Exact enumeration of self-avoiding walks on lattices with random site energies

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The self-avoiding random walk on lattices with quenched random site energies is studied using exact enumeration in $d=2$ and 3. For each configuration we compute the size R and energy E of the minimum-energy self-avoiding walk (SAW). Configuration averages yield the exponents ν and χ, defined by $\overline{R^2}\sim N^{2\nu}$ and $\overline{\delta E^2}\sim N^{2\chi}$. These calculations indicate that ν is significantly larger than its value in the pure system. Finite-temperature studies support the notion that the system is controlled by a zero-temperature fixed point. Consequently, exponents obtained from minimum-energy SAW's characterize the properties of finite temperature SAW's on disordered lattices.

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I. INTRODUCTION

In recent years, there has been considerable interest in the problem of self-avoiding random walks (SAW's) in quenched random environments [1–18]. These studies are motivated in part by questions concerning the behavior of polymers in porous media and in part by the broader aim of elucidating the effect of quenched disorder on critical phenomena. The SAW in a random environment is closely related to other quenched-disorder problems such as spin glasses, random interfaces, and directed walks in random environments. The basic question is how the behavior of the SAW is modified by disorder. A decade of theoretical and numerical studies has led to contradictory answers to this question.

Significant progress was made in the past several years with the hypothesis that the asymptotic properties of the SAW in a quenched random environment are governed by a zero-temperature (strong disorder) fixed point [10–12]. If the finite-temperature problem is controlled by a zero-temperature fixed point, then the critical exponents for finite temperature may be extracted by averaging over minimum-energy SAW's in an ensemble of environments. In the present study exact enumeration methods are employed to investigate the zero-temperature properties of the SAW in a random environment, and to provide evidence that the finite-temperature properties are controlled by a zero-temperature fixed point.

We consider N-step SAW's starting at the origin on the square and simple-cubic lattices. Each lattice site is assigned a random energy $\mathcal{E}_i$, taken from some distribution $p(\mathcal{E})$. The two energy distributions studied here are the Gaussian with mean zero and variance 1 and the uniform distribution on the interval 0 to 1. The energy E of a SAW is the sum of the energies of the visited sites, and the statistical weight of the SAW is given by the Boltzmann factor, $\exp(-E/T)$, at temperature T. In the limit of zero temperature (equivalently strong disorder), the ensemble of SAW's for each environment is dominated by the minimum-energy SAW. Because it is much faster to find the minimum-energy SAW than to sum over all SAW's, most of our efforts are devoted to the zero-temperature problem.

We find the exact minimum-energy configuration for a large number of environments and compute statistics for the end-to-end distance R and energy E of these SAW's. This yields the exponents ν and χ characterizing the size and energy fluctuations of the SAW, defined by

$$\overline{R^2}\sim N^{2\nu} \tag{1a}$$

and

$$\overline{\delta E^2}\sim N^{2\chi}\ , \tag{1b}$$

where the overbar indicates an average over environments. We also study the end-to-end distance at finite temperature by exact enumeration of SAW's weighted by the Boltzmann factor.

Our results show conclusively that the size exponent for the SAW in a random environment in two and three dimensions is larger than the corresponding size exponent for the pure SAW. In order to provide a framework for understanding this conclusion, we review two arguments [12] explaining why the SAW is expanded by quenched disorder. The first argument is of the "Flory" type and is based on the idea that the SAW expands to seek out favorable sites. In a mean-field approximation the fluctuations in site energies available to the SAW increase as the square root of the explored volume. With this in mind one constructs a free energy in which a disorder term of the form $-N/R^{d/2}$ is added to the free energy of pure SAW's, which is $-(R/N^{\nu_{\rm pure}})^{1/(1-\nu_{\rm pure})}$. Minimizing the free energy leads to Flory exponents [12],

$$\nu_F(d)=\frac{1}{1+d(1-\nu_{\rm pure})/2} \tag{2a}$$

and

$$\chi_F(d)=\frac{\nu}{2}(2-d\nu_{\text{pure}}) . \quad (2b)$$

Thus $\nu_F(2)=\frac{4}{5}$, $\nu_F(3)=0.616$, $\chi_F(2)=\frac{1}{5}$, and $\chi_F(3)=0.073$. These values are compared to our numerical results in Tables I and II.

The second argument (also see Ref. [4]) focuses on the probability, with respect to the distribution of environments, that a given SAW is a minimum-energy SAW. It is not difficult to see (e.g., work out the probabilities for two-step SAW's) that a SAW having fewer intersections with all other SAW's has a greater probability of being a minimum-energy SAW. Since SAW's with large end-to-end distances have fewer intersections with other SAW's, they are more likely to be minimum-energy SAW's. This argument shows that the average size of the SAW is increased by quenched disorder, but it does not imply that the size exponent is actually changed.

