LETTER TO THE EDITOR

Monte Carlo study of linear diffusion-limited aggregation

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Abstract. Linear diffusion-limited aggregation is studied on the square lattice. The radius of gyration exponent $\nu = 0.79 \pm 0.01$ is estimated using the Monte Carlo method and a scaling analysis.

Kinetically growing self-avoiding walks (SAW) have been extensively studied recently (see Lyklema (1985a) for a review). In these walks the jump probability depends on the local environment. Some of them have asymptotic properties differing from the usual SAW with $\nu = \frac{3}{4}$ in $d = 2$ and an upper critical dimension $d_c = 4$ above which the walk is Brownian.

In the true SAW (Amit *et al* 1983), which is not strictly self-avoiding, the jump probability depends on the number of times n_i the nearest-neighbour sites (NN) have already been visited:

$$p_i = \exp(-gn_i)\left(\sum_{NN} \exp(-gn_j)\right)^{-1}. \tag{1}$$

It has an upper critical dimension $d_c = 2$ and $\nu = \frac{2}{3}$ in one dimension (Pietronero 1983). The growing self-avoiding trail (Lyklema 1985b), for which bonds are not allowed to be visited more than once and the jump probability $p_i = 1/(\text{number of free bonds})$ allows for self-intersections, has an upper critical dimension $d_c = 3$ and $\nu = 0.535$ in $d = 2$. The indefinitely growing SAW (Kremer and Lyklema 1985) with a jump probability $p_i = 1/(\text{number of jump sites})$, where the jump sites are first-neighbour sites which do not lead into a cage, is truly self-avoiding and never terminates; then $\nu = 0.567$ in $d = 2$ and d_c is unknown. The IGSAW has been generalised (Lyklema and Evertsz 1985) in the Laplacian random walk (LRW). The jump probability is defined as

$$p_i = \phi_i^{\eta}\left(\sum_{NN} \phi_j^{\eta}\right)^{-1} \tag{2}$$

where η is a parameter and the potential ϕ_i is a solution of the discretised Laplace equation which satisfies the boundary conditions $\phi = 1$ on a circle of radius R_c, much larger than the walk radius R, and $\phi = 0$ on the sites already visited. Contrary to the case of the dielectric breakdown problem (Niemeyer *et al* 1984) from which it was inspired, to remain linear, growth only occurs near the last aggregated particle. The IGSAW is recovered when $\eta = 0$ and varies continuously with η as in a recent generalisation of the TSAW (Öttinger 1985).

In this letter we study on the square lattice a new type of kinetically growing SAW in which linear growth occurs via diffusion-limited aggregation (DLA). Although DLA

has been extensively studied since its introduction by Witten and Sander (Witten and Sander 1981, 1983, Meakin 1983), to our knowledge these studies only concern branched structures.

The chains are generated as usual in DLA. A seed particle is placed at the origin of the square lattice and a new particle is launched at random from a distance R_c, performing a random walk on the lattice. The particle is not allowed to visit an occupied site; when it hits the chain, the particle takes another direction in the next step. It aggregates as soon as it reaches a site which is a first neighbour of the active end of the chain. Then a new particle is released and the process is repeated. After the first step the site at the origin becomes inactive and the chain grows only from one end. This convention should not affect the asymptotic properties and it simplifies the calculations. The growth may continue indefinitely since there is always one path leading to the active end, the way followed by the last particle to aggregate.

We chose $R_c = 2R$, where R is the radius of a circle centred at the origin and just enclosing the chain. We have verified, by varying R_c in a preliminary study, that this value is large enough. When a particle goes away, it is eliminated and a new one is started at R_c. In order to avoid long and ineffective trapping along the mazes of the chain, the number of jumps is limited to $2L^2$ where L is the distance, in lattice units, from the starting point to the active end. After that number of steps is exhausted, the particle is eliminated and a new particle is added at R_c. At each step N, the following radii are stored:

$$R_e^2(N) = (\mathbf{r}_N - \mathbf{r}_0)^2 = r_N^2 \tag{3}$$

$$R_a^2(N) = (1/N) \sum_j r_j^2 \tag{4}$$

$$R_g^2(N) = (1/2N^2) \sum_i \sum_j (\mathbf{r}_i - \mathbf{r}_j)^2. \tag{5}$$

R_e is the end-to-end radius, R_a an averaged end-to-end radius and R_g the radius of gyration of the chain. The calculations have been done in assembly language on 8088 and 8087 microprocessors. Limitations on computer time led us to grow chains of up to 45 particles, taking averages over 10^4 samples for each size. A rapid shift-register random number generator was used (Kirkpatrick and Stoll 1981).

