of $\overline{\ln Z_N}$ deviated appreciably from the exact ones.

Our results for χ are qualitatively very similar to those obtained by Le Doussal and Machta on hierarchical lattices. We find a different value for χ when $p \le p_c$ or when $p > p_c$. In Fig. 2(a) we show our results for $2\ln[\mathrm{var}(\ln Z)]$ (in $d=2$) as a function of $\ln N$ at $p = \frac{1}{2}$ ($< p_c$). From these data we find $2\chi = 1.33 \pm 0.04$. A similar value, $2\chi = 1.29 \pm 0.04$ is found at p_c. In contrast, Fig. 2(b) shows the situation at $p = 0.65$ (above p_c). Here we find that there is a crossover in the data when N increases; the data for $N > 8$ fit a straight line leading to the estimate $2\chi = 0.86$ [20].

In $d=3$ (Fig. 3) we encounter a similar situation. For $p \le p_c$ our data lead to $2\chi = 1.28 \pm 0.04$ [Fig. 3(a)] (a value which is surprisingly close to the $d=2$ value), while for $p > p_c$ we find a χ value which is considerably lower, $2\chi = 0.64$ [20] [Fig. 3(b)]. Again, we see a crossover in the data that occurs at lower N values when $p - p_c$ is increased.

In Table I we give a summary of our exponent estimates. Notice that these all satisfy the exact inequality [13,21]

$$(1-\chi)/\nu \le d/2 . \tag{5}$$

When we compare our values for χ with those obtained on hierarchical lattices [13], we see that they are considerably lower, especially for $p \le p_c$.

Our numerical results for χ thus strongly favor the existence of two disorder fixed points, one at $p = p_c$ the other one for $p > p_c$. This is evident from the difference in χ values but also follows from the crossover in the data above p_c. Below the percolation threshold there are few allowed walks on clusters which may look like those at p_c [22]. Because we restrict our averages to those configurations on which at least one N-step SAW can be per-

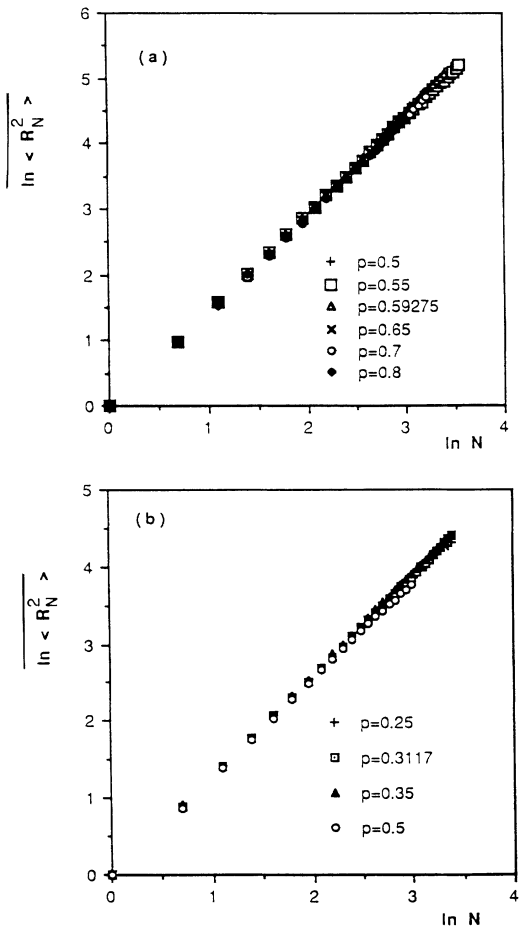

FIG. 1. (a) Numerical results for $\ln\overline{\langle R_N^2\rangle}$ vs $\ln N$ for different p values in $d=2$. (b) The same as in (a), now in $d=3$.

