Collapse transition of linear polymers on a family of truncated n-simplex lattices

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We show that for linear polymers a collapse transition exists on a truncated six-simplex lattice but not on a truncated five-simplex lattice. The existence of the collapsed phase is determined not only by the connectivity but also by the geometrical form of the first-order unit of the fractal lattice. We report exact results for the critical exponents at the transition for the six-simplex lattice.

A lattice model of the self-attracting self-avoiding walk (SASAW) has been the focus of much attention in recent years.[1-6] This is because it simulates a polymer chain in poor solvent that can undergo a collapse transition, where the chain contracts from an expanded state to a globule state when the temperature is lowered. De Gennes[7] has shown that the Flory Θ point[8] of a very long polymer chain is a tricritical point.

In critical phenomena parlance, the infinite random walk (RW) is equivalent to a Gaussian system at its critical point with the radius of gyration exponent $\nu=\frac{1}{2}$, independent of the space dimension d (of a Euclidean lattice). The self-avoiding walk (SAW) is a critical O(n) model, with $n=0$ component. The SASAW changes the behavior of the phase transition of the SAW from continuous (second order) to first order into a collapse phase at low temperatures. At the intermediate temperature (Θ point), its behavior is described by a tricitical point of the O(n), $n\rightarrow 0$ spin system.[7] In this regime, the upper critical dimension changes from four to three with the consequence that, for $d=3$, ν is equal to $\frac{1}{2}$ plus a logarithmic correction.[9] The behavior of the collapse transition of linear and branched polymers on some Euclidean and fractal lattices with "effective" dimension less than three has recently been studied in a number of works.[2-6,10-14] Characteristic exponents of the transition were calculated by real-space renormalization,[2-5,10] Monte Carlo simulation,[11] and transfer-matrix[12] calculations. For the continuous polymer model, the tricritical state of a polymer chain has recently been studied by Duplantier, Jannink, and des Clouizeaux,[15] using renormalized theory.

Interesting results have been reported for the polymer collapse on fractal lattices. For the linear polymer chain, no collapse transition was found to take place on a two-dimensional (2D) Sierpenski gasket.[2,14] The reason for this was thought to be the low ramification number of the lattice. Dhar and Vannimenus[2] have shown that the transition occurs at a finite temperature on a three-dimensional (3D) Sierpenski gasket of base $b=2$ and also on many other fractal lattices of the Hausdorff (fractal) dimension $\bar{d}=2$. No compact globule state was, however, found to occur on a 3D modified Sierpenski gasket of $b=3$. Instead, this lattice exhibits a "frustrated" state (semicompact phase) below a finite critical temperature.[4] These results indicate that the phenomena of polymer collapse can be rather intricate on some fractal lattices. In this paper we study the collapse transition on fractal lattices whose Hausdorff dimensions lie between two and three, and show that collapse transition is found not to occur on some fractals though their ramification numbers are large.

All thermal properties of a polymer on a lattice can be deduced from the generating function $G(x,T)=\sum_{N,P}\Omega(N,P)x^N w^P$, where $\Omega(N,P)$ is the number of different configurations per site of a polymer having N monomers and P number of nearest neighbors. The interaction strength w is related to the temperature T by $w=\exp(E/T)$, $E(>0)$ being the attractive energy associated with a pair of nearest-neighbor bonds. Following Dhar and Vannimenus,[2] we restrict the attractive interaction to bonds within a first-order unit of the fractal lattice. Because of this restriction, w does not appear explicitly in the recursion equations. It appears only in the initial value of the generating functions. By universality, one expects that the qualitative phase diagrams and critical exponents of this system are same as the one with attractive interactions at all bonds. These interactions may, however, affect the location of the critical points and the phase boundaries.

In a previous paper,[16] we reported the critical exponents of the SAW on a family of truncated n-simplex lattices.[17] By means of exact renormalization-group transformations, we calculated the critical exponents ν, α (the specific-heat exponent), and γ (the susceptibility exponent) of the SAW for $n=5$ and 6. In this paper we elaborate on our previous study by including attractive interactions with the constraints mentioned above.