The critical exponent ν may be obtained through a scaling analysis of the data (Botet *et al* 1984)

$$\nu_{N,M} = \tfrac{1}{2}\ln[\langle R^2(N) \rangle / \langle R^2(M) \rangle] / \ln(N/M). \tag{6}$$

When exact averages are used, a better convergence is observed when $M = N - 1$ (Derrida and de Seze 1982). This is no longer true with Monte Carlo data due to statistical fluctuations. In this case better results are obtained when $N - M$ is larger. Here we have used the following definition (Lyklema 1985b):

$$\nu(N) = \tfrac{1}{2}\ln[\langle R^2(N+i) \rangle / \langle R^2(N-i) \rangle] \{\ln[(N+i)/(N-i)]\}^{-1} \tag{7}$$

where i has to be chosen large enough to obtain a smooth variation (figure 1). Assuming the usual asymptotic behaviour for the mean square radius (Privman 1984)

$$\langle R^2(N) \rangle = AN^{2\nu}(1 + BN^{-\Delta} + CN^{-1} + \ldots) \tag{8}$$

equation (7) gives

$$\nu(N) = \nu - \tfrac{1}{2}\Delta BN^{-\Delta} - \tfrac{1}{2}CN^{-1} + \ldots. \tag{9}$$
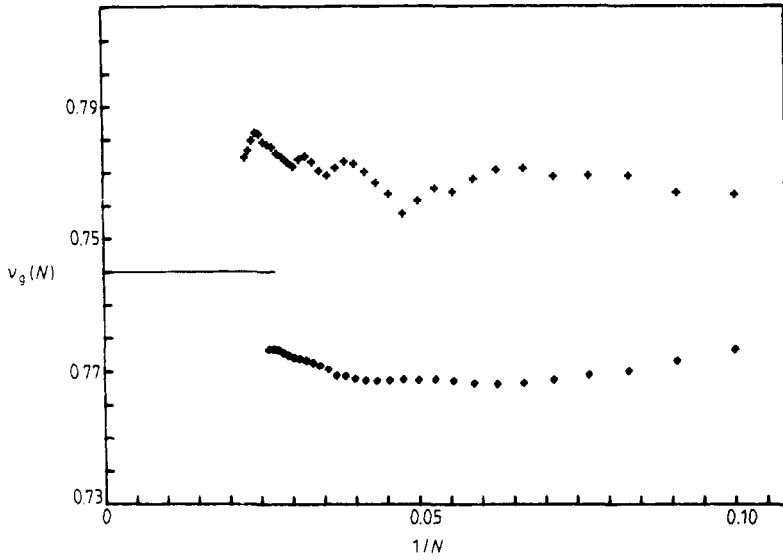
Figure 1. Critical exponent $\nu_g(N)$ of the mean square radius of gyration $\langle R_g^2(N) \rangle$ on the square lattice against $1/N$, obtained using equation (7) with $i = 1$ ($+$) for $4 \leqslant N \leqslant 44$ and $i = 7$ ($\blacklozenge$) for $10 \leqslant N \leqslant 38$.

