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Cell renormalisation of growth processes: 'True' self-avoiding walks and growing animals

Hisao Nakanishi† and Fereydoon Family‡

† Institute for Theoretical Physics, University of California at Santa Barbara, Santa Barbara, CA 93106, USA
‡ Department of Physics, Emory University, Atlanta, GA 30322, USA

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Abstract. We present a generating function formalism for growth processes in general, and introduce a new cell renormalisation scheme. As examples, we treat the 'true' self-avoiding walk and the Eden process (or growing animals) in two and three dimensions using small cells. The results in both cases indicate a substantial increase in the fractal dimension D compared with their equilibrium counterparts. The case of the Eden process may, however, suggest a peculiar convergence behaviour as the cell size b tends to infinity.

1. Introduction

Various models of kinetic aggregation have been studied intensely in recent years due to their presumed relevance to a variety of physical and biological phenomena such as the formation of branched polymers and gels (for recent computer simulations, see Herrmann *et al* (1982), Rushton *et al* (1983) and references therein), coagulation of smoke particles (Witten and Sander 1981, 1983, Meakin 1983a, b, and references therein), and the growth of tumours (Eden 1961, Peters *et al* 1979). These studies have found intrinsic differences in the nature of kinetic aggregates compared with their supposed equilibrium counterparts (when they exist). While these aggregates appear to have *scale invariance* as the size N tends to infinity similarly to the equilibrium clusters at criticality, their structures seem to be quantitatively different.

One important structural characteristic is given by the dependence of the root-meansquare radius of gyration $\xi = \langle R_N^2 \rangle^{1/2}$ on the size N. For aggregates with scale invariance, ξ grows as $\xi \sim N^{\nu}$ where ν is the analogue of the Flory exponent for the correlation length in an equilibrium problem, and $D = 1/\nu$ is the 'fractal' dimension (Mandelbrot 1982) of the aggregate. To illustrate the kind of quantitative differences, let us consider the case of the Eden process versus its equilibrium counterpart, random animals. In the Eden model, one starts from a seed site on a lattice and successively occupies a randomly chosen perimeter site, one at a time. In contrast, random animals are, simply, randomly shaped, connected clusters of sites or bonds on a lattice. The fractal dimension D of the Eden process is expected to be equal to the lattice dimensionality d, i.e. the clusters are compact (Peters et al 1979). For random animals, $D \approx 1.54$ in d = 2 (cf Family 1983) and D = 2 in d = 3 (Parisi and Sourlas 1980).

While the examples discussed above produce branched objects in general, there are other classes of growth processes that are in some sense intrinsically onedimensional; these are called *walks*. The best known example is of course the random

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walk, which, considered as a 'cluster', has D = 2 in all dimensions. The random walk is *Markovian* as a growth process and *local* if viewed as an equilibrium object; thus for this special walk, there is no difference between static and growth models.

However, it is now known (Amit *et al* 1983) that major differences exist for a physically important class of walks called self-avoiding walks. The static self-avoiding 'walk' (sAw) considers random chain *configurations* without self-intersections, while the kinetic or 'true' self-avoiding walk (TSAW) is a growing walk with each step taken randomly but attempting to avoid self-intersections as much as possible. TSAW is thus a process which grows without ever dying out; as a result, self-intersections are possible though not common. SAW has the fractal dimension $D \cong_{3}^{4}$, $\frac{5}{3}$ (or $\nu \cong_{4}^{3}$, $\frac{5}{3}$) in d = 2,3 respectively (see e.g. de Gennes 1979), with the upper marginal dimension of $d_c = 4$; however, Amit *et al* (1983) showed that $d_c = 2$ for TSAW and thus it behaves much like the random walk, with D = 2, for all d > 2! For both models, there are logarithmic corrections at $d = d_c$.

Although there have been real-space renomalisation schemes that effectively deal with *static* versions of both branched aggregates and 'walk' configurations (Stanley *et al* 1982 and references therein), there has been little systematic method for *growth* processes (Gould *et al* 1983). However, their method can be improved in a number of respects. Below, we shall illustrate our renormalisation method by its application to TSAW and the Eden model. This is both because these models allow simple one-parameter approaches and because we can check the reliability of the general method by comparing the results with those of analytic (TSAW) or Monte Carlo (Eden) methods.

