Numerical estimate of a scaling exponent characterizing fluctuating diffusion fronts

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We perform large scale Monte Carlo simulations of the fragmentation of bond percolation cluster perimeters on the square lattice at the percolation threshold. Using our data, we obtain a very accurate estimate for a scaling exponent that characterizes the fluctuations of a diffusion front. Our estimate provides strong support for a prediction made by J. F. Gouyet and Y. Boughaleb [Phys. Rev. B **40**, 4760 (1989)].

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Gouyet and Boughaleb (GB) recently obtained a number of analytical results concerning the temporal fluctuations of diffusion fronts in two dimensions [1]. Of particular interest here is their prediction that the front fragmentation exponent

$$\phi_H = \tfrac{11}{7} = 1.5714\ldots . \tag{1}$$

GB argue that this result is exact. However, they performed small scale numerical simulations of diffusion fronts and found an estimate $\phi_H = 1.40 \pm 0.02$ that does not agree with their own prediction. Moreover, in their arguments in favor of their result, GB make a number of approximations and assumptions. Thus their prediction (1) could be called into question.

In this Brief Report, we will present the results of large scale simulations intended to test GB's prediction (1). Rather than performing simulations of diffusion fronts directly, we instead study the fragmentation of percolation cluster perimeters. We then exploit a relation between this problem and diffusion fronts to obtain an estimate of ϕ_H. In this way, we are able to obtain a much more precise test of GB's prediction than we could have obtained by simulating diffusion fronts directly. Our estimate $\phi_H = 1.570 \pm 0.003$ is in excellent agreement with Eq. (1).

We consider bond percolation on the square lattice at the percolation threshold $p = p_c = \frac{1}{2}$. In order to construct percolation cluster perimeters (or "hulls") without constructing the clusters themselves, we use a perimeter-generating walk due to Gunn and Ortuño [2]. The algorithm used to generate the Gunn and Ortuño walk (GOW) will now be briefly described (for details, see Ref. [2]). GOW's are constructed on the covering lattice of the original square lattice. (The covering lattice is a square lattice obtained by joining the centers of adjacent bonds on the original lattice.) The state of a bond on the original lattice can be unspecified, occupied, or vacant. Initially, all of the bonds are in the unspecified state. The walk starts at the origin of the covering lattice. One of the four possible directions is randomly chosen, and a unit step performed in this direction (Fig. 1). The walk reaches a bond on the original lattice which we will call the target bond. The walk is then constructed step by step. If the target bond's state has not yet been specified, it becomes occupied or vacant with equal probability. On the other hand, if the state of the target bond has previously been designated, its state is left unchanged. A step

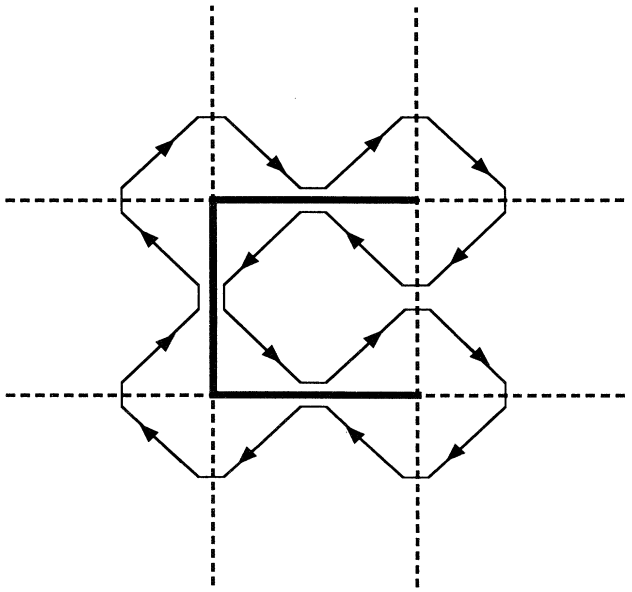

FIG. 1. A clockwise 16-step GOW (thin line) that traces out an external perimeter. The perimeter is made up of three occupied bonds (bold line), plus nine vacant bonds (dotted line). There are four constriction points and three fragmenting bonds on this perimeter.

