

Universality classes for self-avoiding walks in a strongly disordered system

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We study the behavior of self-avoiding walks (SAWs) on square and cubic lattices in the presence of strong disorder. We simulate the disorder by assigning random energy ϵ taken from a probability distribution $P(\epsilon)$ to each site (or bond) of the lattice. We study the strong disorder limit for an extremely broad range of energies with $P(\epsilon) \propto 1/\epsilon$. For each configuration of disorder, we find by exact enumeration the optimal SAW of fixed length N and fixed origin that minimizes the sum of the energies of the visited sites (or bonds). We find the fractal dimension of the optimal path to be $\tilde{d}_{opt} = 1.52 \pm 0.10$ in two dimensions (2D) and $\tilde{d}_{opt} = 1.82 \pm 0.08$ in 3D. Our results imply that SAWs in strong disorder with fixed N are much more compact than SAWs in disordered media with a uniform distribution of energies, optimal paths in strong disorder with fixed end-to-end distance R , and SAWs on a percolation cluster. Our results are also consistent with the possibility that SAWs in strong disorder belong to the same universality class as the maximal SAW on a percolation cluster at criticality, for which we calculate the fractal dimension $d_{max} = 1.64 \pm 0.02$ for 2D and $d_{max} = 1.87 \pm 0.05$ for 3D, values very close to the fractal dimensions of the percolation backbone in 2D and 3D.

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I. INTRODUCTION

The problem of self-avoiding walks (SAWs) in different types of disorder is related to problems such as polymers in porous media and spin glasses. For SAWs in the absence of disorder, the average root mean square of the end-to-end distance R scales with the length N as $R \sim N^\nu$. Hence SAWs are fractals with a fractal dimension $d_{SAW} = 1/\nu$. The values of d_{SAW} in two dimensions (2D) and 3D are well known (see Table I). The effects of disorder on d_{SAW} has been the subject of many studies [1–7]. Recently, there has been much interest in the problem of finding the optimal path in a disordered energy landscape. The optimal path can be defined as follows: consider a d -dimensional lattice, where each site (or bond) is assigned by a random energy ϵ taken from a given distribution. The optimal path is the path for which the sum of the energies along the path is minimal. There are two kinds of the optimal path problems. In the first kind (fixed- R problem), the starting and the ending sites of the path are fixed, but the length of the path N is not fixed. In the second kind (fixed- N problem), the starting site (origin) and the length of the path N are fixed, but the ending point is not fixed. These problems are relevant in many fields such as spin glasses [1], protein folding [2], and the traveling salesman problem [8].

Cieplak *et al.* [4] and Porto *et al.* [5] studied numerically the behavior of the average path length N for the fixed- R minimum-energy SAW. If the distribution of energies ϵ is uniform or Gaussian, N is proportional to R and hence $d_{opt} = 1$. The situation is different in the strong disorder limit. In this case, the total energy E is dominated by the maximum value of ϵ along the path. This case can be realized if the probability density $P(\epsilon) \propto 1/\epsilon$ for an extremely broad range of energies. It was found [4,5] that $N \propto R^{d_{opt}}$, where d_{opt}

≈ 1.22 in 2D and $d_{opt} \approx 1.42$ in 3D. These values are similar to the fractal dimensions of the typical path of a passive tracer in the problem of the ideal flow through the percolation cluster, a problem relevant for oil recovery [9]. This fact is consistent with the possibility that the strong disorder limit is related to the percolation problem.

Smaier *et al.* [3] studied the problem of minimum-energy fixed- N SAWs in which the energies are taken from uniform and Gaussian distributions. This kind of disorder is called weak disorder and is different from the strong disorder case studied here. They studied the asymptotic behavior of the mean square end-to-end distance R versus N and found that the fractal dimension in this case is smaller than in the case of the pure SAW (see Table I). The fixed- N problem for strong disorder has not yet been studied.

Numerical studies of fixed- N SAWs on percolation clus-

TABLE I. Fractal exponents characterizing the end-to-end distance of SAWs as a function of the length as well as the fractal dimension of the backbone, d_B .

