Fragmentation of percolation clusters in general dimensions

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The scaling behavior for binary fragmentation of critical percolation clusters in general dimensions is investigated by Monte Carlo simulation as well as by exact series expansions. We obtain values of critical exponents λ and ϕ describing the scaling of the fragmentation rate and the distribution of cluster masses produced by binary fragmentation. Our results for λ and ϕ in two to nine dimensions agree with the conjectured scaling relation $\sigma=1+\lambda-\phi$ by Edwards and co-workers [Phys. Rev. Lett. **68**, 2692 (1992); Phys. Rev. A **46**, 6252 (1992)], which in turn excludes the other scaling relations suggested by Gouyet (for $d=2$), and by Roux and Guyon [J. Phys. A **22**, 3693 (1989)], where σ is the crossover exponent for the cluster numbers in percolation theory. [S1063-651X(99)51005-2]

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The fragmentation process is widely observed in spatially random objects such as coal particles, branched polymers, atomic nuclei, etc. Understanding the fragmentation property in random porous materials is essential to characterizing a statistical property of degradation in time as well as to probe an internal structure of random materials. Recently there has been great interest in describing this through binary fragmentation of bond percolation clusters because its description is simple and it captures the important scaling properties of the random object [1–6]. Quantities of interest are the fragmentation rate and the mass distribution of fragments after breakup.

The fragmenting bond in a binary fragmentation of bond percolation cluster is a bond whose removal results in two disconnected clusters. The fragmentation rate is proportional to the number a_s of fragmenting bonds of a mother cluster of s bonds, and the mass distribution is a probability distribution $b_{s's}$, which is the probability of finding a daughter cluster of size s' after a binary fragmentation of a mother cluster of s bonds. In one dimension (1D) [6] and on the Bethe lattice [3] the exact results for these quantities show a scaling behavior for large s without dependence on the bond occupation probability p. For dimensions $d>1$, a_s and $b_{s's}$ do not have a scaling behavior at all p due to the p dependence of cluster structure, except at the percolation threshold p_c, where there exists self-similarity. From the scaling behaviors for $d=1$ and Bethe lattice, the generalized scaling forms for $d>1$ were suggested, namely,

$$a_s(p=p_c)\propto s^{\lambda}, \tag{1}$$

$$b_{s's}(p=p_c)=s^{-\phi}g(s'/s) \tag{2}$$

as cluster size increases [7,8] (for $d=1$, $\lambda=1$, $\phi=1$ and for Bethe lattice $\lambda=1$, $\phi=3/2$). Edwards and co-workers performed an intensive Monte Carlo simulation for a binary fragmentation of percolation clusters on the square lattice, and identified these scaling behaviors to provide the critical exponents $\lambda=1.001\pm0.006$, $\phi=1.601\pm0.008$ [7,8]. Their results satisfied the scaling relation

$$\sigma=1+\lambda-\phi, \tag{3}$$

which was derived using the analogy between red and fragmenting bonds, where σ is the crossover exponent of the cluster number in standard percolation theory [9]. Based on this observation they conjectured that these scaling behaviors should exist at p_c with $\lambda=1$ and the scaling relation $\sigma=2-\phi$ must be valid *for all higher dimensions also*. These scaling laws for fragmentation, if applied to Ising models instead of percolation, may also explain the failure of the traditional (Becker-Döring) cluster dynamics right at the Curie point [10].

Two other scaling relations relating the critical exponent ϕ to the standard critical exponents in the percolation theory were also proposed. Gouyet proposed

$$\phi=1+(d_H-1/\nu)/d_f \tag{4}$$

in the limit of a perfectly compressible displaced fluid considering the time fluctuations of the invaded volume in invasion percolation [11]. ν is a critical exponent for the correlation length, and d_H and d_f are the fractal dimensions for the hull and the bulk of percolation clusters, respectively, and we note that $d_H=d_f$ only for $d\geqslant3$. Roux and Guyon proposed

$$\phi=\tau+\sigma-d_H/d_f, \tag{5}$$

where τ is that for the mass distribution [12]. In three and higher dimensions Eqs. (4) and (5) become

$$\phi=2-\sigma, \qquad \phi=\tau-1+\sigma, \tag{6}$$

using $\nu d_f=1/\sigma=\gamma/(3-\tau)$ provided that $\lambda=1$ exactly, and γ is the mean cluster size exponent. Later, Debierre performed Monte Carlo simulations for the three-dimensional percolation clusters on the cubic lattice, and found the critical exponents $\lambda=1.001\pm0.004$, $\phi=1.548\pm0.016$, which supports the scaling relations by Eq. (3) and (4) [13]. The situation, however, is far from clear because the predicted values for ϕ from Eqs. (3)–(5) are 1.604, 1.527, and 1.527 in two dimensions, and 1.548, 1.547, and 1.640 in three dimen-

