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LETTER TO THE EDITOR

Anomalous finite-size effects for the mean-squared gyration radius of Gaussian random knots

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Abstract
Anomalously strong finite-size effects have been observed for the mean square radius of gyration R_K^2 of Gaussian random polygons with a fixed knot K as a function of the number N of polygonal nodes. Through computer simulations with $N < 2000$, we find that the gyration radius R_K^2 can be approximated by a power law, $R_K^2 \sim N^{2\nu_K^{\rm eff}}$, for several knots, where the effective exponents $\nu_K^{\rm eff}$ are larger than 0.5 and less than 0.6. Furthermore, a crossover occurs for the gyration radius of the trivial knot, when N is roughly equal to the characteristic length N_c of random knotting. Assuming an asymptotic fitting formula, we also discuss possible asymptotic behaviours for R_K^2 of Gaussian random polygons.

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1. Introduction

Topological effects on statistical and dynamical properties of ring polymers should be quite nontrivial. The topological state of a ring polymer is described by a knot type, and it is invariant after its synthesis. Knotted ring polymers or knotted DNAs have been discussed theoretically since the 1960s [1, 2], and recently they have been synthesized in several experiments [3, 4]. Various topological effects on ring polymers have been explicitly studied through numerical simulations of random polygons under topological constraints [5–8]. However, many questions still remain unsolved, even on the average size of a knotted ring polymer in solution, which should be the most fundamental quantity in the physics of ring polymers.

Recently, it has been suggested [9–11] that the average size $R_{\rm triv}$ of a random polygon with the trivial knot should scale as N^ν with respect to the number N of polygonal nodes, where the exponent ν is given by the exponent $\nu_{\rm SAW}$ of the asymptotic scaling behaviour of the self-avoiding walk (SAW), where $\nu_{\rm SAW} \approx 0.588$. Here we remark that random polygons correspond to ring polymers with no excluded volume. There has also been a conjecture [9] that the effect of topology on the average size of ring polymers could play a similar role as the excluded-volume effect, since the topological constraint should effectively lead to an entropic repulsion among the monomer segments. Here, we note that the trivial knot (or the unknot) is such a knot that is equivalent to an unknotted circle.

The conjecture on the entropic repulsion seems to be quite interesting and the anomalous scaling behaviour with an enhanced exponent should be effective, at least for some numerical simulations. However, it is not trivial to understand the consequence that the scaling exponent should be enhanced and given by that of the SAW. Furthermore, it is quite nontrivial how the entropic repulsion could lead to finite-size properties on the graph of the average size R_{triv} versus N. The purpose of this letter is to discuss these questions through numerical simulations. We evaluate the mean square radius of gyration R_K^2 of Gaussian random polygons with a fixed knot type K. Discussing the N dependence of R_K^2 for several different knot types, we show that the anomalous scaling behaviour should be considered as a strong finite-size effect which could be valid for very large values of N, such as 2000.

We now review some relevant results on the topological effects of ring polymers. Let us take a model of random polygons of N nodes [6, 7], which describes ring polymers consisting of N Kuhn units at the theta condition. We denote by $P_K(N)$ the probability of a given configuration of the random polygon of N nodes having a fixed knot type K. For the trivial knot, it was numerically shown [7, 8, 12] that the probability is given by an exponential function of N: $P_{\mathrm{triv}}(N) = \exp(-N/N_c)$. For nontrivial knots, the probability is well described by the following function of N: $P_K(N) = C_K\,(N/N_c)^{m(K)} \exp(-N/N_c)$, where we call N_c and $m(K)$ the characteristic length of random knotting and the topological exponent of the knot, respectively [13]. The value of N_c is model-dependent and is roughly given by 340 for the Gaussian random polygon [8, 13]. We remark that the number N_c is important in the analysis of topological effects with the blob picture [11].

The mean-squared gyration radius R_K^2 under the topological constraint of a knot K has been discussed for some models of self-avoiding polygons (SAPs) in [14–20]. In the lattice model, it is shown that the asymptotic behaviour of R_K^2 is consistent with that of the RG theory where, in the large N limit, the ratio R_K^2/R^2 comes close to 1.0 for any knot. However, for the cylinder model of SAPs [21], it is found [20] that the limit of the ratio depends on the cylinder radius which controls the excluded volume. For a lattice model of random polygons [22], R_K^2 has been evaluated for the trivial and trefoil knots with small polygons of $N < 200$.

