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LETTER TO THE EDITOR

Topological frustration and quasicompact phase in a model of interacting polymers

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Abstract. We study the geometric and thermal properties of a model of self-interacting linear polymers (self-avoiding walks) on a fractal lattice, the three-dimensional modified Sierpinski gasket of base $b = 3$. As a consequence of the topological structure of this lattice, the polymer is 'frustrated' and cannot fill the available space with a finite density. When strong attractive interactions between monomers are present the polymer cannot reach the compact globule state usually observed. Rather, it shrinks into a novel phase, the 'semicompact' state, below a finite critical temperature. In this phase, the monomer density per lattice site vanishes asymptotically for large polymers. We give the exact values of the critical exponents at this transition and discuss its possible relevance for polymers placed in a random matrix.

At high temperatures and in good solvents a linear polymer has an extended coil configuration, where the monomer density vanishes asymptotically for large polymers, while at low temperatures and in poor solvents the polymer is found in a compact globule state, with a finite monomer density. This so-called collapse transition has been the subject of continuous investigations (Flory 1966, de Gennes 1979). Using the analogy with a magnetic phase transition it has been pointed out that this transition may be seen as a tricritical point (de Gennes 1975).

Much work has been devoted to the study of lattice models (i.e. self-interacting self-avoiding walks in the case of linear polymers) of this phenomenon, and progress has been made recently for the determination of the critical exponents (Derrida and Saleur 1985, Ishinabe 1985, Saleur 1986, Privman 1986). To each configuration of an N -step self-avoiding walk having K nearest-neighbour pairs of sites one associates the Boltzmann factor $w^P = \exp(P\varepsilon/k_B T)$, $P = K - N$ being the excess number of nearest-neighbour bonds and $\varepsilon > 0$ is the attractive energy per pair. All thermal properties of the polymer can be deduced from the generating function $G(x, T) = \sum \Omega(N, P) x^N w^P$ where $\Omega(N, P)$ is the number of different configurations of an N -step walk having P contacts with itself.

For large N , one expects the following asymptotic behaviour of the mean-squared end-to-end distance $\langle R_N^2 \rangle$:

$$\langle R_N^2 \rangle \sim N^{2\nu} \tag{1}$$

with

$$\nu = \begin{cases} \nu_{SAW} & w < w_c \\ \nu_t & w = w_c \\ 1/d & w > w_c \end{cases} \tag{2}$$

where w_c denotes the critical value of the interaction strength w at the collapse transition and d is the spatial dimension of the lattice.

Despite the apparent simplicity of the lattice model of interacting polymers very few exact results are known. This has motivated recent studies on some fractal lattices where the asymptotic properties of polymers can be obtained by using the *exact* recursion relations (Klein and Seitz 1984, Dhar and Vannimenus 1987, Knežević and Vannimenus 1986, 1987). It was shown that a collapse transition occurs at a finite temperature in the case of polymers on sufficiently ramified lattices. The values obtained for the critical exponents are in qualitative agreement with corresponding estimates for regular lattices (Dhar and Vannimenus 1987, hereafter referred to as DV). Another motivation for these studies comes from the difficult problems associated with polymers in random media: conflicting results have been presented for the effect of disorder on SAW (see Kardar and Zhang 1987 and references therein), and fractal lattices may help understanding these subtle questions (Knežević and Vannimenus 1987).

In the present letter we study the asymptotic properties of a SAW on a three-dimensional, Sierpinski-type fractal of base $b = 3$ (figure 1). The fractal dimension of this lattice is $D = \log 10 / \log 3$, while its spectral dimension is $\tilde{d} = 2 \log 10 / \log(160/9)$ (Hilfer and Blumen 1984). Our approach is very similar to the one which was used in DV to study the collapse transition of linear polymers on the usual ($b = 2$) three-dimensional Sierpinski gasket.