	2D	3D
d_{SAW}	4/3 ^a	1.699 ^b
\tilde{d}_{opt} (weak, fixed N)	1.25 ^c	1.4 ^c
\tilde{d}_{opt} (strong, fixed N)	1.52 ± 0.10^f	1.82 ± 0.08^f
d_{SAW} (percolation at p_c)	1.29 ^d	1.55 ^h
d_{max}	1.64 ± 0.02^f	1.87 ± 0.05^f
d_{opt} (strong, fixed R)	1.21 ^g	1.44 ^g
d_B (backbone)	1.6432 ^e	1.87 ^e

^aRef. [20].

^bRef. [21].

^cRef. [3].

^dRef. [7].

^eRef. [23].

^fRef. [24].

^gRef. [6].

^hRef. [22].

ters at criticality have been performed using exact enumeration [7]. The case of percolation clusters can be regarded as the quenched disorder case in which the energies can take values of 0 with probability $p=p_c$ and ∞ with probability $p=1-p_c$, where p_c is the percolation threshold. The results suggest that the exponents are not significantly different from those of a pure SAW (see Table I).

Here we study the minimum-energy fixed- N SAW in strong disorder. We find that R scales as $N^{1/\tilde{d}_{opt}}$, with $\tilde{d}_{opt}=1.52\pm 0.10$ in 2D and $\tilde{d}_{opt}=1.82\pm 0.08$ in 3D. These values are significantly different from the values of the related problems discussed above [3–7]. We present arguments that optimal SAWs in strong disorder limit belongs to the same universality class as *maximal* SAWs, defined to be the longest SAWs on a percolation cluster. In order to test our hypothesis, we numerically calculate their fractal dimension, d_{max} , for 2d and 3d and find that the value of d_{max} is very close to the value \tilde{d}_{opt} for fixed- N SAW in the strong disorder limit. The numerical value of d_{max} found here is similar to the fractal dimension of the percolation backbone and is significantly larger than the values of d_{max} previously reported [10]. Thus we conjecture that the three models (the fixed- N SAW in strong disorder, the maximal SAW on a percolation cluster, and the percolation backbone) belong to the same universality class, characterized by equal fractal dimensions.

II. METHOD

We consider a N -step SAW with a fixed origin on a d -dimensional hypercubic lattice with strong disorder. We simulate disorder by assigning a random energy ϵ_k ($k=1\cdots L^d$) to each site of the lattice, where L is the linear size of the lattice. We also study the case in which the energies are assigned to the bonds of the lattice. The strong disorder case is simulated by selecting ϵ_k from an extremely broad distribution by generating a random number r_k , uniformly distributed between 0 and 1, and choosing $\epsilon_k=\exp(ar_k)$. The parameter a controls the broadness of the distribution. The probability density of such a distribution is

$$P(\epsilon)=\begin{cases} 1/(a\epsilon) & 1\leq\epsilon\leq\exp(a) \\ 0 & \text{otherwise.} \end{cases} \quad (1)$$

The minimum-energy SAW is the configuration that minimizes the total energy

$$E(N)=\sum_{i=1}^N \epsilon_i \quad (2)$$

among all possible SAWs of length N that start at the origin.

We apply the exact enumeration method to generate each SAW, using the “backtracking algorithm” [11]. At each step, the SAW has z choices for the direction of the next step, where z is the coordination number. If a particular choice of the direction leads to a self intersection, we disregard this choice and take the next possible choice for this step. After the walk reaches the required length N , or if all the choices

for the current step lead to intersection, we backtrack our SAW and find the step for which a new direction is available. In this way, the algorithm constructs the tree of all possible SAWs in a certain order.

For each configuration of disorder, we find the minimum-energy SAW [12]. Using this method, we obtain each minimum SAW of up to 60 steps in 2D and up to 40 steps in 3D, in typically 10^6 realizations of disorder. We apply this method for strong disorder of the site and bond cases [13]. We compute R by averaging the square root of the end-to-end distance of the minimum SAW for each configuration of disorder. We calculated both the end-to-end distance and the average square radius of gyration and find no differences in the values of the exponents.

We also study the infinitely strong disorder limit $a\rightarrow\infty$. In this limit, the sum of energies can be replaced by the largest value of the energy along the path [14]. Our results for the infinite limit coincide with the ones obtained with $a\geq 100$.