2. Anomalous finite-size behaviours

We have constructed $M = 10^5$ samples of the Gaussian random polygon with N nodes [6], where N is given by 20 different values from 50 to 1900. We determine the number M_K of polygons with a knot K, enumerating such polygons in the set of M polygons that have the same set of values of the two knot invariants: the determinant of the knot $\Delta_K(-1)$ and the Vassiliev invariant $v_2(K)$ of second degree [23, 24]. Then, for Gaussian random polygons, numerical estimates of R^2 and R_K^2 have been obtained for the four knots: the trivial, trefoil (3_1) and figure-of-eight (4_1) knots, and the composite knot consisting of two trefoil knots ($3_1\#3_1$). Some of them are shown in figures 1 and 2.

We recall that, under no topological constraint, the mean square radius of gyration R^2 of a random polygon with N nodes is defined by $R^2 = \sum_{n,m=1}^{N} \langle (\vec{R}_n - \vec{R}_m)^2 \rangle / 2N^2$. Here $\vec{R}_n$ is the position vector of the nth node and the symbol $\langle\cdot\rangle$ denotes the statistical average, which is given by the average over M polygons in the simulations. For a knot K, the quantity R_K^2 is

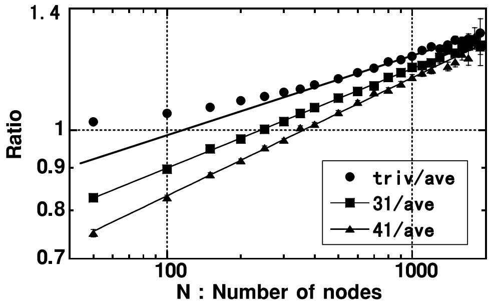

Figure 1. Logarithmic plot of the ratio R_K^2/R^2 versus the number N of polygonal nodes of the Gaussian random polygon for the range from $N = 50$ to 1900. Numerical estimates of R_K^2/R^2 for the trivial, trefoil (31) and figure-of-eight (41) knots are shown by black circles, black squares and black triangles, respectively.

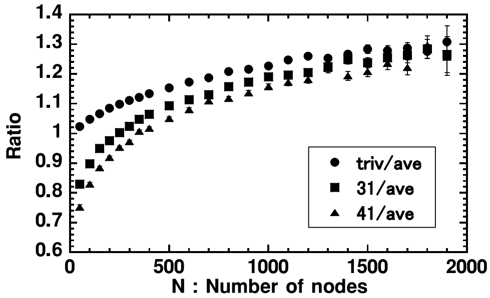

Figure 2. Linear plot of the ratio R_K^2/R^2 versus the number N of polygonal nodes of the Gaussian random polygon. Same symbols as in figure 1.

given by $R_K^2 = \sum_{i=1}^{M_K} R_{K,i}^2/M_K$, where $R_{K,i}^2$ denotes the gyration radius of the ith Gaussian random polygon that has the knot type K, in the set of M_K polygons. In terms of R_K^2, R^2 is given by $R^2 = \sum_K M_K R_K^2/M$.

We see in figure 1 that the ratio R_K^2/R^2 increases monotonically with respect to N for each of the four knots. For the trivial knot, the ratio R_{triv}^2/R^2 is always larger than 1.0. When N is large, however, the ratio R_K^2/R^2 also becomes greater than 1.0 for the other knots. Thus, the topological constraint gives an effective swelling for large N.

There is a nontrivial finite-size behaviour for the trivial knot: in figure 1, the ratio R_{triv}^2/R^2 increases very slowly when $N < N_c$ while, when $N > N_c$, it can be approximated by a scaling behaviour as $R_{\mathrm{triv}}^2/R^2 \sim N^{2\nu_{\mathrm{triv}}^{\mathrm{eff}}}$, at least up to $N = 2000$. This 'crossover phenomenon' should be consistent with the recent theory given by Grosberg [11]. However, the effective exponent $\nu_{\mathrm{triv}}^{\mathrm{eff}}$ is much smaller than the exponent ν_{SAW} with respect to the errors. In fact, we have the numerical estimate: $\nu_{\mathrm{triv}}^{\mathrm{eff}} \approx 0.545$.

