Multiscaling behavior in the crossover between surface and bulk critical exponents for percolation in two dimensions

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The crossover between the surface and bulk values of the order-parameter critical exponent (β) is investigated for the site-percolation model in a rectangular geometry ($L\times M$, $L \ll M$) with free boundary conditions. Due to the reduction in the connectivity, when the space is cut by the surfaces of the sample which cannot be penetrated by the percolating clusters, β decays exponentially from the surface value ($\beta_s \cong 0.40$) to the bulk value ($\beta_b = 5/36$). This decay is interpreted in terms of multiscaling which implies that each row of the percolating cluster (taken in the M direction) has its own scaling and consequently a different fractal dimension.

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I. INTRODUCTION

Percolation theory has applications in diverse areas of physics and physical chemistry such as fluid flow through porous media, gelation, electrical conduction in metal-insulator samples, epidemic growth, etc. (For reviews see, for example, [1–4].) Interest has centered on the properties of percolating clusters at criticality, since this is where universal behavior emerges. Within this context, we have recently studied [5,6] the critical behavior of the site-percolation model in the square lattice using the $L\times M$ ($L \ll M$) geometry and assuming free boundary conditions at the edges of the sample. The study is based upon finite-size scaling arguments and Monte Carlo simulations. The $L\times M$ geometry is particularly useful to the study of the percolative behavior of adsorbed monolayers on regularly stepped surfaces ($M \equiv$ step length, $L \equiv$ terrace width). The same geometry has been used by various authors in order to investigate different properties of the model; see, for example, [7–11] and references therein.

Due to the constraint $L \ll M$ and the free boundary conditions used, the preferential growth of percolating clusters in the L direction is observed not only at criticality but also rather far below the threshold, as is shown in Fig. 1. Due to the reduction in the connectivity, when the space is cut by the surfaces of the sample which cannot be penetrated by the percolating clusters, some features of the critical behavior are modified. In fact, critical behavior at surfaces and the development of methods for calculating the associated critical exponents are subjects of great interest not only in the field of percolation theory ([12–16] and references therein) but also in the study of thermally driven critical phenomena ([17,18] and references therein). The surface exponents are related to each other and to the bulk exponents such that if only one of the surface exponents is known the others may be determined [12–18]. In particular, it is well known that the surface (β_s) and bulk (β_b) critical exponents associated with the order parameter are different, i.e., $\beta_s \cong 0.4$ [14,15] and $\beta_b = 5/36$ [1–4] for percolation in two dimensions. Therefore, the main purpose of the present work is to analyze, at criticality, the crossover behavior between β_s and β_b. Exponents are evaluated computing the pair connectedness function by means of the Monte Carlo method. An interesting feature of the present study is that the crossover between β_s and β_b can be described in terms of a quite general scaling approach called multiscaling [19]. Multiscaling means that an infinity of exponents are obtained by continuously varying a given characteristic parameter. More specifically, in the case studied in this work one has a very rich cluster structure because the percolating cluster fractal dimension crosses over continuously from $D_s = 1-\beta_s/\nu$ to $D_b = 2-\beta_b/\nu$, for the surface and the bulk, respectively, where $\nu = \frac{4}{3}$ is the critical exponent of the correlation length which is the same at the surface and in the bulk.

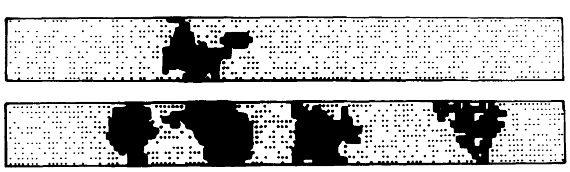
(a)
(b)


FIG. 1. Typical snapshot configurations for rectangular samples of size $L=12$, $M=132$ taken at different values of the occupation probability p. Sites taken by percolating clusters in the L direction are shown in black squares, other occupied sites are shown in black points, and empty sites are left white. (a) $p=0.50$, (b) $p=p_c \cong 0.5927$.

II. RESULTS AND DISCUSSION

The site-percolation model is studied in the square lattice using the $L\times M$ ($L \ll M$) geometry and assuming free boundary conditions at the edges of the sample. In order to appreciate the dramatic effect of the reduction in the connectivity at and close to the surfaces of the sample it is convenient to analyze the density profile of the percolating clusters in the L direction defined as the probability $P(i,L)$ of a site located in the ith row parallel to the M direction belonging to a percolating cluster, i.e.,

$$P(i,L)=(p_c M)^{-1}\sum_{j=1}^{M} c(i,j), \quad i=1,\ldots,L\ , \tag{1}$$

where all lengths, e.g., L, M, i, and j are measured in lattice units, $p_c \cong 0.592\,75$ is the critical occupation probability, and $c(i,j)=1$ $[c(i,j)=0]$ if the site $\{i,j\}$ belongs to a percolating cluster (otherwise). Note that in the limit $L \ll M$ the profiles are independent of M.

