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LETTER TO THE EDITOR

The shell model: a growth model with a tunable fraction of forgotten growth sites

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Abstract. We introduce and discuss a new model in which the growth sites are driven with a power law, r^{α}, away from the original seed. The concept of 'forgotten' growth sites is developed. We find that the fraction of forgotten growth sites, the 'order parameter' for this problem, is zero for α below a critical value $\alpha_c = 1$, and increases sharply for $\alpha > \alpha_c$ with a critical exponent $\beta \simeq \frac{2}{3}$ in two dimensions.

Growth models have been studied intensely in the past year mainly because of the following puzzle: they seem to show scaling behaviour with critical exponents like *equilibrium* critical phenomena, but they are irreversible, *non-equilibrium* phenomena in which the history of each configuration makes it impossible to properly write down a partition function. We are therefore, at the present, confined to study the characteristics of growth models by analysing simple models and for instance to see if by tuning a parameter the behaviour can be changed.

A prominent example for a growth model has been diffusion-limited aggregation, DLA (Witten and Sander 1981). The sites of a cluster where growth takes place are chosen by a diffusion process. Although in this model any site of the surface (with the exception of tiny holes in the cluster) could potentially be chosen by the diffusion process, in practice the growth only takes place at the outer shells of the cluster and the interior growth sites seem completely 'forgotten' by the growth mechanism. The result is so dramatic that asymptotically nearly all sites in the interior remain unoccupied and the result is a fractal cluster.

In order to sharpen this concept of forgotten growth sites, we shall introduce a new model where they appear quite naturally and where the 'forgotten interior' can be quantitatively and precisely measured. Our model is called the shell model because it explicitly contains a growth shell driven by a power law from the original seed.

Let us consider a square lattice. Suppose we grow a percolation cluster as follows: at time $t = 1$, we occupy the site at the origin, which represents the seed of the cluster; the four nearest-neighbour sites are G ('growth') sites. Next choose one of the G sites randomly. With probability p occupy it and with probability $1 - p$ block it forever. If it is occupied, we have formed a two-site cluster with six G sites. If it is blocked, we choose one of the remaining three G sites and continue the process until a two-site cluster is formed or until all G sites are blocked. If all G sites are blocked, the cluster dies and we start a new run. If a two-site cluster is formed, we then choose one of its

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G sites, but not with the same probability to each. Rather, we choose the next G site according to the probability

$$P(r) = \frac{r^\alpha}{\Sigma r^\alpha} \tag{1}$$

where r is the Pythagorean distance of the G site from the *origin* and the sum runs over all G sites.

If $\alpha = 0$, the G site is chosen randomly and the model reduces to a method similar to that proposed by Alexandrowicz (1980) to construct percolation clusters (Family and Vicsek 1985, Bunde *et al* 1984). If $\alpha > 0$, then G sites at larger distance from the seed are preferred, while for $\alpha < 0$ G sites close to the seed are preferred. The chosen G site will be occupied or blocked with probabilities p or $1-p$ and the process is continued. For α positive, the cluster has a seed that repels new sites and drives the cluster outward, leaving many 'forgotten' G sites close to the centre (figure 1(*a*)). For $\alpha < 0$ the seed attracts new sites and G sites close to the centre are rare for large clusters (figure 1(*b*)). The case $\alpha > 0$ has the feature in common with diffusion-limited aggregation (DLA) that the mean distance from the origin of the sites at which growth ('aggregation') takes place *increases in time*; see, e.g., Plischke and Racz (1984), Meakin and Sander (1984), Meakin *et al* (1985). This model is also similar in some respects to the butterfly model of Bunde *et al* (1984) in which the G sites are imagined to be occupied one after another by a butterfly that randomly flies from one G site to another. In the model of Bunde *et al*, P is a function of the previous butterfly position, while in the present model P is a function *only* of the distance of the G sites from the origin of growth. For the case $\alpha = 0$, $P = 1/G$. One could imagine that both models are created by a *charged* butterfly that for the shell model is simply attracted to ($\alpha < 0$) or repelled from ($\alpha > 0$) the origin by a central electrical field. For the model of Bunde *et al*, each G site is itself also charged, and attracts or repels the butterfly with a force that depends on the distance to the G site.

