1995

Mass distribution on clusters at the percolation threshold

Mark F. Gyure

Martin V. Ferer

Boyd F. Edwards

Greg Huber

3-1-1995

Mass Distribution on Clusters at the Percolation Threshold

M. F. Gyure

M. V. Ferer

Boyd F. Edwards
Utah State University

G. Huber

BRIEF REPORTS

Brief Reports are accounts of completed research which do not warrant regular articles or the priority handling given to Rapid Communications; however, the same standards of scientific quality apply. (Addenda are included in Brief Reports.) A Brief Report may be no longer than four printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.

Mass distribution on clusters at the percolation threshold

Mark F. Gyure,* Martin V. Ferer, and Boyd F. Edwards
Department of Physics, P.O. Box 6315, West Virginia University, Morgantown, West Virginia 26506-6315

Greg Huber
Department of Physics and Center for Polymer Studies, Boston University, Boston, Massachusetts 02215
Lawrence Berkeley Laboratory, 1 Cyclotron Road, Berkeley, California 94720
and Department of Mathematics and Department of Physics, University of California, Berkeley, California 94720†
(Received 16 July 1993)

Monte Carlo simulations and a scaling hypothesis are used to study the distribution of blob masses on two-dimensional finite-mass clusters at the percolation threshold. The exponents associated with this distribution function are a combination of backbone and percolation exponents. This work offers insights into the structure and fragmentation properties of percolation clusters in particular, and provides methods applicable to other fractal distribution problems in general.

PACS number(s): 05.40.+j, 82.20.−w, 82.40.Py

A wide variety of fragmentation processes possess no preferred direction. For example, destructive phenomena such as combustion, dissolution, or corrosion occurring both at the external surface and deep within the pores of a random porous solid can cause fragmentation of the solid as the pores widen and fuse [1]. Percolation theory [2] would seem an ideal tool for studying these nearly isotropic random processes. Percolation models of fragmentation [3–5] provide important geometrical information which is absent from rate-equation approaches for fragmentation [6–8]. Moreover, these percolation models raise fundamental questions about the blob-mass distribution on percolation clusters and identify this distribution as a key element in the overall understanding of the structure of percolation clusters. The primary goal of this Brief Report is to understand this distribution using scaling arguments and two-dimensional (2D) Monte Carlo simulations.

Percolation clusters are defined as sets of adjacent occupied sites or bonds (unit line segments) on a lattice randomly occupied with probability p. Above the percolation threshold p_c, a spanning cluster exists on the infinite lattice [9]. The transition at p_c features critical behavior analogous to that of thermal phase transitions, most importantly self-similar clusters with simple scaling properties [2]. The desire to understand transport in random materials has motivated careful studies of the structure of percolation clusters [10,11]. These studies emphasize the cluster surface or "hull" [12] and the cluster backbone [13–17].

The blob-mass distribution on the backbone has been carefully studied at p_c [14]. For bond percolation clusters, the backbone is defined as the subset of bonds carrying current between two designated reference bonds on the cluster. The backbone itself consists of singly connected *red* (cutting) bonds, whose absence would break the backbone, and multiply connected *blue* bonds [10,11,13]. Backbone blobs are defined as connected sets of adjacent blue bonds. Clearly, designating different reference bonds results in a different backbone; the reference bonds define a preferred orientation on the cluster.

For isotropic fragmentation of percolation clusters, it is the overall cluster connectivity, rather than the connectivity of the backbone, that matters. Accordingly, we designate as "fragmenting" those bonds on the cluster that would break the cluster if removed. Cluster blobs are correspondingly defined as groups of adjacent nonfragmenting bonds (Fig. 1). This definition implies a small distinction between cluster blobs and backbone blobs; bond k in Fig. 1 is a member of the cluster blob containing bond i, but is not a member of the corresponding blob on the backbone defined by reference bonds i and j. Only a subset of the blobs and fragmenting bonds on a cluster appear as blobs and red bonds on any particular backbone of the cluster (Fig. 1). The essential connectivity of percolation clusters can be described simply as a branched network or tree of blobs of various masses linked by fragmenting bonds. This network is much like a Bethe lattice (Cayley tree), with blobs occupying the vertices, except here the vertex mass and the coordina-

*Present address: Center for Polymer Studies, Department of Physics, Boston University, Boston, MA 02215.
†Present address.

