

## Semiflexible polymer on an anisotropic Bethe lattice

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The mean-square end-to-end distance of an  $N$ -step polymer on a Bethe lattice is calculated. We consider semiflexible polymers placed on isotropic and anisotropic lattices. The distance on the Cayley tree is defined by embedding the tree on a sufficiently high-dimensional Euclidean space, considering that every bend of the polymer defines a direction orthogonal to all the previous ones. In the isotropic case, the result obtained for the mean-square end-to-end distance turns out to be identical to the one obtained for *ideal* chains without immediate returns on a hypercubic lattice with the same coordination number of the Bethe lattice. For the general case, we obtain asymptotic behavior in both the semiflexible and almost rigid limits.

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### I. INTRODUCTION

Chain polymers are often approximated as self-avoiding and mutually avoiding walks (SAW's) on a lattice, and much information about the behavior of polymers both in a melt or in solution has been understood theoretically through this model [1,2]. One of the characterizations of the conformations of a walk is through its mean-square end-to-end distance  $\langle R^2 \rangle$ , where the mean is taken over all configurations of the  $N$ -step walk on the lattice. In the limit  $N \rightarrow \infty$  a scaling behavior  $\langle R^2 \rangle \sim N^{2\nu}$  is observed, where the exponent  $\nu$  exhibits a universal behavior, with a mean-field value  $\nu = 1/2$  for random walks, which correspond to ideal chains, and  $\nu = 3/4$  for SAW's on two-dimensional lattices [3], for example.

An interesting question arises of whether the chains are not considered to be totally flexible, an energy being associated with bends of the chain. This is often observed for real polymers. Let us, for simplicity, restrict ourselves to SAW'S on hypercubic lattices. In this case, consecutive steps of the walk are either in the same direction or a perpendicular direction. So a Boltzmann factor  $z$  may be associated with each pair of perpendicular consecutive steps of walk. This problem of semiflexible polymers (also called persistent or biased walks) has been studied for some time [4–6], and there occurs a crossover in the behavior of the walk between a rod-like behavior  $\nu_r = 1$  for  $z = 0$ , where the polymer is totally stiff, and the usual behavior with a different exponent  $\nu$  for nonzero values of  $z$ . Stating this point more precisely, the mean-square end-to-end distance displays a scaling behavior in the limit  $N \rightarrow \infty, z \rightarrow 0, N^\psi z = \text{const.}$ , which is given by

$$\langle R^2 \rangle \sim N^{2\nu_r} F(zN^\psi), \quad (1)$$

the observed values being  $\nu_r = 1$  and  $\psi = 1$ .

The scaling function has a behavior  $F(x) \sim x^{(2\nu_r - 2)/\psi}$  in the limit  $x \rightarrow \infty$ . This scaling form has been verified through several techniques, although in three dimensions a mean-field exponent  $\nu = 1/2$  was found for intermediate values of

the number of steps  $N$ , the crossover to the three-dimensional value occurring at rather high values of  $N$  [5].

In this paper, we consider the problem of a semiflexible polymer on a Bethe lattice [7], exactly calculating the mean-square end-to-end distance of walks on the Cayley tree which start at the central site and have  $N$  steps, supposing that the walks will never reach the surface of the Cayley tree, thus remaining in its core. We also calculate the mean-square end-to-end distance in the case when the lattice is considered anisotropic, that is, when the edges of the lattice are not equivalent with respect to their occupation by a polymer bond. The definition of the distance between two sites of the Cayley tree is not obvious, and some possibilities exploring the fact that the tree may be embedded in a hypersurface of a non-Euclidean space have been given [8]. In this paper, however, we used a simpler definition, considering the Cayley tree in the thermodynamic limit to be embedded in an infinite-dimensional Euclidean space. The result for  $\langle R^2 \rangle(N, z)$  for the isotropic case has the scaling form of Eq. (1). Not surprisingly the scaling function  $F(x)$  is equal to the one obtained for random walks with no immediate return on a hypercubic lattice, with the same coordination number of the Bethe lattice considered. This might be expected, since Bethe lattice calculations lead to mean-field critical exponents. Also, in the limit  $N \rightarrow \infty$  for nonzero values of  $z$ , the scaling behavior  $\langle R^2 \rangle \sim N^{2\nu}$  with the classical value  $\nu = 1/2$  is verified in the expression for  $\langle R^2 \rangle(N, z)$ . It should be mentioned that our proposal of defining the Euclidean distance between two points of the Cayley tree is similar to earlier results in the literature relating this distance to the chemical distance, measured along the chain [9]. However, the distinction between the chemical and Euclidean distances is not always properly considered in the literature, and this may lead to contradicting results [10], as we will discuss in more detail in Sec. IV.

