Loop structure of percolation hulls

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The loop structure generated by the percolation hulls in two dimensions is investigated both for random percolation and for the percolation properties of interacting, diffusing particles using the gradient diffusion method. Scaling forms for the loop distribution function are proposed and verified numerically. The results show that while bonding nearby particles on the original hull reduces its fractal dimension from $D_H = \frac{7}{4}$ to $D_{H'} = \frac{4}{3}$, no further change in $D_{H'}$ is observed when additional bonds are placed on the already reduced hull. A similar behavior holds for strongly interacting particles during phase separation on length scales larger than the characteristic droplet size.

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A percolation cluster in two dimensions is a fractal object with fractal dimension $D = \frac{91}{48}$ [1]. A more detailed analysis reveals that it is a closed structure containing loops of all sizes, up to the cluster size itself. As a consequence almost all particles lie in the interior of the cluster. The ensemble of particles accessible from the outside is called hull H_0 or external perimeter [2]. This subset forms a cluster with a smaller fractal dimension, $D_H = \frac{7}{4}$ [3–5]. A second hull $H(r)$ can be constructed by connecting all particles of H_0 that are a distance r apart (r is necessarily larger than r_0, the bond length of the percolation construction). This operation blocks the access to those parts of the hull which are connected to the outside only by narrow channels. The reduced hull $H(r)$, i.e., the particles which are still accessible from the outside after adding the bonds, has an even lower fractal dimension, $D_{H'} = \frac{4}{3}$ [5,6]. The hulls generated by the different rules are illustrated in Fig. 1. The changing of the hull properties due to new bonds is specific to two dimensions and is not observed in three dimensions [7].

The change in fractal dimension from D_H to $D_{H'}$ has been investigated by Monte Carlo simulations [8] for the continuum percolation model [9]. The advantage of continuum percolation is that the bond length r can be varied continuously. The calculation shows that the fractal dimension changes from D_H to $D_{H'}$ for any bond length $r > r_0$, no matter how small $\delta r = (r - r_0)$. A scaling analysis [10] reveals that there exists a crossover length σ^* such that the fractal dimension of a hull of linear size σ is D_H for $\sigma \ll \sigma^*$ and $D_{H'}$ for $\sigma \gg \sigma^*$. σ^* diverges as $\sigma^* \sim \delta r^{\alpha}$ with $\alpha = -1.37$ as $\delta r \to 0$.

The purpose of this investigation is to give a more detailed description of the structure of percolation hulls in two dimensions. Scaling theory proves to be relevant for most properties of the incipient infinite percolation cluster and its hull. Modifying the connectivity of the hull changes its scaling behavior; it necessarily creates loops on all scales. We anticipate that the distribution of these loops also has scaling form.

In the present calculation we study the scaling properties of the loops generated by the reduced hull construction for standard site percolation. We use a square lattice (lattice spacing r_0) and randomly put particles on a fraction p of the sites. Clusters are defined by placing bonds between all particles on nearest-neighbor sites. The hull of a cluster [2] consists of those sites which can be reached from the outside by a continuous path which does not cross any bond of the cluster. A different but equivalent procedure defines the hull as those sites which can be reached from the outside by steps on the empty

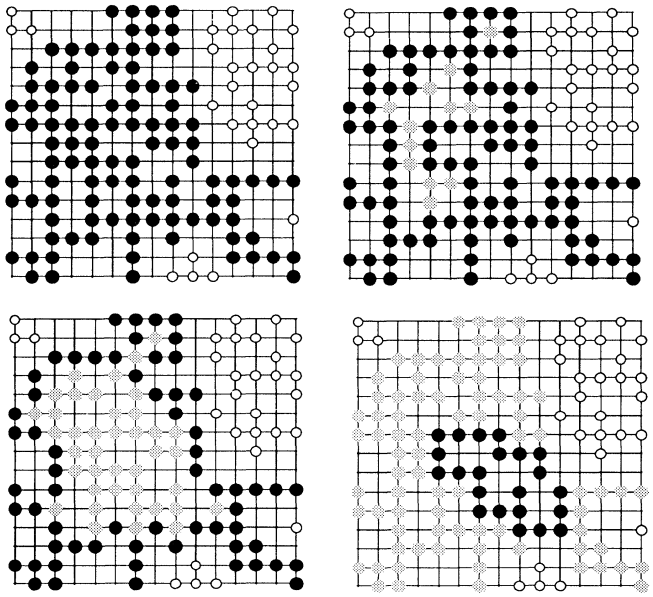

FIG. 1. Percolation structures relevant to the present study. All dots correspond to occupied sites. The filled black dots are the percolation cluster (top left), the standard hull (top right), the reduced hull (bottom left), a loop generated by the reduced hull construction (bottom right).

