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LETTER TO THE EDITOR

Recursion equations for static and kinetic models of branched polymers

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Abstract. A new renormalisation group treatment of bond lattice animals is presented which yields the critical bond fugacity and ν exponent for general dimension d. Good agreement is obtained with predictions based on different methods for all d. In particular $\nu = 1 - \varepsilon + O(\varepsilon^2)$, for $d = 1 + \varepsilon$. Results are also given for a kinetic version of the bond lattice animal problem.

In recent years, cluster renormalisation group methods in real space have been extensively applied to geometrical critical phenomena (Stanley *et al* 1982). In spite of their very intuitive basis and apparent simplicity, these methods suffer rather severe limitations, as far as their range of applicability is concerned. The existing methods for obtaining recursion equations soon become untractable for large cell size (rescaling factor l) and/or space dimension, d because of the difficult enumeration problems.

In particular, for the problem of bond lattice animals, which is related to the conformational statistics of branched polymers in solution (Flory 1969, Stanley *et al* 1982) there exist, up to now, very limited renormalisation group results for the $d = 2$ case (Family 1980).

The situation is somewhat disappointing if one considers the much wider range of results provided e.g. by the simple and powerful Flory approximation (Isaacson and Lubensky 1980). More flexible renormalisation group methods would also be very welcome in the context of further applications to the kinetics of random branched aggregates formed by some irreversible process. Models of these processes are the dynamical counterpart of the static animals and are relevant for the description of several physical and biological situations, such as the coagulation of smoke particles (Witten and Sander 1981) or the growth of tumors (Eden 1961).

In this Letter, following previous analogous developments for self-avoiding random walks (linear polymers) and self-avoiding random surfaces (sheet polymers) (Maritan and Stella 1984a, b), we propose a new version of the cluster renormalisation for bond lattice animals, which yields recursions in closed form for all values of d and l.

When considering random animals on a d-dimensional hypercubic lattice, one is interested in the number of connected clusters of n nearest-neighbour bonds per site, c_n, and on their mean square radius of gyration with respect to the centre of mass, R_n^2.

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One expects that asymptotically, for $n \to \infty$,

$$c_n \propto n^{-\theta} \lambda^n \tag{1}$$

and

$$R_n^2 \propto n^{2\nu}. \tag{2}$$

It is convenient to formulate the problem in a grand canonical context, by associating a fugacity, K, to each bond of the animal, and averaging for unconstrained n. The grand canonical radius of gyration thus becomes

$$\xi^2(K) = \sum_n c_n R_n^2 K^n \Big/ \sum_n c_n K^n. \tag{3}$$

On the basis of (1) and (2) one also obtains

$$\xi(K) \underset{k \to k_c^-}{\sim} (K_c - K)^{-\nu}, \tag{4}$$

with $K_c = \lambda^{-1}$.

The idea of the renormalisation group is to rescale the system by a factor l, so that the new correlation length becomes

$$\xi(K') = l^{-1} \xi(K), \tag{5}$$

where $K' = K_l'(K)$ is a regular function of K. If, as in the cases we consider, the renormalisation transformation involves only one parameter, (5) holds, for $K \leqslant K_c$, only for the leading singular part of $\xi(K)$, given by (4). From (5) and the assumed regularity of $K_l'(K)$, we find that K_c must be a solution of the fixed point equation $K_l'(K_c) = K_c$, and $l^{1/\nu}$ is given by $(\mathrm{d}K_l'/\mathrm{d}K)_{K=K_c}$.

The existing methods for obtaining $K_l'(K)$ in geometrical problems are rather empirical and based on very qualitative arguments (de Queiroz and Chaves 1980, Stanley *et al* 1982). For branched polymers we will essentially follow here the approach of Family (1980). The idea is to partition the lattice into cubic cells of side l (figure 1) and to consider a generating function

$$K_l'(K) = \sum_A K^{|A|}, \tag{6}$$

where the sum is over all animals A (with $|A|$ bonds) in a given cell, which contain a point of the boundary (e.g. the corner C) and go across the cell at least in one given lattice direction.

One expects that $K_l'(K)$, considered as the bond fugacity of a rescaled system, will preserve the long range two-point connectivity of the original system, and satisfy (5) with the aforementioned consequences.

We can also give an heuristic argument, based on the concept of fractal dimension (Mandelbrot 1982), supporting the fact that the exponent associated with the fixed point of the mapping, is indeed ν. It is straightforward to show that

$$\mathrm{d}K_l'/\mathrm{d}K = (K_l'/K)\langle |A| \rangle_l, \tag{7}$$

where $\langle |A| \rangle_l$ is the average obtained from the generating function (6). Because of the last equation, if K_c is a fixed point of $K' = K_l'(K)$, it must also be $\mathrm{d}K'/\mathrm{d}K|_{K_c} \sim l^{1/\nu}$. Indeed $1/\nu$ is the Hausdorff dimension of our random fractals: this means that, for $K \leqslant K_c$, the random animals contributing to (6), which by construction extend over a distance l, will have $\langle |A| \rangle_l \sim l^{1/\nu}$.