sions, respectively. Although the numerical calculations support the scaling relation of Eq. (3) in 2D, and that of Eqs. (3) and (4) in 3D, the discrepancy in two dimensions among these three scaling relations was not discussed clearly. In Ref. [11] Gouyet was originally concerned with the fragmentation of the hull of percolation clusters, and proposed the above scaling relation [Eq. (4)]. Interestingly enough, this scaling relation becomes exactly the same as that of Edwards and co-workers for three dimensions and above because $d_H = d_f$ for $d \geqslant 3$ and $d_H \neq d_f$ for $d=2$. In three and higher dimensions, the empty sites at the percolation threshold penetrate through the whole cluster of occupied sites, and thus hull and perimeter are roughly the same. The perimeter, on the other hand, is known since Leath and others to be proportional to the cluster mass in all dimensions larger than 1 [14]. Therefore, Gouyet's scaling relation can also be applied to the bulk fragmentation of percolation cluster only for $d \geqslant 3$ by simply replacing d_H by d_f, not for the general dimensions because d_H is different from d_f in two dimensions, but it can be applied to the general dimensions for the hull fragmentation. Therefore, the claim made by Debierre that Gouyet's scaling relation is exact for the bulk fragmentations in the general dimensions is not justified [13]. Even in Refs. [11,13] this crucial point was not discussed explicitly. For dimensions higher than 3 there has been no numerical test for these three scaling relations so far.

The validity of these conjectured scaling laws and scaling relations in *general dimensions* is investigated in this Rapid Communication. We report our investigation for the scaling properties of the binary fragmentation of bond percolation clusters in general dimensions by extensive Monte Carlo simulations as well as by exact series expansions. Our results show that the critical exponent for the fragmentation rate is $\lambda = 1.0$ in all dimensions, and for the fragment's mass distribution $\phi = 1.59 \pm 0.02, 1.55 \pm 0.01, 1.53 \pm 0.06, 1.51 \pm 0.08, 1.48 \pm 0.04, 1.52 \pm 0.03$ for two to six and nine dimensions. These values satisfy the scaling relation by Eq. (3) in general dimensions, which consequently excludes the relations by Eq. (4) (for $d=2$) and Eq. (5). Above six dimensions Bethe lattice exponents should be exact.

The Monte Carlo simulations were performed in the hypercubic lattices for two to seven dimensions. The bond percolation clusters were generated at p_c by Leath algorithm at each dimension, and tested for the fragmentation by a burning algorithm [14]. If the removal of a chosen bond on a mother cluster results in two disconnected clusters, such a bond is a fragmenting bond. When the size of a daughter cluster is either zero or $s-1$ or when the other end of a chosen bond is reached in the middle of the burning process, it is not a fragmenting bond. Applying a burning algorithm from either end site of a removed bond gives the size s' and $s-s'-1$ of daughter clusters, if any. Continuing this burning procedure for each bond on the clusters of size s provides the average number of fragmenting bonds per cluster, $a_s(p_c) \propto s^{\lambda}$ for large s. We also calculate the average number $c_{s's} = a_s b_{s's}$ of daughter clusters of size s' from fragmenting a mother cluster of size s in order to calculate the first moment $\mu_s = \Sigma_{s'=1}^{(s-1)/2} s' c_{s's}$. Assuming that the conjectured scaling laws in Eqs. (1) and (2) are valid, the first moment is

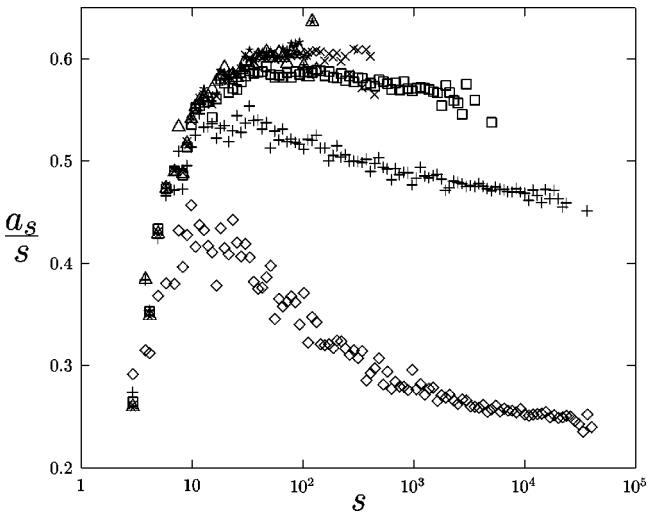

FIG. 1. Ratio a_s/s of the number of fragmenting bonds a_s vs the size s for two to seven dimensions. The marks $\diamond$, $+$, $\square$, $\times$, $\triangle$, $*$ correspond to 2,3,4,5,6,7 dimensions.