lattice sites of length r_0 or $r_0\sqrt{2}$. To construct a reduced hull, additional bonds of length $r=r_0\sqrt{2}$ (second nearest neighbors) are placed between the particles of an *isolated* cluster [5]. The sites that are still accessible from the outside form the reduced hull. Other reduced hulls can be generated by placing bonds of lengths $r=2r_0, r_0\sqrt{5}, r_0\sqrt{8}, \ldots$ on the cluster. The reduced hull construction defines loops in a natural way (Fig. 1).

A hull is a closed linear object. Therefore it is natural to define the length $h_{\rm tot}$ of the original hull as the number of steps of length r_0 needed to "walk" along the hull. The number of bonds may differ slightly from the number of steps but is expected to scale in the same way. The length $h'_{\rm tot}$ of the reduced hull is defined analogously to $h_{\rm tot}$ but allowing for steps of length r whenever possible. Finally, the length h of a loop is equal to the number of steps of length r_0 on the original hull between the two sites that are newly connected by the extra bond of length r.

We first use a scaling argument to calculate the number of loops of length h on the reduced hull $H(r)$. The length $h_{\rm tot}$ of the original hull H_0 (corresponding to the quantity N_f defined in Ref. 3]) is related to its linear size σ by $h_{\rm tot}\sim\sigma^{D_H}$. Correspondingly, the length $h'_{\rm tot}$ of the reduced hull scales as $h'_{\rm tot}\sim\sigma^{D_{H'}}$. The number of loops of length h generated by the reduced hull construction is assumed to have power-law form $N'_h\sim h^{-\tau'_h}$. We furthermore assume that the number of loops per site of the reduced hull does not depend on $h_{\rm tot}$ (this means that $h_{\rm tot}$ only acts as a cutoff). For a reduced hull of linear size σ the number of loops scales as $N'_h\sim h'_{\rm tot}h^{-\tau'_h}\sim\sigma^{D_H}h^{-\tau'_h}$. As the total number of particles on the hull is $h_{\rm tot}=\sum_h hN'_h\sim\sigma^{D_H}$ one finds $\tau'_h=1+D_{H'}/D_H$. Inserting the numerical values for D_H and $D_{H'}$ yields $\tau'_h=\frac{37}{21}\cong 1.76$. This result can also be understood from comparing the total area occupied by the loops with the area occupied by the hull as a whole.

Placing new bonds between *all* sites of a percolation hull that are a distance $r>r_0$ apart not only generates a reduced percolation hull with its loops, but it also creates loops within loops, etc. The total number of loops created by all the new bonds, independent of whether they are on the reduced hull or on a loop is called N_h. It is expected to be related to the fluctuations of the length of the interface, relevant for example for an assembly of randomly diffusing particles, because an extra bond potentially short-circuits a large portion of the hull just as a diffusing particle may clog a bottleneck. Both operations are random and local and therefore they should have the same effect on large scales. These fluctuations have been determined: analytical arguments and numerical simulations agree that they scale as $h_{\rm tot}h^{-11/7}$ [11]. Our numerical results confirm that N_h indeed scales in the same way.

The numerical results were obtained from calculations on a square grid using the gradient percolation method [3,12] in which the average density $p(x,y)$ of occupied sites varies linearly in the x direction and is homogeneous in the y direction (periodic boundary conditions). The boundary of the largest cluster then corresponds to the percolation hull, and the hull width σ plays the role of the correlation length. σ increases as the concentration gradient ∇p decreases, scaling as $\sigma\sim\nabla p^{-1/D_H}$ [3].

Gradient percolation is used for two reasons: (i) it is directly relevant to the formation of rough interfaces [13] and (ii) it is an efficient computational tool which does not require a knowledge of the percolation threshold. This is particularly useful when studying a system in a transitory state where the percolation threshold p_c changes. In the second part of our study the elementary cluster size increases in time, leading to a corresponding decrease of p_c [14,15].