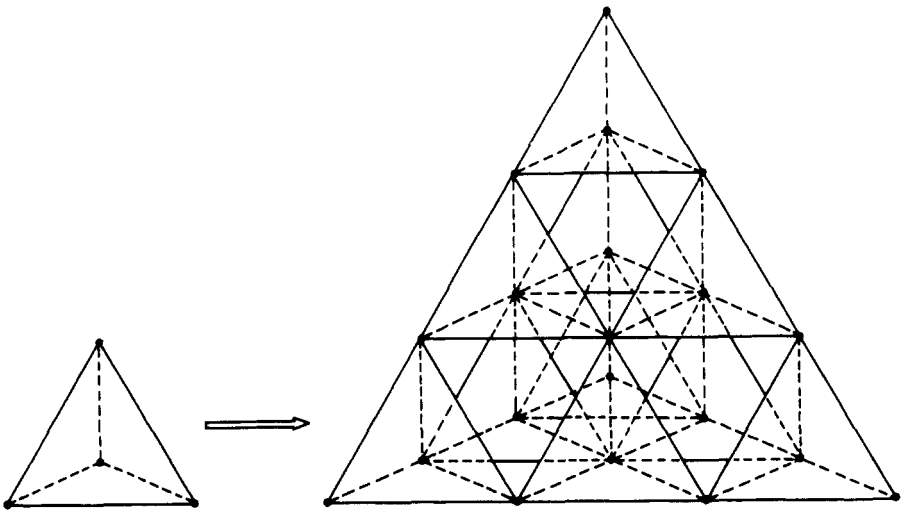


Figure 1. First two stages in the iterative construction of the three-dimensional modified Sierpinski gasket of base $b = 3$. By convention the regions containing matter are represented by full lines and the hidden boundaries are denoted by broken lines. This object has a fractal dimension $D = \log 10 / \log 3 = 2.096$.

To obtain the geometrical critical exponent ν one needs only two restricted generating functions: $A^{(r)}$ counts the number of configurations where the polymer goes once through the r th-order gasket while $B^{(r)}$ counts the configurations where the polymer goes twice through the gasket (see figure 3 of DV). However, the number of polymer configurations is so large here that one has to use computer enumeration to sort them

out. We obtain the following recursion relations:

$$\begin{aligned}
 A^{(r+1)} = & A^3 + 6A^4 + 16A^5 + 34A^6 + 76A^7 + 112A^8 + 112A^9 + 64A^{10} \\
 & + BA^4(8 + 36A + 140A^2 + 292A^3 + 424A^4 + 332A^5) \\
 & + B^2A^3(12 + 12A + 118A^2 + 380A^3 + 806A^4 + 664A^5) \\
 & + B^3A^4(72 + 352A + 704A^2 + 1728A^3) + B^4A^4(344 + 1568A + 848A^2) \\
 & + B^5A^4(264 + 3192A) + 320B^6A^3
 \end{aligned} \tag{3a}$$

$$\begin{aligned}
 B^{(r+1)} = & A^6 + 12A^7 + 40A^8 + 60A^9 + 32A^{10} + BA^6(28 + 88A + 224A^2 + 160A^3) \\
 & + B^2A^6(40 + 496A + 596A^2) + B^3A^5(176 + 768A + 1056A^2) \\
 & + B^4A^3(88 + 264A^2 + 2534A^3) + B^5A^4(1152 + 1888A) \\
 & + 5808B^6A^4 + 1936B^7A^3 + 4308B^8A^2
 \end{aligned} \tag{3b}$$

where we have suppressed the iteration index r on the right-hand side for clarity. The initial values of these functions are

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

$$B^{(1)} = x^4w^4. \tag{4b}$$

For simplicity we have restricted the attractive interactions to bonds within first-order tetrahedral units of the fractal lattice (i.e. the interaction strength w appears only in the initial values of the generating functions, not in the recursion itself). It has been verified in previous work that this restriction plays no role in the determination of critical exponents, as expected on universality grounds. Of course, if one wants to know the precise form of the phase boundaries of the full problem with interactions on all stages, it will be necessary to use more generating functions in the recursion.

We proceed by studying the properties of the recursion equations (3) and (4). One finds three non-trivial fixed points.

