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The collapse transition of linear polymers on fractal lattices

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Abstract. We show that for linear polymers a collapse transition exists on several fractal lattices and obtain exact results for the critical exponents at this transition. A 'rod-like' phase is found in some cases at intermediate temperatures, between the swollen phase and the collapsed phase. We introduce infinitesimal recursion relations with correlation function rescaling as the formal limit of a class of fractals, which give a better approximation to Euclidean 2D lattices. The gyration radius exponent at the transition temperature lies in the range $\nu_t = 0.546 \pm 0.010$, in good agreement with a recent transfer matrix calculation. The possible relevance of anisotropy at the collapse transition is discussed.

1. Introduction

Flexible linear polymers in very dilute solution in a poor solvent can undergo a collapse transition, where an individual polymer chain shrinks from a swollen state to a globule state when the temperature is lowered (see de Gennes (1979) for a general introduction). Much work has been devoted to the study of this transition because of its experimental importance and its possible relevance to protein folding. On the theoretical side, this transition corresponds, in the limit of infinite chain length, to a tricritical point, by analogy with magnetic systems, and renormalisation group methods give predictions differing from those of mean-field-type theories (Stephen 1975, Duplantier 1982, 1986, Kholodenko and Freed 1984).

At the transition temperature T_c for the infinite chain, there is a compensation between the non-crossing constraint that tends to swell the polymer and the short-range attractions that favour a dense state. In the classical picture, the polymer chain becomes ideal (Gaussian) on large length scales and the radius of gyration exponent is $\nu_t = \frac{1}{2}$, as for a purely random walk, independent of the space dimension d . Dimensional arguments show that the upper critical dimension is $d_c = 3$ for this transition, with the consequence that the expression for the radius of gyration contains additional logarithmic factors in three dimensions.

The two-dimensional case is interesting as one expects the collapse transition to occur with non-classical values for the critical exponents. A recent conjecture relates the exponent ν_t to that of an infinitely growing self-avoiding walk (SAW) and also to the exponents describing the geometry of percolation clusters (Coniglio *et al* 1985). Exponents have been determined by real space renormalisation (Marquse and Deutch 1981), Monte Carlo simulations (Baumgärtner 1982) and transfer matrix calculations (Derrida and Saleur 1985, Saleur 1985). It is also feasible to study experimentally

two-dimensional polymer systems (Vilanove and Rondelez 1980, Takahashi *et al* 1983, Granick 1985).

No complete solution of self-avoiding walks with interactions on regular lattices is known. It is therefore instructive to study the problem on some fractal lattices where exact results can be obtained. In general, one can expect a collapse transition with non-ideal behaviour to exist for interacting SAW on fractal lattices, if their effective dimension is less than three. In the present paper, we elaborate on our previous studies of self-avoiding walks on fractal lattices (Dhar 1978, hereafter referred to as I, Rammal *et al* 1984) and show that a collapse transition indeed exists on several lattices of Hausdorff dimension $D_f = 2$. The transition does not occur on the two-dimensional Sierpinski gasket studied earlier by Klein and Seitz (1984) because of its low ramification number. On the fractals studied here, exact recursion relations can be written for the generating function of the polymer and their fixed points correspond to the different phases of the chain. The eigenvalues of the recursion relations at these fixed points yield the gyration radius exponent ν_t and the specific heat exponent α at the collapse transition. In particular, these exponents can be obtained in closed form on the 3D Sierpinski gasket, thus providing a simple example for an *exactly solved model showing a tricritical point*, which may be of pedagogical value.

Our exact calculations show that the phenomenon of polymer collapse can be rather intricate on some fractal lattices. On the modified rectangular lattice (MRL), a fractal introduced in Dhar (1977), we find an intermediate 'rod-like' phase between the swollen phase and the collapsed one. In an effort to understand this unexpected feature, we study a variant with infinitesimal recursion relations, analogous to a Migdal-Kadanoff-type renormalisation, which should give an approximate description of a standard two-dimensional system. We find in this case a normal collapse transition, but anisotropy in the interactions becomes a relevant perturbation precisely at the transition point, which is therefore multicritical.

2. The Sierpinski gasket

The simplest fractal lattice for which the interacting self-avoiding walk may be studied is the Sierpinski gasket, which has now become a standard system for the discussion of many statistical problems. The attractive SAW on this lattice have been studied earlier by Klein and Seitz (1984) who found that on this lattice there is no collapse transition. We consider below a slightly different fractal, the truncated 3-simplex lattice (Dhar 1977, 1978), in order to introduce two very useful and general reductions. The 3-simplex (figure 1) has been shown to belong to the same universality class as the Sierpinski gasket (Rammal *et al* 1984) and it has the advantage of giving simpler equations for the present problem.

The weight of a walk having n steps and r nearest neighbours is $x^n w^r$. Following I, we define $B^{(r)}(x, w)$ as the sum over all walk configurations entering through one corner vertex of an r th order triangle and leaving via a second corner vertex. We also define $B_1^{(r)}(x, w)$ as the restricted sum over all walks entering one vertex of the r th order triangle and leaving via the second vertex having visited the third corner vertex as well (figure 2). The generating function of closed loops is a function of x and w given by

