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Self-directed walk: a Monte Carlo study in two dimensions

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Abstract. A new type of indefinitely growing self-avoiding walk is introduced in which the walker is not allowed to perform a step pointing towards a site he has already visited. This restriction leads to a walk which is a succession of long directed parts. A Monte Carlo study on the square lattice suggests that the radius of gyration exponent $\nu = 1$ in two dimensions. The enhancement factor exponent $\gamma = 1$ in all dimensions. A self-consistent method gives $\nu = 1$ when $1 \leqslant d \leqslant 2$, $\nu = 2/d$ when $2 \leqslant d \leqslant 4$ and $\nu = \frac{1}{2}$ above $d_c = 4$, the upper critical dimension.

1. Introduction

After a long period devoted to the study of the equilibium properties of long polymer chains on the self-avoiding walk model (de Gennes 1979), the field of growing random walks is now extensively explored (see Lyklema (1986) for a review). The interest in such problems originates in the work on the true self-avoiding walk (Amit *et al* 1983) in which the jump probability towards a given site depends on the number of times this site has already been visited. This walk grows for ever (kinetic walk) but is not truly self-avoiding. Among irreversible self-avoiding walks one may mention the indefinitely growing self-avoiding walk (Kremer and Lyklema 1985) which is self-avoiding and truly kinetic. A given site is never visited twice and cages are avoided so that the walk never terminates. This walk has been generalised in the Laplacian random walk (Lyklema and Evertsz 1985) where the jump probability is governed by a potential ϕ which is a solution of the discretised Laplace equation. More recently, we have studied the linear diffusion-limited aggregation (Debierre and Turban 1986) in which aggregates are grown following the rules of Witten and Sander (1981) with the restriction that the growth goes on near to the last occupied site only. In this way chains are generated which may also be considered as kinetically growing self-avoiding walks.

In the present paper, we introduce a new type of growing random walk, the self-directed walk (SDW), in which new steps are allowed when they are directed towards an open path, i.e. in a lattice direction where no site has been already visited. The probability of an allowed step i is then (figure 1)

$$p_i = 1/\text{number of open paths}. \quad (1.1)$$

With these rules the walk is truly kinetic, self-avoiding and built up of long self-directed parts in two dimensions (figure 2).

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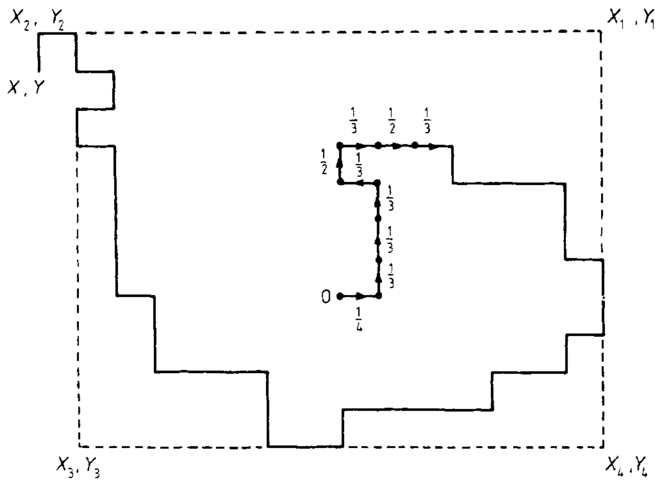

Figure 1. Construction of the self-directed walk: a new step is allowed when it is not directed towards an occupied site. The step probabilities p_i are given for the first steps. When the walker is at X, Y after a downward step, a jump to the right is forbidden as long as $Y_4 \leqslant Y$ and $X_4 > X$. A jump to the left would be forbidden if $Y_3 \leqslant Y$ and $X_3 < X$.

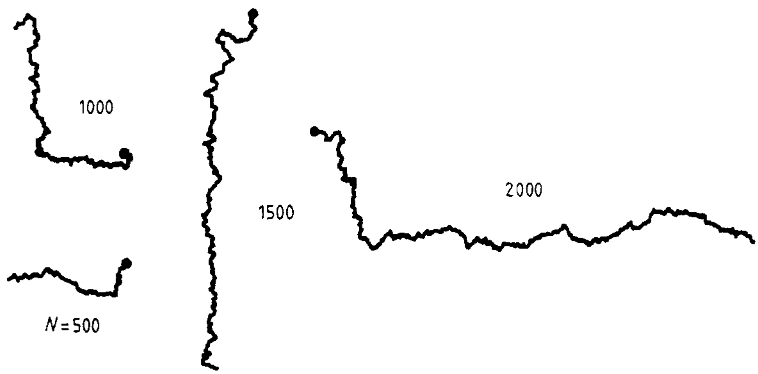

Figure 2. Self-directed walks grown on the square lattice with $N = 500$, 1000, 1500 and 2000 steps. The starting point is indicated by a circle.