Figure 2 shows $N_{\rm tot}$, the *total* number of loops for two different bonding rules, as a function of the concentration gradient ∇p. It scales with an exponent $\alpha_L=0.431$, in close agreement with the exponent $\alpha_N=0.429$ for the total number of particles on the hull. This confirms that the number of loops per hull particle does not depend on the length of the hull.

The number N'_h of loops of length h on the *reduced* hull is presented in Fig. 3 for different bond lengths and gradients. Two bonding rules were used: $r=r_0\sqrt{2}$ and $2r_0$. To make N'_h independent of the sample width it has been normalized by L_y. The curves scale with an exponent $\tau'_h=1.72$ and 1.74, respectively, in good agreement with $\tau'_h=1.76$ from scaling considerations. The data for $r=r_0\sqrt{2}$ is shown for two gradients to illustrate the finite-size effects. The scaling form sets in for very small h and holds up to the rather sharp cutoff just below $h_{\rm tot}$.

An assembly of randomly diffusing particles in a concentration gradient naturally defines a fluctuating interface. One expects that for small concentration gradients the interface defined by the diffusers has the same fractal properties as the percolation hull studied here. In particular, the distribution function of the fluctuations of the

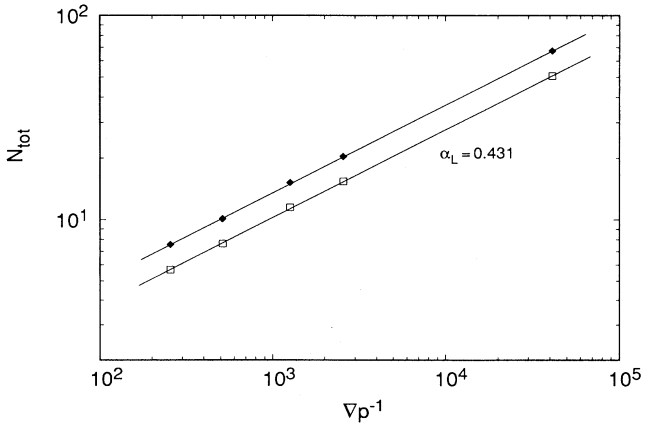

FIG. 2. Total number of loops, $N_{\rm tot}=(1/L_y)\sum_h N_h$, as a function of the inverse concentration gradient ∇p^{-1} (log-log plot). Loops generated by bonds of length $r=r_0\sqrt{2}$ (♦) and $r=2r_0$ (open squares) are compared. The measured exponent $\alpha_L=0.431$ (same for both curves) shows that $N_{\rm tot}$ scales like $h_{\rm tot}$, the total length of the hull.

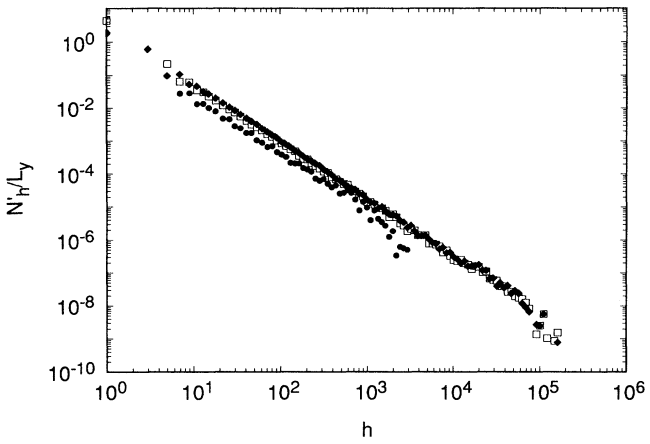

FIG. 3. Normalized number of loops of length h on the reduced hull, $(1/L_y)N'_h$. The different curves correspond to different bond lengths r and gradients: nearest-neighbor bonds ($r=r_0\sqrt{2}$) (open squares), second-neighbor bonds ($r=2r_0$) (♦) with a gradient $\nabla p=\frac{1}{41200}$ [100 independent realizations on a $(1648)^2$ lattice], and $r=r_0\sqrt{2}$ for a larger gradient $\nabla p=\frac{1}{800}$ (filled dots). The exponents determined from the slope are $\tau'_h=1.72$ ($r=r_0\sqrt{2}$) and $\tau'_h=1.74$ ($r=2r_0$). The upper cutoff is determined by the gradient.

