Universality of random knotting

Tetsuo Deguchi [1] and Kyoichi Tsurusaki [2]
[1]*Department of Physics, Ochanomizu University, Ohtsuka, Bunkyo-ku, Tokyo 112, Japan*
[2]*Molecular Engineering Division, Kanagawa Industrial Technology Research Institute, 705-1 Shimoizumi, Ebina-city, Kanagawa 243-04, Japan*
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Knotting probability $[P_K(N)]$ is defined by the probability of an N-noded random polygon being topologically equivalent to a given knot K. For several nontrivial knots we numerically evaluate the knotting probabilities for Gaussian and rod-bead models. We find that they are well approximated by the following formula: $P_K(N)=C(K)[\widetilde{N}/N(K)]^{m(K)}\exp[-\widetilde{N}/N(K)]$ where $\widetilde{N}=N-N_{ini}(K)$, and that the fitting parameters $C(K)$, $N(K)$, and $N_{ini}(K)$ are model dependent, while $m(K)$ is not. We suggest that given a knot K, the exponent $m(K)$ should be universal: it is independent of models of random polygon and is determined only by the knot K. [S1063-651X(97)09004-1]

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Recently knotted ring polymers such as knotted DNA molecules are synthesized in various experiments in chemistry and biology [1–3]. In particular, the formation of knotted species on random ring closure of DNA was observed and their fractions were measured [4,5]. In statistical mechanics, the topological constraint that a ring polymer does not change its topology under any thermal fluctuation leads to a great reduction in the available volume of the configuration space [6]. The topological constraint, or the self-entanglement effect, is derived from the fact that any bond between neighboring monomers in the ring polymer is not disconnected when the bonding energy is very large.

In the 1960s Delbrück formulated a fundamental question about the self-entanglement of a ring polymer: What fraction of permissible configurations of a chain of given length will contain a knot [7,8]? The fraction of knotted ring polymers has been studied from the following three approaches: numerical experiments using certain knot invariants [9–18], mathematical discussion of the self-avoiding polygon [19–21], and biological experiments using DNAs [4,5].

Let us assume that a model of an N-noded random polygon describes a ring polymer with N bonds. Given a knot K, we define knotting probability $P_K(N)$ to the model by the fraction of those configurations of the random polygon that have the same knot type K. The main questions in this paper are how the knotting probability $P_K(N)$ behaves as a function of step number N for each knot K, and how it depends on models of a random polygon.

For the trivial knot $(K=0)$ we call the knotting probability $P_0(N)$ the unknotting probability. It has been evaluated for several different models of random polygons with different lengths N less than about 2000 [9–14]. The exponential decay of $P_0(N)$ with respect to N has been discussed for the molecular dynamical model of ring polymers by Michels and Wiegel, and for the rod-bead model by Koniaris and Muthukumar [11,14].

For nontrivial knots, however, the knotting probabilities have been evaluated only for short polygons with $N<200$, where the graphs of $P_K(N)$ versus N can be approximated by linear functions of N [9]. When we calculate knot invariants for polygons with large N, there are two technical difficulties: memory-size and computation-time problems [22]. For polynomial-valued invariants such as the Alexander polynomial (or Jones polynomial [23], etc.), the size of the memory necessary for computing them will grow exponentially or very rapidly with respect to N. For instance, if we evaluate a term t^N for $N=10^3$ setting 2 to t, then we have a very large number 2^{1000}. Furthermore, for many link polynomials such as Jones, HOMFLY, and Kauffman polynomials, the computation time will grow exponentially with respect to N [22,24].

