Solution of a model of self-avoiding walks with multiple monomers per site on the Bethe lattice

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We solve a model of self-avoiding walks with up to two monomers per site on the Bethe lattice. This model, inspired in the Domb-Joyce model, was recently proposed to describe the collapse transition observed in interacting polymers [J. Krawczyk *et al.*, Phys. Rev. Lett. **96**, 240603 (2006)]. When immediate self-reversals are allowed (reversion-allowed model), the solution displays a phase diagram with a polymerized phase and a nonpolymerized phase, separated by a phase transition which is of first order for a nonvanishing statistical weight of doubly occupied sites. If the configurations are restricted forbidding immediate self-reversals (reversion-forbidden model), a richer phase diagram with two distinct polymerized phases is found, displaying a tricritical point and a critical end point.

I. INTRODUCTION

Since the pioneering work by Flory [1] self-avoiding walks (SAW's) and mutually avoiding walks on lattices have been used extensively to model linear polymer molecules. The realization that the graphs relevant in the high-temperature series expansion of the n-vector model of magnetism correspond to self-avoiding walks in the limit $n \to 0$ [2] made it possible to apply the ideas of the renormalization group to polymer systems, and the concept of scaling has been very important in the later development of this field [3].

If the polymer chains are placed in a solvent, as the temperature is lowered the chains may change from an extended to a collapsed configuration. The temperature where this transition happens was named the θ temperature [1]. This phenomenon was modeled by self-avoiding walks with an attractive interaction between monomers on first-neighbor sites of the lattice [interacting SAW's (ISAW)], and if this problem is considered in an ensemble which is grand canonical with respect to the number of monomers, the θ point of polymer collapse was found to be a tricritical point [4]. Thus, in this generalized parameter space, the transition between a nonpolymerized and a polymerized phase is continuous at high temperatures, but becomes of first order as the temperature is lowered, and a tricritical point separates these two transition lines. The polymer-solvent system may also be treated in more detail, using a lattice gas model with two different particles (polymer monomers and solvent molecules) [5], and such models describe quite well experimental results of equilibrium polymerization in solution [6]. Actually the simpler ISAW model may be obtained as a limiting case of the more general diluted polymer model [7,8], and the tricritical points in the two models apparently belong to the same universality class. In two dimensions, extensive numerical work has been done to calculate the tricritical ex-

ponents of the ISAW model [7,9,10], and for the diluted polymer model the tricritical exponents were calculated exactly [11,12]. Also, it was found that in some cases the ISAW model may display a third phase, besides the nonpolymerized and polymerized phases, which is a dense phase. This behavior seems to be restricted to two-dimensional lattices and was found on the Husimi lattice [13–16] as well as on the square lattice using transfer-matrix and finite-size scaling techniques [17]. From these studies one may conclude that even qualitative aspects of the thermodynamic behavior of interacting polymers may be determined by details of the model. On the square and $q=4$ Husimi lattices, for example, a dense phase exists if the interaction is assumed to be between first-neighbor bonds, but is not stable if interacting monomers are considered.

Including interactions between SAW's is a major complication of the model, both in closed-form approximations and in transfer-matrix calculations. In a recent paper [18], Krawczyk *et al.* proposed an alternative approach which seems to be very promising, since only one-site interactions are present. In this model, $n_i = 0, 1, \ldots, K$ monomers may be placed on site i of the lattice and each site contributes with a factor $\omega_{n_i}(i)$ to the statistical weight of a configuration. Without loss of generalization, we may fix the weight of an empty site to be equal to 1. This model is inspired by a generalization of a model of weighted random walks proposed by Domb and Joyce some time ago [19], and it was also discussed in [20] for the particular choice $\omega_{n_i} = \omega^{-n_i}$ of the weight functions. The model was studied in [18] using simulations for the particular case $K=3$ and as a function of ω_2 and ω_3, fixing $\omega_1 = 1$. With a fixed value for ω_1 only polymerized phases will appear, and the authors look for transitions between those phases. For the particular case of a model where immediate self-reversals are forbidden, simulations on a cubic lattice (model RF3) show a transition between extended and collapsed phases. As the parameters are changed, there are indications in the simulations that the transition changes from second to first order. In another case (RA2-immediate reversals allowed, simulations on the

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square lattice), no evidence of a phase transition is found.