The present investigation differs from most previous numerical studies in two important ways. The first difference is that we consider continuous disorder rather than percolation disorder (site dilution). Above the percolation threshold, percolation disorder and continuous disorder are believed to be in the same universality class [12]. However, there are several advantages in using continuous distributions. First, the averaging procedure is not uniquely defined for percolation disorder. For example, one can average over all environments that support at least one N-step SAW from the origin, or one can average only over environments for which the origin is part of the infinite cluster [7,9,13]. Second, there is no zero-temperature limit for percolation disorder since all allowed SAW's have the same energy. Starting from percolation disorder, the zero-temperature fixed point is approached only at large length scales [10]. Thus we believe that one must go to relatively large N for percolation disorder to obtain good estimates of the asymptotic exponents. By working directly at zero temperature with continuous disorder, we are able to obtain accurate estimates of asymptotic critical exponents from the relatively short SAW's accessible via exact enumeration.

The second important feature that distinguishes the present study from most previous numerical investigations is that we employ exact enumeration rather than Monte Carlo or incomplete enumeration methods. Previous Monte Carlo studies [1,14] and our own preliminary investigations found little or no deviation from pure system behavior. However, we believe this is a consequence of the difficulty of using Monte Carlo methods in a system governed by a strong-disorder fixed point. In this situation, the ensemble for large N is dominated by a small fraction of SAW's that have energy close to the minimum [10–12]. The small sample of SAW's produced by Monte Carlo or incomplete enumeration may entirely miss the regions of configuration space that dominate the ensemble of all SAW's. The fact that finding the minimum-energy SAW is an *NP*-complete problem [15] casts further doubt on whether Monte Carlo or incomplete enumeration can be successfully used to study the equilibrium statistical mechanics of SAW's in quenched random environments. Exact enumeration avoids this pitfall, but is limited to relatively short SAW's.

At least some of the disagreements between previous studies are due to differences in averaging procedures. When the randomness in the lattice is static, one must distinguish between two situations. If one or both ends of the SAW is (are) fixed, there is true quenched disorder. On the other hand, if both ends of the chain are free, the statistics of the SAW is the same as for annealed disorder. This is because the SAW explores many independent environments as it moves around the lattice. Harris [3] showed that disorder is irrelevant for this "annealed" problem, where the chain is free to explore an infinite static lattice. In the present paper we are concerned exclusively with the quenched problem.

Several recent numerical studies of SAW's with quenched percolation disorder have been carried out and suggest that exponents differ from those for the pure SAW. Lam [16] studied SAW's on two-dimensional percolation clusters at p_c using incomplete [17] enumeration and found $\nu=0.81$. Vanderzande and Komoda [18] used exact enumeration to investigate two and three dimensions both at p_c and for $p>p_c$ for SAW's up to $N=30$. In the $d=2$ case they found no significant change from the pure SAW result, but in three dimensions, for $p>p_c$, they reported an increase in the size exponent, $\nu=0.64$ compared to $\nu_{\text{pure}}=0.59$. Grassberger [13] used a recursive incomplete enumeration method for $d=2$ and found $\nu=0.78$ at p_c. For $p<p_c$ he found $\nu=0.81$ averaging over large clusters, while for $p>p_c$ there was significant upward curvature in log-log plots of R versus N out to $N=100$.

Several authors [8,10,12] have pointed out that the SAW in a random environment has much in common with the directed self-avoiding walk (DSAW) in a random environment [19,20]. Both systems are controlled by a strong-disorder fixed point, and both the SAW and DSAW are expanded by quenched disorder. The SAW problem is, however, more complicated than the DSAW problem in several respects. There is an exact solution for the DSAW exponents in $1+1$ dimensions [19] and an exact identity, $\chi=2\nu-1$, which holds in all dimensions. In contrast, no exact results or controlled approximations are known at present for the exponents of the SAW in a quenched random environment in two and three dimensions. From a computational standpoint, finding minimum-energy SAW's is a more difficult problem than finding minimum-energy DSAW's, because the former problem is *NP*-complete [15], while the latter enjoys a polynomial time algorithm [19,20].

