Anomalous finite-size effects and canonical asymptotic behaviors 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 $R^2_K$ 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 for several knots that the gyration radius $R^2_K$ can be approximated by a power law: $R^2_K \sim N^{2\nu_{K}^{\text{eff}}}$, where the effective exponents $\nu_{K}^{\text{eff}}$ for the knots are larger than 0.5 and less than 0.6. 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. For the asymptotic behavior of $R^2_K$, however, we find that it is consistent with the standard one with the scaling exponent 0.5. Thus, although the strong finite-size effects of $R^2_K$ remain effective for extremely large values of $N$, they can be matched with the asymptotic behavior of random walks.

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I. 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 are 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 [3, 4, 5, 6]. 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, 10, 11] that the average size $R_{\text{triv}}$ of a random polygon with the trivial knot should scale as $N^\nu$ with respect to the number $N$ of polygonal nodes, where the exponent $\nu$ is given by the exponent $\nu_{\text{SAW}}$ of the asymptotic scaling-behavior of the the self-avoiding walk (SAW) where $\nu_{\text{SAW}} \approx 0.588$. 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 behavior 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 SAW. First of all, under no topological constraint, the average size $R$ of a random polygon scales as $N^{\nu_{\text{RW}}}$ where $\nu_{\text{RW}} = 0.5$. Furthermore, it is not clear whether the scaling exponents of nontrivial knots should be enhanced similarly as that of the trivial knot. If they might have the same exponent of SAW, then why the total average over all knot types can have the exponent $\nu_{\text{RW}}$ of random walk? The purpose of this paper is to discuss these questions explicitly 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 behavior 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 \( N \):

\[
P_{\text{triv}}(N) = \exp\left(-\frac{N}{N_c}\right).
\]

For nontrivial knots, the probability is well described by the following function of \( N \):

\[
P_K(N) = C_K \left(\frac{N}{N_c}\right)^{m(K)} \exp\left(-\frac{N}{N_c}\right),
\]

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 \( R^2_K \) under the topological constraint of knot \( K \) has been discussed for some models of self-avoiding polygons (SAPs) in Refs. \([14, 15, 16, 17, 18, 19, 20]\). In the lattice model, it is shown that the asymptotic behavior of \( R^2_K \) is consistent with that of the RG theory where in the large \( N \) limit the ratio \( R^2_K/R^2 \) 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 \([22]\), \( R^2_K \) has been evaluated for the trivial and trefoil knots with small polygons of \( N < 200 \).

II. METHODS OF SIMULATIONS

We now introduce the Gaussian random polygon \([3]\). Let \( \vec{X}_1, \ldots, \vec{X}_N \) denote the position vectors of the nodes of a configuration of the Gaussian random polygon of \( N \) segments, and \( \vec{u}_1, \ldots, \vec{u}_N \) the jump vectors such that \( \vec{u}_j = \vec{X}_j - \vec{X}_{j-1} \) for \( j = 1, \ldots, N \). Then, the Gaussian random polygon has the following distribution function of the jump vectors:

\[
P(\vec{u}_1, \ldots, \vec{u}_N) = \text{Const.} \times \exp\left(-\frac{1}{2} \sum_{j=1}^{N} \vec{u}_j^2 + \delta(\vec{u}_1 + \cdots + \vec{u}_N) \right).
\]

Here \( \delta(\vec{x}) \) denote Dirac’s delta function in three dimensions. We construct \( M \) configurations of the Gaussian random polygon with \( N \) nodes by the conditional probability distribution \([3]\)

\[
P(\vec{u}_j; \vec{u}_1, \ldots, \vec{u}_{j-1}) = (2\pi)^{-3/2} \exp\left(-\frac{N - j + 1}{2(N - j)} (\vec{u}_j + \frac{\vec{X}_{j-1}}{N - j + 1})^2\right).
\]

Let us consider \( M \) samples of randomly constructed polygons with \( N \) nodes. We denote
by $M_K$ the number of polygons with knot $K$. We determine the number $M_K$ by enumerating such polygons in the set of $M$ polygons that have the same set of values of the following two invariants for knot $K$: the determinant of knot $\Delta_K(-1)$ and the Vassiliev invariant $v_2(K)$ of the second degree [23, 24].

III. ANOMALOUS FINITE-SIZE BEHAVIORS OF $R_K^2$

Let us discuss the numerical data of our simulations. For Gaussian random polygons with several different numbers $N$ up to 1900, numerical estimates of $R^2$ and $R_K^2$ have been obtained for the four knots: the trivial, trefoil $(3_1)$ and figure-eight $(4_1)$ knots, and the composite knot consisting of two trefoil knots $(3_1\sharp3_1)$. Here, we take $M = 10^5$ in all the simulations.

