Largest and second largest cluster statistics at the percolation threshold of hypercubic lattices

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We investigate the scale invariance of the average ratio between the masses of the largest and second largest clusters at percolation. We employ a finite size scaling method to estimate percolation thresholds based on the simulations of relatively small lattices, and report on estimates for p_c in hypercubic lattices with $d=2-7$, in full agreement with the best literature estimates. Also, we find the critical mass ratio to be strongly dependent on the boundary conditions, decreasing with the lattice dimension. Further, we compute several relevant mass distribution functions associated with the two largest clusters, which approach to limiting distributions for $d>6$. Finally, we discuss the main relevant features of the mass distributions in light of the relative role played by the spanning and nonspanning clusters.

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I. INTRODUCTION

A classic problem in statistical physics concerns the study of percolation in randomly diluted systems. Usually the existence of a percolating process is associated with the presence of an infinite cluster that spans the whole system. Percolation concepts have been widely applied to several phenomena in physics, as for example in fluid flow in random media, dielectric breakdown, and diffusion in disordered media. Moreover, the scaling properties of percolation clusters have also been exploited in order to better understand some features of many chemical, biological, and social phenomena [1]. As such, percolation is a deeply studied phenomenon, and both "static" and "dynamical" [2] variations (i.e., directed percolation) of the problem continue to pose interesting challenges.

Percolation models employed over diluted continuous media are appropriate for describing specific features of real systems that exhibit percolation behavior. However, a large amount of information regarding the scaling of percolation clusters can be captured by simple lattice models that are more suited to extensive studies by means of computational techniques. In random site percolation, every site of a large lattice of linear size L in d dimensions is randomly occupied with probability p, giving rise to clusters of neighboring sites. When the occupation probability is larger than a critical value p_c, a dense infinite cluster arises whose mass (number of connected sites) scales as $m \sim L^d$. In contrast, for $p<p_c$, the cluster masses grow only logarithmically [3–6] with L. At the critical concentration p_c, fractal infinite clusters emerge with $m \sim L^{d_f}$ with a fractal dimension $d_f<d$.

Although many properties of percolating systems are well understood, many questions remain to be addressed. For example, the distribution of ranked cluster masses at the percolation threshold has become a subject of renewed interest among the computational statistical physics community [4,5,7–14]. Recently, it has been shown that all the ranked clusters (largest, second largest, third largest, and so on) have identical fractal dimensions d_f [4,11,15]. Therefore, the largest and second largest clusters, for example, are proportional in mass at p_c. In a previous paper, we have numerically demonstrated that the average ratio of the largest and second largest clusters is drastically dependent on the imposed boundary conditions in $d=2$, and showed the relevance of mass fluctuations at criticality [12]. It is known that the boundary conditions also influence the fraction of spanning clusters at p_c [16,17]. More recently, the universality of the mass distribution of ranked clusters in $d=2$ has also been investigated [13]. It was found that the distribution for any rank shows a universal behavior, but that only in the large rank limit is there a universal Gaussian size distribution. Further, the nature of the largest cluster size distribution was shown to have distinct contributions from the spanning and nonspanning clusters [14]. In $d=2$, the superposition of these contributions results in a well-defined two-peak structure for the size distribution. A single-peak distribution is observed at higher dimensions. The average ratio between the masses of spanning and nonspanning clusters was shown to be roughly independent of the lattice size, dimensionality, and boundary conditions.

Here, we numerically study the relevant quantities related to the scaling behavior of the mass distribution of the largest and second largest clusters at percolation. By defining suitable zero-exponent scaling quantities, we employ a finite size scaling analysis of the data to obtain precise estimates for the percolation threshold up to $d=7$. We also use scaling analysis to determine the average ratio between the largest and second largest clusters, thus allowing us to explore its dependence on dimensionality and on boundary conditions. Further, we report on some mass distribution functions associated with the two largest clusters for distinct boundary conditions and spatial dimension. These results provide a more complete picture concerning the general scaling behavior of mass distribution functions at percolation, and how they evolve to the mean-field distributions at high dimensions.

