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# Mean Square End-to-End Distance of a Semiflexible Polymer on the Bethe Lattice

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A combinatorial method to calculate the mean square end-to-end distance $\langle R^2 \rangle$ of a polymer on a Bethe lattice is used. The case of an anisotropic lattice and semiflexible polymers is considered. The distance on the Cayley tree is defined by embedding the tree on an $N$-dimensional Euclidean space considering that every bend of the polymer defines a direction orthogonal to all the previous ones. The semiflexible polymer is effectively equivalent to a flexible one if one considers an effective (noninteger) coordination number. Although an analytical calculation is performed, a closed expression for $\langle R^2 \rangle$ is possible only for the isotropic case. Numerical results are shown for the anisotropic case. Plots of $\langle R^2 \rangle$ against $N$ for different values of the anisotropy parameter $y$ are shown. The power dependence for $N$ does not depend on the anisotropy as expected, but the linear coefficient increases on increasing the anisotropy. The anisotropy tends to stretch the polymer.

**KEY WORDS:** anisotropy; Bethe lattice; semiflexible polymer; statistical mechanics.

## 1. INTRODUCTION

Chain polymers are extensively discussed in the literature [1–6]. We consider the problem of a semiflexible polymer on a Bethe lattice [7], calculating exactly the mean square end-to-end distance of walks on the Cayley tree which start at the central site and have $N$ steps, assuming 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

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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 assuming that the tree may be embedded in a hypersurface of a non-Euclidean space have been explored [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 $N^2 F(zN)$ in the limit $N \to \infty$; $z \to 0$; $Nz = \text{constant}$. Here $z$ is the Boltzmann factor associated with each pair of perpendicular consecutive steps of walk. 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 $N \to \infty$ for nonzero values of $z$, the scaling behavior $\langle R^2 \rangle \approx N^{2\nu}$ with the classical value $\nu = \frac{1}{2}$ is verified in the expression for $\langle R^2 \rangle(N, z)$. Our definition of the Euclidean distance between two points of the Cayley tree is similar to earlier results relating this distance to the chemical distance measured along the chain [9]. We address the question of the choice of an appropriate nonlinear scaling field $\omega(z)$ for the problem. It should be noted that it has been shown that simulation or exact enumeration results for semiflexible polymers on bidimensional lattices display a much cleaner scaling behavior when convenient nonlinear scaling fields are used [6].

In Section 2 we define the model and show the calculation of the mean square end-to-end distance analytically for the isotropic Bethe lattice. The anisotropy is introduced into the model in Section 3 and the computation of $\langle R^2 \rangle$ is done up to a point, but we were not able to perform a final summation analytically in this case. Thus, for the anisotropic case, we present some numerical results in Section 4, as well as final discussions.

## 2. MODEL

In this section we consider the model that was defined in Ref. 10. For completeness we give here the underlying calculation scheme, showing the combinatorial analysis for the isotropic case. We consider a Cayley tree of coordination number $q$ and place a chain on the tree starting at the central site. Since we want the Cayley tree to be an approximation of a hypercubic lattice in $d$ dimensions, we 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. 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 site of generation $(i+1)$. One of them will be in the same direction as the previous step, while the remaining $(q-2)$ steps 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. Now we assert that the $(q-2)$ bonds orthogonal to the first step are also orthogonal to any bond of the tree connecting sites of 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

$$D = q/2 + (N_g + 1)[(q/2) - 1] \tag{1}$$

The sites of the Cayley tree will be sites of a hypercubical lattice in $D$ dimensions. (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 thermodynamic limit $N_g \to \infty$.