In Sec. II we define the model and calculate the mean-square end-to-end distance recursively on the anisotropic Bethe lattice. The problem is then reduced to finding the general term of a *linear* mapping in six dimensions. In the particular case of an isotropic lattice, we find a closed expression for  $\langle R^2 \rangle$ . In Sec. III the asymptotic behavior is studied for a general case, based on the mapping. In Sec. IV final

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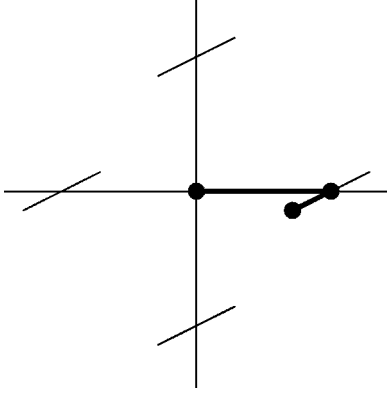


FIG. 1. A four-coordinated Cayley tree with a two step polymer placed on it. The tree has  $N_g=2$  generations, and is embedded on a cubic lattice. For the polymer shown,  $R^2=2$ .

comments and discussions may be found. Finally, in the appendixes we present a combinatorial calculation for  $\langle R^2 \rangle$  in the isotropic case.

## II. DEFINITION OF THE MODEL AND SOLUTION FOR THE ISOTROPIC LATTICE

We consider a Cayley tree of coordination number  $q$ , and place a chain on the tree starting at the central site. Each bond of the tree is supposed to be of unit length. Figure 1 shows a tree with  $q=4$ , and a polymer with  $N=2$  steps placed on it. Since we want the Cayley tree to be an approximation of a hypercubic lattice in  $d$  dimensions, we will restrict ourselves to even coordination numbers  $q=2d$ . As in the hypercubic lattice, the bonds incident on any site of the tree are in  $d$  directions, orthogonal to each other. As may be seen in Fig. 1, the central site of the tree is connected to  $q$  other sites, which belong to the first generation of sites. Each of the sites of the first generation is connected to  $q-1$  sites of the second generation, and this process continues until the surface of the tree is reached, after a number of steps equal to the number of generations in the tree. Upon reaching a site of the  $i$ th generation coming from a site belonging to generation  $i-1$ , there are  $q-1$  possibilities for the next step of the walk toward a site of generation  $i+1$ . One of them will be in the same direction as the previous step, while the remaining  $q-2$  will be in directions orthogonal to *all* previous steps. In the second case, a statistical weight  $z$  is associated with the elementary bend in the walk. Therefore, we admit that the  $q-2$  bonds which are orthogonal to the last step are also orthogonal to *all* bonds of the lattice in earlier generations. Let us stress two consequences of this supposition: (i) A tree of coordination number  $q$  with  $N_g$  generations will be embedded in a space of dimension

$$D = q/2 + (N_g - 1)(q/2 - 1). \quad (2)$$

The sites of the Cayley tree will all be sites of a hypercubic lattice in  $D$  dimensions. This may be seen in Fig. 1, where the sites of a tree with  $q=4$  and  $N_g=2$  are sites of a cubic ( $D=3$ ) lattice. (ii) By construction, there will never be loops in the tree, a property which is true for any Cayley tree. It is well known [7] that it may be shown by other means that the Cayley tree is an infinite-dimensional lattice in the thermo-

dynamic limit  $N_g \rightarrow \infty$ . Finally, the anisotropy is introduced into the model considering that *bonds* of the chain in  $s$  of the  $q/2$  directions (we will call them special) at each lattice site contribute with a factor  $y$  to the partition function, while no additional contribution comes from bonds in the remaining  $t = q/2 - s$  directions at each lattice site.

Usually [7], the calculation of thermodynamic properties of models defined on the Bethe lattice is done in a recursive manner, so we will follow a similar procedure in the calculation of the mean-square end-to-end distance. We define a generalized partition (or generating) function for  $N$ -step chains,

$$g_N = \sum z^m y^{N_e} p^{R^2}, \quad (3)$$

where the sum is over all configurations of the chain,  $z$  is the statistical weight of an elementary bend in the chain,  $y$  is the statistical weight of bonds in special directions, and  $p$  is a parameter associated with the square of the end-to-end distance of the chain. At the end of the calculation, we will take  $p=1$ . The numbers of elementary bends, bonds in special directions, and the square end-to-end distance of each chain are  $m$ ,  $N_e$ , and  $R^2$ , respectively. The mean-square end-to-end distance may then be calculated through

$$\langle R^2 \rangle_N = \frac{1}{g_N} \left( p \frac{\partial g_N}{\partial p} \right) \Big|_{p=1}. \quad (4)$$