II. METHODS

We use an exact enumeration scheme based on the "backtracking" algorithm [21]. At each step after the first, the walker has $Z-1$ choices of direction, with Z the coordination number. An order is imposed among these available directions and the first of the possible steps is attempted. If this leads to a self-intersection, the next possible step is attempted. In this way, the first SAW is grown to the desired length N. When the maximum number of steps has been reached, or when the $Z-1$ choices of directions are rejected, the walker re-

treats a step and tries the next available step from that site. In this way, the algorithm sweeps through the tree of all possible SAW's in a prescribed order.

There are two ways the program can be speeded up to find the minimum-energy SAW. First, the tree of all SAW's can be "pruned" by abandoning all partially grown M-step SAW's ($M<N$) whose energy $E[M]$ exceeds the current minimum N-step energy, $E_{\min}[N]$. This device is useful only when the site energies are positive (e.g., for the uniform distribution), since, otherwise, additional steps in the SAW may lower the total energy. Second, the sequence in which steps are attempted from a given site is chosen according to the energy of the step rather than in a fixed order.

Using this method, we obtained exact minimum-energy SAW's up to $N=20$ steps for order 10^5 environments. Longer minimum-energy SAW's can be readily found for the uniform distribution; for example, on a DECstation 5000/200 (24 MIPS) it takes about 15 min to find a single minimum-energy SAW for 35 steps in two dimensions, and 25 min for 35 steps in three dimensions. However, we chose to study shorter SAW's in order to obtain high-quality statistics. For the Gaussian energy distribution some site energies are negative, so the pruning method does not work and all SAW's must be enumerated, which significantly increases the running time. Similarly, at positive temperatures it is necessary to enumerate all SAW's.

It should be noted that there can be a degeneracy among minimum-energy SAW's since the same set of sites could be visited in a different order by two distinct SAW's. These SAW's will have different end-to-end distances but the same radius of gyration. We also collected statistics for the radius of gyration and found no significant differences in estimates of the size exponent.

III. RESULTS

Figure 1 shows the disorder-averaged end-to-end distance of the minimum-energy SAW on a two-dimensional square lattice with a uniform distribution of site energies. Each data point represents an average of approximately 200 000 configurations. For comparison, the average end-to-end distance for the pure SAW on the same lattice is shown [22]. Figure 1 shows that quenched disorder stretches the SAW and suggests that the size exponent is also increased by disorder. In order to obtain a clearer picture of the value of the size exponent, we define an N-dependent size exponent by the slopes of successive pairs of data points on a double-logarithmic plot, viz.,

$$\nu_N=\frac{1}{2}\frac{\ln(\overline{R_N^2}/\overline{R_{N-2}^2})}{\ln(N/N-2)}\ , \tag{3}$$

where N is the number of bonds in the SAW. In Fig. 2, ν_N is plotted versus $1/N$ for $d=2$. The uniform and Gaussian distributions are shown along with the pure SAW. Our estimates of the asymptotic value of the size exponents and the associated subjective uncertainty are obtained by visually extrapolating $1/N\to 0$ and are listed in Table I. The data points for Gaussian disorder consistently lie above the data for the uniform distribution, but have a smaller slope. This is consistent with the hypothesis that the Gaussian distribution is closer to the fixed distribution than the uniform distribution, so the asymptotic region is reached sooner. In Ref. [12] it was shown that the fixed distribution on hierarchical lattices is qualitatively quite similar to a Gaussian. The close correspondence between the Gaussian and uniform distribution suggests that a single zero-temperature fixed point controls both cases.

Figure 3 shows the size exponent versus $1/N$ for the

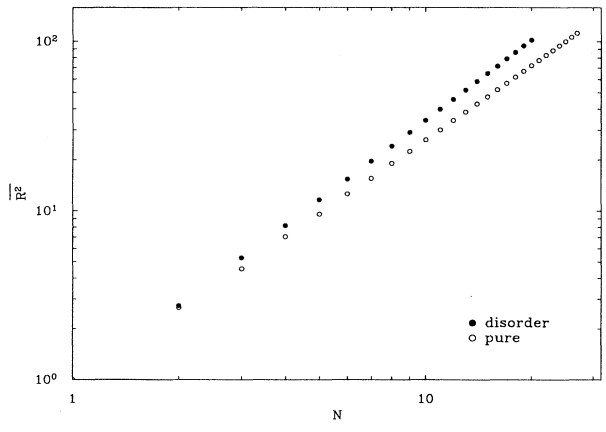

FIG. 1. Double-logarithmic plot of the average squared end-to-end distance for minimum-energy SAW's on a square lattice with a uniform distribution of site energies, compared with the average squared end-to-end distance for a pure SAW on the same lattice (Ref. [22]).