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 those 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 a $N$-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 $\vec{R}$. For a polymer with $m$ bends, the number of components of this vector will be equal to $m+1$. For simplicity, we assume 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:

$$\langle R^2 \rangle = \frac{\sum_{\vec{R}_m^N} z^m R^2}{\sum_{\vec{R}_m^N} z^m} \tag{2}$$

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 and $m$ bends and over the numbers of bends. Besides the first and the last components, the values of the other

$m-1$ components of $R$ are the numbers of steps between successive bends in the walk. We should remember that there are $q-2$ possibilities for each bend. So we may rewrite Eq. (2) as

$$\langle R^2 \rangle = \frac{\sum_{m=0}^{N-1} a^m B_{N,m}}{\sum_{m=0}^{N-1} a^m A_{N,m}} \tag{3}$$

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

$$A_{N,m} = \sum_{\vec{R}_m^N} 1 \tag{4}$$

and

$$B_{N,m} = \sum_{\vec{R}_m^N} \sum_{i=0}^{m+1} R_i^2 \tag{5}$$

Here the sum is made with $m$ fixed. Also, $R_i$ is the number of steps in each stretch made of consecutive steps without bends. The sums in $A_{N,m}$ and $B_{N,m}$ are explicitly calculated in Ref. 10 and are given by

$$A_{N,m} = \frac{(N-1)!}{m!\,(N-m-1)!} \tag{6}$$

and

$$B_{N,m} = \frac{(m+1)(2N-m)\,N!}{(m+2)!\,(N-m-1)!} \tag{7}$$

Performing the sum in the denominator of Eq. (3) while taking Eq. (6) into account, we have

$$\langle R^2 \rangle = \frac{N}{[1+a]^{N-1}} \left[ 2(N+1) \sum_{m=0}^{N-1} \binom{N-1}{m} \frac{a^m}{m+2} - \sum_{m=0}^{N-1} \binom{N-1}{m} a^m \right] \tag{8}$$

The first sum gives [10]

$$\sum_{m=0}^{N-1} \binom{N-1}{m} \frac{a^m}{m+2} = \frac{[1+a]^N\,[aN-1]+1}{N(N+1)\,a^2} \tag{9}$$

Substituting this result into Eq. (8) and performing the second sum, we finally, get the expression

$$\langle R^2 \rangle = \frac{2[1+a]}{a^2}\left[ Na - 1 + \frac{1}{[1+a]^N} \right] - N \tag{10}$$

The properties of the mean square end-to-end distance, Eq. (10) in some limiting cases, show that our result has the expected behavior. First, we observe that when the bend statistical weight $z$ vanishes, we have

$$\lim_{z \to 0} \langle R^2 \rangle = N^2 \tag{11}$$

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

$$\lim_{z \to \infty} \langle R^2 \rangle = N \tag{12}$$

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 $N \to \infty$ we get, for nonzero $z$,

$$\lim_{N \to \infty} \langle R^2 \rangle = \frac{(2+a)\,N}{a} \tag{13}$$

and we note that the expected scaling behavior $\langle R^2 \rangle \approx N^{2\nu}$ is obtained with the mean-field exponent $\nu = \frac{1}{2}$. The asymptotic behavior of $\langle R^2 \rangle$ is different for zero and nonzero $a$, as may be appreciated by comparing Eqs. (12) and (13), respectively. So we may look for the crossover between both behaviors in the limit of $N \to \infty$; $z \to 0$; $Nz = \text{constant}$, getting the result

$$\lim_{N \to \infty;\, a \to 0;\, aN = x} \langle R^2 \rangle = N^2 F(x) \tag{14}$$

with a scaling function

$$F(x) = \frac{2(x - 1 + \exp(-x))}{x^2} \tag{15}$$

It should be stressed that this scaling function is the same as the one obtained by taking the limit of $N \to \infty$, $z \to 0$, $Nz = \text{constant}$ on the calculation of the

mean square end-to-end distance for random walks on a hypercubic lattice without immediate return, which may be obtained from Flory's general result for semiflexible polymers [1].