The partition function may then be calculated in a recursive way if we define partial partition functions  $a_N^l$  and  $b_N^l$  such that the first ones include all  $N$ -bond chains whose last  $l$  bonds are collinear and in one of the special directions (there is necessarily a bend before the  $l$  bonds, if  $l < N$ ), while the last  $l$  bonds of the chains contributing to  $b_N^l$  are collinear and in one of the nonspecial directions. The partition function may then be written as

$$g_N = \sum_{l=1}^N (a_N^l + b_N^l). \quad (5)$$

Due to the fact that there are no closed loops on the Cayley tree, it is quite easy to write down recursion relations for the partial partition functions:

$$a_{N+1}^1 = 2syzp \sum_{l=1}^N b_N^l + 2(s-1)yzp \sum_{l=1}^N a_N^l, \quad (6a)$$

$$a_{N+1}^{l+1} = yp^{2l+1} a_N^l, \quad (6b)$$

$$b_{N+1}^1 = 2tzp \sum_{l=1}^N a_N^l + 2(t-1)z p \sum_{l=1}^N b_N^l, \quad (6c)$$

$$b_{N+1}^l = p^{2l+1} b_N^l, \quad (6d)$$

with the initial conditions

$$a_1^1 = 2syp, \quad (7a)$$

$$b_1^1 = 2tp. \quad (7b)$$

For example, in the first expression above, the new bond may be preceded by a bond in a special direction, with  $2s$  possibilities, or by a bond in a nonspecial direction, with  $2(s-1)$  possibilities. In both cases a factor  $p$  is present, since the bond added is in a direction perpendicular to all previous ones, and thus  $R^2$  is increased by one unit. Finally, the inclusion of the new bond introduces one bend in the chain, thus explaining the factor  $z$ , and since the bond is in a special direction the factor  $y$  is justified. In the second expression, it should be mentioned that  $R^2$  is increased by  $(l+1)^2 - l^2$ , thus explaining the exponent of  $p$ . If we now define

$$a_N = \sum_{l=1}^N a_N^l, \quad (8a)$$

$$b_N = \sum_{l=1}^N b_N^l, \quad (8b)$$

the mean-square end-to-end distance will be

$$\langle R^2 \rangle_N = \frac{1}{a_N + b_N} \left[ p \frac{\partial}{\partial p} (a_N + b_N) \right] \Big|_{p=1} = \frac{c_N + d_N}{a_N + b_N}. \quad (9)$$

The recursion relations for  $a_N$  and  $b_N$ , as well as the ones for the new variables  $c_N$  and  $d_N$ , may be written, for  $p=1$ , as

$$a_{N+1} = 2z \sum_{l=0}^N y^{l+1} [(s-1)a_{N-l} + sb_{N-l}], \quad (10a)$$

$$b_{N+1} = 2z \sum_{l=0}^N [ta_{N-l} + sb_{N-l}], \quad (10b)$$

$$c_{N+1} = 2z \sum_{l=0}^N y^{l+1} [(s-1)(l+1)^2 a_{N-l} + s(l+1)^2 b_{N-l} + (s-1)c_{N-l} + sd_{N-l}], \quad (10c)$$

$$d_{N+1} = 2z \sum_{l=0}^N [t(l+1)^2 a_{N-l} + (t-1)(l+1)^2 b_{N-l} + tc_{N-l} + (t-1)d_{N-l}], \quad (10d)$$

with the initial conditions

$$a_0 = \frac{2s}{z(q-2)}, \quad (11a)$$

$$b_0 = \frac{2t}{z(q-2)}, \quad (11b)$$

$$c_0 = d_0 = 0. \quad (11c)$$

An undesirable feature of the recursion relations [Eqs. (10)] is that the new values of the iterating variables depend on all previous values. This dependence, however, is rather simple, and it is possible, introducing two more variables  $e_N$  and  $f_N$ , to rewrite the recursion relations as a mapping involving only one previous value of each variable, valid for  $N \geq 1$ :

$$a_{N+1} = ya_N + 2zy[(s-1)a_N + sb_N], \quad (12a)$$

$$b_{N+1} = b_N + 2z[ta_N + (t-1)b_N], \quad (12b)$$

$$c_{N+1} = yc_N + 2zy[(s-1)(a_N + c_N) + s(b_N + d_N)] + (2N+1)ya_N - 2ye_N, \quad (12c)$$

$$d_{N+1} = d_N + 2z[t(a_N + c_N) + (t-1)(b_N + d_N)] + (2N+1)b_N - 2f_N, \quad (12d)$$