$$P(x, w) = \sum_r 3^{-r} [B^{(r)}(x, w)]^3. \quad (2.1)$$

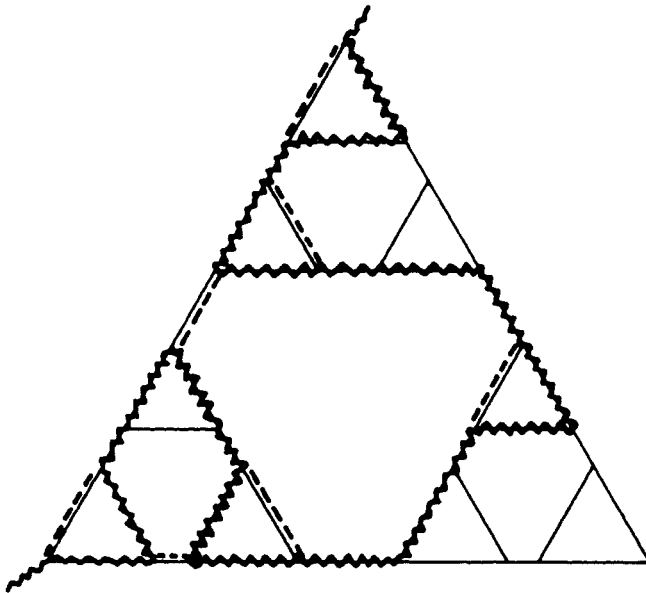


Figure 1. A self-avoiding polymer (~~~~) on a 3-simplex lattice at the third stage of construction ($r=3$). The attractive interactions between neighbouring sites are denoted by broken lines.

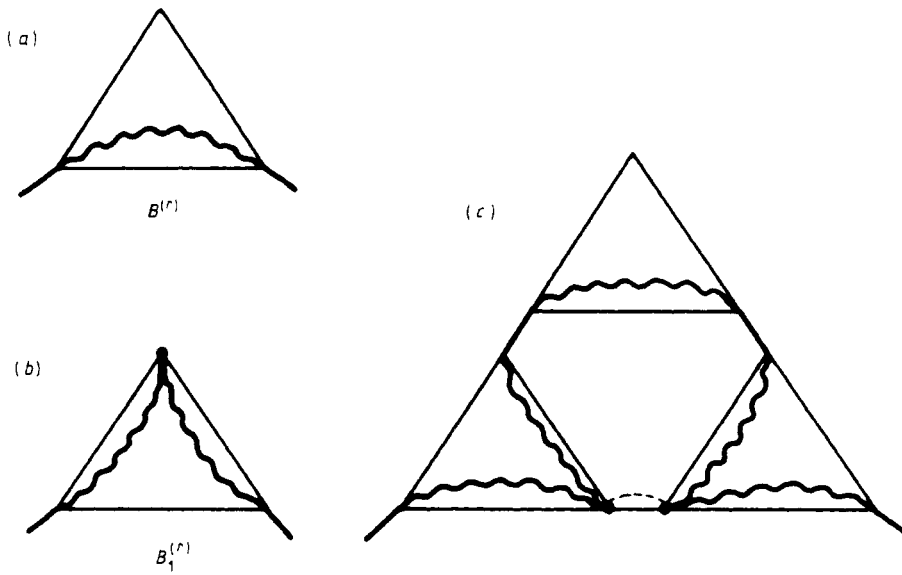


Figure 2. Diagrammatic representation of the weights $B^{(r)}$ and $B_1^{(r)}$. The configuration shown in (c) contributes a term $wB^{(r)}[B_1^{(r)}]^2$ to $B^{(r+1)}$ on the 3-simplex lattice (note that $B^{(r)}$ contains $B_1^{(r)}$).

The recursion equations for $B^{(r)}$ and $B_1^{(r)}$ are easily written down:

$$\begin{aligned} B^{(r+1)} &= B^{(r)2} + B^{(r)}[(B^{(r)} - B_1^{(r)})^2 + 2B_1^{(r)}(B^{(r)} - B_1^{(r)})] + wB^{(r)}B_1^{(r)2} \\ &= B^{(r)2} + B^{(r)3} + (w - 1)B_1^{(r)2}B^{(r)} \end{aligned} \tag{2.2}$$

and

$$B_1^{(r+1)} = B_1^{(r)}B^{(r)2} + (w - 1)B_1^{(r)3} \tag{2.3}$$

noting that B contains B_1 with our notation and that one has to avoid double counting of configurations. The initial weights are

$$B^{(1)} = x^2 + x^3w \tag{2.4}$$

$$B_1^{(1)} = x^3w \tag{2.5}$$

assigning, as in I, a weight x to every vertex that the walk passes through (and a weight $x^{1/2}$ to each of the endpoints of the chain).

These equations are exact for the 3-simplex lattice. We define new variables $\tilde{B}_1^{(r)} = (w - 1)^{1/2}B_1^{(r)}$ and the recursion equations become

$$B^{(r+1)} = B^{(r)2} + B^{(r)3} + B^{(r)}\tilde{B}_1^{(r)2} \tag{2.6}$$

$$\tilde{B}_1^{(r+1)} = \tilde{B}_1^{(r)}[B^{(r)2} + \tilde{B}_1^{(r)2}]. \tag{2.7}$$

Thus the weight factor $(w - 1)$ can be absorbed in the definition of variables of recursion and does not appear explicitly in the recursion equations. This is the first reduction.

Also, from equations (2.6) and (2.7), we have

$$\tilde{B}_1^{(r+1)}/B^{(r+1)} < \tilde{B}_1^{(r)}/B^{(r)}. \tag{2.8}$$

Thus, if $B^{(r)}$ stays finite as r tends to infinity, then $\tilde{B}_1^{(r)}$ must tend to zero. Then these variables drop out of the recursion equations, and the recursion equations for $B^{(r)}$ are the same as in the non-attractive case. This is the second reduction. This implies that, to find the fixed points and critical exponents in the case of walks with interactions, an analysis of recursion equations for the non-attractive walks is sufficient.

