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Knot complexity and the probability of random knotting

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The probability of a random polygon (or a ring polymer) having a knot type K should depend on the complexity of the knot K. Through computer simulation using knot invariants, we show that the knotting probability decreases exponentially with respect to knot complexity. Here we assume that some aspects of knot complexity are expressed by the minimal crossing number C and the "rope length" of K, which is defined by the smallest length of rope with unit diameter that can be tied to make the knot K.

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I. INTRODUCTION

Various species of knotted polymers have been synthesized and observed in chemistry and biology in the last two decades [1–4]. Once a ring polymer is formed, its topological state is unique and invariant. The topological constraint on the ring polymer should be nontrivial. It may restrict the available degrees of freedom in the configuration space of the polymer, to a great extent. Consequently, it may lead to a large entropic reduction, which is related to the probability of random knotting, as we shall see shortly.

For a knot K, we define the knotting probability $P_K(N)$ by the probability that the topology of a random polygon with N nodes is given by the knot K. If a ring polymer is under the topological constraint of the knot K, then the decrease of the polymer entropy is given by $\Delta S_K = -k_B \ln P_K(N)$, where $P_K(N)$ is the ratio of the volume of the configuration space under the topological constraint to that of no topological constraint. The knotting probability $P_K(N)$ should also correspond to the probability that a ring polymer of N Kuhn units have the knot K when it is closed randomly during its synthesis. The knotting probabilities have been measured as the fractions of knotted species of circular DNAs [3,4].

Let us now discuss how to express the complexity of knots. We could classify knots completely, if we might know all the topological properties that are invariant under any continuous deformation of the spatial configurations. The topology of a given polygon can be effectively detected by calculating some topological invariants such as the Alexander polynomial $\Delta_K(t)$ and the Vassiliev-type invariants $v_n(K)$. Although the invariants are practically useful for computer simulations [5,6], it is not easy to derive any explicit topological properties or meanings from them. Let us consider the minimal number of crossing points in the knot diagram of a knot K. We denote it by C, or $|K|$ for the knot K. The minimal crossing number C should be a measure on the complexity of knots. The number C is useful in studying statistical or dynamical properties of knotted ring polymers [7,8]. There is some argument on the mean-square radius of gyration of knotted ring polymers with respect to C [7]. However, C is rather weak as a topological invariant. The number of knots that have the same number C increases rapidly: there are 165 primes knots which have ten crossings.

Recently, the concept of ideal knots has attracted much interest [9–11]. One of the most ideal (or elegant) geometric representations of a knot should be given by such a closed tube with uniform diameter that gives the largest ratio of the diameter to the tube length. We call such geometric representations *ideal knots*, briefly. Given a knot K, the ratio of the tube length to the diameter of its ideal knot is called the rope length $\ell(K)$ of the knot K [12]. For a ring polymer with a knot type K, Grosberg *et al.* [11] discussed a topological invariant p of K, which is defined by the aspect ratio of the length to the diameter of such a geometric tubular representation of K that is maximally inflated, i.e., the ideal knot of K. The invariant p of K is thus nothing but the rope length $\ell(K)$. The rope length $\ell(K)$ should be a measure of knot complexity. It could be more powerful than C: we have a conjecture that different knots should have different values of $\ell(K)$. Katritch *et al.* have obtained ideal knots for 42 different knots [9,10]. The rope length $\ell(K)$ should be useful for describing flexible DNA knots in thermal equilibrium [9]. Furthermore, it should also be useful for statistical or dynamical studies on knotted ring polymers [13,14].

The N dependence of the knotting probability has been studied through computer simulations, [5,15–23] and it is found that the probability of the unknot (the trivial knot) decreases exponentially with respect to N,

$$P_0(N) = C_0 \exp(-N/N_c), \tag{1}$$

where C_0 and N_c are fitting parameters. For some nontrivial knots ($3_1, 4_1, 5_1, 5_2$), knotting probabilities have been evaluated numerically for several different models of random polygons and self-avoiding polygons [19–23]. Through the simulations using the Vassiliev-type invariants, it is found that the probability $P_K(N)$ as a function of N can be expressed as

$$P_K(N) = C_K \left(\frac{N}{N_K}\right)^{m_K} \exp\left(-\frac{N}{N_K}\right). \tag{2}$$

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Here C_K, N_K, and m_K are fitting parameters to be determined from the numerical results. The expressions (1) and (2) should correspond to the asymptotic expansion of renormalization group arguments. Numerically, we see that the estimates of N_K should be given by almost the same value for any knot K [20–22], and therefore the N_K's are almost equal to N_c, which depends on the model. We also observe that the value m_K of a knot K should be universal for the different models [21].

