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Critical behavior of an interacting polymer chain in a porous model system: Exact results for truncated simplex lattices

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We present an exact and a Flory-type study of thermal and geometrical properties of interacting chain polymers situated on a class of porous model systems represented by the truncated simplex lattices. Within the exact approach, we have developed a systematic use of recursion relations for both the partition functions and their various derivatives. We have thereby been able to obtain a proper solution of the polymer problem, demonstrating that the studied model has a finite critical temperature ($\Theta \neq 0$ K, with well-defined critical exponents), in the cases of the truncated 4-simplex and 6-simplex lattices. However, we show that in the 5-simplex case there is no finite Θ temperature. This finding is in contrast with the generally accepted qualitative argument that leads to the conclusion that the more ramified lattices are more likely to allow of existence of the Θ point. The same finding shows that the problem of existence of a collapse transition on regular fractals is more intricate than one could expect, and hence one can infer that for stochastic fractals (such as the critical percolation clusters) the same problem should be approached rather cautiously. Besides, our results for the 4-simplex case demonstrate that the model under study is in the same class of universality as a model, studied previously, with a restricted set of interactions, which should be relevant to the problem of the possible difference between the Θ and Θ' point.

I. INTRODUCTION

The equilibrium properties of a polymer chain in a quenched random environment, such as a porous medium, appear to be both potentially relevant to various experimental situations and a controversial theoretical problem for more than a decade. Porous media are often fractals, which means that they display a self-similar distribution of voids over three to four orders of magnitude in length scale.[1] In this paper we model the porous media by a class of fractal lattices and study the statistics of a polymer chain situated on such lattices. These statistics can be captured by the self-avoiding random walk model and may be related to the critical phenomena of magnetic model systems.[2] The relation is useful in the case when one studies geometrical properties of the linear polymers in a good solvent. On the other hand, it appears that in a poor solvent linear polymers exhibit at a certain temperature (Θ point) their own thermal-like critical behavior, in addition to geometrical critical properties. Indeed, at high temperatures the excluded volume repulsion is the dominant constraint and the polymer chain is in an extended (swollen) state. When the temperature T is sufficiently lowered, the attractive interactions between the segments of the chain become important and thereby the chain is in a compact state. These two temperature regions are separated by a critical temperature Θ, which appears to be a tricritical point.[3]

In what follows we first outline a general theoretical framework needed for the study of the polymer chain statistics. The basic property of a polymer chain comprised of N monomers is its mean squared end-to-end distance $\langle R_N^2 \rangle$, which scales in the following way

$$\langle R_N^2 \rangle \cong \mathcal{B} N^{2\nu} , \tag{1}$$

where $\mathcal{B}$ is the critical amplitude, and ν is the geometrical critical exponent. In general, ν assumes distinct values in different temperature regions

$$\nu = \begin{cases} \nu, & T > \Theta , \\ \nu_\Theta, & T = \Theta , \\ 1/d, & T < \Theta , \end{cases} \tag{2}$$

where d is dimension of the space in which the chain is embedded.

To describe linear polymers we consider the usual lattice model in which the polymers are represented by the self-avoiding random walk (SAW) paths. Within the SAW model, relation (1) may be interpreted as the mean squared displacement that the walker makes after N steps on a lattice. In order to study thermal properties, we attribute an attractive energy $-\varepsilon$ ($\varepsilon > 0$) to each pair of neighboring occupied sites that are not adjacent on the chain. All thermal properties can be deduced from the knowledge of the number $\Omega(N,P)$ of different walks of N steps with P pairs of the neighboring sites. The corresponding generating function is defined by

$$G(x,T) = \sum_{N,P} \Omega(N,P) x^N w^P , \tag{3}$$

where w is the Boltzmann factor $w=\exp(\varepsilon/T)$ with the Boltzmann constant k_B being set equal to unity, and x is the one-step weight (fugacity). The free energy per site $f(T)$ is determined by the radius of convergence

$$x_c(T)=1/\mu \tag{4}$$

of the sum (3); that is,

$$f(T)=-T\lim_{N\to\infty}\left[\frac{1}{N}\ln Z_N\right]=-T\ln\mu(T)\ , \tag{5}$$

where Z_N is the partition function

$$Z_N=\sum_P \Omega(N,P)w^P\ . \tag{6}$$

It turns out that in most cases instead of the generating function (3), it is sufficient to study the following generating function[4]

$$g_{\vec{0}\vec{R}}(x,T)=\sum_{N,P}\mathcal{G}_{\vec{0}\vec{R}}(N,P)x^N w^P\ , \tag{7}$$

where $\mathcal{G}_{\vec{0}\vec{R}}(N,P)$ is the number of all different chain configurations that, having N monomers and P neighboring sites, span the points $\vec{0}$ and $\vec{R}$. It has been shown[5] that for $x<x_c$ the function (7) decreases exponentially for large R,

$$g_{\vec{0}\vec{R}}(x,T)\sim\exp[-R/\xi(x,T)]\ , \tag{8}$$

where $\xi(x,T)$ is the geometrical correlation length of the polymer chain. When $x\to x_c$ the correlation length diverges according to the power law

$$\xi(x,T)\sim(x_c-x)^{-\nu}\ , \tag{9}$$

where ν is given by (2).

It is important to notice that the generating (correlation) function is, in fact, the grand canonical partition function of a chain polymer that spans points $\vec{0}$ and $\vec{R}$. Thus, knowing g one can get the thermodynamical potential

$$\Psi=-T\ln g_{\vec{0}\vec{R}}(x,T)\ , \tag{10}$$

which is related to the free energy f_N of the N-monomer chain via the Legendre transformation

$$f_N=T\ln x+\Psi/N\ . \tag{11}$$

Investigation of the statistics of the interacting polymer chains within the outlined framework has been approached in various ways, including exact enumerations on lattices,[6] computer simulations,[7] renormalization group (RG) approaches,[8,9] and the transfer matrix calculations.[10] However, there is no complete solution of the problem on a regular lattice.

In this paper we study thermal and geometrical properties of chain polymers whose constituting monomers are situated on a fractal lattice represented by the truncated 4-simplex.[11] We have been able to obtain a complete solution of the polymer problem, demonstrating that the studied model has a finite critical temperature ($\Theta\neq 0$), with well-defined critical exponents. A similar problem has been studied by Klein and Seitz,[12] in the case of the Sierpinski gasket lattice, who found that there is no finite critical temperature. The same conclusion has been reached by Dhar and Vannimenus[13] in the case of the truncated 3-simplex lattice. In both cases, absence of the critical temperature has been attributed to low ramifications of the underlying lattices. On the other hand, a finite critical temperature has been found[13] for the truncated 4-simplex lattice, by studying a model with a restricted set of attractive interactions. In our model, however, we do not impose restrictions on the attractive interactions; furthermore, we make a complete study of the polymer thermal properties within a wide temperature range. In addition, we analyze the relevant problem in the cases of 5- and 6-simplex lattice, and find a surprising fact in that the 5-simplex lattice, in contrast to the 4- and 6-simple lattice, does not allow the existence of the collapse transition.

The present paper is organized as follows. In Sec. II we describe our model and a method of treating it exactly. In Sec. III we analyze the low-temperature behavior of the model, while in Sec. IV we present its high-temperature properties, including the Θ-point singularities. Then in Sec. V we develop the Flory-type approach to the problem of collapse transition of linear chains on fractal lattices. Finally, in Sec. VI we present an overall discussion of the obtained results. In the Appendix we elaborate the polymer problem in the case of the 5-simplex lattice.

II. THE MODEL AND BASIC RECURSION RELATIONS

We assume that the self-interacting polymer chain is situated on the truncated 4-simplex lattice. This is a fractal lattice[11] (see Fig. 1), with the fractal dimension $d_f=2$ and the spectral dimension $d_s=2\ln 4/\ln 6$. Within the accepted model, a polymer chain can be visualized as a SAW path. To each walk of N sites we attribute the weight x^N, and if there are P neighboring sites (which are not adjacent along the path) we add the weight w^P.