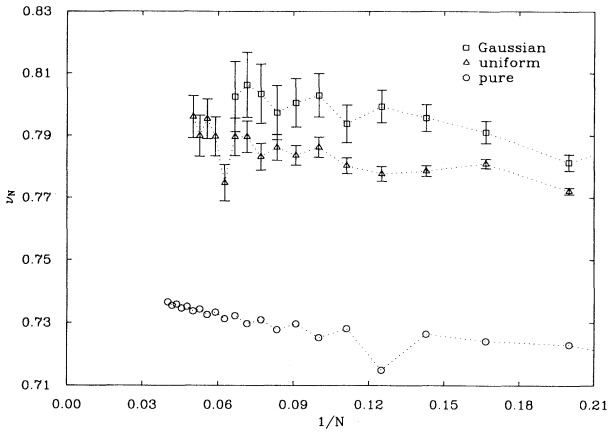

FIG. 2. Size exponent ν_N [see Eq. (3)] for the minimum-energy SAW in $d=2$ with the uniform and the Gaussian site-energy distributions, compared with the pure SAW.

TABLE I. Estimates of the exponents ν and χ for uniform and Gaussian disorder for $d=2$ compared with values for the pure system (Ref. [22]) and a Flory approximation (Ref. [12]).

$d=2$	Pure	Uniform	Gaussian	Flory
ν	0.75	0.80±0.02	0.81±0.02	0.8
χ		0.28±0.03	0.28±0.02	0.2

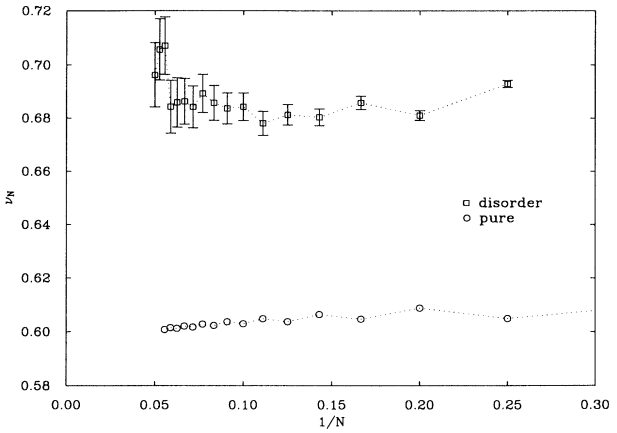

FIG. 3. Size exponent ν_N vs $1/N$ in $d=3$ for the uniform distribution, compared with the pure SAW.

uniform distribution compared to the corresponding curve for the pure SAW on a three-dimensional simple-cubic lattice. 70 000 configurations are averaged to obtain these data points. The estimate of the asymptotic size exponent is given in Table II.

The approach of ν_N to its asymptote depends on the definition of N; the number of sites and the number of bonds are two obvious choices ($N_s=N_b-1$). In general, if $N=N_b$, the curve approaches the asymptotic value from below; if $N=N_s$, from above. The data for R^2 are better behaved for the choice $N=N_b$.

Next, we consider the energy and its fluctuations. For Gaussian distributions with mean zero and standard deviation σ the average energy of the minimum-energy SAW should grow linearly in both the number of steps and in the standard deviation. For the two-dimensional square lattice we find $\bar{E}\sim -0.84N_s\sigma$.

Figure 4 shows the N-dependent energy-fluctuation exponent versus $1/N$ for the square lattice with the uniform and Gaussian distributions of site energies. Here $N=N_s$ is the number of sites visited by the SAW. The N-dependent energy-fluctuation exponent χ_N is defined as in Eq. (3) with δE^2 replacing $\overline{R^2}$. The data points for the Gaussian have a smaller slope than the data points for the uniform distribution, reinforcing the view that the Gaussian is closer to the zero-temperature fixed distribution than the uniform distribution. Since the energy of a SAW directly probes the distribution of site energies, it is not surprising that differences between the two distributions in the N-dependent exponents are more evident in χ_N than in ν_N. Figure 5 shows χ_N versus $1/N$ for the cubic lattice and the uniform distribution. Our best estimates of the asymptotic energy-fluctuation exponents and their uncertainties are given in Tables I and II for $d=2$ and 3, respectively.

TABLE II. Estimates of the exponents ν and χ for uniform and Gaussian disorder for $d=3$ compared with the values for the pure system (Ref. [22]) and a Flory approximation (Ref. [12]).

