



Distribution of dangling ends on the incipient percolation cluster

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Abstract

We study numerically and by scaling arguments the probability $P(M)dM$ that a given dangling end of the incipient percolation cluster has a mass between M and $M+dM$. We find by scaling arguments that $P(M)$ decays with a power law, $P(M) \sim M^{-(1+\kappa)}$, with an exponent $\kappa = d_f^B/d_f$, where d_f and d_f^B are the fractal dimensions of the cluster and its backbone, respectively. Our numerical results yield $\kappa = 0.83$ in $d = 2$ and $\kappa = 0.74$ in $d = 3$ in very good agreement with theory. © 1999 Published by Elsevier Science B.V. All rights reserved.

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Percolation is a standard model for structural disordered systems, its applications range from amorphous and porous media and composites to branched polymers, gels, and complex ionic conductors [1–3]. The origin of anomalous diffusion in the incipient percolation cluster (i.e. in structural disordered system) is still challenging and an analytical treatment is still not available. Its complexity arises from different contribution from the backbone and the dangling ends of the cluster, which together slow down, in a self-similar fashion, the motion of a random walker. The backbone of a cluster is defined as all sites carrying current when a voltage difference is applied between two arbitrary sites, the dangling ends are the remaining sites, each one singly connected to the backbone. Considerable effort was expended to map percolation cluster to comb-like structures, see e.g. [4] for an overview. To find suitable simple models and to understand anomalous diffusion better, a detailed knowledge about the internal

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structure of the percolation cluster is required, including distribution of masses and lengths of dangling ends, that represents the teeth in the comb-like structures.

In this paper we concentrate on the incipient percolation cluster at p_c , which is known to be self-similar on all length scales. The mass S within Euclidean distance r scales as $S \sim r^{d_f}$, where d_f is the fractal dimension. A second useful metric is the so-called ‘chemical’ distance ℓ , which is defined as the length of the shortest path on the structure. This chemical distance ℓ scales as $\ell \sim r^{d_{\min}}$, where d_{\min} is the fractal dimension of the shortest path. As a result, the mass within chemical distance ℓ scales as $S \sim \ell^{d_\ell}$, with $d_\ell = d_f/d_{\min}$. The dangling ends are known to have the same fractal dimension as the cluster, being larger than the fractal dimension d_f^B of the backbone (and consequently $d_\ell^B = d_f^B/d_{\min} < d_\ell$).

To study the distributions numerically we generated large critical percolation cluster in $d = 2$ and 3 using the well-known Leath algorithm [5,6]. The maximum size of the cluster is $\ell_{\max} = 2000$ in $d = 2$ ($p_c \cong 0.5927460\dots$) and $\ell_{\max} = 1000$ in $d = 3$ ($p_c \cong 0.311606\dots$). For each of the about 10^5 configurations the backbone is extracted using the improved ‘burning’ algorithm [7] (for the original burning algorithm see [8]). Then the mass M and the chemical size L of all dangling ends are determined, as well as their total number N . The chemical size L is defined as the maximum chemical distance available on the dangling end, measured from the point where it is connected to the backbone.

We are interested in the distributions $P(M)$ and $P(L)$ of dangling ends. Here $P(M) dM$ gives the probability that a given dangling end has a mass between M and $M + dM$ which is expected to behave as

$$P(M) \sim M^{-(1+\kappa)} \tag{1}$$

with an exponent κ to be determined. Accordingly, $P(L) dL$ is the probability that the dangling end has a chemical size between L and $L + dL$. Since $M(L) \sim L^{d_\ell}$, both quantities are related by

$$P(L) \propto P(M) \frac{dM}{dL} \sim L^{-(1+\kappa)d_\ell + (d_\ell - 1)}. \tag{2}$$

For relating the exponent κ to known exponents, let us first consider the total number of dangling ends N on a certain cluster. It is natural to assume that this total number increases linearly with the mass of the cluster’s backbone S_B , i.e. $N \sim S_B$. Since the backbone mass scales with the cluster mass S as $S_B \sim S^{d_f^B/d_f}$, we obtain for the total number of dangling ends $N(S) \sim S^{d_f^B/d_f}$ as a function of the cluster mass S . Numerical results for this quantity are shown in Fig. 1. The obtained slopes 0.86 ($d = 2$) and 0.74 ($d = 3$) fit perfectly with the ratio d_f^B/d_f . Hence, d_f^B is a very good approximation for the fractal dimension of the number of dangling ends, i.e. $N \sim r^{d_f^B}$.