Due to the finite ramification of the truncated 4-simplex, the statistics of the polymer model can be studied exactly within a scheme of finite number of the restricted partition functions. In what follows it will be sufficient to study four restricted partition functions (generating functions). These functions are defined recursively as weighted sums over the SAW paths within a finite stage of construction of the fractal lattice. Their

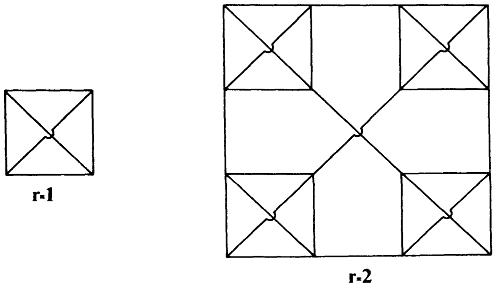

FIG. 1. The truncated 4-simplex lattice at the first ($r=1$) and second ($r=2$) stage of construction.

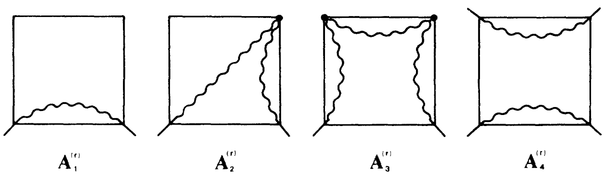

FIG. 2. The four restricted partition functions used in the study of the interacting SAW problem in the case of the truncated 4-simplex lattice. It should be noted that the sets of walks described by A_2 and A_3 are contained in the set of walks described by A_1. Similarly, the set of walks described by A_2 contains all walks described by A_3.

schematic representation is depicted in Fig. 2. The generating function $A_1^{(r)}$ is the weighted sum over all walks that enters the rth stage fractal lattice at one vertex and leaves it at the other vertex, without specifying whether the walker visits the other two vertices. On the other hand, the function $A_2^{(r)}$ is defined quite similarly, but with the proviso that the walker must visit at least one extra vertex. In the case of the function $A_3^{(r)}$, it is assumed that the walker obligatory visits two extra vertices. Thus, one can notice that the function $A_1^{(r)}$ contains both the sum $A_2^{(r)}$ and the sum $A_3^{(r)}$, in addition to the term which describes the walks that pass through the rth stage fractal lattice without visiting the two extra corners. Finally, the function $A_4^{(r)}$ represents walks that pass twice through the rth stage fractal lattice.

In Fig. 3 we show an example of the walk within the second stage of the fractal construction. It can also be considered as an example of the coarse-grained SAW path within two arbitrary successive stages (r and $r+1$) of the fractal construction. Hence, if we denote the generating functions that correspond to the $(r+1)$-th stage with primes, and those that correspond to the first lower stage without superscripts, then the walk shown in Fig. 3 contributes the term $(A_2)^2A_3A_4w$ to the function A_2'. By drawing all other similar configurations one can find the exact relation between the function A_2' and the generating functions A_1, A_2, A_3, and A_4. In practice, due to the very large number of all possible configurations, one uses computer facilities to establish such a relation. Here we present the complete system of the recursion relations

$$A_1'=A_1^2+2A_1^3+2A_1^4+4A_1^3A_4+6A_1^2A_4^2+2vA_2^2[3A_1^2+3A_4^2+4A_1A_4+A_1+vA_2^2+2vA_3(A_1+A_4)+v^2A_3^2]\,, \tag{12}$$

$$\begin{aligned}A_2'=&A_1A_2(A_1+4A_1A_4+2A_1^2+6A_4^2)\\&+vA_2[4A_1A_3A_4+4A_1A_2^2+4A_2^2A_4+2A_1^2A_3+6A_3A_4^2+A_2^2+2vA_3(2A_3A_4+2A_2^2+A_1A_3+vA_3^2)]\,,\end{aligned} \tag{13}$$

$$A_3'=2A_2^2(A_1^2+2A_1A_4+3A_4^2)+v[6A_4^2A_3^2+2A_2^4+4A_2^2A_3(A_1+2A_4)+vA_3^2(4A_4A_3+6A_2^2+2vA_3^2)]\,, \tag{14}$$

$$A_4'=A_1^4+4A_1^3A_4+22A_4^4+4vA_1A_2^2(A_1+3A_4)+v^2[2A_2^4+4A_2^2A_3(A_1+3A_4)+4vA_3^2(A_2^2+A_4A_3)+v^2A_3^4]\,, \tag{15}$$

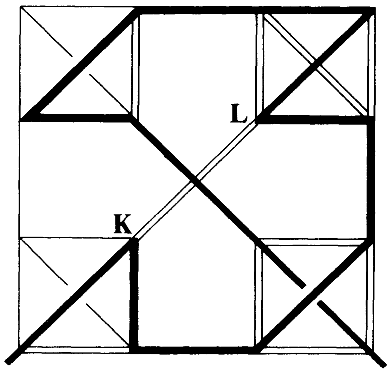

FIG. 3. A linear polymer chain situated on the second stage of construction of the truncated 4-simplex lattice. The polymer configuration is represented by the sequence of solid segments, whereas the interactions between the neighboring sites (which are not adjacent on the chain) are depicted by adding parallel lines to the corresponding bonds. The associated SAW path contributes the term $(A_2^{(1)})^2A_3^{(1)}A_4^{(1)}w$ to the function $A_2^{(2)}$. It should be noted that in this study we assume the presence of the interaction among all neighboring sites on all stages of the iterative construction of the lattice; that is, we do not confine interaction only to bonds that lie within the first stages of the construction. Consequently, there appears, for instance, the interaction between the K and L sites.

where $v=w-1$. In fact, the system of equations should be supplemented with the starting values conditions

$$A_1^{(1)}=x^2+2x^3w+2x^4w^3\,, \tag{16}$$

$$A_2^{(1)}=x^3w+2x^4w^3\,, \tag{17}$$

$$A_3^{(1)}=2x^4w^3\,, \tag{18}$$

$$A_4^{(1)}=x^4w^4\,, \tag{19}$$

where x is a weight associated with each vertex that the walk passes through. We may observe here that in the case of chains without self-interaction ($w=1$, that is $v=0$) our system of recursions equations [(11)–(15)] reduces to equations originally obtained for simple SAW on the truncated 4-simplex lattice.[11,13]

Concerning the general framework outlined in Sec. I, it is important to emphasize that the restricted partition function $A_1^{(r)}$ can be identified with the correlation function (7), so that the distance $|\vec{R}|$ corresponds to the extent between two vertices at the ends of an external edge of the r-th stage of the construction of the lattice. Thus, the analysis of the polymer statistics within the framework of the partition functions defined by Eqs. (12)–(19) is equivalent to a grand-canonical ensemble analysis. For a given interaction parameter w, the radius of convergence $x_c(w)$ of the partition function $A_1^{(r)}$ can be determined as the maximum value of the fugacity x for which the partition functions remain finite after many iterations of the system of the recursion relations (12)–(19).

In order to find explicit statistical properties of the polymer system it is profitable to derive recursion relations for derivatives of the partition functions A_1, A_2, A_3, and A_4. For instance, the average number $N^{(r)}$ of monomers that comprise a polymer chain lying within the rth stage fractal lattice is given by the expression

$$N^{(r)}=\frac{x}{A_1^{(r)}}\frac{\partial A_1^{(r)}}{\partial x}\ , \tag{20}$$

while the average number $P^{(r)}$ of neighboring pairs of monomers that are not adjacent along the chain can be expressed as

$$P^{(r)}=\frac{w}{A_1^{(r)}}\frac{\partial A_1^{(r)}}{\partial w}\ . \tag{21}$$

It should be noticed that the average attractive energy for the chain is given by $E^{(r)}=-\varepsilon P^{(r)}$. Besides, the average monomer density is determined by

$$\rho^{(r)}=N^{(r)}/(R^{(r)})^{d_f}\ , \tag{22}$$

where $R^{(r)}$ is the distance between two vertices at the ends of an external edge of the rth stage of the construction of the lattice. Therefore, in what follows we need the partial derivatives of the partition functions with respect to x and w. Using the system of the recursion relations (12)–(15), the requisite derivatives with respect to x can be expressed in terms of a column vector $\mathbf{K}^{(r)}$ whose four components are given by