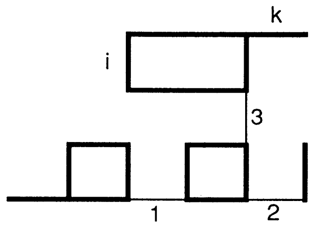

FIG. 1. Sample cluster of mass 20 on a square bond lattice with three fragmenting bonds (thin lines) and cluster blobs (groups of adjacent nonfragmenting bonds) of masses 1, 4, 5, and 7. Fragmenting bonds 2 and 3 serve as red bonds on the backbone defined by reference bonds i and j. Bond k, bond 1, and the blob to its left are not on this backbone.

tion number (the number of links per vertex) can vary. By contrast, the blobs and red bonds on a backbone form a branchless, one-dimensional path between the two reference bonds.

What is the form of the cluster blob-mass distribution and how does it differ, if at all, from the backbone blob-mass distribution? What is the dependence of the coordination number on the blob mass? As will be seen, the answers to these questions provide fundamental information about the internal structure of percolation clusters relevant to the fragmentation of random porous solids.

It is natural to define the cluster blob-mass distribution as the average number density n_{sb} of blobs of mass b on clusters of mass s at p_c, where number density means the number of such blobs per cluster bond and mass refers in both cases to bonds, not sites. In this Brief Report, we propose the scaling form

$$n_{sb} = b^{-\tau'} f(b/s^z) \tag{1}$$

and the scaling relationship

$$\tau' - 1 = 1/z = D/\widetilde{D} \ , \tag{2}$$

which involve new exponents τ' and z as well as the known cluster and backbone fractal dimensions D and $\widetilde{D}$. That $D > \widetilde{D}$ in all dimensions greater than one demands that $\tau' > 2$ and $z < 1$.

To test Eqs. (1) and (2) and to determine the exponents numerically, we performed 2D Monte Carlo simulations involving 42 861 clusters generated using the Leath method [18] on a square bond lattice at $p_c = 1/2$. Once the fragmenting bonds are identified on a particular cluster [5], one more pass through the list of cluster bonds is sufficient to determine the blob-mass distribution for that cluster. This is done using a burning algorithm [14], which starts at one end of a fragmenting bond and burns only nonfragmenting bonds until all of these are burned, thereby counting the number of bonds burned in this process (the blob mass). Figure 2 shows a log-log plot of n_{sb} as a function of b for four different cluster masses. Evident in the figure are a power-law decay for small b and a cutoff at large b consistent with Eq. (1).

Moments $\mu_s^{(k)} = \sum_b b^k n_{sb}$ of the distribution allow us to determine τ and z precisely from the Monte Carlo simulations. These moments scale as [19]

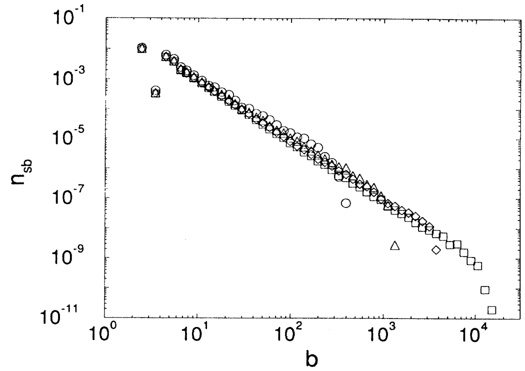

FIG. 2. Distribution of blob masses for clusters in the mass ranges 32 768–35 734 (squares), 8192–8933 (diamonds), 4096–4467 (triangles), and 512–558 (circles).

$$\mu_s^{(k)} = a_k + b_k s^{-z} + c_k s^{z(k-\tau'+1)} \ . \tag{3}$$

The last term comes by direct integration of Eq. (1) and dominates as $s \to \infty$ for $k \geq 2$, whereas the first (constant) term dominates for $k = 0$ and $k = 1$. Consequently, the average blob mass $\mu_s^{(1)}/\mu_s^{(0)} = a_1/a_0$ representing the ratio of the total blob mass on a cluster to the number of blobs on the cluster is a constant for large s, as is evident in Fig. 3. The weighted average blob mass $\mu_s^{(2)}/\mu_s^{(1)} \sim s^\gamma$ with $\gamma = z(3-\tau')$ is analogous to the average cluster size as it is usually defined [2]. The moment ratio $\mu_s^{(3)}/\mu_s^{(2)} \sim s^z$ scales as the cutoff blob mass $B \sim s^z$ and involves a "gap" exponent z. Fits to the highly linear data in Fig. 3 yield $\gamma = 0.721 \pm 0.008$ and $z = 0.856 \pm 0.018$, from which $\tau' = 2.16 \pm 0.02$ follows immediately.

These computed scaling exponents agree with Eq. (2) to high precision. With the known 2D values $D = 91/48$ [2] and $\widetilde{D} = 1.64 \pm 0.01$ [16,17], Eq. (2) implies $z = 0.865 \pm 0.005$ and $\tau' = 2.16 \pm 0.01$, in precise agreement with the computed exponents.