2. Generating functions

To illustrate our approach, it is convenient first to review the conventional way to study lattice animals and (static) 'walk' configurations. Generating functions are introduced there as a means to convert the 'canonical' problem into one of grand canonical ensemble with fugacity K: let C_N be the number of animals of N sites containing the origin (or of 'walks' of N steps starting at the origin). Then the (static) generating function is given by

$$S(K) = \sum_{N} C_{N} K^{N}.$$
 (1)

Since the asymptotic behaviour of C_N for these problems is typically

$$C_N \sim \mu^N N^{-\theta}, \qquad N \to \infty,$$
 (2)

where μ , θ are constants appropriate for the problem, we may conclude for the singular behaviour

$$[S(K)]_{s} \sim (K_{c} - K)^{\theta - 1}$$
(3)

with $K_c \equiv 1/\mu$. The numerical values of θ are, e.g., $\frac{3}{2}$ for random animals in d = 3 (Parisi and Sourlas 1981) and about -0.16 for the sAW in d = 3 (Le Guillou and Zinn-Justin 1980). We can then write for the 'average' size of the objects

$$\langle N \rangle = \left(\sum_{N} N C_{N} K^{N} \right)_{s} / \left(\sum_{N} C_{N} K^{N} \right)_{s} \sim (K_{c} - K)^{-1}$$
(4)

irrespective of θ . Similarly, more detailed information (than C_N 's) leads to the root-mean-square radius of gyration ξ ,

$$\boldsymbol{\xi} \sim (\boldsymbol{K}_{\mathrm{c}} - \boldsymbol{K})^{-\nu},\tag{5}$$

and from (4) and (5), we write

 $\xi \sim \langle N \rangle^{\nu}$ or $\langle N \rangle \sim \xi^{D}$ (6)

with $D = 1/\nu$ as mentioned before.

Let us now take, as the simplest example of 'walk' configurations, the random walk. Then, in (2), we have $\mu = z$ (the coordination number of the lattice) and $\theta = 0$. Thus for this case S(K) = zK/(1-zK), and if we relabel $zK \rightarrow K$, $S(K) = K/(1-K) = \sum_{N} K^{N}$ simply. Since we can also consider the random walk to be a growth process, this generating function should also be appropriate for a growth process. In this case, the interpretation of K should be that it is the *total* weight placed on taking a step (any step). Thus, the probability of taking a step in a given direction is 1/z, and the weight associated with such a step is K/z; since there are z possible directions, the weight of one step will total K.

Indeed, in general for a process with objects growing with varying probabilities for particular steps, there is no other sensible way to assign a fugacity than to assign K to the *total* event of taking one step at all. Since in perpetual growth processes there are just as many *n*-step processes as one-step ones, the value K = 1 arises naturally as a 'critical' point. Therefore, we propose to take the ('growth') generating function for *all* growth processes to be

$$G(K) = \sum_{N} K^{N} = K/(1-K).$$
 (7)

Simple though equation (7) may be, it does not by itself allow the calculation of D; we still need to calculate the radius of gyration ξ (cf equation (5)) consistent with the statistical weight as given in (7). This is illustrated for TSAW and the Eden model below.

3. Renormalisation of TSAW

In order to calculate D, we resort to simple cell renormalisation which approximately conserves the generating function under rescaling by a linear factor b. First we present the case of TSAWS with small b. Following de Queiroz and Chaves (1980) and Family (1980), we take a b^d cell, and use a *corner rule* to calculate recursion relations; i.e. TSAWS starting from the origin at the corner (cf figure 1) and traversing the cell in a given direction contribute to the renormalised fugacity K'.

Thus, for example, on a 2×2 cell, the walks that contribute to K' are exactly the same as those for static sAWS (de Queiroz and Chaves 1980 and Family 1980); however, their weights are entirely different (cf figure 1):

$$\frac{1}{2}K' = \frac{1}{4}K^2 + \frac{1}{6}K^3 + \frac{1}{12}K^4.$$
(8)

These weights arise from calculating the relative probability of the spanning processes over all processes of a given number of steps. Hence we obtain $K^* = 1$ and the eigenvalue $\lambda = \frac{8}{3}$ computed in the usual manner as the derivative $dK'/dK|_{K^*}$, which yields $\nu \approx 0.707$ and $D \approx 1.415$ in comparison with the similar 2×2 result of $\bar{\nu} \approx 0.715$



Figure 1. Shown in (a)-(d) are the spanning *configurations* of TSAWs in a 2×2 cell which renormalise to the one in (e). The relative probabilities of these walks among all TSAWs of the same length (in the quadrant containing the cell) are $\frac{1}{4}$ for (a) and $\frac{1}{12}$ for each of (b), (c) and (d).

and $\overline{D} \approx 1.40$ for static sAWS. Even though this estimate of ν is not very close to $\frac{1}{2}$ expected from analytic work (Amit *et al* 1983, Obukhov and Peliti 1983), this could be a reflection of the expected logarithmic correction at d = 2. Our 3×3 recursion relation indicates a slight increase of D in contrast to the slightly decreasing trend for \overline{D} in the case of sAWS. Using the rule that self-intersection is allowed only when a walk is surrounded by its own previous steps within the cell (this occurs twice for 3×3), the recursion relation for 3×3 is

$$\frac{1}{2}K' = \frac{1}{8}K^3 + \frac{7}{72}K^4 + \frac{4}{27}K^5 + \frac{1}{24}K^6 + \frac{19}{432}K^7 + \frac{5}{576}K^8 + \frac{23}{1728}K^9 + \frac{1}{648}K^{10}.$$
(9)

This leads to $K^* \cong 1.01$ (away from 1), $\lambda \cong 4.75$, and $\nu \cong 0.705$, D = 1.419.