For the case of nontrivial knots (3_1, 4_1, $3_1\#3_1$), the ratio R_K^2/R^2 is well approximated by the power law: $R_K^2/R^2 \approx \Gamma_K N^{2\Delta\nu_K^{\mathrm{eff}}}$ for the range from $N = 100$ to 2000. Furthermore, there is no crossover for the nontrivial knots: we do not find any change in the slope near $N \sim N_c$ for each of the graphs. It is also remarkable from table 1 that the exponent $\Delta\nu_K^{\mathrm{eff}}$ strongly depends on the knot type. In particular, the effective scaling exponent of the composite knot $3_1\#3_1$ is almost as large as the exponent ν_{SAW}, while that of the trefoil knot is given by 0.561, which is rather smaller than ν_{SAW} with respect to the errors.

Table 1. Best estimates for the fitting lines in figure 1 describing the anomalous scaling behaviour: $R_K^2/R^2 = \Gamma_K\, N^{2\Delta\nu_K^{\mathrm{eff}}}$. Here $\Delta\nu_K^{\mathrm{eff}} = \nu_K^{\mathrm{eff}} - \nu_{\mathrm{RW}}$. For the trivial knot, the fit is obtained from the data points with $N \geqslant 400$. For the trefoil (3_1) and figure-of-eight (4_1) knots, and the composite knot of $3_1\#3_1$, the fitting lines are obtained from the data for $N \geqslant 100$.

Knot type	Γ_K	$2\Delta\nu_K^{\mathrm{eff}}$	χ^2
triv/ave	0.600 ± 0.012	0.090 ± 0.003	6
tre/ave	0.514 ± 0.004	0.121 ± 0.001	14
4_1/ave	0.431 ± 0.006	0.143 ± 0.002	11
$3_1\#3_1$/ave	0.398 ± 0.005	0.153 ± 0.002	25

The three fitting lines of figure 1 become very close to each other at around $N = 2000$. We see in figure 2 that, when N becomes close to 2000, the values of R_K^2 for the four knots (K = trivial, 3_1, 4_1 and $3_1\#3_1$) should become almost equal to each other. In fact, up to $N = 1900$, the values of R_K^2 for the nontrivial knots are always smaller than or equal to that of R_{triv}^2 in our simulations. If the power-law approximation might be valid also for $N > 2000$, then R_{triv}^2 would become much smaller than R_K^2 for the three nontrivial knots for large N and it would be inconsistent with the numerical results obtained so far. Thus, we may conclude that the approximation of R_K^2 by the power law should be valid only when $N < 2000$. Therefore, in order to study the N dependence of R_K^2 for $N > 2000$, we need another independent analysis.

3. Asymptotic behaviour of R_K^2

Let us discuss a possible asymptotic behaviour of R_K^2 through the following expansion: $R_K^2 = A_K N^{2\nu_K}(1 + B_K N^{-\Delta} + \mathrm{O}(1/N))$. It may be nontrivial to assume it for the Gaussian polygons with $N < 2000$, since there are various finite-size effects as discussed in section 2. Furthermore, in the case of cylindrical SAPs, a large-N plateau region appears in the graph of R_K^2/R^2 versus N [20, 25] for any of the knots, while in figure 2 the plateau tendency is not very clear when $N < 2000$. However, we discuss the best estimates given by the formula, since they are quite useful in comparing the data of R_K^2 of Gaussian polygons with those of other models. In fact, the formula is quite effective for R_K^2 of the lattice SAPs [17, 19] and the cylindrical SAPs [20, 25].

For each of the four knots, we have applied the asymptotic formula to the 13 data points of the ratio R_K^2/R^2 with $N \geqslant 700$ shown in figures 1 and 2, and we have obtained the estimates of $\Delta\nu_K = \nu_K - \nu_{\mathrm{RW}}$, where $\nu_{\mathrm{RW}} = 0.5$. Here, we assign the condition of $N \geqslant 700$, considering the strong finite-size effects of R_K^2 such as the crossover of the trivial knot.

