Exponents of intrachain correlation for self-avoiding walks and knotted self-avoiding polygons

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Abstract
We show numerically that critical exponents for two-point intrachain correlation of an infinite chain characterize those of finite chains in self-avoiding walk (SAW) and self-avoiding polygon (SAP) under a topological constraint. We evaluate short-distance exponents \( \theta(i, j) \) through the probability distribution functions of the distance between the \( i \)th and \( j \)th vertices of \( N \)-step SAW (or SAP with a knot) for all pairs \((1 \leq i, j \leq N)\). We construct the contour plot of \( \theta(i, j) \), and express it as a function of \( i \) and \( j \). We suggest that it has quite a simple structure. Here exponents \( \theta(i, j) \) generalize des Cloizeaux’s three critical exponents for short-distance intrachain correlation of SAW, and we show the crossover among them. We also evaluate the diffusion coefficient of knotted SAP for a few knot types, which can be calculated with the probability distribution functions of the distance between two nodes.

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(Some figures may appear in colour only in the online journal)

1. Introduction
Polymers with nontrivial topology such as cyclic polymers have attracted much interest in several fields. Ring polymers are observed in nature such as circular DNA whose topology is given by the trivial knot (figure 1), while DNA with nontrivial knots are derived in experiments [1–3]. Naturally occurring proteins whose ends are connected to give a circular topology have been recently discovered [4]. Due to novel developments in experimental techniques, ring polymers are now effectively synthesized in chemistry [5–9]. Moreover, polymers of topologically complex structures, which are sometimes called topological polymers, have been synthesized and separated with respect to their hydrodynamic radii such as through GPC [10, 11]. It is thus an interesting theoretical problem to calculate physical quantities such as the hydrodynamic radius, i.e. the diffusion coefficient, of each topological type. It can be derived...
through intrachain correlation of the polymer chain by Kirkwood’s approximation. Here we remark that the topology of a ring polymer is specified by a knot, and it gives the simplest and most fundamental example of nontrivial topologies.

Topological constraints often play a central role in the statistical and dynamical properties of ring polymers in solution [12–14]. For instance, the mean-square radius of gyration of ring polymers under a topological constraint can be much larger than that of no topological constraint, in particular, at the $\theta$ temperature of the corresponding linear polymers [15–21]. We call the phenomenon topological swelling. It is also confirmed in an experiment [22]. Due to the strong finite-size effect, however, it is not easy to determine numerically the exponent of the mean-square radius of gyration for knotted ring polymers in $\theta$ solution [20]. It is thus interesting to study topological effects on the scaling behavior of two-point correlations for self-avoiding polygons (SAPs) or random polygons through simulation.

The self-avoiding walk (SAW) and SAP are fundamental theoretical models for linear and ring polymers in good solution, respectively [23–26]. The exact enumeration, the Monte Carlo simulation and the renormalization group (RG) are important methods for studying the SAW model [26]. The scaling behavior of SAW is studied through the Monte Carlo simulation and the RG approach [27]. Correlations among configurations of SAW and SAP are nontrivial due to the excluded volume effect, and have attracted much interest in theoretical studies [28–39]. SAP has several different points from SAW: it is not only that SAP has cyclic symmetry while SAW has two ends and no translational symmetry, but also that SAP has a topological constraint specified by a knot. However, we shall show that several short-chain scaling properties of SAW are useful for describing those of SAP.

In this paper, we study the scaling behavior of intrachain correlation for SAW and off-lattice SAP with a fixed knot type through the Monte Carlo simulation. In particular, we evaluate exponents for short-distance correlation for any pair of segments in a SAW or SAP under a topological constraint. We numerically determine the probability distribution function of the distance between two vertices $i$ and $j$ of the chain, from which we evaluate the exponent $\theta_{ij}$ for short-distance correlation and the exponent $\delta$ for long-distance asymptotic behavior. The estimates of exponents $\theta_{ij}$ and $\delta$ are useful for expressing physical quantities such as the diffusion coefficient and the structure factor of SAW or SAP as an approximate integral form. For SAW, exponents $\theta_{ij}$ generalize des Cloizeaux’s three exponents $\theta_s$ ($s = 0, 1, 2$) for short-distance intrachain correlation of an infinite chain, which we shall define shortly. We shall show that the estimates of exponents $\theta_{ij}$ corresponding to $\theta_s$ ($s = 0, 1, 2$) are roughly similar to or a little smaller than the theoretical values of $\theta_s$. The difference may be due to the finiteness of the chain investigated. We also show the crossover among them. For SAP consisting of cylindrical segments, we show that exponents $\theta_{ij}$ and $\delta$ of SAP with large excluded volume are close to those of SAW, while exponents $\theta_{ij}$ and $\delta$ for SAP with small excluded volume are much smaller than those of SAW and close to those of random walks.

Let us briefly review the scaling behavior of intrachain correlation of SAW. We denote by $p_{ij}(r; N)$ the probability distribution function of the end-to-end vector $r$ of an $N$-step SAW.
Considering the rotational symmetry we express it also as \( p_0(r; N) \) where \( r \) is the end-to-end distance: \( r = |r| \). The large-\( r \) asymptotic behavior of \( p_0(r; N) \) was argued [28] as

\[
p_0(r; N) \sim R_N^{-d}A(r/R_N)\exp(-(r/R_N)^\delta)
\]

(1)

where \( R_N = R_0N^\nu \) and \( \delta = 1/(1-\nu) \). Here the scaling exponent \( \nu \) is given by \( \nu \approx 0.588 \). The small-\( r \) behavior of \( p_0(r; N) \) was studied analytically [29]. By assuming a scaling function \( F_0(y) \) satisfying \( p_0(r; N) = R_N^{-d}F_0(r/R_N) \), it was shown that the short-distance behavior is given by

\[
F_0(y) \sim y^g \quad \text{as} \quad y \to 0,
\]

(2)

with \( g = (\gamma + 1 - d\nu - \alpha)/\nu \). The exponent \( g \) was also derived through RG arguments [30]. Here we have \( g = (\gamma - 1)/\nu \) through the scaling relation: \( \alpha = 2 - d\nu \). It is also derived via RG arguments with the blob picture [23].