Recently, new methods have been independently proposed for computing certain knot invariants in polynomial time [22,25]. Thanks to these methods, we can practically determine the knot types of given large polygons. The purpose of the paper is to show some universal properties of the knotting probability $P_K(N)$ regarded as a function of step number N. We discuss them from computer simulations on $P_K(N)$ of several nontrivial knots for different models of random polygons. We apply to the data the formula [16]

$$P_K(N)=C(K)[\widetilde{N}/N(K)]^{m(K)}\exp[-\widetilde{N}/N(K)], \qquad (1)$$

where the symbol $\widetilde{N}$ denotes $\widetilde{N}=N-N_{ini}(K)$, and $C(K)$, $m(K)$, $N(K)$, and $N_{ini}(K)$ are fitting parameters. We con-

TABLE I. The values of the determinant of the knot $|\Delta_K(-1)|$ and that of the jth coefficient $v_j(K)$ in the expansion of the Jones polynomial for $j=2$, 3, and 4. Symbols $3_1(+)$ and $3_1(-)$ denote the mirror images of the trefoil knot. Symbol $K_1\sharp K_2$ denotes the product (or the composite knot) of K_1 and K_2.

Knot K	$\lvert\Delta_K(-1)\rvert$	$v_2(K)$	$v_3(K)$	$v_4(K)$
$3_1(+)$	3	−12	60	−199
$3_1(-)$	3	−12	−36	−55
4_1	5	12	−12	31
$5_1(+)$	5	−36	276	−1365
$5_1(-)$	5	−36	−204	−645
$5_2(+)$	7	−24	168	−758
$5_2(-)$	7	−24	−120	−326
$3_1(+)\sharp 3_1(+)$	9	−24	120	−254
$3_1(+)\sharp 3_1(-)$	9	−24	24	−110
$3_1(-)\sharp 3_1(-)$	9	−24	−72	34
$3_1(+)\sharp 4_1$	15	0	48	−312
$3_1(-)\sharp 4_1$	15	0	−48	−168
$4_1\sharp 4_1$	25	24	−24	208

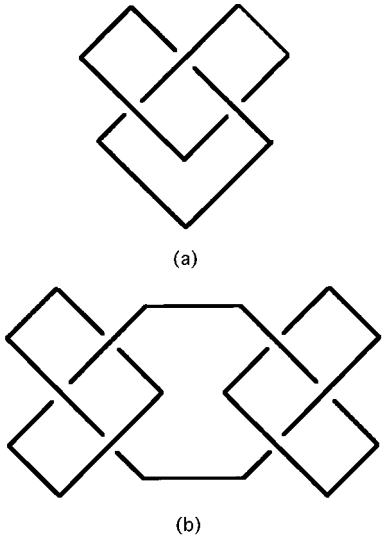

FIG. 1. (a) A diagram of prime knot 3_1 with 3 crossing points. (b) A diagram of composite knot $3_1\sharp 3_1$.

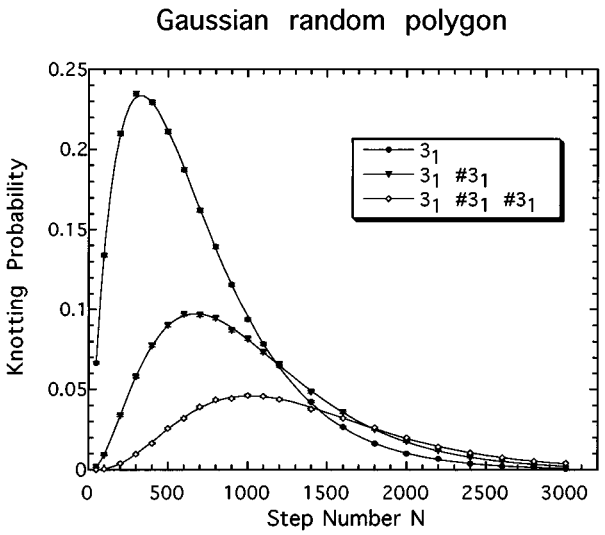

FIG. 3. Knotting probability of the Gaussian model for knots 3_1, $3_1\sharp 3_1$, and $3_1\sharp 3_1\sharp 3_1$.

sider two types of random polygon models, the Gaussian model [10] and the rod-bead model [12]. For the rod-bead model we change the bead radius r which describes the self-avoiding effect.