Figure 2 shows plots of density profiles vs $(i-L/2)$ obtained using lattices of different sizes. Due to the missing neighbors effect at $i=1$ and L the profiles are depleted close to those boundaries. This effect propagates into the bulk, and the profiles are symmetric around $i=L/2$, as is shown in Fig. 2. This fact can be understood because the correlation length ξ, which would become $\xi=\infty$ in an infinite system at criticality, stays at the order $\xi \cong L$ in the present case due to the geometric constraint. Density profiles obtained for $p<p_c$ are also symmetric and peaked at $i=L/2$. Because of the symmetry, the data corresponding to rows equidistant from $i=L/2$ are averaged over in the following. It should be noted that the order-parameter profiles of the ferromagnetic Ising model in the absence of magnetic field [18] (or equivalently the coverage profiles of the lattice gas model [20]) also exhibit a similar symmetry, but in contrast to the density profiles shown in Fig. 2 the former profiles smoothly flatten out close to the critical temperature.

Critical exponents of the order parameter are determined by computing the pair connectedness function $G(r,i)$, which is also known as the correlation function. $G(r,i)$ is defined as the probability that two sites of the ith row $(i=1,\ldots,L)$ at a distance r belong to the same percolating cluster. Note that due to the geometry used $(L\times M,\ L\ll M)$ it is only interesting to study the pair connectedness function calculated parallel to the M direction. At p_c one has that $G(r,i)$ behaves as [1–4]

$$G(r,i)\propto r^{-\beta(i)/\nu}\ , \tag{2}$$

where the dependence of the exponent β on the distance to the surface has been written explicitly. Note that, as quoted in the Introduction, $\nu=4/3$ is the critical exponent of the correlation length. The physical reason why this exponent is the same at the surface and in the bulk follows from the fact that only a single divergent length, namely, $\xi\propto|p-p_c|^{-\nu}$, has to be considered in order to describe both the bulk and surface critical behavior [12].

Figure 3 shows log-log plots of $G(r,i)$ vs r evaluated for $i=1$ and $L/2$. Here two different regimes characteristic of $G(r,i)$ can clearly be observed: (i) the algebraic regime for $r<L$ and (ii) the exponential decay for $L<r<M$ [21]. So, it is worth mentioning that only the obtained straight lines within the algebraic regime of $G(r,i)$ allow us to evaluate reliable critical exponents. In fact, for $i=1$ one gets $\beta_s/\nu\cong 0.30\pm 0.03$, in good agreement with Monte Carlo results 0.31 [14] and 0.299 ± 0.005 [15], and in marginal agreement with the (presumable) exact value $\beta_s/\nu=\frac{1}{3}$ [16]. On the other hand, for $L/2=50$ one gets $\beta(50)/\nu\cong 0.104\pm 0.005$, which means that the bulk value $\beta_b/\nu=5/48\cong 0.104$ is practically recovered.

The crossover of the critical exponent between the surface and the bulk behavior becomes evident in Fig. 4(a), which shows a plot of $\beta(i)/\nu$ vs i. A more detailed view of the crossover is shown in Fig. 4(b). From Figs. 4(a) and 4(b) it follows that $\beta(i)/\nu$ drops drastically close to

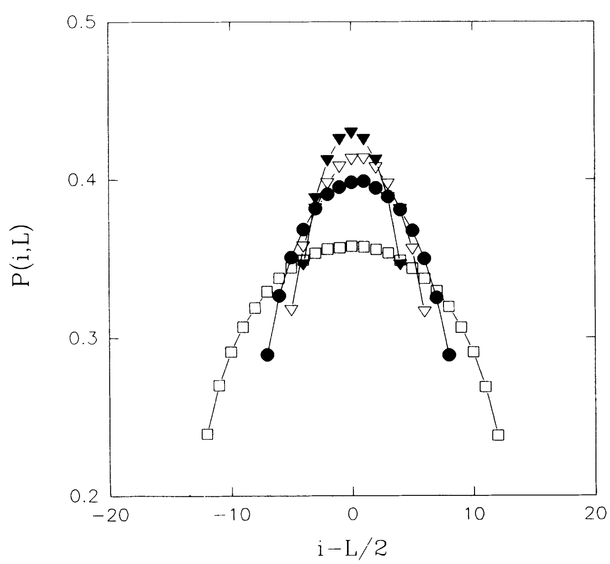


FIG. 2. Plots of the density profiles $P(i,L)$ vs $i-(1/2)L$ for lattices of different size $(L\times m)$: ▼, 9×420; ▽, 12×440; ●, 16×576; and □, 25×150. All lengths are measured in lattice units. Lines have been drawn to guide the eyes.