For the d = 3 case, our recursion relation for $2 \times 2 \times 2$ cell reads

$$\frac{1}{3}K' = \frac{1}{9}K^2 + \frac{1}{9}K^3 + \frac{11}{180}K^4 + \frac{29}{1080}K^5 + \frac{127}{8640}K^6 + \frac{79}{12960}K^7 + \frac{61}{25920}K^8.$$
(10)

This gives $K^* = 1$, $\lambda \approx 3.25$, $\nu \approx 0.588$ and $D \approx 1.70$ reasonably close to the expected values $\nu = \frac{1}{2}$, D = 2. However, these values are also close to those of the sAW problem, and the real test must await the results of large cell calculations. In the above calculations, the deviations of K^* from unity arise from the finite probability allowed for the escape of the walk away from the quadrant containing the cell when all other avenues are blocked.

4. Renormalisation of growing animals

The renormalisation of growing animals proceeds essentially along the same lines. One apparent concern here is the basic requirement for a cell renormalisation, i.e. that of the equivalence of all the cells covering the lattice. Upon further consideration, however, this turns out not to be a problem. The apparent 'difficulty' rises from the fact that, at any given instance (in units of the time to add one site), growth is occcuring only at the periphery of the animal *and* that a given perimeter site becomes occupied with a progressively smaller probability as the animal grows larger. (We note that such a property is shared by the diffusion limited aggregation model of Witten and Sander (1981, 1983) as well.) This is, however, not a real problem since we are interested in a purely *spatial* property, and thus our rescaling must be spatially uniform. Spatially uniform rescaling corresponds, e.g., to the simultaneous rescaling of cells

whose growth has taken place at various different times, and to the treatment of cells further away from the seed as if they were grown at a much greater rate. Not only does all of this not interfere with our aim of calculating spatial properties, but it is in fact essential.

In practice, we again employ a 'corner rule' in which a cell is counted occupied if an animal grown from a corner seed spans the cell in all directions (corresponding to ' r_2 ' and ' r_3 ' for square and simple cubic lattices respectively, of Family (1983); see also Reynolds *et al* (1980)). For 2×2 cell on the square lattice, we thus obtain

$$K' = K^3 + K^4, (11)$$

i.e. all three- and four-site processes span the cell in both directions. This recursion relation results in $K^* \cong 0.755$, $\lambda \cong 3.43$, and $\nu \cong 0.562$, $D \cong 1.778$. These estimates are considerably different from the similar 2×2 results for the (static) random animals (Family 1983), $\bar{\nu} \cong 0.604$, $\bar{D} \cong 1.66$, and already relatively close to the compact cluster values of $\nu = \frac{1}{2}$, D = 2.

We may remark at this point on the difference between our recursion relation (11) and that of Gould *et al* (1983):

$$K' = 4K^3 + 4K^4. (12)$$

Gould *et al* do not make clear what their generating function is and their procedure consists of counting the *number* of growth processes that span the cell. Thus, they implicitly weight each process of the same size equally. While this assumption is correct at the level of 2×2 , as we shall see, it breaks down already for 3×3 cells. In addition, since the number of processes are counted, terms of higher order in K naturally occur with much larger coefficients. This contrasts with the original problem in which there are equal numbers of animals of all sizes in the 'ensemble', leading to a generating function with a singularity at K = 1.

Now for a 3×3 cell, we obtain

$$K' = \sum_{N} C_{N} K^{N} = \frac{329}{1080} K^{5} + \frac{20239}{25920} K^{6} + K^{7} + K^{8} + K^{9},$$
(13)

which leads to $K^* \cong 0.797$, $\lambda \cong 7.03$, and $\nu \cong 0.563$, $D \cong 1.776$. Thus, the estimate of D has a slightly larger deviation from D = d = 2 than for 2×2 cells. While this is somewhat discouraging, such non-monotonicity was already encountered in Monte Carlo simulations (Peters *et al* 1979).