interface for the diffusers should be equal to the loop size distribution calculated here for gradient percolation. To verify that the number of *all* the loops of length h (including loops within loops) scale with the same power as the statistics of the hull fluctuations, the total loop distribution was computed for the same types of bonds as in Fig. 3. Figure 4 shows the data. The measured exponents $\tau_h=1.56$ and 1.54 for $r=r_0\sqrt{2}$ and $2r_0$, respectively, are in good agreement with the scaling exponent $\frac{11}{7}\cong 1.57$ of the diffusion problem [11]. The static calculations performed here improve the statistics and allow for larger systems than the direct observation of the fluctuations. Comparing the data for different gradients shows that the scaling prediction is approached from below. The effective exponents obtained here coincide very well with the ones obtained from the fluctuation measurements for the same gradient.

In order that the fractal dimension changes when passing from the standard to the reduced hull the exponent τ'_h of the loop size distribution must be smaller than 2. To check whether the fractal dimension changes further when reducing an already reduced hull, bonds of length $r=2r_0$ were placed on a hull which was already reduced by bonds of length $r=r_0\sqrt{2}$. The number of such loops is shown in Fig. 5. The statistics is less good than in Fig. 4 as there are fewer loops altogether. Nevertheless the corresponding exponent can be estimated as $\tau''_h=2.28(10)$. It is clearly larger than 2 which confirms that there is no further change in $D_{H'}$.

So far we have considered hulls generated by random percolation on a lattice which describe a random diffusion process with a concentration gradient. It is interesting to extend the study of the hull to systems of interacting particles because then the lattice spacing and the elementary length of the percolation structure no longer coincide. Earlier work [15] on diffusion with interaction in the gradient geometry has shown that the connectivity properties of strongly interacting particles during phase separation can be described in terms of random percolation on length scales larger than the characteristic droplet radius.

We have studied the hull properties for diffusing particles under the influence of a strong attraction between the particles such that phase separation takes place. The initial configuration is the same as in the noninteracting case described above. Particles then diffuse by hopping to empty nearest-neighbor sites. The jump rate W is determined by the interaction $J<0$, $W\sim e^{(J/k_BT)n_{NN}}$, where n_{NN} is the number of particles on nearest-neighbor sites of the diffuser before the jump. The temperature is chosen such that $J/k_BT=-2.0$ (the critical temperature

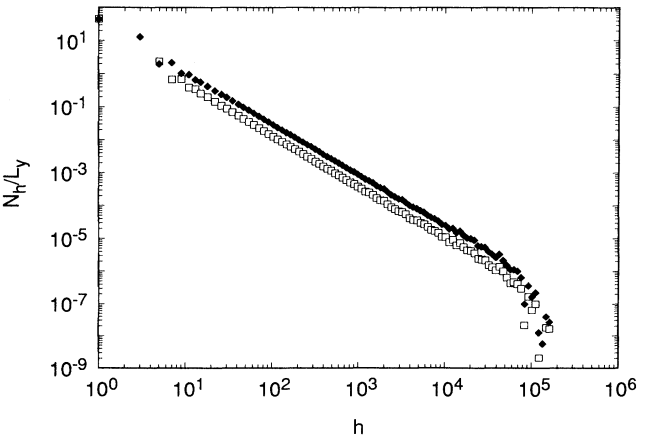

FIG. 4. Normalized total number of loops, $(1/L_y)N_h$, as a function of its length h on the original hull. The same symbols are used as in Fig. 2. The measured values for the exponent τ_h are $\tau_h=1.56$ ($r=r_0\sqrt{2}$) and $\tau_h=1.54$ ($r=2r_0$).

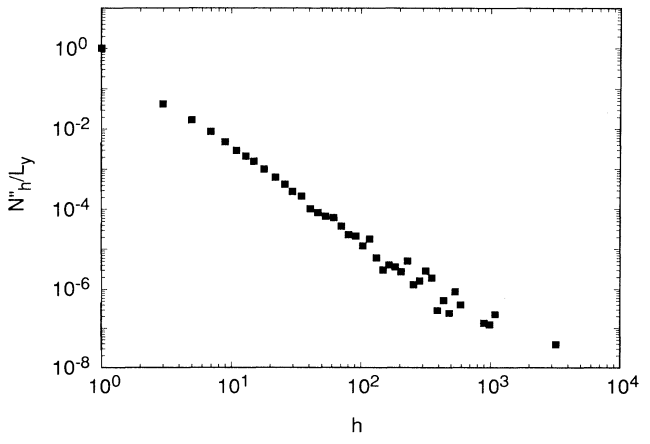

FIG. 5. Number of loops, $(1/L_y)N''_h$ of length h generated by bonds of length $r=2r_0$ placed on the hull already reduced by bonds of length $r=r_0\sqrt{2}$. The slope determines the exponent $\tau''_h=2.28$.