$d=3$	Pure	Uniform	Flory
ν	0.592	0.71±0.03	0.62
χ		0.15±0.03	0.073

The results for positive temperatures in two dimensions are shown in Fig. 6, where ν_N versus $1/N$ is plotted for $T=0.5$ and 1.0 and compared with the zero-temperature and pure SAW data. Each positive-temperature point corresponds to an average over 500 environments with Gaussian disorder. As expected, the lower temperature is closer to the zero-temperature limit. Both positive-temperature curves lie significantly above the pure SAW curve. This result supports the hypothesis that the positive-temperature (i.e., weak-disorder) and zero-temperature (i.e., strong-disorder) problems lie in the same universality class, which differs from the pure SAW universality class.

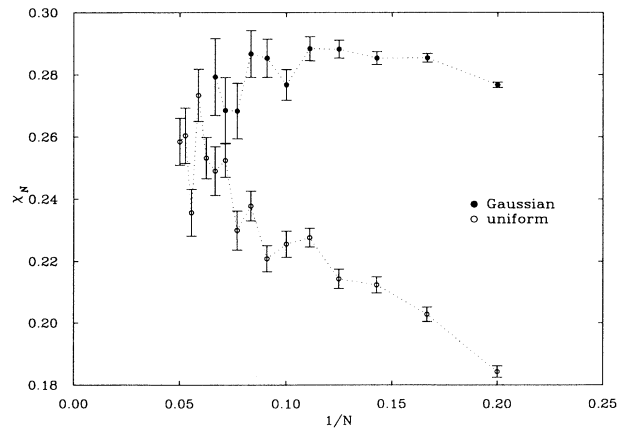

FIG. 4. Energy-fluctuation exponent χ_N vs $1/N$ in $d=2$ for the uniform and Gaussian distributions.

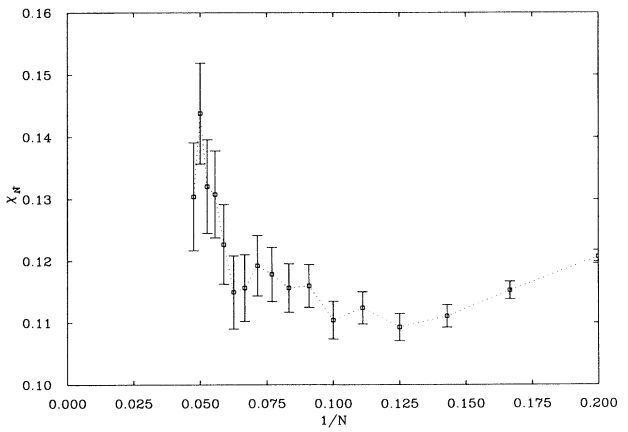

FIG. 5. Energy-fluctuation exponent χ_N vs $1/N$ in $d=3$ for the uniform distribution.

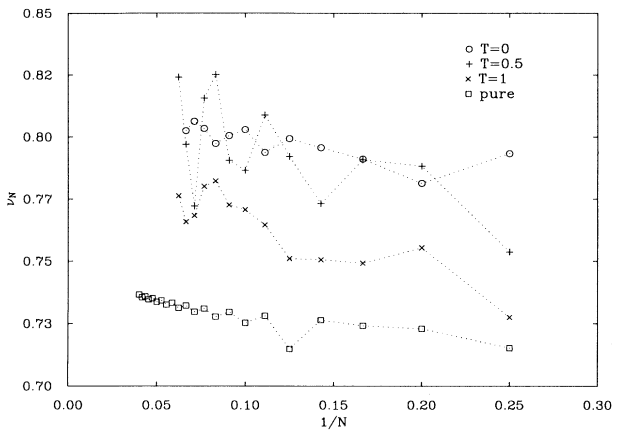

FIG. 6. Size exponent ν_N vs $1/N$ in $d=2$ for runs performed at temperatures $T=0$, 0.5, and 1.0 with the Gaussian distribution.

IV. DISCUSSION

Our results provide strong evidence that the self-avoiding walk in a random environment at zero temperature is in a different universality class than the pure self-avoiding walk in both $d=2$ and 3. The positive-temperature results suggest that the weak- and strong-disorder problems are in the same universality class for these dimensions. The critical exponent for the size in $d=2$ is close to the Flory approximation and to the $d=2$ percolation-threshold results of Refs. [13] and [16]. For $d=3$ we find that the size exponent is considerably larger than either the Flory prediction or that of Ref. [18]. We find values of the energy-fluctuation exponent that are quite small, though larger than the Flory values. We believe that the values recorded in Tables I and II are the best measurements to date of these exponents, although it would be useful to have good statistics for larger SAW's, especially for the evaluation of χ, which can be expected to be more sensitive than ν to deviations from the fixed-point distribution.

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