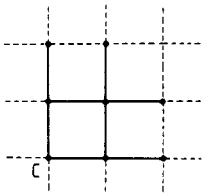

Figure 1. 2×2 cell in the square lattice. The continuous links belong to the cell, the broken ones to the neighbouring cells.

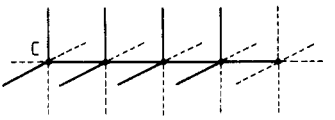

Figure 2. Anisotropic cell in $d=3$ (continuous links) corresponding to a rescaling factor $l=4$ in the longitudinal direction.

The computation of (6) for a 2×2 cell (see figure 1) already implies a total of 73 contributing animals.

Indeed, summing over all animals which contain the lower-left corner (C) and go across the cell, e.g. horizontally, one gets (Family 1980)

$$K_2'(K)=K^2+4K^3+14K^4+24K^5+21K^6+8K^7+K^8, \tag{8}$$

which leads to $K_c=0.270$ and $\nu=0.57$, to be compared with $K_c=0.192$ and $\nu=0.61$, as estimated by series expansions analysis (Gaunt 1980), and field theoretical arguments (Parisi and Sourlas 1981), respectively.

To obtain recursion equations for generic d and l is obviously very difficult. The strategy we propose for overcoming this difficulty is to rescale the lattice successively, one direction at a time, using the anisotropic cell shown in figure 2 for $d=3$.

The rule for renormalising the fugacity K is essentially the same as the one used for obtaining (8) in the isotropic case; now however, we obtain different recursions, according to whether the renormalised bond considered is perpendicular ($K_\perp'$) or parallel ($K_\parallel'$) to the rescaling direction.

Summing over all animals which contain C and cross the cell longitudinally, we get, for general d and l,

$$K_\parallel'=K^l(1+K)^{D(l-1)} \tag{9}$$

where $D=d-1$. In this last equation we exclude animals containing any transverse bond at the origin: this ensures that, for $l=1$, $K_\parallel'\equiv K$, as it should.

The expression for $K_\perp'$ is slightly more complicated. Considering one of the D transverse directions, we sum over all animals which contain C and cross the cell in that direction, with at least one bond. Also in this case, to ensure that the transformation is identical for $l=1$, we have to exclude the $D-1$ bonds at the origin, parallel to the other transverse directions; furthermore we prevent the possibility of a full longitudinal connection, by excluding the longitudinal bond most remote from C.

Using these rules we obtain

$$K_\perp'=\frac{[K(1+K)^D]^l-1}{K(1+K)^D-1}(1+K)-\frac{[K(1+K)^{D-1}]^l}{K(1+K)^{D-1}-1}=R_l(K). \tag{10}$$

For $d=1$ only $K_\parallel$ exists and equation (9) gives the correct results: $K_c=1$ and $\nu=1$. For $d>1$ we choose to work still with an isotropic fugacity and take as renormalised K' the result of applying to the original fugacity transformations (10) and (9) D and one times, respectively†. This is certainly a source of further approximation in the

† It turns out that the actual order in which the transformations are applied does not very sensitively affect the results.

method, because it amounts to disregarding the anisotropies generated at each successive rescaling. We can however reasonably hope that this approximation will not be too crude, at least for low d, as previous experience with other geometrical problems has shown (Maritan and Stella 1984a, b). We thus choose as renormalised fugacity

$$K' = [R_l^D(K)]^l [1 + R_l^D(K)]^{D(l-1)}. \tag{11}$$

In table 1 we report the fixed points and ν exponents of (11) for $l = 2, 3$ and $2 \leqslant d \leqslant 8$. Results for different l values are slightly different†. It should be noted that K_c and ν for $d = 2$ are very close to the results of (8). This indicates that our anisotropic rescalings do not introduce too heavy approximations. Independent estimates of K_c for lattice animals have been obtained from series analysis and are reported in table 1. Our estimates are systematically above the series one.

Table 1. The results for rescalings 2 and 3 are reported in the first and second row, respectively. In the third row results are reported from series and a conjectured relation between θ and ν exponents. In the last row the Flory values of ν are reported.

d		2	3	4	5	6	7	8
$l=2$	K_c	0.269	0.144	0.0959	0.0714	0.0567	0.0469	0.0399
	ν	0.58	0.46	0.39	0.35	0.32	0.30	0.29
$l=3$	K_c	0.263	0.140	0.0936	0.0698	0.0555	0.0459	0.0392
	ν	0.61	0.48	0.42	0.38	0.36	0.34	0.32
	K_c	0.192[a]	0.0942[a]	0.0613[a]	0.0452[a]	0.0360[a]	0.0301[a]	0.0256[a]
	ν	0.61[b]	0.50[b]	0.45[c]	0.40[c]	0.32[c]	0.28[c]	0.25[d]
Flory value		0.62	0.50	0.42	0.36	0.31	0.28	0.25

[a] Gaunt (1980), [b] Parisi and Sourlas (1981), [c] Family (1982), [d] Isaacson and Lubensky (1979).