In this paper, we solve the model proposed in [18] on a Bethe lattice with coordination number q. Although the critical exponents are classical for Bethe lattice solutions, they may provide better information on the thermodynamic behavior of models than simpler mean-field approximations, particularly for polymer models, since first-neighbor correlations are included [21]. For the sake of simplicity, we restrict our calculation to the case $K=2$, where collapse may already occur, but we will not assume $\omega_1=1$, so that transitions between polymerized and nonpolymerized phases may be found. Similar to what happens in studies of the ISAW model and in simulations of the model with multiple monomers per site [18], qualitative differences are found on the Bethe lattice solutions of the reversion-allowed and reversion-forbidden (RA and RF) models. In the more restrictive RF model, we find two distinct polymerized phases, one of them with double-occupied sites only. This phase does not appear in the RA model. For $q>2$, no qualitative differences in the phase diagrams are found as q is changed. Although a tricritical point is found in the RF model, as expected, in the RA model the transition between the nonpolymerized and polymerized phases is always discontinuous for nonvanishing values of ω_2.

In Sec. II the model is defined in greater detail and its solution of the Bethe lattice in terms of recursion relations is presented. The thermodynamic properties of the model are obtained from the recursion relations and presented in Sec. III. Final conclusions and a discussion are in Sec. IV.

II. DEFINITION OF THE MODEL AND SOLUTION IN TERMS OF RECURSION RELATIONS

We consider linear polymers formed by monomers linked by bonds. The monomers are placed on the sites of a lattice and the chains are self-avoiding and mutually avoiding walks on this lattice. Up to K monomers may be located at the same lattice site. All monomers are supposed to be distinguishable. The polymeric chains are linear self-avoiding and mutually avoiding walks, each step linking two monomers located on first-neighbor sites. Thus multiple steps of the walk may be placed on the same bond of the lattice. The chains are not allowed to form rings. The statistical weight of a configuration will be a product over site configuration weights $\omega_{n_i}(i)$, where i labels the site and $n_i=0,1,\ldots,K$ is the number of monomers located on site i. We assume the weight of an empty site to be unitary ($\omega_0(i)=1$) and the weights to be independent of the site ($\omega_{n_i}(i)=\omega_{n_i}$). The model may be interpreted as an interacting polymer model, so that $\omega_1=z=\exp(\mu/k_BT)$ is the fugacity of a monomer and $\omega_n=z^n\exp[-\epsilon(n)/k_BT]$, ϵ_n being the interaction energy of the set of n monomers located on the same site. Monomers on different sites do not interact. Usually, if we are interested in the collapse transition, the monomer-monomer interactions should be attractive, and thus $\epsilon(n)<0$. For $K=1$ the usual polymerization model in the grand-canonical ensemble is recovered, which has been much studied as a model for equilibrium polymerization [5]. The model described here is the same studied by Krawczyk et al. [18], with a slight generalization,
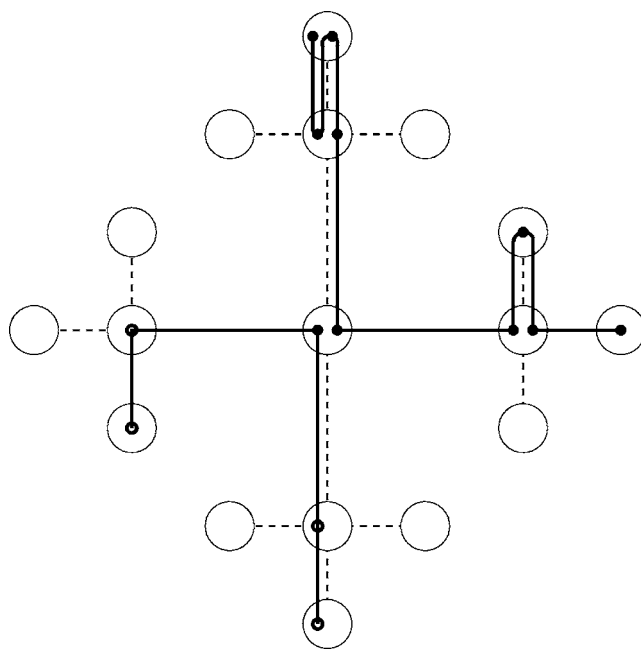

FIG. 1. Example of a configuration of the Cayley tree with $q=4$ and 3 generations. This configuration is allowed in the RA model, but not in the RF model. Polymer bonds (steps of the walks) are represented by solid lines, while the lattice bonds are dashed lines.

since they fixed $z=1$ in their simulations. With the parametrization adopted by them, the polymerization transition between a nonpolymerized and a polymerized phase is not found. Following Krawczyk et al. [18], we consider two versions of the model. In the RA variant, all walks which obey the self-avoidance restraint are included, whereas in the RF variant, only walks without immediate self-reversals are allowed. In other words, in the RF case configurations such that the walk reaches a site and immediately leaves this site through the same bond are prohibited.