III. RESULTS

We study the asymptotic value of \tilde{d}_{opt} for the minimum-energy SAW in the strong disorder limit in two and three dimensions. In order to find \tilde{d}_{opt} we use successive slopes [3] defined as

$$\tilde{d}_{opt}(N)\equiv 2\frac{\ln(N+1)-\ln(N-1)}{\ln(R_{N+1}^2)-\ln(R_{N-1}^2)}. \quad (3)$$

We estimate the errors for $\tilde{d}_{opt}(N)$ as the standard deviations of the values $\tilde{d}_{opt}(N)$ computed for 10 independent sets of 10^4 configurations.

Figures 1(a) and 1(b) show the value of $\tilde{d}_{opt}(N)$ vs $1/N$ for 2D and 3D, respectively, in comparison with the behavior of these values for fixed- N SAWs in the weak disorder and for regular SAWs. Both results are for the site case. In contrast with regular SAWs and SAWs in weak disorder, the values of $\tilde{d}_{opt}(N)$ in strong disorder have strong corrections to scaling, manifesting in the nonlinear behavior of $\tilde{d}_{opt}(N)$ versus $1/N$ for $1/N\rightarrow 0$. Our attempt to achieve better straight line fits by plotting $\tilde{d}_{opt}(N)$ vs $1/N^\alpha$ for various $0<\alpha<1$ suggests that the limiting value of $\tilde{d}_{opt}(N)$ for $N\rightarrow\infty$ may be significantly larger than the values obtained in Fig. 1. As a result of these estimates, we report $\tilde{d}_{opt}=1.52\pm 0.10$ in 2D and $\tilde{d}_{opt}=1.82\pm 0.08$ in 3D. This shows the minimum energy fixed- N SAWs in strong disorder to be more compact than other types of SAWs studied earlier (see Table I).

In order to better understand this type of SAW we study the distribution of the maximum value r_m of random variables $r_i=a^{-1}\ln\epsilon$, $i=1,\dots,N$, for the minimum-energy SAW of different length N . This distribution is bell shaped, narrow, and has a maximum at $r_m=r^*$ [see Fig 2(a)]. We find that for $N\rightarrow\infty$ the distribution becomes steeper in the vicinity of r^* . Moreover, we find that