The best estimates of the fitting parameters and the χ^2 values are listed in table 2. From the results, we may conclude that the asymptotic expansion is consistent with the numerical values of R_K^2 for $N \geqslant 700$. It is remarked that the χ^2 values in table 2 are less than 20 for the four knots. Moreover, the best estimates are compatible with several different viewpoints. For instance, the estimate of $2\Delta\nu_K$ is given by about 0.03 and is independent of the knot type. This leads to an estimate of the exponent, $\nu_K \approx 0.515$, which could be consistent with the exponent ν_{RW} with respect to the errors of the analysis. The fact that the exponent ν_K is independent of the knot type is consistent with the interpretation on the lattice model of [17, 19]. The estimated values of the amplitude ratio A_K/A for the four knots also seem to be independent of the knot type.

Let us consider a formula which effectively describes the N dependence of R_K^2 for $N > 2000$. Assuming $\nu_K = \nu_{\mathrm{RW}}$ in the asymptotic expansion, we have the following: $R_K^2/R^2 = \alpha_K(1 + \beta_K\, N^{-\Delta} + \mathrm{O}(1/N))$. Here we have replaced by α_K and β_K, A_K/A

Table 2. Best estimates of the fitting parameters of the asymptotic formula: $R_K^2/R^2 = (A_K/A)N^{2\Delta\nu_K}(1 + (B_K - B)N^{-\Delta})$. Here $\Delta\nu_K = \nu_K - \nu_{\mathrm{RW}}$. We set $\Delta = 0.5$.

Knot type	A_K/A	$B_K - B$	$2\Delta\nu_K$	χ^2
triv/ave	1.146 ± 0.838	-3.628 ± 4.151	0.028 ± 0.084	4
tre/ave	1.122 ± 0.526	-4.973 ± 2.468	0.033 ± 0.054	11
4_1/ave	1.112 ± 1.102	-5.232 ± 5.113	0.032 ± 0.115	12
$3_1\#3_1$/ave	1.115 ± 0.313	-5.952 ± 1.404	0.034 ± 0.033	13

Table 3. Best estimates of the fitting parameters of the formula effectively describing the large-N behaviour of the ratio: $R_K^2/R^2 = \alpha_K\,(1 + \beta_K\,N^{-\Delta})$.

Knot type	α_K	β_K	χ^2
triv/ave	1.459 ± 0.018	-4.925 ± 0.308	4
tre/ave	1.486 ± 0.012	-6.335 ± 0.198	12
4_1/ave	1.460 ± 0.025	-6.517 ± 0.414	8
$3_1\#3_1$	1.495 ± 0.007	-7.283 ± 0.121	13

and $B_K - B$, respectively. Applying the formula to the numerical data of R_K^2 of the Gaussian random polygon for $N \geqslant 700$, we see that it gives good fitting curves to the data. The best estimates of the parameters are shown in table 3. Interestingly, they are rather close to the best estimates for the cylinder model of SAPs with a very small cylinder radius, which are obtained by applying the same formula to the data of R_K^2 in [20]. In table 3, the parameter α_K is roughly given by 1.5 for the Gaussian random polygon. On the other hand, we have the similar value for the cylinder model with the cylinder radius $r = 0.001$, as shown in figure 3 of [20]. We also find in table 3 that $\alpha_K \approx 1.5$ for the four knots. It follows that the mean size R_K of random polygons with a specified knot K, such as the trivial, 3_1, 4_1 and $3_1\#3_1$ knots, is larger than the average size R of random polygons over all knots in the asymptotic regime. However, it is consistent with the observation in figure 1 that the ratio R_K^2/R^2 increases monotonically and approaches 1.3 or 1.4 when $N \sim 2000$ (see also [20]).

4. Conclusion

We have shown that R_K^2 of Gaussian random polygons have strong finite-size effects which should be valid for extremely large values of N, such as $N = 2000$. Thus, the studies [9–11] associated with the conjecture of effective entropic repulsion should be important for describing the strong finite-size effects of random polygons, which could appear practically in any system of ring polymers in solution at the theta condition.

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