The physical argument used to understand this phenomenon is the following. By universality, one expects that a SAW with attractive interactions only on bonds lying within first-order triangles will have the same phase transition as one with attractive interactions at all bonds. But for the former problem, the recursion equations are the same as for the non-attractive case. The attraction strength w appears only in the initial values of the weights (equations (2.4) and (2.5)). These are needed to determine the location of critical points and the phase boundaries but not to determine the qualitative phase diagram and critical exponents.

In this specific case, as $B_1^{(r)}$ tends to zero for large r , equation (3.6) reduces to

$$B^{(r+1)} = B^{(r)2} + B^{(r)3}. \tag{2.9}$$

This equation has only one non-trivial positive real fixed point $B^* = (\sqrt{5} - 1)/2$ corresponding to the swollen phase of the chain. Thus, we find no collapsed phase, in agreement with the result of Klein and Seitz (1984).

3. The three-dimensional Sierpinski gasket

In order to get a collapsed phase, we have to consider a lattice with higher ramification number to allow for extended contact between different segments of the chain. The

ramification number of the three-dimensional Sierpinski gasket is four and we show below that it is sufficient to ensure the existence of a collapsed phase. The 3D gasket has a self-similar tetrahedral structure which generalises the triangular structure of the 2D gasket. It is in the same universality class as the truncated 4-simplex lattice (Dhar 1977, 1978) and here we restrict our attention to the 4-simplex, which gives simpler equations. The recursion relations are, in that case,

$$A^{(r+1)} = A^2 + 2A^3 + 2A^4 + 4A^3B + 6A^2B^2 \quad (3.1)$$

$$B^{(r+1)} = A^4 + 4A^3B + 22B^4 \quad (3.2)$$

where $A^{(r)}$ (respectively $B^{(r)}$) is the partial generating function for chains going once (twice) through an r th order tetrahedron (figure 3). We restrict the attractive interaction to bonds within the first-order gasket. Then the starting values of these weights are

$$A^{(1)} = x^2 + 2x^3w + 2x^4w^3 \quad (3.3)$$

$$B^{(1)} = x^4w^4. \quad (3.4)$$

Equations (3.1) and (3.2) have three non-trivial positive real fixed points.

(i) The fixed point $(A^*, B^*) \approx (0.4294 \dots, 0.04998 \dots)$, corresponding to the swollen state of the chain. The end-to-end distance for a chain of N steps in this phase varies as N^ν with $\nu = 0.7294 \dots$. For $x = x_c(w)$, this fixed point is reached for all $w < w_c = 2 + 3^{1/4} = 3.316 \dots$.

(ii) The fixed point $(A^*, B^*) = (0, 22^{1/3})$. Linearising recursion relations about this fixed point, we find the largest eigenvalue $\lambda_1 = 4$, corresponding to $\nu = 1/D_f = \frac{1}{2}$. This phase therefore has a finite density of monomers per site and is the collapsed phase. For all $w > w_c$ and $x = x_c(w)$, the recursion equations iterate to this fixed point.

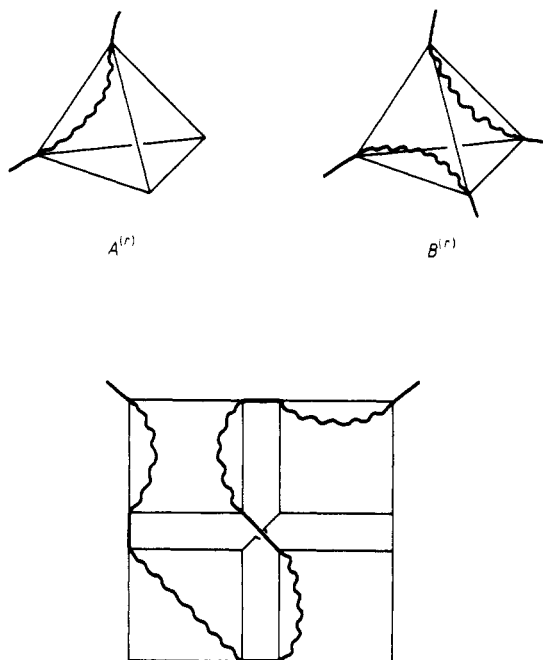


Figure 3. Diagrams defining the weights $A^{(r)}$ and $B^{(r)}$ for the 3D Sierpinski gasket (or 4-simplex lattice). The particular configuration shown in projection gives a contribution $A^{(r)3}B^{(r)}$ to $A^{(r+1)}$.

(iii) If $w = w_c$ and $x = x_c(w_c)$, then the equations (3.1) and (3.2) remain at the fixed points $(A^*, B^*) = (\frac{1}{3}, \frac{1}{3})$. The linearised renormalisation transformation near this fixed point has both eigenvalues greater than 1. We get $\lambda_1 = \frac{100}{27}$, $\lambda_2 = \frac{20}{9}$. This is a tricritical point, the third relevant eigenvalue being the 'magnetic field' scaling eigenvalue corresponding to the renormalisation of the endpoints of chains.

The behaviour of thermodynamic quantities near this transition, which corresponds to the infinite-chain θ temperature, can be determined by arguments similar to those of Derrida and Herrmann (1983) in their discussion of the collapse of branched polymers. One finds that the specific heat of the polymer chain diverges as $|w - w_c|^{-\alpha}$ with $\alpha = 2 - (\log \lambda_1 / \log \lambda_2) \approx 0.36027$, and the thermal correlation length diverges as $|w - w_c|^{-\nu_2}$ where $\nu_2 = \log 2 / \log \lambda_2 \approx 0.8680$. At the transition the end-to-end length of the chain scales as N^{ν_1} with $\nu_1 = \log 2 / \log \lambda_1 \approx 0.52939$. In the compact phase near the critical temperature, the average density of the polymer vanishes as $(w - w_c)^\beta$ with $\beta = \nu_2(2 - \nu_1) \approx 0.09638 \dots$

The fact that the tricritical fixed point $(\frac{1}{3}, \frac{1}{3})$ and its eigenvalues can be obtained in closed form is a pleasant surprise. It can also be used to study the specific heat near the transition in detail and determine the region where the asymptotic form $|w - w_c|^{-\alpha}$ is valid. Numerically, one finds that $|w - w_c|$ has to be as small as 10^{-4} - 10^{-5} to obtain, on a log-log plot, a value of α within less than 10% of the exact value.