Short-distance correlation between two points of a long polymer in a good solvent was studied by des Cloizeaux with the RG techniques [31]. The exponents of the short-distance correlation, \( \theta_s \) for \( s = 0, 1, 2 \), were defined through the probability distribution functions \( p_s(r, N) \) of the distance between two given vertices of an \( N \)-step SAW in the large-\( N \) limit as follows. We denote by \( p_1(r, N) \) the probability distribution function of the distance between an end point and a middle point of the SAW, and by \( p_0(r, N) \) that of the distance between two points in the middle region of the SAW. Assuming that \( p_s(r, N) \approx R_N^{-d}F_s(r/R_N) \), we define the critical exponents \( \theta_s \) for short-distance correlation by

\[
F_s(y) \sim y^{\theta_s} \quad \text{as} \quad y \to 0, \quad \text{for} \quad s = 0, 1, 2.
\]

(3)

Here we remark that exponent \( g \) in equation (2) corresponds to \( \theta_0 \). The exponents \( \theta_s \) for \( s = 0, 1, 2 \) were calculated by des Cloizeaux with RG techniques in terms of the \( \epsilon \)-expansion up to the second order [31]. The estimates for \( d = 3 \) are given by

\[
\theta_0^{(RG)} = 0.273, \quad \theta_1^{(RG)} = 0.46, \quad \theta_2^{(RG)} = 0.71.
\]

(4)

In the RG derivation of \( \theta_0 \) it is assumed that the SAW is infinitely long. Here we remark that making use of the estimates of critical exponents \( \gamma \) and \( \nu \) of the \( O(N) \) model with higher loop corrections, we evaluate \( \theta_0 \) through the relation \( \theta_0 = g = (\gamma - 1)/\nu \) as follows. We have \( \theta_0 = 0.2713 \pm 0.0039 \) from the estimates \( (d = 3 \text{ expansion}) \) in figure 1 of [27], and \( \theta_0 = 0.2672 \pm 0.0056 \) from the estimates \( (\epsilon\text{-expansion, bc}) \) in figure 2 of [27].

As the first result of this paper, we numerically evaluate the critical exponents \( \theta_s \) for \( s = 0, 1, 2 \), by evaluating \( \theta(i, j) \) in the simulation of \( N \)-step SAW on the cubic lattice with \( N = 8000 \), and compare them with the theoretical values obtained by des Cloizeaux. Moreover, we show the crossover among exponents from \( \theta_1 \) and \( \theta_2 \) to \( \theta_0 \), and that between \( \theta_1 \) and \( \theta_2 \). Let us denote the estimates of \( \theta_s \) \( (s = 0, 1, 2) \) by \( \theta_i^{(MC)} \) \( (s = 0, 1, 2) \). They are given by

\[
\theta_0^{(MC)} = 0.23 \pm 0.02, \quad \theta_1^{(MC)} = 0.35 \pm 0.03, \quad \theta_2^{(MC)} = 0.74 \pm 0.03.
\]

(5)

The estimate of \( s = 0 \) is roughly the same but a little smaller than the RG value with respect to errors. It may be due to the finiteness of the chain. We have estimated exponent \( \theta_0 \) for several different numbers of steps, \( N \), in appendix A. We suggest from the data that the estimate of \( \theta_0 \) increases quite slowly with respect to \( N \). The estimate of \( s = 1 \) is clearly smaller than the RG value; The estimate of \( s = 2 \) is roughly the same with the theoretical value within errors. For SAP with knot \( K \) the estimates of the exponent for short-distance correlation, denoted by \( \theta_k \) or \( \theta_k(\lambda) \), are a little smaller than the RG value of \( \theta_2 \) for SAW. We have \( \theta_k = 0.679 \pm 0.004 \) for SAP of the trivial knot \( K = 0 \) with \( N = 3000 \) between two nodes separated by 900 steps along the chain \( \text{(i.e.,} \lambda = 0.3) \).
The estimates of critical exponents of a finite chain are useful, although the simulation values may be slightly different from the theoretical values due to the finiteness of the chain. For instance, with the estimates $\theta^{\text{MC}}(i, j)$ for exponents $\theta(i, j)$ we have good fitting curves to the probability distribution function of the distance between two vertices $i$ and $j$ of SAW. We can thus approximate it by an analytic function in terms of $\theta^{\text{MC}}(i, j)$. Moreover, polymers in reality are always of finite length, which can be compared with simulation results of finite chains.

For SAW the end-to-end distance distribution [36, 37] and the probability distribution functions of the internal distances [32, 38] have been evaluated numerically in simulation. However, the critical exponent of the short-distance correlation has not been evaluated in simulation with high numerical precision, yet.