We will here discuss the solution of the model for the particular case $K=2$ on the Bethe lattice. This is the smallest value for K for which the collapse may be found, so we have chosen it for simplicity. The Bethe lattice is the core of a Cayley tree, and the exact solution of statistical models on it may be viewed as an approximation of the solutions of the same models on regular lattices with the same coordination number [22]. We consider a Cayley tree of coordination number q and place the end points of the walks on the surface of the tree. In Fig. 1(a) configuration which contributes to the partition function of the RA model is shown for a tree with $q=4$ and three generations. This walk would not be considered in the RF model, since two immediate self-reversals are present. The statistical weight of the depicted configuration is $\omega_1^6\omega_2^4$.

The solution of the model on the Bethe lattice is obtained by defining partial partition functions for rooted subtrees and realizing that a subtree with $n+1$ generations may be obtained through the connection of $q-1$ n-generation subtrees to a new site and bond [21]. This operation leads to recursion relations for the partial partition functions. We start with the more restrictive RF model. One should be careful with the
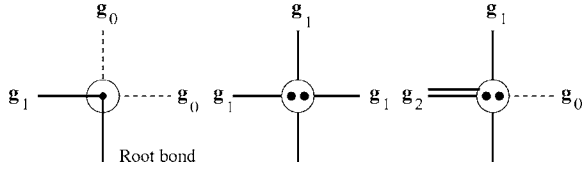
FIG. 2. Contributions to the recursion relation for the partial partition function g_1 (RF model).

multiplicity of each contribution to the recursion relations, recalling that even monomers placed on the same site of the lattice should be considered distinguishable. The partial partition functions for the model are g_0, g_1, and g_2, where the subscript denotes the number of polymer bonds on the root bond of the subtree. In Fig. 2 the contributions to the recursion relation for g_1 are shown graphically, in the order they appear in Eqs. (2).

Below, the recursion relations are presented. In general, we have $g_i' = \Sigma_j g_{i,j}'$, and whenever appropriate, the terms in the sums begin with a product of two numerical factors, the first of which is the multiplicity of the configuration of the incoming bonds and the second is the multiplicity of the connections with the monomers located at the new site. The recursion relation for g_0' is

$$g_{0,1}' = g_0^{q-1}, \tag{1a}$$

$$g_{0,2}' = \binom{q-1}{2} \times 1 \omega_1 g_0^{q-3} g_1^2, \tag{1b}$$

$$g_{0,3}' = \binom{q-1}{4} \times 6 \omega_2 g_0^{q-5} g_1^4, \tag{1c}$$

$$g_{0,4}' = 3\binom{q-1}{3} \times 4 \omega_2 g_0^{q-4} g_1^2 g_2, \tag{1d}$$

$$g_{0,5}' = \binom{q-1}{2} \times 4 \omega_2 g_0^{q-3} g_2^2. \tag{1e}$$

The terms of the recursion relation for g_1' are

$$g_{1,1}' = (q-1) \times 1 \omega_1 g_0^{q-2} g_1, \tag{2a}$$

$$g_{1,2}' = \binom{q-1}{3} \times 6 \omega_2 g_0^{q-4} g_1^3, \tag{2b}$$

$$g_{1,3}' = 2\binom{q-1}{2} \times 4 \omega_2 g_0^{q-3} g_1 g_2. \tag{2c}$$

For g_2' we find two terms

$$g_{2,1}' = \binom{q-1}{2} \times 2 \omega_2 g_0^{q-3} g_1^2, \tag{3a}$$

$$g_{2,2}' = (q-1) \times 2 \omega_2 g_0^{q-2} g_2. \tag{3b}$$

We may now define the ratios of the partial partition functions $R_1 = g_1/g_0$ and $R_2 = g_2/g_0$. Any expected value in the

center of the tree may be expressed as a function of these ratios, so that if we are interested in the behavior of the model in the center of the tree and in the thermodynamic limit, we should find the fixed point of the recursion relations for the ratios, which are

$$R_1' = \left[(q-1)\omega_1 + 6\binom{q-1}{3}\omega_2 R_1^2 + 8\binom{q-1}{2}\omega_2 R_2 \right] \frac{R_1}{D}, \tag{4a}$$

$$R_2' = 2\left[\binom{q-1}{2}R_1^2 + (q-1)R_2 \right] \frac{\omega_2}{D}, \tag{4b}$$

where

$$D = 1 + \binom{q-1}{2}\omega_1 R_1^2 + 6\binom{q-1}{4}\omega_2 R_1^4 + 12\binom{q-1}{3}\omega_2 R_1^2 R_2$$
$$+ 4\binom{q-1}{2}\omega_2 R_2^2. \tag{5}$$

