Characteristic length of random knotting for cylindrical self-avoiding polygons

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Abstract

We discuss the probability of random knotting for a model of self-avoiding polygons whose segments are given by cylinders of unit length with radius $r$. We show numerically that the characteristic length of random knotting is roughly approximated by an exponential function of the chain thickness $r$.

Keyword: characteristic length, random knotting, self-avoiding polygons, knot invariants, knots

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1 Introduction

Knotted ring polymers such as knotted DNA molecules are synthesized in various experiments in chemistry and biology [1, 2, 3]. The question on the topological constraint of the macromolecules was first formulated by Delbrück, Frisch and Wasserman in the ’60s [4, 5]. Then, topological properties of ring polymers have been studied through numerical simulations [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. Furthermore, the fractions of knotted species synthesized after the random cyclization of the circular DNAs are experimentally measured, and they give an experimental estimate on the effective diameter of the DNA molecules surrounded by the counterions [7, 8, 9]; it is estimated so that the experimental values of fractions of some knots are consistent with the theoretical values of the fractions obtained for the hedgehog model [11] of self-avoiding polygons. The model gives self-avoiding polygons consisting of cylindrical segments, where the length and the radius of the cylindrical segments correspond to the Kuhn length and the effective radius, respectively.

Let us introduce the probability of random knotting. First, we assume an algorithm of constructing random polygons (or self-avoiding polygons) of $N$ polygonal nodes. Then, for a given knot $K$, we define knotting probability $P_K(N)$ by the probability of observing a random polygon (or a self-avoiding polygon) of the knot $K$. When $K$ is trivial ($K = 0$), we denote it by $P_0(N)$. It has been found [8, 13] that the probability of unknot has a decreasing-exponential dependence on the nodes $N$:

$$P_0(N) = C_0 \exp(-N/N_0).$$  \hspace{1cm} (1)

For the different models of random polygons and self-avoiding polygons, knotting probabilities of some nontrivial knots have been evaluated numerically [6, 11, 14, 15]. Through the simulations with the Vassiliev-type knot invariants, it has been found that for a given knot type $K$, the probability $P_K(N)$ as a function of the number $N$ of nodes can be well described by the following formula [14, 15]

$$P_K(N) = C_K \left( \frac{N}{N_K} \right)^{m(K)} \exp(-N/N_K).$$ \hspace{1cm} (2)

From the numerical results, it is found that the parameter $N_K$ should have almost the same value for any knot [14, 15]. The result is also consistent with the simulation of self-avoiding polygons on the cubic lattice [16]. Thus, we may assume that $N_K$ should be given by a constant $N_c$ for any knot $K$: $N_K = N_c$. We call $N_c$ the characteristic length of random knotting.

In this paper, we discuss how the characteristic length $N_c$ depends on the excluded-volume parameter of self-avoiding polygons. We introduce a new
method for constructing self-avoiding polygons with cylindrical segments with radius \( r \). The method is a variant of the dimerization algorithm. It seems that the algorithm is more efficient than that of the hedgehog model. Then, we study the characteristic length \( N_c(r) \) as a function of the cylinder radius \( r \) for the self-avoiding polygons. We give the estimates of the characteristic length by applying the formula (1) to the numerical values of the probability of unknot. Here the fitting parameters \( C_0(r) \), \( N_0(r) \) are determined by the least square method.

The numerical study on the characteristic length of random knotting as a function of the thickness parameter of polymer chains should be important in the study of knotted DNAs where the effective diameter can be changed according to the concentration of the counter ions. Furthermore, it could be also important in other systems of polymer rings. The length and the radius of the cylindrical segments of the model correspond to the two fundamental parameters of polymer chains, i.e., the Kuhn length (the statistical length) and the stiffness (or the excluded-volume parameter), respectively. \([19]\) In association with the numerical result of the rod-bead model \([13]\), Nechaev and Grosberg have addressed a conjecture \([24]\) that the characteristic length \( N_0 \) as a function of some thickness parameter \( d \) should be given by the following:

\[
N_0(d) = N_0(0) \exp(d/\ell).
\]

Here \( \ell \) denotes the Kuhn length. As we shall see later, however, the conjecture \([24]\) does not hold for the rod-bead model. On the other hand, the numerical simulation in this paper shows that the exponential behavior \([3]\) gives a rough approximation for the new cylinder model of self-avoiding polygons.

