Exact Scaling Law for the Fragmentation of Percolation Clusters: Numerical Evidence

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We perform large-scale numerical simulations to generate and fragment three-dimensional bond percolation clusters on the cubic lattice. We compute very accurately the standard exponents τ and γ, as well as an exponent ϕ which characterizes the binary fragmentation of the clusters. Two published scaling laws which relate ϕ to τ and γ are tested. Excellent agreement is obtained with one of these relations, indicating that it is possibly exact in any dimension, while the other relation is shown to be in error. [S0031-9007(97)02946-3]

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Fragmentation is a very wide area of science in which applications range from subatomic scales, with the fragmentation of atomic nuclei [1], to planetary scales, with the fragmentation of asteroids [2]. It is of special importance in materials science, where particular attention is devoted to the fragmentation of random porous materials [3,4]. Recently, there has been an increasing interest in binary fragmentation of percolation clusters [5,6], probably because it is a rare example of a model for the fragmentation of disordered porous solids providing analytical results. Usually bond percolation clusters are studied, since removing a single bond from a cluster produces two fragments at most. Thus, fragmentation is automatically binary, which is not true for site percolation. The bond which is removed can be arbitrarily chosen among all the bonds in the cluster [5]. Alternatively, this choice can be restricted to the bonds that belong to the cluster external surface (the "hull") [6]. In the latter case, the quantity of interest is the probability $P_{s',s}$ that a fragment of s' bonds is obtained when a bond is removed at the hull of a s-bond cluster. This quantity is expected to scale with s' as

$$P_{s',s} \sim (s')^{-\phi} G(s'/s)\,, \tag{1}$$

where the scaling function $G(x)$ is finite and nonzero for $x = 0$, and is zero for $x \geq 1$ [5,6].

Two analytical expressions relating the fragmentation exponent ϕ to the standard exponents of the percolation transition have been recently proposed in the literature. Considering the time fluctuations of the invaded volume in invasion percolation, Gouyet obtained [7]

$$\phi = 1 + (d_H - 1/\nu)/d_f\,, \tag{2}$$

in the limit of a perfectly compressible displaced fluid, i.e., in the limit of standard kinetic percolation. In this relation, ν represents the critical exponent for the correlation length of the percolation clusters. The fractal dimensions for the hull and for the bulk of the clusters are denoted by d_H and d_f, respectively. The second relation, found by Roux and Guyon in a very similar context [8] reads

$$\phi = \tau + \sigma - d_H/d_f\,, \tag{3}$$

where τ and σ, respectively, are the mass distribution and the characteristic mass exponents for regular percolation. In the following, Eqs. (2) and (3) will be referred to as (G) and (RG), respectively. In two dimensions, the numerical values of ϕ given by (G) and (RG) coincide. Using the exact values of the critical exponents [9], we have then $\phi = 139/91 = 1.527\ldots$. On the other hand, as first noticed by Gouyet [7], the two relations give different results in three dimensions (3D). As a consequence, one (or both) of these relations is not exact. Since most applications of fragmentation are in 3D, this point is of practical importance. However, to our knowledge, there has been no numerical test of (G) and (RG) in 3D so far. The reason is probably that conclusive numerical results are difficult to obtain.

In this Letter, we will present the results of intensive numerical simulations intended to test the validity of (G) and (RG) in 3D. Since the standard critical exponent γ of percolation is not known very precisely in 3D, we begin by computing it more accurately by constructing bond percolation clusters on the cubic lattice. Our results are then used in conjunction with (G) and (RG) to produce precise estimates for ϕ. In parallel, we independently compute the exponent ϕ by fragmenting a large set of percolation clusters. An efficient fragmentation algorithm is designed to perform this task. Our results support Gouyet's relation with remarkable precision, suggesting that (G) is indeed exact in any dimension. On the other hand, Roux and Guyon's prediction [8] is found to be invalid and we offer an insight into why this is so.