$$e_{N+1} = ye_N + 2Nzy[(s-1)a_N + sb_N], \quad (12e)$$

$$f_{N+1} = f_N + 2Nz[ta_N + (t-1)b_N], \quad (12f)$$

with the initial conditions

$$a_1 = c_1 = 2sy, \quad (13a)$$

$$b_1 = d_1 = 2t, \quad (13b)$$

$$e_1 = f_1 = 0. \quad (13c)$$

The value for  $\langle R^2 \rangle$  may be found by iterating the mapping above through Eq. (9). In principle, since the mapping is *linear*, it is solvable. One starts finding the general term of the first two equations, then solving the last two equations, and finally solving the two remaining relations. A software for algebraic computing is helpful, but we realized that the general answer will be too large to be handled, and also the computer time and memory required are beyond the resources we have available. We therefore restrict ourselves to a complete solution of the isotropic case  $y=1$ , and to an exact study of the asymptotic properties of the solution for the general case. It is worthwhile to observe in the mapping equations (12) that under transformations

$$s' = t, \quad (14a)$$

$$t' = s, \quad (14b)$$

$$y' = 1/y, \quad (14c)$$

$\langle R^2 \rangle$  will be invariant, as expected.

For the isotropic case ( $y=1$ ) mapping equations (12) are reduced to three variables

$$\alpha_N = a_N + b_N, \quad (15a)$$

$$\beta_N = c_N + d_N, \quad (15b)$$

$$\gamma_N = e_N + f_N, \quad (15c)$$

and may be written as

$$\alpha_{N+1} = [1 + z(q-2)]\alpha_N, \quad (16a)$$

$$\beta_{N+1} = [1 + z(q-2)]\beta_N + [2N+1 + z(q-2)]\alpha_N - 2\gamma_N, \quad (16b)$$

$$\gamma_{N+1} = \gamma_N + Nz(q-2)\alpha_N. \quad (16c)$$

The initial conditions are

$$\alpha_1 = \beta_1 = q, \quad (17)$$

$$\gamma_1 = 0. \quad (18)$$

It is easy to find general solutions for this mapping:

$$\alpha_N = qk^{N-1}, \quad (19a)$$

$$\beta_N = \frac{q}{(k-1)^2} [N(k^2-1)k^{N-1} + 2 - 2k^N], \quad (19b)$$

$$\gamma_N = \frac{q}{k-1} [N(k^2-1)k^{N-1} + 1 - k^N], \quad (19c)$$

where  $k = 1 + (q-2)z$ . The substitution of these solutions into Eq. (9) results in

$$\langle R^2 \rangle = \frac{2[1+a]}{a^2} \left[ Na - 1 + \frac{1}{[1+a]^N} \right] - N, \quad (20)$$

where  $a = k - 1 = (q-2)z$ .

The properties of the mean square end-to-end distance [Eq. (20)] in some limiting cases show that our result has the expected behavior. First, we notice that when the bend statistical weight  $z$  vanishes, we have

$$\lim_{z \rightarrow 0} \langle R^2 \rangle = N^2 \quad (21)$$

for any number of steps  $N$ . This rodlike behavior is expected, since no bend will be present in the walk. In the opposite limit of infinite bending statistical weight, the result is

$$\lim_{z \rightarrow \infty} \langle R^2 \rangle = N, \quad (22)$$

which is also an expected result, since in this limit there is a bend at every internal site of the chain, so that, according to the definition of the end-to-end distance we are using, the vector  $\vec{R}$  in this situation will have  $N$  components, all of them being equal to 1.

In the limit of an infinite chain  $N \rightarrow \infty$ , for nonzero  $z$ , we obtain

$$\lim_{N \rightarrow \infty} \langle R^2 \rangle = \frac{(2+a)N}{a}, \quad (23)$$

and we note that the expected scaling behavior  $\langle R^2 \rangle \sim N^{2\nu}$  is obtained with the mean-field exponent  $\nu = 1/2$ . The asymptotic behavior of  $\langle R^2 \rangle$  is different for zero and nonzero  $a$ , as may be appreciated comparing Eqs. (21) and (23), respectively. So we may look for the crossover between both behaviors in the limit of Eq. (1), obtaining the result

$$\lim_{N \rightarrow \infty; a \rightarrow 0; aN = x} \langle R^2 \rangle = N^2 F(x), \quad (24)$$

with a scaling function

$$F(x) = \frac{2[x-1 + \exp(-x)]}{x^2}. \quad (25)$$

It should be stressed that the square end-to-end distance given in Eq. (20) is the same as that obtained by adapting the general result of Flory for random walks without immediate return [1] to hypercubic lattices. In general, it may be shown that an exact solution of statistical models with first neighbor interactions on the Bethe lattice is equivalent to the Bethe approximation on the Bravais lattice with the same coordination number [7]. The random walk without immediate returns corresponds to the Bethe approximation of the  $n \rightarrow 0$  model associated with the self-avoiding walk problem [11], and here we show that the analogy may be extended to the mean-square end-to-end distance if we define distances on the Bethe lattice as was done above. Although the results on the Bethe lattice as calculated here, and the ones for ideal chains without immediate return on a hypercubic lattice with the same coordination number, should have the same asymptotic behaviors, it is at first surprising that they are actually identical. However, it turns out that the mean value of the angle between successive bonds, as calculated by Flory in his original work [1], is actually *exact* for chains on the Bethe lattice as we considered.