The paper is organized as follows. In §2 we introduce the cylinder model and explain the method of our numerical experiment of random knotting. In §3 we show the numerical data of our simulations and discuss possible relations between the characteristic length and the cylinder radius. We also discuss for the rod-bead model how the characteristic length depends on the bead radius. Finally, we give some discussion in §4.

2 The methods of simulations

2.1 New method for constructing self-avoiding polygons of cylindrical segments

Let us explain the new method for constructing self-avoiding polygons of cylindrical segments. In this method, each segment of a polygon consists of a cylinder of unit length with radius \( r \). The main structure of the algorithm is given by the following: (1) we generate a set of chains with cylindrical segments by the dimerization method; (2) we construct polygons by connecting two cylindrical self-avoiding chains with the concatenating method of Ref. \([1]\). In this method, we also calculate the statistical weight related to the probability of successful concatenation.

Let us define the condition of an overlap between a given pair of segments for our model of self-avoiding polygons. First, we assume that there is no overlap between any pair of adjacent segments. Second, for a pair of two segments which are not next-neighboring to each other, we assume that the two segments have no overlap if and only if the distance between the central axes of the two cylinders is larger than \( 2r \). Here we have considered that a central axis of a cylinder is given by the line segment between the centers of the upper and lower disks of the cylinder.

In the step (1) of the algorithm, we construct a chain with cylindrical segments randomly, and then we check whether there is an overlap or not for all unadjacent pairs of cylinders of the chain. If there is an overlap, then we give up the chain and construct a new chain from the beginning. If there is no overlap, then we keep the chain in the computer memory.

The new model of self-avoiding polygons produces free-joint rings with thickness parameter \( r \), systematically. We can construct very long self-avoiding polygons with the cylinder radius \( r \). It is known that the thickness of polymer chains plays an important role in the study of stiff polymers such as DNAs. \([21, 22, 23]\) We may assume that negatively charged DNA molecules with surrounding counter ions can be approximated by impermeable cylinders with the effective radius given by the screening effect. Thus, the new algorithm can be applied to the study of knotted closed DNAs.

2.2 The method for simulation of random knotting

Let us describe the algorithm of our numerical simulation of random knotting. For a given number \( N \) of polygonal nodes, we construct \( M \) polygons. Here the number \( M \) should be very large, such as \( M = 10^4 \). Then, for a fixed knot type \( K \), we enumerate the number \( M_K \) of such polygons out of the \( M \) polygons that have the same set of values of the knot invariants with the knot \( K \). We estimate the probability \( P_K(N) \) of knot \( K \) by the following

\[
P_K(N) = \frac{M_K}{M}.
\]

We employ two knot invariants, the determinant \( \Delta_K(-1) \) of knot and the Vassiliev-type invariant \( v_2(K) \) of the second degree, as the tool for detecting the knot type of a given polygon. \([24, 25]\) The values
Table 1: Values of the determinant of knot $\Delta_K(-1)$ and the second Vassiliev invariant $v_2(K)$ for some simple knots.

| Knot $K$ | $\Delta_K(-1)$ | $v_2(K)$ |
|----------|-----------------|-----------|
| 0        | 1               | 0         |
| $3_1$    | 3               | -12       |
| $4_1$    | 5               | 12        |
| $5_1$    | 5               | -36       |
| $5_2$    | 7               | -24       |
| $3_{10}$ | 9               | 24        |

Figure 1: Probability $P_0(N)$ of unknot versus number $N$ of nodes for the cylinder model: the numerical estimates of $P_0(N)$ for $r = 0.01, 0.03$ and $0.05$ are shown by black circles, black triangles, and black diamonds, respectively, with error bars given by their standard deviations. Number $N$ of nodes are given by $10j + 1$ with $j = 2, 3, \ldots, 15$.

of the invariants for some typical knots are given in Table 1.

3 Characteristic lengths of random knotting

3.1 The exponential decay of the probability of unknot

Let us discuss the numerical results of our simulations. Employing the cylinder model introduced in §2, we construct self-avoiding polygons with $N$ polygonal nodes where the cylinder radius is given by $r$. For a given number $N$ and a given value of $r$, we construct four sets of $10^4$ polygons. ($M = 4 \times 10^4$.) We consider for the polygonal nodes $N$ fourteen different numbers from 20 to 150, and for the radius $r$ 10 different values from 0.0 to 0.09.