II. METHODS

We focus our computational efforts towards the study of the traditional site percolation problem on a hypercubic lat-

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tice in d dimensions, under either open or periodic boundary conditions (BC). Specifically, in our numerical simulations, we randomly distribute active sites with probability p in a hypercubic lattice with linear size L. In order to identify the largest and second largest clusters, we employ standard random percolation algorithms. For a given disorder distribution, we measure the size of the largest cluster M_1 and of the second largest cluster M_2. A configurational average over the disorder is then performed. Hence we effectively measure $\langle M_1 \rangle$, $\langle M_2 \rangle$, and $\langle M_1/M_2 \rangle$ as a function of p and L.

The same random distribution of active sites can represent distinct cluster distributions when different BC are considered. This is because two clusters at opposite extremes with open BC may become a single larger cluster if periodic BC are used instead. Therefore, the largest clusters masses can be significantly affected by the imposed BC even in the thermodynamic limit $L \to \infty$.

According to the finite size scaling hypothesis, the average size of the largest cluster near the percolation threshold scales as

$$\langle M_1 \rangle \sim L^{d-\beta/\nu}. \tag{1}$$

As has been recently demonstrated [4,11], the same scaling behavior stands for $\langle M_2 \rangle$. The ratio $\langle M_1/M_2 \rangle$ behaves as a zero-exponent critical quantity scaling as

$$\langle M_1/M_2 \rangle = g[(p-p_c)L^{1/\nu}]. \tag{2}$$

A similar scaling relation also holds for $\langle M_1 \rangle / \langle M_2 \rangle$. According to the above scaling behavior these ratios are size independent at the critical percolation threshold.

In a previous work, we employed the above scaling hypothesis to analyze data from the site percolation problem in a square lattice. We showed that a very precise estimate of the percolation threshold can be achieved with a relatively small computational effort, and that $\langle M_1/M_2 \rangle$ is strongly dependent on the imposed boundary condition [12]. Here, we extend our results by considering high-dimensional lattices up to $d=7$, which is above the upper critical dimension $d_c=6$ for the percolation problem. Further, we will also measure the mass distribution function of the two largest clusters at p_c, as well as the distribution functions of the mass ratio M_1/M_2, exploring their sensitivity on BC and convergence to the mean-field behavior.

III. RESULTS

In our simulations, we measured the size of the two largest clusters for each disordered configuration with a concentration p of active sites. In order to obtain good statistics, we generated 10^4 distinct configurations for each concentration in hypercubic lattices with periodic BC. For lattices with open boundaries, we needed to perform a more extensive statistical analysis (with 10^5 configurations) since larger fluctuations are present in this case. The largest lattice size $L_{\max}$ simulated for each dimension d contained about 10^6 sites ($L_{\max}$=1000, 100, 40, 20, 11, 9; for $d=2$, 3, 4, 5, 6, 7, respectively). To measure the probability distribution of the two largest clusters and the ratio between the largest and second largest cluster sizes at $p=p_c$ for each dimension, we ran 5×10^4 configurations of size $L_{\max}$ to obtain the mass distributions for open and periodic BC.

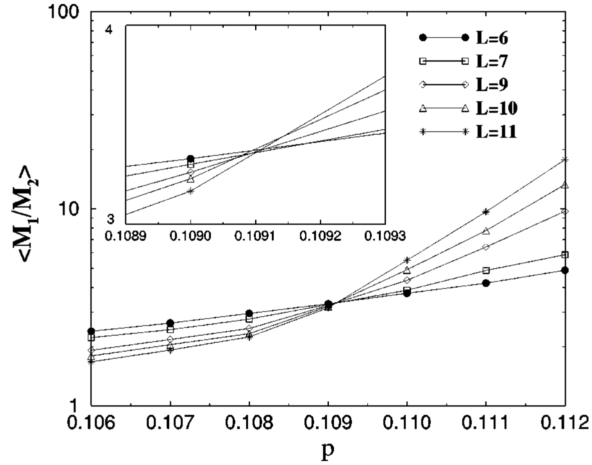

FIG. 1. $\langle M_1/M_2 \rangle$ versus p for $d=6$ and periodic BC. Data were obtained after a configurational average over 10 000 samples. Error bars are much smaller than symbols size. The common point determines p_c and the scale invariant average mass ratio at percolation.