4. The modified rectangular lattice (MRL)

This lattice has a self-similar rectangular structure (figure 4) and its fractal dimension $D_f = 2$ is equal to the space dimension, but it has interesting properties, in particular for self-avoiding walks (Dhar 1977, 1978). In this case, the number of variables in the

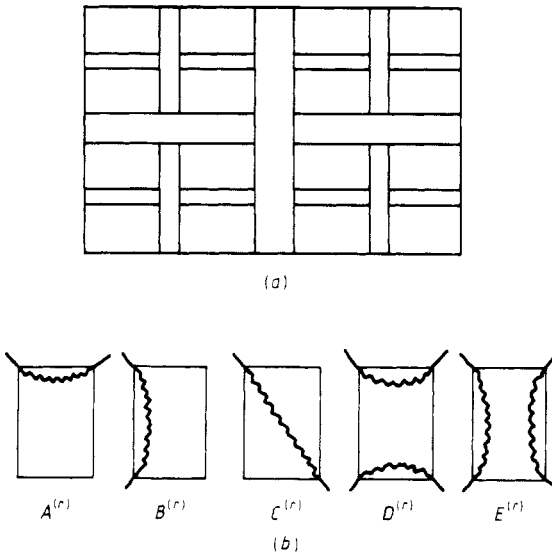


Figure 4. (a) Modified rectangular lattice at the fifth order of construction. (b) Diagrams representing the restricted partition functions for the various ways the polymer can cross the r th order rectangle.

recursion equations is larger and their analysis much more complicated. The non-attractive case involves recursions in nine variables for a complete treatment. To describe interacting walks, we have to introduce additional variables. For example, to describe closed loops it is necessary to introduce additional weights $A_1^{(r)}, B_1^{(r)}, C_1^{(r)}, A_2^{(r)}, B_2^{(r)}, C_2^{(r)}$, where the subscript 1(2) indicates a restricted summation over configurations where 1(2) extra corner sites of the r th-order rectangle are visited (figure 5). This gives a total of eleven variables. To describe open chains, we would need 17 additional variables, making a total of 28 variables—a rather formidable number.

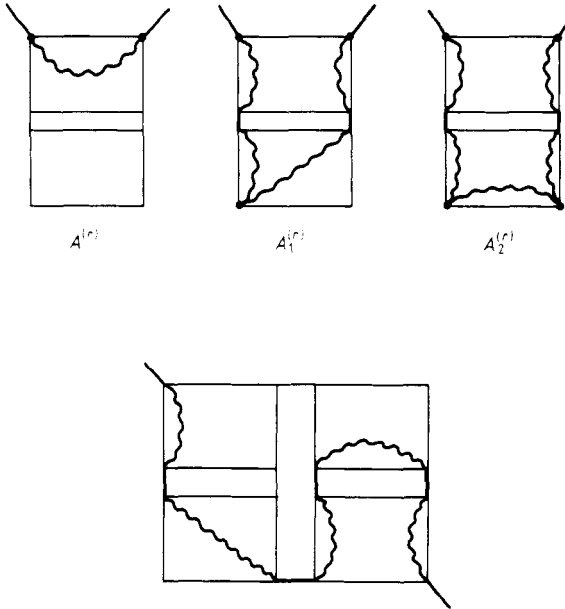


Figure 5. Diagrams defining the weights A, A_1 and A_2 for the modified rectangular lattice. The lower diagram corresponds to a term $A^{(r)}B^{(r)}C^{(r)}D^{(r)}$ and contributes to $C^{(r+2)}$.

However, as shown in § 2 for the gasket, most of these variables are irrelevant and may be set equal to zero. This can be shown explicitly for the additional weights $A_1^{(r)}, B_1^{(r)}, \dots$ (d’Humières 1985). Furthermore, except for calculating the susceptibility exponent γ (which is not directly determinable by experiments) the analysis of closed polygons is sufficient, which requires only five variables $A^{(r)}, B^{(r)}, C^{(r)}, D^{(r)}$ and $E^{(r)}$ (figure 4).

In the case where attractive interactions are restricted to bonds within the first-order rectangle, the initial values of these weights are

$$(A, B, C, D, E)^{(r)} = (x^2 + x^4w, x^2 + x^4w, 2x^3, x^4w^2, x^4w^2) \tag{4.1}$$

and the recursion equations are

$$A^{(r+1)} = B(1 + D) \tag{4.2}$$

$$B^{(r+1)} = A^2 + C^2 \tag{4.3}$$

$$C^{(r+1)} = 2AC \tag{4.4}$$

$$D^{(r+1)} = B^2 + 2DE \tag{4.5}$$

$$E^{(r+1)} = D^2. \tag{4.6}$$

We determined numerically the critical value $x_c(w)$ for which the recursion equations tend to a non-trivial fixed point and we studied the fixed points so obtained as a function of w . The full system of eleven equations was also studied. It gives different values for the transition points, but the structure of the phase diagram and the critical exponents are unchanged. The following behaviour is observed.