$$|r^*-p_c|\sim A/N^{\tilde{\sigma}}, \quad (4)$$

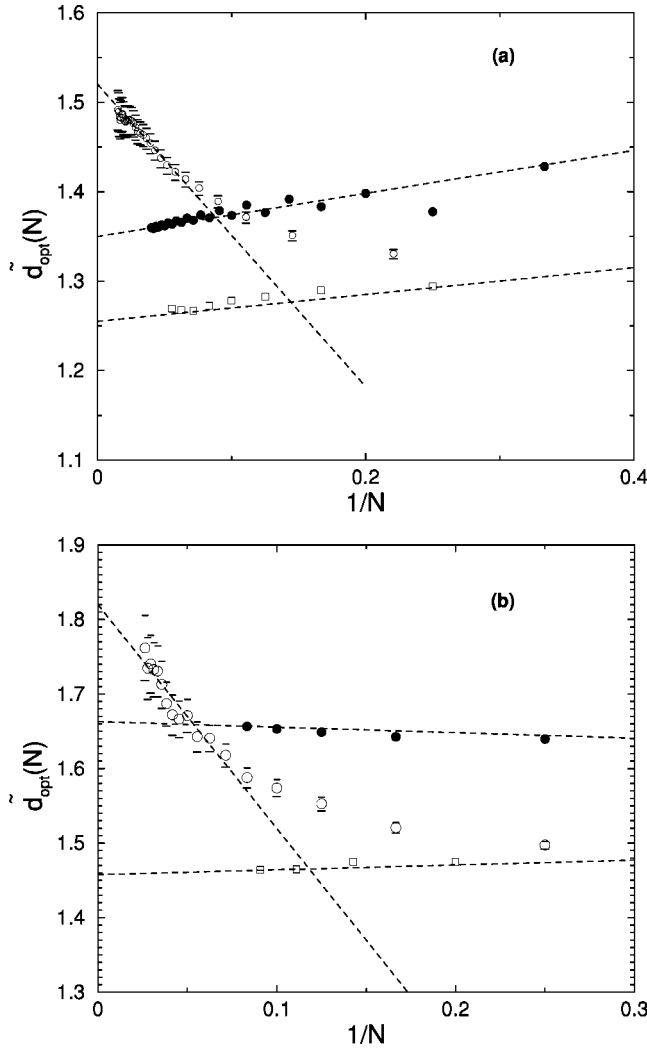


FIG. 1. Effective exponent \tilde{d}_{opt} as a function of $1/N$ for the minimum-energy SAW, in (a) $d=2$ and (b) $d=3$, with strong site disorder of strength $a=100$ (\circ) with error bars (—) compared with the same problem in weak disorder (\square) and with the pure SAW (\bullet). The dashed lines are used as a guide for the eye to show the extrapolated values of the effective exponent in the limit $1/N \rightarrow 0$. Note that since the dependence of \tilde{d}_{opt} on $1/N$ is not linear, the results of linear extrapolation can be significantly smaller than the actual limiting value.

where p_c is the percolation threshold for bond or site percolation, A is a positive constant and $\tilde{\sigma} \approx 0.5$ [see inset of Fig. 2(a)].

The behavior of the distribution of r_m resembles the behavior of the distribution of the maximal threshold value in the invasion percolation model [15,16] for different cluster sizes S_I [see Fig 2(b)]. In the invasion percolation model, each site of the lattice is assigned a random threshold r , uniformly distributed on the interval $0 < r < 1$. Initially, a site at the origin is invaded and the invaded cluster is generated from it. At each stage of the process, the boundary of the invaded cluster consists of the sites not yet invaded, which are the nearest neighbors of the invaded sites. The next site invaded is the boundary site with the smallest value of r .

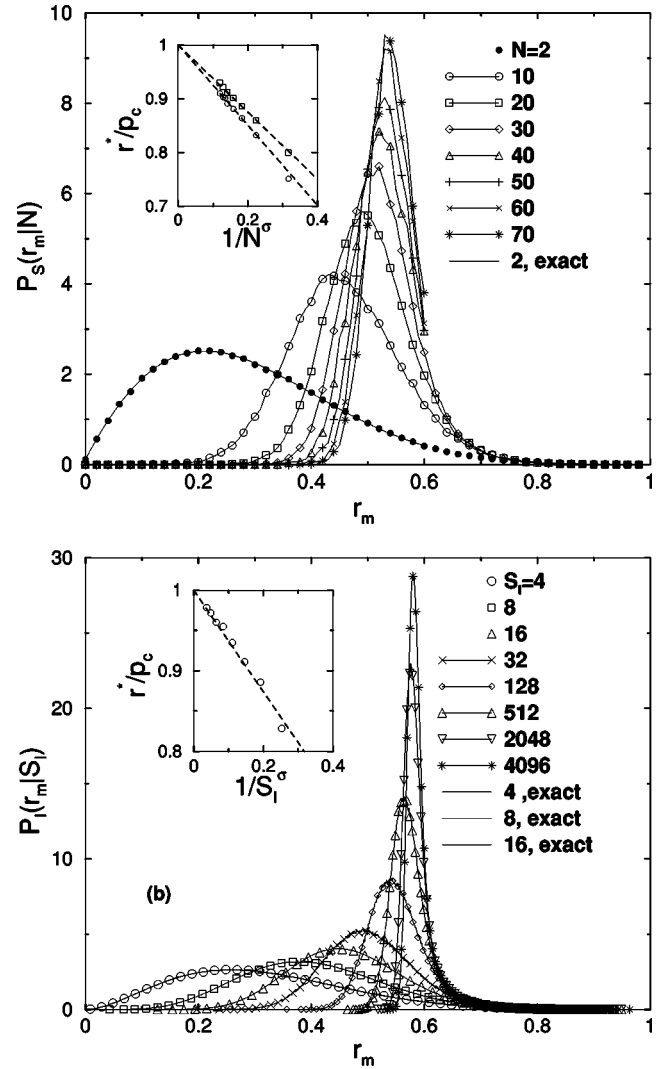


FIG. 2. (a) Plot of the distribution $P(r_m|N)$ of the maximum random numbers r_m (associated with the energies along the optimal path) for different values of N (different symbols) in 2D (bond case). The lines are used as a guide except for $N=2$ that indicates the result of Eq. (13). The inset figure shows the maximum values of the distribution r_m^* divided by p_c ($p_c =$ critical probability) as a function of $1/N^\sigma$, with $\sigma=1/2$ for sites (\circ) and bonds (\square). Here we use $a=100$. (b) Plot of the distribution of the maximal threshold values r_m overcome in the invasion percolation clusters of size S_I indicated in the graph. The lines are used as a guide except for $S_I = 4, 8, 16$ that show the analytical results of Eq. (5). The inset figure shows the maximum values of the distribution r_m^* divided by p_c ($p_c =$ critical probability) as function of $1/N^\sigma$, where $\sigma=36/91$ [15].

