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A re-examination of diffusion-limited aggregation with a finite lifetime

Jean-Marc Debierre† and R Mark Bradley
Department of Physics, Colorado State University, Fort Collins, CO 80523, USA

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Abstract. We study generalized diffusion-limited aggregation with a lifetime τ, a model introduced by Miyazima *et al*. Our Monte Carlo simulations for $\tau = 1$ and for $\tau = 2$ indicate that the asymptotic behaviour is most likely to be identical for all finite values of τ. Our estimate for the exponent ν characterizing the asymptotic regime is in strong disagreement with that found by Miyazima *et al*.

1. Introduction

At high temperatures, diluted polymers at equilibrium are well described by two basic models: self-avoiding walks (SAWs) in the case of topologically linear polymers and lattice animals for branched polymers. In two dimensions, the fractal dimension d_f of a SAW is exactly 4/3 [1], while the best estimate known for lattice animals is $d_f \simeq 1.56$ [2]. Thus, branching appears to be a relevant parameter for these equilibrium models.

The situation is somewhat similar in the case of the irreversible growth of clusters. Whereas diffusion-limited aggregation (DLA) produces ramified clusters with $d_f \simeq 1.71$ [3, 4], the diffusion-limited self-avoiding walk (DLSAW) has a much lower fractal dimension, $d_f \simeq 1.3$ [5–7]. The DLSAW differs from DLA in that, each time a new particle is added to the cluster, it becomes the only active tip. The next particle must adhere in turn to this tip and then becomes active itself. This restrictive rule automatically prevents branching from occuring. This model was initially introduced to describe rapid linear polymerization in a diluted solution of monomers. The first two studies of the DLSAW led to the estimates $d_f = 1.27 \pm 0.02$ [5] and $d_f = 1.29 \pm 0.01$ [6]. These results were obtained by performing a finite-size analysis of the data for 10^4 chains of 45 and 32 particles, respectively. A subsequent study of 800 chains of 1000 particles gave the more precise result $d_f = 1.305 \pm 0.002$ [7], which is in fair agreement with the earlier estimates.

More recently, Miyazima *et al* [8] have modified DLA by assigning a finite lifetime τ to the particles in the cluster. Each time a new particle is added to the cluster, it remains active while the next τ particles are added, and then it becomes inactive. This generalized version of DLA (GDLA) must be equivalent to DLA when $\tau \to \infty$ and to the DLSAW when $\tau = 1$. When τ is greater than 1 but is finite, a crossover from DLA to the DLSAW is expected as the clusters grow larger than a crossover size

† Permanent address: Laboratoire de Physique du Solide, Université de Nancy I, BP 239, F-54506 Vandoeuvre-lès-Nancy, France.

$N^* \sim \tau^\phi$. Performing numerical simulations for $\tau = 5$, 10, 20, 50 and 100, Miyazima *et al* [8] indeed observed a crossover from DLA to a regime with a smaller fractal dimension, $d_f = 1.04 \pm 0.03$. In a related study by Bunde and Miyazima [9], the particles were assigned a finite lifetime τ with probability p and an infinite lifetime with probability $1 - p$. The same estimate, $d_f = 1.04 \pm 0.03$, was found in the whole range $p > 0.5$ [9].

The value of d_f obtained by Miyazima *et al* for $\tau > 1$ is considerably smaller than all the estimates of d_f for $\tau = 1$ listed above. On the other hand, it seems very unlikely that the three independent estimates for the fractal dimension of the DLSAW are all grossly overestimated. There are two possible resolutions to this impasse. One is that the estimate of Miyazima *et al* is too low. Another possibility is that the asymptotic behaviour for $\tau > 1$ differs from that for $\tau = 1$.

In this paper, we investigate this question further by performing intensive Monte Carlo simulations of GDLA for $\tau = 1$ and $\tau = 2$. We obtain strong numerical evidence that the fractal dimension d_f is the same in both cases, and our estimate of d_f is in good agreement with the results obtained earlier for the DLSAW. Thus, our work strongly suggest that the estimate $d_f = 1.04 \pm 0.03$ proposed by Miyazima *et al* [8, 9] for GDLA is in error.