For the RA model, where immediate self-reversals are allowed, three other root configurations for subtrees are possible. The additional partial partition functions are g_3 (two polymer bonds at the root, connected to the same monomer above), g_4 (same as for g_3, but with more than one monomer in the closed path), and g_5 (three polymer bonds at the root, two of them connected to the same monomer above). The recursion relations for this generalized model are

$$g_{0,1}' = g_0^{q-1}, \tag{6a}$$

$$g_{0,2}' = \binom{q-1}{2} \times 1 \omega_1 g_0^{q-3} g_1^2, \tag{6b}$$

$$g_{0,3}' = \binom{q-1}{4} \times 6 \omega_2 g_0^{q-5} g_1^4, \tag{6c}$$

$$g_{0,4}' = 3\binom{q-1}{3} \times 6 \omega_2 g_0^{q-4} g_1^2 g_2, \tag{6d}$$

$$g_{0,5}' = \binom{q-1}{2} \times 6 \omega_2 g_0^{q-3} g_2^2, \tag{6e}$$

$$g_{0,6}' = (q-1) \times 1 \omega_1 g_0^{q-2} g_2, \tag{6f}$$

$$g_{0,7}' = 3\binom{q-1}{3} \times 2 \omega_2 g_0^{q-4} g_1^2 g_3, \tag{6g}$$

$$g_{0,8}' = 3\binom{q-1}{3} \times 4 \omega_2 g_0^{q-4} g_1^2 g_4, \tag{6h}$$

$$g_{0,9}' = 2\binom{q-1}{2} \times 2 \omega_2 g_0^{q-3} g_2 g_3, \tag{6i}$$

$$g_{0,10}' = 2\binom{q-1}{2} \times 4 \omega_2 g_0^{q-3} g_2 g_4, \tag{6j}$$

$$g'_{0,11} = 2\binom{q-1}{2} \times 2\omega_2 g_0^{q-3} g_1 g_5. \tag{6k}$$

Notice that, although the first five terms are similar to the ones in the RF model, the multiplicities related to the connections of the two additional monomers may be larger in the less restrictive RA model. The contributions to g'_1 are

$$g'_{1,1} = (q-1) \times 1\omega_1 g_0^{q-2} g_1, \tag{7a}$$

$$g'_{1,2} = \binom{q-1}{3} \times 6\omega_2 g_0^{q-4} g_1^3, \tag{7b}$$

$$g'_{1,3} = 2\binom{q-1}{2} \times 6\omega_2 g_0^{q-3} g_1 g_2, \tag{7c}$$

$$g'_{1,4} = 2\binom{q-1}{2} \times 2\omega_2 g_0^{q-3} g_1 g_3, \tag{7d}$$

$$g'_{1,5} = 2\binom{q-1}{2} \times 4\omega_2 g_0^{q-3} g_1 g_4, \tag{7e}$$

$$g'_{1,6} = (q-1) \times 2\omega_2 g_0^{q-2} g_5, \tag{7f}$$

The contributions to g'_2 identical to the ones in the RF model, shown in Eqs. (3). For g_3 we find

$$g'_{3,1} = \omega_1 g_0^{q-1}, \tag{8a}$$

$$g'_{3,2} = \binom{q-1}{2} \times 2\omega_2 g_0^{q-3} g_1^2 \tag{8b}$$

$$g'_{3,3} = (q-1) \times 2\omega_2 g_0^{q-2} g_2. \tag{8c}$$

The contributions to g'_4 are

$$g'_{4,1} = (q-1) \times 1\omega_2 g_0^{q-2} g_3, \tag{9a}$$

$$g'_{4,2} = (q-1) \times 2\omega_2 g_0^{q-2} g_4. \tag{9b}$$

Finally, a single contribution to g'_5 was found:

$$g'_{5,1} = (q-1) \times 2\omega_2 g_0^{q-2} g_1. \tag{10}$$

In the recursion relations for the RA model, we notice that the partial partition functions g_3 and g_4 always appear in the combination $g_3 + 2g_4$. We therefore define the following ratios for this model: $R_1 = g_1/g_0$, $R_2 = g_2/g_0$, $R_3 = (g_3+2g_4)/g_0$, and $R_4 = g_5/g_0$. The recursion relations for the ratios are

$$R'_1 = \left[(q-1)\omega_1 R_1 + 6\binom{q-1}{3}\omega_2 R_1^3 + 12\binom{q-1}{2}\omega_2 R_1 R_2 \right.$$
$$\left. + 4\binom{q-1}{2}\omega_2 R_1 R_3 + 2(q-1)\omega_2 R_4 \right]\frac{1}{D}, \tag{11a}$$

$$R'_2 = 2\left[\binom{q-1}{2} R_1^2 + (q-1) R_2 \right]\frac{\omega_2}{D}, \tag{11b}$$

$$R'_3 = \left[\omega_1 + 2\binom{q-1}{2}\omega_2 R_1^2 + 2(q-1)\omega_2(R_2 + R_3) \right]\frac{1}{D}, \tag{11c}$$

$$R'_4 = \frac{2(q-1)\omega_2 R_1}{D}, \tag{11d}$$

where

$$D = 1 + \binom{q-1}{2}\omega_1 R_1^2 + 6\binom{q-1}{4}\omega_2 R_1^4 + 18\binom{q-1}{3}\omega_2 R_1^2 R_2$$
$$+ 6\binom{q-1}{2}\omega_2 R_2^2 + (q-1)\omega_1 R_2 + 6\binom{q-1}{3}\omega_2 R_1^2 R_3$$
$$+ 4\binom{q-1}{2}\omega_2 R_2 R_3 + 4\binom{q-1}{2}\omega_2 R_1 R_4. \tag{12}$$