Let us explain our method for evaluating the knotting probability [16,22]. We first construct many configurations of an N-noded random polygon, for example, M configurations. For each one of the configurations we calculate both Vassiliev-type knot invariants of order less than 4 and the Alexander polynomial evaluated at $t=-1$, and then we practically enumerate the number M_K of those configurations that have the same knot type K: for a given configuration C we search such a knot K_1 that has the same set of values of the invariants with that of C, and we assume that the knot type K of C is given by the knot K_1. We evaluate the knotting probability $P_K(N)$ by the ratio M_K/M.

The Alexander polynomial $\Delta_K(t)$ is a topological invariant (isotopy invariant) of knots and links, which is given by a Laurent polynomial of variable t [27]. For the knot K, we call $|\Delta_K(-1)|$ the determinant of the knot. We can calculate the Alexander polynomial in polynomial time with respect to the number S of the double points of a given link diagram, since the invariant is defined as a determinant of an $S\times S$ matrix [27]. In the previous numerical works [9–14], all the authors employed the Alexander polynomial evaluated at special values of t, in particular, the determinant of the knot. It seems that the determinant of the knot $|\Delta_K(-1)|$ was the only known invariant practically useful for search of the knot types of large polygons.

Vassiliev-type (or finite-type) invariants are topological invariants of knots and links defined by some recurrence relations [28,29]. It is known that the coefficients of the quasiclassical expansion of the link polynomials associated with the quantum groups give Vassiliev-type invariants [28]. Let $V_K(q)$ denote the Jones polynomial of a knot K [23]. Its quasiclassical expansion is given by the expansion around $q=1$,

$$V_K(q)=1+v_2(K)\epsilon^2+v_3(K)\epsilon^3+v_4(K)\epsilon^4+\cdots, \quad (2)$$

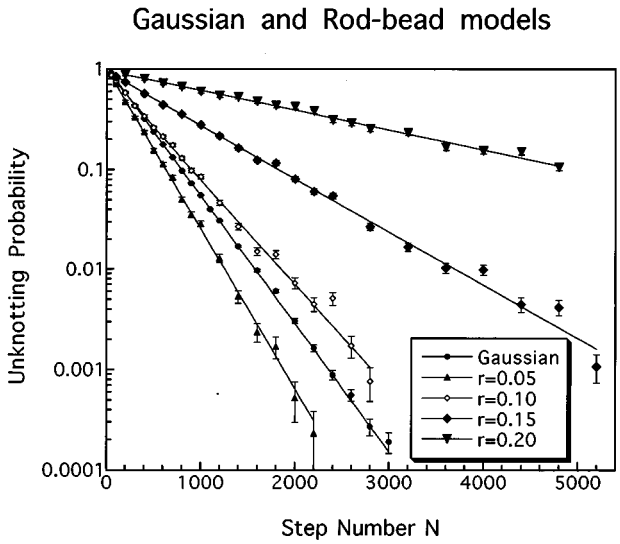

FIG. 2. Semilogarithmic plot of the unknotting probability versus step number N (the number of nodes N) for the Gaussian model and the rod-bead models with $r=0.05$, 0.10, 0.15, and 0.20.

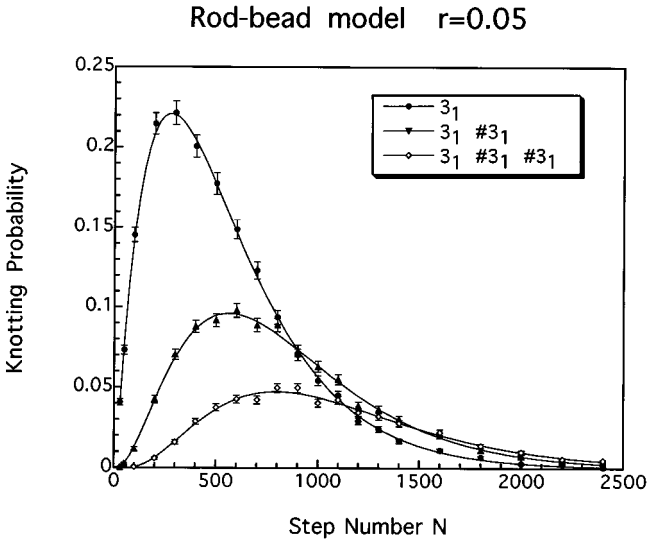

FIG. 4. Knotting probability in the case of the rod-bead model with $r=0.05$, for knots 3_1, $3_1\sharp 3_1$, and $3_1\sharp 3_1\sharp 3_1$.