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is made to the right if the target bond is vacant, and to the left it if is occupied. The walk stops when it attempts to retraverse the initial step, forming a closed loop. In practice, we stopped constructing the GOW if the number of steps performed (s) exceeded a cutoff value $s_{\max}$.

It is straightforward to see that the GOW generates the perimeter of a percolation cluster. With our conventions, GOW's that close in a clockwise (counterclockwise) fashion trace out external (internal) perimeters.

The occupied bonds on the original lattice that are touched by the GOW are the perimeter bonds. One of these perimeter bonds is now chosen at random, and is replaced by a vacant bond. This replacement may or may not result in the fragmentation of the percolation cluster. A *fragmenting bond* will be defined to be an occupied bond on the original lattice that the GOW visits twice (see Fig. 1). The replacement of the chosen occupied bond by a vacant bond only results in the fragmentation of the percolation cluster if the chosen bond is a fragmenting bond. If the chosen bond is indeed a fragmenting bond, the GOW is modified to reflect the fact that the chosen bond is now vacant. This results in the fragmentation of the parent GOW into two loops that trace out the perimeters of the cluster fragments.

Suppose that the original GOW of s steps is fragmented into two loops of s' and $s-s'$ steps, respectively, and let $s' \leq s-s'$, so that the loop of s' steps is the smaller of the two fragments. We define $P_{s',s}$ to be the probability that a daughter GOW of s' steps is obtained from a parent loop of length s when the replacement is made. Note that the probability that this event actually fragments a GOW of s steps, $P_f(s) \equiv \sum_{s'=4}^{s/2} P_{s',s}$, is in general different from unity.

Let us define a *constriction point* to be any point touched twice by the GOW (see Fig. 1). A constriction point can lie at the center of either an occupied or a vacant bond. We will denote the number of constriction points and fragmenting bonds touched by a GOW of s steps by $N_c(s)$ and $N_f(s)$, respectively. There is a simple relation between their average values $\langle N_c(s) \rangle$ and $\langle N_f(s) \rangle$, as we now show. When the direction of a GOW that traces out an external perimeter is reversed, it becomes a GOW that follows an internal perimeter, and vice versa. To see this, we transform the simple graph in Fig. 1 in the following way. First, any bond (whether it be occupied or vacant) is replaced by its dual bond. The dual bond is obtained by a $\pi/2$ rotation of the original bond about its center. Next, occupied bonds on the dual lattice are replaced by vacant bonds, and vice versa. Finally, the direction of the GOW is reversed. It is straightforward to see that this two-step operation transforms Fig. 1 to Fig. 2, and vice versa. The square lattice is self-dual. As a consequence, the *total* number of constriction points in Figs. 1 and 2 is exactly equal to twice the *total* number of fragmenting bonds. Moreover, occupied and vacant bonds are equally likely for $p = p_c = \frac{1}{2}$, and so both graphs occur with the same probability. These considerations apply equally well to arbitrary closed GOW's. Therefore, $\langle N_c(s) \rangle = 2 \langle N_f(s) \rangle$.

A closed Gunn and Ortuño walk can be mapped onto a self-attracting self-avoiding loop on the Manhattan lattice at its θ point (θ-MSASAL) [3]. A number of exact results are known for the latter model (for a recent review, see Ref. [4]). In particular, the average energy of a θ-MSASAL of s steps scales as $\frac{2}{3}\epsilon s + 2\epsilon A s^{3/7}$ as s tends to infinity [3,4]. Here ϵ is the energy assigned to each unbonded nearest-neighbor pair, and A is a nonzero constant. Under the mapping, a θ-MSASAL with s steps and energy $2\epsilon N$ is transformed into a GOW with s steps and N constriction points. Thus the average number of constriction points in a GOW of s steps scales as $\frac{1}{3}s + A s^{3/7}$ and, consequently,

$$\langle N_f(s) \rangle \sim \frac{1}{6}s + \frac{A}{2}s^{3/7} \tag{2}$$

when s is large.