In analogy with our optimization problem, one can construct the distribution of the maximal value of r_m of the threshold of the invaded cluster of size S_I . This distribution can be explained in terms of the usual percolation theory. Let us assume that we select unblocked sites if $r \leq r_m$ and blocked sites otherwise. Thus the value of r_m can be interpreted as the occupancy probability p of a percolating site. Suppose that in invasion percolation, we obtain a cluster of size S_I with a value of $r_m \leq p$. This configuration, in terms of

a regular percolation problem, corresponds to a percolation cluster with size $S_p \geq S_I$ for a given percolation probability $p = r_m$. Hence, the probability $P(r_m \leq p | S_I)$ in an invasion percolation problem is equal to the probability $P(S_p \geq S_I | p = r_m)$ in the conventional percolation problem. The latter probability has been computed analytically for small cluster sizes S_I using exact enumeration [17],

$$P(S_p \geq S_I | p) = 1 - \sum_{s=1}^{S_I-1} \sum_{t=4}^{2s+2} s p^{s-1} (1-p)^t g_{s,t}, \quad (5)$$

where $g_{s,t}$ is the number of different clusters of size s and perimeter t ($g_{1,4}=1$, $g_{2,6}=2$, $g_{3,7}=4$, $g_{3,8}=2, \dots$). Thus the probability density of r_m , $P_I(r_m | S_I)$, in invasion percolation can be expressed as

$$P_I(r_m | S_I) = \frac{dP(S_p \geq S_I | p = r_m)}{dr_m} \quad (6)$$

and is shown in Fig. 2(b) for small S_I .

For $S_I \rightarrow \infty$, we have

$$P(S_p \geq S_I | p = r_m) \rightarrow P_\infty(r_m), \quad (7)$$

where $P_\infty(r_m)$ is the probability of an infinite cluster, which is the order parameter of the percolation problem, characterized by the critical exponent β :

$$\begin{aligned} P_\infty &\sim |r_m - p_c|^\beta & r_m > p_c, \\ P_\infty &= 0 & r_m \leq p_c. \end{aligned} \quad (8)$$

Thus

$$\lim_{S_I \rightarrow \infty} P_I(r_m | S_I) = \left. \frac{dP_\infty(p)}{dp} \right|_{p=r_m}. \quad (9)$$

This limiting distribution is strictly equal to zero for $r_m < p_c$ and diverges as $(r_m - p_c)^{\beta-1}$ as $r_m \rightarrow p_c + \varepsilon$.

For large finite S_I , the distribution $P_I(r_m | S_I)$ is not strictly equal to zero for $r_m < p_c$, but rapidly decays as r_m decreases. It is known [15] that in the regular percolation problem, for $p < p_c$,

$$P(S_p \geq S_I | p) \sim f((p_c - p) S_I^\sigma), \quad (10)$$

where $f(x)$ decays exponentially as $x \rightarrow \infty$, $\sigma = 1/(\nu_p d_f)$, ν_p is the percolation correlation exponent, and d_f is the fractal dimension of the percolation cluster. Hence for $r_m < p_c$,

$$P(r_m \leq p | S_I) \sim f((p_c - r_m) S_I^\sigma), \quad (11)$$

which means that the distribution of r_m rapidly approaches zero for $r_m < p_c - A S_I^{-\sigma}$, where A is some positive coefficient. The maximum of the probability density $P(r_m)$ is reached at the point r^* , such that $d^2 f(x)/dx^2|_{x^*} = 0$, where $x^* = (p_c - r^*) S_I^\sigma$. Hence $r^* = p_c - x^* S_I^{-\sigma}$. In our problem, $\tilde{d}_{opt} \approx 1.52$ in 2D, $\nu_p = 4/3$ thus we can expect $\tilde{\sigma} = 1/(\nu_p \tilde{d}_{opt}) \approx 0.5$ in good agreement with our numerical results in Fig. 2(a).