2. Results and discussion

We performed Monte Carlo simulations on the square lattice using a DLA algorithm modified to incorporate the finite lifetime of the particles in the cluster. This algorithm is described in detail in [8] and will only be outlined here. The seed particle is placed at the origin of the lattice and it is assigned a lifetime τ. Each time a new particle is added to the cluster, it is assigned a lifetime τ and all the other active particles have their lifetime reduced by one (a particle with lifetime zero becomes inactive). The release and killing radii for the diffusing particle are set to $d = R_{max} + 5$ and $D = 10d$ respectively, where R_{max} is the largest distance from the seed to any particle in the cluster. The diffusion step is fixed to one lattice unit inside the release circle. When the diffusing particle moves outside the release circle, its distance from the origin, δ, is computed. The step size is set to 1 whenever $\delta - d \leqslant 2$ and to $\delta - d$ otherwiswe. Finally, reflecting boundary conditions are imposed on the cluster [5, 6], so that any step in which the diffusing particle would land on a cluster particle is forbidden. Except for minor details (such as the values of d and D we have employed), our algorithm is identical to that described in [8].

We have grown 2000 independent clusters, each containing 500 particles, for both $\tau = 1$ and for $\tau = 2$. We looked at $\tau = 2$ because this is the smallest τ value greater than 1, and hence this is the τ value where the asymptotic behaviour of GDLA will set in first, since the crossover from DLA to the DLSAW occurs for N comparable to $N^* \sim \tau^\phi$ with $\phi > 1$ [8]. The mean radius of gyration $R_\tau(N)$ was computed as a function of the number N of particles in the cluster. Figure 1 is a log–log plot of R_1/N^ν as a function of N for two different choices of the exponent $\nu = d_f^{-1}$. Since we expect R_1 to vary as N^ν [5–7], the curve will be flat when the correct value of ν is chosen. From this figure, one can immediately rule out the estimate $\nu = 0.962 = (1.04)^{-1}$ proposed by Miyazima *et al* [8, 9] for the DLSAW. On the other hand, the best fit to a horizontal line for $N \geqslant 20$ is obtained for $\nu = 0.760$. This estimate is close to, but slightly lower than, the value $\nu = 0.766 \pm 0.001$ obtained

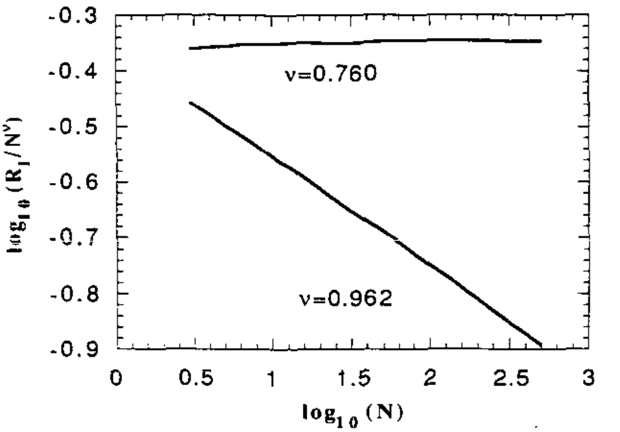

Figure 1. $\log_{10}(R_1/N^\nu)$ as a function of $\log_{10} N$ for $\nu = 0.962$ and $\nu = 0.760$.

by Meakin [7]. This kind of direct analysis does not give satisfactory results when applied to the data for $\tau = 2$, because the crossover between the DLA and DLSAW regimes persists until N values close to 500 are reached. A finite-size analysis is thus necessary to extract the real asymptotic behaviour from our data for $\tau = 2$.

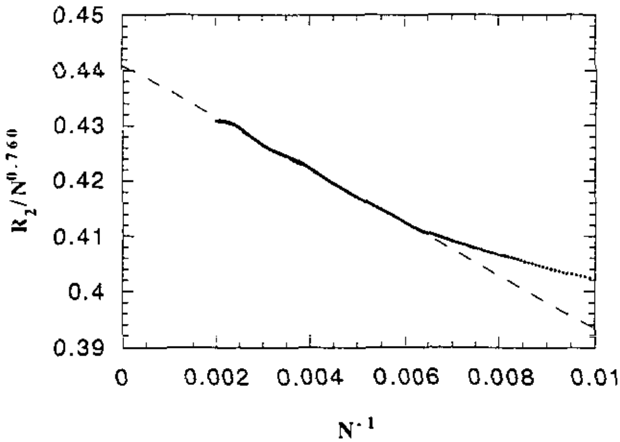

Figure 2. The ratio $R_2/N^{0.760}$ as a function of N^{-1}. The broken line is a linear least-squares fit to the data points for $N^{-1} \leqslant 0.006$.

