Harmonic Measure for Percolation and Ising Clusters Including Rare Events

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We obtain the harmonic measure of the hulls of critical percolation clusters and Ising-model Fortuin-Kastelyn clusters using a biased random-walk sampling technique which allows us to measure probabilities as small as 10^{-300}. We find the multifractal $D(q)$ spectrum including regions of small and negative q. Our results for external hulls agree with Duplantier's theoretical predictions for $D(q)$ and his exponent $-23/24$ for the harmonic measure probability distribution for percolation. For the complete hull, we find the probability decays with an exponent of -1 for both systems.

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The harmonic measure is a fundamental property of geometric objects. It may be defined by considering the object to be a grounded conductor with fixed charge of unity. The harmonic measure, μ, specifies the normal derivative of the potential (a harmonic function) on the surface. That is, it is the distribution of electric field on the hull (surface) of the object. We may also allow many random walkers to start far away from the object and record where they land. The probability density of hitting the hull at a point is μ. This quantity is the focus of much theoretical activity [1–4], and it is of considerable practical interest because it predicts where particles will diffuse to for adsorption, catalytic reaction, etching, etc. See also [5]. If the shape in question is fractal, μ shows interesting scaling properties.

Here, we show how to find μ numerically for two systems that produce fractal clusters in two dimensions, percolation [6] and Fortuin-Kasteleyn (FK) [7] clusters in the Ising model. Our method allows us to sample very small probabilities (of order 10^{-300}) using random walker simulations. In these cases, μ is *multifractal*. Our large dynamic range allows us to explore this property fully.

The function μ is non-negative and normalized on the hull: $\int d\mu = 1$. A partition function [8] can be defined by dividing the hull into j boxes of length l,

$$Z_q = \sum_j p_j^q, \tag{1}$$

where $p_j = \int d\mu$ over box j. For large fractals, Z_q obeys

$$Z_q \approx (l/R)^{(q-1)D(q)}, \tag{2}$$

where R is the length scale of the cluster. $D(q)$ is called the generalized dimension. In our simulations, we choose the smallest l to be the lattice spacing, and use $2l$, $4l$, etc., until a sufficient range is available to fit Eq. (2). We recall some special values of $D(q)$: $D(0)$ is the fractal dimension of the support of the measure, which describes the region the hull covers. Additionally, $D(1) = 1$ is known from Makarov's theorem [9]. A related quantity is the curve $f(\alpha)$, which is the Legendre transform of $\tau(q) \equiv (q-1)D(q)$,

$$f(\alpha) = q\frac{d\tau}{dq} - \tau, \qquad \alpha = \frac{d\tau}{dq}. \tag{3}$$

We will focus on $D(q)$ in this Letter.

The exact spectrum of $D(q)$ for percolation [2] and the more general Q-state Potts model [3] can be derived from generalized conformal invariance in terms of a central charge c,

$$D(q) = \frac{1}{2} + \left(\sqrt{\frac{24q+1-c}{25-c}} + 1\right)^{-1} \quad q \in \left[-\frac{1-c}{24}, +\infty\right). \tag{4}$$

Percolation and FK-Ising clusters correspond to $c = 0$ and $c = 1/2$, respectively.

Equation (4) was derived for the *accessible* or *external* hull of the clusters [10,11]. For a finite system, the external hull is approximately produced by closing all fjords on the complete hull with a neck size of order unity. This reduces the dimension for percolation and the Ising model from $7/4$ and $5/3$ for the complete hull to $4/3$ and $11/8$ for the external hull, respectively [3].

We should note that Eq. (4) is based on a computation about a continuum model; in principle, it might not actually apply to the scaling limit of lattice percolation. The prediction was made nearly ten years ago and has never been reliably tested in the significant small-q regime. For percolation, and for large q, it agrees with results [1] on relatively small systems, $\approx 10^5$ sites. These simulations did not probe deep into the fractal surface, which is necessary for the small q regime.

The authors of Ref. [1] used the method mentioned above: a large number of walkers were allowed to diffuse until they were absorbed on the hull. This method is able to measure μ to an accuracy of $\approx 10^{-10}$. However, percolation clusters with 10^5 sites can have regions of the hull with probabilities per lattice site smaller than 10^{-100}. Although these regions do not contribute to $D(q)$ for large q, they dominate for small and negative q.