In this paper, we discuss how the knotting probability $P_K(N)$ of a knot K should depend on its complexity while N being fixed, or in short, the knot dependence of the normalization constant C_K. Evaluating the knotting probabilities of several prime knots for Gaussian random polygons, we observe a rough tendency that the amplitude C_K decreases exponentially with respect to the rope length $\ell(K)$. The numerical result seems to be favorable to Grosberg's conjecture [13] that the probability $P_K(N)$ as a function of the aspect ratio p (i.e., rope length $\ell(K)$) should be given by an exponential function

$$P_K(N) \sim \exp(-N/N_c - sp). \tag{3}$$

Here s is a constant. At this stage, however, we could not judge whether the conjecture is valid, since the data points scatter outside the range of statistical errors. However, we show another explicit statistical behavior for a version of the knotting probability. Let us define the average knotting probability $P_{ave}(N,C)$ by

$$P_{ave}(N,C) = \sum_{K:|K|=C} P_K(N)/A_C. \tag{4}$$

Here the sum is over such knots that have the same minimal crossing number C, and A_C denotes the number of prime knots that have the same minimal crossing number C. For instance, we have $A_3 = A_4 = 1$, $A_5 = 2$, and $A_6 = 3$. Then, we shall see from the data that the average knotting probability decreases exponentially with respect to C. Furthermore, if we consider the average of the rope lengths over such knots that have the same C,

$$\langle \ell \rangle = \sum_{K:|K|=C} \ell(K)/A_C, \tag{5}$$

then we see that the average knotting probability also decays exponentially with respect to the average $\langle \ell \rangle$.

II. THE METHOD OF SIMULATIONS

Using the conditional probability [15], we construct a large number of Gaussian random polygons, say M polygons, of N nodes for $N=300$, 500 and 1000. Then, the knotting probability of a knot K is evaluated by $P_K(N) = M_K/M$. Here M_K is the number of polygons with the knot K, and M is given by $M = 10^5$ to each of the three numbers of N.

In order to detect the knot type of a give polygon, we employ three knot invariants: the determinant $|\Delta_K(t=-1)|$ of a knot K, the Vassiliev-type invariants $v_2(K)$, and $|v_3(K)|$ of the second and third degrees, respectively. We evaluate M_K, after enumerating the number of the polygons that have the same set of the values of the three invariants for the knot K. Using $|v_3(K)|$, we do not distinguish the chirality of the knot, i.e., the right-handed knots and the left-handed ones [6,24]. Furthermore, we do not consider six knots (8_9, 8_{10}, 8_{11}, 8_{18}, 8_{20}, and 8_{21}) in any of the simulations in the paper. They have the same values of the three invariants as those of some composite knots.

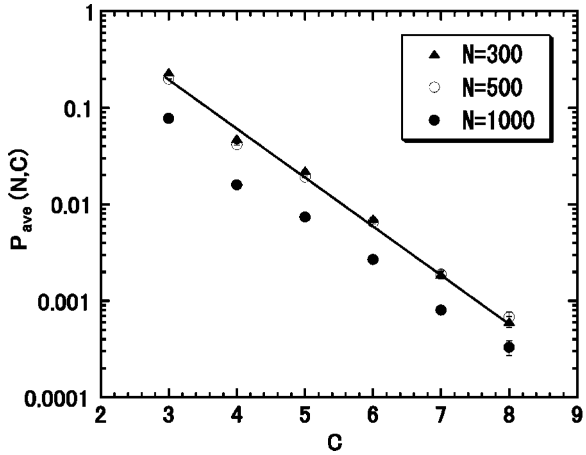

FIG. 1. Average knotting probability $P_{ave}(N,C)$ vs the minimal crossings C for 29 prime knots with up to $C=8$. The line is given by $P_{ave}(N,C) = P_{ave}(N,0)\exp(-\alpha C)$ with $\alpha = 1.16$.

III. RESULTS AND DISCUSSION

The estimates of the average knotting probability $P_{ave}(N,C)$ are plotted in Fig. 1 against the minimal crossing number C, up to $C=8$. It is clear in Fig. 1 that the average knotting probability $P_{ave}(N,C)$ decreases exponentially with respect to C. We remark that error bars correspond to one standard deviation in all the four figures in the paper.

Let us now discuss the knotting probability in terms of the rope length. In Fig. 2, the knotting probabilities $P_K(N)$ for some prime knots are plotted against the rope length $\ell(K)$, where N is kept constant. We note that the values of $\ell(K)$

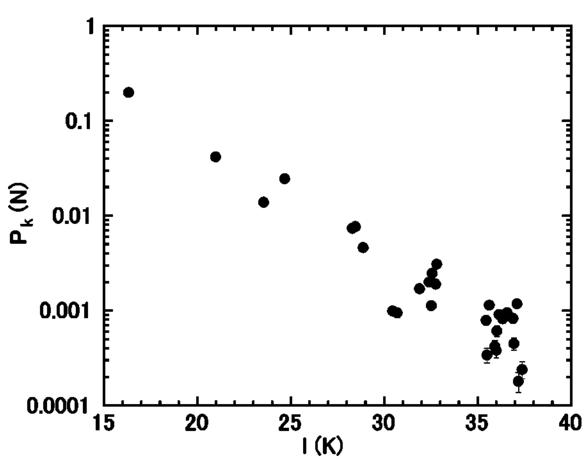

FIG. 2. Knotting probability $P_K(N)$ with $N=500$ vs the rope length $\ell(K)$ for 29 prime knots with up to $C=8$.