(i) For weak attractions, $w < w_c \approx 3.2023$ and $x = x_c(w)$, the fixed point reached is

$$(A^*, B^*, C^*, D^*, E^*) = \left(\frac{1}{2}, \frac{1}{2(1+D^*)}, \frac{1}{2} \left(\frac{1-D^*}{1+D^*} \right)^{1/2}, D^*, D^{*2} \right)$$

where D^* is the smaller of the two positive real solutions of the equation

$$D^* = \frac{1}{4(1+D^*)^2} + 2D^{*3}. \tag{4.7}$$

Numerically $D^* \approx 0.190\ 24$. This is the fixed point corresponding to the swollen phase of the polymer and linearised recursion equations near this point have only one relevant eigenvalue $\lambda_1 \approx 1.683\ 94$. This corresponds to

$$\nu = \log 2 / 2 \log \lambda_1 \approx 0.665\ 03 \tag{4.8}$$

the same exponent as in the case of no interaction ($w = 1$).

(ii) For large interactions $w > w_{c_2} \approx 3.2341$, one tends to an oscillatory fixed point characterised by vanishing values of $A^{(r)}, B^{(r)}, C^{(r)}$ and non-vanishing values of $D^{(r)}$ and $E^{(r)}$. The fixed point can be characterised by a parameter α which is a continuous function of w and is given by

$$(0, 0, 0, \alpha/\sqrt{2}, 1/2\alpha^2) \leftrightarrow (0, 0, 0, 1/\sqrt{2}\alpha, \alpha^2/2).$$

This is thus a line of fixed points of period 2. Small perturbations around this solution are simpler to study if we iterate the recursion relations once. This has the effect of multiplying the lattice dimension by a factor 2 in both directions. Then each of the period-2 points becomes a simple fixed point. Linear analysis about any of these fixed points gives a relevant eigenvalue $\lambda_1 = 4$, which corresponds to the collapsed phase with $\nu = \frac{1}{2}$. A second eigenvalue is marginal, $\lambda_2 = 1$, corresponding to displacement along the line of fixed points.

The period-2 nature of this fixed point shows that in this phase the horizontal and vertical directions are not equivalent and the average extents of the polymer in the two directions are not equal (though both vary as $N^{1/2}$, where N is the number of links in the chain). As w tends to w_{c_2} from above, α increases continuously to infinity and thus the anisotropy increases as we approach w_{c_2} .

Between the swollen and collapsed phase, we do not find a standard collapse transition, but a more complicated behaviour.

(iii) For $w_{c_1} < w < w_{c_2}$, one tends to the period-2 fixed points

$$(1, 0, 0, 1, 0) \leftrightarrow (0, 1, 0, 0, 1).$$

It is easy to verify that in this case the largest eigenvalue of the linearised recursion relations is 2, corresponding to $\nu = 1$. Thus the polymer is in an extended ‘rod-like’ phase with the average end-to-end length proportional to N . The rapid convergence to zero observed for the two-point correlation function in the perpendicular direction implies that the average width of the polymer stays finite.

(iv) For $w = w_{c_1}$, the variables iterate to cycle-2 fixed points:

(0.259 72; 0.944 75; 0.259 77; 0.018 86; 0.855 28)

\leftrightarrow (0.962 57; 0.134 93; 0.134 93; 0.924 82; 0.000 36).

Linearising the once iterated recursion equations about any one of these two points, we find that there are two relevant eigenvalues, $\lambda_1 \approx 2.365 57$ and $\lambda_2 \approx 1.593 99$. Analysis of thermodynamic quantities is as in the case of the 3D Sierpinski gasket. We get $\nu \approx 0.805 03$ and the specific heat singularity exponent $\alpha \approx 0.153 27$. Note that the value of ν at this point is intermediate between those for the non-attractive and the 'rod-like' phases.

(v) If $w = w_{c_2}$, the behaviour of recursion equations is more complicated. Firstly, we have even-odd oscillations as in the previous three cases. Confining our attention to even iterates (the behaviour of odd iterates is determined by a simple recursion), we find the following behaviour to lowest order in r when r goes to infinity:

$$A^{(2r)} = 1 - 3/2r + \dots \quad (4.9)$$

$$B^{(2r)} = C^{(2r)} = 0 \quad (4.10)$$

$$D^{(2r)} = r/3 + \dots \quad (4.11)$$

$$E^{(2r)} = 9/4r^2 + \dots \quad (4.12)$$

It is easy to verify that equations (4.9)-(4.12) are consistent with the iteration equations (4.2)-(4.6). Higher-order terms in a systematic expansion involve logarithms.

If, instead of the variables $D^{(r)}$ and $E^{(r)}$, we choose variables $X^{(r)} = 4D^{(r)2}E^{(r)}$ and $Y^{(r)} = 1/D^{(r)}$ then the fixed point occurs for $X^* = 1$, $Y^* = 0$. Eigenvalues of the linearised iterated renormalisation transformation near this point are 4, 2, 1. Thus at this point we have $\nu = \frac{1}{2}$ and the specific heat singularity exponent $\alpha = 0$ (logarithmic singularity).

5. Infinitesimal recursions

The surprising feature of the calculations in the previous section is the existence of the intermediate rod-like phase. In this phase the average extent of the polymer in the two directions varies as different powers of N (N^1 and N^0) for large N . This is quite different from the usual behaviour of anisotropic systems where the correlation lengths in different directions have different amplitudes but diverge with the same exponent near criticality. Different exponents in different directions are known in systems with preferred orientation (directed percolation (Kinzel 1983)) or in systems at disorder points or at Lifschitz points (Hornreich 1980). Our problem is distinct from these and it is desirable to understand the origin of two correlation lengths in this system better.