The partition function of the model on the Cayley tree may be obtained if we consider the operation of attaching q subtrees to the central site of the lattice. The result for the RF model will be

$$Y^{(RF)} = g_0^q + \binom{q}{2}\omega_1 g_0^{q-2} g_1^2 + 6\binom{q}{4}\omega_2 g_0^{q-4} g_1^4$$
$$+ 12\binom{q}{3}\omega_2 g_0^{q-3} g_1^2 g_2 + 4\binom{q}{2}\omega_2 g_0^{q-2} g_2^2. \tag{13}$$

For the RA model, a similar calculation leads to the partition function

$$Y^{(RA)} = g_0^q + \binom{q}{2}\omega_1 g_0^{q-2} g_1^2 + 6\binom{q}{4}\omega_2 g_0^{q-4} g_1^4$$
$$+ 18\binom{q}{3}\omega_2 g_0^{q-3} g_1^2 g_2 + 6\binom{q}{2}\omega_2 g_0^{q-2} g_2^2 + q\omega_1 g_0^{q-1} g_2$$
$$+ 6\binom{q}{3}\omega_2 g_0^{q-3} g_1^2(g_3 + 2g_4) + 4\binom{q}{2}\omega_2 g_0^{q-2} g_2(g_3$$
$$+ 2g_4) + 4\binom{q}{2}\omega_2 g_0^{q-2} g_1 g_5. \tag{14}$$

In the thermodynamic limit, the solution of a model on the Cayley tree usually shows a behavior which is quite different from the one expected on regular lattices, since the number of surface sites represents a nonzero fraction of the total number of sites, even in the thermodynamic limit. We therefore study mean values calculated at the central site of the tree. The behavior of a model in the thermodynamic limit and in the central region of the Cayley tree has been named the Bethe lattice solution of this model [22]. Using the partition functions above, we then proceed calculating the densities at the central site of the tree. The density of monomers is given by

$$\rho = \frac{P + 2Q}{1 + P + Q}, \tag{15}$$

where for the RF model we have

$$P^{(RF)} = \omega_1 \binom{q}{2} R_1^2, \qquad (16a)$$

$$Q^{(RF)} = \omega_2 \left[6\binom{q}{4}\omega_2 R_1^4 + 12\binom{q}{3}R_1^2 R_2 + 4\binom{q}{2}R_2^2 \right]. \qquad (16b)$$

For the RA model, we have the results

$$P^{(RA)} = \omega_1 \left[\binom{q}{2}R_1^2 + qR_2 \right], \qquad (17a)$$

$$Q^{(RA)} = \omega_2 \left[6\binom{q}{4}R_1^4 + 18\binom{q}{3}R_1^2 R_2 + 6\binom{q}{2}R_2^2 + 6\binom{q}{3}R_1^2 R_3 \right.$$
$$\left. + 4\binom{q}{2}R_2 R_3 + 4\binom{q}{2}R_1 R_4 \right]. \qquad (17b)$$

It is supposed in the expressions above for the density of monomers at the central site that the ratios R_i have their fixed-point values, so that the thermodynamic limit results are obtained. Since P and Q are non-negative, the density of monomers will be in the interval $[0,2]$, as expected. The probability that the central site is occupied by a single monomer will be $\rho_1 = P/(1+P+Q)$, and the probability to find two monomers at the central site is $\rho_2 = Q/(1+P+Q)$.

III. THERMODYNAMIC PROPERTIES OF THE MODEL

As discussed above, the thermodynamic properties of the model on the Bethe lattice are determined by the fixed-point values of the ratios, defined by the recursion relations, for fixed values of the parameters ω_1 and ω_2. For the RF model, an inspection of the recursion relations (4) shows that a fixed point with $R_1 = R_2 = 0$ may exist. Equations (15) and (16) show that in such a phase the density of monomers vanishes, so that we may recognize it as the nonpolymerized (NP) phase. The next step is to identify the region of the parameter space (ω_1, ω_2) where this phase is stable. We thus calculate the jacobian in the NP phase, whose elements are

$$J_{i,j} = \left. \frac{\partial R_i'}{\partial R_j} \right|_{R_1 = R_2 = 0}, \qquad (18)$$

and the NP phase will be stable in the region of the parameter phase where the absolute values of both eigenvalues of the jacobian are smaller than 1. The Jacobian matrix is diagonal and the result of this calculation shows that the NP phase is stable when the conditions $\omega_1 < 1/(q-1)$ and $\omega_2 < 1/[2(q-1)]$ are both satisfied.