The paper is organised as follows: in § 2 we present the Monte Carlo procedure which is used to grow the SDW; the numerical results are given in § 3 and discussed in § 4.

2. The Monte Carlo procedure

The walks are grown on the square lattice using a Monte Carlo method. At each step N, the following radii are stored:

$$R_e^2(N) = (\boldsymbol{r}_N - \boldsymbol{r}_0)^2 = r_N^2 \tag{2.1}$$

$$R_a^2(N) = (1/N) \sum_j r_j^2 \tag{2.2}$$

$$R_g^2(N) = (1/N^2) \sum_{i<j} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2. \tag{2.3}$$

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 walk. The calculations have been done in assembly language on 8088 and 8087 microprocessors.

The step direction is chosen at random, using a rapid shift-register random number generator (Kirkpatrick and Stoll 1981), from among the three possible ones since a backstep is forbidden. A step in the forward direction is automatically allowed. When there is a turn, in order to see whether the new step is allowed, one need only compare the position of the walker to the coordinates of one of the four corners on a convex open polygon drawn around the walk (figure 1). This procedure spares a lot of computer time since it avoids the examination of the preceding steps but it cannot be used in higher dimensions. The polygon may be modified at each new turn of the walk.

Typical SDW generated in this way are displayed in figure 2 for increasing numbers of steps ($N = 500$, 1000, 1500, 2000). It is clear in this figure that the walks are built up of successive directed parts. Walks of up to 1500 steps were generated to obtain averaged values of the radii $R_\alpha(N)$ ($\alpha = \mathrm{e, a, g}$). Averages were taken over 16 500 samples for $N \leq 500$, 6500 samples for $500 < N \leq 1000$ and 3000 samples for $N > 1000$.

3. Numerical results

The averaged radii are expected to grow with N like $\langle R_\alpha^2(N)\rangle \sim N^{2\nu}$ ($\alpha = \mathrm{e, a, g}$) for large N values. This is verified in figure 3 where $\frac{1}{2}\ln\langle R^2(N)\rangle$ is plotted against $\ln(N)$. The asymptotic behaviour sets in rather slowly only when N is greater than 150-200 steps.

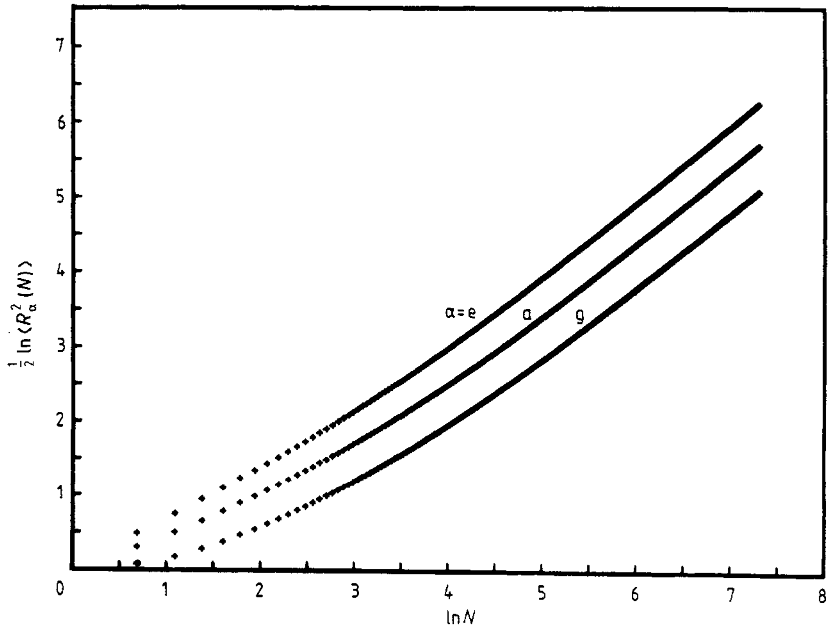

Figure 3. Plot of $\frac{1}{2}\ln\langle R_\alpha^2(N)\rangle$ against $\ln(N)$ ($\alpha = \mathrm{e, a, g}$). The asymptotic behaviour sets in slowly for $N \sim 150$-200. The slope of the linear part gives an exponent ν near to 1.