A possible origin for the strong anisotropy displayed in our case may be the asymmetry between the horizontal and vertical directions in the MRL. There are more horizontal than vertical bonds on this lattice at any stage of iteration. It is, however, possible to eliminate this anisotropy in the MRL by a formal device. We consider the generalised MRL with arbitrary index p (figure 6), which retains the same fractal

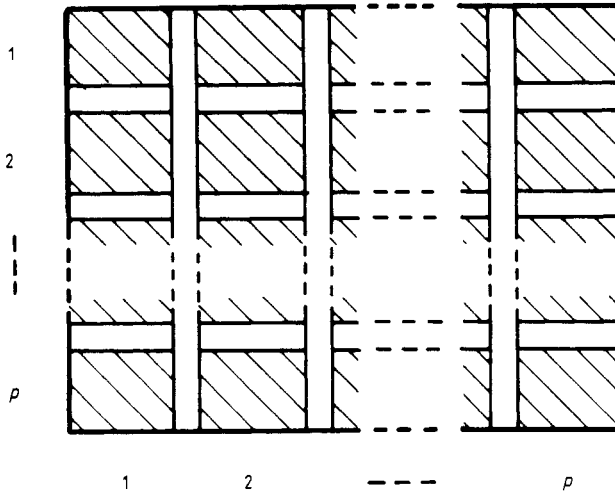


Figure 6. A graphical representation of the recursive construction of the modified rectangular lattice of index p .

dimension $D_f = 2$. We obtain for the recursion equations, for any integer value of p ,

$$A' = B(1 - D^p)/(1 - D) \tag{5.1}$$

$$B' + C' = (A + C)^p \tag{5.2}$$

$$B' - C' = (A - C)^p \tag{5.3}$$

$$D' = pD^{p-1}E + B^2 \left(\frac{1 - D^p}{(1 - D)^2} - p \frac{D^{p-1}}{(1 - D)} \right) \tag{5.4}$$

$$E' = D^p. \tag{5.5}$$

It is easy to verify that for $p = 2$ these equations reduce to equations (4.2)-(4.6). The case $p = 3$ has been discussed earlier in I. For larger values of p , the lattice becomes more and more anisotropic. These equations are continuous functions of p and we may formally continue them analytically for all real (positive) values and put $p = 1 + \epsilon$ with ϵ infinitesimal. Then, iterating these equations twice, we get a lattice whose linear extent is $(1 + \epsilon)$ times larger in both horizontal and vertical directions. The equations then become differential equations for the change in the weights with the length scale L . Simple algebra gives

$$dA/d \log L = \frac{1}{2}[(A + C) \log(A + C) + (A - C) \log(A - C)] - (AE \log E)/(1 - E) \tag{5.6}$$

$$dB/d \log L = \frac{1}{2}[(B + C) \log(B + C) + (B - C) \log(B - C)] - (BD \log D)/(1 - D) \tag{5.7}$$

$$dC/d \log L = \frac{1}{2}[(A + C) \log(A + C) - (A - C) \log(A - C)] + (B + C) \log(B + C) - (B - C) \log(B - C) \tag{5.8}$$

$$dD/d \log L = -A^2[1 + (\log E)/(1 - E)]/(1 - E) + D(1 + \log DE) \tag{5.9}$$

$$dE/d \log L = -B^2[1 + (\log D)/(1 - D)]/(1 - D) + E(1 + \log DE). \tag{5.10}$$

Note that if the starting system is symmetric in the horizontal and vertical directions, so that if $A = B$ and $D = E$ at some length scale $L = L_0$, then by equations (5.6)–(5.10) the system will remain symmetric under renormalisation. We have thus recovered the symmetry between x and y directions in the recursion equations by the formal trick of letting $p \rightarrow 1$.

6. Analysis of the phase diagram for the infinitesimal recursions

We now introduce anisotropic interactions in the two directions $w_x = w\theta$ and $w_y = w/\theta$, where the parameter θ measures the strength of the anisotropy, with $\theta = 1$ corresponding to the isotropic system. The starting values of the weights (A, B, C, D, E) may then be taken as

$$(x^2 + x^4 w\theta, x^2 + x^4 w/\theta, 2x^3, x^4 w^2 \theta^{-2}, x^4 w^2 \theta^2)$$

and the whole problem has a symmetry ($\theta \leftrightarrow 1/\theta, A \leftrightarrow B, D \leftrightarrow E$).

The analysis of these equations gives us the following phase diagram for this problem (figure 7).

(i) For w and θ lying in region I and x equal to its critical value $x_c(w, \theta)$, we tend to the non-trivial fixed point (0.455 194; 0.455 194; 0.420 751; 0.099 446; 0.099 446). Linearised renormalisation equations about this fixed point have only one relevant eigenvalue $\lambda = 1.5114 \dots$. For infinitesimal recursions, one readily sees that $\nu = 1/\lambda$ in general, so $\nu = 0.6616 \dots$ here. This fixed point describes the swollen phase of the SAW.

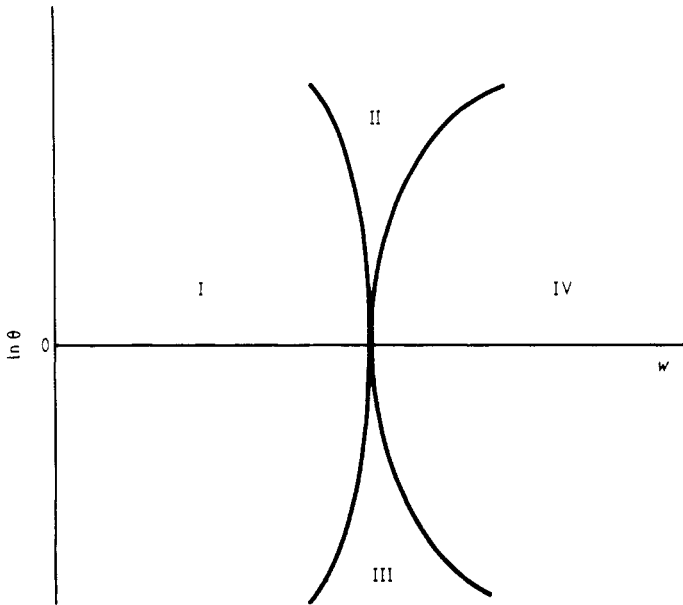


Figure 7. Schematic phase diagram given by the infinitesimal recursions (5.6)–(5.10): w is the mean interaction strength and θ the anisotropy parameter ($\theta = (w_x/w_y)^{1/2}$). Region I corresponds to a swollen (SAW) phase, regions II and III to rod-like phases and region IV to a collapsed phase.