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 $n$-th 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 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 $i$-th Gaussian random polygon that has the knot type $K$, in the set of $M$ polygons. In terms of $R_K^2$, $R^2$ is given by $R^2 = \sum_K M_K R_K^2 / M$.

In Fig. 1, the graphs of the ratio $R_K^2/R^2$ against the the number $N$ are depicted for the trivial, trefoil and figure-eight knots. The fitting curves in Fig. 1 are given by $R_K^2/R^2 = \Gamma_K N^{2\nu_{eff} K}$. The best estimates of the fitting parameters are given in Table 1.

We see in Fig. 1 that the ratio $R_K^2/R^2$ is not constant with respect to $N$. The ratio $R_K^2/R^2$ increases monotonically for all the knots. For the trivial knot, the ratio $R_{triv}^2/R^2$ is always larger than 1.0. On the other hand, for the other three knots ($K=3_1, 4_1, 3_1\sharp3_1$), the ratio $R_K^2/R^2$ is smaller than 1.0 when $N$ is small. However, the ratio $R_K^2/R^2$ becomes larger than 1.0 when $N$ is large. Thus, the topological constraint gives an effective swelling for the case of large $N$. Here we have a conjecture that for any nontrivial knot $K$, $R_K^2$ should be larger than $R^2$ if $N$ is large enough.

Let us consider the plot of the trivial knot shown in Fig. 1. There is a nontrivial finite-size behavior: the ratio $R_{triv}^2/R^2$ is constant with respect to $N$ when $N$ is very small, while when $N > N_c$, it can be approximated by a scaling behavior as $R_{triv}^2/R^2 \sim N^{2\nu_{triv}}$, at least up to
$N = 2000$. This crossover phenomenon should be consistent with the recent theory given by Grosberg. However, the effective exponent $\nu_{\text{eff}}^{\text{triv}}$ is much smaller than the exponent $\nu_{\text{SAW}}$ with respect to the errors. In fact, we have the numerical estimate: $\nu_{\text{eff}}^{\text{triv}} \approx 0.545$.

For the case of nontrivial knots (3_1, 4_1, 3_1#3_1), the ratio $R_{2K}/R^2$ is well approximated by the power law: $R_{2K}/R^2 \approx \Gamma_N N^{2\Delta\nu_{\text{eff}}^K}$ for the range from $N = 100$ to $N = 2000$. Furthermore, there is no crossover for the nontrivial knots: we do not find any change in the slope of the graphs near $N \sim N_c$. It is also remarkable from Table 1 that the exponent $\Delta\nu_{\text{eff}}^K$ 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 $\nu_{\text{SAW}}$, while that of the trefoil knot is given by 0.561, which is rather smaller than $\nu_{\text{SAW}}$ with respect to the errors.

Let us consider the three fitting lines of Fig. 1. Then, we see that the three lines become very close to each other at around $N = 2000$. Furthermore, it is suggested from the simulations that when $N$ becomes close to 2000, the values of $R_{2K}^2$ 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 $R_{2K}^2$ for the nontrivial knots are always smaller than or equal to that of $R_{\text{triv}}^2$ in our simulations. If the power-law approximation might be valid also for $N > 2000$, then $R_{\text{triv}}^2$ would become much smaller than $R_{2K}^2$ of 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 $R_{2K}^2$ with the power law should be valid only when $N < 2000$. Therefore, in order to study the $N$-dependence of $R_{2K}^2$ for $N > 2000$, we need another independent analysis.

**IV. ASYMPTOTIC BEHAVIOR OF $R_{2K}^2$.**

Let us discuss the asymptotic behavior of $R_{2K}^2$. When $N$ is very large, we may assume the following expansion: $R_{2K}^2 = A_K N^{2\nu_K} (1 + B_K N^{-\Delta} + O(1/N))$. It is consistent with renormalization group arguments, and hence it should be valid when $N$ is asymptotically large. For the ratio $R_{2K}^2/R^2$ we have the following expansion:

$$R_{2K}^2/R^2 = (A_K/A) N^{2\Delta\nu_K} (1 + (B_K - B) N^{-\Delta} + O(1/N)),$$

where $\Delta\nu_K = \nu_K - \nu_{\text{RW}}$. Here we recall that $\nu_{\text{RW}} = 0.5$. For each of the four knots, we have applied the formula (2) to the 10 data points with $N \geq 1000$ shown in Fig. 1. Here,
when we assign the condition of $N \geq 1000$, we have taken into account the strong finite-size effects of $R_{K}^{2}$ such as the crossover of the trivial knot. Another recent study [25] on the cylinder model of SAPs [20, 21] shows that the asymptotic scaling behavior is seen only when $N > 1000$ for the case of very thin cylinders with the cylinder radius $r = 0.001$.