As a first step, we performed the finite size scaling analysis of the average ratio $\langle M_1/M_2 \rangle$. According to Eq. (2), this ratio is size independent at the percolation threshold. Therefore, the curves $\langle M_1/M_2 \rangle$ versus p, as obtained from distinct lattice sizes, must intersect at a common point that defines p_c and the average ratio at criticality. In Fig. 1, we show the result of the above analysis for $d=6$ and periodic BC. From this we estimate $p_c=0.109\,10(5)$ and $\langle M_1/M_2 \rangle=3.27(3)$, for $d=6$. In these estimates we are not considering any possible correction to scaling. We notice that our estimate for p_c is relatively above the previous numerical estimate $p_c(d=6)=0.107(1)$ [1], but is quite close to the value obtained from the conjecture of Galam and Mauger [18]. From $d=2$–7, all estimated values are in fully agreement with the best ones previously reported in the literature [1,18–21].

In Table I, we summarize our best estimates for the critical concentration and the critical values of $\langle M_1/M_2 \rangle$ and $\langle M_1 \rangle / \langle M_2 \rangle$. These results confirm the strong dependence on the imposed BC of the average mass ratio of the two largest clusters. These averages monotonically decrease with the lattice dimension d, and seem to saturate above $d=6$. The fact that $\langle M_1/M_2 \rangle \neq \langle M_1 \rangle / \langle M_2 \rangle$ reflects the relevance of mass fluctuations at criticality. These fluctuations decrease with increasing d and are larger for periodic BC.

In Fig. 2, we report on the mass distribution of the largest cluster at the percolation threshold for periodic [Fig. 2(a)] and open [Fig. 2(b)] BC. For periodic BC [Fig. 2(a)], the shape of the distribution in $d=2$ is quite distinct from those at higher dimensions. This feature was previously observed by Sen [14], and related to the distinct scaling behavior of the spanning and nonspanning cluster distributions. We observed that in $d=2$, the distribution has a peak near the average cluster size and rapidly decreases for larger clusters. At higher dimensions, the distributions evolve to a broader one peaked around $\langle M_1 \rangle/2$ with a slowly decaying tail. No-

TABLE I. Summary of the dependence on BC of the ratio between the masses of the first and second largest clusters. The observed behavior is nonuniversal with respect to the BC.

Dimension	$p_c \pm \Delta p$	Periodic boundary $\langle M_1/M_2\rangle \pm \Delta$	Periodic boundary $\langle M_1\rangle/\langle M_2\rangle \pm \Delta$	Open boundary $\langle M_1/M_2\rangle \pm \Delta$	Open boundary $\langle M_1\rangle/\langle M_2\rangle \pm \Delta$
2	0.59272 ± 0.00005	25.1 ± 0.1	10.1 ± 0.1	6.7 ± 0.1	3.51 ± 0.07
3	0.31161 ± 0.00003	7.51 ± 0.04	4.38 ± 0.04	2.50 ± 0.05	2.12 ± 0.04
4	0.19687 ± 0.00006	4.68 ± 0.03	3.30 ± 0.06	1.84 ± 0.02	1.74 ± 0.04
5	0.14081 ± 0.00004	3.72 ± 0.03	2.79 ± 0.05	1.62 ± 0.02	1.57 ± 0.07
6	0.10910 ± 0.00005	3.27 ± 0.03	2.61 ± 0.05	1.49 ± 0.03	1.46 ± 0.03
7	0.08888 ± 0.00006	3.20 ± 0.06	2.53 ± 0.07	1.44 ± 0.01	1.42 ± 0.01

tice also that, in all dimensions, the distribution is vanishingly small for $M_1 < 0.15\langle M_1\rangle$. For open boundaries, the distinction between the $d=2$ distribution is not very much pronounced, given that the spanning probability at p_c is smaller than in the periodic case. However, a two-peak structure is still clearly identified in agreement with Ref. [14]. The distribution is wider and therefore larger deviations from the mean are more probable to occur than in the periodic lattices. At higher dimensions, the largest cluster distribution in lattices with open and periodic BC has similar trends. The distinct features that can be observed in open BC as compared with periodic BC concern the peak position (closer to the average value) and a rapidly decaying tail.