(ii) In region IV, we find a *line* of fixed points describing the collapsed phase:

$$(A^*, B^*, C^*, D^*, E) = (0, 0, 0, e^{-1/2}\alpha, e^{-1/2}/\alpha)$$

where the parameter α varies continuously with θ and is equal to 1 for $\theta = 1$. Linearised renormalisation equations about this fixed point have one relevant eigenvalue $\lambda_1 = 2$ ($\nu = 1/D_f = \frac{1}{2}$) and a marginal operator (corresponding to anisotropy) with eigenvalue 0.

(iii) Regime II is the region of attraction for the fixed point $(0, 1, 0, 0, 1)$. Again for this fixed point there is only one positive eigenvalue $\lambda_1 = 1$, corresponding to $\nu = 1$, so it describes a rod-like phase. Regime III is obtained by symmetry, so the rods there are aligned in the other direction.

(iv) For initial values of (w, θ) lying on the boundary between phase I and II, the variables tend to the fixed point $(0.193\ 59; 0.956\ 22; 0.193\ 56; 0.004\ 436; 0.902\ 48)$. This is a tricritical point, with two relevant eigenvalues: $\lambda_1 \approx 1.2463$ and $\lambda_2 \approx 0.671\ 999$. At this boundary, the mean size of polymer varies as $N^{\nu'}$ with $\nu' \approx 0.8024$ and the specific heat singularity is given by $\alpha = 2 - \lambda_1/\lambda_2 \approx 0.1454$.

(v) The point $w = w_c \approx 3.1782$, $\theta = 1$, which is the common point on the boundaries of the four phases I, II, III and IV, corresponds to the fixed point

$$(0.394\ 95; 0.394\ 95; 0.261\ 64; 0.546\ 26; 0.546\ 26).$$

This point is the analogue of the usual tricritical point found in studies of the collapse transition, but here it is a multicritical point where four eigenvalues of the linearised recursions are relevant. The largest one is $\lambda_1 = 1.8653$ corresponding to $\nu_1 = 0.5361$ at this point. The next largest eigenvalue λ_2 describes the rescaling of the interactions and the corresponding value of the specific heat exponent α is 0.204. The other two relevant eigenvalues are complex ($\lambda = 0.2402 \pm 0.250i$) and are associated to the fact that *anisotropy is a relevant operator at this point*.

(vi) The boundary between regions II and IV is described by an anisotropic tricritical point. The behaviour of variables A, B, C, D, E for large L in this case is quite similar to that in the case $p = 2$, except that there are more logarithmic correction terms.

In detail:

$$A(L) \approx 1 - 2/(e \log L) + \dots \quad (6.1)$$

$$B(L) \approx C(L) \approx 0 \quad (6.2)$$

$$D(L) = 1/2 \log L \log(\log L) + \dots \quad (6.3)$$

$$E(L) \approx (e D(L))^{-1}. \quad (6.4)$$

The largest eigenvalue is $\lambda_1 = 2$ (i.e. $\nu = \frac{1}{2}$), as in the case $p = 2$.

Notice that the critical exponents and the values of fixed points are not very different from the case $p = 2$. The insensitivity of the exponents to the value of p is an *a posteriori* justification of the formal analytic continuation in p .

7. Approximate recursions with Green functions rescaling

For $p = 1 + \varepsilon$, we cannot give a graphical representation of the lattice. This is, however, a special limit of a class of planar lattices with rectangular symmetry and should imitate a two-dimensional square lattice. However, the value $\nu_1 = 0.6616$ should be compared

with the exact value $\frac{3}{4}$ known for the square lattice, and clearly the values are quite different.

The reason for the difference is clear: our calculation is essentially a real space renormalisation group calculation which, while exact on fractals, cannot give correct results for two-dimensional systems unless we introduce 'spin rescaling' in the problem (Van Leeuwen 1975, Griffiths 1981). In two dimensions at the critical point, the two-point Green functions A , B , C are expected to vary as L^{-x} , and the four-point functions D and E as L^{-2x} where x is some exponent which depends on the scaling power of the *corner* spin variables.

However, on finitely ramified fractal lattices, these functions at the critical point go to a constant for large distances. In order to obtain reasonable estimates of the exponents in two dimensions, we must devise a renormalisation prescription that allows power-law decay of the correlation functions at the critical point. This can be done approximately by rescaling the variables $A(L)$, $B(L)$, $C(L)$ by a factor L^x and $D(L)$ and $E(L)$ by L^{2x} , after renormalisation by a scale factor L . The new equations will have fixed points (A^* , B^* , ...) so that the unscaled $A(L)$, $B(L)$... decay as A^*L^{-x} , B^*L^{-x} , ... for large L . Several different criteria may be chosen to determine the value of x within the renormalisation scheme and it is difficult to choose amongst them, so we prefer to treat it as a free parameter.

