

## Average size of random polygons with fixed knot topology

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We have evaluated by numerical simulation the average size  $R_K$  of random polygons of fixed knot topology  $K = \emptyset, 3_1, 3_1 \# 4_1$ , and we have confirmed the scaling law  $R_K^2 \sim N^{2\nu_K}$  for the number  $N$  of polygonal nodes in a wide range;  $N = 100$ – $2200$ . The best fit gives  $2\nu_K \approx 1.11$ – $1.16$  with good fitting curves in the whole range of  $N$ . The estimate of  $2\nu_K$  is consistent with the exponent of self-avoiding polygons. In a limited range of  $N$  ( $N \geq 600$ ), however, we have another fit with  $2\nu_K \approx 1.01$ – $1.07$ , which is close to the exponent of random polygons.

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### I. INTRODUCTION

The topology of polymers is an important issue in understanding the physical properties of polymer materials, such as the viscoelasticity of polymer solutions [1]. It is also relevant to fundamental problems in biology [2]; the enzymes can cut and reconnect DNA strands, which are crucial functions in the mechanism of the complex processes of reproduction, transcription and recombination of DNA strands [3]. The topology of DNA rings can be used as a probe to detect the action of the enzymes on the DNA strands by observing the change of their knot type. The recent experimental observation [4] reports that the average polymer size depends on the topology of polymers.

One important quantity in the study of ring polymers is their average size with fixed knot type. This quantity has been estimated in several numerical methods [5–12]. The renormalization group argument leads to the power law scaling for the average size of linear polymers as their length increases [13–15],

$$R^2(N) = AN^{2\nu}(1 + BN^{-\Delta} + \dots), \quad (1)$$

where  $N$  is the number of segments, and  $R^2(N)$  is the mean square size of polymers. The same scaling law should hold for ring polymers without topological constraint with the same value of the exponent  $\nu$ . It is commonly accepted that the size of ring polymers with fixed knot topology  $K$  is given by the same scaling relation as Eq. (1),

$$R_K^2(N) = A_K N^{2\nu_K}(1 + B_K N^{-\Delta_K} + \dots). \quad (2)$$

This conjecture is supported by numerical simulations [7–12].

The scaling law of form (1) has already been discussed in connection with random walks (RW) and self-avoiding walks (SAW). Closed paths of RW and SAW are, respectively, random polygons and self-avoiding polygons (SAP). The exponents in these two cases are well established:  $\nu_{RW} = \frac{1}{2}$  and  $\nu_{SAW} \approx 0.588$  [16,17]. The central question regarding the

scaling (2) is: What is the value of  $\nu_K$ ? Is  $\nu_K$  related to either  $\nu_{RW}$  or  $\nu_{SAW}$ ? Note that the exponent  $\nu_K$ , or the coefficient  $A_K$  or  $B_K$ , should depend on the knot type  $K$ .

It has been found by numerical analysis that, in the case of SAP, the exponent  $\nu_K$  does not depend on the knot type  $K$ , and is given by  $\nu_{SAW}$  [7,8]. The question is then whether the effect of topology appears in  $A_K$  or at the level of correction to scaling (2), i.e., in  $B_K$  [18]. Simulations by van Rensburg and co-workers [7,8] support the conjecture that knot topology does not affect coefficient  $A_K$ .

For the model of random closed curves, des Cloizeaux made the conjecture that the constraint of topology should lead effectively to the growth of their average size, so called the “topological excluded volume effect,” even though it has no excluded volume interactions [19]. It is predicted that exponent  $\nu_\emptyset$  for polymers with trivial knot topology  $\emptyset$  obeys  $\nu_\emptyset \leq \nu_{SAW}$ . Deutsch has performed a simulation for random polygons in the case of trivial knot  $\emptyset$  and obtained the value of  $\nu_\emptyset$  consistent with this inequality [9]. The conjecture is also supported by a phenomenological argument [20] for  $\emptyset$  and other knots.

Recently, Shimamura and Deguchi have evaluated the exponent  $\nu_K$  for the radius of gyration for knot types  $\emptyset, 3_1$ , and  $4_1$  in the case of the Gaussian random polygons [11]. Taking into account the correction term in scaling (2), they have found that the fit gives  $\nu_K \approx \nu_{RW}$ .