Another fixed point of the recursion relations for the RF model is such that $R_1 = 0$ and $R_2 \neq 0$. In this phase ρ_1 vanishes but ρ_2 not, so it is a polymerized phase in which only double occupied (DO) sites are present. The fixed-point value for R_2 is given by

$$R_2^{DO} = \sqrt{\frac{2(q-1)\omega_2 - 1}{2(q-1)(q-2)\omega_2}}, \qquad (19)$$

and from 16 we have $P = 0$ and

$$Q = 4[2(q-1)\omega_2 - 1],$$

which leads to the density of doubly occupied sites:

$$\rho_2^{DO} = \frac{8(q-1)\omega_2 - 4}{8(q-1)\omega_2 - 3}. \qquad (20)$$

The Jacobian matrix is also diagonal in the DO phase, and the nonzero elements are

$$J_{1,1} = \frac{\omega_1}{2\omega_2} + \sqrt{\frac{2(q-2)[2(q-1)\omega_2 - 1]}{(q-1)\omega_2}}, \qquad (21a)$$

$$J_{2,2} = \frac{1}{(q-1)\omega_2} - 1. \qquad (21b)$$

The DO phase is stable if the absolute value of both eigenvalues of the Jacobian is less or equal to 1, which leads to the conditions

$$\frac{1}{2(q-1)} \leq \omega_2 \leq \frac{2(q-2)}{(q-1)(4q-9)}, \qquad (22)$$

and for a value of ω_2 in the range above, we have

$$\omega_1(\omega_2) \leq 2\omega_2 - 2\sqrt{\frac{2[2(q-1)\omega_2 - 1](q-2)\omega_2}{(q-1)}}. \qquad (23)$$

It may be observed that this phase has a nonvanishing region of stability for any value of the lattice coordination number. For large values of q we may expand the limits of the stability interval in powers of $1/q$, finding that

$$\frac{1}{2(q-1)} \underset{q\to\infty}{\sim} \frac{1}{2q}\left(1 + \frac{1}{q} + \cdots\right),$$

$$\frac{2(q-2)}{(q-1)(4q-9)} \underset{q\to\infty}{\sim} \frac{1}{2q}\left(1 + \frac{5}{4q} + \cdots\right).$$

We conclude that the NP-DO phase transition is continuous, at $\omega_2 = 1/[2(q-1)]$. For $\omega_2 > 1/[2(q-1)]$ the other stability limit of the DO phase is given by expression (23).

A third fixed point of the recursion relations (4), which we may associate with the regular polymerized phase (P), corresponds to both ratios at nonzero values. The analytic study of this fixed point is harder, but with the help of a formal algebra software we may conclude that the stability limit of the DO phase is never coincident with the stability limit of the P phase, and thus the DO-P transition is always of first order. The stability limits of the NP and P phases are the same for $\omega_2 < 1/[2(q-1)^2]$; henceforth, the transition between these phases is continuous in this region. For larger values of ω_2, this transition becomes discontinuous. A tricritical point is found at

$$\omega_1^{TC} = \frac{1}{q-1}, \qquad (24a)$$

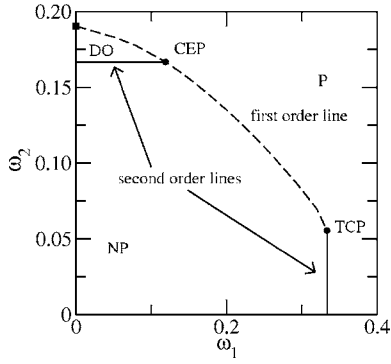$$\omega_2^{TC} = \frac{1}{2(q-1)^2}. \qquad (24b)$$

FIG. 3. Phase diagram for the RF model on a Bethe lattice with $q=4$. Solid lines are continuous transitions and on the dashed lines two phases coexist. NP denotes the nonpolymerized phase ($\rho_1=\rho_2=0$), DO the double-occupancy phase ($\rho_1=0,\rho_2\neq 0$), and P the regular polymerized phase ($\rho_1,\rho_2\neq 0$).