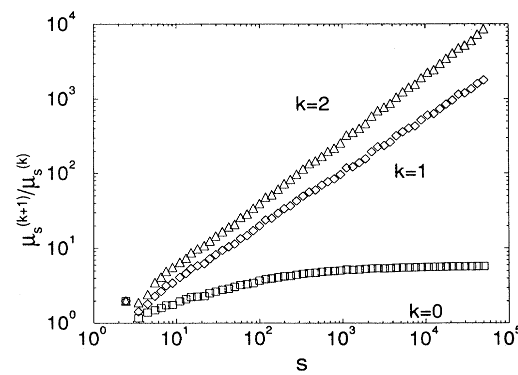

FIG. 3. Computed ratios of moments of the blob-mass distribution vs cluster mass. Shown are the ratio of the third to second moment (triangles), the second to first moment (diamonds), and the first to zeroth moment (squares) whose asymptotic slopes are the exponents z, γ, and zero, respectively.

Figure 4 shows the scaled distribution $b^{\tau'} n_{sb}$ as a function of the ratio $x = b/s^z$ of the blob mass to the cutoff blob mass, with $\tau' = 2.16$ and $z = 0.856$. The striking collapse of the data further confirms Eq. (1) and defines the shape of the scaling function $f(x)$. This function measures the deviations of n_{sb} from the pure power-law behavior $b^{-\tau'}$. The peak near $x = 1$ implies an excess of blobs just below the cutoff, whereas the sharpness of the cutoff at higher x reflects an extreme sensitivity of the cluster blob-mass distribution to the blob mass in the vicinity of the cutoff.

Fractal concepts provide a deeper understanding of the cluster blob-mass distribution and drive a scaling argument for the second equality in Eq. (2). In a box of edge L, the cutoff cluster of mass $s \sim L^D$ has a cutoff blob mass $B \sim s^z \sim L^{Dz}$. This can be related to the corresponding cutoff blob mass on the backbone. The fractal dimension of backbone blobs equals the fractal dimension $\widetilde{D}$ of the backbone itself because the red bonds contribute insignificantly to the backbone mass [11,14]. Hence the cutoff backbone blob mass in a box of edge L scales as $B_{bb} \sim L^{\widetilde{D}}$. The small distinction between cluster and backbone blobs is not expected to affect the scaling of the cutoff blob mass. Accordingly, taking $B \sim B_{bb}$ produces $z = \widetilde{D}/D$, the second equality in Eq. (2).

The scaling relation $\tau' - 1 = 1/z$ can be derived from a hyperscaling argument similar to the original Widom hyperscaling argument for thermal critical points [20]. A slight variant of this argument hypothesizes that the scaling part of the free-energy density $F_{\rm sc} \sim t^{2-\alpha}$ in a volume defined by the correlation length approaches a constant at criticality. That is, $F_{\rm sc}\xi^d \sim t^{2-\alpha-d\nu}$ is a constant at reduced temperature $t = |T - T_c| = 0$, requiring that $d\nu = 2 - \alpha$. For the cluster distribution function at $p = p_c$, the number density of percolation clusters on a lattice of size L^d should scale as [2] $n_s(L) = s^{-\tau} f(s/L^D)$. The total density of these clusters, given by the integral of $n_s(L)$ over all cluster masses, has a singular part which scales as $L^{(1-\tau)D}$. This singular part measures the density of only the largest clusters on the lattice since it arises from the integration over the largest cluster masses. That is, the integration of the cluster distribution function is performed over the largest cluster masses only, say,

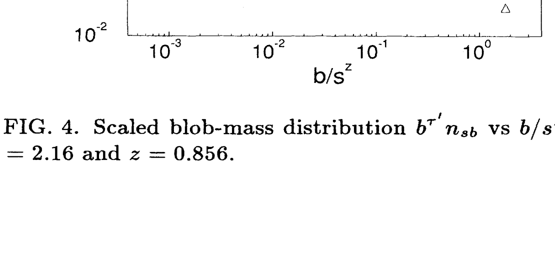

FIG. 4. Scaled blob-mass distribution $b^{\tau'} n_{sb}$ vs b/s^z with $\tau' = 2.16$ and $z = 0.856$.

from a fraction of the cutoff mass $s_c = \sigma L^D$ to infinity

$$\int_{s_c}^{\infty} n_s(L) ds = L^{(1-\tau)D} \int_{\sigma}^{\infty} u^{-\tau} f(u) du \sim L^{(1-\tau)D} \ . \quad (4)$$

It seems natural to hypothesize that there should be a finite number of these largest clusters for any size lattice in two dimensions. Then as criticality is approached (here, as $L \to \infty$), the total number of these largest clusters approaches a constant $L^{d+(1-\tau)D}$, requiring that $\tau - 1 = d/D$. This is the familiar hyperscaling relation for the cluster number exponent τ in terms of the fractal dimension.