## 3. ANISOTROPY IN THE BETHE LATTICE

Let us now turn our attention to the calculation of the mean square end-to-end distance of a polymer with an intrinsic anisotropy on the Bethe lattice. This anisotropy will come into play through an additional statistical weight $y$ ascribed for any link in a particular direction. Upon every $q/2$ bend directions at each step of the polymer, one may be a particular direction. The vector $\vec{R}$ with $m$ bends has $m+1$ linear stretches. The binary variable is now ascribed for each step $i$ so that $v_i$ is 1 if the stretch is in the particular direction and $v_i$ is 0 for the other $(q-2)/2$ directions. The averaging will be done with the statistical weight

$$z^m \prod_{i=1}^{m+1} y^{v_i R_i} \tag{16}$$

The quadratic end-to-end distance will be obtained as

$$\langle R^2 \rangle = \frac{\sum_{m=0}^{N-1} z^m \sum_{\vec{R}_m^N} \sum_{v_m} \prod_{i=1}^{m+1} c(v_{i-1}, v_i)\, y^{v_i R_i} \sum_{i=1}^{m+1} R_i^2}{\sum_{m=0}^{N-1} z^m \sum_{\vec{R}_m^N} \sum_{v_m} \prod_{i=1}^{m+1} c(v_{i-1}, v_i)\, y^{v_i R_i} \sum_{i=1}^{m+1} 1} \tag{17}$$

Here $c(v_{i-1}, v_i)$ are multiplicity coefficients for successive stretches. For the first stretch we define

$$c(v_{-1}, 0) = (q-2), \qquad c(v_{-1}, 1) = 2 \tag{18}$$

where the labels 0 and 1 refer to nonparticular and particular directions, respectively. For the next bends the factors will be

$$c(0, 0) = (q-4), \qquad c(0, 1) = 2, \qquad c(1, 0) = q-2, \qquad c(1, 1) = 1 \tag{19}$$

The sums over $\vec{R}_m^N$ take into account all conformations of the polymer with $(m+1)$ stretches and $N$ links, but the sums over $v_m$ count the $2^{m+1}$ different configurations described by the binary variables $v_i = 0, 1$, which take values for each $m+1$ stretch.

The sum over the conformations will be best performed introducing the variables

$$S_{m+1}(j) = \left( \prod_{k=1}^{m} \sum_{v_k = 0, 1} \right) \prod_{i=0}^{m+1} c(v_{i-1}, v_i)\, y^{v_i R_i}|_{v_{m+1} = j} \tag{20}$$

where $j=1$ if the last stretch is on the particular direction and $j=0$ otherwise. These variables may also be defined recursively as

$$S_{m+2}(0)=(q-4)\,S_{m+1}(0)+(q-2)\,S_{m+1}(1) \tag{21}$$

$$S_{m+2}(1)=2y^{R_{m+2}}S_{m+1}(0) \tag{22}$$

It is quite difficult to obtain explicit expressions for the sums $S_{m+1}(0)+S_{m+1}(1)$ for general values of $q$. Let us first consider the case $q=4$, for which the set of recursive definitions for $S$ decouples. The sum then becomes

$$S_{m+1}(0)+S_{m+1}(1)=2^{m+1}\left[\prod_{\substack{i\\ \text{even}}}^{m+1} y^{R_i}+\prod_{\substack{i\\ \text{odd}}}^{m+1} y^{R_i}\right] \tag{23}$$

Considering $k$ links in the even stretches and $(N-k)$ in the odd ones, this equation is rewritten

$$S_{m+1}(0)+S_{m+1}(1)=2^{m+1}[\,y^k+y^{N-k}] \tag{24}$$

Now we define

$$B_{N,m}(y)=\sum_{\vec{R}_m^N}\sum_{v_m}\prod_{i=1}^{m+1} c(v_{i-1},v_i)\,y^{v_iR_i}\sum_{i=1}^{m+1} R_i^2 \tag{25}$$