The first-order transition lines may be found through a Maxwell construction [13], but this procedure may be difficult to converge numerically if more than two phases are present. For simplicity, we thus adopted an alternative procedure [14], iterating the recursion relations starting with the physical values for the partial partition functions for a subtree of generation "zero," which are $g_0^{(0)}=1$, $g_1^{(0)}=\omega_1$, and $g_2^{(0)}=\omega_2$. With these starting values, the recursion relations do converge to the stable thermodynamic phase and therefore do converge to the stable thermodynamic phase and therefore we may obtain the first-order transition lines. In Fig. 3 we show the phase diagram of the RF model for $q=4$. The solid lines are second-order transitions and at the dashed lines two distinct phases coexist. The continuous NP-P transition line ends at a tricritical point located at $\omega_1=1/(q-1)=1/3$ and $\omega_2=1/2(q-1)^2=1/18$. The second-order NP-DO transition ends at a critical end point at $\omega_1=0.119\ 036\ 5$ and $\omega_2=1/6$ (ω_1 was determined numerically). It is worth mentioning that there is no discontinuity at the point where the P-DO coexistence line touches the $\omega_1=0$ axis, denoted by a square in the phase diagram. Also, the fact that the DO phase becomes unstable as ω_1 is increased for fixed ω_2 may be understood noting that although it is energetically more favorable to have doubly occupied sites at high values of ω_2, a nonzero density of simply occupied sites increases the entropy.

In Fig. 4 the densities of single- and double-occupied sites are shown as functions of ω_2 for a fixed value $\omega_1=0.09$, again for a lattice with $q=4$. For low values of ω_2 the NP phase is stable. At $\omega_2=1/2(q-1)=1/6$, a continuous transition to the DO phase occurs, followed by a discontinuous transition to the P phase at $\omega_2\approx 0.17503$.

Turning our attention to the more general RA model, we notice from the recursion relations (11) that the nonpolymerized phase has now the fixed-point values $R_1=R_2=R_4=0$ and

$$R_3=\frac{\omega_1}{1-2(q-1)\omega_2}. \tag{25}$$

These values for the ratios actually correspond to $\rho=0$, as may be seen using Eq. (15) for the density of monomers. The stability limit of the NP phase is obtained requiring that the
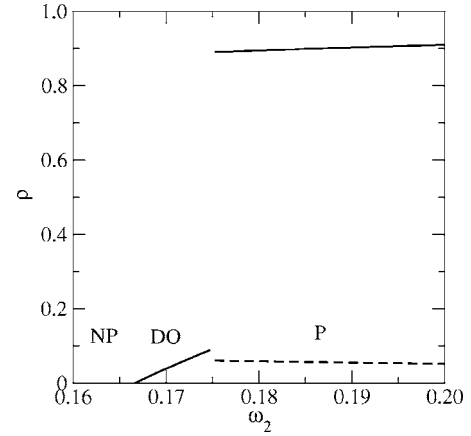

FIG. 4. Densities for the RF model with $q=4$ as functions of ω_2, for $\omega_1=0.09$. The solid line is the density of double-occupied sites (ρ_2), and the dashed line corresponds to the density of single-occupied sites (ρ_1).

largest eigenvalue of the Jacobian, calculated at the fixed-point values of the ratios above, have an absolute value equal to 1. This leads to the following condition:

$$\omega_1^{(NP)}=\frac{[1-2(q-1)\omega_2]^2[1+2(q-1)\omega_2]}{1-2\omega_2}. \tag{26}$$

We may search for a DO fixed point, which should have the values $R_1=R_4=0$ and $R_2,R_3\neq 0$. However, writing the equation for the fixed-point value of the ratio R_2/R_3, we reach the unphysical conclusion $R_2=-\omega_1/[2(q-1)\omega_2]$, indicating that such a phase does not appear in the RA model for $\omega_1\neq 0$, since the ratios of partial partition functions should be non-negative. We may have some physical understanding of the nonexistence of a region where the DO phase is stable in the RA model if we notice that the DO phase found in the RF model is composed by linear chains with double polymer bonds between first-neighbor sites occupied by two monomers, which are constrained to have end points at the surface of the tree. We may notice that in the RF model, for $\omega_1=0$, we have a continuous transition from the NP phase to the DO phase at $\omega_2=1/[2(q-1)]$. If we take into account that at each lattice site there are two ways to connect the bonds to the monomers on this site for a linear DO polymer, this corresponds exactly to the well-known result that the polymerization transition for linear chains on a Bethe lattice occurs when the statistical weight of a monomer is equal to $1/(q-1)$ [21], as may be also seen in our results for the RF model in the particular case $\omega_2=0$. If we allow immediate self-reversals, these chains may end at any step inside the tree. Therefore, this corresponds to allow for *end points* in the problem of polymerization of linear chains, and it is known that this effect eliminates the polymerization transition. It is possible to map the equilibrium polymerization model into the *n*-vector model of magnetism in the formal limit $n\rightarrow 0$, and if this is done, the statistical weight of monomer at the end of chains is proportional to the magnetic field in the *n*-vector model [23]. The continuous ferromagnetic transition in the *n*-vector model exists only when no magnetic field is
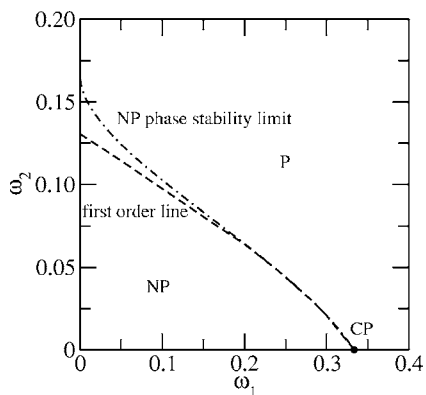
FIG. 5. Phase diagram for the RA model on a Bethe lattice with $q=4$. Only the nonpolymerized (NP and the regular polymerized (P) phases appear. For nonzero ω_2, the phase transition is always discontinuous. The stability limit of the NP phase is shown as a dash-dotted line.