(i) The high-temperature fixed point $(A, B)^* = (0.341\ 96, 0.023\ 95)$ is reached for small values of the interaction $w < w_c = 5.63$. Linearising around the fixed point we find only one eigenvalue larger than one, $\lambda = 5.362\ 01$. We identify this point as a SAW fixed point, corresponding to the extended states of the chain. The critical exponent $\nu_{\text{SAW}} = \log 3 / \log \lambda = 0.6542$ is larger than the value $\nu \approx 0.588$ for three-dimensional Euclidean space (Le Guillou and Zinn-Justin 1985). This is in contrast to the behaviour of a random walk on the fractal lattice, for which $\nu_{\text{RW}} = d/2D = 0.3817$ is less than the corresponding Euclidean value $\frac{1}{2}$. The critical exponent α which controls the singular behaviour of the generating function $P(x)$ for closed polygons is given by the scaling law $\alpha = 2 - D\nu_{\text{SAW}} = 0.6288$ (Dhar 1977).

(ii) The tricritical fixed point $(A, B)^* = (0.207\ 17, 0.430\ 75)$ is reached when starting with $w = w_c$. We obtain both eigenvalues greater than one: $\lambda_1 = 8.723\ 08$, $\lambda_2 = 2.450\ 12$, and the geometric exponent is $\nu_t = \log 3 / \log \lambda_1 = 0.5072$ (the third relevant eigenvalue for this tricritical point would correspond to the renormalisation of endpoints of the chain, which involves additional generating functions). The free energy per site f has a singular behaviour at this point:

$$f \sim |w - w_c|^{2-\alpha_t} \quad \text{with} \quad \alpha_t = 2 - \log \lambda_1 / \log \lambda_2 = -0.4170.$$

The exponent is negative and therefore the specific heat is smooth at this transition, which is analogous to the standard collapse transition.

(iii) The fixed point $(A, B)^* = (0, \infty)$ can be analysed by keeping the dominant terms in the right-hand side of (3):

$$A_{r+1} \sim 320B^6A^3 \quad B_{r+1} \sim 4308B^8A^2 \quad \text{as } x \rightarrow x_c(w) \text{ and } w > w_c.$$

Making the change of variables $A = A$, $y = BA^2$, with $z = (\sqrt{73} - 5)/12$, one obtains asymptotically

$$y_{r+1} \approx Cy_r^{(11+\sqrt{73})/2}$$

where C is a constant. Linearising this equation around the fixed point (y^* , $A = 0$), we find one relevant eigenvalue $\lambda = (11 + \sqrt{73})/2$, corresponding to $\nu' = 0.48195$. The fractal dimension of the chain in this phase, $D_{\text{ch}} = 1/\nu' = 2.07491$, is larger than for the two other states, but it is still *less* than the fractal dimension of the lattice $D = 2.09590$. This is in contrast with the case of linear polymers on regular lattices and on the other fractal lattices previously studied, where one finds $D_{\text{ch}} = D$ for $w > w_c$. The density of monomers per site vanishes asymptotically in the new phase, so we propose to call it the 'semicompact' phase.

It is easy to understand the physical origin of such a behaviour. The topological structure of the lattice of figure 1 does not allow polymer configurations where all vertices would be occupied. This appears in equation (3b) through the absence of terms of order B^{10} which could give rise to a standard compact phase with $D_{\text{ch}} = D$. For $w > w_c$ the polymer chain is 'frustrated' on this lattice: it cannot realise the state of minimum energy, in close analogy with the situation for frustrated lattice spin systems, e.g., the Ising antiferromagnet on a triangular lattice. Even a state with a finite monomer density is not allowed, because the topological obstruction occurs on *all* scales. The ramification of the basic tetrahedron is sufficiently high, however, to allow strong local self-interaction effects and the polymer reaches a compromise through the 'semi-compact' state.

It has been suggested recently that the collapse transition in lattice models of polymers could be interpreted as some kind of a spin-glass transition (Derrida and Saleur 1985, Saleur 1986, Privman 1986 and references therein). Let us emphasise that the frustration effect that appears here is of a different nature and is due to the topology of the lattice; it does not exist on Euclidean lattices but it might be relevant to polymers placed in random media, when the local potential energy of the monomers varies rapidly from place to place. The favourable regions then have a geometry similar to percolation clusters and become fractal close to the percolation threshold. It is known that such clusters have a rather low ramification but their topology is not known in enough detail to predict if the effect we have discovered on a deterministic fractal also occurs in such more realistic situations. Anyway, little work has been devoted to self-interacting polymers in disordered systems and it would be very interesting to investigate this problem in more detail.

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