### III. ASYMPTOTIC BEHAVIOR IN THE GENERAL CASE

In this section we develop a study of the asymptotic solution of the mapping Eqs. (12) for  $N \gg 1$ . Let us reduce the dimension of the mapping by one defining new iteration variables

$$B_N = \frac{b_N}{a_N}, \quad (26a)$$

$$C_N = \frac{c_N}{a_N}, \quad (26b)$$

$$D_N = \frac{d_N}{a_N}, \quad (26c)$$

$$E_N = \frac{e_N}{a_N}, \quad (26d)$$

$$F_N = \frac{f_N}{a_N}. \quad (26e)$$

From Eqs. (12) and the initial conditions [Eqs. (13)] it is easy to write the recursion relations and initial conditions for the new iterative variables in the mapping above. In the limit of large values of  $N$ , for fixed  $z$  and  $y$ , the following asymptotic behaviors are observed:

$$B_N \sim B^0, \quad (27a)$$

$$C_N \sim C^0 + C^1 N, \quad (27b)$$

$$D_N \sim D^0 + D^1 N, \quad (27c)$$

$$E_N \sim E^0 + E^1 N, \quad (27d)$$

$$F_N \sim F^0 + F^1 N. \quad (27e)$$

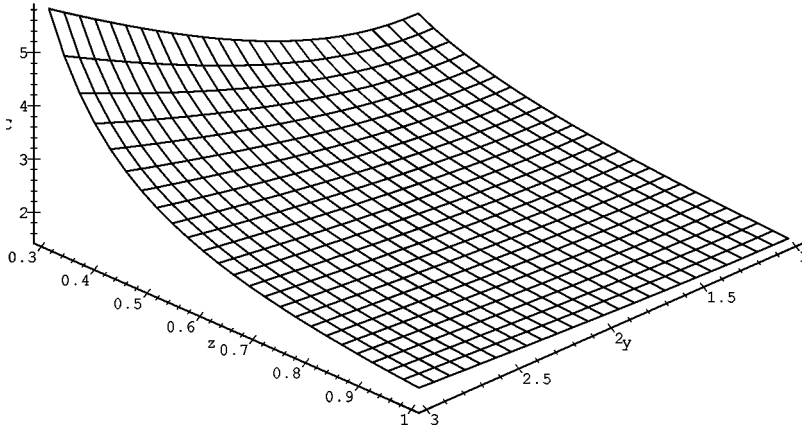


FIG. 2. The amplitude of  $\langle R^2 \rangle$  as a function of  $z$  and  $y$  for a lattice with  $s=1$  and  $t=2$  ( $q=6$ ). As expected, the amplitude diverges as  $z \rightarrow 0$ . Since  $s=1$ , a divergence is also observed as  $y \rightarrow \infty$ .

The substitution of these expressions into the recursion relations for the variables defined in Eqs. (26), obtained from the general mapping Eqs. (12), leads to a determination of the constants in the asymptotic behavior, thus we obtain

$$\langle R^2 \rangle = \frac{C_N + D_N}{1 + B_N} \sim \frac{C^1 + D^1}{1 + B^0} N = CN, \quad (28)$$

where the amplitude  $C = C^1$  is given by

$$C = \frac{sy(B^0)^2 \left[ \frac{y(1+\epsilon)+1}{y(1+\epsilon)-1} \right] + t \left[ \frac{2+\epsilon}{\epsilon} \right]}{sy(B^0)^2 + t}, \quad (29)$$

where

$$\epsilon = 2z(s-1 + sB^0), \quad (30)$$

and  $B^0$  is the positive root of

$$2zsy(B^0)^2 + [y-1 + 2z(sy-t-y+1)]B^0 - 2zt = 0. \quad (31)$$

The amplitude of the asymptotic behavior of  $\langle R^2 \rangle$  thus may be obtained exactly in the general case and, as may be seen in Fig. 2, diverges as  $z \rightarrow 0$ , as expected. Also, in the limit  $y \rightarrow \infty$  the problem reduces to a walk on an isotropic lattice with coordination number equal to  $2s$ , and we obtain

$$C = \frac{2z(s-1) + 2}{2z(s-1)}, \quad (32)$$

which agrees with Eq. (19) for the isotropic case.