The best estimates of the fitting parameters of the formula (2) and the $\chi^{2}$ values are listed in Table 2. From the results, we may conclude that the asymptotic expansion (2) is consistent with the numerical values of $R_{K}^{2}$ for $N \geq 1000$. It is remarked that the $\chi^{2}$ values in Table 2 are less than 10 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 independent of the knot type. This leads to an estimate of the exponent: $\nu_{K} \approx 0.515$. The value can be considered as equivalent to the exponent $\nu_{RW}$, with respect to the errors of the analysis. The fact that the exponent $\nu_{K}$ is independent of the knot type is consistent with the interpretation on the lattice model of Refs. [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. We note that we have assumed $\Delta = 0.5$ in constructing Table 2. When we set $\Delta = 1.0$, similar values are obtained for the best estimates of the fitting parameters.

Let us consider a formula which effectively describes the $N$-dependence of $R_{K}^{2}$ for $N > 2000$. Assuming $\Delta \nu_{K} = 0$ in the asymptotic formula (2), we have the following: $R_{K}^{2}/R^{2} = \alpha_{K}(1 + \beta_{K} N^{-\Delta} + O(1/N))$. Here we have replaced by $\alpha_{K}$ and $\beta_{K}$, $A_{K}/A$ and $B_{K} - B$, respectively. Applying the formula to the numerical data of $R_{K}^{2}$ of the Gaussian random polygon for $N \geq 1000$, 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 Ref. [20]. In Table 3, the parameter $\alpha_{K}$ 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 Fig. 3 of Ref. [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 Fig. 1 that the ratio $R_{K}^{2}/R^{2}$ increases monotonically and approaches 1.3 or 1.4 when $N \sim 2000$ (see also Ref. [20]).
V. CONCLUSION

We have shown that $R^2_K$ of Gaussian random polygons have strong finite-size effects which should be valid for extremely large values of $N$ such as $N = 2000$. If we remove the finite-size effects from the data analysis, then the asymptotic behavior of $R^2_K$ is given by the standard one with the critical exponent $\nu_{RW}$ of random walks. Here we note that the main result should be valid also for the numerical data of other models of random polygons [23, 26]. Thus, the studies [9, 10, 11] associated with the conjecture of the 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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TABLE I: Best estimates for the fitting lines in Fig.1 describing the anomalous scaling behavior: $R_K^2/R^2 = \Gamma_K N^{2\Delta\nu_{K}^{\text{eff}}}$. Here $\Delta\nu_{K}^{\text{eff}} = \nu_{K}^{\text{eff}} - \nu_{\text{RW}}$. For the trivial knot, the fit is obtained from the data points with $N \geq 400$. For the trefoil ($3_1$) and figure-eight ($4_1$) knots, and the composite knot of $3_1 \# 3_1$, the fitting lines are obtained from the data for $N \geq 100$.

| knot type | $\Gamma_K$  | $2\Delta\nu_{K}^{\text{eff}}$ | $\chi^2$ |
|-----------|-------------|-------------------------------|-----------|
| 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        |

TABLE II: 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 $\Delta\nu_{K} = \nu_{K} - \nu_{\text{RW}}$.

| knot type | $A_K/A$    | $B_K - B$     | $2\Delta\nu_{K}$ | $\chi^2$ |
|-----------|------------|---------------|-------------------|-----------|
| triv/ave  | 1.163±3.22 | -3.746±17.609 | 0.027±0.309       | 3         |
| tre/ave   | 1.131±1.837| -5.333±9.486  | 0.033±0.183       | 9         |
| $4_1$/ave | 1.129±3.837| -5.860±19.170 | 0.033±0.385       | 7         |
| $3_1\#3_1$/ave | 1.166±1.662 | -5.928±8.071  | 0.028±0.161       | 9         |

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

| knot type | $\alpha_K$  | $\beta_K$  | $\chi^2$ |
|-----------|-------------|-------------|-----------|
| triv/ave  | 1.472±0.042 | -5.187±0.833| 3         |
| tre/ave   | 1.516±0.026 | -6.923±0.483| 10        |
| $4_1$/ave | 1.507±0.0056| -7.375±1.1010| 7         |
| $3_1\#3_1$/ave | 1.493±0.024 | -7.270±0.446| 9         |
FIG. 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 $N = 100$ to $N = 1900$. Numerical estimates of $R_K^2/R^2$ for the trivial, trefoil (31) and figure-eight (41) knots are shown by black circles, black squares and black triangles, respectively. In the inset, the enlarged figure shows the logarithmic plot of the estimates of $R_K^2/R^2$ from $N = 1000$ to 1900 for the trivial, trefoil and figure-eight knots.