$$K_i^{(r)}=\frac{\partial A_i^{(r)}}{\partial x}\quad (i=1,2,3,4)\ ,$$

so that the following recursion relation is valid

$$\mathbf{K}^{(r+1)}=\underline{Q}^{(r)}\mathbf{K}^{(r)}\ , \tag{23}$$

where $\underline{Q}^{(r)}$ is a 4×4 matrix. The elements of the matrix $\underline{Q}^{(r)}$ are given by

$$Q_{ij}^{(r)}=\frac{\partial A_i^{(r+1)}}{\partial A_j^{(r)}}\ . \tag{24}$$

Therefore, one can, for instance, obtain the monomer density from formulas (20) and (22) by iterating the recursion relation (23), with the initial conditions being the first derivatives of (16)–(19) with respect to x. To study critical properties of the system, one should approach the thermodynamic limit by performing large numbers of the iterations, and, at the same time one should calculate all relevant quantities at $x=x_c(w)$. Here we can add that in order to learn the average energy $E^{(r)}$ one should iterate the recursion relation

$$\mathbf{L}^{(r+1)}=\underline{Q}^{(r)}\mathbf{L}^{(r)}+\mathbf{M}^{(r)}\ , \tag{25}$$

which is analogous to (23). The elements of the column vector $\mathbf{L}^{(r)}$ are the partial derivatives of $A_i^{(r)}$ with respect to w, assuming that only x is fixed, whereas the elements of the vector column $\mathbf{M}^{(r)}$ are the partial derivatives of $A_i^{(r)}$ with respect to w, assuming that all $A_i^{(r-1)}$ and x are fixed.

III. THE LOW-TEMPERATURE BEHAVIOR

We start our discussion of the behavior of the polymer system introduced in the preceding section by an analysis of its low-temperature properties. Due to the dominant influence of the attractive interactions at very low temperatures, the model being studied should be expected to display statistical properties of the Hamiltonian walks, that is, of the SAW that visit every site of the lattice. Such walks comprise a subset of all possible walks described by the four generating functions A_i (see Fig. 2). The corresponding recursion relations can be obtained, for instance, by substituting A_3 for A_1 and A_2 in relations (14) and (15). Consequently, one obtains

$$\begin{aligned} A_3' &= 2w^3A_3^4+4w^2A_3^3A_4+6wA_3^2A_4^2\ ,\\ A_4' &= 22A_4^4+w^4A_3^4+4w^3A_3^3A_4\ , \end{aligned} \tag{26}$$

which are relevant to the interacting Hamiltonian walks on the truncated 4-simplex. Here we want to emphasize that in a conventional treatment of the Hamiltonian walks one does not consider any interaction (except the excluded-volume interaction), and in such an approach w is equal to 1. Thus, if we set $w=1$ in (26) we can see that the latter acquire the form of renormalization group (RG) relations obtained by Bradley[14] in the case of noninteracting Hamiltonian walks.[15] These RG relations have one nontrivial fixed point given by $A_3^*=0$ and $A_4^*=(22)^{-1/3}$, with only one relevant eigenvalue $\lambda=4$ and with the critical exponent ν being equal to $\frac{1}{2}$.

The Hamiltonian walks have certain interesting properties that deserve to be studied in their own right. For example, in order to learn thermodynamic properties of these walks, with an arbitrary interaction w, it is necessary to determine the radius of convergence $x_H=1/\mu_H$ of the corresponding generating functions. This can be achieved by starting with the initial conditions (18) and (19), and by iterating the recursion relations (26). Thus we have found $1/\mu_H$ as a function of temperature (see Fig. 4). It is not difficult to check that the closed form of this function is $x_H(T)=\exp(-\varepsilon/T)/\omega$; that is, $x_H(T)=1/w\omega$, where $\omega=1.399\,710\,173$ is the limiting value of the reciprocal of the radius of convergence $x_H(T)$ when $T\to\infty$. Knowing the function $x_H(T)$, we can learn that the entropy of the Hamiltonian walks is the constant $\sigma=\ln\omega$ for all temperatures. Besides, it should be observed that the low-temperature behavior of our polymer system is properly described by the function $x_H(T)$ for small values of T. Indeed, we can obtain the same low-temperature values of $x_H(T)$ also by iterating (for large values of w) the system of Eqs. (12)–(15) with the initial conditions (16)–(19). This observation implies, among other things, that our polymer system has the finite entropy $\sigma=\ln\omega$ at $T=0$, which is reminiscent of a glasslike behavior.

Before leaving the subject related to the Hamiltonian walks, we would like to point out interesting properties of the case with a repulsive interaction ($\varepsilon<0$; that is,

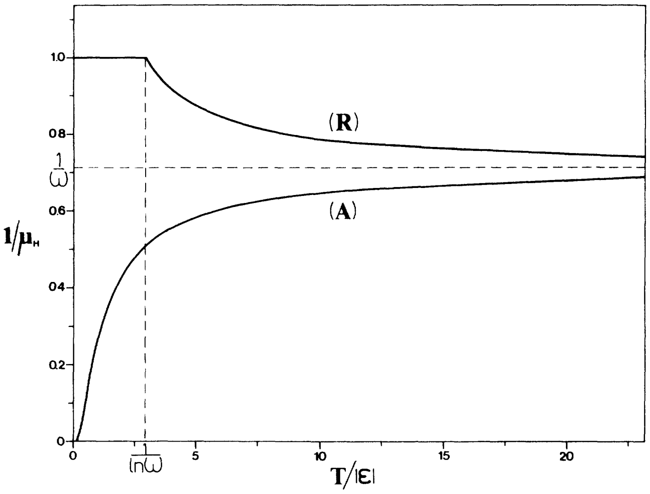

FIG. 4. Radius of convergence $1/\mu_H$ of the interacting Hamiltonian walks-generating function. (A) The case of attractive interactions ($\varepsilon > 0$). (R) The case of repulsive interactions ($\varepsilon < 0$). One can observe that, when $T \rightarrow \infty$, both curves approach the limiting value relevant to the noninteracting case.

$w < 1$). In this case we have found that the radius of convergence $x_H(T)$ is equal to one, for T less than $|\varepsilon|/\ln\omega$, whereas for $T \geq |\varepsilon|/\ln\omega$ the radius of convergence is given by $x_H(T) = w/\omega$ (see Fig. 4). Since the radius of convergence determines the free energy of the model system, this peculiar behavior of $x_H(T)$ implies a first-order phase transition at the finite temperature $T_0 = |\varepsilon|/\ln\omega$ (see Fig. 4), which was not observed in the case of an attractive interaction. The phase transition at T_0 can be described as a change from the low-temperature state, being rich in configurations depicted by the function A_4 (see Fig. 2), to the high-temperature state in which both types of configurations A_3 and A_4 are present.

The presence of monomer-monomer repulsive interactions ($w < 1$), in addition to the excluded-volume effect, is relevant to the case of a "super-good" solvent in which the nearest-neighbor contacts of nonconsecutive elements of the polymer must not occur ($w = 0$; that is, $v = -1$). Thus, if we let $v = -1$ ($w = 0$) in our recursion relations (12)–(14), we obtain a system of RG equations that describes a polymer chain in a "super-good" solvent. For this RG system of equations, with the initial conditions (15)–(19), it can be verified that only one nontrivial fixed point can be reached. The fixed point is given by $A_1^* = 0.429\,44$, $A_2^* = 0$, $A_3^* = 0$, and $A_4^* = 0.049\,98$. An analysis of this fixed point reveals that the corresponding critical exponent ν is equal to 0.674 022, which coincides with the value pertinent to the case of noninteracting SAW on the same lattice.[11] Therefore, increasing the self-avoiding constraint in the described way does not change the SAW class of universality. Of course, the same conclusion can be corroborated under the weaker constraint $w < 1$.

Now we turn to the case of attractive interactions ($w > 1$). The critical exponent ν for the entire low-temperature region can be obtained by using the general (valid for any temperature) formula

$$\nu^{(r)} = \ln 2 / \ln(N^{(r+1)}/N^{(r)}) , \tag{27}$$

which follows from the scaling law (1) and from the fact that within the rth stage of the fractal lattice the polymer chain's end-to-end distance is given by $R^{(r)} = 2^r$. The average number of monomers $N^{(r)}$ can be calculated by an iterative application of formula (20), so that (27) provides a sequence of values $\nu^{(r)}$. It turns out that the latter sequence converges quite rapidly to $\frac{1}{2}$ in the entire low-temperature region.