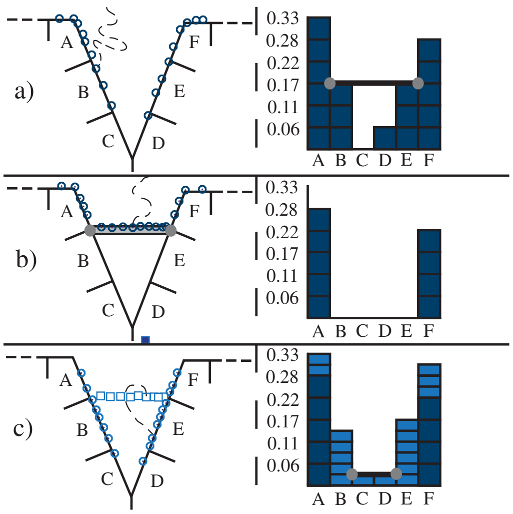

FIG. 1 (color online). Signpost algorithm. Left: hull of the cluster divided into boxes A–F. Absorbed walkers are the $N = 18$ dots. Right: histogram of probability in each box. The initial threshold is $1/6$. (a) Probe step: walkers absorb onto the hull. Below the heavy black line on the histogram $p < 1/6$. Thus, boxes B–E should be behind a signpost. (b) N more walkers are released and absorb onto the hull and the signpost (horizontal gray line). In this case, there are $N/2$ walkers on the signpost; histogram shows the probability on the hull. (c) Next probe step: N walkers are released from the signpost where walkers in the step (b) landed (squares). These walkers have half the weight as the ones released in parts (a) and (b). The heavy line on the histogram shows the new threshold, $1/36$. In the next step, boxes C, D must be behind a signpost.

The computation of $D(q)$ is a very difficult numerical problem (as emphasized in [4]). We have solved this once and for all for arbitrary shapes; the algorithm of this Letter can measure probabilities down to 10^{-300}. This accuracy completely samples lattice systems with $\sim 10^4$ hull sites. We have applied the method on systems as large as $\sim 10^6$ hull sites. Here, we consider only percolation and Ising clusters on a lattice. Our method is quite general and can also be applied to off-lattice clusters. Reference [4] is our only real competitor for finding the complete harmonic measure; however, it relies on a technique that is only applicable for small DLA [12] clusters.

To treat rare events, we use *iterative biased sampling* to keep track of the "lucky" walkers that penetrate deep into the fjords of the hull; see Fig. 1. In the first iteration, N random walkers with weight $1/N$ are released from outside the cluster and allowed to diffuse until they are absorbed on the hull. The weights of the walkers are temporarily added to the probability of the site where they land. This step probes the cluster to find regions of small measure. The hull sites that bound regions below a threshold (say $1/10$) are used as the end points of absorbing lines (*signposts*) which mark the depth of our current sampling. Then the probability added in the first step is removed and N more random walkers are released. These walkers can either be absorbed on the hull or on a signpost. The weights of the walkers that touch the hull in this step are permanently added to the probability distribution. After all walkers have been absorbed, the signposts are removed.

Next, the probe step is repeated with N walkers released from the locations along the signposts where walkers absorbed previously. The threshold for small probability is reduced by a constant factor, e.g., 10. These walkers carry a weight given by the fraction of the walkers in the last step that touched a signpost. The method is repeated until small probabilities are sampled. We find that errors build up slowly in the method: even for probabilities of order 10^{-300}, the fractional standard deviation over the ensemble is only 10–20%.

In effect, we find the Green's function for the random walkers by summing over intermediate positions. At the intermediate points where the sampling is poor, we enrich it. This is similar to methods used in chemical physics [13]. Figure 2 shows the harmonic measure of the complete hull of a percolation cluster obtained using this method.

Our simulations are performed on a periodic triangular lattice with height h and width w such that $h = 100w$ so that we obtain clusters that wrap around in width but not in height. One ambiguity which must be resolved is the definition of random walkers touching the hull. Here, we interpret this as the walker hopping *onto* a hull site.

The percolation clusters are grown using the Leath algorithm [14], with p equal to the site threshold for the triangular lattice, $p_c = 1/2$. If a given cluster spans the width of the system, the top hull of the cluster is found using a simple border walking algorithm related to the method of generating percolation cluster perimeters by random walks [15]. The list of complete hull sites of the cluster is then used in the signpost method to obtain the harmonic measure. If the topmost vacant sites bordering

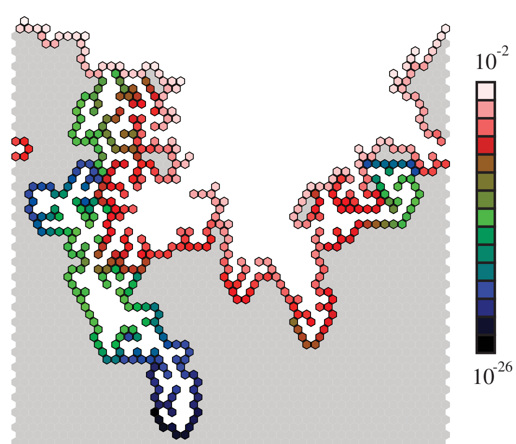

FIG. 2 (color online). Harmonic measure on the complete hull of a percolation cluster. The hull sites are outlined in black, and the harmonic measure goes from high to low: light colors are high and dark, low. The scale is given by the color thermometer on the right. Sites outside the cluster are white, and inside, gray.

the cluster are used instead of the occupied sites as the absorbing sites, one obtains the external hull.

