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LETTER TO THE EDITOR

On the position-space renormalisation group approach to diffusion-limited cluster growth problems

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Abstract. We investigate the application of position-space renormalisation group methods to the Witten–Sander model of diffusion-limited cluster growth. We show that this method cannot be used to investigate the asymptotic behaviour of the Witten–Sander model in three and higher dimensions, even though it yields satisfactory results in two dimensions with small cells.

A wide variety of problems such as the growth of crystals from an undercooled melt or a supersaturated solution (for a review see Langer (1980) and references therein), coagulation of smoke particles (Forrest and Witten 1979), growth of tumours (Williams and Bjerknes 1972) and turbulence (Hentschel and Procaccia 1982) have a common root in the physical mechanisms that govern the structure of randomly branched clusters. Most of these processes are governed by diffusion and surface tension. Surface tension favours compact clusters, i.e. clusters that fill their surrounding space, with a minimum area to volume ratio. On the other hand, because surface sites deep inside the cluster are connected to the surrounding environment by narrow paths, they are screened. Thus the rate of growth of the cluster at such sites is reduced.

The recent popularity of the study of the kinetics of formation of randomly branched clusters is largely due to the paper by Witten and Sander (1981). In their model the initial state at time $t = 1$ is a seed particle located at the centre of a large hypersphere. A second particle is released at the surface of this sphere at time $t = 2$. The particle then performs a random walk until it reaches a site adjacent to the seed site, where it stops its random walk and joins the cluster. The process of releasing the particles on the surface of the sphere is continued until a large cluster of occupied sites is formed. Witten and Sander (1981) performed computer simulations of such a cluster growth process on a lattice, and by ignoring surface tension and treating the random walk (diffusion) on the lattice exactly, showed that the resulting clusters are extremely branched. A fundamental measure of the structure of a randomly formed cluster is the manner in which R, the linear dimension of the cluster, scales with n, the total number of particles in the cluster. If

$$R \sim n^{\nu}, \tag{1}$$

then $D = 1/\nu$ is the Hausdorff or fractal dimensionality of the cluster (see Mandelbrot 1982). Witten and Sander called this growth process a new kind of critical phenomenon,

mainly because the density–density correlation function

$$c(r) = n^{-1} \sum_{r'} \rho(r')\rho(r+r') \tag{2}$$

seems to obey a power-law relationship,

$$c(r) \sim r^{-\alpha}, \tag{3}$$

similar to usual critical phenomena. Here α and D are related through $D = d - \alpha$. Meakin (1983) has studied the Witten–Sander (ws) model extensively by computer simulations. He has found that the ratio D/d, where d is the Euclidean dimensionality, is a superuniversal value, i.e. its value is independent of dimension and details of the lattice, and is close to $\frac{5}{6}$ for $d = 2$–6. However, his results for three- and higher-dimensional systems are not conclusive since they contain large statistical uncertainties. Muthukumar (1983) has developed mean-field theory for the ws model which predicts that $D = (d^2+1)/(d+1)$. This formula yields results which are in good agreement with the computer simulation results of Meakin (1983). Rosenstock and Marquardt (1980) developed upper and lower limits on the rate of cluster growth in the ws model by using concepts from random-walk theory.

Computer simulations have been the major tool in studying the formation of randomly branched clusters. However, one may also study these models by renormalisation group approach. Because a Hamiltonian formulation of these processes is not available, and because it appears that the ws model does not have an upper critical dimensionality (Witten and Sander 1983), a momentum-space renormalisation group approach and ε expansion ($\varepsilon = d_u - d$, where d_u is the upper critical dimensionality) is not possible. Very recently Gould *et al* (1983) developed a position-space renormalisation group (PSRG) approach to study the ws model. They studied this model in two dimensions and showed that it is in a different universality class from the lattice animals. One might hope that this method can be used to study the ws model in three- and higher-dimensional systems to obtain accurate estimates of D. In this letter we explore the applicability of this method to the study of the ws model in three and higher dimensions.