In Fig. 1, the estimates of the probability of unknot for the cylinder model with $r = 0.01, 0.03, 0.05$ are shown against the number $N$ of polygonal nodes. The error bars are given by the standard deviations. For the cylinder model, we evaluate the variance of the values of the probability $P_0(N)$ of unknot by taking into account both the statistical fluctuation of the number $M_K$ and that of the statistical weight $|v_2(K)|$ appearing in the ring-dimerization procedure.

From Fig. 1, we may confirm the exponential decay of $P_0(N)$ for the cylinder model. We note that the result is consistent with all the numerical simulations for other models such as the Gaussian dynamical model [1], the Gaussian random polygon model [2], the hedgehog model [3], and the rod-bead model [13]. The lines in Fig. 1 are theoretical curves given by the formula (1). The estimates of the parameters $C_0$ and $N_0(r)$ for the ten different values of the radius $r$ from $r = 0$ to $r = 0.9$ are given in Table 1.

3.2 The characteristic length of the cylinder model

A semilogarithmic plot of the numerical estimates of the characteristic length $N_0(r)$ is given in Fig. 2 against the cylinder radius $r$ for the ten different values from $r = 0.0$ to $r = 0.9$. From Fig. 2, we see that the characteristic length $N_0(r)$ as a function of the cylinder radius $r$ can be roughly approximated by an increasing exponential function of $r$. Let us consider a fitting formula in the following

$$N_0(r) = N_0(0) \exp (\alpha r). \quad (5)$$

Here, there are two parameters to fit, i.e., $N_0(0)$ and $\alpha$. Applying the formula (5) to the numerical estimates of the characteristic lengths, we have the fitting line drawn in Fig. 2. The estimates of the fitting parameters are given by $N_0(0) = 292\pm 5$ and $\alpha = 43.5 \pm 0.6$. From the viewpoint of the $\chi^2$ test,
numerical simulations. Larger than the polygonal nodes ($N < M$) covers most important cases. Furthermore, when recall that even for the case of tic length becomes technically more difficult. We recall the formula (6).

\[ N_0(r) = N_0(0) \exp(\beta r^\nu), \]  

(6)

where there are three parameters $N_0(0)$, $\beta$ and $\nu$. The new fitting curve is shown in Fig. 3 to the same numerical data points with Fig. 2. The best estimates of the fitting parameters are given by $N_0(0) = 271 \pm 6$, $\beta = 29 \pm 2$ and $\nu = 0.85 \pm 0.02$. It seems that the curve fits well to the data, although the value of $\chi^2$ might be a little too small: $\chi^2 = 2.2$. Thus, we may conclude that for the cylinder model, the characteristic length of the probability of unknot as a function of the cylinder radius is given by the formula (6).

We have evaluated the characteristic length $N_0(r)$ for $r < 0.1$. For stiff chains such as DNAs, the radius $r$ can be rather small such as $r = 0.003$. We thus consider that the range: $0.0 \leq r < 0.1$ covers most important cases. Furthermore, when $r \geq 0.1$, numerical evaluation of the characteristic length becomes technically more difficult. We recall that even for the case of $r = 0.09$, the estimates $N_0(r)$ is of the order of $10^3$, which is much larger than the polygonal nodes ($N < 160$) of our numerical simulations.

### 3.3 The characteristic length of the rod-bead model

Let us now discuss the characteristic length for the rod-bead model. Here we assume that the parameter $r$ denotes the bead radius. (Fig. 4) In Fig. 4, for the rod-bead model, the numerical estimates of the characteristic length $N_0$ are plotted against the bead radius $r$. For an illustration, the estimates of the characteristic length $N_0$ for the cylinder model are also shown in Fig. 4 against the cylinder radius $r$. We note that when $r = 0$, the characteristic lengths of the two models should coincide. The two algorithms are essentially equivalent for $r = 0$. We have evaluated the characteristic length $N_0(r)$ for $0.0 \leq r < 0.1$. For stiff chains such as DNAs, the radius $r$ can be rather small such as $r = 0.003$. We thus consider that the range: $0.0 \leq r < 0.1$ covers most important cases. Furthermore, when $r \geq 0.1$, numerical evaluation of the characteristic length becomes technically more difficult. We recall that even for the case of $r = 0.09$, the estimates $N_0(r)$ is of the order of $10^3$, which is much larger than the polygonal nodes ($N < 160$) of our numerical simulations.