Now we will study the asymptotic behavior in the quasirigid limits  $N \rightarrow \infty$ ,  $z \rightarrow 0$ , and  $N(q-2)z = x$ . We thus expand  $\langle R^2 \rangle$  for small values of  $z$ :

$$\langle R^2 \rangle(z, y, N) \sim \langle R^2 \rangle(0, y, N) + \left. \frac{\partial \langle R^2 \rangle}{\partial z} \right|_{z=0} z. \quad (33)$$

For  $z=0$  the solutions of the mapping equations (12) are

$$a_N = 2sy^N, \quad (34a)$$

$$b_N = 2t, \quad (34b)$$

$$c_N = 2sy^N N^2, \quad (34c)$$

$$d_N = 2tN^2, \quad (34d)$$

$$e_N = f_N = 0, \quad (34e)$$

and we have  $\langle R^2 \rangle = N^2$ , as expected. From the mapping equations (12), the recursion relations for the derivatives of the variables with respect to  $z$  (at  $z=0$ ) may be seen to be

$$a'_{N+1} = ya'_N + 4ys[(s-1)y^N + t], \quad (35a)$$

$$b'_{N+1} = b'_N + 4t(sy^N + t - 1), \quad (35b)$$

$$c'_{N+1} = yc'_N + 4ys(1+N^2)[(s-1)y^N + t] + y(2N+1)a'_N - 2ye'_N, \quad (35c)$$

$$d'_{N+1} = d'_N + 4t(1+N^2)(sy^N + t - 1) + (2N+1)b'_N - 2f'_N, \quad (35d)$$

$$e'_{N+1} = ye'_N + 4Nys[(s-1)y^N + t], \quad (35e)$$

$$f'_{N+1} = f'_N + 4Nt(sy^N + t - 1), \quad (35f)$$

where the values for the variables [Eqs. (34)] have already been substituted and the initial conditions are  $a'_1 = b'_1 = \dots = f'_1 = 0$ . The general solution of the recursion relations [Eqs. (35)] is not difficult to obtain with the aid of an algebra software. Considering the invariance described in Eqs. (14), we will restrict our discussion to the case  $y > 1$ , without loss of generality. For large values of  $N$ , the dominant terms of the solution of the mapping are

$$a_N + b_N \sim 2sy^N, \quad (36a)$$

$$c_N + d_N \sim 2sy^N N^2, \quad (36b)$$

$$a'_N + b'_N \sim \begin{cases} 4s(s-1)y^N N & \text{if } s > 1 \\ \frac{8ty^N}{y-1} & \text{if } s = 1, \end{cases} \quad (36c)$$

$$c'_N + d'_N \sim \begin{cases} \frac{8}{3}s(s-1)y^N N^3 & \text{if } s > 1 \\ \frac{8ty^N N^2}{y-1} & \text{if } s = 1. \end{cases} \quad (36d)$$



The leading term in the derivative of the mean-square end-to-end distance will be

$$\left. \frac{\partial \langle R^2 \rangle}{\partial z} \right|_{z=0} \sim -\frac{2}{3}(s-1)N^3. \quad (37)$$

Therefore, up to first order in  $x$ , the scaling function  $F(x)$  in the quasirigid limit is found to be  $F(x) \sim 1 - F_1(s, t)x$ . Considering the symmetry equation (14) and the solution for the isotropic case [Eq. (20)], we have

$$F_1(s, t) = \begin{cases} \frac{2(t-1)}{3(q-2)} & \text{if } y < 1 \\ \frac{1}{3} & \text{if } y = 1 \\ \frac{2(s-1)}{3(q-2)} & \text{if } y > 1. \end{cases} \quad (38)$$

We thus conclude that the scaling function in general displays a discontinuous derivative at  $y = 1$ .

#### IV. CONCLUSION

We formulated the problem of the calculation of the mean-square end-to-end distance of semiflexible polymers placed on a  $q$ -coordinated anisotropic Bethe lattice as a linear mapping, whose general term may in principle be obtained. In the isotropic case, the mapping may easily be solved, and leads to an expression for  $\langle R^2 \rangle$  which is *identical* to the one obtained for random walks without immediate return on a hypercubic lattice with the same coordination number [1]. The identity between the two problems regarding thermodynamic properties derived from the free energy is well known [11], and here is extended for a thermodynamic average of a geometric property. One point which should be stressed is that the definition of the Euclidean distance between two points on the Bethe lattice is rather arbitrary. Here we defined the distance by embedding the Cayley tree in a hypercubic lattice of sufficiently high dimensionality. In the thermodynamic limit the dimensionality of this lattice diverges, as expected [7]. Other definitions of distance may be proposed [8]. The simple one we adopted here leads to meaningful conclusions. Since calculations on the Bethe lattice are usually done recursively, and one step in the recursion relations corresponds to adding another generation to the tree, it is tempting to define the distance between two sites on the tree as the difference between the numbers of the generations they belong to. This definition, although simple and operational, has serious drawbacks. This is quite clear for the particular problem we looked at here, since it implies that  $\langle R^2 \rangle$  for *any*  $N$ -step chain is equal to  $N^2$ . We would thus have  $\nu = 1$ , the one-dimensional value, and the identity between the results for the Bethe lattice and for walks without immediate return on hypercubic lattices would break down. This definition of distance was used recently in the exact calculation of correlation functions for a general spin- $S$  magnetic model [10], leading to  $\nu = 1$ , in opposition to the generally accepted mean-field value  $\nu = 1/2$  [12].