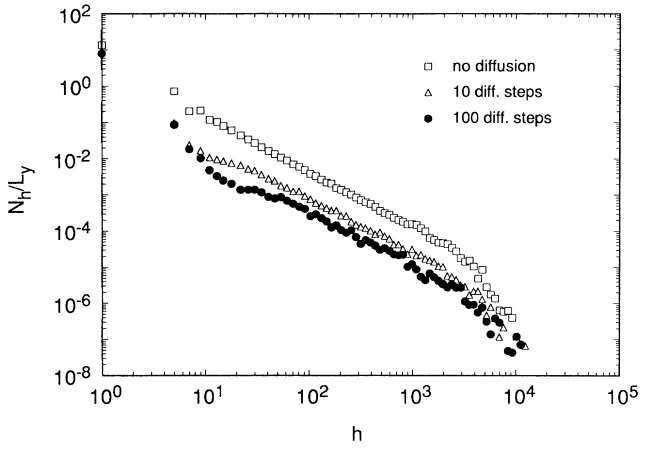

FIG. 6. Hull of diffusing particles during coarsening. The size distribution of total number of loops on the *original* hull (i.e., before diffusion) is shown for comparison. The different curves correspond to different times τ (Monte Carlo diffusion steps): $\tau=0$ (open squares), 10 (open triangles), 100 (filled dots). The asymptotic (large h) slope is unchanged but the total number of loops decreases with time. 100 samples were averaged on a $(512)^2$ lattice. The gradient for the original hull is $\nabla p=\frac{1}{2560}$.

T_c corresponds to $J/k_B T_c=-1.76$). Coarsening leads to droplets whose radius R evolves in time according to $R\sim t^{1/3}$ [16]. During this evolution, the percolation threshold decreases from the value $p_c=0.593$ for the square lattice to $p_c=0.5$ anticipated for large droplets by the particle-hole symmetry [14,15]. The percolation properties are extracted at different times during the coarsening process in exactly the same way as for the noninteracting system.

The analysis of the loop structure of the interacting system is presented in Figs. 6 and 7. Figure 6 shows the change of the loop size distribution for all loops during coarsening. The following changes occur: (i) for small fixed h the number of loops drops rapidly with time, (ii) the number of loops of the coarsened system is lower than for the noninteracting case, and (iii) for large h the slope of the coarsened system approaches the same value as for the noninteracting case. These properties can be explained in terms of the droplet picture. The lack of small loops is due to the surface tension induced by the interaction. This effect prevents the formation of loops of linear size up to $\sim R$. No change in the scaling law is expected for $h\gg 1$ if the droplets of size R are distributed randomly. The scaling of the hull structure can then be compared with the one found for continuum percolation [10]. R increases with time and the crossover towards the asymptotic (noninteracting or $T=\infty$) regime shifts to larger and larger values. The data of Fig. 6 is consistent with this picture.

Figure 7 shows the data of the interacting system for the loops on the reduced hull (due to the interaction the reduced hull changes). For small h, corresponding to loops of radius less than R, the curves are qualitatively similar to those of Fig. 6. For intermediate h a change of the slope from τ'_h to τ_h is observed. This is due to the fact that in this range the probability for two droplets of size R to be bonded is small and the hull behaves like the fluctuation problem. For larger h one expects a second crossover at R^* back to the reduced hull exponent, analogous to continuum percolation. With time R and R^* shift to larger values.