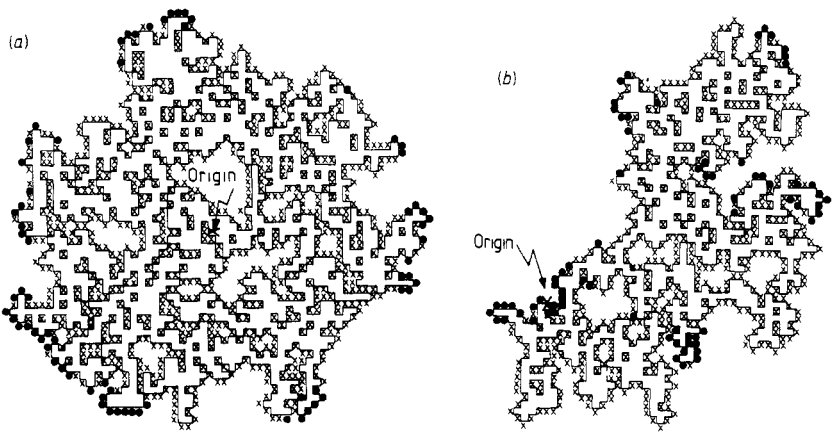

Figure 1. Characteristic clusters for (*a*) $P(r) \sim r^4$ (size 720) and (*b*) $P(r) \sim r^{-12}$ (size 1200). p is chosen to be the percolation threshold $p_c = 0.592\,77$. The occupied sites are white sites surrounded by the closed line which is the borderline of the cluster. Outside this borderline there are the blocked sites (crosses) and the growth sites (black dots). The origin is marked.

Static properties. Some of the geometrical properties of the large clusters are reflected in the fractal dimension d_f, which governs how the cluster mass s increases with its radius of gyration

$$s \sim r^{d_f}. \tag{2}$$

Let us first consider $p = 1$, i.e., no blocked sites. If $\alpha = 0$, our model reduces to the much-studied Eden model. If $\alpha = -\infty$, the shells around the seed are successively filled and the growth process resembles the Leath method for $p = 1$ (Leath 1976). If $\alpha > 0$ but is still *finite*, clusters are grown that take the form of a stick for small sizes and a 'club' for larger sizes. In all cases the dimension of the clusters is $d_f = d$. For $\alpha = \infty$, a one-dimensional chain is formed.

In general, for $\alpha < \infty$ the clusters stop growing if and only if all G sites are exhausted. These finite clusters that are not growing anymore are just clusters of random percolation at the probability p and $d_f = \frac{91}{48}$. Henceforth we will choose $p = p_c$.

Kinetic properties. In addition to the static properties of this growth process, we consider the kinetic properties. Information about the growth process is obtained from the G sites. The G sites themselves form a fractal† with a fractal dimension d_G given by

$$G \sim r^{d_G} \sim s^{d_G/d_f}. \tag{3}$$

For a range of α values between -12 and $+12$, we have calculated G (for $p = p_c$ and s up to 4000); we averaged over typically 10^5 configurations. We find $d_G/d_f = 0.40 \pm 0.02$, irrespective of α. Thus we find that the overall growth mechanics of what are ultimately percolation clusters does not depend sensitively on the 'central field' and is the same for both repulsive and attractive 'forces'. This finding is in sharp contrast to the butterfly in a *non-central* field (Bunde *et al* 1984, Family and Vicsek 1985), for which d_G/d_f has one value (0.40) for $\alpha \leqslant 1$ and a completely different value ($\simeq 0.6$) for $\alpha \geqslant 2$. In addition to the standard 'static' method of determining the fractal dimension by calculating the mass as a function of the radius, we have two kinetic ways to determine d_f for the growth process.