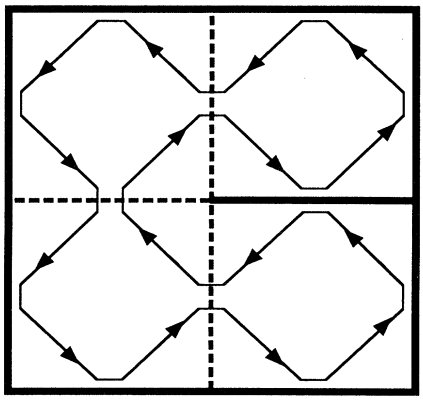

FIG. 2. The counterclockwise version of the GOW shown in Fig. 1. This GOW traces out an internal perimeter. The perimeter is made up of nine occupied bonds (bold line), plus three vacant bonds (dotted line). There are four constriction points and one fragmenting bond on this perimeter.

We now turn to the relationship between our model for the fragmentation of percolation hulls and the problem studied by GB [1]. GB's work concerns the diffusion of a set of noninteracting particles in the presence of a concentration gradient in the strip $\{(x,y) | 0 \leq x \leq L' \text{ and } 0 \leq y \leq L\}$. The length of the strip L' is assumed to be large compared to the width L. The concentration of diffusers p is fixed at one for $x=0$ and at zero for $x=L'$. This problem is also known as gradient percolation since at any time the problem is equivalent to site percolation in which the fraction of occupied sites p varies linearly from one end of the strip to the other [5]. The large cluster of particles that has one edge on the end of the strip with concentration $p=1$ is called the parent cluster. The frontier of the parent cluster within the strip is the diffusion front. Since the particles are all diffusing, the diffusion front is constantly fluctuating, and small clusters are continually joining and separating from the parent cluster at the diffusion front. It is these fluctuations that GB chose to study.

Let $N_{\text{frag}}(\sigma)$ be the number of clusters with an external perimeter of length σ that disconnect from the parent

cluster in a unit time. GB argued that $N_{\rm frag}(\sigma)$ follows the scaling form $N_{\rm frag}(\sigma)=L\sigma^{-\phi_H}(L')^{3/7}F(\sigma/L')$, where F is a scaling function [1]. Note that $F(0)$ is a finite, nonzero constant and that $F(x)\to 0$ as $x\to\infty$. Let $P_{\rm frag}(\sigma)\Delta y$ be the probability that an external perimeter of length σ is disconnected from the parent cluster per unit time within the strip $\{(x,y)|0\le x\le L'$ and $y_0\le y\le y_0+\Delta y\}$. Here y_0 is a constant lying between zero and L and $a\ll\Delta y\ll L$. Clearly, $P_{\rm frag}(\sigma)=\sigma^{-\phi_H}(L')^{3/7}F(\sigma/L')$. If $\sigma\ll L'$, then $P_{\rm frag}(\sigma)$ scales as $\sigma^{-\phi_H}$ as a function of σ. On length scales small compared to the width of the diffusion front $w\sim(L')^{4/7}$, the diffusion front has the same geometry as the infinite percolation cluster at threshold in percolation without a concentration gradient [5]. Therefore, $P_{\sigma,s}\sim\sigma^{-\phi_H}$ for $\sigma\ll s$. Now a fragment cannot have a perimeter longer than its parent, which means that this scaling behavior must be cut off when σ approaches s. We conclude that $P_{\sigma,s}$ obeys the scaling law

$$P_{\sigma,s}\simeq\sigma^{-\phi_H}G(\sigma/s)\ , \tag{3}$$

where the scaling function $G(x)$ is finite and nonzero for $x=0$, and is zero for $x\ge 1$.