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

$$\nu_{N,M} = \tfrac{1}{2}\ln(\langle R^2(N)\rangle/\langle R^2(M)\rangle)/\ln(N/M). \tag{3.1}$$

With exact averages the best convergence is generally obtained when $M = N+1$ (Derrida and de Sèze 1982). This is not true for Monte Carlo data due to the statistical fluctuations. Better results are then obtained with larger $M-N$ values. Following Lyklema (1986) we use the following estimate:

$$\nu(N) = \tfrac{1}{2}\ln(\langle R^2(N+i)\rangle/\langle R^2(N-i)\rangle)/\ln[(N+i)/(N-i)] \tag{3.2}$$

where i is chosen in order to obtain a smooth variation with $1/N$. Large i values are needed for $\nu_e(N)$ since the fluctuations are strong in this case (figure 4). For $\nu_g(N)$ and $\nu_a(N)$, the fluctuations are much weaker and no marked evolution with i is observed for i varying between 1 and 20. The results for $\nu_e(N)$, $\nu_a(N)$ and $\nu_g(N)$ are reported in figure 5 against $1/N$ with $i=10$.

Assuming a power law correction to scaling, the mean-square radius is given by

$$\langle R^2(N)\rangle = AN^{2\nu}(1+BN^{-\Delta}+\ldots) \tag{3.3}$$

which together with equation (3.2) leads to

$$\nu(N) = \nu - \tfrac{1}{2}\Delta BN^{-\Delta}+\ldots. \tag{3.4}$$

The exponent ν may be obtained through a least-squares fit of $\nu(N)$ against $N^{-\Delta}$. This has been done for the three radii in the asymptotic regime ($N = 200$–1500) with

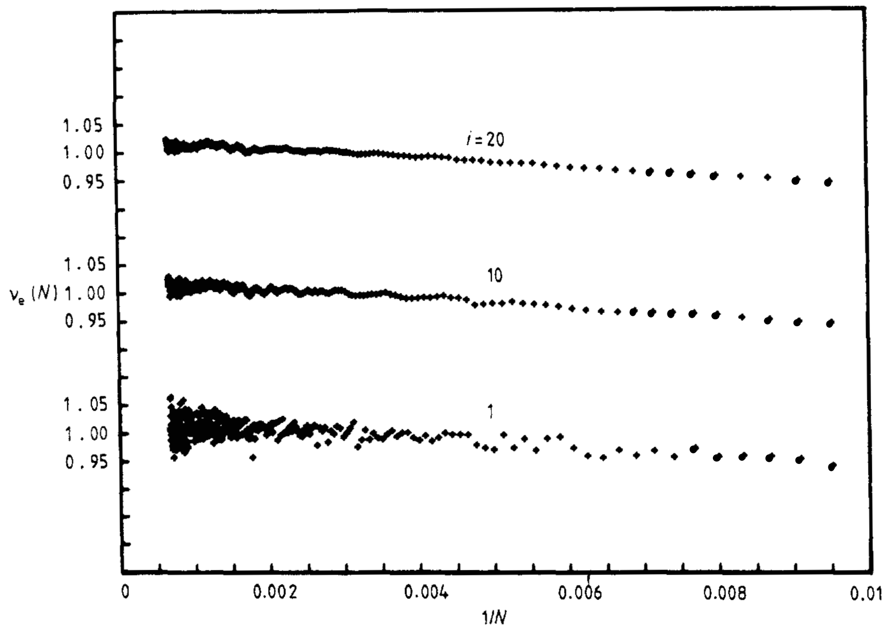

Figure 4. Plot of $\nu_e(N)$, critical exponent of the end-to-end radius, estimated using equation (3.2) with $i = 1$, 10 and 20. The effect of the statistical fluctuations is reduced by increasing i.