This study of the two-point correlations of SAW is also important in expressing topological effects of knotted ring polymers in $\theta$ solution [40–45]. It has been shown that the average size of a ring polymer with a fixed knot in $\theta$ solution becomes enhanced due to the topological entropic force acting among the segments of the ring polymer. Furthermore, it has been suggested in several researches that the universality class of ring polymers in $\theta$ solution should be given by that of SAW [16, 19–21]. However, the distribution function of the distance between two vertices of a random polygon with fixed knot type is close to the Gaussian one [41, 44]. Thus, the method of this paper for determining the exponents of two-point correlation of SAW or SAP is useful for investigating the critical behavior of ring polymers with a fixed knot in $\theta$ solution more explicitly.

The contents of the paper consist of the following. In section 2, we explain the numerical methods of simulation in this research. We introduce normalized distance $x$, which is given by the distance between two points of SAW divided by the root-mean-square distance. We then define the probability distribution function of variable $x$. In section 3, we define exponents $\theta(i, j)$ between the $i$th and $j$th vertices of SAW, and give the numerical results. We show that the fitting formula for the probability distribution function of the distance between two vertices of SAP as a function of normalized distance $x$ gives good fitting curves to the numerical data. We then derive numerical estimates of exponents $\theta(i, j)$ for all pairs of vertices $i$ and $j$, and express them as a function of $i$ and $j$. In particular, we present the contour plot of exponents $\theta(i, j)$ for all vertices $i$ and $j$ ($0 \leq i, j \leq N$), and show that it has a simple structure. In section 4, we briefly review the topological swelling, i.e., the enhancement of the mean-square radius of gyration due to topological constraints. Then, we show the scaling behavior of intrachain correlation of SAP under a given topological constraint. In section 5, we evaluate the diffusion coefficient of SAP with a fixed knot through Kirkwood’s approximation for a few knots. In section 6, we give concluding remarks.

2. Numerical methods and important notation

2.1. Pivot algorithm for generating self-avoiding walks

We have generated $10^5$ configurations of the $N$-step SAW on the cubic lattice by the pivot algorithm [46, 47] for several values of $N$ with $N \leq 8000$. For a given initial configuration of the $N$-step SAW we pick up the configuration of SAW after every $8N$ Monte Carlo procedures, and assume that it is independent from the previous one. Here, in the cubic lattice each edge has unit length. We made an autocorrelation plot for the correlation between the relative position vectors from the center of mass of SAW at the initial time $t = 0$ and those of SAW at later time $t$, in appendix B. We observe that the correlation decays fast with respect to the Monte Carlo time.
The mean-square radius of gyration, $R_g^2$, for SAW on the cubic lattice is evaluated for several different numbers of $N$. The fitting curve in figure 2 is given by

$$R_g^2 = AN^{2\nu} (1 + B/\sqrt{N}).$$

(6)

Here the estimate of exponent $\nu$ is given by $\nu = 0.5899 \pm 0.0004$, which is consistent with exponent $\nu_{\text{SAW}}$ of SAW.

### 2.2. Distance between two vertices of SAW

For a given three-dimensional configuration of SAW with $N$ steps on the cubic lattice, we take a pair of integers $i$ and $j$ such that $0 \leq i < j \leq N$ (see, figure 3). There are $N + 1$ vertices in total from the zeroth to the $N$th vertex with position vectors $\vec{R}_j$ for $j = 0, 1, \ldots, N$. To the given configuration of SAW we calculate the distance between the $i$th and $j$th vertices

$$r(i, j) = |\vec{R}_j - \vec{R}_i|.$$  

(7)

We shall denote $r(i, j)$ also by $r_{ij}$, briefly.

For integers $i$ and $j$ satisfying $1 \leq i < j \leq N$, let $N_1$, $N_2$ and $N_3$ denote the number of steps in the first, second and third part of an $N$-step SAW, respectively, as shown in figure 3. We have $N_1 = i$, $N_2 = j - i$, and $N_3 = N - j$.
We denote by $R_N(i, j)$ the average distance between the $i$th and $j$th vertices of an $N$-step SAW, i.e. the root-mean-square distance between the $i$th and $j$th vertices of SAW with $N$ steps:

$$R_N(i, j) = \sqrt{\langle r^2_{ij} \rangle}.$$  

It is approximated by

$$(R_N(i, j))^2 = A_{ij}|j-i|^{2\nu}(1 + B_{ij}/\sqrt{|j-i|}).$$  

(8)

Here $A_{ij}$ and $B_{ij}$ are fitting parameters. The estimates are given in table 1.

We introduce parameter $\lambda$ such that the selected two points $i$ and $j$ are separated by $\lambda N$ steps $(0 \leq \lambda \leq 1)$: $N_2 = \lambda N$. We define parameter $\mu$ by $N_1 = \mu N_2$. We have

$$N_1 = \mu N_2 = \mu \lambda N.$$  

(9)

In terms of parameters $\lambda$ and $\mu$, integers $i$ and $j$ are given by $i = N_1 = \mu \lambda N$ and $j = N_1 + N_2 = (1 + \mu)\lambda N$, respectively. The integer $N_1$ is given by $N_1 = N - j = N - (1 + \mu)\lambda N$. In the case of $s = 2$ where $N_1 = N_2$, we have $(1 + 2\mu)\lambda = 1$.

The data of the mean-square distance $\langle r^2_{ij} \rangle$ versus $\lambda$ are shown in figure 4. The data points of different values of parameter $\mu$ almost coincide with each other for $0 \leq \mu \leq 0.5$ in figure 4. It is thus suggested that the fitting parameters of (8) are continuous with respect to the change of parameter $\mu$.

