Large-Scale Properties and Collapse Transition of Branched Polymers: Exact Results on Fractal Lattices

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(Received 23 December 1985)

The asymptotic properties of branched polymers are studied on the two- and three-dimensional Sierpinski gaskets, with use of exact recursion equations. It is shown that loops are irrelevant on large scales and the exponents θ and ν for lattice animals are obtained exactly. In the presence of self-interactions, a collapse transition occurs at a nonzero critical temperature. At the transition the value ν_t of the gyration-radius exponent is very close to its value in the compact phase, in analogy with recent numerical results on two-dimensional branched polymers.

PACS numbers: 61.41.+e, 05.50.+q, 64.60.Cn, 75.40.−s

The study of models of branched polymers on Euclidean lattices has been very fruitful in the recent years. Deep connections have been discovered between this problem and other areas of statistical mechanics, such as lattice animals, percolation,[1] and the Lee-Yang edge singularity for Ising magnetic systems.[2] This progress has led to specific predictions, e.g., for the average gyration radius of polymers in dilute solution.[2]

There are several motivations to extend the study of polymer statistics to fractal lattices. First, exact solutions may be obtained for some simple fractals, giving the possibility to investigate the range of validity of general results derived, for regular lattices, by the field-theory and renormalization-group approaches. For example, the number of different branched polymers made of N monomers and their average gyration radius are expected to grow as $\mu^N N^{-\theta}$ and N^{ν}, respectively, for large N: θ and ν are universal exponents, which are different from the analogous quantities for linear polymers but are invariant when configurations containing loops are taken into account or are discarded in the statistics.[1] We provide here a direct verification on exactly solvable models that these asymptotic behaviors and the universality properties also hold on fractals. A second motivation comes from the remarkable relation[2] $\theta - 1 = (d-2)\nu$ for Euclidean lattices. It appears to hold exactly for all $d \leq 8$,[3] and the question arises of how this relation is modified on fractal lattices. Our results show that the exponents θ and ν no longer obey as simple a relation and are now independent.

Our final, and strongest, justification has to do with the collapse transition that branched polymers may undergo in dilute solution in a poor solvent when the temperature is lowered.[4,5] We show in the present Letter that such a transition also exists for polymers with attractive self-interactions on two- and three-dimensional Sierpinski gaskets. This result is of great significance because fractal lattices have been advocated as a new field for the study of phase transitions.[6] Up to now, however, the actual situation was disappointing: Solvable models had transitions only at zero temperature, as for Ising and Potts spin systems on Sierpinski gaskets,[6,7] and models of physical significance with nontrivial transitions could only be treated by approximate methods.[8,9] The models considered here show a phase transition at finite temperature, for which the critical behavior may be determined exactly and compared to the numerical results available for Euclidean lattices.

The fractal lattices treated here are defined recursively and exact renormalization equations (RE) may be written down in terms of a small number of coupling constants. Several studies have been devoted to the problem of linear polymers on these lattices, in the self-avoiding walk limit,[10,11] i.e., without self-interactions between monomers, or in the interacting case.[12] A collapse transition can also exist for linear polymers on sufficiently ramified fractals; it will be the subject of a separate publication.[13] The generalization to branched polymers of the methods first used in Ref. 10 for a self-avoiding walk is straightforward in principle but raises some difficulties in practice. The related technical points will be discussed in a more complete publication, including results on other fractals.

All thermal properties of a polymer on a lattice 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 per site of a polymer having N monomers and P pairs of nearest neighbors. The interaction strength w is related to the temperature T by $w = \exp(\epsilon/T)$, ϵ (>0) being the attractive energy associated with a pair of nearest-neighbor bonds. For simplicity, in the following we restrict the attractive interactions to bonds within first-order units of the fractal lattice. In several models of linear polymers it can be demonstrated explicitly[13] that this restriction plays no role in the determination of the critical exponents. One expects this result to be quite general, on universality grounds, and the restriction has the advantage that the recursion equations do not contain the interac-

tion strength w explicitly (it appears only in the initial values of the generating functions). An analysis of the equations established for noninteracting polymers is therefore sufficient to obtain the critical exponents for the full problem. Anyway, it is clear that if a collapse transition exists with restricted interactions, it will also exist when attractive interactions are present on all scales. Of course, to obtain the precise form of the phase boundaries, of the specific heat, etc., it would be necessary to use the full equations with interactions on all stages.