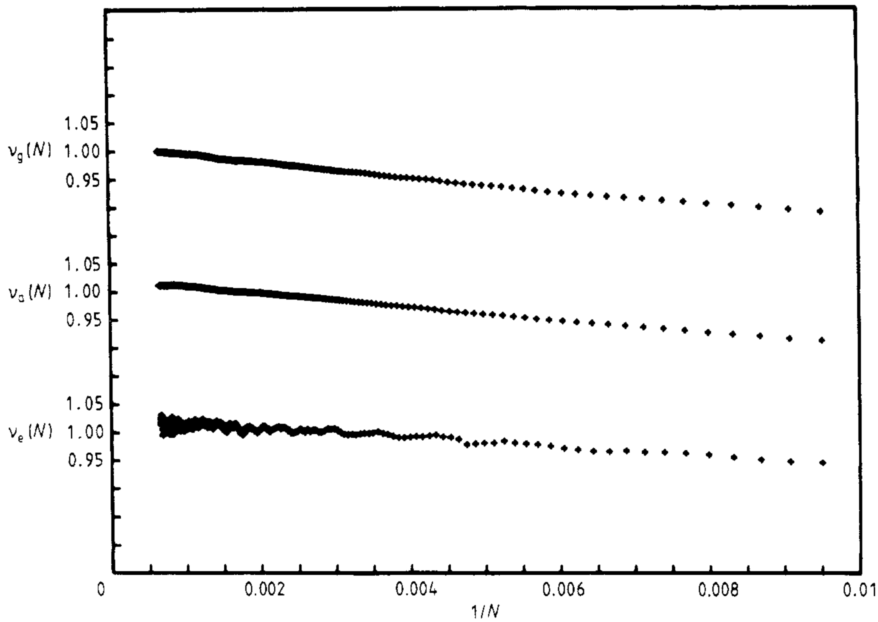

Figure 5. Plots of $\nu_e(N)$, $\nu_a(N)$ and $\nu_g(N)$ against $1/N$ with $i = 10$. The extrapolated values are given in equations (3.5), (3.6) and (3.7) in the text.

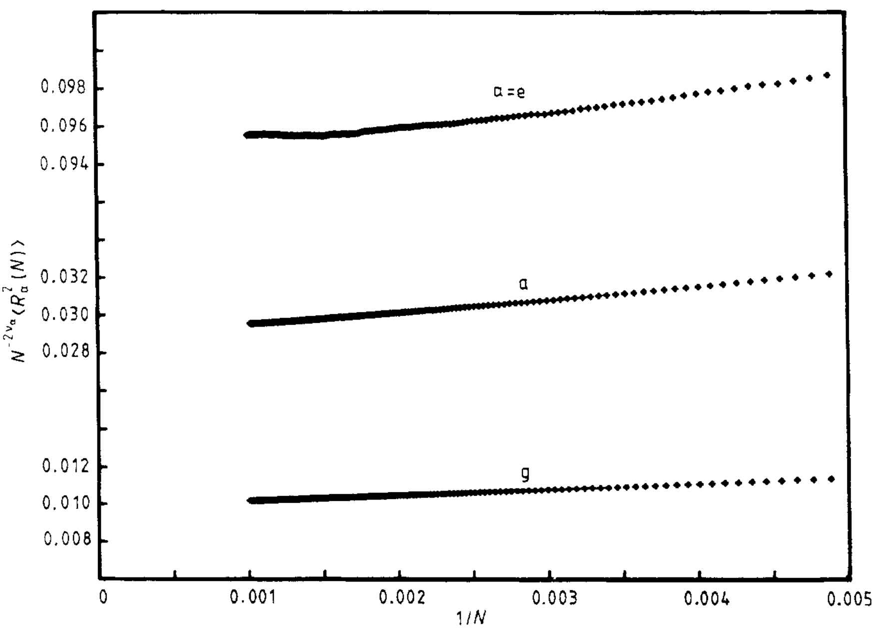

Figure 6. Plots of $N^{-2\nu_\alpha}\langle R_\alpha^2(N)\rangle$ against $1/N$ ($\alpha = \mathrm{e, a, g}$). The extrapolated values are the amplitudes A given in equations (3.8), (3.9) and (3.10) in the text.

the following results for the extrapolated values:

$$\nu_e = 1.014 \pm 0.03 \qquad \Delta_e = 1.7 \tag{3.5}$$

$$\nu_a = 1.019 \pm 0.02 \qquad \Delta_a = 1.2 \tag{3.6}$$

$$\nu_g = 1.009 \pm 0.01 \qquad \Delta_g = 1.0. \tag{3.7}$$

When the fit is done keeping only the last 1000 steps, ν_a and ν_g both decrease ($\nu_a = 1.014$, $\nu_g = 1.002$) but it is not very sensitive to the choice of Δ.