expected to scale as $\mu_s(p_c) \sim s^{\psi}$, where $\psi = 2 + \lambda - \phi$, from which one can find the critical exponent ϕ. From now on we assume $\lambda = 1$ [11].

In two to seven dimensions at the percolation threshold, our Monte Carlo simulations made 15 000, 27 800, 64 700, 0.45 million, 0.236 million, and 1.8 million attempts to grow a bond percolation cluster by the Leath algorithm in hypercubic lattices of L^d sites, with L up to 400, 100, 31, 13, 9, and 9 for $d=2$ to 7. About 7000 processor hours were spent on a Cray T3E. Here, the effects of the finite lattice sizes are strong for the cluster size distribution (not shown) but statistically insignificant for the fraction a_s/s of fragmenting bonds (Fig. 1) and the first moment μ_s (Fig. 2). Figure 1 suggests that the fraction of fragmenting bonds approaches for large clusters a constant near 0.25, 0.44, 0.56, 0.60, 0.61, and 0.62 for $d=2$ to 7, with a typical error of 0.02; Edwards and co-workers gave 0.24 for $d=2$ and 0.6321 for $d=\infty$.

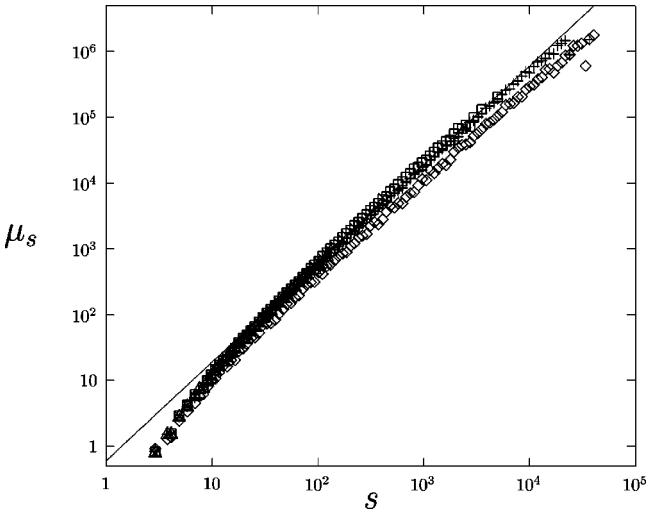

FIG. 2. First moment μ_s vs the size s in log-log scale. The slope gives $3-\phi$. The marks $\diamond$, $+$, $\square$, $\times$, $\triangle$, $*$ correspond to 2,3,4,5,6,7 dimensions. The straight line is drawn with a slope 1.5 for eye guidance.

The fraction of fragmenting bonds a_s/s versus s in a cluster increases rapidly for the small s and saturates from above to a constant value for the large s consistent with the large-s scaling behavior $a_s \propto s^{1}$, which thus results in the peak in between for all dimensions. The nonlinear behavior of a_s (Fig. 1) and μ_s (Fig. 2) versus the small s is due to the finite cluster size effect, which illustrates the importance of the correction-to-scaling especially for the small size clusters [7,8]. The higher the dimension is, the larger the constant value of a_s/s is for the large s. This shows that the critical percolation clusters in higher dimensions are easier to fragment, because the loops in critical percolation clusters become irrelevant in higher dimensions on which most nonfragmenting bonds exist.