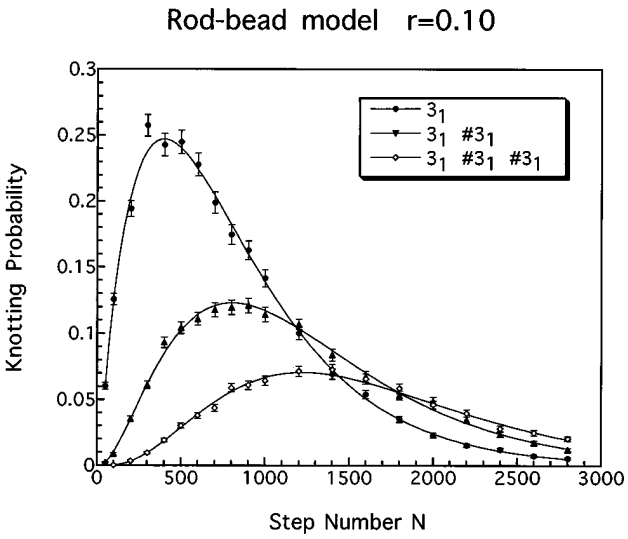

FIG. 5. Knotting probability in the case of the rod-bead model with $r=0.10$, for knots 3_1, $3_1\#3_1$, and $3_1\#3_1\#3_1$.

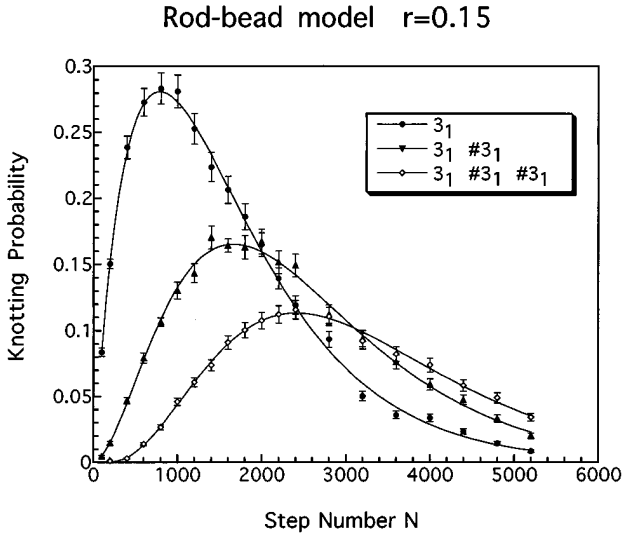

FIG. 6. Knotting probability in the case of the rod-bead model with $r=0.15$, for knots 3_1, $3_1\#3_1$, and $3_1\#3_1\#3_1$.

where $\epsilon=q-1$. The coefficients $v_2(K)$, $v_3(K)$, and $v_4(K)$ give Vassiliev-type invariants of order 2, 3, and 4, respectively.

Utilizing oriented state sum models we can calculate the Vassiliev-type invariants derived from the quasiclassical expansion of quantum link invariants [16,22]. The method has the following advantages: (i) we can calculate the invariants in polynomial time with respect to N, and (ii) we can calculate them without using a large memory area. We note that there are other methods for polynomial-time computation of

TABLE II. The estimates of $m(K)$, $C(K)$, $N(K)$, $N_{ini}(K)$, and the χ^2 values of the fitting curves to the data of $P_K(N)$ for the Gaussian model and the rod-bead models with $r=0.05$, 0.10, 0.15, and 0.20. For the rod-bead model with $r=0.20$ the order of the values of $N(K)$ and $N_{ini}(K)$ is given by 10^3. For the other models it is given by 10^2, e.g., $N(0)=340\pm4$ for the Gaussian model. The parameters of the fitting curves in Figs. 2–6 are given here.