(i) At p_c the fraction N_{surv} of clusters containing at least s sites is not constant for large s (as it is for $p > p_c$) but decays to zero with a power law

$$N_{surv} \sim s^{-1+d/d_f}. \tag{4}$$

(ii) As noted above, the cluster growth arises from the trajectory of a butterfly that always moves from G site to G site, creating cluster sites each time it touches a G site subject only to the condition (1). The time t is increased by one unit whenever the butterfly visits a new G site; hence $s = tp$ and

$$\langle r^2 \rangle \sim t^{2/d_f}. \tag{5}$$

We have used both methods to calculate d_f for $-12 \leqslant \alpha \leqslant +12$ and have always obtained $d_f \simeq \frac{91}{48}$, the value for percolation, irrespective of α. In order to get a more microscopic insight into the growth process we have calculated the radial distribution function of the growth sites. Figure 2 shows, for several different cluster sizes s, the

† Note that the fractal formed by the G sites is a 'volatile fractal', a term proposed by Herrmann and Stanley (1984) for fractals whose identity changes with time. Two other familiar volatile fractals are cluster-cluster aggregation, where the cluster identity changes in time, and the blobs (of multiply connected bonds) in a cluster backbone, whose identity changes not with time but with system size (Herrmann and Stanley 1984). The scaling functions for volatile fractals have power law singularities.

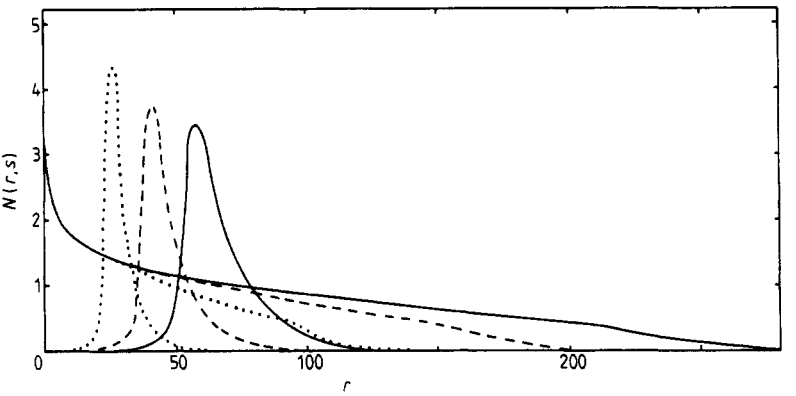

Figure 2. $N(r, s)$ for $P(r) \sim r^{-12}$ (peaked functions) and $P(r) \sim r^{12}$ (monotonic functions) for $s = 800$ (· · · ·), $s = 2000$ (- - -) and $s = 4000$ (——).

dependence on r of $N(r, s)$, the (averaged) number of G sites of an s cluster at distance r from the seed. Shown are results for strongly *attracting* ($\alpha = -12$) and strongly *repulsive* seeds ($\alpha = +12$). For $\alpha = -12$ the distribution function shows a narrow peak that broadens with increasing cluster size; within a certain core around the seed there exist practically no G sites. The radius of the core as well as the position of the peak increases with s. For $\alpha = +12$, $N(r, s)$ decays monotonically and becomes, at a given value of r, independent of s for large s†. For large s and $r \ll s^{1/d_f}$ the distribution function decays with the power law

$$N(r, s) \sim r^{d_G - 1} \tag{6}$$

where $d_G - 1 \simeq -\frac{1}{4}$ independent of s.