The PSRG treatment of the ws model is a two-parameter model. A fugacity S is associated with each occupied site of the cell, and another fugacity W is assigned to each step of the random walk of the added particle. Thus the recursion relation for S', the renormalised site occupation fugacity, is written as (Gould *et al* 1983)

$$S' = \sum_{s,t} C_{st} S^s W^t \tag{4}$$

where C_{st} is the number of different ways of growing a spanning cluster of s sites generated by random walks with total number of steps t. This is somewhat similar to the PSRG treatment of lattice animals (Family 1980, 1983). One has to develop also a recursion relation for W', the fugacity of a single-step random walk on the renormalised lattice. This relation is of the form

$$W' = \sum_{m} b_m W^m, \tag{5}$$

where b_m is the total number of walks of m steps that span the cell in a given direction. For dimensions $d \geqslant 2$ equation (5) cannot be determined exactly, even for the smallest cell, because there are an infinite number of spanning walks that exist for a finite cell and thus contribute to (5).

In an attempt to circumvent this difficulty, Family and Gould (1983) developed a PSRG procedure that avoids this difficulty. They noted that after a larger number n of random walk steps is taken, the length ξ of the random walk obeys the equation

$$\xi \sim n^{1/2} \tag{6}$$

since the random walk would be diffusive. Thus at the critical fugacity W^* (i.e. in the limit $n \to \infty$), only those random walks whose number of steps obey (6) contribute significantly to (5). Thus the summation in (5) is restricted to spanning random walks whose number of steps n satisfies the relation $n \leqslant \xi^2$, where ξ is the end-to-end length of the walk on the cell. Our procedure for calculation of W' is somewhat different from that of Family and Gould (1983) in that we enumerate longer walks (see below) and thus obtain a better approximation to ν.

In figure 1 we show the smallest cell that we used in two dimensions. The seed particle is located at A, and another particle can enter the cell from the 'north' or 'east'. For a cell of this type on a d-dimensional simple cubic lattice, with linear dimension b we enumerate walks with up to $\xi^2 = (d-1)(b-1)^2 + b^2$ steps. Thus for $b = 2$ we have

$$S' = 6S^3W^2(1+2W) + 8S^4W^3(1+2W) \tag{7}$$

$$W' = W^2 + 2W^3 + 5W^4 + 14W^5. \tag{8}$$

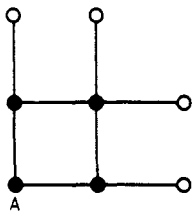

Figure 1. The smallest ($b = 2$) cell used in the PSRG treatment of the Witten–Sander model in two dimensions. A denotes the seed particle.

Equations (7) and (8) have the fixed points $S = S^*$ and $W = W^*$. Thus the fractal dimensionality of the WS model is given by

$$D = \ln \lambda / \ln b \tag{9}$$

where λ is the eigenvalue of the linearised transformation S', i.e. $\lambda = \partial S'/\partial S$ evaluated at $S = S^*$ and $W = W^*$. One may also define a cell-to-cell transformation (Reynolds *et al* 1978) in which an implicit transformation from a cell of size b to a cell of size b' is constructed. One may interpret this as an infinitesimal transformation whose results will improve as $b/b' \to 1$, in contrast to the cell-to-site (or bond) transformation whose results are expected to improve with increasing cell size. We have used cells of up to $b = 4$ in two dimensions and the results are displayed in table 1. The results agree very well with the Monte Carlo result of Meakin (1983), $D = 1.67$.

We note that equation (5) describes the PSRG treatment of an unbiased, nearest-neighbour random walk on a lattice. Because such a walk is Markovian, the fractal dimensionality of the walk is $D_{RW} = 2$, independent of the dimension. The inverse μ of the 'critical' fugacity W^* is also an estimate of the connective constant

Table 1. Results of cell-to-site and cell-to-cell PSRG calculations of the fractal dimensionality D of the Witten–Sander model. The expected value is $D \simeq 1.67$.

b \ b'	1	2	3
2	1.7067		
3	1.6740	1.6510	
4	1.67380	1.6421	1.6703

of the random walk. For the random walks considered in this paper $\mu = Z$ exactly, where Z is the coordination number of the lattice. We have determined the renormalisation transformation for W' for cell sizes up to $b = 6$, the results of which are presented in table 2. As can be seen, for $b = 6$ and with a cell-to-bond transformation, we have obtained $\nu = 0.5040$, in excellent agreement with the exact value of $\frac{1}{2}$. The connective constant $\mu = 1/W^*$ converges more slowly to its exact value of 4 because of the truncation that we imposed on equation (5). Previous application of the PSRG method to the random walk problems had been restricted to one dimension (Høye and Napiórkowski 1980, Muto 1981).