Keeping only the leading correction term in equation (9), the exponent ν is obtained through a least squares fit of $\nu(N)$ against N^{-y} ($N > 25$). The fit is not very sensitive to the choice of y so we assumed an analytic correction, $y = 1$ (figure 2). The extrapolated values (table 1) are $\nu_{e,a} \simeq 0.784$, $\nu_g = 0.795$ with $i = 7$. One may notice that although $\nu_e(N)$ and $\nu_a(N)$ decrease, $\nu_g(N)$ increases with N for large N values;
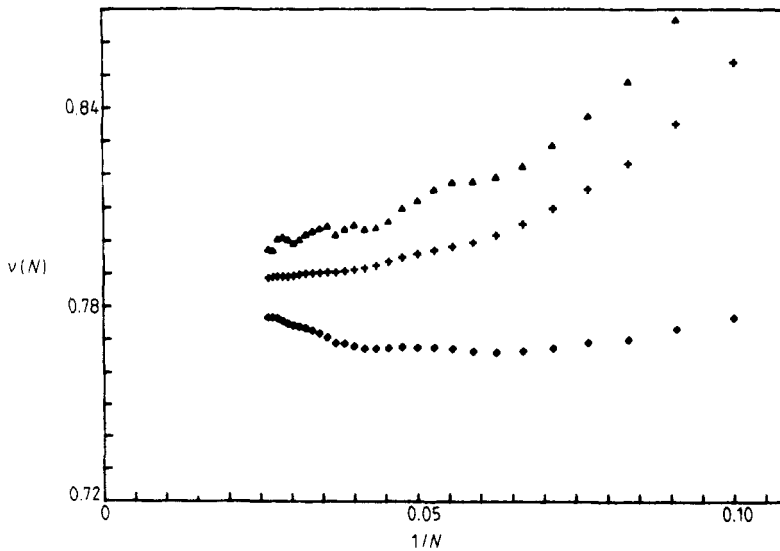

Figure 2. Critical exponents $\nu_e(N)$ ($\blacktriangle$), $\nu_a(N)$($+$) and $\nu_g(N)$ ($\blacklozenge$) of the mean square radius $\langle R_\alpha^2(N) \rangle$ ($\alpha =$ e, a, g) on the square lattice, against $1/N$, obtained using equation (7) with $i = 7$.

Table 1. Extrapolated values of the mean square radius exponent ν_α ($\alpha = $ e, end-to-end radius; a, averaged end-to-end radius; g, radius of gyration). The first column gives the first value of N in the fit to a N^{-1} variation.

N	ν_e	ν_a	ν_g
25	0.786	0.784	0.795
26	0.786	0.784	0.796
27	0.784	0.784	0.796
28	0.780	0.784	0.794
29	0.780	0.784	0.794
30	0.781	0.784	0.793
31	0.782	0.784	0.794
32	0.784	0.785	0.795

this seems to exclude the possibility of the linear DLA belonging to the SAW universality. From the extrapolated values, one may estimate that $\nu = 0.79 \pm 0.01$. A least squares fit of $N^{-2\nu}\langle R^2(N)\rangle$ against N^{-y} gives the amplitude A (equation (8)) which is also not very sensitive to the value of y. The following estimates may be given: $A_e = 0.73 \pm 0.01$, $A_a = 0.280 \pm 0.005$, $A_g = 0.155 \pm 0.005$ with the central value corresponding to $y = 1$.

The fractal dimension $D = \nu^{-1} = 1.27$ is lower than in the IGSAW, a result which is not unexpected since the chain is 'attracted' outwards by the diffusion field. Our result agrees with the LRW with $\eta = 1$ (Lyklema and Evertsz 1985) for which $\nu = 0.8$. The two problems are equivalent except for the boundary conditions. In the linear DLA the particle is reflected by the chain whereas in the LRW it is absorbed. This difference in the boundary conditions is probably irrelevant.

One may expect that the upper critical dimension will be reached when the chain is transparent to the random walk and transparent to itself (Witten and Sander 1983). According to the rule of fractal codimension additivity (Mandelbrot 1982), the first condition requires $d > D$ (walk) $+ D$, where D is the chain fractal dimension and D (walk) $= 2$ for a random walk and the second requires $d > 2D$. Since the diffusion field is then essentially uniform near the active end and self-intersections are negligible, the chain will perform a random walk with $D = 2$. Both conditions are satisfied at $d_c = 4$.

To end, let us mention that the $d = 2$ linear DLA may find a physical realisation in the diffusion-limited growth of a polymer chain adsorbed on a surface, provided the adsorption is strong enough to prevent the relaxation.

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