In Fig. 3, the distribution of the second largest cluster size is reported. For periodic BC [Fig. 3(a)], the $d=2$ distribution is also quite distinct from those of higher dimensions. This

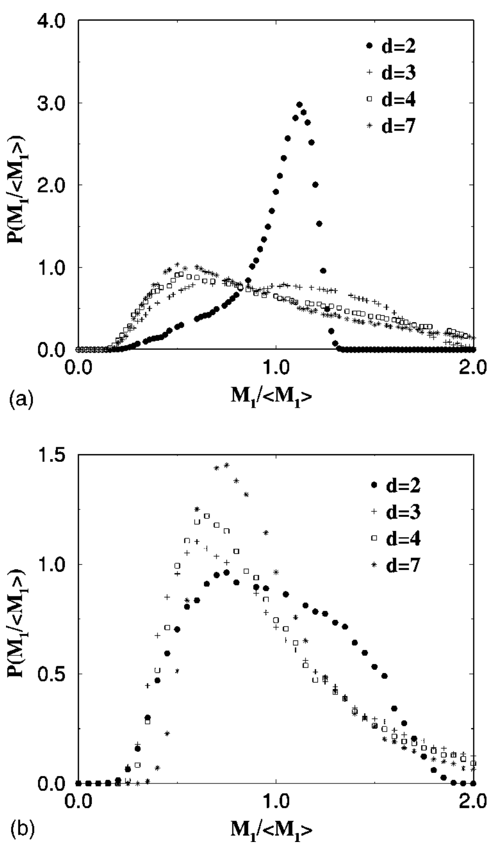

FIG. 2. The mass distribution of the largest cluster at the percolation threshold is shown for $d=2$, 3, 4, and 7 with (a) periodic BC and (b) open BC. We performed 50 000 measures for each dimension d simulated with $L_{\max}=1000$, 100, 40, and 9, respectively. Our data indicate that the convergence to the limiting distribution for high dimensions is faster for periodic BC.

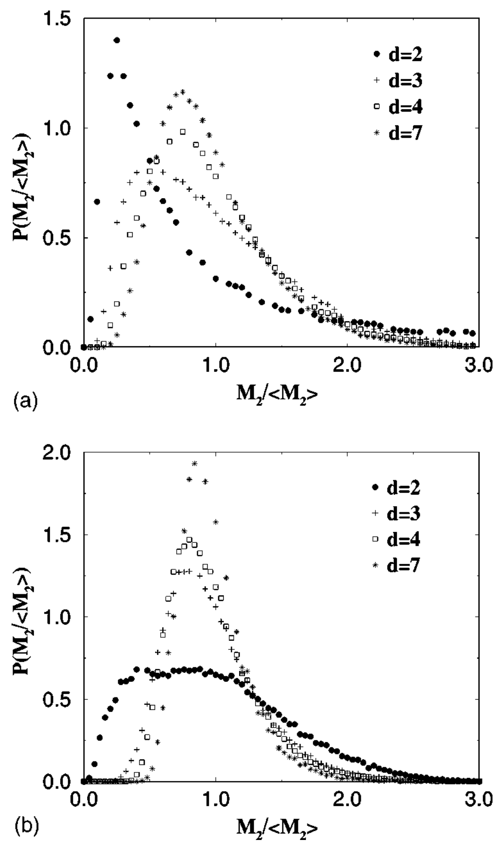

FIG. 3. The mass distribution of the second largest cluster at the percolation threshold is shown for $d=2,3,4$, and 7 with (a) periodic BC and (b) open BC. We performed 50 000 measures for each dimension d simulated with $L_{\max}=1000$, 100, 40, and 9, respectively. Notice that at high dimensions, these distributions are similar to those for the largest cluster. However, at low dimensions (specially at $d=2$) and periodic BC, the largest and second largest clusters have quite distinct mass distributions, once the spanning and nonspanning clusters have well-distinguishable distributions in this case.

finding is related to the very small probability of the second largest cluster to span the lattice in $d=2$ [17]. This feature makes $P(M_2)$ to become wider and to show a peak at a typical cluster size considerably smaller than the average size. At higher dimensions, the distribution of the second largest cluster is more similar to the largest cluster size distribution. For open BC [Fig. 3(b)], the second largest cluster in $d=2$ has a higher probability to span the lattice and the distribution shows a two-peak structure. As the lattice dimensionality grows, the second largest cluster size distribution becomes sharper.