In this paper, we reexamine the radius of gyration for random polygons. For the topological effect on the size of random polygons, two different answers have been presented. Furthermore, other possibilities are not excluded. The topological effect should also be investigated in different models. We employ the pivot algorithm which is a modification of the original one [9] so that the possible bias is reduced. The simulation procedure used in Ref. [9], which is a kind of pivot algorithm [21,22] for continuum models, tends to pick up extended conformation more frequently. It is conceivable that this bias leads to an artificial expansion of chains and raises the exponent  $\nu_K$  from  $\nu_{RW}$ . We have evaluated the radii of gyration for the range of chains  $N$

=100–2200 for three knot types: trivial knot, trefoil knot, and composite knot, denoted by  $\emptyset$ ,  $3_1$ , and  $3_1\#4_1$ . Here,  $3_1$  and  $4_1$  are the first two simplest knots, while trivial knot  $\emptyset$  is the unknotted polygon. The shapes  $3_1$  and  $4_1$  can be pictured on paper to look like a trefoil and figure eight, respectively. A concatenation of two knots,  $3_1$  and  $4_1$ , makes composite knot  $3_1$  shape  $4_1$ . In the case of  $\emptyset$ , our improved algorithm has given a result consistent with that of Ref. [9]. We have further results in other cases.

We have found two good fits to our simulation data. The best fit gives  $2\nu_K \approx 1.11$ – $1.16$ . It is consistent with  $\nu_{SAW}$ , which also agrees with the result of Deutsch:  $\nu_{\emptyset} \approx 1.17$  [9]. The second fit gives  $2\nu_K \approx 1.01$ – $1.07$ , which is in accordance with  $\nu_{RW}$ . The first fit gives good fitting curves for the whole range of  $N$  investigated in simulation:  $N = 100$ – $2200$ .

## II. MODEL

We consider random polygons in three dimensions, consisting of  $N$  line segments of length  $a$ . We call them  $N$ -node polygons. We assume that the polygons have no excluded volume. It means that the nodes and segments of the polygon are purely geometrical points and line segments, respectively [9]. This model may be regarded as a model for polymers at the  $\theta$  point or a polymer in a melt.

A polygon  $\mathcal{P}_N$  is defined by the set of position vectors of its nodes,  $\mathcal{P}_N = (R_1, R_2, \dots, R_N)$ . All cyclic permutations of one position vectors correspond to the same polygon. The vectors satisfy the geometrical constraint  $|R_{i+1} - R_i| = a$  for  $1 \leq i \leq N$  ( $R_{N+1} = R_1$ ). Each polygon is topologically equivalent to a knot  $K$  in three dimensions. The configuration space  $\mathcal{C}$  of the model is divided into subspaces  $\mathcal{C}_K$  in which all polygons have a fixed knot type  $K$ ,  $\mathcal{C} = \sum_K \mathcal{C}_K$ .

The radius of gyration of polygons is given by

$$R^2(\mathcal{P}_N) = \frac{1}{2N^2} \sum_{i,j=1}^N (R_i - R_j)^2. \quad (3)$$

This definition is different from that of the polygon size employed in Ref. [9] but their asymptotic behaviors in the limit of large  $N$  are the same. We set the segment length  $a$  to unity; macroscopic properties are independent of the microscopic parameter  $a$ .

We generate a large number  $M$  of polygons with length  $N$ . They are used to evaluate the mean square size of polygons without topological constraint,

$$R^2(N) = \frac{1}{M} \sum_{i=1}^M R^2(\mathcal{P}_{N,i}), \quad (4)$$

and the same quantities for fixed knot topology,

$$R_K^2(N) = \frac{1}{M_K} \sum_{i=1}^M R^2(\mathcal{P}_{N,i}) \chi(\mathcal{P}_{N,i}, K). \quad (5)$$

Here the indicator function  $\chi(\mathcal{P}, K)$  takes value 1 if  $\mathcal{P} \in \mathcal{C}_K$  and zero otherwise. The number of polygons,  $M_K$ , with fixed topology  $K$  is  $M_K = \sum_i \chi(\mathcal{P}_{N,i}, K)$ .

We are concerned with the scaling relation

$$\frac{R_K^2}{R^2} = \frac{A_K}{A} N^{2\Delta\nu_K} [1 + \Delta B_K N^{-1/2} + O(N^{-1})], \quad (6)$$

where  $\Delta\nu_K = \nu_K - \nu$ ,  $\Delta B_K = B_K - B$ . It follows from the scaling laws (1) and (2) with  $\Delta = \Delta_K = 1/2$  [8]. We perform the fit simulation data using Eq. (2)

## III. SIMULATION PROCEDURE

Our sampling of the polygons follows the dynamic Monte Carlo method using the pivot algorithm [21,22], applied to the continuum model by Deutsch [9]. In the continuum model, a pivot move for a polygon is a rotation of a chain of segments randomly chosen from the polygon around the axis passing the two endmost nodes of the chain by a random amount of angle  $\theta$ .