The foregoing result ($\nu = \frac{1}{2}$) can be related to the fact that the average monomer density is finite in the entire low-temperature region, that is to say, for all temperatures below the Θ point. This fact can be checked by calculating the monomer-density $\rho^{(r)}$ limiting values, when $r \rightarrow \infty$, via an iterative application of formula (22). Besides, an analysis of (22), together with the basic recursion relations (12)–(19), reveals the asymptotic form

$$\rho^{(r)} \cong \rho^{(\infty)} + \mathcal{C}/2^r ,$$

valid for sufficiently large r. In this formula $\mathcal{C}$ is a constant independent of r. Besides, henceforth we are going to denote without the superscript (∞) all quantities that are relevant to the thermodynamic limit $r \rightarrow \infty$. When temperature increases the average monomer density decreases and vanishes, at the Θ point, according to the power law $\rho \sim t^{\beta_T}$, where t is the reduced temperature $t = (\Theta - T)/T$ and β_T is the thermal critical exponent. Within our analysis we have found the value of Θ/ε with 22 correct digits, and here we quote the first few digits $\Theta/\varepsilon = 0.785\,89\ldots$. The preceding accuracy allowed us to determine the critical exponent β_T (by plotting $\ln\rho$ versus $\ln t$) with the five correct digits $\beta_T = 0.096\,38$. This result coincides with the value found by Dhar and Vannimenus[13] in the case of a model system in which the attractive interactions are restricted to bonds within only the first-order 4-simplex lattice, whereas the corresponding critical temperatures are found to be different, as should have been expected.

The critical exponent β_T can be related to the geometrical critical exponent ν_Θ and to the thermal critical exponent ν_T that appears in the scaling law of the thermal correlation length $\xi_T \sim (\Theta - T)^{-\nu_T}$. Specifically, using formulas (1), (22), and the expression $R^{(r)} = 2^r$ for the polymer end-to-end distance within the rth stage of the fractal lattice, we can obtain the result

$$\rho^{(r)} \sim 2^{\delta r} \quad (\delta = 1/\nu_\Theta - d_f) . \tag{28}$$

On the other hand, using the power law $\rho \sim \xi_T^{-\beta_T/\nu_T}$ and the finite-size scaling argument $\xi_T = 2^r$ we obtain

$$\rho^{(r)} \sim 2^{-r\beta_T/\nu_T} . \tag{29}$$

Combining (28) and (29) we finally obtain

$$\beta_T = \nu_T(d_f - 1/\nu_\Theta) . \tag{30}$$

We shall see later that our results for the critical exponents do confirm this relation.

IV. THE Θ POINT AND HIGH TEMPERATURE BEHAVIOR

In the preceding section we determined the Θ-point temperature, $\Theta/\varepsilon = 0.785\,89$, as a temperature at which the average monomer density vanishes. As was mentioned in the Introduction, at the Θ point the fractal dimension ($D = 1/\nu$) of the polymer chain changes abruptly from the compact-phase value 2 to the new value $1/\nu_\Theta$. Above the Θ point, it again changes (abruptly) to a value that is the characteristic of the swollen phase. We have determined ν_Θ by successive application of formula (27), together with the basic iterative relations (12)–(19), for the critical value of the Boltzmann factor $w_c = \exp(\varepsilon/\Theta)$. Thereby we have found $\nu_\Theta = 0.529\,39$, which coincides with the value found by Dhar and Vannimenus.[13] For all $w < w_c$ (that is, $T > \Theta$) we have obtained, by using a similar procedure, the expected[11] value $\nu = 0.674\,022$. Thus, we have learned the entire scaling behavior (2) of the average end-to-end distance.

In order to achieve a complete picture about the critical behavior of the polymer system, we should determine the thermal correlation length exponent ν_T. The latter can be found by studying the polymer heat capacity and the corresponding critical exponent α_T, since the following scaling relation $\nu_T = (2 - \alpha_T)\nu_\Theta$ can be established.[4,16] The heat capacity can be determined by calculating the second derivative of the free energy (5) with respect to temperature. However, this direct approach cannot be sufficiently precise as it implies a numerical differentiation. For this reason, we have applied the framework of the grand-canonical ensemble. Thus we start with the thermodynamic relation

$$C_N = \left[\frac{\partial E}{\partial T}\right]_x - \frac{\left[\dfrac{\partial E}{\partial x}\right]_T \left[\dfrac{\partial N}{\partial T}\right]_x}{\left[\dfrac{\partial N}{\partial x}\right]_T} , \qquad (31)$$

which we are going to use for calculating the specific heat C_N of our model system for a given number N of monomers (at a constant volume V). Within the framework of the grand canonical ensemble, the derivatives on the right-hand side of (31) can be expressed in terms of fluctuations of the number of contacts P and the number of monomers N, with the result

$$C_N = \frac{\varepsilon^2}{T^2}\left[\langle P^2\rangle - \langle P\rangle^2 - \frac{(\langle PN\rangle - \langle P\rangle\langle N\rangle)^2}{\langle N^2\rangle - \langle N\rangle^2}\right] . \qquad (32)$$

Here the bracketed quantities are the corresponding grand-canonical averages. For example, $\langle P\rangle$ is given by

$$\langle P\rangle = \frac{\sum_{N,P} P\,\mathcal{G}_{\vec{0}\vec{R}}(N,P)\,x^N w^P}{\sum_{N,P} \mathcal{G}_{\vec{0}\vec{R}}(N,P)\,x^N w^P} ,$$

where $\mathcal{G}_{\vec{0}\vec{R}}(N,P)$ is the number of all different chain configurations having N monomers and P contacts and span the points $\vec{0}$ and $\vec{R}$. The standard deviations of P and N that appear in (32) can be expressed in terms of first and second derivatives of the generating functions A introduced in Sec. II. For instance, the following relation is valid:

$$\langle N^2\rangle - \langle N\rangle^2 = \frac{x}{A_1}\frac{\partial A_1}{\partial x} - \left[\frac{x}{A_1}\frac{\partial A_1}{\partial x}\right]^2 + \frac{x^2}{A_1}\frac{\partial^2 A_1}{\partial x^2} , \qquad (33)$$

where the first two terms on the right-hand side of (33) can be calculated by applying the recursion relation (23), while for the third term we need the recursion relation

$$M_i^{(r+1)} = \sum_{j=1}^{4} Q_{ij}^{(r)} M_j^{(r)} + \sum_{j,k} \frac{\partial Q_{ij}^{(r)}}{\partial A_k^{(r)}} M_j^{(r)} M_k^{(r)} . \qquad (34)$$

Here $M_i^{(r)}$ is the second derivative of the generating function $A_i^{(r)}$ with respect to x.

Using the method presented in the preceding paragraph we have calculated the specific heat per monomer C_N/N of the model under study (a similar method can be applied to calculate other response functions). The obtained results are shown in Fig. 5. One can notice a pronounced divergence of the polymer system specific heat at the critical temperature $\Theta/\varepsilon = 0.785\,89\ldots$, which was previously located as a point where the order parameter (monomer density) vanishes. The method we have applied allows us to approach the critical point with a very high accuracy (of order 1 part in 10^{16}, and, if necessary, even better). Thus we have been able to determine the specific-heat critical-point exponent α_T with five correct digits $\alpha_T = 0.360\,27$. As we mentioned before, the knowledge of α_T, together with the scaling relation $\nu_T = (2 - \alpha_T)\nu_\Theta$, renders it possible to learn the thermal-correlation-length critical exponent $\nu_T = 0.868\,05$. With this result we have completed the picture about the critical behavior of the polymer system. Consequently, after inserting our findings for β_T, ν_Θ, and ν_T in relation (30),