For all values of α considered here we have also calculated the mean $\bar{r}$ and the variance Δ of the positions of the G sites. We found that both also scale with the cluster radius. This finding is in agreement with the results from other percolation growth processes (Stanley *et al* 1984, Bunde *et al* 1984, Family and Vicsek 1985), is in contrast to the case of the Eden model where the width increases less quickly than the radius (Jullien and Botet 1984, Dhar 1984), and should be compared with the case of DLA where this question has not yet been satisfactorily settled (Plischke and Racz 1984, Meakin and Sander 1984). We also confirmed that $N(r, s)$ obeys scaling in the two active parameters r and s, according to

$$N(r, s) = s^{(d_G - 1)/d_f} f_\alpha(r s^{-1/d_f}). \tag{7}$$

Figure 3 shows two representative examples $\alpha = \pm 12$. The scaling functions describe the two different typical situations. If $\alpha = 12$ most of the G sites are 'forgotten' and do not actively participate in the growth process, while for $\alpha = -12$ practically all G sites are either active or become active in the course of the cluster growth. We have varied α gradually from -12 to $+12$ and calculated the *scaled* distribution function $f_\alpha(x)$. The result is shown in figure 4, in the upper three curves. The peak at $r = 0$, characteristic of the forgotten G sites, is present for $\alpha > 1$, and is absent for $\alpha \leqslant 1$.

† This part of the distribution function describes the 'forgotten' G sites that do not actively participate in the growth process.

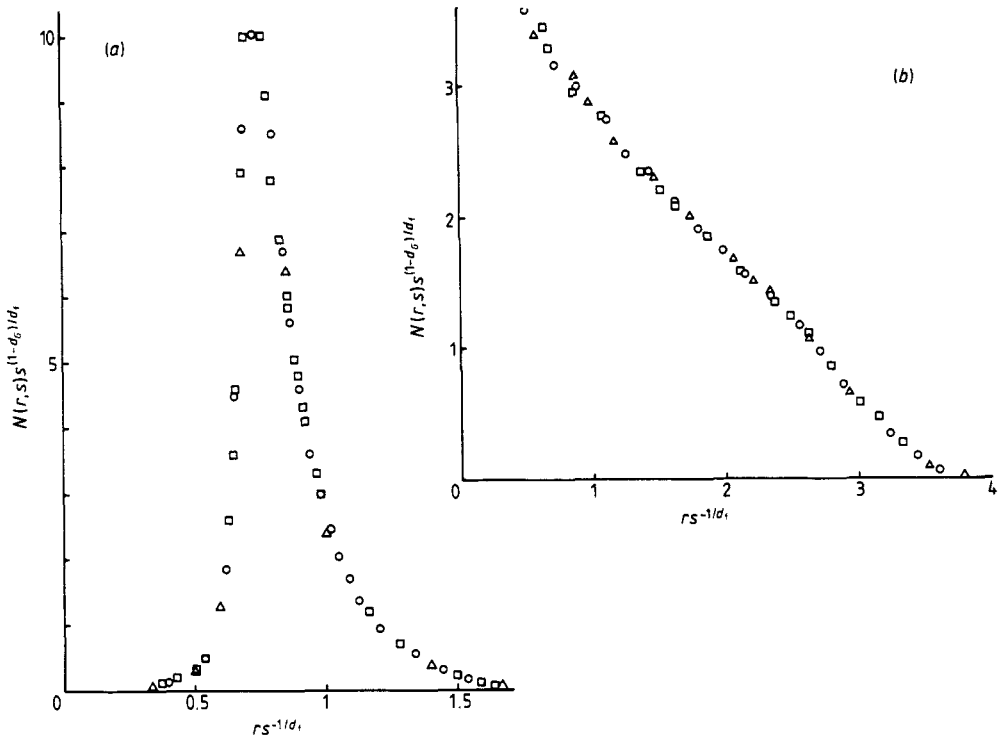

Figure 3. The number $N(r, s)$ of G sites of a primary s-site cluster at a distance r from the seed scaled such that all curves collapse on a single curve ($s = 800$: Δ; $s = 2000$: $\circ$; $s = 4000$: $\square$). (*a*) $P(r) \sim r^{-12}$, (*b*) $P(r) \sim r^{12}$.