In practice the method used in Ref. [9] imposes two restrictions on pivot moves: (1) the banning of self-intersections during the move and (2) the range of angle  $\theta$ . There is a possibility that these may cause a virtual expansion of polygons due to these restrictions. The transformation process of the pivot move prohibits those moves in which self-intersections of polygonal segments occur. The angle  $\theta$  is selected from the range  $-90^\circ \leq \theta \leq 90^\circ$ , excluding rotations with  $\theta > 90^\circ$ . This tends to bring polygons to less folded conformations, and hence the polygon size is increased. Furthermore, the rotations are not completely randomly distributed over the range of  $\theta$ , since the rotations are limited to those which make no change of the knot topology.

In this paper, we modify the algorithm in two respects: We allow the selected chain of segments to rotate by an angle  $\theta$  between  $0^\circ$  and  $360^\circ$ . We do not check the self-intersections during the process of rotation of the chain. In addition, we neglect the possibility of self-intersections occurring in the configuration after a pivot move is completed, since such configurations are negligible in space  $\mathcal{C}$ .

With this algorithm, the topology of a polygon may change by a pivot move. We estimate the knot type of polygons by calculating several topological invariants [23], the value of the Alexander polynomial  $\Delta_K(t)$  at  $t = -1$  [24], and the Vassiliev invariants of the second and third order,  $v_2(K)$  and  $v_3(K)$ , respectively [25]. The chance of miss identification is negligible for the simple knots we are concerned with.

We choose a certain conformation of a polygon as an initial state of the Markov process. The mean deflection angle between adjacent segments is equal to  $90^\circ$  in the thermal equilibrium. We prepare seeds on the cubic lattice as an equilibrium conformation of a polygon, exploiting the method used for the SAP on the cubic lattice [26]. Starting from a seed, we generate a sequence of polygons by applying the pivot moves repeatedly. After discarding the initial 2000 transient conformations, we take samples of polygons at every 200 pivot moves.

The simulation has been performed for polygons with

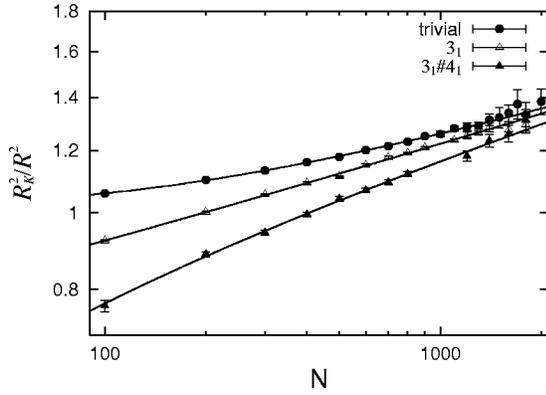


FIG. 1. Simulation data on the ratios  $R_K^2/R^2$  for the knot types  $\emptyset$ ,  $3_1$ ,  $3_1\#4_1$  and the best fit curves (solution 1) using Eq. (6). The scales are double logarithmic.

length  $N$  between 100 and 2200 and for each of three knot types  $\emptyset$ ,  $3_1$ , and  $3_1\#4_1$ . We have collected  $10^5$  polygons for each given length  $N$  and for each given knot type, and we have evaluated the radii of gyration (4) and (5). We put a lower bound  $N_{min}$  in fitting the simulation results using the scaling formula (6). Thus we make the fit in the range  $N_{min} \leq N \leq N_{max} (=2200)$ , varying the value of  $N_{min}$  from 100 to 600.

#### IV. RESULTS OF THE SIMULATION

We now discuss the results of our simulation for the three knot types. The best fit curve for each knot type together with the data on the ratio  $R_K^2/R^2$  are shown in Fig. 1. We have found that the scaling relation (6) fits the simulation data very well for all three cases in the range of  $N$  from  $N_{min} \geq 100$  to  $N_{max} = 2200$ . The estimated values of the parameters in (6) are shown in Table I. The  $\chi^2$  values remain small,  $\chi^2 \approx 1-2$  per datum, even if  $N_{min}$  is lowered to 100. In the case of  $3_1$ , however, the  $\chi^2$  values become small for  $N \geq 600$ .