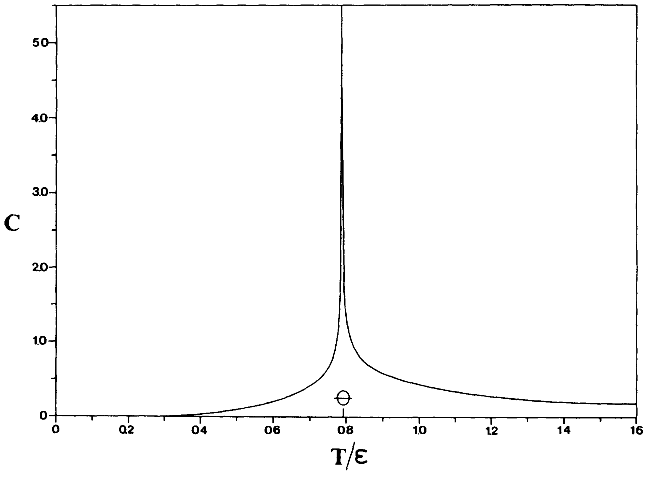

FIG. 5. The specific heat per monomer $C = C_N/N$ as a function of temperature. It should be emphasized that a log-log plot of the specific-heat data (taken from the region very close to the Θ point) vs the reduced temperature t reveals a well-defined straight line, with the slope $\alpha_T = 0.360\,27$.

we can now see that this relation (which was obtained after certain scaling assumptions) is satisfied. Besides, we would like to mention two additional relevant results. First, we have found that the specific-heat critical exponent α_T has the same value below and above the Θ point. Second, we have found that the ratio $\mathcal{A}_-/\mathcal{A}_+$ of the specific-heat critical amplitudes below and above the Θ point (which is a universal quantity in the case of the Euclidean lattices) for the truncated 4-simplex lattice has the value 0.514 45.

It is interesting to examine the place of the Θ point in relation to the phase diagram in the (x,T) plane. Within this plane the phase diagram is determined by a line of the critical values $x_c(T)$ that represent radii of convergence of the generating function $A_1(x,T)$. Our results are shown in Fig. 6. The Θ point divides the $x_c(T)$ curve into two parts. The low-temperature part $(T<\Theta)$ corresponds to the first-order phase transitions, which means that a crossing of the $x_c(T)$ curve below the Θ point corresponds to a discontinuous change of the polymer density $\rho(x)$ (see Fig. 7). On the other hand, a crossing of the $x_c(T)$ curve above the Θ point corresponds to a continuous vanishing of $\rho(x)$ [when $x(T)$ tends to $x_c(T)$ from higher values], which can be related to a second-order phase transition. Thus, the Θ point itself represents merging of the first- and second-order phase-transition lines, and for this reason it is a tricritical point.

General behavior of the order parameter ρ as a function of the fugacity x is shown in Fig. 7. There are several curves for several different temperatures. For $T\geq\Theta$ one can see that the corresponding curves continuously vanish at $x_c(T)$, whereas for $T<\Theta$ there is a discontinuous vanishing of $\rho(x)$. The continuous vanishing of ρ can be described as a power law of the type

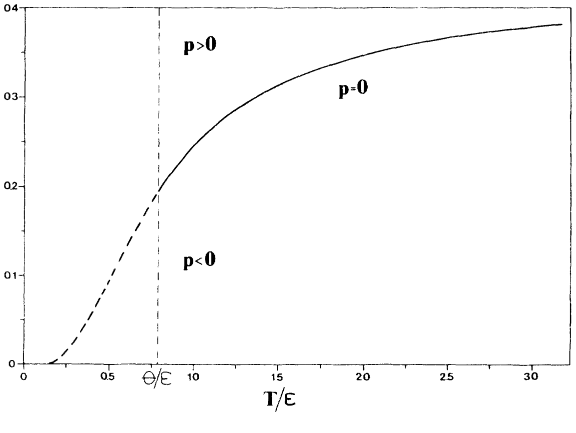

FIG. 6. The phase diagram depicted in the fugacity-temperature plane. The solid part of the $x_c(T)$ curve represents points of the second-order phase transitions, whereas the dashed part corresponds to points of the first-order phase transitions. Points that lie in the region below the $x_c(T)$ curve represent the swollen polymer states. In this phase the pressure of the polymer system is negative, which can be related to the exponential decreasing of the type (8) of the correlation function $A_1(x,T)$. Above the $x_c(T)$ curve the correlation function $A_1(x,T)$ increases exponentially with the system volume, implying densed polymer states with positive pressure.

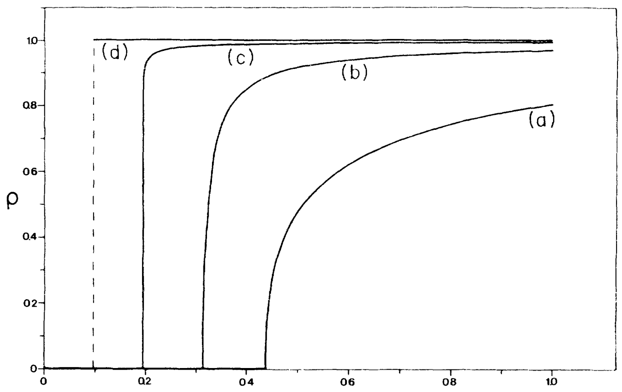

FIG. 7. The order parameter ρ as a function of the fugacity. The curves have been obtained by using expression (22) for different values of T. The (a) and (b) curves correspond to $T/\varepsilon=\infty$ and $T/\varepsilon=1.5$, respectively. The Θ temperature case corresponds to the (c) curve $(\Theta/\varepsilon=0.786)$. Finally, the (d) curve represents a case that corresponds to temperatures lower than Θ, when $\rho(x)$ has a steplike behavior.

$$\rho(x)\sim(x-x_c)^{\beta}\ , \tag{35}$$

where x_c and β take different values for different temperatures, and x approaches x_c from higher values. The critical exponent β can be related to the geometrical critical exponent (2) via the scaling relation

$$\beta=d_f\nu-1\ , \tag{36}$$

which can be obtained by using arguments that are similar to those presented in the last paragraph of Sec. III. On the other hand, by a numerical analysis of the curves depicted in Fig. 7, we have been able to determine precisely the values $\beta=0.348\,04$ and $\beta=0.058\,78$ for $T>\Theta$ and $T=\Theta$, respectively. These values of β, together with the previously obtained values of ν, are in agreement with the scaling relation (36). In the low-temperature region ($T<\Theta$, when $\nu=1/d_f$), the scaling relation (36) implies $\beta=0$, which is in accord with the steplike behavior of the function $\rho(x)$ (see Fig. 7).

Within this section we would like to present also a short discussion of the case of interacting ring polymers situated on the truncated 4-simplex lattice. The appropriate generating function $P(x,T)$ for these types of polymers may be expressed in terms of the generating functions A_1 and A_2, whose recursion relation are given by (12) and (13), respectively. We have found the explicit expression

$$P(x,T)=\sum_{r=0}^{\infty}4^{-4-1}[4(A_1^{(r)})^3+3(A_1^{(r)})^4 +6v(A_1^{(r)})^2(A_2^{(r)})^2+3v^2(A_2^{(r)})^4]\ ,$$

where $v=w-1$. It is expected that $P(x,T)$ has a singular behavior of the power-law type $P(x,T)\sim(x-x_c)^{2-\alpha}$, where x_c is the same function of T that is depicted in Fig. 6. Thus, the thermal properties of these types of polymers, in the thermodynamic limit, are the same as properties of the open chain polymers discussed above. As regards the critical exponent α, it should be related to the geometrical critical exponent (2) via the scaling relation $d_f\nu=2-\alpha$. Indeed, by studying the exact second derivative of $P(x,T)$, with respect to x, we have determined numerical values of α, which, together with previously found values of ν, are in accord with the latter scaling relation in all regions of temperature.

V. FLORY THEORY OF THE Θ POINT BEHAVIOR

Having developed an exact theory of interacting linear polymers on a fractal lattice, it is interesting to compare the obtained results with the corresponding Flory-type theory. Recently many attempts have been made to establish a proper Flory-type theory for the problem of SAW on fractals (see, for instance, Ref. 17 and references quoted therein). Here we shall first make a similar attempt in the case of the interacting SAW at the Θ point, and afterwards we shall compare the consequent findings with the available exact results.