We have seen in figure 2 that for $\alpha = 12$ a large fraction of the G sites remain close to the origin. These forgotten growth sites are essentially never visited again by the butterfly since $N(r, s)$ becomes independent of s for large s. As a consequence, the functional form of the scaling function f_α is not universal anymore as seen in figure 4 though d_G is universal. This behaviour is opposed to the behaviour usually found in critical phenomena (Betts *et al* 1971). To better describe the G sites, we introduce the *new* function

$$\mathcal{P}(r, s) = \frac{r^\alpha N(r, s)}{\Sigma r^\alpha N(r, s)}. \tag{8}$$

While $N(r, s)$ is the number of G sites *present* at distance r, $\mathcal{P}(r, s)$ is the probability that the butterfly actually *visits* such a G site (Plischke and Racz 1984), i.e., $\mathcal{P}(r, s)$ may be thought of as the radial distribution function for the 'active' G sites, and a suitable quantity for growth models with forgotten G sites. We find that $\mathcal{P}(r, s)$ also scales in s and r similar to $N(r, s)$

$$\mathcal{P}(r, s) = s^{-1/d_f} g_\alpha(rs^{-1/d_f}). \tag{9}$$

In the three lower curves of figure 4, g_α is shown for different values of α. We see that the form of the scaling function g_α does not change with α: it is universal. This is in contrast to the shape of the scaling function f_α of $N(r, s)$, which is shown also in figure 4 (upper curves). The physical difference between $N(r, s)$ and $\mathcal{P}(r, s)$ is just

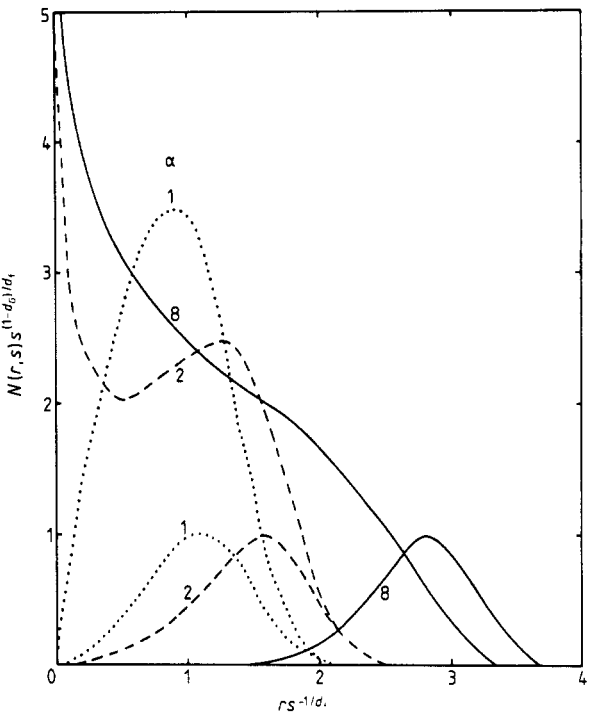

Figure 4. The scaling functions $f_\alpha(x)$ (upper curves) and $g_\alpha(x)$ (lower curves) of distributions of growth sites and active growth sites respectively, for $\alpha = 1$ (· · · ·), $\alpha = 2$ (- - -) and $\alpha = 8$ (——).

the forgotten G sites and the fact that for increasing $\alpha > 0$ we expect more and more forgotten G sites to apparently account for the development of the maximum of $N(r, s)$ at the origin (or its scaling function in figure 4). This maximum seems to disappear at $\alpha_c = 1$.