We consider two special types of intrachain distance: $R_{s\lambda}(\lambda)$ for $s = 1, 2$. We define $R_{s\lambda}(\lambda)$ by the root-mean-square distance between the zeroth and $\lambda N$th vertices. Here we
recall \( i = 0 \) and \( j = \lambda N \): \( R_{N,1}(\lambda) = \sqrt{\langle r^2(0, \lambda N) \rangle} \). We define \( R_{N,2}(\lambda) \) by the root-mean-
square distance between the \(((1 \pm \lambda)N/2)\)th vertices. Here, we have \( i = (1 - \lambda)N/2 \) and \( j = (1 + \lambda)N/2 \), and parameter \( \mu \) is given by \( \mu = (1 - \lambda)/(2\lambda) \). Thus, we have \( R_{N,2}(\lambda) = \sqrt{\langle r^2((1 - \lambda)N/2, (1 + \lambda)N/2) \rangle} \). The square roots of intrachain distances \( R_{N,s}(\lambda) \) for \( s = 1, 2 \) are well approximated by

\[
(R_{N,s}(\lambda))^2 = A_s(\lambda N)^{2s}(1 + B_s/(\lambda N)^{1/2}),
\]

where \( A_s \) and \( B_s \) are fitting parameters. We shall often neglect the correction term \( B_s/(\lambda N) \).

### 2.3. Probability distribution function of the distance between two vertices of SAW

Let us denote by \( p(r; i, j; N) \) the probability of finding the \( j \)th vertex in the region \( d^3r \) at a position \( r \) from the \( i \)th vertex of an \( N \)-step SAW. It is expressed in terms of the average over all configurations of SAW, \( \langle \cdots \rangle \), as follows:

\[
p(r; i, j; N) = \delta(r - (R_j - R_i)).
\]

Here we recall that \( R_i \) and \( R_j \) are the position vectors of the \( i \)th and \( j \)th vertices of the SAW, respectively. Due to the rotational symmetry, the probability distribution function \( p(r; i, j; N) \) depends only on the distance \( r = |r| \), and we denote it simply by \( p(r; i, j; N) \).

We shall show that good fitting curves are given by the following formula:

\[
p(r; i, j; N) = c_{i,j}(r/R_N(i, j))^{\delta(i,j)} \exp(-(D_{i,j}/R_N(i, j))^\delta).
\]

Here exponent \( \delta \) is related to the exponent \( \nu \) by \( \delta = 1/(1 - \nu) \), and \( R_N(i, j) \) are given by the root-mean-square distance between the two vertices \( i \) and \( j \). Applying it to the numerical data of \( p(r; i, j; N) \), we evaluate exponents \( \theta(i, j) \) by the best estimates of parameters for fitting curves.

Let us consider two special types of the probability distribution functions of the distance \( r \) between two vertices of an \( N \)-step SAW: \( p_s(r; \lambda, N) \) for \( s = 1, 2 \). For \( s = 1 \), \( p_1(r; \lambda, N) \) is defined for the distance \( r \) between the vertex of an end point and another vertex of SAW, say, the \( n \)th vertex with \( n = \lambda N \); for \( s = 2 \), \( p_2(r; \lambda, N) \) is defined for the distance \( r \) between the \(((1 - \lambda)N/2)\)th and \(((1 + \lambda)N/2)\)th vertices of SAW. Here we recall that for \( s = 0 \), the probability distribution function \( p_0(r; N) \) has been defined for the distance \( r \) between two ends of an \( N \)-step SAW. It corresponds to \( p_s(r; \lambda, N) \) for \( s = 1, 2 \) in the case of \( \lambda = 1 \).

We shall also show that \( p_s(r; \lambda, N) \) for \( s = 1, 2 \) are well approximated by

\[
p_s(r; \lambda, N) = c_s(r/R_{N,s}(\lambda))^{\delta_s(\lambda)} \exp(-(D_s r/R_{N,s}(\lambda))^\delta).
\]

We shall evaluate exponents \( \theta_s(\lambda) \) for \( s = 1, 2 \) by the fitting formula of \( p_s(r; \lambda, N) \) for \( s = 1, 2 \), respectively.

### 2.4. Distribution function of the normalized distance

Let us assume an ensemble of SAW where there are \( W = 10^5 \) random configurations of \( N \)-step SAW on the cubic lattice. For the distance between the \( i \)th and \( j \)th vertices, \( r_{i,j} \), we introduce the normalized distance \( x_{i,j} \) by

\[
x_{i,j} = r_{i,j}/\sqrt{\langle r_{i,j}^2 \rangle}.
\]

We set the length \( \Delta x \) of intervals by \( \Delta x = 10^{-1} \). We enumerate the number of configurations of SAW such that the normalized distance \( x_{i,j} \) between the \( i \)th and \( j \)th vertices satisfies the conditions \( x < x_{i,j} < x + \Delta x \). We express the number by \( n_{i,j}(x, \Delta x) \). We define the probability
distribution function \( f(x; i, j; N) \) of the normalized distance \( x \) between the \( i \)th and \( j \)th vertices by

\[
x^2 f(x; i, j; N) \Delta x = n_{ij}(x, \Delta x)/W.
\]

In terms of \( p(r; i, j; N) \) we have \( f(x; i, j; N) = 4\pi R_N^3(i, j) p(r; i, j; N) \). Hereafter, we also call \( f(x; i, j; N) \), the distribution function.