As a rough estimation from Fig. 2, the exponent $3-\phi \simeq 1.5$ for the first moment is the same for $d=2$–7, and apart from two dimensions, this ''superuniversality'' seems to hold also for the proportionality factor (''amplitude'') and correction to the asymptotic behavior. However, a careful analysis for $d=2, 3, 4$, and 5 gave an exponent of 1.41 ± 0.02 for $d=2$, 1.45 ± 0.01 for $d=3$, and 1.50 ± 0.05 for $d=4$ and 5, which is also compatible with the two-dimensional estimates 1.40 of both Edwards and co-workers [7,8] and Cheon and Chang [15] and the three-dimensional estimate 1.452 of Debierre [13]. It agrees with the scaling prediction $1+\sigma = 1.396, 1.452, 1.488, 1.495, 1.5$, and 1.5 of Edwards and co-workers, but agrees only for $d \geqslant 3$ with 1.473, 1.453, 1.48, 1.49, 1.50, and 1.50 of Gouyet for $d=2$–7, respectively. The prediction 1.473, 1.36, 1.2, 1.1, 1.0, and $1.0\,(=4-\tau-\sigma$ for $d \geqslant 3)$ of Roux and Guyon, already excluded by Debierre for $d=3$, is violated even more strongly in higher dimensions [12]. Thus our data are compatible with $\lambda = 1$, and with one of the three competing scaling relations.

We also applied exact series expansions to calculate the critical exponents λ and ϕ in general dimensions. Given the occupation probability p of a bond, each realization of the random system consists of clusters (Γ) of sites interconnected by bonds. We define the low concentration series expansions for the average number of fragmenting bonds as

$$Q_a(p) = \sum_{\Gamma} W(d,\Gamma) a_s(\Gamma) s^2(\Gamma) p^{n_b(\Gamma)} (1-p)^{n_p(\Gamma)}, \quad (7)$$

and that for the first moment of the sum of daughter cluster size as

$$Q_\mu(p) = \sum_{\Gamma} W(d,\Gamma) \mu_s(\Gamma) s^2(\Gamma) p^{n_b(\Gamma)} (1-p)^{n_p(\Gamma)}, \quad (8)$$

which is the weighted sum of a_s and μ_s on the cluster Γ, respectively. Here $W_d(\Gamma)$ is the embedding weight of Γ on the d-dimensional hypercubic lattice, while $n_b(\Gamma)$ and $n_p(\Gamma)$ are the numbers of bonds in Γ and on its perimeter. The generation of series for $Q_a(p)$ and $Q_\mu(p)$ only requires the topology of clusters, since the fragmentation process is not affected by the geometry of clusters. We generated these series in general dimensions up to 13 bonds, which required 20 724 clusters of different topologies, and our series contains exact averages over all the random configurations. Now, assuming Eqs. (1) and (2), the singular behavior for $Q_a(p)$ and $Q_\mu(p)$ at $p=p_c$ is expected to be $Q_a(p) \propto |p-p_c|^{-\zeta_a}$, $Q_\mu(p) \propto |p-p_c|^{-\zeta_\mu}$, with $\zeta_a = -\beta + (\beta+\gamma)(\lambda+1)$ and $\zeta_\mu = -\beta + (\beta+\gamma)(3+\lambda-\phi)$ from standard percolation theory. Here β is the percolation order parameter exponent. Since the values of β, γ are known numerically in general dimensions, the values of λ, ϕ can be calculated directly from ζ_a and ζ_μ.

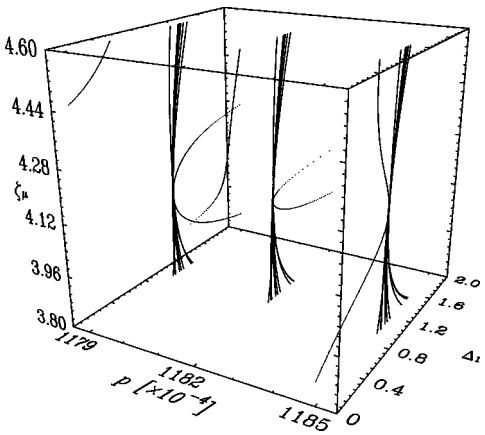

FIG. 3. $M1$ analysis of the $Q_\mu(p,d=5)$ series. The best convergence from different Padé approximants is achieved at $p_c = 0.1182 \pm 0.0003$.