In the spirit of the standard Flory theory,[18] we construct the free energy F of a polymer chain in a solvent as the sum of two parts $F=F_1+F_2$. The first part (sometimes called energetic term) can be written in the form

$$F_1=N[b_2(T)\rho+b_3(T)\rho^2+\cdots] , \tag{37}$$

where ρ is the monomer density ($\rho=N/R^{d_f}$), and b_2 and b_3 are the virial coefficients. In the extended state of the polymer chain the first term in the expression (37) dominates, while at the Θ point the second virial coefficient $b_2(T)$ vanishes and the energetic part of the total free energy acquires the simple form $F_1=b_3(T)N^3/R^{2d_f}$. On the other hand, the second part of the total free energy (the entropic term) F_2 can be written[17] in the form $F_2=c(T)(R^{d_{w,B}}/N)^{\tau}$, where $d_{w,B}$ is the fractal dimension of the random walk path made on the backbone of the fractal under study, and τ is a random walk exponent. Aharony and Harris[17] have shown that τ can be expressed in terms of two other scaling exponents $\tau=d_{\min}/(d_{w,B}-d_{\min})$, where $d_{\min}$ is the fractal dimension of the shortest (chemical) path on the fractal under study. Minimization with respect to R of the total free energy F yields the following expression for the geometrical critical exponent ν_F at the Θ point

$$\nu_F=\frac{3+\tau}{d_{f,B}(2+2\tau/d_{s,B})} , \tag{38}$$

where $d_{f,B}$ and $d_{s,B}$ are the fractal and spectral dimensions of the backbone, respectively. The obtained formula can be applied to the case of the critical percolation cluster, as well as to the case of a deterministic fractal. Besides, in the case of the Euclidean lattices, formula (38) reduces to the result found in Ref. 19. Furthermore, by imposing on ν_F that it be equal to $d_{s,B}/2d_{f,B}$ in (38) one neglects the excluded-volume effects, and thereby one can find that the spectral dimension value $d_{s,B}=3$ determines the upper critical dimension for the Θ-point behavior on fractals.

Now we are going to compare predictions that follow from (38) with the exact results found in the case of deterministic fractals. In particular, we are concerned here with the class of fractal objects that are their own backbone, which means that $d_{f,B}=d_f$ and $d_{s,B}=d_s$. Thus, for the truncated 4-simplex lattice, formula (38) implies $\nu_F=0.644\,82$, whereas the exact result is $\nu_\Theta=0.529\,39$. The second exact result can be obtained in the case of the truncated 6-simplex lattice,[11,20] which is characterized by $d_f=\ln 6/\ln 2$ and $d_s=2\ln 6/\ln 8$. It turns out that a description of an appropriate model system, in which the attractive interactions are limited to bonds within only the first-order 6-simplex lattice, can be achieved by using only three restricted partition functions.[21] An analysis of the corresponding recursion relations reveals the existence of three relevant fixed points. Two of these fixed points describe low- and high-temperature behavior (with the respective geometrical critical index ν being equal to $\ln 2/\ln 6$ and $0.550\,18$), while the third one describes a Θ-point behavior with the following exact critical exponent $\nu_\Theta=0.401\,38$. This finding should be compared with the value $0.524\,74$ which follows from (38). Therefore, one can see that in the case of the truncated 4-simplex, as well as in the case of the truncated 6-simplex, the Flory-type formula (38) overestimates the critical exponent ν_Θ. The case of the truncated 5-simplex lattice is not discussed here since this lattice does not allow the existence of the Θ point (see Sec. VI and the Appendix).

The observed discrepancy between the exact values for ν_Θ and the corresponding Flory-type predictions, in the case of fractal lattices, could have been anticipated because the same type of discrepancy appears in the case of regular lattices.[19,22] One may try to lessen the discrepancy (in a phenomenological manner) by relaxing the choice of the exponent τ for the problem of interacting linear polymers on fractals at the Θ point. Accordingly, by taking a value of τ that satisfies the inequality $\tau>1/(d_w-1)$ one can bring about a better agreement with the available exact results. Of course, there are many other phenomenological ways to achieve various closed-form expressions for ν_Θ. For instance, by using a correspondence (in two dimensions) between the percolation hull and the polymer conformation at the Θ point,[23] it has been learned that $\nu_\Theta=5/(d_{f,B}+7)$, which fits the exact results reasonably well (although it cannot be expected[23] that the latter formula works well for higher dimensional systems). Therefore, it appears that in the case of the Θ-point behavior on fractals, similarly to the SAW problem on fractals, it is hardly possible to find the critical exponents closed-form expressions that are both simple and accurate.

VI. SUMMARY

In this paper we have presented results of our study of thermal and geometrical properties of interacting chain polymers situated on a class of fractal lattices represented by the truncated 4-simplex. In order to achieve a complete picture of the corresponding thermodynamical behavior (including the critical behavior), we have developed a systematic use of the recursion relations for both the partition functions *and* their various derivatives, which makes possible the avoiding of difficulties related to numerical differentiation. We have thereby been able to obtain a proper solution of the polymer problem, demonstrating that the studied model has a finite critical temperature ($\Theta \neq 0$), with well-defined critical exponents. A finite critical temperature has been found[13] also for the truncated 4-simplex lattice, by studying a model with a restricted set of attractive interactions. In our model, however, we do not impose restrictions on the attractive interactions. The critical temperatures found in the two cases (the restricted set[13] of interactions and the entire set of possible interactions) are different, as could have been expected. On the other hand, the set of exponents calculated in Ref. 13, as well as those exponents whose values follow from the scaling relations, agree with our results, which indicates that the models (with two different sets of interactions) belong to the same universality class. This finding should be a relevant piece of information within the context of the problem of equivalence of the Θ and Θ' point.[7,24]

The method developed in the case of the truncated 4-simplex lattice can be applied to any fractal lattice with a finite order of ramification. In this manner, we have studied the polymer-chain problem on a lattice with a higher order of ramification, that is, on the truncated 5-simplex lattice (see Appendix) and found no collapse transition. This finding is in contrast with the generally accepted qualitative argument[12] that leads to the conclusion that the more ramified lattices are more likely to allow the appearance of a polymer phase with a finite-monomer density. On the other hand, a study of the available recursion relations for the truncated 6-simplex lattice,[20,21] obtained for a restricted set of the attractive interactions, reveals the existence of a finite-temperature collapse transition. This fact demonstrates that the problem of existence of collapse transition is more intricate than one could have expected. Consequently, keeping in mind that the fractals under study are more regular objects than stochastic fractals (like the critical percolation clusters), one can infer that for the latter the same problem should be approached rather cautiously.

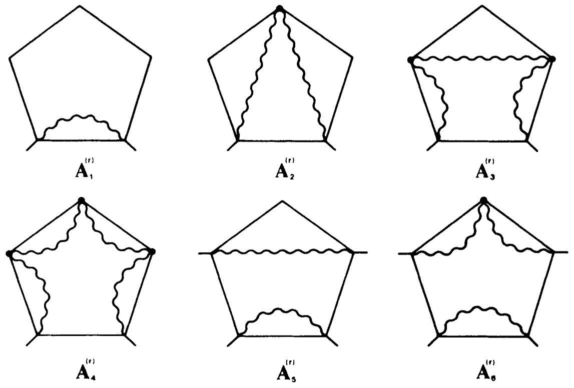

FIG. 8. The six restricted partition functions used in the study of the interacting SAW problem in the case of the truncated 5-simplex lattice.