Let us now introduce symbols \( f_s(x; \lambda, N) \) for \( s = 0, 1, 2 \). We denote by \( f_0(x; N) \) the probability distribution function of the normalized end-to-end distance \( x = r/R_N \). We then denote by \( f_1(x; \lambda, N) \) the probability distribution function of the normalized distance between an end point (the zeroth vertex) and the \( \lambda N \)th vertex of SAW of \( N \) steps and by \( f_2(x; \lambda, N) \) that of the normalized distance between two vertices separated by \( \lambda N \) steps in a middle region of SAW.

2.5. Algorithm for constructing off-lattice SAP

We generated \( 2 \times 10^5 \) configurations of SAP consisting of \( N \) cylindrical segments with cylindrical radius \( r_{ex} \) of unit length for various number of nodes \( N \). Each cylinder segment has the excluded volume of \( \pi r_{ex}^3 \). In the model of cylindrical SAP, we assume that neighboring segments have no excluded volume interaction: neighboring cylinder segments may overlap each other.

In the Monte Carlo procedure we first select two nodes of SAP randomly and consider a subchain between the two nodes. We then construct the ensembles of cylindrical SAP by combining the crank-shaft move and the rotation of a subchain of cylindrical SAP around an axis at the center of the axis by 180 degrees. Here, the axis is orthogonal to the end-to-end vector of the subchain. We apply the crank-shaft move \( 2N \) times, and then we apply the rotation of subchains \( 2N \) times in the Monte Carlo algorithm.

3. Scaling behavior of intrachain correlation of SAW

3.1. Distribution functions \( f_s(x; \lambda, N) \) of the distance between two vertices of SAW and short-distance exponents \( \theta_s \)

Let us introduce the formula for fitting curves to the data of the probability distribution functions \( f_s(x; \lambda, N) \) for \( s = 1, 2 \) as follows:

\[
f_s(x; \lambda, N) = C_s x^{\theta_s(\lambda)} \exp(-D_s x^\delta),
\]

where \( \delta = 1/(1 - \nu) \). The constants \( D_s \) and \( C_s \) are given by

\[
D_s = \left( \frac{\Gamma((5 + \theta_s)/\delta)}{\Gamma((3 + \theta_s)/\delta)} \right) \delta \left( \frac{\Gamma((5 + \theta_s)/\delta)}{\Gamma((3 + \theta_s)/\delta)} \right)^{(3+\theta_s)/2},
\]

Here we recall that \( x \) denotes the normalized distance: \( x = r/R_{N,ex}(\lambda) \), where \( R_{N,ex}(\lambda) = \sqrt{A_0(\lambda N)^{\nu}} \). For \( s = 0 \), we assume that \( R_{N,ex}(\lambda) \) denotes the end-to-end distance \( R_N \), and apply the formula which is obtained by replacing all \( \theta_s(\lambda) \) of (16) and (17) with \( \theta_0 \).

Formula (16) has two fitting parameters \( \theta_s(\lambda) \) and \( \delta \) for each \( s \) of \( s = 1, 2 \). The constants \( C_s \) and \( D_s \) satisfy the following constraints for \( s = 1, 2 \):

\[
\int_0^\infty x^2 f_s(x; \lambda, N) \, dx = 1, \quad \int_0^\infty x^4 f_s(x; \lambda, N) \, dx = 1.
\]

We made the graphs of the distribution function of the end-to-end distance \( f_0(x; N) \) \( (s = 0) \) and those of the distribution functions \( f_s(x; \lambda, N) \) of the distance between two vertices
separated by $\lambda N$ steps for $s = 1, 2$ with 45 different values of $\lambda$ from 0.10 to 0.98 by 0.02 against normalized distance $x$. Each graph has 20 data points from $x = 0.05$ to 1.95. Here we recall that $10^5$ SAWs of $N$ steps are generated by the pivot algorithm for $N = 8000$.

Formula (16) gives good fitting curves to the data of the probability distribution functions $f_s(x; \lambda, N)$ of the distance between two vertices of SAW for several different values of $\lambda$ and $N$ and over almost the entire region of normalized distance $x$. The $\chi^2$ value per datum is less than 2.0 for all fitting curves (in total, 91 curves).

The fitting curves of the end-to-end distance distribution function are fitted uniformly well to the data points with respect to errors. In fact, the estimate of exponent $\theta_0$ does not depend on the plot range. The estimate of exponent $\theta_0$ and the $\chi^2$ value do not change much for various different ranges of data points, for which we apply fitting formula (16). For asymptotically large distances, in the factor of the power of distances in equation (16) we may have a different exponent from $\theta_0$, since exponent $\theta_0$ is originally defined for short distances. However, the estimate of the exponent where the plot range is shifted to large distances is not numerically distinct from exponent $\theta_0$ with respect to errors. We therefore conclude that fitting formula (16) is practically good for describing the end-to-end distance distribution function with respect to the size of errors in the present simulation.

We have thus shown that the probability distribution function of the distance between two vertices of type $s$ ($s = 0, 1, 2$) is given by

$$p_s(r; \lambda, N) = f_s(r/R_{N,s}(\lambda); \lambda, N)/(4\pi R_{N,s}(\lambda)^3),$$

(19)

where $R_{N,s}(\lambda) = \sqrt{\lambda_s}(\lambda N)^{\nu(s)}$ for $s = 1, 2$.