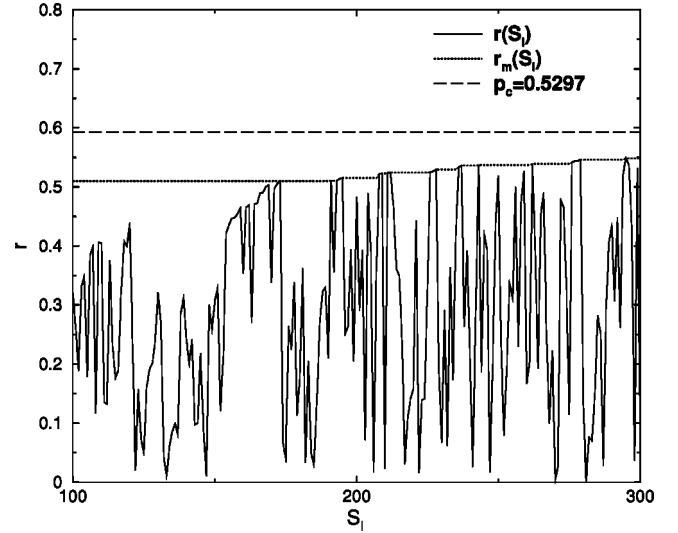


FIG. 3. Linear plot of the random values r as a function of the cluster size S_I for invasion percolation (site case). The solid line shows r as a function of the cluster size S_I . The dotted line shows the maximum value r_m as a function of S_I . The dashed line shows p_c . As the cluster size increases, $r_m \rightarrow p_c$.

The similarities between invasion percolation and fixed- N SAWs in strong disorder are not surprising, since for large a , our algorithm essentially selects the walks that minimize the largest value of r [14]. In invasion percolation, the value of $r(S_I)$ for the last selected site S_I fluctuates, sometimes reaching the value r_m , which is the largest value among all previously invaded sites (see Fig. 3). Suppose that the longest possible SAW starting at the origin and staying inside this invaded cluster has a length $N_{max}(S_I)$. Then all optimal SAWs of lengths $N \leq N_{max}(S_I)$ must stay inside this cluster too. Moreover, the optimal SAW of length $N = N_{max}(S_I)$ must exactly coincide with the maximal SAW in the cluster of size S_I . For $N > N_{max}(S_I)$, the optimal SAWs will achieve the maximal r_m and stay inside the percolation cluster corresponding to a new record value of the percolation probability $r'_m > r_m$ (see Fig. 4). As N grows, the record value of r_m approaches the percolation threshold p_c . In Fig. 5, we show a typical configuration of an optimal SAW in a strong site disorder in 2D. We assign to each site white color if the site has a value $r < r_m$ and gray color otherwise.

Sometimes, however, the record value r_m exceeds the percolation threshold. In this case, r_m may become an absolute maximal record that is never overcome for larger N or S_I . In this case, the optimal SAW will try to minimize the second largest value of energy and continue to stay inside the invasion percolation cluster corresponding to the second largest value of r_m achieved after the absolute record.

In a full analogy with Eq. (6), the probability distribution of the maximum value for the optimal SAW of length N is