The analysis for singular behaviors of $Q_a(p)$ and $Q_\mu(p)$ involves a d log Padé analysis to locate the rough position of poles (p_c) and the residues ζ_a and ζ_μ in each dimension [16]. We employed the recently developed efficient three-dimensional visualization methods [17] together with the $M1$ and $M2$ analysis algorithms [18], which allow a very accurate determination of the threshold p_c, the leading critical exponent (denoted by h below), and the confluent correction-to-scaling exponent Δ_1 simultaneously. Denoting the general series by $H(p)$, we assume the form $H(p) = A(p_c-p)^{-h}[1 + a(p_c-p)^{\Delta_1} + \cdots]$. In the $M1$ method, we study the logarithmic derivative of $B(p) = hH(p) - (p_c - p)[dH(p)/dp]$, which has a pole at p_c with residue $-h + \Delta_1$. For a given value of p_c we obtain graphs of Δ_1 versus input h for all Padé approximants, and we choose the triplet (p_c, h, Δ_1) where a selection of high, near-diagonal Padés converge to the same point. In the $M2$ method, we first transform the series in p into a series in the variable $y = 1 - (1-p/p_c)^{\Delta_1}$ and then take the Padé approximants to $G(y) = \Delta_1 (y-1) d/dy \ln[H(p)]$, which should converge to $-h$. Here we plot graphs of h versus the input Δ_1 for different values of p_c and choose again the triplet (p_c, h, Δ_1), where the Padés converge to the same point.

In Fig. 3 we present three slices from the $M1$ analysis of the $Q_\mu(p, d=5)$ series. The best convergence from different Padé approximants is achieved at $p_c = 0.1182 \pm 0.0003$. Figure 4 shows a slice at $p_c = 0.1182$, from which we read the value of the leading critical exponent $\zeta_\mu = 4.12$ as well as the correction to scaling exponent $\Delta_1 \approx 1.02$. We repeated these analyses many times for $Q_a(p,d)$ and $Q_\mu(p,d)$ in other general dimensions, and found average values $p_c = 0.2488 \pm 0.0010, 0.1600 \pm 0.0005, 0.1182 \pm 0.0003, 0.0942 \pm 0.0005, 0.0595 \pm 0.0002$, $\phi = 1.55 \pm 0.05, 1.53 \pm 0.06, 1.51 \pm 0.08, 1.48 \pm 0.04, 1.52 \pm 0.03$, $\lambda = 1.0 \pm 0.04$, and $\Delta_1 \approx 1.0$ from $M1$ and $M2$ analyses of two series for 3,4,5,6,9 dimensions, respectively. This directly shows the validity of the

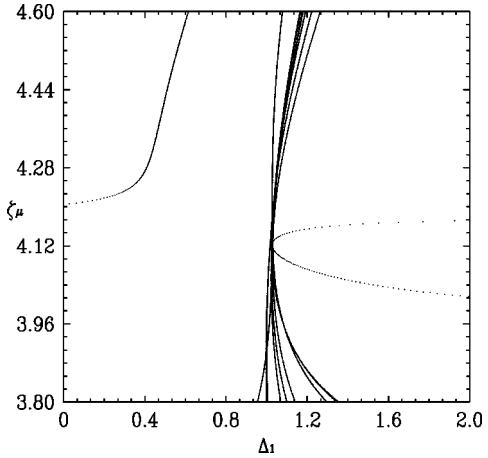

FIG. 4. $M1$ analysis of the $Q_\mu(p,d=5)$ series at $p_c=0.1182$. The value of the leading critical exponent $\zeta_\mu=4.12$ and the correction to scaling exponent $\Delta_1\approx 1.02$.

scaling relation by Eq. (3), although the error bar of ϕ is not small enough to distinguish ϕ's in different dimensions. In view of the relatively short length of our series, our result, however, is quite satisfactory since it shows a nice trend of ϕ from 1.55 to 1.50 for three to six dimensions and above. The series in two dimensions do not behave well in the Padé analysis because they are too short to show a strong singularity. Overall our estimate for λ and ϕ from the series expansions agrees with those from our current Monte Carlo simulation in every dimension, with Edwards and co-workers for 2D [7,8], with Debierre for 3D [13], and with Cheon and Chang for 2D and 3D [15]. Although our numerical values of ϕ support Edwards and co-workers' scaling relation Eq. (3), we cannot exclude the possibility of super-universality for $d\geqslant 3$ because they are indistinguishable within our numerical error bars.

To summarize, we have investigated the scaling behavior for binary fragmentation of critical bond percolation clusters in general dimensions by extensive Monte Carlo simulation as well as by exact series expansions. The critical exponent for a fragmentation rate is $\lambda=1.0$ in all dimensions, and for a fragment's mass distribution $\phi=1.59, 1.55, 1.53, 1.51, 1.48, 1.52$ for two to six and nine dimensions. These values are clearly consistent with the Edwards and co-workers' scaling relation $\sigma=1+\lambda-\phi,\lambda=1$ in general dimensions, which consequently excludes the relations by Gouyet (for $d=2$) and Roux and Guyon. Above six dimensions Bethe lattice exponents should be exact.

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