The expected changes in the reduced hull structure during coarsening can also be observed in the properties of the second hull placed on top of the first one. Figure 8 shows data for interacting particles when a hull with $r=2r_0$ is placed on a hull with $r=r_0\sqrt{2}$. Again, as the particles diffuse several different regimes appear. For small h the surface tension lets the number of loops drop very rapidly. For intermediate h (on scales larger than the droplet size R) the surface tension renders the bonds of length $r=r_0\sqrt{2}$ ineffective in closing loops. The

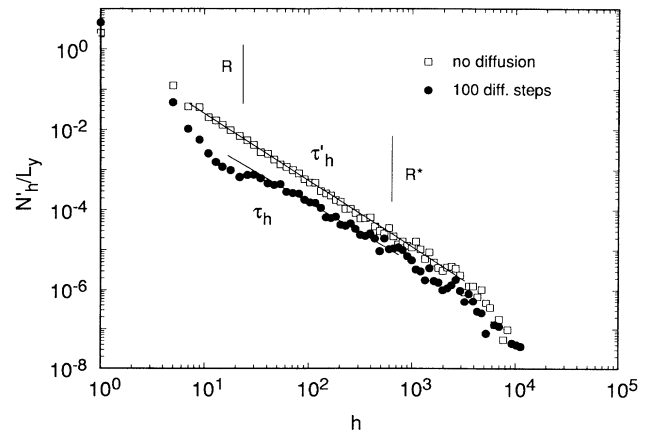

FIG. 7. Size distribution of the loops on the *reduced* hull during coarsening (same symbols as in Fig. 6). In the intermediate range indicated by the vertical bars the slope changes from τ_h to τ'_h. The position labeled R corresponds to the size of the droplets, whereas the position R^* corresponds to the distance beyond which the reduced hull properties are recovered.

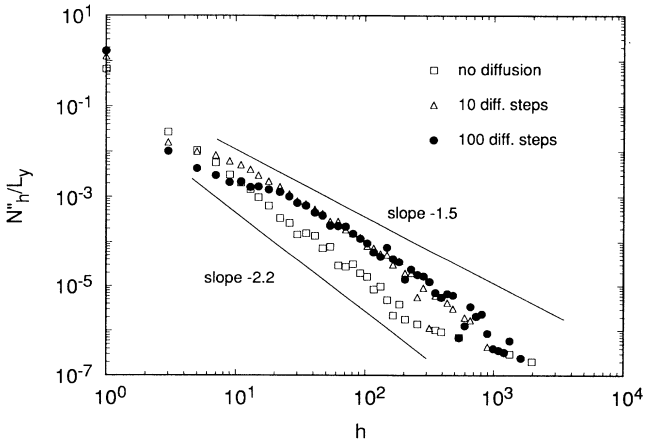

FIG. 8. Loop distribution generated by placing bonds of length $r=2r_0$ on top of a hull generated by bonds of length $r=r_0\sqrt{2}$, during phase separation (same symbols as in Fig. 6). See discussion in text.

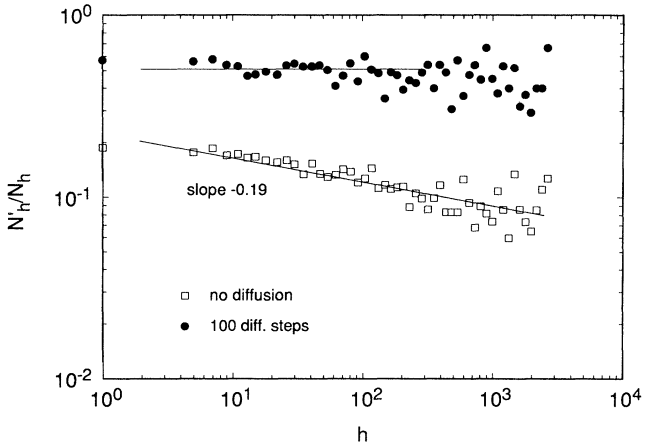

FIG. 9. Ratio N'_h/N_h of the number of loops on the reduced hull with $r=r_0\sqrt{2}$ over the number of loops on the original hull during coarsening, as a function of time. The noninteracting system (open squares) scales with an exponent $\tau_h-\tau'_h=-0.19$, the interaction (filled dots) "opens up" the loops for small h. This leads to an increase of the number of loops with time.