Knot K	$m(K)$	$C(K)$	$N(K)\times10^{-2}$	$N_{ini}(K)\times10^{-2}$	χ^2
	Gaussian random polygon (22 data points)				
0	-0.0051 ± 0.0190	1.05 ± 0.87	3.40 ± 0.04	-0.01 ± 2.84	37
3_1	0.888 ± 0.024	0.631 ± 0.004	3.50 ± 0.04	0.19 ± 0.02	24
4_1	0.91 ± 0.05	0.130 ± 0.002	3.49 ± 0.09	0.28 ± 0.04	30
$3_1\#3_1$	1.85 ± 0.05	0.198 ± 0.005	3.51 ± 0.05	0.24 ± 0.04	16
$3_1\#4_1$	1.90 ± 0.07	0.078 ± 0.003	3.49 ± 0.08	0.27 ± 0.06	26
$3_1\#3_1\#3_1$	2.80 ± 0.11	0.042 ± 0.005	3.54 ± 0.09	0.23 ± 0.12	20
	Rod-bead model with $r=0.05$ (21 data points)				
0	0.00 ± 0.10	1.0 ± 51.0	2.7 ± 0.2	0.0 ± 136.0	16
3_1	0.98 ± 0.09	0.60 ± 0.02	2.7 ± 0.1	0.1 ± 0.1	16
4_1	1.1 ± 0.2	0.12 ± 0.01	2.5 ± 0.2	0.2 ± 0.1	14
$3_1\#3_1$	1.9 ± 0.2	0.19 ± 0.02	2.8 ± 0.2	0.2 ± 0.1	13
$3_1\#4_1$	2.1 ± 0.3	0.070 ± 0.015	2.7 ± 0.3	0.0 ± 0.2	14
$3_1\#3_1\#3_1$	2.4 ± 0.4	0.065 ± 0.019	3.1 ± 0.3	0.6 ± 0.3	13
	Rod-bead model with $r=0.10$ (20 data points)				
0	-0.08 ± 0.26	1.1 ± 1.6	4.2 ± 0.4	-0.1 ± 6.2	32
3_1	0.91 ± 0.10	0.67 ± 0.02	4.2 ± 0.2	0.2 ± 0.1	14
4_1	0.8 ± 0.2	0.12 ± 0.01	4.4 ± 0.4	0.3 ± 0.1	17
$3_1\#3_1$	1.8 ± 0.2	0.26 ± 0.02	4.4 ± 0.3	0.3 ± 0.1	16
$3_1\#4_1$	1.8 ± 0.2	0.094 ± 0.011	4.4 ± 0.4	0.3 ± 0.2	18
$3_1\#3_1\#3_1$	2.6 ± 0.3	0.079 ± 0.023	4.4 ± 0.5	0.6 ± 0.3	12
	Rod-bead model with $r=0.15$ (20 data points)				
0	-0.01 ± 0.10	0.9 ± 2.2	8.2 ± 0.5	-0.1 ± 19.3	27
3_1	0.90 ± 0.11	0.76 ± 0.03	8.5 ± 0.5	0.2 ± 0.3	23
4_1	0.9 ± 0.2	0.10 ± 0.01	8.5 ± 0.9	0.3 ± 0.5	6
$3_1\#3_1$	2.0 ± 0.2	0.30 ± 0.04	8.3 ± 0.6	-0.1 ± 0.4	10
$3_1\#4_1$	1.9 ± 0.3	0.082 ± 0.017	8.5 ± 1.0	0.1 ± 0.7	18
$3_1\#3_1\#3_1$	2.7 ± 0.5	0.11 ± 0.05	8.3 ± 1.1	1.4 ± 1.0	14
	Rod-bead model with $r=0.20$ (20 data points)				
Knot K	$m(K)$	$C(K)$	$N(K)\times10^{-3}$	$N_{ini}(K)\times10^{-3}$	χ^2
0	0.01 ± 0.35	1.0 ± 6.5	2.2 ± 0.6	-0.1 ± 13.1	15
3_1	0.9 ± 0.2	0.84 ± 0.04	2.3 ± 0.5	0.0 ± 0.1	8
$3_1\#3_1$	2.1 ± 0.4	0.38 ± 0.14	2.2 ± 0.7	0.0 ± 0.1	36

certain knot invariants [25,26].