The fact that all walks we considered here have their initial sites located at the central site of the Cayley tree is of

course convenient for the calculations, and may be seen as a particular case. A closer consideration of this point, however, leads to the conclusion that our results are exact for any chains such that the assertion that at any bend the new direction is perpendicular to *all* previous directions of bonds holds. Thus it is clear that if the whole chain is contained in one of the  $q$  rooted subtrees attached to the central site, the results are still the same. If portions of the chain are located on two of these subtrees the calculation becomes more complicated since, as may be seen in Fig. 1, there are bonds in the same direction in different subtrees. However, this problem may be easily avoided by enlarging the dimension of the Euclidean space in which the tree is embedded, thus assuring that any two bonds in the same direction are necessarily connected by a walk without any bend. For such a tree, our results hold for any chain, regardless of the location of its endpoints.

In the general anisotropic case, we restricted ourselves to the discussion of the asymptotic behavior of  $\langle R^2 \rangle$ , which was studied in the semiflexible case and also in the quasirigid limit. The expected scaling behavior was obtained in both cases, and an interesting discontinuity in the quasirigid limit amplitude is observed as the isotropic value  $y = 1$  is crossed.

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#### APPENDIX A: COMBINATORIAL SOLUTION IN THE ISOTROPIC CASE

Any  $N$ -step walk on the Cayley tree will visit a subset of sites of the  $D$ -dimensional hypercubic lattice defining a subspace whose dimensionality is between 1 and  $N$ . The limiting cases are the ones of a polymer without any bend (rod), which is one dimensional, and a polymer where we have a bend at every internal site, and since at each bend the new bond is in a direction orthogonal to all precedent bonds of the polymer, the polymer is embedded in an  $N$ -dimensional subspace. Since the initial site of the chain is supposed to be at the central site of the tree, the end-to-end distance will be given by the modulus of the position vector of the final site, denoted by  $\vec{R}$ . For a polymer with  $m$  bends, the number of components of this vector will be equal to  $m + 1$ . For simplicity, we will admit that each bond is of unit length, so that the components of  $\vec{R}$  will be integers. We want to compute the mean value of  $\vec{R}$  over all polymers with  $N$  steps,

$$\langle R^2 \rangle = \frac{\sum_{\vec{R}_m^N} z^m R^2}{\sum_{\vec{R}_m^N} z^m}, \quad (A1)$$

where  $m$  is the number of bends in the walk and the sum is over all configurations  $\vec{R}_m^N$  of polymers with  $N$  steps. Besides the first and last components the values of the other  $m - 1$  components of  $R$  are the numbers of steps between succes-

sive bends in the walk. We should remember that there are  $q-2$  possibilities for each bend. So we may rewrite Eq. (A1) as

$$\langle R^2 \rangle = \frac{\sum_{m=0}^{N-1} a^m B_{N,m}}{\sum_{m=0}^{N-1} a^m A_{N,m}}, \quad (\text{A2})$$

where  $a = (q-2)z$  embodies all dependence on coordination number and statistical weight as long as  $q \geq 4$ ,

$$A_{N,m} = \sum_{\vec{R}_m^N} 1, \quad (\text{A3})$$

and

$$B_{N,m} = \sum_{\vec{R}_m^N} \sum_{i=0}^{m+1} R_i^2. \quad (\text{A4})$$

Note that the effect of the bending energy can be described by introducing an effective coordination number  $q' = a + 2$  for an associated totally flexible polymer. The sums in  $A_{N,m}$  and  $B_{N,m}$  are over all possible values for  $\vec{R}$  with  $m+1$  components and subjected to the constraint of the total number of steps being equal to  $N$ ; that is,

$$\sum_{i=1}^{m+1} R_i = N. \quad (\text{A5})$$

The sum in Eq. (A3) is just the number of vectors  $\vec{R}$  with  $m+1$  components which obey constraint (A5). Since the minimum value of each component of  $\vec{R}$  is equal to 1, it is convenient to define  $r_i = R_i - 1$  and therefore  $A_{N,m}$  is the number of ways to put the  $N - m - 1$  remaining steps into the  $m+1$  components of  $\vec{R}$ :