$$P_S(r_m | N) = \frac{dP(N_{max} \geq N | p = r_m)}{dr_m}, \quad (12)$$

where

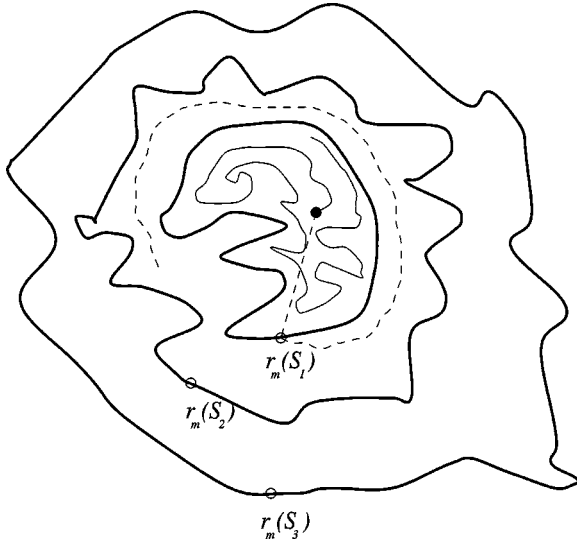


FIG. 4. Schematic picture of invasion clusters at three different successive record values of $r_m(S_l) = r(S_l)$. The positions of the maximal threshold $r_m(S_l)$ are shown by open circles. Two optimal SAW of different lengths start from the origin (closed circles). One SAW with $N = N_{max}(S_1)$ (thin solid line) fits inside the cluster S_1 . Another SAW of length $N > N_{max}(S_1)$ (dashed lines), achieves the maximal $r_m(S_1)$ and stays inside the cluster S_2 corresponding to a new record value of the percolation probability $r_m(S_2) > r_m(S_1)$.

$$P(N_{max} \geq N | p = r_m) = 1 - \sum_0^{N-1} b_n(p), \quad (13)$$

and $b_n(p)$ is the probability of finding a maximal walk of length n starting from the origin at percolation probability p . One can show that $b_n(p)$ are polynomials with respect to p

$$b_n(p) = \sum_{t,s} b_{n,s,t} p^{s-1} (1-p)^t, \quad (14)$$

where $b_{n,s,t}$ are integers such that $\sum_{n=0}^{\infty} b_{n,s,t} = s g_{s,t}$. The coefficients $b_{n,s,t}$ can be found by exact enumeration similar white Ref. [10]. Analyzing all clusters of size $s \leq 5$, one can easily find that

$$b_0(p) = (1-p)^4, \quad (15)$$

and

$$b_1(p) = 4p(1-p)^6 + 2p^2(1-p)^8 + 4p^2(1-p)^7 + 4p^3(1-p)^8 + p^4(1-p)^8. \quad (16)$$

In summary, the behavior of the optimal SAW path can be explained in terms of connected basins with energy $\epsilon \leq \epsilon_c \equiv \exp(ap_c)$, where p_c is the critical value for percolation. In order to minimize the energy, the SAW tries to fill the entire basin. When the length of the SAW is larger than the maximal size that may fit into the basin, the SAW jumps to another basin and tries to fill it. For very large N , the SAW is almost completely confined to a finite percolation cluster at

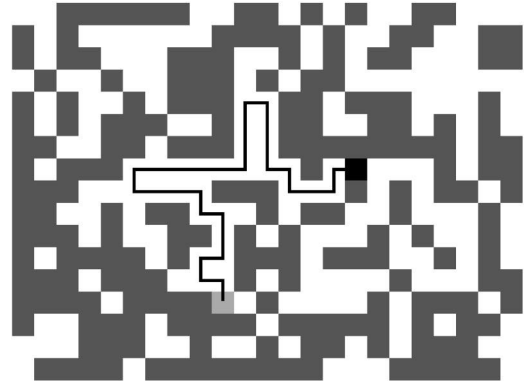


FIG. 5. A typical optimal SAW of length $N = 30$ in the strong disorder limit in 2D. The sites with random numbers $r < r_m = 0.46$ are white, the sites with random numbers $r > r_m$ are dark gray and the site with $r = 0.46$ is light gray. The optimal SAW in this configuration is shown as a black line. The origin is marked by the black square. One can see that the path stays within the percolation cluster for $p = r_m$. Moreover, visual inspection shows that this path coincides with the longest possible SAW inside the cluster.

criticality and will often coincide with the longest possible SAW inside this cluster. Thus the fractal dimension d_{max} of the longest SAW inside the finite percolation cluster at criticality must be a rigorous upper bound for d_{opt} .