Let us further assume that the main contribution to the cluster mass S is given by the sum of the N dangling end masses M_i and that it is possible, in a good approximation, to neglect the backbone mass. Under this assumption we can write approximately $S \cong \sum_{i=1}^N M_i$. When rewriting this sum by an integral using the distribution $P(M)$, we get $S \sim N \int_1^{M_{\max}} MP(M) dM \sim NM_{\max}^{1-\kappa}$, where M_{\max} is the maximum dangling end

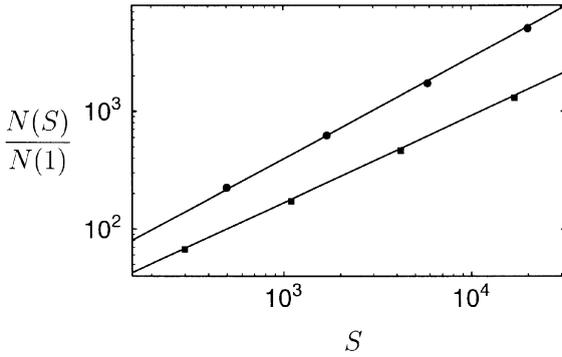


Fig. 1. Plot of the mean number $N(S)$ of dangling ends on a cluster of mass S in the cases $d = 2$ (full circle) and $d = 3$ (full square). The lines have the slope 0.86 ($d = 2$) and 0.74 ($d = 3$).

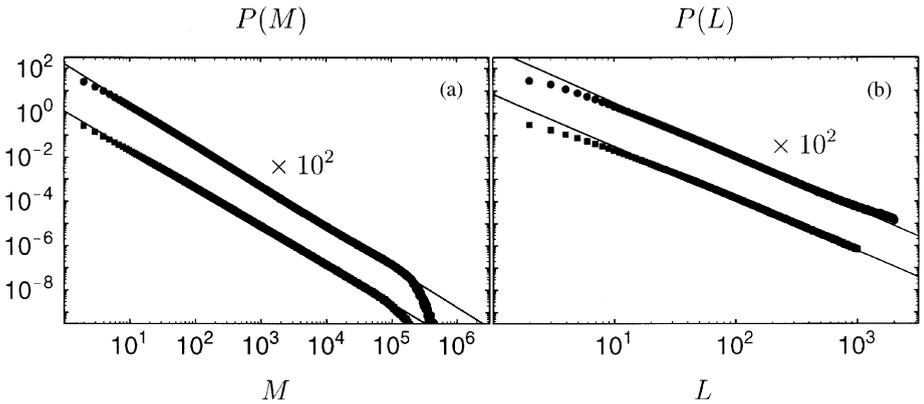


Fig. 2. Plot of the probability distribution functions (a) $P(M)$ vs. mass M and (b) $P(L)$ vs. size L , in both cases for $d = 2$ (full circle, multiplied by 10^2) and $d = 3$ (full square). The lines have the slope (a) -1.83 ($d = 2$) and -1.74 ($d = 3$), and (b) -2.42 ($d = 2$) and -2.36 ($d = 3$).

mass that appears as the average on a cluster of mass S . When taking N dangling end masses out of the distribution $P(M) \sim M^{-(1+\kappa)}$, the largest one on an average will be $M_{\max} \sim N^{1/\kappa}$. Putting both together we get $S \sim NN^{(1-\kappa)/\kappa} \sim N^{1/\kappa}$ or $N \sim S^\kappa$. Comparing this with the result $N \sim S^{d_f^B/d_f}$ obtained above, it follows that $\kappa = d_f^B/d_f$. We note that a more general derivation relating fractal dimension and distribution was presented in [9,10], which yields an identical result under the same assumption that the backbone mass is negligible compared to the cluster mass.

The results of the numerical simulation for $P(M)$ and $P(L)$ are shown in Fig. 2. For $P(M)$, we obtain a slope of -1.83 in $d = 2$ and -1.74 in $d = 3$, which has to be compared to $-(1 + d_f^B/d_f)$ being -1.87 in $d = 2$ and -1.74 in $d = 3$. Concerning $P(L)$, we find a slope of -2.42 in $d = 2$ and -2.36 in $d = 3$, which has to be compared to $-(1 + d_f^B/d_f)d_\ell + (d_\ell - 1) = -(1 + d_f^B)$ being -2.44 in $d = 2$ and -2.36 in $d = 3$.

As a conclusion, we see that $\kappa = d_f^B/d_f$ is a very good approximation in $d = 2$ and fits even better in $d = 3$. For the critical dimension $d = 6$ we recover the known result $P(M) \sim M^{-3/2}$ [1].

Concerning the problem of diffusion on percolation cluster and its mapping to comb-like structures, we see that the distribution of masses $P(M)$ of dangling ends is singular. A random comb with such a singular distribution of teeth lengths yields anomalous diffusion [4]. Different from this, the non-singular distribution of lengths $P(L)$ of dangling ends may be the key quantity in the case of strong topological bias, since we expect only the chemical size of the dangling ends to control the time the random walker spends inside, and not their mass nor their internal structure.

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