ACKNOWLEDGMENTS

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APPENDIX: THE 5-SIMPLEX CASE

The following remarks concern the existence of the Θ point in the case of the truncated 5-simplex lattice. This is a self-similar (fractal) lattice, with the fractal and spectral dimension being equal to ln5/ln2 and 2 ln2/ln7, respectively.[11,20] The problem of the interacting SAW on this lattice can be studied by introducing the six restricted generating functions represented in Fig. 8, whose meaning is similar to the meaning given to the functions (see Fig. 2) used in the 4-simplex case. These functions satisfy the following set of the recursion relations:

$$\begin{aligned}
A_1' = {} & 132A_5^4(A_1+A_5)+A_1^2(1+18A_5^2+96A_5^3)+A_1^3(3+12A_5+78A_5^2)+6A_1^4(1+A_1+5A_5) \\
& +v[528A_5^3A_6(A_2+A_6)+A_1A_2A_6(384A_5^2+216A_1A_5+48A_1^2)+A_1A_2^2(3+24A_5+198A_5^2) \\
& \quad +A_1^2A_2^2(18+126A_5+36A_1)+A_2^2A_5^2(18+96A_5)+24A_1^3A_6^2 \\
& \quad +v(384A_2A_5A_6(A_3A_5+A_2A_6)+A_2A_3A_6(72A_1^2+288A_1A_5)+A_3A_5^2(528A_6^2+162A_2^2) \\
& \qquad +A_1A_2^2A_3(12+156A_5+54A_1)+A_2^2(216A_1A_6^2+12A_3A_5)+A_2^3A_6(216A_5+120A_1) \\
& \qquad +6A_2^4(1+6A_1+8A_5)+v\{96A_2A_3^2A_6(A_1+3A_5)+24A_1(A_3^3A_5+A_2^2A_4A_6) \\
& \qquad\qquad +A_2^2(60A_1A_3^2+360A_3A_6^2+72A_4A_5A_6+6A_3^2+108A_3^2A_5) \\
& \qquad\qquad +12A_2^3(A_1A_4+14A_3A_6+2A_4A_5)+6A_3^3(A_1^2+7A_5^2)+384A_3^2A_5A_6^2 \\
& \qquad\qquad +42A_2^4A_3+v[6A_2A_3^2(2A_1A_4+4vA_3A_4+6A_4A_5+20A_3A_6) \\
& \qquad\qquad\qquad +6A_3^2(A_1A_3^2+vA_5A_4^2+8vA_3A_4A_6+vA_3^3) \\
& \qquad\qquad\qquad +6A_2^2A_3(vA_4^2+12A_4A_6+8A_3^2+4A_2A_4) \\
& \qquad\qquad\qquad +6A_3^2(v^2A_3A_4^2+12A_4A_5A_6+28A_3A_6^2+3A_3^2A_5)]\})] \, ,
\end{aligned}$$

$$\begin{aligned}
A_2' = {} & A_2^2(6A_1^3+6A_5^2+4A_1A_5+54A_1A_5^2+2A_1^2+26A_1^2A_5)+A_1A_5^2A_6(128A_2+176A_6) \\
& +8A_1^2A_2A_6(6A_5+A_1)+A_5^3(176A_2A_6+32A_2^2+528A_6^2) \\
& +2v[A_2^4(7A_1+11A_5+1)+A_2^3A_6(28A_1+60A_5)+352A_5A_6^2(A_3A_5+A_2A_6)+A_1A_3^2A_5(21A_5+6A_1) \\
& \quad +A_3^2(A_1^3+3A_5^2+16A_5^3)+A_2^2A_6^2(60A_1+128A_5)+A_2^2A_3(2A_1+36A_1A_5+4A_5+10A_1^2+42A_5^2) \\
& \quad +A_5A_6^2(128A_1A_3+1056A_6^2)+A_2A_3A_6)(96A_1A_5+128A_5^2+16A_1^2) \\
& \quad +v(A_2A_3A_4(12A_1A_5+2A_1^2+30A_5^2)+A_2A_3A_6^2(256A_6+168A_2)+A_3A_4A_5A_6(24A_1+64A_5) \\
& \quad\quad +A_2^3A_3(64A_6+13A_2)+352A_6^3(A_4A_5+A_3A_6)+A_2^2A_3^2(3+24A_1+48A_5) \\
& \quad\quad +A_2A_3^2A_6(180A_5+60A_1)+A_5A_6^2(128A_2A_4+192A_3^2)+A_3^3(12A_1A_5+2A_5+2A_1^2+15A_5^2) \\
& \quad\quad +A_2^2A_4A_6(12A_1+48A_5)+A_2^3A_4(4A_1+10A_5)+84A_1A_3^2A_6^2 \\
& \quad\quad +v\{A_3^4(1+5A_1+10A_5)+A_2^2A_4^2(A_1+4A_5)+A_3A_4(216A_2A_6^2+72A_2^2A_6+16A_2^3+256A_6^3) \\
& \quad\quad\quad +A_5A_4^2(2A_1A_3+9A_3A_5+24A_2A_6)+A_3^2A_4(12A_1A_2+42A_2A_5+24A_1A_6+108A_5A_6) \\
& \quad\quad\quad +A_2A_3^3(88A_6+26A_2)+A_6^2(64A_4^2A_5+108A_3^3) \\
& \quad\quad\quad +v[A_3A_4^2(6vA_2A_4+52A_2A_6+28vA_4A_6+10A_2^2+3v^2A_4^2+132A_6^2)+A_4^3A_5(2A_2+vA_4+12A_6) \\
& \quad\quad\quad\quad +A_3^2A_4^2(3A_1+15A_5)+A_3^3(28A_2A_4+12vA_4^2+64A_4A_6+4A_3^2)]\})] ,
\end{aligned}$$

$$\begin{aligned}
A_3' = {} & 8A_1A_2A_6(16A_5^2+6A_1A_5+A_1^2)+176A_5^3A_6(A_2+3A_6) \\
& +A_2^2(2A_1^2+4A_1A_5+54A_1A_5^2+26A_1^2A_5+6A_1^3+6A_5^2+32A_5^3)+176A_1A_5^2A_6^2 \\
& +v[2A_2^4(1+7A_1+11A_5)+A_2^3A_6(56A_1+120A_5)+A_2^2A_6^2(120A_1+256A_5) \\
& \quad +A_3^2(12A_1^2A_5+2A_1^3+6A_5^2+32A_5^3+42A_1A_5^2)+704A_5A_6^2(A_3A_5+A_2A_6+3A_6^2) \\
& \quad +4A_2^2A_3(A_1+18A_1A_5+2A_5+5A_1^2+21A_5^2)+32A_2A_3A_6(A_1^2+6A_1A_5+8A_5^2)+256A_1A_3A_5A_6^2 \\
& \quad +v(4A_2A_3A_4(A_1^2+6A_1A_5+10A_5^2)+128A_2A_3A_6(A_2+4A_6^2)+704A_6^3(A_3A_6+A_4A_5) \\
& \quad\quad +48A_4A_5A_6(A_1A_3+2A_2^2)+4A_3^3(4A_5+4A_1^2+24A_1A_5+30A_5^2)+A_2^3A_4(8A_1+20A_5) \\
& \quad\quad +120A_3^2A_2A_6(A_1+3A_5)+6A_2^2A_3^2(1+8A_1)+24A_2^2A_6(A_1A_4+14A_3A_6) \\
& \quad\quad +96A_3^2A_5(A_2^2+4A_6^2)+128A_4A_5A_6(A_5A_3+2A_2A_6)+26A_3A_4^4+168A_1A_3^2A_6^2 \\
& \quad\quad +v\{144A_2A_3A_4A_6(A_2+2A_6)+2A_3^4(1+5A_1+10A_5)+2A_2^2A_4^2(A_1+4A_5) \\
& \quad\quad\quad +A_3^3(176A_2A_6+52A_2^2+216A_6^2)+4A_3^2A_4(6A_1A_2+21A_2A_5+12A_1A_6+54A_5A_6) \\
& \quad\quad\quad +128A_4A_6^2(A_4A_5+4A_3A_6)+4A_3A_4(A_1A_4A_5+8A_2^3)+A_4^2A_5(18A_3A_5+48A_2A_6) \\
& \quad\quad\quad +v[A_2A_3A_4^2(104A_6+20A_2)+vA_3A_4^3(12A_2+56A_6+6vA_4)+4A_4^3A_5(A_2+6A_6) \\
& \quad\quad\quad\quad +6A_3^2A_4^2(A_1+5A_5)+A_3^3A_4(56A_2+24A_4+128A_6)+264A_3A_4^2A_6^2+2vA_4^4A_5+8A_3^5]\})] ,
\end{aligned}$$