A hyperscaling argument identical to the one for cluster numbers leads to the scaling relation in Eq. (2). At $p = p_c$, we have argued that the number density of blobs on a cluster of mass s should scale as $n_{sb} = b^{-\tau'} f(b/s^z)$. Now consider the total density of these blobs [the zeroth moment $k = 0$ in Eq. (3)] whose singular part scales as $s^{(1-\tau')z}$. The scaling part in Eq. (3) measures the density of the largest blobs on the cluster since the other terms arise from the lower limit of the integral over the cluster masses. In analogy with Eq. (4), the scaling part of the blob distribution function is integrated over the largest blobs, i.e., from a fraction of the cutoff blob size ($b_c = \sigma s^z$) to infinity. It seems natural to hypothesize that there should be a finite number of largest blobs for any size cluster so that as criticality is approached ($s \to \infty$), the total number of these largest blobs $s^{1+(1-\tau')z}$ should approach a constant, requiring that $\tau' - 1 = 1/z$.

Introducing a "cluster granularity" further illuminates this hyperscaling relation as well as the finite-s scaling of the total fraction $\mu_s^{(1)} = c_1 s^{z(2-\tau')} + a_1$ of blob bonds on a cluster. The granularity G of blobs on percolation clusters is defined as the ratio of the cutoff blob mass to the cluster mass $G = B/s \sim s^{z-1}$. Since the scaling part of this total blob fraction arises from the finite number of largest blobs whose mass approximately equals the cutoff mass, the scaling part of the total fraction should differ from the granularity only by a factor of the constant number of these largest blobs; this also leads to $\tau' - 1 = 1/z$. Furthermore, the cluster granularity plays an important role in $\mu_s^{(1)}$, even to rather large s (Fig. 3, $k = 0$) since $1 - z = z(2 - \tau')$ is small.

Although individual cluster and backbone blobs are nearly identical, their mass distributions are quite different. The backbone blob-mass distribution [14] is defined as the average number density n_{Lb} of blobs of mass b on a backbone contained in a d-dimensional box of edge L at p_c. It scales as $n_{Lb} = L^{D_r - d} b^{-\tilde{\tau}} \tilde{f}(b/L^{\widetilde{D}})$, where D_r is the fractal dimension of the red bonds. Whereas fragmenting and blob bonds each comprise finite mass fractions of large clusters, the inequality $D_r < \widetilde{D}$ implies that red bonds comprise an insignificant mass fraction of large backbones. Furthermore, since $\tilde{\tau} < 2$, the moments $m_L^{(k)} = \sum_b b^k n_{Lb} \sim L^{D_r - d} \left[\tilde{a}_k + \tilde{b}_k L^{\widetilde{D}(k-\tilde{\tau}+1)}\right]$ are dominated by the first term only for $k = 0$. The scaling relationship $\tilde{\tau} - 1 = D_r/\widetilde{D}$ analogous to Eq. (2) follows by simply demanding that $m_L^{(1)}$ scale as the total blob-mass density $L^{\tilde{D}-d}$. Finally, whereas the average mass $\mu_s^{(1)}/\mu_s^{(0)}$ of cluster blobs is constant, the average mass $m_L^{(1)}/m_L^{(0)} \sim L^{\tilde{D}-D_r}$ of backbone blobs *increases* with increasing L. Consequently, large cluster blobs (of mass $b > \mu_s^{(1)}/\mu_s^{(0)}$) have a higher likelihood of appearing on the backbone than small cluster blobs; the backbone is populated preferentially with large cluster blobs. In fact, the granularity of blobs on the backbone is a constant of order unity, being the ratio of the cutoff blob mass to the backbone mass, which both scale as $L^{\tilde{D}}$; in contrast, the granularity of blobs on clusters goes to zero for large clusters.

The coordination number Z_b, defined as the average number of fragmenting bonds attached to blobs of mass b, is interesting because it describes the overall connectivity of percolation clusters. Its scaling [21] $Z_b \sim b$, independent of cluster mass, indicates that the average number of links emanating from a blob is proportional to the blob mass. This is in contrast to backbone blobs where only the two links to the backbone are relevant. This result, coupled with the results on the blob-mass distribution, constitutes an important addition to the nodes, links, and blobs picture of percolation clusters [10,11]. Studies of the distribution of the number of fragmenting bonds per link might further illuminate the structure of percolation clusters.