The value $\alpha_c = 1$, i.e., the critical α above which forgotten growth sites appear and below which forgotten growth sites are irrelevant can be obtained from the following argument. Our growth mechanism can be viewed as the growth of an Eden model (with the condition of equation (1)) not on a Euclidean lattice but on a percolation cluster at p_c. When will the forgotten G sites appear? Suppose we start with a cluster of radius R with a given homogeneous density ϕ of forgotten G sites; i.e., ϕ is the number of *forgotten* G sites divided by the number of *occupied* sites. Pick any G site near the origin, i.e., $r \simeq 1$, and ask for the probability that it will chosen by the butterfly at the next time step. By equation (1) this probability will be of the order of $R^{-d_f+1-\alpha}$. To see this, note that the sum over all G sites in (1), the ones that contribute most (for $\alpha > 0$) are those on the surface (fractal cut) of the cluster:

$$\frac{r^\alpha}{\Sigma r^\alpha} \sim \frac{1}{\Sigma_{\text{surf}} R^\alpha} \sim 1/R^{d_f-1+\alpha}. \tag{10}$$

Suppose that at each time step we create with a fixed probability ϕp new G sites that later will be forgotten. In order that the number of forgotten G sites decreases one must compensate via equation (10) for this creation of new forgotten G sites. The

butterfly creates new G sites by picking a chosen G site with a probability at least of the order of $1/R^{d_f}$, since the probability of picking a specific G site is proportional to the inverse of the volume R^{d_f}. Equating both probabilities gives the marginal value for α: $\alpha_c = 1$.

From the scaling function g_α of figure 4 we see another interesting fact. The functional form of the curves $g_\alpha(x)$ seems identical for all α, except for a shift in the position of maximum x_N if $\alpha > 1$. How do we understand this remarkable feature? Let us for a given s consider two active G sites, one in the small r tail and one in the large r tail of g_α. The difference in probability to visit these G sites can be calculated according to equation (1) and one finds that it does not depend on α. This explains why the width of the function g_α is the same for all α. It is very surprising to find that the maximum $x_N(\alpha)$ scales like a power law

$$x_N(\alpha) - x_N(\alpha_c) \sim (\alpha - \alpha_c)^{2/3}. \tag{11}$$

This has the physical implication that the fraction of sites ϕ of the cluster that are forgotten G sites scales within the accuracy of our data as

$$\phi \sim (\alpha - \alpha_c)^{2/3} \tag{12}$$

because the maximum x_N described in equation (11) is proportional to the radius of the cluster as seen in figure 4.

In conclusion, by driving the active growth sites away from the original seed with a power law r^α we find, at $\alpha_c = 1$, the onset to a different behaviour. We investigate intermediate stages for $\alpha > 1$; the clusters (percolation clusters at p_c) are not grown completely but a finite fraction ϕ of forgotten growth sites is 'left behind'. However the overall fractal dimension d_f—even the fractal dimension of growth sites d_G—remains unchanged. The fraction ϕ of forgotten growth sites increases with $\alpha - \alpha_c$ with a power law as if ϕ were the order parameter of a critical behaviour at $\alpha_c = 1$.

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References

Alexandrowicz Z 1980 *Phys. Lett.* **80A** 284
Betts D D, Guttmann A J and Joyce G S 1971 *J. Phys. C: Solid State Phys.* **4** 1994
Bunde A, Herrmann H J, Margolina A and Stanley H E 1984 *Preprint*
Dhar D 1984 *Preprint*
Family F and Vicsek T 1985 *J. Phys. A: Math. Gen.* **18** L75
Herrmann H J and Stanley H E 1984 *Phys. Rev. Lett.* **53** 1121
Jullien R and Botet R 1984 *Preprint*
Leath P L 1976 *Phys. Rev.* B **14** 5046
Meakin P and Sander L M 1984 *Preprint*
Meakin P, Sander L M and Po J K 1985 *Preprint*
Plischke M and Racz Z 1984 *Phys. Rev. Lett.* **53** 415
Stanley H E, Majid I, Margolina A and Bunde A 1984 *Phys. Rev. Lett.* **53** 1706
Vicsek T and Family F 1984 *Phys. Rev. Lett.* **52** 1669
Witten T A and Sander L M 1981 *Phys. Rev. Lett.* **47** 1400