For the truncated five-simplex lattice, the recursion relations relevant to our present study are[16]

$$A_{r+1}=A^2+3A^3+6A^4+6A^5+18A^2B^2+96A^2B^3+12A^3B+78A^3B^2+30A^4B+132AB^4+132B^5\,, \tag{1}$$

$$B_{r+1}=A^4+2A^5+13A^4B+4A^3B+32A^3B^2+88A^2B^3+22B^4+220AB^4+186B^5\,. \tag{2}$$

These recursion relations correspond to the configurations shown in Fig. 1. As emphasized in Ref.

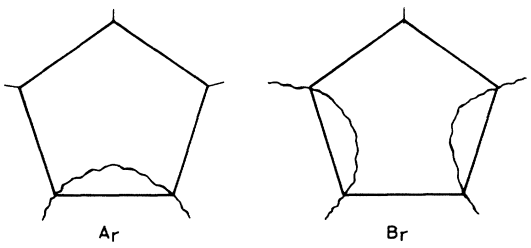

FIG. 1. Diagrams defining the weights A_r and B_r for the five-simplex lattice.

16, these recursion relations are sufficient to calculate the exponents ν and α. The starting weights for SASAW's (see Fig. 2) are

$$A_1 = x^2 + 3x^2 w + 6x^4 w^3 + 6x^5 w^6 ,$$
$$B_1 = x^4 w^4 + 2x^5 w^7 . \tag{3}$$

Equations (1) and (2) have only one nontrivial positive real fixed point, respectively,

$$A^* = 0.3265, \quad B^* = 0.0279 , \tag{4}$$

that corresponds to the swollen state of the chain with $\nu = 0.6049$ and $\alpha = 0.5954$.

Thus we find no collapse phase for the five-simplex lattice, where the coordination number is 5, the connectivity (for the SAW) $\mu = 2.9760$, $\bar{d} = 2.3219$, and the spectral dimension $\tilde{d} = 1.6541$. It is easy to understand the physical origin of such a behavior. The topological structure of the lattice is such that it does not allow polymer configuration where all vertices would be occupied. This situation is reflected by the term $132B^5$ in Eq. (1). In order to see the effect of this term on the fixed-point structure, we associated it with a factor ϵ, which varies between 0 and 1. At $\epsilon = 0$, we get three fixed points corresponding to the (i) expanded state, (ii) semicompact state,[4] and (iii) tricritical point. As ϵ is increased from zero, the fixed points (ii) and (iii) move closer to each other and finally merge at $\epsilon \sim 0.3$. For $0.39 < \epsilon < 1$, we find only one fixed point corresponding to the expanded state. It is, however, not obvious how to modify the fractal lattice, so that the term involving B^5 in Eq. (1) becomes much smaller than its present value. No effect on the fixed point was found when a particular bond of the simplex was removed from all orders of iteration stages. The other possibility is to dilute each bond with a given probability. Recently, Meir and Harris[18] have shown that the exponent ν, in a diluted lattice at a percolation threshold, is determined by a fixed point different from the pure-lattice one.

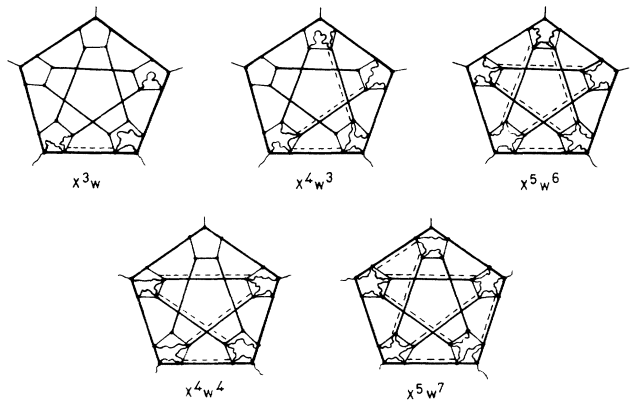

FIG. 2. Diagrams defining the initial weights for the SASAW's on a five-simplex lattice. The attractive interactions between neighboring sites are denoted by dashed lines.