The coefficients C_N are obtained, as before, by the relative probability of those growth processes of N-site animals that satisfy the spanning rule. The calculation of these weights is normally quite non-trivial; however, for small cells the task is greatly simplified by looking at $(1-C_N)$. In the 3×3 case, no processes of seven or more sites fail to span, leading to $C_7 = C_8 = C_9 = 1$, and $(1-C_5)$ and $(1-C_6)$ are each obtained as the sum of just 48 terms (cf figure 2).

For d = 3, the result from a $2 \times 2 \times 2$ cell on the simple cubic lattice is

$$K' = \frac{3}{4}K^4 + K^5 + K^6 + K^7 + K^8.$$
(14)

This leads to $K^* \cong 0.723$, $\lambda \cong 5.51$, and $\nu \cong 0.406$, $D \cong 2.46$, still fairly far from compact clusters ($\nu = \frac{1}{3}$, D = d = 3). In comparison, for the random animal case one finds (Family 1983) $\bar{\nu} \cong 0.459$, $\bar{D} \cong 2.18$ on a 2×2×2 cell.



Figure 2. Just three of the ten *non-spanning configurations* of the five-site animals in a 3×3 cell are shown. For the Eden model, we must consider the relative probability of each *growth* process among those of the same size. Thus, for (*a*), there is only one way to grow it from the corner seed and the probability is $\frac{1}{2} \times \frac{1}{3} \times \frac{1}{4} \times \frac{1}{5} = \frac{1}{120}$. For (*b*), there are four ways to grow it with a total probability of $\frac{23}{27}$; for (*c*), four ways to grow it with total probability of $\frac{53}{564}$. The remaining seven configurations (not shown) have 39 ways to grow among them with varying probabilities totalling $\frac{2483}{4370}$.

Our final comment concerns the peculiar limiting property of our recursion relations for the Eden process. As remarked already, on a b^d cell, all b^{d-1} terms C_N with $N > b^d - b^{d-1}$ are equal to 1. Thus, the eigenvalue λ_b satisfies

$$\lambda_{b} \equiv \frac{\mathrm{d}K'}{\mathrm{d}K} \bigg|_{K^{*}} > \sum_{N=b^{d-1}-b^{d-1}+1}^{b^{d}} NK^{*N-1}.$$
(15)

Hence, as $b \rightarrow \infty$, we have

$$\lambda_b > b^{2d-1} K^{*b^d}. \tag{16}$$

Let

$$K^* \sim 1 - f(b) \tag{17}$$

with $f(b) \rightarrow 0$. Normally, we would expect $f(b) \sim b^{-1/\nu} \sim b^{-D}$ with the *true D*; however, since K^* is raised to b^d in (16), even asymptotically small deviation of f(b) from b^{-d} is important here.

In fact, if we let $f(b) \sim b^{-D}$ with D = d (as expected for the Eden process), then the factor $K^{*b^d} \rightarrow O(1)$ in (16), and $\nu_b^{-1} = (\ln \lambda_b)/\ln b \ge 2d - 1$, which is in contradiction with the assumption. This appears to suggest either a fault in the construction of our renormalisation scheme *or* one in our assumption of $f(b) \sim b^{-D}$ with D = d. Our point of view is that, because of the sensitivity of the rate of convergence of K^* to 1 here, we must allow for a correction of the type

$$f(b) \sim (\ln b)^{x} b^{-d}.$$
 (18)

Note that this may be due either to a real logarithmic correction in D (unlikely from the Monte Carlo data of Peters *et al* (1979)) *or*, if we take $f(b) \sim b^{-1/\nu_b}$ where ν_b is the b^d cell estimate of ν for self-consistency, then to a peculiarly slow convergence of $1/\nu_b \sim d-x \ln \ln b/\ln b$ to the limit $1/\nu \equiv D \equiv d$. At any rate, for (18) to be compatible with D = d in a sensible way, we must still have

 $x > 1, \tag{19}$

since the term

$$[1 - (\ln b)^{x} b^{-d}]^{b^{d}} \sim b^{-(\ln b)^{x-1}}$$
⁽²⁰⁾

must win over the prefactor b^{2d-1} in (16) to render this contribution to λ_b (from C_N with large N) negligible in the large b limit.

5. Summary

In summary, we have proposed a generating function for all growth processes that start from a seed site on a lattice, and constructed a new cell renormalisation scheme consistent with this generating function. This scheme is illustrated for TSAWS and the Eden model where the results are in good agreement with analytic and Monte Carlo expectations considering the small cell sizes employed. Moreover, since our method is based on *relative* probabilities of spanning processes, it is fairly straightforward to extend it to much larger cell sizes by using Monte Carlo techniques to evaluate C_{N} . Our preliminary results with relatively small cell sizes already indicate the reversal of the slightly decreasing trend of D found for b = 2 and 3 for the Eden process. This program is now in progress, and results will be reported subsequently.

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