Table 2. Results of cell-to-bond PSRG calculations of the exponent ν and the connective constant μ for random walks on a square lattice. The exact results are $\nu = \frac{1}{2}$ and $\mu = 4$.

b	2	3	4	5	6
ν	0.5853	0.5392	0.5215	0.5109	0.5040
μ	2.8818	3.2938	3.4818	3.6004	3.6813

We now turn our attention to the WS model on the simple cubic lattice in three dimensions. For the $b = 2$ cell we have

$$W' = W^2 + 4W^3 + 14W^4 + 52W^5 + 180W^6. \tag{10}$$

The corresponding renormalisation transformation for S' is too long to be given here, but the fractal dimensionality of the WS model with the $b = 2$ cell is found to be $D = 2.31$. This must be compared with the Monte Carlo simulation result of Meakin (1983) $D \simeq 2.51$. One may think that larger and larger cells will improve the result obtained with the smallest cell. Although it is not possible to determine exactly the recursion relations for S' for the $b = 3$ cell and larger ones, because of the enormous number of possible configurations and walks, we show below that we do not expect that such a procedure will yield satisfactory and *meaningful* results for the fractal dimensionality D. In fact we believe that this PSRG treatment of the WS model breaks down in three- and higher-dimensional lattices.

It is very easy to calculate the recursion relations for W' for larger cells. For example, for $b = 3$ on a simple cubic lattice in three dimensions we have

$$\begin{aligned} W' = {} & W^3 + 6W^4 + 39W^5 + 188W^6 + 988W^7 + 4380W^8 + 21\,471W^9 + 92\,742W^{10} \\ & + 450\,627W^{11} + 1887\,328W^{12} + 9084\,700W^{13} + 37\,709\,040W^{14} \\ & + 180\,703\,717W^{15} + 746\,728\,150W^{16} + 3570\,464\,863W^{17}. \end{aligned} \tag{11}$$

We determined W' for cells up to $b = 5$ and the results are presented in table 3. As can be seen for the $b = 3$ cell we already have $\nu = 0.4818$ and larger cells decrease ν further. It may be thought that if we enumerate longer walks the results will improve.

Table 3. Results of cell-to-bond PSRG calculations of the exponent ν and connective constant μ for random walks on a simple cubic lattice in three dimensions. The exact results are $\nu = \frac{1}{2}$ and $\mu = 6$.

b	2	3	4	5
ν	0.5236	0.4818	0.4664	0.4423
μ	4.1356	4.7619	5.0890	5.1312

We enumerated much longer walks (longer than the maximum number of steps ξ^2) and the results became poorer, i.e. ν decreased. Cell-to-cell renormalisation procedure did not improve the results either. We do not believe that if we use much larger cells this trend will reverse itself and ν will increase again and approach its asymptotic value of $\frac{1}{2}$. But even if this could happen one would have to use several very large cells and calculate ν and extrapolate the results to an infinite cell. As Reynolds *et al* (1980) pointed out this procedure is equivalent to the finite-size scaling approach. It has been established by Brézin (1982) that the finite-size scaling approach breaks down at and above the upper critical dimensionality of the system considered because of singularity of the scaling function. Though there is no Hamiltonian formulation of a nearest-neighbour and unbiased random walk (as used here to deduce the fractal dimensionality of the ws model), one can conceivably assume that the upper critical dimensionality of such a random walk is two (Barber and Ninham 1970), since the statistics of the walk do not change qualitatively in dimensions higher than two. Thus any attempt to exploit the finite-size scaling approach or one of its equivalents for deducing asymptotic properties of the random walk at three and higher dimensions by PSRG treatment would fail. Consequently we do not expect to obtain satisfactory and *meaningful* results for the recursion relation for S' with larger cells, and thus the fractal dimensionality D of the ws model.

As a further test we also determined the recursion relations for W' for $b = 2$ and 3 cells for a simple cubic lattice in four dimensions. For $b = 2$ we obtained

$$W' = W^2 + 6W^3 + 29W^4 + 138W^5 + 637W^6 + 2898W^7. \tag{12}$$

The results for ν for cell-to-bond transformation are $\nu = 0.4813$ and 0.4438 for $b = 2$ and 3 respectively. The cell-to-cell transformation yields $\nu = 0.4410$. These results support our view expressed above.