| $r$    | $C_0$    | $N(K)$     |
|--------|----------|------------|
| 0.0    | 1.05±0.004 | (2.7±0.06)×10^2 |
| 0.01   | 1.07±0.01  | (2.6±0.08)×10^2 |
| 0.03   | 1.06±0.01  | (2.6±0.09)×10^2 |
| 0.05   | 1.05±0.01  | (2.8±0.1)×10^2  |
| 0.1    | 1.04±0.03  | (4.2±0.1)×10^2  |
| 0.15   | 1.00±0.03  | (9.0±0.3)×10^2  |
| 0.2    | 1.0±0.03   | (2.2±0.6)×10^3  |
Figure 4: Two series of estimates of the characteristic length $N_0(r)$ are shown by black triangles for the rod-bead model and by black circles for the cylinder model, respectively. The estimates for the cylinder model is given in Table 2, and those of the rod-bead model in Table 3. The two estimates for the two models coincide for $r = 0$.

From Fig. 4, we see that the numerical estimates of the two models really coincide for $r = 0$, which gives a partial consistency check of our numerical simulations.

Nechaev and Grosberg discussed a conjecture that the characteristic length $N_0$ as a function of the “chain thickness” $d$ should be given by an exponential form: $N_0(d) = N_0(0) \exp(27d/\ell)$, where $\ell$ is the Kuhn length. [20] It seems that their conjecture is based on the numerical result [13] of the rod-bead model. However, we see from Fig. 4 that the characteristic length $N_0(r)$ for the rod-bead model is not given by an exponential function of the bead radius $r$ with $0.0 \leq r \leq 0.2$. Let us consider a part of the range such as $0.1 \leq r \leq 0.2$, and apply for the rod-bead model an exponential approximation: $N_0(r) = N_0(0) \exp(\gamma r)$. Then, we find that the parameter $\gamma$ is roughly given by 15. Thus, for the rod-bead model, the conjecture of the exponential dependence could be valid only for a limited range of the bead radius. Furthermore, it seems that the estimate of the coefficient $\gamma$ is not consistent with the conjectured value of 27.

### 4 Discussion

Finally, we discuss a possible connection of the cylinder model of this paper to the hedgehog model. Klenin et al. [11] studied the probability of unknot for the hedgehog model of ring polymers. The algorithm of the model is given by the following: (1) generating a set of vectors of unit length with a common origin (a “hedgehog”); and (2) setting the minimal distance between any two unadjacent segments larger than the segment diameter.

It seems that the hedgehog model and the cylinder model introduced in this paper produce almost the same results for the self-avoiding polygons with cylinder radius $r$. It is our conjecture that the two models should give the same results, although the two algorithms themselves are quite different. For the probability of unknot, the two values obtained by the two different methods are rather close. However, it is not easy to see whether they are exactly the same or not. We shall discuss much more precise comparison between the two models in our future publications.

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**Figure captions**

Fig. 1: Probability $P_0(N)$ of unknot versus number $N$ of nodes for the cylinder model: the numerical estimates of $P_0(N)$ for $r = 0.01, 0.03$ and $0.05$ are shown by black circles, black triangles, and black diamonds, respectively, with error bars given by their standard deviations. Number $N$ of nodes are given by $10j + 1$ with $j = 2, 3, \ldots, 15$.

Fig. 2: Characteristic length $N_0(r)$ versus cylinder radius $r$ for the cylinder model. The numerical estimates of $N_0(r)$ listed in Table 2 are depicted by black circles together with their errors. The fitting line of eq. (5) is determined by the least square method with $\chi^2 = 42$.

Fig. 3: Fitting curve of eq. (6) to the data of $N_0(r)$ versus radius $r$ for the cylinder model. The three fitting parameters of eq. (6) are determined by the least square method, which gives $\chi^2 = 2.2$. The data points and their error bars are given in Table 2.

Fig. 4: Two series of estimates of the characteristic length $N_0(r)$ are shown by black triangles for the rod-bead model and by black circles for the cylinder model, respectively. The estimates for the cylinder model is given in Table 2, and those of the rod-bead model in Table 3. The two estimates for the two models coincide for $r = 0$. 