This spin rescaling adds terms xA , xB , xC , $2xD$ and $2xE$ to the right-hand sides of equations (5.7)-(5.10) respectively. For $x=0$, we get no spin rescaling. For $x=1$, the effect of rescaling may be interpreted as a Migdal-Kadanoff type bond-moving approximation in which the *weight* of a bond connecting two r th-order rectangles is $x2^{r/2}$ instead of being simply x . We consider for concreteness the case $p=2$. (Notice that the modified rectangular lattice can be obtained by a particular bond-moving transformation applied on the square lattice (as in Berker and Ostlund 1979) but then it is the interaction strengths and not the bond weights which are multiplied by the number of bonds moved.) Then the analogue of equation (4.3) for instance is

$$B^{(r+1)} = 2^{r/2}(A^2 + C^2) \quad (7.1)$$

and similar equations hold for the other variables. Redefining new variables $\hat{B}^{(r)} = B^{(r)}2^{r/2}$ and similarly \hat{A} and \hat{C} , we get the recursion equations with bond moving as

$$\hat{B}^{(r+1)} = 2^{1/2}(\hat{A}^2 + \hat{C}^2) \quad (7.2)$$

and similar equations for the other variables. These equations do not depend explicitly on r and show that this type of bond moving is equivalent to spin rescaling with $x=1$. At a non-trivial fixed point we have $\hat{B}^{(r)}$ independent of r and $B^{(r)}$ decreases as the inverse of the size of the system.

The general features of the phase diagram are not sensitive to the particular choice of x between 0 and 1, but the values of the exponents depend on x . For $x=1$, we get $\nu \approx 0.68756$ for the pure SAW fixed point. For the tricritical point $\nu_t \approx 0.55638$ and the crossover exponent $\varphi_t = \nu_1/\nu_2 \approx 0.5418$. These values are close to the estimates obtained recently by a transfer matrix method on the square lattice, $\nu_t = 0.55 \pm 0.01$ (Derrida and Saleur 1985) and $\varphi_t = 0.48 \pm 0.05$ (Saleur 1985).

8. Discussion

The first important qualitative conclusion one may draw from our results is that a collapse transition exists on fractal lattices as soon as the connectivity is sufficient to

allow different parts of the polymer to come into close contact on every length scale. This is not the case for the 2D Sierpinski gasket, because once the chain has gone through an r th-order triangle it cannot cross it again (there is only one open vertex left), but transitions exist for the closely related 3D Sierpinski gasket and for the modified rectangular lattice, where the four vertices are sufficient to allow two chain segments to live in the same r th-order unit.

It should be emphasised that the behaviour of the polymers at these collapse transitions is very far from Gaussian: on fractal lattices, a purely random walk is described by an exponent ν_{RW} smaller than $\frac{1}{2}$ (Alexander and Orbach 1982, Rammal and Toulouse 1983), e.g. $\nu_{\text{RW}} = \ln 2 / \ln 6 \approx 0.3869$ for the 3D Sierpinski gasket and $\nu_{\text{RW}} = \frac{3}{8}$ for the family of modified rectangular lattices. Of course, a polymer cannot have a gyration radius exponent smaller than $\nu_c = 1/D_f = \frac{1}{2}$ for the lattices studied here, so Gaussian behaviour corresponds to a case in which any point of the walk is visited many times. The collapse transition corresponds to a new fixed point, intermediate between the SAW (swollen) phase and the collapsed phase, and cannot be viewed as a perturbation of the Gaussian fixed point describing random walks. The case of 2D Euclidean lattices is in a sense degenerate, because $\nu_{\text{RW}} = \nu_c = \frac{1}{2}$, but the result for ν_l given by our infinitesimal recursions for spin rescaling (§ 7) is very close to the numerical value obtained by Derrida and Saleur (1985) and this may indicate that the situation there is not so different from the fractals. We note that in our calculation the critical exponent ν_c of the polymer in the collapsed phase is obtained exactly, which was not the case in the calculation of Marquse and Deutch (1981).

The rod-like phase found in our calculations raises several questions: its existence in a model with only excluded-volume and short-range attractive interactions is surprising, even taking into account the slight overall anisotropy of the modified rectangular lattice. The possibility suggested by the infinitesimal recursions, that anisotropy in the interactions might be a relevant perturbation, is opposite to the conventional pictures. Usually, one argues that anisotropy effects can be absorbed into a redefinition of the length scales, so that the correlation functions keep the same qualitative dependence on system size—no phase transition is expected and the operator is marginal, as we find for the collapsed phase. This is verified in the exactly solved cases, i.e. the Ising model. To explain the coil to rod transitions experimentally observed (Lim *et al* 1983), one usually invokes effective long-range interactions, e.g. mediated by phonons (Goldenfeld and Halley 1985). The situation in our models is quite different and clearly the lattice geometry plays a role in stabilising a rod-like phase, but the balance of effects is subtle.

A useful comparison can be made with the behaviour of purely random walks. On Euclidean lattices, anisotropy of the jump probabilities is a *marginal* perturbation, in the sense that the walks just become elliptical. On fractal lattices, this problem is equivalent, through Einstein's relation, to the conductivity of the lattice viewed as a network of resistors with anisotropic values. It can be shown that this anisotropy is irrelevant for the family of Sierpinski gaskets (Vannimenus and Knezevic 1984) and that the conductivity tensor asymptotically has a finite anisotropy for the modified rectangular p lattices, stable against small perturbations, so the operator is irrelevant (Knezevic 1985). In any case, anisotropy does not have a stronger effect for random walks on fractals than on regular lattices.

A similar remark holds for polymers in the swollen phase, at least within the infinitesimal recursion relations studied above, since anisotropy is irrelevant at the SAW fixed point. It then seems reasonable to argue that the polymer chain will in

general be *more sensitive to anisotropy in the vicinity of the collapse transition* than in the other regions of the phase diagram. Whether anisotropy is relevant at the transition for Euclidean lattices is a delicate point which needs more investigation.

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