3.2. Independence of estimates $\theta_s(\lambda)$ and $\nu(\lambda)$ of parameter $\lambda$

We have evaluated parameters $\delta(\lambda)$ (or $\nu(\lambda)$) and $\theta_s(\lambda)$ for $s = 1, 2$ with the least-square method by applying formula (16) to the data plots of the probability distribution functions $f_s(x; \lambda, N)$ for $s = 1, 2$ as functions of the normalized distance $x$ over the entire region of $x$ for various values of $\lambda$ ($0.1 < \lambda < 1.0$). The estimates are given in table 2. Here, $N = 8000$. For a given value of $\lambda$ and each of $s = 1, 2$, we make a fitting curve to the data points of the distribution function $f_s(x; \lambda, N)$ of the distance between two vertices, and evaluate fitting parameters $\delta(\lambda)$ and $\theta_s(\lambda)$.

The estimates of $\nu(\lambda)$ evaluated from formula (16) of distribution functions $f_s(x; \lambda, N)$ for $s = 1, 2$ via relation $\nu = 1 - 1/\delta$ are plotted against parameter $\lambda$ in figure 6. They are almost completely constant with respect to $\lambda$, and consistent with the exponent of SAW, $v_{SAW} \approx 0.588$.

For an illustration, we presented in figure 5 fitting curves to distribution functions $f_s(x; \lambda, N)$ for $s = 1$ and $2$, respectively. In the cases of $s = 1$ and $2$ the curves for the data points of $\lambda = 0.30$ coincide within errors for any value of $x$.

The exponents $\theta_s$ for $s = 0, 1, 2$ are in increasing order: $\theta_0 < \theta_1 < \theta_2$. We observe in figure 5 that in small $x$ region, the fitting curve of $s = 0$ is higher in position than $s = 1$, and

| $s = 0$ | $s = 1$ | $s = 2$ |
|--------|--------|--------|
| $\theta_0$ | 0.23 ± 0.02 | 0.33 ± 0.03 | 0.73 ± 0.03 |
| $\nu$ | 0.589 ± 0.005 | 0.608 ± 0.005 | 0.604 ± 0.005 |
| $\chi^2$/datum | 0.786 | 0.887 | 1.07 |

Table 2. Estimates of fitting parameters and the $\chi^2$ value per datum for the fitting curves in figure 5: $\theta_s(\lambda)$ and $\delta$ for $s = 1, 2$. Here $N = 8000$ and $\lambda = 0.3$.  

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Figure 5. Distribution function $f_s(x; \lambda, N)$ of the distance between two vertices of SAWs of $N$ steps separated by $\lambda N$ steps for $s = 1, 2$, with $\lambda = 0.3$ and $N = 8000$. Distribution function of the end-to-end distance, $f_0(x; N)$, is also plotted. Each distribution function has 20 data points.

Figure 6. Exponents $\nu(\lambda)$ evaluated through the distribution functions $f_s(x; \lambda, N)$ of the distance between two points separated by $\lambda N$ steps of SAW with $N = 8000$ for $0.1 \leq \lambda < 1$. Here, $\nu$ is calculated from $\delta$ by $\nu = 1 - 1/\delta$.

The fitting curve of $s = 1$ is higher in position than the fitting curve of $s = 2$. In fact, by taking the derivative of fitting formula (16), we can show that the peak position of the fitting curve (16) becomes larger as the parameter $\theta_s$ increases.

The critical exponents $\theta_1(\lambda)$ and $\theta_2(\lambda)$ are plotted against parameter $\lambda$ over a wide range such as $0.1 \leq \lambda < 1$ in figure 7 for SAW of $N = 8000$ steps. They are given by the best estimates that are obtained by applying formula (16) to the data. Here we recall that formula (16) has only two fitting parameters, $\theta$ and $\delta$.

We observe that the estimates of $\theta_1(\lambda)$ are independent of the parameter $\lambda$ for $0.1 < \lambda < 0.8$. The constant value of $\theta_1(\lambda)$ is given by 0.35 (see also equation (5), which is a little smaller than the theoretical value: $\theta_1 = 0.46$. Here we remark that in the theoretical derivation [31] the remaining part of the chain is assumed to be infinitely long; i.e., $N_3 \to \infty$. However, when $\lambda < 0.8$, the remaining part of the SAW is more than 20% of the SAW, which may be long enough in the case of $N = 8000$. We also observe that for $0.1 < \lambda < 0.5$, the estimates of $\theta_2(\lambda)$ do not depend on the parameter $\lambda$, and they are close to the theoretical value: $\theta_2 = 0.71$ with respect to errors, as shown in figure 7.
3.3. Distribution functions \( f(x; i, j; N) \) of the distance between vertices \( i \) and \( j \) of SAW and exponent \( \theta(i, j) \)

In figure 8, distribution functions \( f_s(x; \lambda, N) \) with \( \lambda = 0.30 \) and \( N = 8000 \) for \( s = 1, 2 \) and distribution function \( f(x; i, j; N) \) with \( i = \mu \lambda N \) and \( j = (1+\mu)\lambda N \) with \( \lambda = 0.30 \) are plotted against normalized distance \( x \). Here we recall \( N = 8000 \). In the small \( x \) region, the fitting curve of \( \mu = 0.1 \) is located between those of \( s = 1 \) and \( s = 2 \). In the large \( x \) region, the three fitting curves overlap each other for \( s = 1, 2 \) and \( \lambda = 0.3 \). We therefore suggest that the asymptotic behavior for large \( x \) is the same among the three cases of \( f_s(x; \lambda, N) \) with \( \lambda = 0.30 \) for \( s = 1, 2 \) and \( f(x; i, j; N) \) with \( i = \mu \lambda N \) and \( j = (1+\mu)\lambda N \) with \( \lambda = 0.30 \).