We now consider the six-simplex lattice with fractal and spectral dimensions of $\bar{d} = 2.5849$ and $\tilde{d} = 1.7233$, respectively, and the connectivity (for the SAW) $\mu = 3.6810$. The recursion relations for the configurations shown in Fig. 3 are[16]

$$A_{r+1} = A^2(1 + 36B^2 + 384B^3 + 5544B^4 + 4992B^2C) + 4A^3(1 + 6B + 78B^2 + 648B^3 + 432B^2C)$$
$$+ 12A^4(1 + 10B + 80B^3 + 10C^2 + 40BC) + 24A^5(1 + A + 2C + 9B)$$
$$+ 24AB^3(1 + 22B + 362B^2 + 636BC + 472C^2) + 48B^4(11B + 137B^2 + 521C^2 + 428BC) , \tag{5}$$

$$B_{r+1} = A^4(1 + 26B + 144BC + 324B^2 + 6A^2) + 4A^5(1 + 4C + 16B) + 4A^2B^2(44B + 905B^2 + 1272BC + 708C^2)$$
$$+ 4A^3B(1 + 16B + 308B^2 + 208BC) + 8AB^3(55B + 822B^2 + 2140BC + 2084C^2)$$
$$+ B^2(22B^2 + 372B^3 + 5440B^4 + 23\,520B^3C + 48\,160B^2C^2 + 76\,800BC^3 + 94\,336C^4) , \tag{6}$$

$$C_{r+1} = A^6 + 6A^5(C + 2B) + 4A^2B^2(9A^2 + 52AB) + 18A^2B^3(159B + 236C) + AB^4(2568B + 6252C)$$
$$+ 14\,448B^5C + 43\,200B^4C^2 + 94\,336B^3C^3 + 541\,568C^6 . \tag{7}$$

The initial weights for the SASAW's are found to be

$$A_1 = x^2 + 4x^3 w + 12x^4 w^3 + 24x^5 w^6 + 24x^6 w^{10} ,$$
$$B_1 = x^4 w^4 + 4x^5 w^7 + 6x^6 w^{11} , \tag{8}$$
$$C_1 = x^6 w^{12} .$$

Equations (5)–(7) have been analyzed, and the general flow diagram is shown in Fig. 4. There are five different positive real fixed points whose features are discussed below.

(i) The fixed point $(A^*, B^*, C^*) = (0.262\,352, 0.017\,588, 0.000\,701)$ corresponds to the expanded state

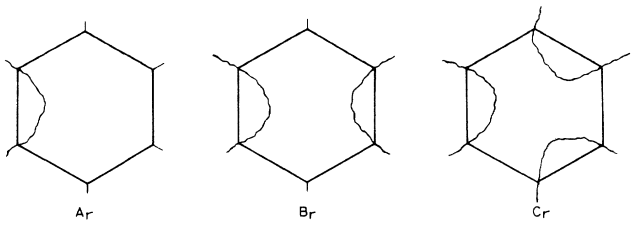

FIG. 3. Diagrams defining the weights A_r, B_r, and C_r for the six-simplex lattice.

of chain,[16] with $\nu=0.5506$ and $\alpha=0.5767$. For $x=x_c(w)$, this fixed point is reached for all $w<w_c=3.499\,984\,7$.

(ii) The fixed point $(A^*,B^*,C^*)=(0,0,0.713\,29)$ is reached for all $w>w_c$ (at low temperatures), and $x=x_c(w)$. Linearizing the recursion relation about this fixed point, we find the largest eigenvalue, $\lambda_1=6$, corresponding to $\nu_c=1/\bar{d}=0.3869$. This phase has a finite density of monomers per site when $N\to\infty$. This is a compact fixed point, which describes the collapsed phase of the polymer.

(iii) The fixed point $(A^*,B^*,C^*)=(0.129\,48, 0.095\,72, 0.053\,44)$ is obtained for $w=w_c$. The linearized renormalization transformation near this fixed point yields eigenvalues $\lambda_1=5.4492$, $\lambda_2=1.9049$, and $\lambda_3=0.4286$. Since the point has two eigenvalues greater than 1, we identify this tricritical point as corresponding to the collapse transition. The average radius of the polymer scales N^{ν_t}, with

$$\nu_t=\frac{\ln 2}{\ln\lambda_1}=0.4088$$

close to the value ν_c for the collapsed phase.

The singular part of the free energy per site varies as $(w-w_c)^{2-\alpha}$, with

$$\alpha=2-\frac{\ln\lambda_1}{\ln\lambda_2}=0.6309\ .$$

Thus the transition is weak with smooth specific heat.

The second positive exponent controls the divergence of the "thermal correlation:"

$$\xi_{\rm th}=(w-w_c)^{-\nu_{\rm th}}\ ,$$

where $\nu_{\rm th}=\ln 2/\ln\lambda_2=1.0755$.