applied. Accordingly, no polymerization transition is found for nonzero statistical weight of monomers at the end points of chains.

The phase diagram for the RA model is shown in Fig. 5. The coexistence line between the NP and P phases was again found iterating the recursion relations 11 with initial values $g_0^{(0)}=1$, $g_1^{(0)}=\omega_1$, $g_2^{(0)}=\omega_2$, $g_3^{(0)}=\omega_1$, $g_4^{(0)}=0$, and $g_5^{(0)}=\omega_2$. In the RA model, the NP-P transition was found to be continuous only at vanishing values of ω_2, so that the phase diagram is qualitatively different from the one found for the RF model. At $(\omega_1=1/(q-1), \omega_2=0)$ we have, therefore, a critical point and no tricritical point is present in the phase diagram.

IV. CONCLUSION

A model of self-avoiding and mutually avoiding chains which allows for up to $K=2$ monomers per lattice site was solved on the Bethe lattice with general coordination number q. End points of the chains are allowed only at the surface of the tree. Following [18], besides the general model (RA), a restricted version (RF), where immediate self-reversals of the chains are forbidden, was also considered. Although in some respects this model resembles models for branched polymers which were already studied on the Bethe lattice [24], the multiplicities of the contributions to the partition functions are different, since each configuration has to be a self-avoiding walk passing through all monomers placed on the lattice. The statistical weight of a configuration is $\omega_1^{N_1}\omega_2^{N_2}$, where N_1 (N_2) is the number of lattice sites with one (two) monomers. For low values of ω_1 and ω_2, a nonpolymerized phase is stable for both models. The phase diagram for the RF model displays two distinct polymerized phases, one of

which (DO) with double-occupied sites only. In this model, the transition between the NP phase and the regular polymerized (P) phase may be of first or second order, and therefore a tricritical point is found, which could be associated with the θ point. Also, the second-order transition between the NP and DO phases ends at a critical end point. In the solution of the more general RA model only one polymerized phase is found, and the transitions between it and the NP phase are always discontinuous for nonzero ω_2. Thus, no tricritical point is found in this case. In both models no dense phase was found, similar the one found for the ISAW model with interacting bonds on the $q=4$ Husimi lattice [13,14,16].

One conclusion of this study is that both versions of the model have qualitatively different phase diagrams on the Bethe lattice. It is worth mentioning that simulations of the model for $K=3$ also presented results which were strongly dependent upon the restrictions of the model [18], although no direct comparison can be done between our results and the simulations, since they correspond to different values of the maximum number of monomers per lattice site K. Although at least for the RF model a tricritical point is found which may be associated to the collapse transition of the chains, if we consider the location of this point we are led to an inconsistency. We may adopt a physically reasonable parametrization of the two statistical weights, stating that $\omega_1 = z = \exp(\beta\mu)$ is the fugacity of one monomer and $\omega_2 = z^2\omega$, where ω is the Boltzmann factor associated with the interaction of the two monomers placed on the same site (interactions between monomers at different sites are not considered in the model). The tricritical point, whose location is given by Eqs. (24), corresponds to a fugacity $z=1/(q-1)$ and a Boltzmann factor $\omega=1/2$. Since $\omega<1$, the collapse transition would occur for *repulsive* interactions between monomers occupying the same site. For the ISAW model on the Bethe lattice, the tricritical point is located at $z=1/(q-1)$ and $\omega=(q-1)/(q-2)>1$ [8], in the attractive region. It should be mentioned, however, that the solution of the ISAW model (interaction between monomers) on the Husimi lattice with $q=4$ leads to a tricritical point at $\omega\approx1.54$ [14], which is somewhat higher than the Bethe lattice result. It may be interesting to see if the solution of the RF model on the Husimi lattice (which is supposed to be closer to the solution on regular lattices) displays a tricritical point in the physically expected attractive region. We are presently working on this problem.

ACKNOWLEDGMENTS

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