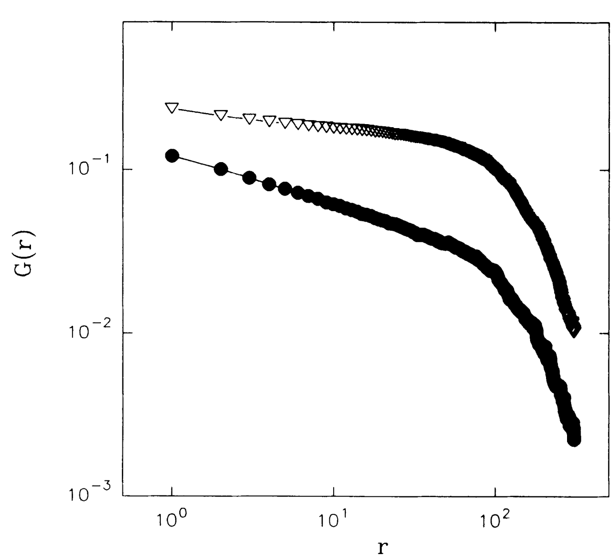


FIG. 3. Plots of the pair connectedness function $G(r,i)$ vs r for $i=1$ (●) and $i=L/2$ (▽), respectively. All lengths are measured in lattice units. The lattice size is $L=100$, $M=700$ and data are averaged over 200 different samples.

the surface and then approaches the bulk value. This behavior suggests an exponential decay of the form

$$[\beta(i/L)-\beta_b]/\nu=\{[\beta_s-\beta_b]/\nu\}\exp[-C(i-1)/L], \tag{3}$$

where for $i=1$ ($i\rightarrow\infty$) the values $\beta(i)=\beta_s$ [$\beta(i)=\beta_b$] are recovered, respectively, and C is a constant. Note that the multiscaling hypothesis has been drawn explicitly by assuming $\beta(i,L)=\beta(i/L)$ [19]. In order to test the conjecture of Eq. (3), Fig. 5 shows plots of $[\beta(i,L)-\beta_b]/\nu$ vs $(i-1)/L$ for lattices of different size. The obtained straight line and the excellent data collapsing strongly support the validity of Eq. (3) and the multiscaling behavior. From the slope of the straight line the value $C\cong-5.5$ is obtained by a mean-square fit of the data. Also, the intersection gives $[\beta_s-\beta_b]/\nu\cong0.200\pm0.005$, in excellent agreement with the expected value, namely, $[\beta_s-\beta_b]/\nu\cong0.1958$.