A least-squares fit of $N^{-2\nu}\langle R^2(N)\rangle$ against $N^{-\Delta}$ (figure 6) with $N = 200$–1000 gives the following amplitudes:

$$A_e = 0.095 \pm 0.001 \qquad \Delta_e = 1.9 \tag{3.8}$$

$$A_a = 0.0290 \pm 0.0001 \qquad \Delta_a = 1.2 \tag{3.9}$$

$$A_g = 0.009\,90 \pm 0.000\,05 \qquad \Delta_g = 1.1. \tag{3.10}$$

An analytic correction to scaling of order N^{-1} is expected and the analysis should give either $\Delta = 1$ or $\Delta < 1$ when the leading term is non-analytic. The values obtained for Δ_e are clearly not reliable; this is probably due to the large fluctuations observed with the end-to-end radius. The errors in Δ_a and Δ_g are smaller.

4. Discussion

For large N values, the partition function $Z(N)$ behaves like (de Gennes 1979)

$$Z(N) \propto q^N N^{\gamma-1} \tag{4.1}$$

where $N^{\gamma-1}$ is the enhancement factor. For indefinitely growing self-avoiding walks, a simple argument (Kremer and Lyklema 1985) may be used to obtain exact values for γ and q in all dimensions.

Let $P\{r_N\} = \Pi_{i=1}^{N} p_i$ be the probability of a walk of N steps with a configuration $\{r_N\}$; since the SDW never stops, the partition function

$$Z(N) = \sum_{\{r_N\}} P\{r_N\} \equiv 1 \tag{4.2}$$

where each walk is weighted by its probability P. Using equation (4.1) one obtains $\gamma = 1$ and $q = 1$. The generating function (or susceptibility) is given by

$$G(K) = \sum_N Z(N) K^N \overset{K \to K_c^-}{\propto} (K_c - K)^{-\gamma}. \tag{4.3}$$

With $Z(N) = 1$, equation (4.3) leads to $\gamma = 1$, $K_c = q^{-1} = 1$.

q in equation (4.1) is not the connective constant of the SDW since in $Z(N)$ each walk is weighted by its probability P which is generally not the same for all the N-step walks (see figure 1). It follows that $Z(N)$ no longer gives the number of walks of N steps as in the self-avoiding walk where the weight, which is the same for all the walks, may be taken to be unity.

On a Cayley tree with coordination number z each step of the SDW is done in a new lattice direction in a space of infinite dimension. Each step has a probability $p_i = (z-1)^{-1}$ and the $(z-1)^N$ walks of N steps have the same weight $P\{r_N\} = (z-1)^{-N}$ so that we recover $Z(N) = 1$; the contribution of the connective constant, which is $z - 1$ in this case, is compensated by the weight factor.

Since on a Cayley tree with $d=\infty$ the SDW is also a self-avoiding walk, one obtains $\gamma=1$ and $\nu=\frac{1}{2}$ above the upper critical dimension d_c of the SDW.

A walk cannot be more extended than a line; as a consequence one obviously has $\nu\leqslant 1$. The numerical results of § 3 suggest that $\nu=1$ for the SDW in two dimensions. This conjecture is supported by the following self-consistent calculation of ν for all d (see Pietronero 1983 for a similar treatment of the true self-avoiding walk).

Let us consider the radial motion of a random walker with asymmetric jump probabilities. After N steps, the walker is at a distance R from the origin O. Let p_{out} and p_{in} be the probabilities for a jump outside or inside the d-dimensional sphere of radius R (figure 7). When ΔN steps are added to the walk, R is changed by

$$\Delta R\sim\delta p\Delta N \qquad (4.4)$$

where $\delta p=p_{\text{out}}-p_{\text{in}}$. In the SDW δp will be proportional to the probability of having at least one visited site inside the sphere on the line MM' in the new step direction. This probability will be given by the density $\rho_p(R)$ of the projection of the walk on a $(d-1)$-dimensional surface S_{d-1} which is orthogonal to the jump direction. If $D=1/\nu$ is the fractal dimension of the walk, the dimension of the projection D_p is given by (Mandelbrot 1982)

$$D_p=\min(D, d-1) \qquad (4.5)$$

and we obtain

$$\delta p\sim\rho_p^{(R)}=\frac{R^D}{R^{d-1}}\sim N^{1-\nu(d-1)} \qquad (D\leqslant d-1) \qquad (4.6)$$