The simplest fractal lattice on which we find a collapse transition is the 2D Siepinski gasket.[6] A closed set of RE is obtained with six restricted generating functions which are described in Fig. 1. These functions obey the following equations[14]:

$$A^{(r+1)} = A[1+2B+2B^2] + 2B^2C + F[B^2+A^2+2BD], \tag{1a}$$

$$B^{(r+1)} = B^2 + B^3 + F[4BC+2AB] + F^2[B+D], \tag{1b}$$

$$C^{(r+1)} = AB^2 + 3B^2C + F[7C^2+2BD] + F^2[C+E], \tag{1c}$$

$$D^{(r+1)} = A^2 + B[6C^2+4AC+2A^2] + D[2D+3B^2] + 2F[2CD+AD+BC+BE], \tag{1d}$$

$$E^{(r+1)} = A^3 + 14C^3 + 12BCD + 6ABD + 3B^2E + 3F[C^2+D^2+4CE], \tag{1e}$$

$$F^{(r+1)} = 3FB^2 + 6F^2C + F^3, \tag{1f}$$

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

$$(A,\ B,\ C,\ D,\ E,\ F)^{(0)} = (1,\ x,\ xw^2,\ w,\ w^3,\ x^3+3wx^2). \tag{2}$$

For a given interaction w there exists a critical value $x_c(w)$ above which the iterations diverge. For $x = x_c(w)$, we found that the recursion system (1)–(2) has the following general asympotic behavior for branched polymers:

$$A^{(r)} \sim A^* k^r, \quad B^{(r)} \sim B^*, \quad C^{(r)} \sim C^* k^r, \quad D^{(r)} \sim D^* k^{2r}, \quad E^{(r)} \sim E^* k^{3r}, \quad F^{(r)} \sim F^* k^{-r}, \tag{3}$$

where $A^*, B^*, \ldots, F^*$ and k (>1) are finite constants. It is more convenient to work with new, nondiverging variables, and the form of (3) suggests the choice

$$a = AF, \quad b = B, \quad c = CF, \quad d = DF^2, \quad e = EF^3, \quad f = F. \tag{4}$$

In terms of these variables, we find that three fixed points are relevant.

(1) The fixed point $(a, \ldots, f)^* = (0.2009, 0.3276, 0.0231, 0.0232, 0.0022, 0)$. This is reached for small values of the interaction, $w < w_t \simeq 5.5$. We identify it as a random-animal fixed point $(T \to \infty)$, corresponding to the swollen phase of the polymer. The critical exponents are obtained from the linearized recursion equations around the fixed point (4). Only one eigenvalue is greater than 1: $\lambda = 2.630\,93\ldots$. The average size of the polymer varies as N^{ν}, with $\nu = \ln 2/\ln\lambda = 0.716\,55$. The exponent θ can be obtained most directly by a finite-size scaling argument for $G_L(x_c)$, the generating function of animals on a gasket of size L at the critical value x_c $(w=1)$. This is expected to diverge as $L^{(1-\theta)/\nu}$, and a direct evaluation of the dominant terms in $G(x)$ gives

$$G_L(x_c) \sim \sum_{r=1}^{R} \left(\frac{k^2}{3}\right)^r,$$

where $L = 2^R$ and k is the constant defined in Eq. (3). Comparing the behavior of the two sides for large k, we get

$$(\theta-1)/\nu = D - \ln(k^2)/\ln 2 = D - \delta, \tag{5}$$

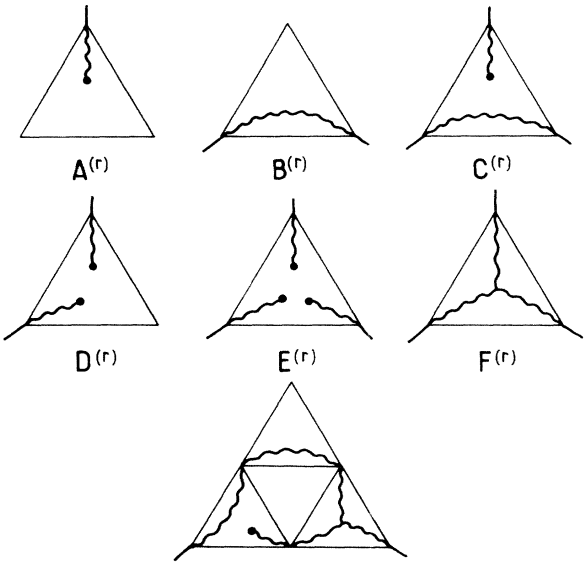

FIG. 1. Diagrams representing the six restricted generating functions for branched polymers on the two-dimensional Sierpinski gasket. $C^{(r)}$ corresponds, for instance, to configurations where a part of the polymer joins two vertices of an rth-order triangle while one of its ends penetrates through the third vertex. The bottom diagram shows a term $B^{(r)}C^{(r)}F^{(r)}$ contributing to $B^{(r+1)}$.

$D = \ln 3/\ln 2$ being the fractal dimension of the gasket. The numerical values are $\theta = 0.5328$ and $\delta = 2.2370$. A calculation of the leading singularity of $G(x)$ when $x \to x_c$, along the lines of Ref. 10, gives the same result for θ.

(2) The fixed point $(a, \ldots, f)^* = (0, 0, \sqrt{15}/30, 0, \frac{1}{20}, 0)$ is reached when starting with large values of the interaction strength, $w > w_t$ (low temperatures). It gives one relevant eigenvalue $\lambda = 3$, corresponding to $\nu_c = 1/D = 0.63093$ and therefore to a finite monomer density per site when $N \to \infty$. This is a compact fixed point which describes the collapsed phase of the polymer.