Using Eqs. (20) and (24), we obtain the following relation:

$$B_{N,m}(y)=2^{m+1}\sum_{k=n_e}^{N-n_o}[\,y^k+y^{N-k}]\left(\sum_{\vec{R}_{n_e-1}^k}\sum_{\substack{i\\ \text{even}}} R_i^2+\sum_{\vec{R}_{n_o-1}^{N-k}}\sum_{\substack{i\\ \text{odd}}} R_i^2\right) \tag{26}$$

Here $n_o(n_e)$ means the total number of links in the odd(even) stretches. The sum over $\vec{R}_{n_e-1}^k(\vec{R}_{n_0-1}^k)$ takes into account the configuration of the part of the polymer with only even(odd) stretches which have the total of $k(N-k)$ links. These sums coincide with the ones for the isotropic polymer performed in the first section. We obtain the expression

$$B_{N,m}(y)=2^{m+1}\sum_{k=n_e}^{N-n_o}[\,y^k+y^{N-k}]\left\{\frac{n_e k!\,(2k-n_e+1)(N-k-1)!}{(n_e+1)!\,(k-n_e)!\,(n_o-1)!\,(N-k-n_o)!}\right.$$
$$\left.+\frac{n_o(N-k)!\,(2N-2k-n_o+1)(k-1)!}{(n_o+1)!\,(N-k-n_o)!\,(n_e-1)!\,(k-n_e)!}\right\} \tag{27}$$

The sums are quite distinct for the cases when the total number of bends $m$ is odd or even. For the case $m$ odd ($m=2n-1$), the variable $n_e(n_o)$ reduces to $m/2((m/2)+1)$. In this case simple algebraic manipulations give

$$B_{N,\,2n-1}(y)=\frac{n2^{2n+1}y^n}{(n+1)!\,(n-1)!} \times [\,-4yP_n^{N-2n-2}+(2N^2-5Nn+4n^2+N)\,P_{n-1}^{N-2n}] \tag{28}$$

where the sums over $k$ have all been encoded on

$$P_n^N=\sum_{j=0}^{N}\frac{(j+n)!\,(N-j+n)!}{j!\,(N-j)!}\,y^j \tag{29}$$

In the case of $m$ even, we have obtained

$$B_{N,\,2n}(y)=\frac{2^{2n+1}}{(n-1)!\,(n+2)!} \times \sum_{j=0}^{N-2n-1}\frac{(j+n+1)!\,(N-n-j-1)!}{j!\,(N-2n-1-j)!}\,x_{N,\,n,\,j}[\,y^{j+n}+y^{N-n-j}] \tag{30}$$

where

$$x_{N,\,n,\,j}=(4n+6)\,j^2-(2+4(N-2n-1)(n+1))\,j +(n+1)(n(n+2)+(N-n)(2N-3n+1)) \tag{31}$$

An analytical summation on both the $j$ and the $n$ variables seems to be very difficult. We are thus led to a numerical analysis.

## 4. RESULTS AND DISCUSSION

Let us study the dependence of the mean square end-to-end distance of the polymer as a function of $N$. The isotropic case for $q=4$ and nonzero bend fugacity $z$ presents the scaling as

$$\lim_{N\to\infty}\langle R^2\rangle=cN \tag{32}$$

with $c=1$. The power of $N$ in this behavior was expected for the Bethe lattice and should not depend on the introduction of the anisotropy, as discussed earlier. The linear coefficient $c$, on the other hand, could depend on details of the model. We then plot the $\langle R^2\rangle$ variable against $N$ for different