$$\begin{aligned}
A_4' = {} & 6A_2^3(4A_1A_5+A_1^2+7A_5^2)+528A_5^2A_6^2(A_2+2A_6)+12A_2^2A_6(A_1^2+6A_1A_5+16A_5^2) \\
& +6v[A_2A_3A_5(128A_6^2+6A_1A_3)+A_2A_3^2(A_1^2+15A_5^2)+352A_6^3(2A_6^2+A_3A_5)+12A_2^2A_3A_6(A_1+4A_5) \\
& \quad +A_3^2A_5A_6(12A_1+32A_5)+A_2^3A_3(4A_1+10A_5)+A_2^3(A_2^2+6A_2A_6+28A_6^2) \\
& \quad +v(A_2^2A_3^2(8A_2+36A_6)+A_2^3A_4(A_2+8A_6)+A_3A_4A_5A_6(48A_2+128A_6)+4A_1A_3^3(A_2+2A_6) \\
& \quad\quad +2A_2^2A_3A_4(A_1+4A_5)+A_3^3A_5(14A_2+36A_6)+A_3^2A_4A_5(2A_1+9A_5) \\
& \quad\quad +A_3^2A_6^2(108A_2+128A_6)+352A_4A_6^4 \\
& \quad\quad +v\{A_3^4(7A_2+16A_6)+2A_3^3A_4(A_1+5A_5)+6A_3A_4^2A_5(A_2+6A_6) \\
& \quad\quad\quad +A_3^2A_4(52A_2A_6+10A_2^2+132A_6^2)+A_4^2(A_2^3+A_4A_5^2+128A_6^3) \\
& \quad\quad\quad +v[6A_3^4A_4+A_3^2A_4^2(9A_2+42A_6)+A_4^3(4A_3A_5+6vA_3^2+52A_6^2)+10vA_4^4A_6+v^2A_4^5]\})] ,
\end{aligned}$$

$$\begin{aligned}
A_5' = {} & 22A_5^4(1+10A_1)+4A_1^3A_5(1+8A_5)+A_1^4(1+13A_5)+2A_1^5+88A_1^2A_5^3+186A_5^5 \\
& +v\{A_1A_2A_5A_6(528A_5+128A_1)+24A_2A_6(A_1^3+44A_5^3)+A_1^2A_2^2(4+66A_5)+12A_1A_2^2A_5(1+8A_5) \\
& \quad +A_2^2(14A_1^3+88A_5^3)+A_5^2A_6^2(528A_1+1488A_5) \\
& \quad +v[A_2A_3A_5A_6(256A_1+528A_5)+A_3A_5A_6^2(352A_1+1584A_5)+A_5A_6^3(2112A_2+2976A_6) \\
& \qquad +4A_1A_2^2A_3(1+27A_5)+A_2^4(2+27A_5+16A_1)+A_2^3A_6(72A_1+128A_5) \\
& \qquad +A_2^2A_6^2(128A_1+704A_5)+12A_2^2A_3A_5(1+8A_5)+A_1A_2A_3(48A_1A_6+26A_1) \\
& \qquad +v(A_1A_3^2A_6(96A_2+128A_6)+352A_2A_6^2(A_4A_5+2A_3A_6)+256A_2A_3A_6(A_3A_5+A_2A_6) \\
& \qquad\quad +28A_5(A_1A_3^3+A_2^3A_4)+704A_6^3(A_4A_5+3A_3A_6)+A_2^2A_4A_6(24A_1+128A_5) \\
& \qquad\quad +A_2^2A_3^2(4+36A_1+84A_5) \\
& \qquad\quad +8A_2^3(A_1A_4+15A_3A_6)+4A_3^2A_5(A_3+176A_6)+4A_3^3(A_1^2+8A_5^2)+22A_2^4A_3 \\
& \qquad\quad +v\{128A_3^2A_6(A_4A_5+A_3A_6)+A_3^4(1+15A_5)+24A_3^2A_6(A_1A_4+5A_2A_3) \\
& \qquad\qquad +32A_2^2A_3(A_3^2+3A_4A_6)+A_2A_3A_4(12A_1A_3+256A_6^2) \\
& \qquad\qquad +20A_2A_3A_4(A_2^2+3A_3A_5)+6A_1A_3^4+704A_3A_4A_6^3 \\
& \qquad\qquad +v[24A_3A_4^2A_6(vA_4+2A_2)+A_3^3A_4(28A_2+72A_6)+2A_3^2A_4^2(A_1+5vA_3) \\
& \qquad\qquad\quad +vA_4^4(A_5+2vA_3)+8A_4^2A_3(A_2^2+16A_6^2)+4A_3^5+4vA_2A_3A_4^3+18A_3^2A_4^2A_5]\})]\}\,, \\[2ex]
A_6' = {} & A_1^4(A_2+A_6)+44A_1A_5^3(A_2+2A_6)+A_5^4(66A_2+186A_6)+A_1^2A_2A_5(6A_1+16A_5) \\
& +v\{A_2A_3A_5(32A_1A_5+44A_5^2+12A_1^2)+88A_3A_5^2A_6(A_1+3A_5)+16A_2^2A_5^2(A_2+11A_6) \\
& \quad +A_1A_2^3(5A_1+18A_5)+A_5^2A_6^2(792A_2+1488A_6)+A_1A_2^2A_6(18A_1+64A_5)+2A_1^3A_2A_3 \\
& \quad +v[A_2A_3A_5(24A_1A_3+528A_6^2+32A_3A_5+128A_2A_6+30A_2^2)+A_2^2A_4(A_1^2+6A_1A_5+16A_5^2) \\
& \qquad +88A_4A_5A_6(A_2A_5+3A_5A_6)+A_3^2A_5A_6(64A_1+176A_5)+A_1A_2^2A_3(14A_2+60A_3) \\
& \qquad +A_2^3A_6(15A_2+64A_6)+2112A_3A_5A_6^3+2976A_6^5+4A_1^2A_2A_3^2+2A_2^5 \\
& \qquad +v(A_1A_3^2(10A_2A_3+6A_4A_5+28A_3A_6)+352A_6^3(A_3^2+5A_4A_6)+16A_3^2A_5(A_4A_5+4A_3A_6) \\
& \qquad\quad +A_3A_4A_5(24A_2^2+128A_2A_6+528A_6^2)+A_2A_3^2A_6(84A_2+192A_6)+A_2^3(28A_4A_6+16A_3^2) \\
& \qquad\quad +3A_2^2A_4(A_2^2+2A_1A_3)+30A_2A_3^3A_5 \\
& \qquad\quad +v\{12A_2A_3A_4(A_4A_5+9A_3A_6)+11A_2A_3^4+4A_1A_3^3A_4+64A_3A_4^2A_5A_6 \\
& \qquad\qquad +18A_2^2A_3^2A_4+2A_2^3A_4^2+192A_3^2A_4A_6^2+18A_3^3A_4A_5+27A_3^4A_6+352A_4^2A_6^3 \\
& \qquad\qquad +v[13A_2A_3^2A_4^2+13vA_4^4A_6+7vA_3^2A_4^3+6A_3A_4^3A_5+v^2A_4^5+66A_3^2A_4^2A_6 \\
& \qquad\qquad\quad +8A_3^4A_4+64A_3^3A_6^2]\})]\}\,.
\end{aligned} \tag{A1}$$

This system of equations should be supplemented by the initial conditions

$$\begin{aligned}
A_1^{(1)} &= x^2+6x^5w^6+3x^3w+6x^4w^3\,, \\
A_2^{(1)} &= x^3w+4x^4w^3+6x^5w^6\,, \\
A_3^{(1)} &= 2x^4w^3+6x^5w^6\,, \\
A_4^{(1)} &= 6x^5w^6\,, \\
A_5^{(1)} &= x^4w^4+2x^5w^7\,, \\
A_6^{(1)} &= x^5w^7\,,
\end{aligned} \tag{A2}$$

which make the definition of the polymer chain model complete.

An analysis of (A1), by applying the method described in Sec. II, reveals that the corresponding model system cannot reach a phase characterized by a finite monomer density starting with the initial conditions (A2). In addition, within the same analysis we have shown that, in the 5-simplex case, the geometrical critical exponent ν has the single value 0.600 32 in the entire temperature region, which, among other things, means that the model under study does not display the Θ point at a finite temperature. This finding should be contrasted with the results obtained for the 4-simplex and 6-simplex lattices.

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