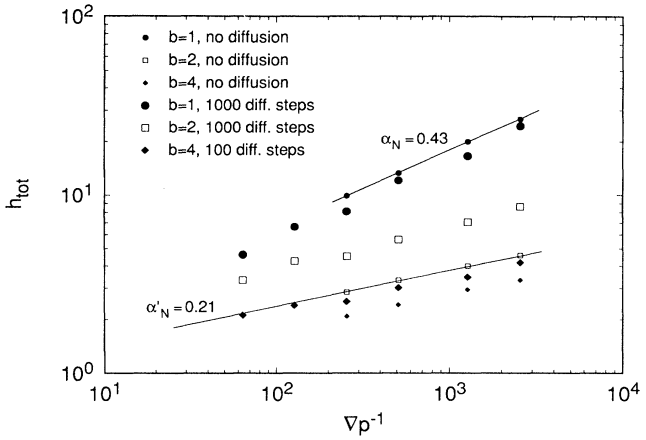

FIG. 11. Total length of the hull, generated by the block method, as a function of the inverse concentration gradient. Both for the nondiffusing and for the diffusing cases, the original hull ($b=1$, filled dots) is compared with block hulls for $b=2$ (open squares) and $b=4$ (♦). The interaction diminishes the total length of the original hull but increases it for the blocked hulls. The measured slopes for the original (reduced) hulls are $\alpha_N=0.43$ ($\alpha'_N=0.21$).

second hull effectively acts like the first hull with an exponent τ'_h. This is clearly visible: the number of $r=2r_0$ loops increases and the slope decreases. On a very large scale the $r=r_0\sqrt{2}$ loops become effective again and the original τ''_h ought to be recovered.

A particularly clear way to see the effect of the interaction is presented in Fig. 9. The ratio of the number of loops of length h on the reduced hull over the number of loops of length h on the original hull (both generated by bonds of length $r=r_0\sqrt{2}$) is plotted for different times. The noninteracting case (which, for small gradients, is equivalent to gradient percolation) follows a straight line with slope $\tau'_h-\tau_h=0.19$. Because of the interaction this ratio is expected to become constant for small h (due to the opening up of the hull as R increases) and introduces a crossover towards the noninteracting behavior for larger h. The same effect is also observed for the ratio of the number of loops generated by $r=2r_0$ on the external hull over those generated by $r=r_0\sqrt{2}$ loops on the total hull. In both cases the ratio increases with time as the closing of r becomes less and less effective. Correspondingly, the crossover size R^* shifts to larger values.

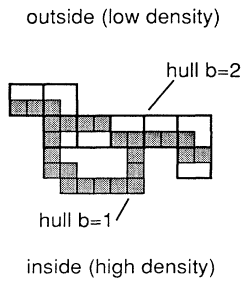

FIG. 10. Schematic representation of the renormalization procedure to generate reduced hull ($b=2$): a part of the original hull is shown as filled gray squares, the corresponding block hull after renormalization is shown as large open squares.

According to general renormalization considerations, scaling results usually do not depend on microscopic details. This means that the rule to construct reduced hulls by placing bonds between nearby sites of the percolation cluster can be modified without changing the essential results. In this spirit we therefore consider the following new method to construct a coarse-grained percolation hull (Fig. 10): a block site is associated with every square of side length b (b^2 sites). The site is occupied if at least one of the associated sites on the original lattice is occupied. The block cluster is necessarily connected on the block lattice. The sites which are accessible from the outside then play the role of the external hull. One expects that the block side length b corresponds to the bond length r. We have calculated the total length of the hull h_{tot} for the original hull ($b=1$) and for two blocked hulls, with $b=2$ and 4, respectively, and present it in Fig. 11. The slope of the hulls on the block lattices have slopes 0.206 ($b=2$) and 0.205 ($b=4$), in close agreement with the results from the bonding method. Furthermore, the interaction has a very different effect on the original hull and on the blocked hulls. The former decreases, essentially due to straightening of fractal segments on scales smaller than R, whereas the block hulls become longer due to the opening up of loops which were closed by the block building process.

In conclusion, the results obtained from simulations of percolation hulls in two dimensions show that reducing hulls either by bridging or by block building generates a power-law distribution of loops. The closing of very large parts of the front during the first reduction step leads to a drop in the fractal dimension but there is no further change as subsequent reduction steps only close small parts of the remaining hull.

Counting all the loops generated by bonding nearby particles can be compared with the fluctuations of an inhomogeneous distribution of diffusing particles. Letting them interact (attraction) permits separation of the droplet size R and the elementary percolation length r_0. The bonding length r (or b for the block building method) then can be chosen such that $r/R \ll 1$ and the problem becomes comparable to continuum percolation (provided that the droplets of size R are only weakly correlated—which is confirmed by the simulations). The fluctuations are visible from the outside up to a distance R^*, and increase with R^* during coarsening.

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