It has recently been shown that in 3D the hull and the bulk of percolation clusters have the same fractal dimension, i.e., that $d_H = d_f$ [10]. Using in addition the scaling laws $\nu d_f = 1/\sigma = \gamma/(3 - \tau)$ [9], (G) and (RG), respectively, become

$$\phi = 2 - \frac{3 - \tau}{\gamma} \tag{4}$$

and

$$\phi = \tau - 1 + \frac{3 - \tau}{\gamma}\,, \tag{5}$$

where γ is the critical exponent associated with the mean cluster mass. The most accurate estimates of τ and γ

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published so far are $\gamma = 1.805 \pm 0.020$ [11], obtained by performing series expansions, and $\tau = 2.188 \pm 0.003$ [12], obtained in Monte Carlo simulations [13]. With these estimates, Eqs. (4) and (5), respectively, give $\phi = 1.550 \pm 0.007$ and $\phi = 1.638 \pm 0.007$. The gap between the two central values is about 12 standard deviations. This is definitely sufficient to allow a conclusive comparison with an independent estimate for ϕ. Let us remark, however, that the main contribution to the error on ϕ comes from the estimate for γ. In the following, we compute a more precise estimate for γ which allows us to obtain the exponent ϕ even more accurately.

With this aim, a large number of bond percolation clusters were constructed on the 3D cubic lattice. We used a Leath-Alexandrowicz algorithm [14] which constructs the clusters one by one. Starting from a single occupied bond, this algorithm repeatedly adds either a new occupied bond with probability p or a new vacant bond with probability $1 - p$, until the cluster surface is saturated with vacant bonds. As new occupied or vacant bonds are added to the cluster, their locations are stored in a list. Using a hashing technique [15], only two attempts are necessary on the average to locate a given bond in the list. This algorithm allows us to get rid of any finite-size effect due to the underlying lattice and to save computer memory. The maximum number of occupied bonds in a cluster is set to $s_{\max} = 2^{18}$ in the simulations.

A total of 10^5 clusters were constructed at the percolation threshold, $p = p_c = 0.248\,813$. This value is an average of the estimates $0.248\,814 \pm 0.000\,003$ and $0.248\,812 \pm 0.000\,002$ given in Refs. [12] and [16], respectively. As a preliminary test, the fraction $F(s)$ of clusters containing at least s bonds was computed. At $p = p_c$, this quantity is expected to scale with s as $F(s) \sim s^{2-\tau}$. In Fig. 1, the finite-size estimator $\tau_s = 2 - \log_{10}[F(as)/F(s)]/\log_{10}(a)$ is plotted as a function of s, for $a = 2^{1/8}$. We observe that τ_s is roughly constant for $s \geq 50$. A statistical average of the corresponding data points gives $\tau = 2.188 \pm 0.001$. In order to take into account the error on p_c explicitly, we repeated the same calculations for $p_c = 0.248\,810$ and $p_c = 0.248\,817$, the lower and upper bounds of the error range on p_c. We obtained $\tau = 2.189 \pm 0.002$ and $\tau = 2.188 \pm 0.003$, respectively. Our final estimate is thus $\tau = 2.188 \pm 0.003$, in very good agreement with the estimate quoted above [12].

The exponent γ was determined by considering 20 p values below p_c, $p_1 = 0.217 < p_2 < \cdots < p_{20} = 0.245$ and by constructing 10^6 clusters for each p_i $(i = 1, 2, \ldots, 20)$. All the clusters constructed stopped growing before reaching the maximum mass $s_{\max}$, so that no bias was introduced by this cutoff. The average cluster mass, $\chi(p) = \sum_{s=1}^{s=\infty} F(s)$, is expected to scale with p as $\chi(p) \sim (p_c - p)^{-\gamma}$. Finite-size corrections are usually important for χ and we found it to be indeed the case with our data, $\chi_i = \chi(p_i)$. To minimize these corrections, a finite-size estimator, $\gamma_k(p_i) = \log_{10}(\chi_{i+k}/\chi_{i-k})/\log_{10}[(p_c - p_{i-k})/(p_c - p_{i+k})]$, was computed and plotted as a function of $(p_c - p_i)$. As observed in Fig. 2, the data points for $\gamma_5(p)$ fall on a straight line. Linear extrapolation to $p = p_c$ gives $\gamma = 1.794 \pm 0.004$. The robustness of this method was tested by repeating the procedure with $k = 3, 4, 6, 7$. The same result was found in each case. Here again, the same analysis was repeated for $p_c = 0.248\,810$ and $p_c = 0.248\,817$, which gave $\gamma = 1.793 \pm 0.003$ and $\gamma = 1.796 \pm 0.004$, respectively. Altogether, our final estimate is $\gamma = 1.794 \pm 0.006$. This estimate is in good agreement with the γ value quoted above [11] but is significantly more precise. As a matter of fact, our estimates for τ and γ are very close to unpublished results obtained by Ziff and Stell [16].