We now investigate briefly a variation of the ws model which might be useful in probing the structure of the percolation clusters (for a review of percolation theory see Stauffer (1979, 1981)). If the growth process is considered in a lattice in which a fraction p of sites (or bonds) have been removed at random, then an interesting situation arises. If $p > p_c$ where p_c is the percolation threshold of the lattice, then the infinite percolation cluster is compact, i.e. its fractal dimensionality is the same as the Euclidean dimensionality of the space embedding the lattice. Thus we may expect no fundamental change in the structure of the growing cluster. However, at $p = p_c$ the lattice is barely connected and the infinite percolation cluster has a ramified

structure. Therefore we may expect that the structure of the growing cluster will be different from the one above the percolation threshold. Random walks on percolation clusters at the percolation threshold are not diffusive, and the fractal dimensionality of the walks depends upon the dimensionality of the system (Rammal and Toulouse 1983, Sahimi and Jerauld 1983). Thus it is possible to investigate the ws model in such a system with the PSRG method.

In this case we need a three-parameter PSRG as opposed to the two-parameter one for the growth process on compact clusters that we discussed above. The third parameter is the probability p that a site is present in the lattice. Within the PSRG framework one has to find p', the probability that a site in the renormalised cell is present. We define a cell to be percolating if and only if it contains a set of connected sites that span the cell. Following Reynolds *et al* (1978) we can use several rules to define percolation of the cell. We may consider a cell as percolating if a connected path of occupied sites exists which spans the cell either horizontally or vertically; we call this rule r_0. Rule r_1 requires spanning in a particular direction, while rule r_2 requires spanning of the cell in both directions. These rules define the renormalisation transformation p' for site probability p. We consider all three rules in this paper. Because a site in the renormalised cell can become part of the growing cluster if and only if it is present with probability p', the recursion relation for S', the renormalised site fugacity, is written as

$$p'S' = \sum_{i}^{m} p^i (1-p)^{n-i} \left(\sum_{s,t} C^{\mathrm{R}}_{ist} S^s W^t \right), \tag{13}$$

where m is the total number of sites in the cell ($m = b^2$) and i the number of present sites. A similar procedure is also necessary for W', the renormalised walk fugacity.

We determined the fractal dimensionality D of the ws model at the site percolation threshold of the square lattice for cells of size $b = 2$ and 3 using the closed form formulae for p' which are given by Reynolds *et al* (1980). The results are listed in table 4. As can be seen, the results are insensitive to the different rules that were used to determine p'. Thus we calculated the fractal dimensionality D of the ws model for a cell of size $b = 4$ using only the recursion relation for p' that corresponds to rule r_1. This value is also listed in table 4 and it is clear that D is decreasing with increasing cell size. Reynolds *et al* (1980) showed that the error in the cell-to-site transformation results with finite b vanishes as $b \to \infty$ in the form

$$D(b) = D + C_1/\ln b + C_2/(\ln b)^2. \tag{14}$$

Table 4. Results of cell-to-site and cell-to-cell PSRG calculations of the fractal dimensionality D of the Witten–Sander model on a percolation cluster at the site percolation threshold of the square lattice.

Rule	b	b' 1	2	3
r_0		1.714		
r_1	2	1.711		
r_2		1.709		
r_0		1.691	1.661	
r_1	3	1.684	1.660	
r_2		1.681	1.660	
r_1	4	1.672	1.652	1.640

We used the data of table 4 to determine the best estimate of D. We obtained $D = 1.55$ which should be compared with $D \simeq 1.67$ for the growth process on compact clusters. This large difference means that the infinite percolation cluster whose fractal dimensionality is $\frac{91}{48} \simeq 1.896$ at p_c in two dimensions (Stauffer 1981) contains many deadend branches whose sites are screened during the growth process, and thus the fractal dimensionality D of the WS model is very low at p_c.

In conclusion we have demonstrated that the PSRG treatment of the Witten–Sander model of cluster growth is not a useful and *consistent* method for three- and higher-dimensional systems. Even though small cell PSRG yields satisfactory results in two dimensions, the applicability of this method to obtain very accurate and *meaningful* estimates of the 'critical' exponents that characterise this model in three and higher dimensions is questionable.

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Note added in proof. After this work was accepted we received a preprint by H Nakanishi and F Family in which they discussed some other difficulties of the PSRG method of Gould *et al.* We thank them for timely correspondence.

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