Moreover, the longest SAW must stay inside the percolation backbone connecting the origin and the last step of the SAW. If the SAW enters a singly connected “dangling end,” it cannot come back to the position of the last step without self-intersection. Thus the fractal dimension of the percolation backbone d_B is a rigorous upper bound for both d_{max} and d_{opt} . Since the optimal SAW tries to be as compact as possible in order to “fit” inside the cluster [18] and the long-

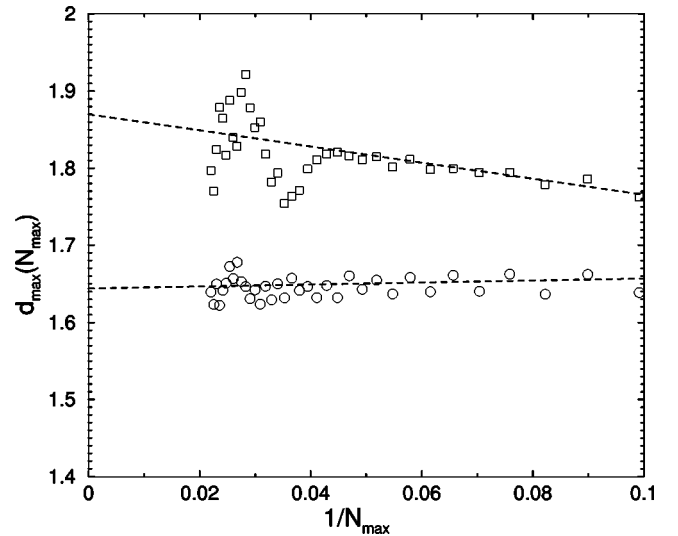


FIG. 6. Log-Log of the effective exponent $d_{max}(N_{max})$ as a function of $1/N_{max}$ of a SAW in a finite percolation cluster at the criticality in 2D (\circ) and 3D (\square). The symbols are the results of simulations, the dashed line is used as a guide to show the asymptotic value.

est SAW tries to fill the entire backbone, it is plausible that $\tilde{d}_{opt} = d_{max} = d_B$.

In order to verify this hypothesis, we simulate the longest SAW on a cluster at criticality and study by exact enumeration R as a function of the maximum length N . We use the Leath [19] algorithm to generate finite clusters at criticality. We find by exact enumeration the longest SAW that starts from the origin of each Leath cluster. We perform the simulation over 5×10^6 realizations of disorder in $d=2$ and 10^6 in $d=3$. We average the square of the end-to-end distance of the longest SAW for each value of the maximum length N_{max} . In Fig. 6, we plot the effective exponent $d_{max}(N_{max})$ [see Eq. (3)] as a function of $1/N_{max}$. We find

$$d_{max} = \begin{cases} 1.64 \pm 0.02 & \text{in } d=2 \\ 1.87 \pm 0.05 & \text{in } d=3. \end{cases} \quad (17)$$

These values are within the error bars with the values we find for \tilde{d}_{opt} . The values of d_{max} found here coincide with the fractal dimension of the backbone and are significantly larger than the values previously reported [10].

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- [12] In order to speed up the calculation, we abandoned all the SAW's for which the sum of the energies $E(M) = \sum_{i=1}^M \epsilon_i$, $M \leq N$ exceeds the actual minimum energy $E_{min}(N)$ of the previous explored N -steps SAWs.
- [13] In the site-disorder case there exists a degeneracy for the minimum SAWs. The same set of sites may be visited in a different order by several different SAWs. Those SAWs may have different end-to-end distances and in that case, we compute the average square distance.
- [14] Consider two closest random values for the energies $\epsilon_1 = \exp(ar_1)$ and $\epsilon_2 = \exp(ar_2)$ such that $r_2 = r_1 + 1/\Pi$, where Π is the period of the random generator number ($\Pi \gg L^d$). We

have $\epsilon_2 = \epsilon_1 \exp(a/\Pi)$. If $\exp(a/\Pi) = 2$, the sum of the energies can be represented as a binary number in which each binary digit represents an energy value of a different order of magnitude. In this limit, the sum of the energies of the path is completely governed by the largest energy. Any SAW i is characterized by a set of its energy values $S_i = \{\epsilon_{i1}, \epsilon_{i2}, \dots, \epsilon_{iN}\}$, sorted in decreasing order, so that $\epsilon_{ij} > \epsilon_{ij+1}$. We define that $S_k < S_i$ if there exists a value of m , $1 \leq m \leq N$, for which

$$e_{ij} = e_{kj} \quad \text{for } j < m \quad \text{and}$$

$$e_{kj} < e_{ij} \quad \text{for } j = m.$$

Using exact enumeration, we find the SAW with the minimal S_i . The results for these SAWs coincide with the results for finite $a \geq 100$. See also [5].

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