With our estimates for τ and γ, Gouyet's and Roux and Guyon's relations give $\phi = 1.547 \pm 0.003$ and $\phi = 1.641 \pm 0.003$, respectively. These two values of ϕ differ now by more than 30 standard deviations. Comparing them to a value of ϕ computed independently should thus definitely allow us to discriminate between Eqs. (4)

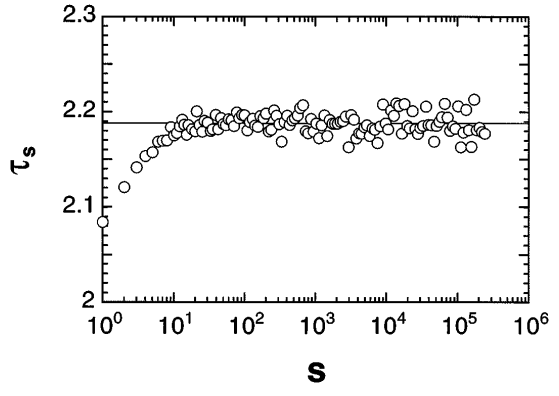

FIG. 1. The finite-size estimator for the exponent τ plotted as a function of the cluster mass s. The horizontal line is to the average value of the data points for $s \geq 50$.

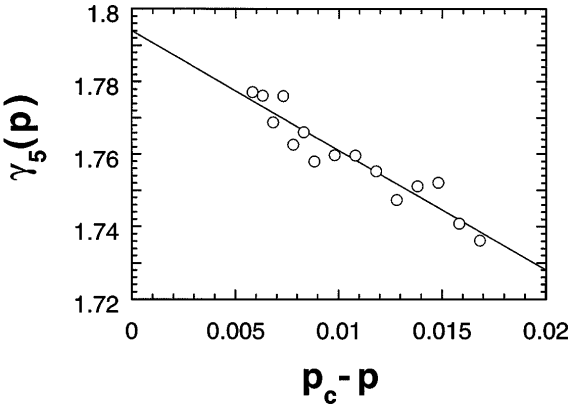

FIG. 2. The finite-size estimator for the exponent γ plotted as a function of $p_c - p$. The line is a linear least-squares fit to the data points.

and (5). With this aim, we constructed and fragmented exhaustively a set of 5×10^4 clusters with a cutoff mass $s_{\max} = 2^{16}$. In order to exhaustively fragment a given cluster, each of its s occupied bonds is replaced in turn with a vacant bond. A test is then performed to decide whether this substitution causes a binary fragmentation. If it does, the selected bond is called a fragmenting bond. When the test is completed, the selected bond is replaced again by an occupied bond and the next cluster bond is processed. It is worth noting that all the bonds in the cluster, and not only the bonds in the hull, are tested in our algorithm. However, since the hull and the bulk fractal dimensions are equal in 3D, this only introduces a constant factor in the fragmentation probability, so that Eqs. (4) and (5) apply equally well in both cases.

Fragmentation is usually tested by using a simple burning algorithm [5]: One end of the selected bond is randomly chosen and an occupied bond adjacent to this end is set alight. Burning then propagates from bond to bond until none is left unburnt. On the average, this simple algorithm needs a total number of operations of order s^2 for a s-bond cluster. On the other hand, if burning is started and propagated *simultaneously* on both ends of the selected bond, it can be shown [17] that the order of the algorithm reduces to $s^{3-\phi}$. Since ϕ is roughly equal to 1.5, the double-burning algorithm is significantly faster than the simple one. Qualitatively, this is so because a percolation cluster is much more likely to give fragments of very different masses than fragments of comparable masses. The double-burning algorithm was used to compute the average number of fragmenting bonds, $\langle N_f(s)\rangle$, as well as the average cumulative mass of the smaller fragments, $M(s) = (\sum_{s'=1}^{(s-1)/2} s' \langle N_f(s)\rangle P_{s',s})\,(\sum_{s'=1}^{(s-1)/2} P_{s',s})^{-1}$. In these expressions, the angular brackets represent statistical averages over all the s-bond clusters constructed.