In conclusion, we have described the distribution of blobs on critical percolation clusters using a scaling theory and numerical simulations. The blob-mass distribution exponent $\tau' = 1 + D/\tilde{D}$, being a combination of the percolation cluster dimension D and the backbone dimension $\tilde{D}$, reflects the geometry of fractal clusters (blobs) embedded in a fractal substrate (the percolation cluster).

We gratefully acknowledge discussions with Mark Bradley, Stefan Schwarzer, Gene Stanley, and Dietrich Stauffer. This work was supported by Department of Energy Grants Nos. DE-FG22-89PC-89791 and DE-AC03-76SF-00098, National Science Foundation Grant No. RII-8922106, and the National Research Center for Coal and Energy.

[1] D. Dunn-Rankin and A. R. Kerstein, Combust. Flame **74**, 207 (1988); **69**, 193 (1987); A. R. Kerstein and B. F. Edwards, Chem. Eng. Sci. **42**, 1629 (1987).
[2] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, 2nd ed. (Taylor and Francis, London, 1992); *Fractals and Disordered Systems*, edited by A. Bunde and S. Havlin (Springer, Berlin, 1991).
[3] M. Sahimi, Phys. Rev. A **43**, 5367 (1991); M. Sahimi, G. R. Gavalas, and T. T. Tsotsis, Chem. Eng. Sci. **45**, 1443 (1990), and references therein.
[4] A. R. Kerstein, J. Phys. A **22**, 3371 (1989).
[5] M. F. Gyure and B. F. Edwards, Phys. Rev. Lett. **68**, 2692 (1992); B. F. Edwards, M. F. Gyure, and M. Ferer, Phys. Rev. A **46**, 6252 (1992).
[6] S. Redner, in *Statistical Models for the Fracture of Disordered Media*, edited by H. J. Herrmann and S. Roux (Elsevier Science, Amsterdam, 1990), Chap. 10, and references therein; Z. Cheng and S. Redner, Phys. Rev. Lett. **60**, 2450 (1988).
[7] E. D. McGrady and R. M. Ziff, Phys. Rev. Lett. **58**, 892 (1987); R. M. Ziff, J. Phys. A **24**, 2821 (1991).
[8] M. Cai, B. F. Edwards, and H. Han, Phys. Rev. A **43**, 656 (1991); J. Huang, B. F. Edwards, and A. D. Levine, J. Phys. A **24**, 3967 (1991).
[9] R. M. Ziff, Phys. Rev. Lett. **69**, 2670 (1992).
[10] H. E. Stanley, J. Phys. A **10**, L211 (1977).
[11] A. Coniglio, J. Phys. A **15**, 3829 (1982).
[12] P. N. Strenski, R. M. Bradley, and J.-M. Debierre, Phys. Rev. Lett. **66**, 1330 (1991); R. M. Bradley, P. N. Strenski, and J.-M. Debierre, Phys. Rev. B **44**, 76 (1991).
[13] R. Pike and H. E. Stanley, J. Phys. A **14**, L169 (1981).
[14] H. J. Herrmann and H. E. Stanley, Phys. Rev. Lett. **53**, 1121 (1984).
[15] T. Ohtsuki and T. Keyes, J. Phys. A **17**, L267 (1984).
[16] D. Laidlaw, G. MacKay, and N. Jan, J. Stat. Phys. **46**, 507 (1987).
[17] M. D. Rintoul and H. Nakanishi, J. Phys. A **25**, L945 (1992).
[18] P. L. Leath, Phys. Rev. B **14**, 5046 (1976).
[19] Computing the moments directly as $\mu_s^{(k)} = s^{z(k-\tau+1)} \int_0^\infty x^{k-\tau} f(x)dx$ produces an $x = b/s^z \to 0$ divergence for $k = 0$ and $k = 1$ because $f(x) \to$ const as $x \to 0$. To obtain the correct scaling for $k = 0$ and $k = 1$, we use an inverse cutoff blob mass $\xi = s^{-z}$ to write $\mu_s^{(k)} = \tilde{\mu}_\xi^{(k)} = \int b^{k-\tau} f(b\xi)db$. Equation (3) follows immediately by integrating $d^2\tilde{\mu}_\xi^{(k)}/d\xi^2 = \xi^{-k+\tau-3} \int x^{k-\tau+2} f''(x)dx$.
[20] B. Widom, J. Chem. Phys. **43**, 3892 (1965).
[21] M. F. Gyure, B. F. Edwards, and M. V. Ferer (unpublished).