We should note that the fact that two knots have the same value of a certain computable knot invariant does not imply that they are topologically equivalent. If we combine several independent knot invariants together, then we can determine the knot type of a given polygon more exactly. For instance, the determinant of the knot has the same value 5 for knots 4_1 and 5_1, while the Vassiliev-type invariant $v_2(K)$ gives different values for them (see Table I and Fig. 1).

Let us discuss the numerical results. For a given step number N we have constructed 10^5 polygons for the Gaussian model ($M=10^5$), and 10^4 polygons for each of the rod-bead models ($M=10^4$). For the Gaussian polygon we make use of the conditional probability distribution of the jth step ($1 \leqslant j \leqslant N$) [10]. For the rod-bead models, we first construct $2M$ chains with step number $N/2$ by the dimerization method, and then make M polygons with N (or $N+1$) nodes by the concatenating procedure [12].

In Fig. 2, the unknotting probabilities for the Gaussian model and the rod-bead models with four different values of the bead radius $r=0.05$, 0.10, 0.15, and 0.20 are shown. The error bars denote the standard deviations. For the Gaussian model the errors are estimated by applying the binomial distribution to the number M_K of polygons of knot K. For the rod-bead models we estimate the variance of $P_K(N)$ of knot K by the sum of the contribution due to the fluctuation of M_K and that of the weights in the concatenating procedure. From Fig. 2 we confirm the exponential decay of $P_0(N)$ for the rod-bead model shown by Koniaris and Muthukumar [14].

We now consider the case of nontrivial knots. For knots 3_1, $3_1\sharp 3_1$, and $3_1\sharp 3_1\sharp 3_1$, the data of the knotting probabilities $P_K(N)$ are plotted against the step number N for the Gaussian polygon and the three rod-beam models with $r=0.05$, 0.10, and 0.15 in Figs. 3, 4, 5, and 6, respectively. From Figs. 3–6 we find that the theoretical curves given by formula (1) fit well to the numerical data.

Table II gives the least-squares estimates of the parameters $C(K)$, $m(K)$, $N(K)$, and $N_{ini}(K)$ together with the χ^2 values of the fitting curves. The χ^2 values are consistent with the above observation that the fitting curves are good. The error estimates in Table II correspond to 68.3% confidence intervals. For the trivial knot the errors of $C(0)$ and $N_{ini}(0)$ do not make sense since $m(0) \cong 0$; we consider only those of $N(0)$ and $m(0)$, which are not too large.

From the estimates of $N(K)$ in Table II we see that for each of the models the parameter $N(K)$ of any knot K is almost equal to that of the trivial knot $[N(0)]$ with respect to the confidence intervals, where $N(0)$ gives different values to the different models. From Table II we also find that the parameter $m(K)$ of any knot K does not change for the Gaussian model or the rod-bead models with the different bead radii, with respect to the error bars.

The fitting variable $N_{ini}(K)$ is important when N is small [i.e., for $N<N(0)$] [4]. When N is large, however, it seems that $N_{ini}(K)$ does not change the fitting curves very much. In fact, the fitting curves in this paper are consistent with those of the previous work [16–18] that were given by formula (1) with $N_{ini}(K)=0$.

From all the numerical results, we suggest that formula (1) of the knotting probability $P_K(N)$ can be applied to any model of a random polygon with $N(K)=N(0)$ for any knot K where $N(0)$, $N_{ini}(K)$, and $C(K)$ are model dependent, and that given a knot K, the exponent $m(K)$ should be universal: for any random polygon model $m(K)$ is given by the same value and is determined only by the knot K. The exponent $m(K)$ should be important to the topological entanglement effect on the entropy of the ring polymer.

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