Our data for $\langle N_f(s)\rangle$ and $M(s)$ were binned, according to the method described in Refs. [5,6]. The binned values are denoted by $\langle N_f^B(s)\rangle$ and $M^B(s)$, respectively. In 2D, analytical and numerical results showed that $\langle N_f(s)\rangle \sim s$ [5,6] and it was argued that this is true in any dimension [5,18]. A careful finite-size analysis of our data gave $\langle N_f^B(s)\rangle \sim s^{1.001\pm0.004}$ [17], providing extra support to the relation $\langle N_f(s)\rangle \sim s$.

Using this last relation in conjunction with Eq. (1), we find $M(s) \sim s^{3-\phi}$. Figure 3 is a plot of the finite-size estimator $\phi_s = 3 - \log_{10}[M^B(4s)/M^B(s)]/\log_{10}(4)$ as a function of $1/s$. A linear behavior is obtained and extrapolation to $s \to \infty$ gives the estimate $\phi = 1.548 \pm 0.008$. Let us remark that a direct fit of *all* the data points for $M(s)$ in the range $s \geq 10^4$ gave a comparable, though less precise, estimate [17]. Our fragmentation program was run again for $p_c = 0.248\,817$, the upper boundary of the error range on p_c. The exponent ϕ extracted from the corresponding data was found to be equal to 1.545 ± 0.009. Assuming a symmetric behavior for $p_c = 0.248\,810$, the lower bound of the error range on p_c, we finally obtained

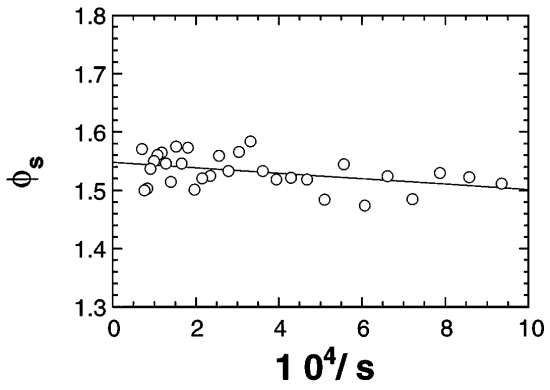

FIG. 3. Extrapolation of the finite-size estimator for the exponent ϕ to the limit $1/s \to 0$. The solid line is a linear least-squares fit to the data points.

$$\phi = 1.548 \pm 0.016\,. \tag{6}$$

This direct estimate of ϕ is in excellent agreement with the value $\phi = 1.547 \pm 0.003$ obtained from Eq. (4). Conversely, it definitely rules out Eq. (5) which gave $\phi = 1.641 \pm 0.003$. Thus, (RG) is found to be in error in 3D. Since this relation does not give the expected mean field behavior either [19], its validity can be called into question. The derivation of (RG) is actually based on the observation that the bursts which form at the front in invasion percolation are equivalent to percolation clusters [8]. Roux and Guyon [8] then make several assumptions to arrive at (RG). One of these assumptions is that the probability for a burst of s sites to grow is proportional to the number of sites which belong to its hull. Since this number varies with s like s^{d_H/d_f}, the term $T = -d_H/d_f$ which appears in (RG) is obtained. However, we believe that this assumption is not correct because only a subset of all the sites which belong to the hull can be the root of the burst. This subset is found by considering only the configurations where the burst and the front are linked by a *single* bond. This bond is thus a red bond for the ensemble composed of the burst and the parent cluster behind the front. Within the region of space occupied by the burst, the number of red bonds is proportional to $s^{1/\nu d_f}$ [20]. In (RG), T should then be replaced with $T' = -(\nu d_f)^{-1}$, in agreement with an intermediate result found by Gouyet in the derivation of (G) [7]. Since one term appears to be wrong in (RG), the fact that this relation gives the correct value for ϕ in 2D is probably just a mere coincidence.

In summary, our numerical results confirm the validity of Gouyet's scaling law (G) in 3D. Since this law was also successfully tested in two dimensions [5,6] and, in addition, is exact in one dimension and on the Bethe lattice [5,19], we conclude that it is very likely exact in any dimensions.

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