$$A_{N,m} = \frac{(N-1)!}{m!(N-m-1)!}. \quad (\text{A6})$$

The sum  $B_{N,m}$  may then be rewritten as

$$B_{N,m} = \sum_{\vec{r}_m^N} \sum_{i=1}^{m+1} (1+r_i)^2, \quad (\text{A7})$$

where each component  $r_i$  assumes values between 0 and  $N - m - 1$  subject to the constraint of Eq. (A5):

$$\sum_{i=1}^{m+1} r_i = N - m - 1. \quad (\text{A8})$$

The calculation of  $B_{N,m}$  is given in Appendix B, and the result is

$$B_{N,m} = \frac{(m+1)(2N-m)N!}{(m+2)!(N-m-1)!}. \quad (\text{A9})$$

Performing the sum in the denominator of Eq. (A2) taking Eq. (A6) into account, we have

$$\langle R^2 \rangle = \frac{N}{[1+a]^{N-1}} \left[ 2(N+1) \sum_{m=0}^{N-1} \binom{N-1}{m} \times \frac{a^m}{m+2} - \sum_{m=0}^{N-1} \binom{N-1}{m} a^m \right]. \quad (\text{A10})$$

The first sum may be calculated by noting that

$$\int_0^A x(1+x)^{N-1} dx = A^2 \sum_{m=0}^{N-1} \binom{N-1}{m} \frac{A^m}{m+2}, \quad (\text{A11})$$

and, therefore

$$\sum_{m=0}^{N-1} \binom{N-1}{m} \frac{a^m}{m+2} = \frac{[1+a]^N [aN-1] + 1}{N(N+1)a^2}. \quad (\text{A12})$$

Substituting this result into Eq. (A10) and performing the second sum, we finally obtain the expression

$$\langle R^2 \rangle = \frac{2[1+a]}{a^2} \left[ Na - 1 + \frac{1}{[1+a]^N} \right] - N. \quad (\text{A13})$$

## APPENDIX B: DERIVATION OF $B_{N,m}$

In this appendix we want to derive Eq. (A9) for  $B_{N,m}$ . Using Eq. (A8) and defining for convenience  $\mathcal{N} = N - m - 1$ , Eq. (A7) is rewritten as

$$B_{N,m} = (m+1) \sum_{j=0}^{\mathcal{N}+1} \frac{(\mathcal{N}+m-j)! j^2}{(\mathcal{N}+1-j)!(m-1)!}. \quad (\text{B1})$$

Redefining the summation variable with  $i = \mathcal{N} + 1 - j$ , this equation turns out to be

$$B_{N,m} = (m+1) \sum_{i=0}^{\mathcal{N}} (\mathcal{N}+1-i)^2 \frac{(i+m-1)!}{i!(m-1)!}. \quad (\text{B2})$$

Using the equality

$$\sum_{i=0}^{\mathcal{N}} \frac{(m+i)!}{m!i!} = \frac{(m+N+1)!}{(m+1)!N!}, \quad (\text{B3})$$

after some manipulation we obtain

$$B_{N,m} = (m+1) \left\{ (\mathcal{N}+1) \frac{(\mathcal{N}+1+m)!}{\mathcal{N}!m!} - 2(\mathcal{N}+1) \times \frac{m(\mathcal{N}+1+m)!}{\mathcal{N}!(m+1)!} + \sum_{i=1}^{\mathcal{N}+1} \frac{(i+m-1)!i}{(i-1)!(m-1)!} \right\}. \quad (\text{B4})$$

The last summation to be dealt with is just

$$\sum_{i=1}^{\mathcal{N}+1} \frac{(i+m-1)!i}{(i-1)!(m-1)!}. \quad (\text{B5})$$

Defining  $j = i - 1$ , it follows that

$$\sum_{j=0}^{\mathcal{N}} \frac{(j+m)!(j+1)}{j!(m-1)!} = \frac{m(\mathcal{N}+m+1)!}{\mathcal{N}!(m+1)!} + m(m+1) \frac{(\mathcal{N}+m+1)!}{(\mathcal{N}-1)!(m+2)!}. \quad (\text{B6})$$

Substitution into Eq. (B4) leads to

$$B_{N,m} = \frac{(m+1)(\mathcal{N}+m+1)! [2\mathcal{N}+m+2]}{(m+2)! \mathcal{N}!}. \quad (\text{B7})$$

Substituting  $\mathcal{N} = N - m - 1$ , we obtain

$$B_{N,m} = \frac{(m+1)(2N-m)N!}{(m+2)!(N-m-1)!}. \quad (\text{B8})$$

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