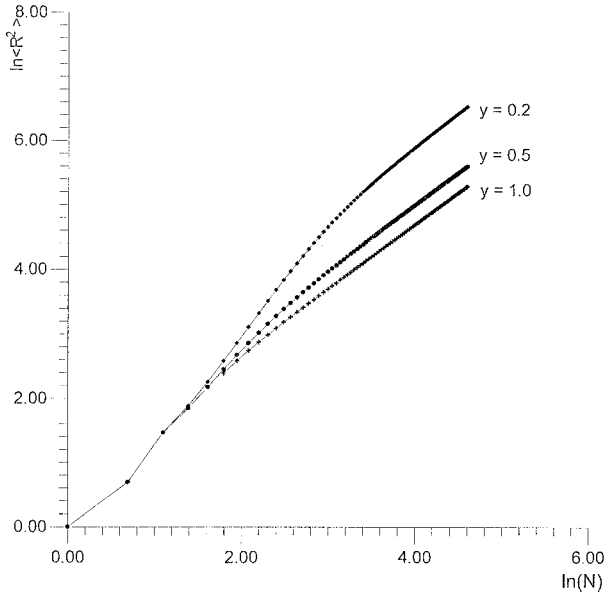


**Fig. 1.** Plot of $\ln \langle R^2 \rangle$ versus $\ln N$ for different anisotropy parameter values and for $z = 0.5$.

values of the anisotropy parameter $y$. We fix the representative value $z = 0.5$. In Fig. 1 we have done this for two values of $y$ other than the value $y = 1$, which reproduces the isotropic case.

Two aspects of this plot are most noticeable. First, although the power dependence for large $N$ is the same for any value of $y$, the straight curves they reach differ asymptotically. This means that the linear coefficient $c$ increases as $y$ becomes different from 1. The anisotropy tends to straighten the polymer, increasing its size while at the same time maintaining the critical exponent 1. On the other hand, the value of $N$ for which the scaling regime is achieved also increases with the value of $y$ getting far from 1. This means that the regime where the detailed behavior of the polymer size with the number of points is important persists more for the anisotropic case. Figure 2 shows more clearly the larger is the value of $N$ necessary for reaching the scaling region, as $y$ becomes more different from 1.

Another interesting behavior appears if we take values of $y$ larger than 1. We have noticed the equivalence between the cases $y$ and $y'$ whenever $y = 1/y'$. This can be understood as a peculiarity of $q = 4$. Taking $y$ greater than 1 actually represents a preference for the other directions. Since for $q = 4$ there are only two directions, the case with $y$ greater then 1 turns out to be equivalent to the case with $y \to (1/y)$.

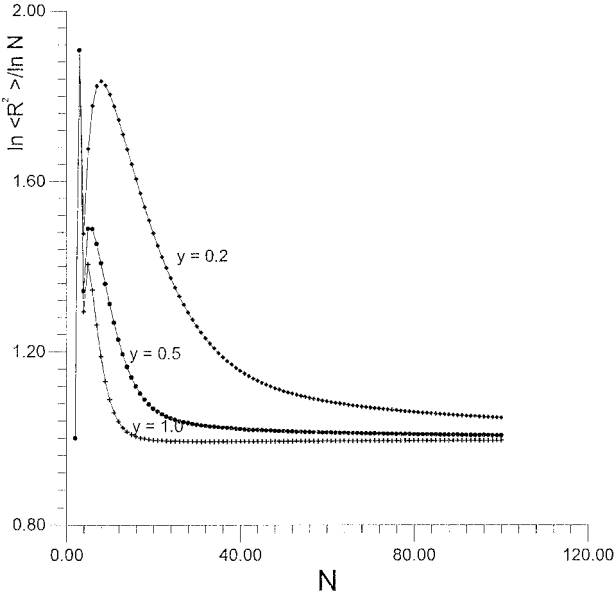


**Fig. 2.** Plot of $\ln(\langle R^2 \rangle)/\ln N$ versus $N$ for different anisotropy parameter values and for $z = 0.5$.

It would be interesting to continue this work in two directions. First, it seems feasible, although not trivial, to perform the analytical treatment of the anisotropic case, if we consider $y = 1 - x$ and perform an expansion in the small variable $x$. Another interesting direction would be to consider the effect of anisotropy for polymers with coordination numbers randomly distributed.

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