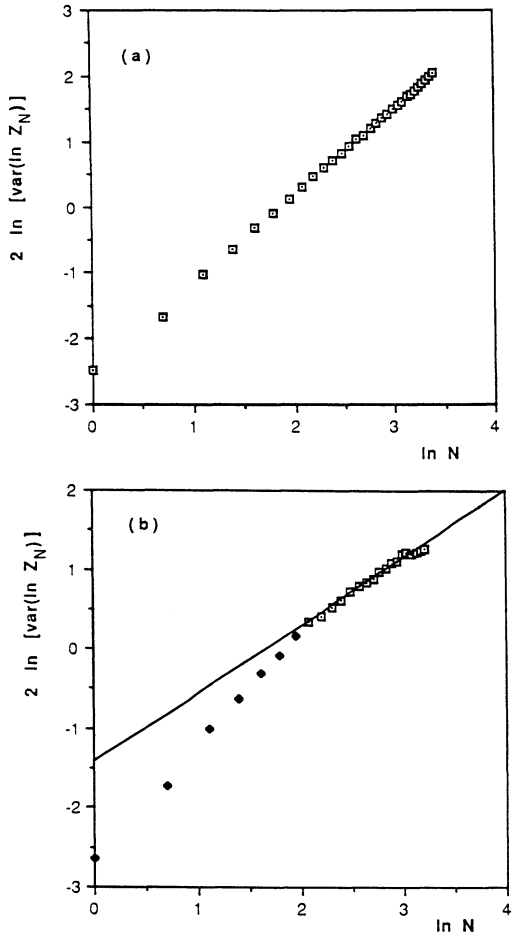

FIG. 2. (a) Numerical results for $2\ln[\mathrm{var}(\ln Z_N)]$ vs $\ln N$ in $d=2$ at $p=\frac{1}{2}$. (b) The same as in (a), now at $p=0.65$. The straight line gives the best fit through the data for $N \geq 8$.

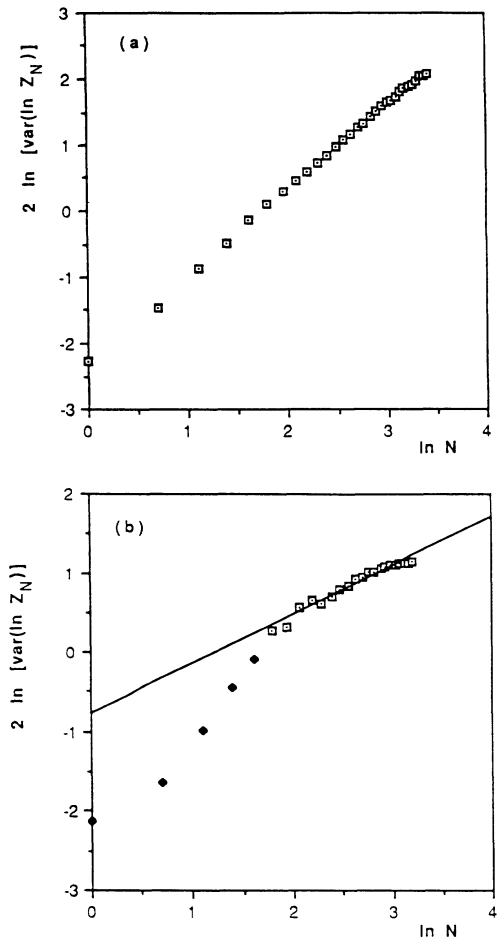

FIG. 3. (a) Numerical results for $2\ln[\mathrm{var}(\ln Z_N)]$ vs $\ln N$ in $d=3$ at $p=p_c \simeq 0.3117$. (b) The same as in (a), now at $p=0.4$. The straight line gives the best fit through the data for $N \geq 6$.

formed, this may explain why our data at and below the threshold give the same results.

It is our feeling that the ν exponent is also different in the two regimes but that the difference is too small to be detected with the present numerical accuracy (for example, on one of the hierarchical lattices considered by the authors of Ref. [13], one has $\nu=0.8488$ at p_c, $\nu=0.86$ for $p > p_c$, while $\nu_p=0.8465$), though of course there is no *a priori* reason why ν could not be the same at two different fixed points.

In conclusion, we have presented extensive numerical calculations for the SAW on percolation clusters using exact enumerations. These calculations are very time consuming. Our results clearly show that, at least in $d=3$, the ν exponent increases with respect to its value in a pure system, and is not too different from the Flory estimate, $\nu=\frac{2}{3}$. Results for the exponent χ which describe the zero-temperature energy fluctuations clearly point to the existence of two distinct low-temperature phases for the problem, one for small disorder ($p > p_c$), the other one for strong disorder. It is now clear why previous calculations which only looked at the behavior of the distance failed. Indeed, it turns out that the exponent ν does not discriminate (or only a very little bit) between the two phases. However, these phases do show up very clearly in the free-energy fluctuations. We feel that in this way the problem of a SAW in a quenched random environment is much better understood. We are currently further extending our calculations in order to determine also the crossover exponent at the percolation threshold fixed point. Of course, the understanding gained here is only numerical, and one needs also to get a better analytical understanding of the problem.

TABLE I. Overview of exponent values.

	ν	χ	$\omega=\chi/\nu$
	$d=2$		
$p \leq p_c$	0.745 ± 0.01	0.65 ± 0.02	0.87
$p_c < p < 1$	0.75 ± 0.01	0.43	0.57
	$d=3$		
$p \leq p_c$	0.635 ± 0.01	0.64 ± 0.02	1.01
$p_c < p < 1$	0.645 ± 0.01	0.33	0.50

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