For the FK clusters on the Ising model, bonds are placed between adjacent same-spin sites with probability $p_c = 1 - e^{-\beta J_c}$, where on the triangular lattice $p_c = 1 - 1/\sqrt{3}$. We use the Swendsen-Wang method [16] to equilibrate the system and simultaneously generate the FK clusters. After the system is sufficiently equilibrated, we attempt to find a spanning cluster. These spanning bond clusters must be converted to site clusters if they are to be used with our algorithm. We do this by making another triangular lattice with half the lattice spacing. Bonds are copied to the new lattice at the even sites on which they are centered. Odd sites are added to the cluster if two adjacent bonds meet at the odd site. Next, the perimeter-walk algorithm is used to record the locations of the hull sites; then, we use the signpost method to find the harmonic measure. As in percolation, an external hull can be obtained. However, for Ising clusters, we need to add artificial vacancies to all sites bordering the cluster.

The signpost method iteratively obtains smaller and smaller probabilities by reducing the weight of the random walkers released in each round, in our case by a factor of 10, on average. We took the number of walkers, N, to depend on the system width, w. For example, for $w = 400$, we use $N = 2 \times 10^6$ and for $w = 4000$, $N = 2 \times 10^7$. The signpost method is performed until all probabilities have been measured or until the minimum measurable probability 10^{-300} has been reached. This minimum is close to the smallest value that can be stored in a double precision floating point number. Smaller values could, in principle, be obtained by storing the logarithm of the probability instead of the probability itself.

The locations of the sites and their associated probabilities are then used to obtain $D(q)$ and the histogram of the probability distribution (see below). $D(q)$ is obtained by applying a linear fit to $\log Z_q$ in Eq. (1) versus $\log l$, where l is the box length. The fit was performed for a range of l over which the function was linear.

Simulations of percolation and Ising clusters were performed for a number of system widths. Our results are for $w = 400$, 1000, 2000, and 4000. Small systems, $w = 400$, have $\approx 5 \times 10^5$ hull sites in the cluster and large systems, $w = 4000$, have $\approx 5 \times 10^6$ hull sites. $D(q)$ and the slope of the power-law fit to the probability distribution were obtained for the complete and external hulls of both percolation and the Ising clusters.

Figure 3 shows a comparison between the results of the complete and external hulls of percolation clusters with the theory for the external hulls, Eq. (4). There is good agreement among all three for large q, which is not surprising as the complete hull fjords contribute negligibly to $D(q)$ in this case. For small q, there is significant disagreement between the complete hull and the theory as the two must approach different values for $D(0)$. Previous simulations

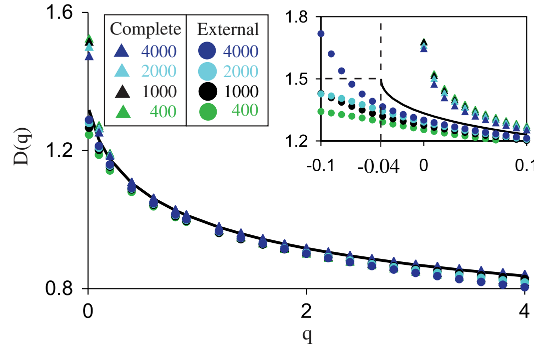

FIG. 3 (color online). $D(q)$ vs q for the complete and external hulls of percolation clusters for four different widths compared to theory, Eq. (4) [2] (black line). Inset: small q behavior of $D(q)$. Dashed lines are the theoretical limit for the external hull; the vertical dashed line is at $-1/24$.

[10] have shown that $D(0)$ increases with increasing width; however, we see a peak at a width of 1000; see Fig. 3. This is because there is a non-negligible fraction of the hull sites with probabilities less than 10^{-300} for large widths. We expect for very large systems, if we are able to record all probabilities, that the complete hull $D(q)$ will be nearly identical to the theory for $q > 0$ because the small probabilities do not contribute. But at $q = 0$, there will be a jump to $D(0) = 7/4$ because we are finding all the sites. For $q < 0$, $D(q)$ will be ill-defined (unbounded). In comparison, for the external hull, we see good agreement between the data and the theory (4) over the entire range of $D(q)$, especially for largest system sizes.