The ratios  $R_K^2/R^2$  increase as functions of  $N$ , and they become larger than that for large  $N$ . The same behavior has been observed in other models, such as the Gaussian random polygon model [11] and the cylindrical SAP model [12]. The above observation tells that the average size of polygons grows due to the topological constraint. The exponents  $\nu_K$  obtained in the fit are insensitive to the change of  $N_{min}$ , showing the validity of the scaling relation  $R_K^2 \approx N^{2\nu_K}$ . The resulting values  $2\nu_K \approx 1.11-1.16$  are consistent with  $\nu_{SAW}$ , supporting the assertion in papers [9,19].

We have found another optimal fit to our simulation data, as shown in Fig. 2. The curves represent the second fit in which only data for  $N \geq 600$  are used in Fig. 2. The estimated values of the parameters are given in Table II. The  $\chi^2$  values for these fits grow rapidly as  $N_{min}$  is lowered less than about 400. It implies that formula (6) does not give a good approximation in the range  $N \leq 400$ .

The second solution implies that the asymptotic behavior of the average size of polygons is scarcely affected by the topological constraint. It gives  $2\nu_K \approx 1.01-1.07$ , which is not much different from  $2\nu = 1$ . Another noticeable differ-

TABLE I. The value of the parameters of the scaling relation (6) of the ratio  $R_K^2/R^2$  obtained from the best fit.

$N_{min}$	$A_{\emptyset}/A$	Trivial/all $\Delta B_{\emptyset}$	$2\Delta\nu_{\emptyset}$	$\chi^2$
100	$0.471 \pm 0.014$	$2.197 \pm 0.159$	$0.133 \pm 0.004$	0.86
200	$0.405 \pm 0.027$	$3.172 \pm 0.429$	$0.151 \pm 0.008$	0.69
400	$0.376 \pm 0.079$	$3.779 \pm 1.619$	$0.159 \pm 0.024$	0.70
600	$0.242 \pm 0.154$	$7.812 \pm 6.457$	$0.207 \pm 0.068$	0.679
$N_{min}$	$A_{3_1}/A$	$3_1$ /all $\Delta B_{3_1}$	$2\Delta\nu_{3_1}$	$\chi^2$
100	$0.494 \pm 0.030$	$0.258 \pm 0.269$	$0.130 \pm 0.008$	6.26
200	$0.455 \pm 0.064$	$0.722 \pm 0.782$	$0.140 \pm 0.017$	6.56
400	$0.624 \pm 0.221$	$-1.281 \pm 1.973$	$0.104 \pm 0.0420$	6.54
500	$0.578 \pm 0.262$	$-1.041 \pm 2.683$	$0.114 \pm 0.053$	5.15
600	$0.793 \pm 0.277$	$-2.417 \pm 2.022$	$0.074 \pm 0.041$	1.30
$N_{min}$	$A_{3_1\#4_1}/A$	$3_1\#4_1$ /all $\Delta B_{3_1\#4_1}$	$2\Delta\nu_{3_1\#4_1}$	$\chi^2$
100	$0.460 \pm 0.048$	$-1.229 \pm 0.443$	$0.140 \pm 0.013$	1.68
200	$0.389 \pm 0.064$	$-0.369 \pm 0.831$	$0.160 \pm 0.020$	1.52
400	$0.378 \pm 0.159$	$-0.110 \pm 2.559$	$0.163 \pm 0.049$	1.64
600	$0.293 \pm 0.335$	$1.670 \pm 8.634$	$0.192 \pm 0.128$	1.46

ence is in the value of  $A_K/A$ .  $A_K/A < 1$  for the solution 1, whereas  $A_K/A \approx 1$  for solution 2.

If we assume  $A_K/A = 1$ , then the effect of the topological constraint could only appear in the coefficients  $B_K$ . It is noted that the sign of  $\Delta B_K$  is negative for each knot type with large statistical errors. This observation supports the result derived by the perturbation argument in the limit of large characteristic length of random knotting [27].

Let us explicitly discuss physical implications of the present numerical result; both  $\nu_{SAW}$  and  $\nu_{RW}$  are consistent with the simulation data. The fitting curves with  $\nu_{SAW}$  are better at describing the data points. However, we could not consider it as the conclusion of the present study, since  $\nu_{RW}$  is also consistent with the same data. The numerical analysis

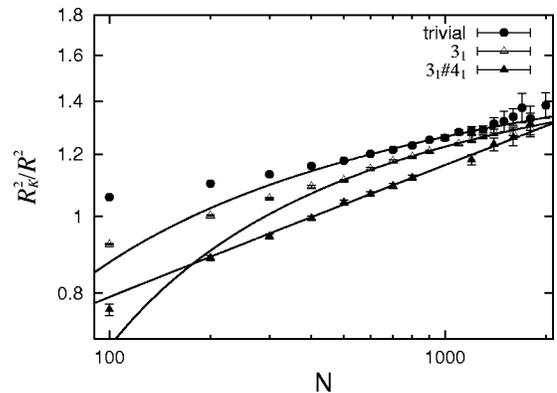


FIG. 2. Simulation data on the ratio  $R_K^2/R^2$  for the knot types  $\emptyset$ ,  $3_1$ ,  $3_1\#4_1$  and the curves of the second optimal fit (solution 2) using Eq. (6). The curves represent the second fit in which only data for  $N \geq 600$  are used.