In figure 2, the ratio $R_2/N^{0.760}$ is plotted as a function of N^{-1} for $N \geqslant 100$. For sufficiently large N, the curve becomes straight, indicating that the leading correction-to-scaling term varies as N^{-1}. As a consequence, the intercept is non-zero and we have the asymptotic behaviour $R_2 \sim N^{0.760}$ for $\tau = 2$, just as for $\tau = 1$. An alternative way to determine the asymptotic behaviour is to compute a finite-size estimator for the exponent ν. For this purpose, we first plotted $\log R_\tau$ as a function of $\log N$ and then performed linear fits to all the data points except those with $N < N_0$. The resulting slope gives the finite-size estimator $\nu_\tau(N_0)$. This estimator is plotted in figure 3 as a function of N_0, for both $\tau = 1$ and $\tau = 2$. For $\tau = 1$, the

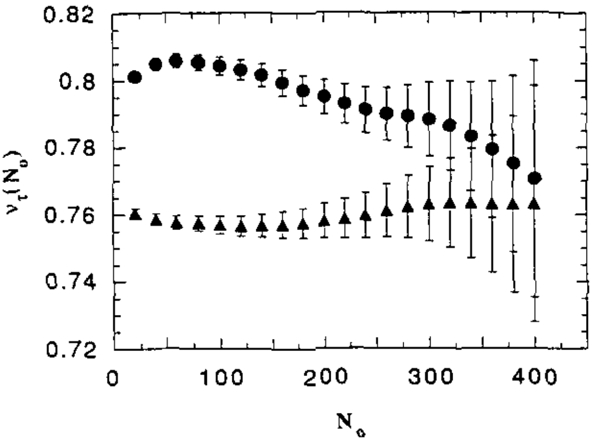

Figure 3. The finite-size estimator $\nu_\tau(N_0)$ as a function of N_0. The error bars are included for both ν_1 (▲) and ν_2 (●). Only the points with a relative error smaller than five per cent are displayed.

fluctuations about the mean value $\nu = 0.760$ were taken into account to determine an error bar for ν, and our final estimate is $\nu = 0.760 \pm 0.003$. On the other hand, the curve for $\tau = 2$ is monotonically decreasing and, for $N_0 > 300$, the error bars for $\nu_1(N_0)$ and $\nu_2(N_0)$ overlap. We thus conclude that $\nu_2(N_0) \to \nu_1(N_0)$ as $N_0 \to \infty$, which confirms our previous conclusion that the asymptotic behaviour is identical for $\tau = 1$ and $\tau = 2$.

(*a*) (*b*)

Figure 4. Two typical large clusters generated with our algorithm. (*a*) 2500 particles for $\tau = 1$ and (*b*) 4000 particles for $\tau = 2$.

One can be further convinced that this result is correct by looking at figure 4, where two large clusters grown with $\tau = 1$ and $\tau = 2$ are shown. This plot also makes it hard to believe that a fractal dimension as low as $d_f = 1.04$ can be obtained for either $\tau = 1$ or $\tau = 2$. Finally, it is worth noting that the corresponding cluster for $\tau = 2$ obtained by Miyazima *et al* appears to be much more linear than ours (see [8, figure 1(*g*)]). This suggests that a subtle bias toward radial growth was accidentally introduced into the algorithm used by Miyazima *et al*. Since the DLSAW is known to be very sensitive to any change in the boundary conditions [7, 10], any such bias is likely to dramatically affect the value of d_f.

To conclude this section, let us mention that qualitatively similar, although much less precise, results were obtained by using the mean end-to-end radius instead of the radius of gyration.

3. Summary

We have performed Monte Carlo simulations for DLA with a finite lifetime τ. Our data strongly suggest that the asymptotic behaviour is identical for $\tau = 1$ (DLSAW) and $\tau = 2$ (GDLA), lending support to the idea that it is identical for any finite value of $\tau \geqslant 1$. Our final estimate for the exponent $\nu = d_f^{-1}$ ($\nu = 0.760 \pm 0.003$) is in good agreement with those found in earlier studies of DLSAW. The present study also rules out the result $\nu = 0.926 \pm 0.03$ obtained by Miyazima *et al* for GDLA with $\tau > 1$.

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