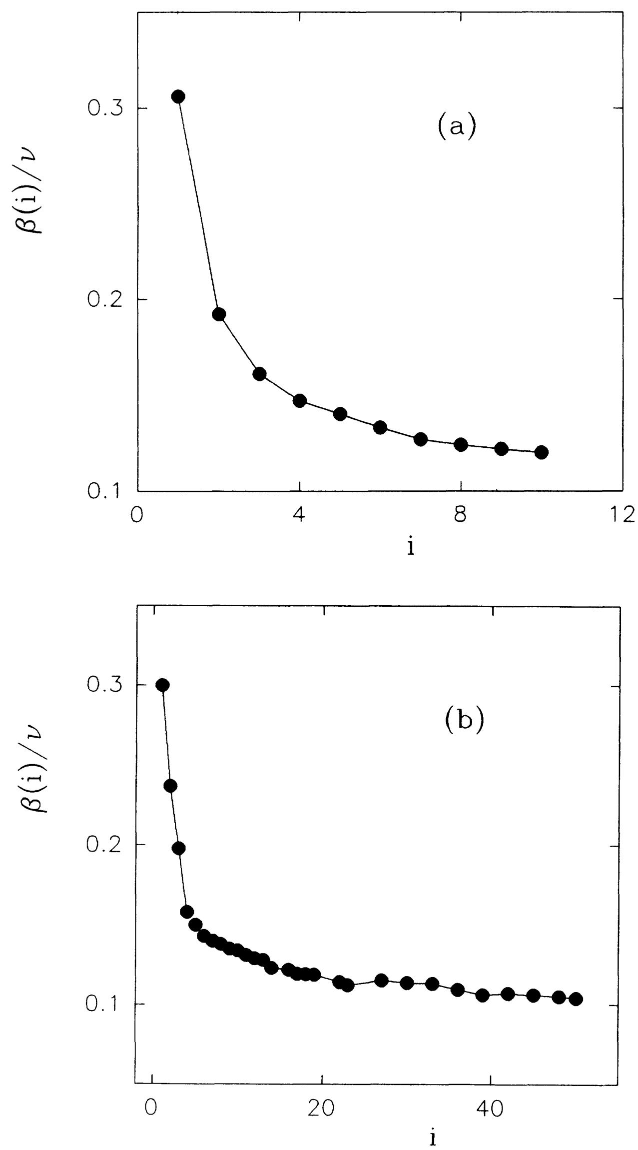


FIG. 4. Plots of the critical exponent ratio $\beta(i)/\nu$ vs i. The exponent values were obtained from the correlation function calculated over the ith row ($i=1,\ldots,L$) in the M direction. All lengths are measured in lattice units. (a) The lattice size is $L=20$, $M=600$ and data are averaged over 8×10^3 different samples. (b) The lattice size is $L=100$, $M=600$ and data are averaged over 3×10^2 different samples.

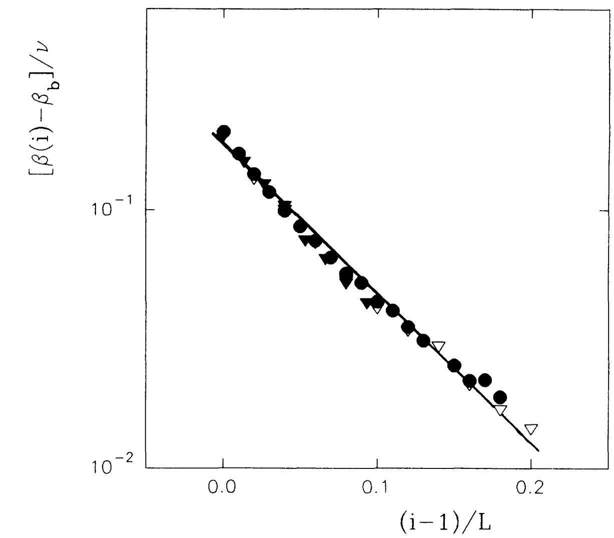


FIG. 5. Semilogarithmic plot of $[\beta(i)-\beta_b]/\nu$ vs $(i-1)/L$ obtained using data from different lattice sizes: $L=50$, $M=700$ (●); $L=100$, $M=600$ (▽); and $L=70$, $M=900$ (▼). All lengths are measured in lattice units. Exponents are obtained after averaging over 10^2-10^3 different samples.

Multiscaling behavior is expected to be a general feature of many dynamic processes such as diffusion-limited aggregation (DLA) [19], spinoidal decomposition, when a system initially disordered at high temperature is suddenly quenched below the critical point [19], damage spreading in magnetic systems, such as the three-dimensional ferromagnetic Ising model [22], etc. In order to understand the physical picture behind multiscaling behavior let us analyze the growth of a DLA. According to the discovery of Plischke and Racz [23] one has to make the distinction between two regions: a frozen region characterized by practically zero growth probability and an active region where most of the growth occurs. Consequently, the density profile exhibits a different power-law decay at different distances from the center of the aggregate, and therefore the outer (active) regions of the DLA have lower fractal dimensions than the inner (frozen) regions [19]. Let us now reconcile the fact that the percolating clusters studied in the present work are "static" aggregates while the above physical picture holds for dynamic growth. For this purpose we consider a percolating cluster at criticality and in the $L=\infty$ limit. After fixing arbitrarily a certain origin at 0, let us cut the cluster by an edge at a distance L_1 from 0. The reduction in the connectivity caused by the cut will propagate up to 0 (remember that the correlation length is infinite). So, we will measure β_s at L_1 and a β value close to β_b at 0. If we perform a second cut at $L_2>L_1$, we observe that some mass of the cluster already mutilated by the first cut will now contribute to $G(r)$ at

0. So, we will again measure β_s at L_2 but a β value closer than in the previous case, to β_b at 0. This process can continue indefinitely, but even for very large L distances one has, due to the infinite correlation length, a small but finite probability of growth at 0 and consequently the β values measured at the origin will asymptotically approach β_b. Therefore, the inner and outer regions of the DLA are qualitatively similar to the region close to 0 and that close to L in the present case, respectively.

The observed multiscaling behavior implies that each row i of the percolating cluster (taken in the M direction) has its own scaling and consequently different fractal dimension.

III. CONCLUSIONS

Evaluation of the pair connectedness function parallel to the M direction on percolating clusters at p_c allows us to determine the dependence of the exponents ratio β/ν on the distance to the edge of the sample. For $i=1$ and $L\rightarrow\infty$ the surface and bulk order-parameter exponents β_s and β_b are obtained, respectively. Furthermore, evidence is presented to show an exponential crossover from β_s to β_b which is interpreted in terms of a multiscaling behavior.

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