(3) The fixed point $(0.0592, 0.0750, 0.1253, 0.0225, 0.0474, 0)$ is obtained for $w = w_t$ and has two eigenvalues greater than 1: $\lambda_1 = 2.99181$ and $\lambda_2 = 1.19941$. We identify this tricritical point as corresponding to the collapse transition of the branched polymer. The average radius of the polymer then scales as N^{ν_t} with $\nu_t = \ln 2/\ln \lambda_1 = 0.63250$, extremely close to the value ν_c for the collapsed phase. The behavior of thermodynamic quantities near the transition can be easily deduced from the free energy per site,[4] whose singular part varies as $|w - w_t|^{2-\alpha}$, with $\alpha = 2 - \ln\lambda_1/\ln\lambda_2 = -4.0269$. The transition is very weak and the specific heat very smooth. On periodic lattices the numerical value for 2D lattice animals $\nu_t = 0.509 \pm 0.003$ is also quite close to the value $\nu_c = \frac{1}{2}$ for collapsed polymers. Our results suggest that this proximity is not accidental and has a deeper and general origin.

Several remarks are in order.

One can check explicitly that discarding in Eq. (1) the terms due to configurations with loops does not affect the asymptotic behavior and the value of ν. Lattice animals *with* and *without* loops belong to the same universality class, in agreement with the field-theory argument for regular lattices.[1] Also, the value $\nu = 0.71655$ is *larger* than the value $\nu \simeq 0.641$ for animals on 2D Euclidean lattices[15]: The polymer is swollen on the gasket, contrary to what happens for random walks.

The problem of linear polymers is recovered if all terms containing the functions E and F are suppressed in Eqs. (1) and (2). The truncated equations have only one fixed point, corresponding to the swollen phase of the chain[11] with $\nu = 0.7986$. There is no collapsed phase, in agreement with earlier results.[12]

The relation (5) generalizes the relation $(\theta - 1)/\nu = d - 2$ for Euclidean lattices.[2] It shows that on fractals the two exponents θ and ν are independent in general. The quantity δ appearing in (5) is a new fractal exponent, not reducible to previously defined quantities. Equivalently, we may define a new dimension d_a, specific to the animal problem, by requiring that the form of the Parisi-Sourlas relation be preserved and by writing

$$(\theta - 1)/\nu = d_a - 2. \tag{6}$$

On all other fractals that we have studied δ is also larger than 2, suggesting that in general $d_a \leq d$. No simple relation seems to exist between d_a and the spectral dimension.

The problem of branched polymers is much more difficult on 3D Sierpinski gaskets. To obtain a closed set of RE one needs eleven restricted generating functions (taking symmetries into account) and we had to use computer enumeration to sort the large number of polymer configurations ($\sim 10^7$) to be considered. We report here only the main results, which are qualitatively similar to the 2D case. The three different regimes expected for branched polymers are identified:

(i) At infinite temperature ($w = 1$), the configuration energies play no role and the problem reduces to the random-animal model. We find that $\nu = 0.6057$, $\theta = 0.7567$, and $\delta = 2.4018$. This fixed point is reached for all values of $w < w_t \sim 2$, when interactions are restricted to first-order units.

(ii) When the temperature is lowered a transition occurs for $w = w_t$. At this tricritical point, the geometrical polymer exponent is $\nu_t = 0.5055$ and the thermal exponent is $\alpha = -2.9267$. The transition is less weak than for the 2D case, but the exponent ν_t is still close to the value $\nu_c = 1/D = \frac{1}{2}$ corresponding to a compact phase.

(iii) Finally, at low temperatures ($w < w_t$) the polymer is in a collapsed phase, with $\nu_c = \frac{1}{2}$.

It is to be noted that, as in the 2D case, the equations for the linear polymer problem are contained in the general system by our keeping only a restricted set of recursion equations, with appropriate boundary conditions. In fact, the system has probably additional fixed points, but they cannot be reached when starting from initial conditions corresponding to attractive monomer-monomer interactions. Other fractals with finite ramification order[6] allow a similar exact treatment of the polymer problem. In general, the recurrence equations will be quite complex and will have to be generated by computer: An interesting direction for future work will be to see if simple approximations of the real-space renormalization-group type can give accurate results for these systems.

In conclusion, we have studied the large-scale properties of branched polymers on simple fractals, the 2D and 3D Sierpinski gaskets. A collapse transition has been found at a finite temperature in both cases, with a geometrical exponent ν_t at the transition only slightly larger than for a compact polymer, in close analogy with recent findings on 2D Euclidean lattices.[4] The present work provides a concrete example of an exactly solvable nontrivial phase transition on a fractal. The approach may be applied to other problems, like linear

polymers,[13] and to other fractal lattices, opening the way to various extensions and confirming that fractals may help gain insight into critical phenomena.

We thank D. Dhar for his many suggestions and V. Hakim and N. Sourlas for useful discussions during the course of this work. The numerical calculations were made possible by the Groupement de Recherches Coödonnées de Experimentation Numerique (supported by the Centre National de la Recherche Scientifique) and greatly benefitted from the advice of D. d'Humieres.

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