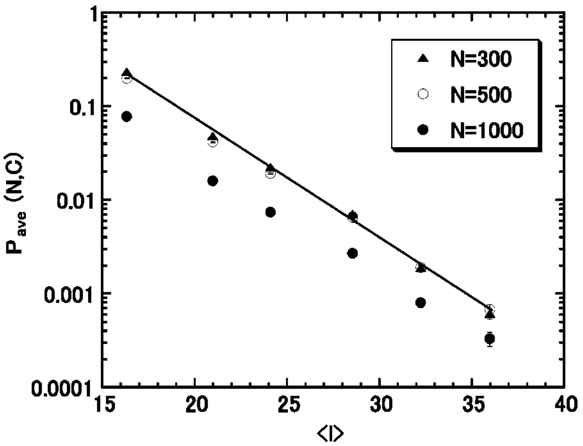

FIG. 3. Average knotting probability $P_{ave}(N,C)$ vs the average $\langle \ell \rangle$ for 29 prime knots with up to $C=8$. The line is given by $P_{ave}(N,C)=P_{ave}(N,0)\exp(-\beta\langle \ell \rangle)$ with $\beta=0.30$.

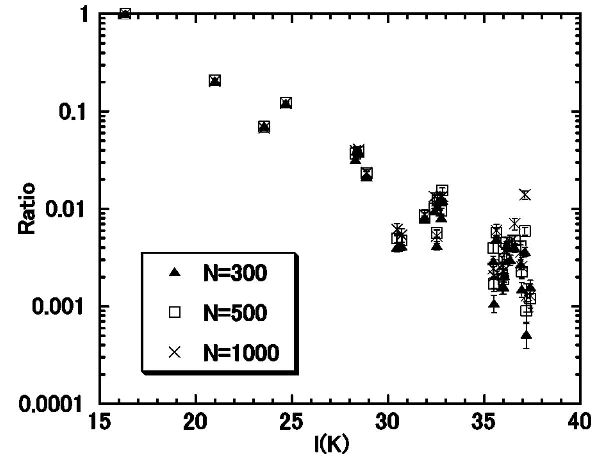

FIG. 4. The ratio of knotting probabilities $P_K(N)/P_{3_1}(N)$ vs the rope length $\ell(K)$ for $N=300$, 500, and 1000.

for the 42 knots are listed in Table 1 of Ref. [10], which are used in the paper. We see in Fig. 2 that there is a rough tendency that the knotting probability of a prime knot decrease exponentially with respect to the rope length $\ell(K)$. The observation should be useful. However, it seems that there is no clear relation between the knotting probability $P_K(N)$ and the rope length $\ell(K)$ (i.e., the aspect ratio p), since the data points of larger values of $\ell(K)$ deviate from the possible regression line, considerably. Here we recall that error bars correspond to one standard deviation.

Let us discuss the knotting probability for such knots that have the same minimal crossing number. For instance, there are two knots with five minimal crossings: 5_1 and 5_2. For Gaussian polygons, the knotting probability of 5_2 is always larger than that of 5_1. This is consistent with the simulation of the cylindrical self-avoiding polygons [23]. Let us consider the three prime knots with $C=6$. We observe that the knotting probabilities of 6_1 and 6_2 are almost the same, while that of 6_3 is always smaller than the other two. For prime knots with $C=7$ or 8, the data points are so close to each other that it is difficult to give any definite ranking on them.

In terms of the average value $\langle \ell \rangle$, which is a function of C, the estimates of the average knotting probability $P_{ave}(N,C)$ are expressed in Fig. 3. We clearly see the exponential decay of the average knotting probability $P_{ave}(N,C)$ with respect to $\langle \ell \rangle$. It is similar to Fig. 1. This result shows that the entropy of a ring polymer with knot K decreases with respect to knot complexity expressed in terms of $\langle \ell \rangle$ or C. Here it is also suggested that $\langle \ell \rangle$ should be approximately linear to C.

Let us discuss the N dependence of the knotting probability in terms of knot complexity. The ratio $P_K(N)/P_{3_1}(N)$ of a knot K against the rope length $\ell(K)$ is plotted in Fig. 4 for the three numbers of N: $N=300$, 500, and 1000. Here we note that the trefoil knot (3_1) is dominant among the nontrivial prime knots for the three N's. We find again the rough tendency that the ratio $P_K(N)/P_{3_1}(N)$ decays exponentially with respect to the rope length $\ell(K)$. Moreover, for any knot K, the ratio $P_K(N)/P_{3_1}(N)$ is given by almost the same value for the three numbers of N, with respect to error bars as seen in Fig. 4. Thus, the ratios $P_K(N)/P_{3_1}(N)$ are independent of N.

The above observation in Fig. 4 can be explained by using the fitting formula (2). Let us assume that for a prime knot K, the exponent m_K of Eq. (2) should be given by almost the same value. Then, we have $P_K(N)/P_{3_1}(N) \sim C_K/C_{3_1}$, which is clearly independent of N. Thus, in terms of the formula (2), the rough exponential decay of the knotting probability with respect to p is closely related to the knot complexity-dependence of the amplitude C_K.

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