In figures 7 we observe that as the parameter \( \lambda \) increases up to \( \lambda = 1 \), the exponents \( \theta_s(\lambda) \) for \( s = 1, 2 \) are decreasing and become close to the value of the exponent \( \theta_0 \). Here we remark that at \( \lambda = 1 \), the distance between the two vertices is nothing but the end-to-end distance. Therefore, we may expect that the values of exponents \( \theta_s(\lambda) \) for \( s = 1, 2 \) approach the value of \( \theta_0 \) when we send \( \lambda \) to 1.

Let us now introduce the exponent \( \theta(i, j) \) in order to describe the short-distance correlation of the distribution function \( f(x; i, j; N) \) for normalized distance \( x \) between the \( i \)th and \( j \)th
Figure 9. Exponents $\theta(i, j)$ for the distance between the two points separated by $\lambda N$ steps where one point is located at $\mu \lambda N$ steps from an end point of SAW, i.e. $N_1 = \mu \lambda N$. Here, $N = 8000$.

vertices of an $N$-step SAW. We introduce the fitting formula for the distribution functions $f(x; i, j; N)$ as follows:

$$f(x; i, j; N) = C_{i, j} x^{\theta(i, j)} \exp(-D_{i, j} x^\delta)$$

(20)

where $\delta = 1/(1 - \nu)$. The constants $D_{i, j}$ and $C_{i, j}$ are given by

$$D_{i, j} = \sqrt{\frac{\Gamma((5 + \theta(i, j))/\delta)}{\Gamma((3 + \theta(i, j))/\delta)}}, \quad C_{i, j} = \frac{\delta \Gamma((5 + \theta(i, j))/\delta)}{\Gamma((3 + \theta(i, j))/\delta)} \frac{\Gamma((5 + \theta(i, j))/\delta)}{\Gamma((3 + \theta(i, j))/\delta)}^{(3+\theta(i, j))/2}$$

(21)

Here we recall that $x$ denotes the normalized distance: $x = r/R_N(i, j)$, where $R_N(i, j) = \sqrt{A_{ij}(\lambda N)^\nu}$.

Let us express vertices $i$ and $j$ of a SAW in terms of parameters $\lambda$ and $\mu$ as

$$i = \mu \lambda N, \quad j = (1 + \mu) \lambda N.$$  

(22)

If we fix the parameter $\mu$, vertices $i$ and $j$ satisfy the following relation:

$$j = i(1 + \mu^{-1}).$$  

(23)

Here we recall that for a pair of vertices $i$ and $j$ of a SAW, the numbers $N_1$ and $N_2$ are expressed in terms of parameters $\lambda$ and $\mu$ by $N_1 = \mu \lambda N$ and $N_2 = \lambda N$, as shown in figure 3.

We now show numerically that for a given value of $\mu$, the exponent $\theta(i, j)$ is constant with respect to the parameter $\lambda$ on the straight line segment: $0 \leq \lambda \leq 1/(1 + 2\mu)$. In figure 9 we observe that for given values of parameter $\mu$ such as 0.05, 0.1, 0.2, 0.3, 0.4, estimates of exponents $\theta(i, j)$ are independent of the parameter $\lambda$ for $0.1 < \lambda < 0.5$.

Furthermore, in figure 9 we observe the crossover phenomenon such that if one of the two points separated by $\lambda N$ steps along SAW is close to an end point of SAW with less than 0.4$\lambda N$ (or 0.5$\lambda N$) steps (i.e. $\mu < 0.4$ or $\mu < 0.5$), then the value of the exponent $\theta(i, j)$ changes from $\theta_2$ to $\theta_1$ as the parameter $\mu$ approaches 0.

3.4. Contour plot of exponent $\theta(i, j)$

Let us now show that the exponent $\theta(i, j)$ as a function of $i$ and $j$ has a simple structure. The contours of the exponent $\theta(i, j)$ are shown in figure 10. The region where exponents $\theta(i, j)$ are larger than 0.7 and less than 0.8 is colored by magenta. The magenta region of $\theta(i, j)$,
Figure 10. Exponent $\theta(i, j)$ for $0 < i, j < 8000$. In colored areas with red, yellow, green, cyan, blue, magenta and rose pink, we have $0.1 \times k \leq \theta(i, j) < 0.1 \times (k + 1)$ for $k = 2, 3, \ldots, 8$, respectively. The estimate of $\theta(i, j)$ is constant in the magenta rhombus region, where we have $\theta(i, j) \approx 0.7$; i.e., we have $\theta(i, j) \approx \theta_2$, denoted by $s = 2$; two corners with red color correspond to the areas of the exponent $\theta_0$ and denoted by $s = 0$; four edges with yellow color correspond to the areas of the exponent $\theta_1$ and denoted by $s = 1$. The blank (or empty) region around the diagonal area where $|i - j|$ are small has no data due to poor statistics.

where $0.7 \leq \theta(i, j) < 0.8$, is approximately given by a rhombus with four black edges in figure 10. We thus observe that the contour plot of $\theta(i, j)$ has a plateau region on the rhombus of figure 10 where the estimate of $\theta(i, j)$ is constant: $\theta(i, j) \approx 0.7$.

It is natural to interpret that the constant value of the exponent $\theta(i, j)$ in the large rhombus region of $(i, j)$ in figure 10 corresponds to the exponent $\theta_2$, since the estimate of $\theta(i, j)$ is almost constant and it is approximately equal to the theoretical value $\theta^{\text{RG}}_2$ given in equation (4). Thus, it is practically straightforward to estimate the exponent $\theta_2$, although it is defined through the double asymptotic behavior where both $N_1$ and $N_3$ given in figure 3 are taken to be very large.