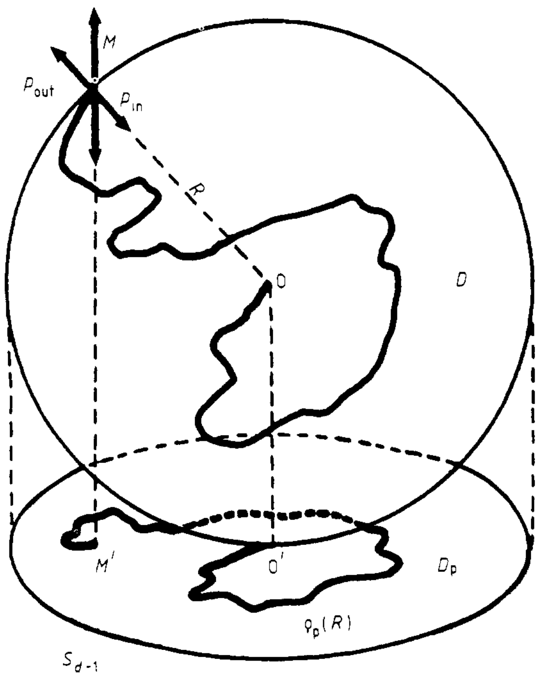

Figure 7. When the walker is at M, at a distance R from the origin O, the asymmetry δp in the jump probabilities p_{out} and p_{in} outside or inside the d-dimensional sphere of radius R is proportional to the density $\rho_p(R)$ of the projection of the walk on a surface S_{d-1} which is orthogonal to the jump direction MM'.

and

$$\delta p \sim N^0 \qquad (D \geqslant d-1). \tag{4.7}$$

When ΔN steps are added to an N-step walk, the radius $R \propto N^\nu$ is changed by

$$\Delta R \sim N^{\nu-1}\Delta N \tag{4.8}$$

and according to equations (4.4), (4.6) and (4.7)

$$\Delta R \sim N^{1-\nu(d-1)}\Delta N \qquad (1/\nu \leqslant d-1) \tag{4.9}$$

$$\Delta R \sim N^0 \Delta N \qquad (1/\nu \geqslant d-1). \tag{4.10}$$

Equation (4.9) remains valid as long as ΔR is larger than the Gaussian contribution ΔR_g which is superposed to the biased motion

$$\Delta R_g \sim N^{-1/2}\Delta N \tag{4.11}$$

so that we have three cases to consider:

(a) $-\frac{1}{2} > 1 - \nu(d-1)$: then equations (4.8) and (4.11) give $\nu = \frac{1}{2}$ and the inequality gives the upper critical dimension. The walk is Gaussian when $d > d_c = 4$.

(b) $d < 4$; $1/\nu \leqslant d-1$: equations (4.8) and (4.9) lead to $\nu = 2/d$ and the last inequality gives a lower critical dimension $d_l = 2$ at and below which the walk is cojmpletely directed ($\nu = 1$).

(c) $1 \leqslant d \leqslant 2$: then equations (4.8) and (4.10) give $\nu = 1$.

References

Amit D J, Parisi G and Peliti L 1983 *Phys. Rev.* B **27** 1635
Botet R, Jullien R and Kolb M 1984 *J. Phys. A: Math. Gen.* **17** L75
Debierre J-M and Turban L 1986 *J. Phys. A: Math. Gen.* **19** L131
de Gennes P G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
Derrida B and de Sèze L 1982 *J. Physique* **43** 475
Kirkpatrick S and Stoll E P 1981 *J. Comput. Phys.* **40** 517
Kremer K and Lyklema J W 1985 *J. Phys. A: Math. Gen.* **18** 1515
Lyklema J W 1986 *Proc. 6th Int. Symp. on Fractals in Physics* ed L Pietronero and E Tossati (Amsterdam: North-Holland) p 93
Lyklema J W and Evertsz C 1986 *Proc. 6th Int. Symp. on Fractals in Physics* ed L Pietronero and E Tossati (Amsterdam: North-Holland) p 87
Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
Pietronero L 1983 *Phys. Rev.* B **27** 5887
Witten T A and Sander M 1981 *Phys. Rev. Lett.* **47** 1400