The crossover exponent at the tricritical point is

$$\Phi=\frac{\nu_t}{\nu_{\rm th}}=0.3801$$

The other two fixed points, $(A^*,B^*,C^*)=(0.254037,0.022159,0.07098)$ and $(0.200,0.0666, 0.0666)$, cannot be reached starting with the initial condition, so they are spurious. All these fixed points are shown in the flow diagram (Fig. 4).

The first important qualitative conclusion one may draw from our results is that the ramification number of a fractal lattice is not enough to control the existence of the collapse transition or, more importantly, the geometrical form of the first-order unit of the lattice. The absence of collapse transition on the truncated three- and five-simplex lattices strongly suggests that the transition may not be found to occur on all odd-simplex lattices. The collapsed phase occurs when different parts of the polymer chain come into close contact on every length scale. Because of the geometric nature of the odd-simplex lattices, at least one vertex of each first-order unit of the lattice is left unoccupied. The semicompact state was also found not occur at finite temperatures on the five-simplex lattice.

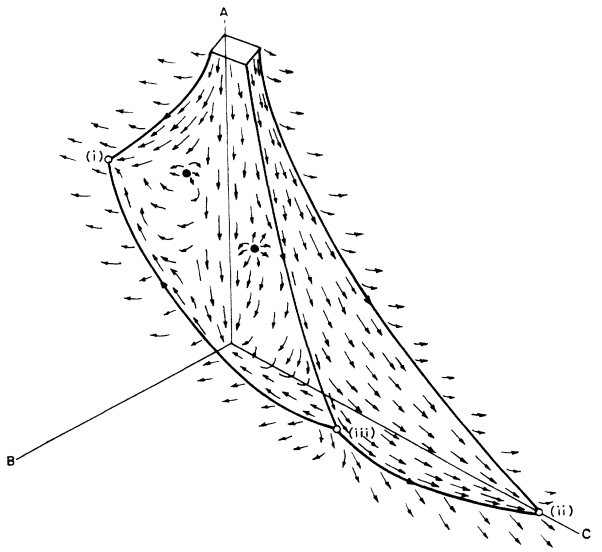

FIG. 4. Flow diagram in parameter space for the six-simplex lattice. The fixed points discussed in the text are shown. The two unstable fixed points are shown by open circles.

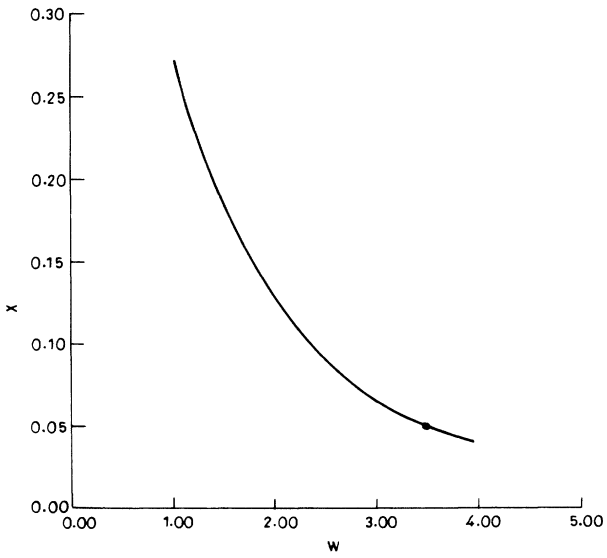

FIG. 5. Critical fugacity x_c for linear polymers on the six-simplex lattice as a function of the self-attraction parameter w. The collapse transition occurs for $w=\omega_c\simeq 3.5$.

The collapse transition corresponds to a new fixed point, intermediately between the SAW (expanded) phase and the collapsed phase. In Fig. 5 we plot the radius of convergence w_c of $G(x,w)$ as a function of the interaction strength w. This gives the phase diagram for polymers in solution in a fractal environment. This figure also gives the internal energy per site U of the polymer, through the following simple relation:

$$U = -wd(\ln x_c)/dw \ .$$

A final remark is that the two fixed points, which are regarded as spurious, might be reached if other constraints or more complicated interactions are included. In that case, the qualitative nature of the phase diagram of Fig. 5 would change.

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