We constructed a total of 10^6 GOW's of maximum length $s_{\rm max}=2^{20}$. The 819 338 GOW's that closed before reaching a length $s_{\rm max}$ were fragmented exhaustively. This task was made possible through the use of a very efficient fragmentation algorithm [6]. For the perimeters of length s, we computed the average number $F_{s',s}$ of fragmenting bonds whose replacement by a vacant bond gives a daughter perimeter of length s'. Note that

$$F_{s',s}=\langle N_f(s)\rangle P_{s',s}/P_f(s)\ . \tag{4}$$

The first moment of $F_{s',s}$ was then calculated for the smaller fragments:

$$M_1(s)=\sum_{s'=4}^{s/2}s'F_{s',s}\ . \tag{5}$$

The lower limit for this summation, $s'=4$, corresponds to the smallest fragment that can be produced by removing a fragmenting bond in a GOW. According to Eqs. (2)–(4), $M_1(s)$ has the asymptotic behavior.

$$M_1(s)\cong A's^{3-\phi_H}+B's\ . \tag{6}$$

The second term on the right hand side of Eq. (6) is a correction that arises because the lower limit in Eq. (5) is nonzero. To avoid large fluctuations, we binned our data for $M_1(s)$. The binned quantity is defined as

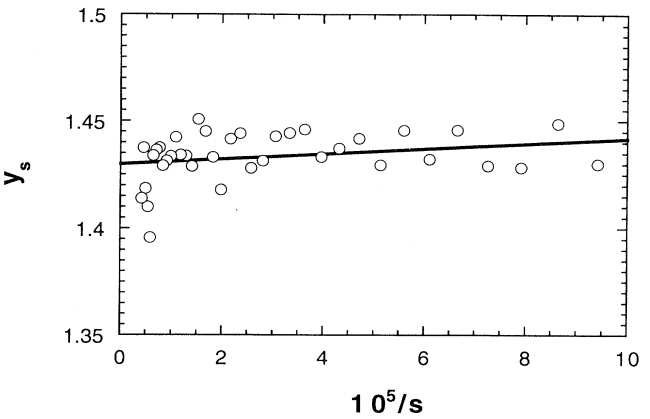

FIG. 3. Extrapolation of the finite-size estimator y_s to the limit $1/s\to 0$. The solid line is a linear least-squares fit to the data points.

$$\mu_s=\left[\sum_{\sigma=s}^{\alpha s}N_\sigma\right]^{-1}\sum_{\sigma=s}^{\alpha s}M_1(\sigma)N_\sigma\ , \tag{7}$$

where $\alpha=2^{1/8}$, and N_σ is the number of σ-step perimeters constructed. The influence of the correction to scaling on the asymptotic behavior of M_1 was found to persist over the whole range of s values. To determine the asymptotic behavior of μ_s, we computed a finite-size estimator $y_s=\log_{10}(\mu_{4s}/\mu_s)/\log_{10}4$ and plotted it as a function of $1/s$ (Fig. 3). A linear least-squares fit to the data points for $s>10^4$ gave $y_\infty=1.430\pm0.003$. Then, from Eq. (5) we deduced the estimate

$$\phi_H=1.570\pm0.003\ ,$$

which is in excellent agreement with GB's prediction $\phi_H=\frac{11}{7}=1.571\ldots$.

Our numerical results span over six decades in s, and as a result we were able to obtain a very precise estimate for ϕ_H. In contrast, GB's estimate for ϕ_H was extracted from data ranging over two decades in s only. As we have seen, corrections to scaling persist up to very large values of s. Therefore, GB's estimate of ϕ_H was very likely biased by finite-size effects.

In summary, the goal of the present work was to carry out a very precise numerical test of Gouyet and Boughaleb's prediction that ϕ_H is exactly $\frac{11}{7}$. Our numerical estimate of ϕ_H, which has an accuracy of 0.2%, is in excellent agreement with this prediction.

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