As far as the ν exponent is concerned, information is available either on the basis of the Flory approximation, or of series estimates (Gaunt 1980) of the entropic θ exponent (Parisi and Sourlas 1981, Family 1982) (see table 1). The Flory approximation (Isaacson and Lubensky 1980) gives

$$\begin{aligned} &\nu = 5/[2(d+2)] && d \leqslant 8 \\ &\nu = \tfrac{1}{4}, && d > 8. \end{aligned} \tag{12}$$

An upper critical dimensionality $d_c = 8$ with $\nu = \frac{1}{4}$ is also predicted on the basis of field theoretical techniques (Isaacson and Lubensky 1979).

Our renormalisation group results compare rather nicely, even if qualitatively, with Flory and series values over all the range of dimensionalities considered. For high values of d the decrease of ν is rather slow. Of course a real space calculation like ours cannot produce a ν exponent which stays constant above the critical dimension, $d_c = 8$, of the problem (Isaacson and Lubensky 1979).

The above results are rather remarkable for such a relatively simple recursion scheme.

† A systematic improvement of the results is not to be expected for increasing l, because the effect of anisotropies becomes stronger.

An important advantage of (11) is that, unlike (12), it allows us to gain insight into the problem for d close to its lower critical value, i.e. $d = 1$.

Considering a rescaling $l = 1 + \delta$, as customary in such a type of renormalisation calculations, and $d = 1 + \varepsilon$, one gets, after some algebra,

$$\left.\frac{dK'}{d\ln l}\right|_{l=1} = K \ln K\left(1 - \frac{2K\varepsilon}{1-K}\right) + O(\varepsilon^2), \tag{13}$$

from which we obtain $\nu = 1 - \varepsilon$, and $K_c = 1 - 2\varepsilon$. These results, which are certainly exact for $\varepsilon = 0$, have a reasonable chance of being correct also to first order in ε, as similar ones obtained for percolation and self-avoiding walks (SAWs) (Redner and Reynolds 1981, Maritan and Stella 1984a, b). For SAWs one obtains $\nu = 1 - \frac{1}{2}\varepsilon$: so, to first order in ε, lattice animals are space filling, whereas SAWs have a fractal dimension lower than the euclidean one.

In view of its relative simplicity, one is naturally tempted to extend the above renormalisation scheme to the kinetic case. One can conceive an aggregation process in which our animals grow by attaching bonds (one at a time) randomly to lattice links adjacent to the already occupied ones. This is a bond analogue of the more familiar Eden model, in which site aggregation occurs (Eden 1961). Even if the conjecture that these two dynamical models belong to the same universality class appears rather plausible, this is not strictly guaranteed, *a priori*.

In the dynamical case the computations are analogous to those described above (Gould *et al* 1983). The only difference is that now each animal contributing to the static recursion, has a multiplicity $\geqslant 1$, which accounts for the several different ways in which it can be grown starting from C.

Without entering into further details, we just give the formulae for $l = 2$ and general d†

$$K'_{\parallel} = K^2 \sum_{p=0}^{D} \binom{D}{p} (p+1)!\, K^p \tag{14}$$

$$K'_{\perp} = \sum_{p=0}^{D} \binom{D}{p} [(K^2+K)p! + K^2(p+1)!] K^p. \tag{15}$$

Following the previous procedure we computed the values of ν for the kinetic animals.

For $d = 2$ we get $\nu = 0.54$, which implies a fractal dimension, $1/\nu$, very close to d itself.

It should be noticed that for the Eden model the ν exponent is also found to be close to $\frac{1}{2}$ for $d = 2$ (Peters *et al* 1979). This result could support the hypothesis that our model and the Eden one belong indeed to the same universality class. We must however mention the fact that, on the basis of (14) and (15), the ν exponents in higher d turn out to be definitely above those conjectured for the Eden model ($\nu = 1/d$) (Peters *et al* 1979). In particular we find $\nu = 0.42$ and 0.35 in $d = 3$ and 4, respectively, while ν is close to $\frac{1}{4}$ for d close to 8, as is expected for static animals.

Of course we cannot exclude the fact that the discrepancy between what is expected for the Eden model and the results for our model could be due to an inadequacy of our approximations in the dynamics.

In summary we have presented new renormalisation recursions both for static and kinetic bond lattice animals. At least for the static case, our approach appears extremely

† In the dynamical case we were not able to obtain recursions in closed form for general l and d simultaneously.

powerful and allows us to gain new insight into the behaviour close to the lower critical dimension, $d = 1$.

Further investigation will be needed to test the validity of the approach in the kinetic case, especially for high dimensionality.

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