To further characterize the above trends of the cluster size statistics, we measured the normalized probability density distribution of the ratio between the largest and second largest cluster sizes (see Fig. 4). For periodic BC, we clearly see that the probability of the second largest cluster to have a size of the order of the largest one is significantly smaller in $d=2$ as shown in Fig. 4(a). Thus, it corroborates the proposed relation between the sharp peak depicted by $P(M_2/\langle M_2\rangle)$ and the predominant nonspanning character of the second largest cluster in $d=2$. The mass ratio distribution converges with increasing lattice dimensionality to a power-law distribution for small ratios in the form $P(M_1/M_2)\propto(M_1/M_2)^{-3/2}$ crossing over to an exponential decay for large size ratios. With open BC, the size ratio distribution is narrower and the initial power-law regime at high dimensions is not well characterized, as shown in Fig. 4(b). Also, for the two-dimensional lattice, $P(1)$ is larger than in the corresponding distribution for periodic BC, which agrees with the shift of the peak of $P(M_2/\langle M_2\rangle)$ to a larger cluster size as reported in Fig. 3(b).

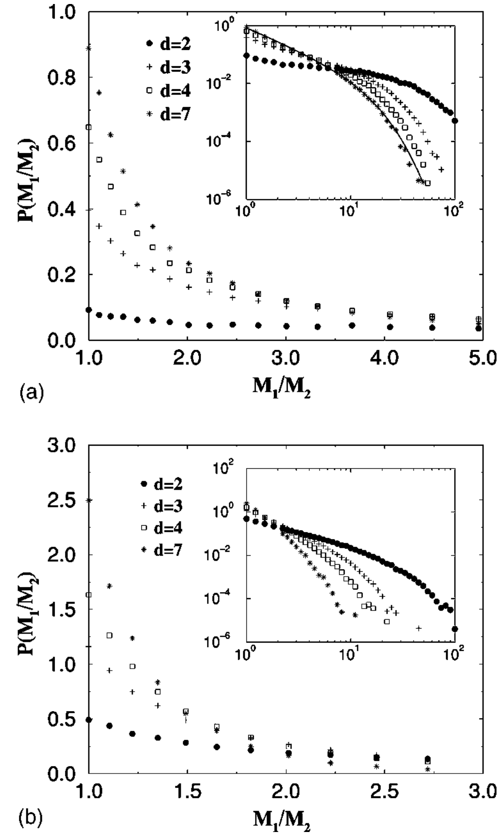

FIG. 4. The distribution of the ratio between the masses of the largest and second largest clusters at the percolation threshold are shown for $d=2,3,4$, and 7 with (a) periodic BC and (b) open BC. We performed 50 000 measures for each dimension d simulated with $L_{max}=1000$, 100, 40, and 9, respectively. Notice also that the convergence to the high-d limiting distribution is faster for periodic BC. The insets show the same data in log–log scale. The solid line in (a) corresponds to a fit from an initial power law $P(x)\propto x^{-3/2}$ crossing over to an exponential decay

IV. CONCLUSION

In summary, we have reported on several statistical properties related to the mass distribution of the largest and second largest clusters at the percolation threshold in hypercubic lattices up to $d=7$. We have explored the scale invariance of the average mass ratio at percolation to provide accurate estimates of the critical percolation threshold and the critical average mass ratio. By comparing the critical values of $\langle M_1/M_2\rangle$ with $\langle M_1\rangle/\langle M_2\rangle$, we showed that size fluctuations progressively decrease, with increasing lattice dimensionality, and are larger for periodic boundary conditions. We also reported on the probability density for the largest and second largest cluster sizes, as well as for the mass ratio between the two largest clusters. We identified several peculiar features in the two-dimensional distributions and related them with the very small probability of coexistence of more than one spanning cluster in $d=2$. Furthermore, we showed how these distributions evolve to limiting distributions characterizing the main behavior above the upper critical dimension $d=6$. To the best of our knowledge, the analytical expressions for these limiting distributions are still unknown. We hope that the present work can stimulate future efforts along this direction.

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