TABLE II. The value of the parameters of the scaling relation (6) of the ratio  $R_K^2/R^2$  obtained from the best fit.

$N_{min}$	$A_{\emptyset}/A$	Trivial/all $\Delta B_{\emptyset}$	$2\Delta\nu_{\emptyset}$	$\chi^2$
200	$1.720 \pm 0.464$	$-3.731 \pm 0.915$	$-0.029 \pm 0.035$	49.42
400	$1.736 \pm 0.585$	$-4.820 \pm 1.37$	$-0.023 \pm 0.042$	7.24
500	$1.359 \pm 0.270$	$-5.345 \pm 0.844$	$0.012 \pm 0.024$	1.91
600	$1.203 \pm 0.514$	$-3.884 \pm 2.214$	$0.026 \pm 0.050$	1.66
$N_{min}$	$A_{3_1}/A$	$3_1$ /all $\Delta B_{3_1}$	$2\Delta\nu_{3_1}$	$\chi^2$
200	$1.273 \pm 0.340$	$-3.867 \pm 0.941$	$0.012 \pm 0.034$	61.19
400	$1.117 \pm 0.370$	$-4.181 \pm 1.461$	$0.034 \pm 0.040$	9.17
500	$1.286 \pm 0.261$	$-5.107 \pm 0.882$	$0.019 \pm 0.025$	1.92
600	$1.095 \pm 0.360$	$-4.180 \pm 1.684$	$0.037 \pm 0.039$	1.50
$N_{min}$	$A_{3_1\#4_1}/A$	$3_1\#4_1$ /all $\Delta B_{3_1\#4_1}$	$2\Delta\nu_{3_1\#4_1}$	$\chi^2$
200	$0.926 \pm 0.306$	$-4.056 \pm 1.137$	$0.050 \pm 0.043$	12.22
400	$0.997 \pm 0.432$	$-4.992 \pm 1.787$	$0.047 \pm 0.053$	3.80
600	$0.877 \pm 0.827$	$-5.021 \pm 4.623$	$0.066 \pm 0.111$	2.67

suggests that the topological effect on the average size  $R_K$  of fixed knot  $K$  has not been understood completely, yet. In fact, the present numerical data are consistent with all the previous results, at least partially. The plots of Fig. 1 confirm the enhancement of the average size observed for the trivial knot in Ref. [9], and extend it to the case of the nontrivial knots. Furthermore, the fitting curves in Fig. 1 seem to be favorable to the scaling argument given in Ref. [20]. On the other hand, the fitting curves of Fig. 2 are consistent with those of Ref. [11] for the Gaussian random polygons.

The present numerical data also suggest that finite-size

effects should be significant for the average size  $R_K$  of knot  $K$ . For instance, the ratio  $R_K^2/R^2$  of the trefoil knot is smaller than 1.0 when  $N \leq 300$ , as shown in Figs. 1 and 2. We may consider it as a finite-size effect: the average size of random polygons with a nontrivial knot should be very small when length  $N$  is small, while the knot dependence of the average size  $R_K$  should become relatively less significant as the length  $N$  increases. Furthermore, the number about 300 may correspond to the characteristic length  $N_c$  of random knotting for the model of random polygons consisting of cylindrical segments in the case of zero cylinder radius [27].

To summarize, we have confirmed that the simulation data on the average size  $R_K$  of ring polymers can be fitted by the scaling relation (6). We have found two solutions. The best fit solution (solution 1) is good for  $100 \leq N \leq 2200$  with quite small  $\chi^2$  ( $\chi^2 \approx 1$ ) while the second solution (solution 2) becomes good for  $N_{min} \geq 600$ . The two solutions lead to two different interpretations regarding the effect of fixed knot topology on the average size of ring polymers as their length  $N$  increases. We may thus conclude that the topological effects of random polygons have not been completely understood, yet, probably due to the large finite-size effects. Further investigation should be necessary to understand completely the topological effects, which may be quite nontrivial and rather deep.

*Note added in proof.* Recently the authors came to know that results similar to ours had been obtained independently [28].

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