The histogram of the frequency of occurrence of the p_j was tallied using exponentially distributed bin sizes, e.g., the first box has size 1/2, the next 1/4, then 1/8, etc. The histogram is a power law over, (incredibly) more than 150 orders of magnitude. The exponent of the power law is fit at different probabilities using 5 points which roughly span an order of magnitude in probability. It is shown for the complete and external hull (inset) in Fig. 4. The exponent

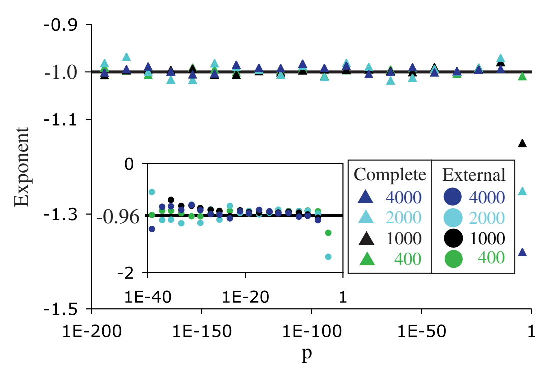

FIG. 4 (color online). Exponent of a power-law fit to the histogram of the probabilities as a function of p for the complete hull of a percolation cluster for several different widths. Inset: a similar plot for the external hull with the associated theoretical prediction (black line) [2].

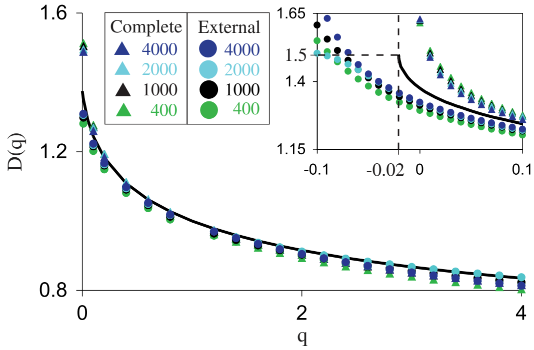

FIG. 5 (color online). $D(q)$ vs q for the complete and external hulls of Ising clusters for four different widths compared to theory from Eq. (4) (black line). Inset: small q behavior of $D(q)$. Dashed lines at $(-1/48, 3/2)$ are the theoretical limit for the external hull.

for the complete hull is -0.996 ± 0.01. We presume that the exact value of the exponent is -1, which implies that $D(q)$ is undefined for $q < 0$. Previous simulations [1] were unable to obtain this result because the smallest probability that could be measured, $\approx 10^{-10}$, is still in the transient regime. The initial overshoot of the power for small systems corresponds to the probability distribution for the *external* hull being picked up by the complete hull. The power-law exponent is also obtained for the external hull, -0.93 ± 0.05, which is consistent with the theoretical prediction of $-23/24 \simeq -0.958$.

Similar results were obtained for the Ising model. Figure 5 shows the comparison between the complete and external hulls of Ising clusters with the theory [3] for $D(q)$. As with percolation, there is good agreement with theory for large q for both the complete and external hulls but significant disagreement at small q for the complete hull, where Eq. (4) does not apply. The probability power-law exponents for the complete and external hull are -0.997 ± 0.012 and -0.920 ± 0.048, respectively, for the Ising model. The complete hull exponent again points to $q = 0$ as the discontinuity point for $D(q)$. The external hull exponent agrees roughly with theory which gives $-47/48 = -0.979$.

In summary, we have described a method to obtain precise values of $D(q)$ by including events of extremely low probability. We probed the internal structure of percolation and Ising model complete cluster hull. We observe the histogram of occurrences of probability p to be $\sim p^{-1}$. We are not aware of any prediction for this case.

In future work [17], we plan to apply the continuous version of this algorithm to obtain the harmonic measure for Diffusion Limited Aggregation (DLA) [12] for which there are no exact results, though there are several conjectures for the form of $D(q)$ for small and negative q [4]. For DLA, the harmonic measure plays a central role because it represents the growth probability at every point on the cluster at a given time. The best current results for $D(q)$ use iterative conformal maps [18,19] and are restricted to clusters of $\approx 10^4$ sites. Our method can go to much larger sizes, $\approx 10^7$ sites. This is important because the slow crossover of some length scales in DLA [20] suggests large clusters are necessary to approximate the scaling limit. Our method could shed light on the internal structure of DLA about which little is known.

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