The contour plot of figure 10 clearly illustrate the following two observations. (i) In figure 9 we observe that the exponent $\theta(i, j)$ does not depend on the parameter $\lambda$ in the region $0 \leq \lambda \leq 1/(1 + 2\mu)$; (ii) in figure 9 we observe the crossover phenomenon: from $\theta_2$ to $\theta_1$ as $\mu$ approaches 0, and then from $\theta_1$ to $\theta_0$ as $\lambda$ approaches 1.0.

The graph of $(i, j)$ for the parameter $\lambda$ satisfying $0 \leq \lambda \leq 1/(1 + 2\mu)$ is given by the straight line with gradient $1 + \mu^{-1}$ from the origin $(0,0)$ to the crossing point $(i_c, j_c)$ in the graph of $i + j = N$. The crossing point $(i_c, j_c)$ is given by

$$
(i_c, j_c) = \left( \mu N \frac{1 + \mu}{1 + 2\mu}, \frac{(1 + \mu)N}{1 + 2\mu} \right). 
$$

In figure 10 we observe that the value of the exponent $\theta(i, j)$ is constant on the line segment from the origin to the crossing point $(i_c, j_c)$. It depends on the parameter $\mu$. Here we recall equation (23).
Let us describe the magenta rhombus region in figure 10, where the estimate of \( \theta(i, j) \) is constant and approximately equal to \( \theta_1^{(RG)} \). The line of \( \mu = 0.5 \) corresponds to the straight line from the origin \((0,0)\) to \((2000, 6000)\) in the coordinate of \((i, j)\) with \( N = 8000 \). It is given by one of the four edges of the magenta rhombus where we have \( \theta(i, j) \approx \theta_2 \) in figure 10. If \( \mu \) becomes smaller than 0.5, then the gradient of the straight line increases and \( \theta(i, j) \) becomes smaller than \( \theta_2 \). Finally, we have \( \theta(i, j) = \theta_1 \) at \( \mu = 0 \). Around at the two edges of \((0, 8000)\) and \((8000, 0)\) we have \( \theta(i, j) = \theta_0 \).

We now give an approximate expression for exponent \( \theta(i, j) \) as a function of \( i \) and \( j \) as follows. For \( 0 \leq \lambda \leq 1/(1 + 2\mu) \), we have

\[
\theta(i, j) = \begin{cases} 
\theta_0^{(MC)} & \text{for } \mu = 0 \text{ and } 0.8 < \lambda \leq 1.0 \\
\theta_1^{(MC)} + \frac{4\mu}{1 + 2\mu} (\theta_2^{(MC)} - \theta_1^{(MC)}) & \text{for } 0 < \mu \leq 0.5 \\
\theta_2^{(MC)} & \text{for } 0.5 \leq \mu < \infty.
\end{cases}
\]  

(25)

Here, estimates \( g_s^{(MC)} \) for \( s = 0, 1, 2 \) are given in equation (5).

### 3.5. Correlation functions through exponents \( \theta(i, j) \) of SAW

The estimates of short-distance exponents \( \theta(i, j) \) shown in figure 10 are useful for constructing various quantities of SAW. In fact, formula (20) has only two parameters \( \theta(i, j) \) and \( \delta \) (or \( \nu \)), and the probability distribution function \( p(r; i, j; N) \) is determined if we give parameter \( A_{i,j} \) (or \( R_N(i, j) \)) in addition to \( \theta(i, j) \) and \( \delta \).

For instance, the pair correlation function of SAW, \( g(r) \), is given by the sum of the distribution functions of the distance between two vertices \( i \) and \( j \), \( p(r; i, j; N) \), over all vertices \( i \) and \( j \) of SAW:

\[
g(r) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} p(r; i, j; N).
\]  

(26)

In terms of parameters \( \lambda \) and \( \mu \) we have

\[
g(r) = 4N \int_0^\infty \mu \int_0^\mu d\lambda \int_0^{1/(1+2\mu)} \lambda \ d\lambda \ p(r; i, j; N) d\mu.
\]  

(27)

We define the static structure factor of SAW, \( g(q) \), by

\[
g(q) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle \exp(iq \cdot (r_i - r_j)) \rangle.
\]  

(28)

Assuming the rotational symmetry we have

\[
\langle \exp(iq \cdot (r_i - r_j)) \rangle = \int_0^\infty \sin qr \ \frac{qr}{qr} \ p(r; i, j; N)4\pi r^2 \ dr.
\]  

(29)

where \( r = |r_i - r_j| \) and \( q = |q| \). We have the following expression of the static structure factor of SAW:

\[
g(q) = \frac{1}{N} \int_0^N \int_0^N dm \int_0^N \int_0^\infty \sin qr \ \frac{qr}{qr} \ p(r; m, n; N)4\pi r^2 \ dr
\]

\[
= 4N \int_0^\infty \mu \int_0^{1/(1+2\mu)} d\lambda \int_0^\infty \sin qr \ \frac{qr}{qr} \ p(r; \lambda, \mu; N)4\pi r^2 \ dr.
\]  

(30)
3.6. Diffusion coefficients of polymers through intrachain correlation of SAW

The diffusion coefficient of a linear polymer in a good solvent, $D_{G,L}$, can be evaluated through the probability distribution functions of the distance between two points through the method of Kirkwood’s approximation [24].

The Brownian motion of polymers in a good solvent can be experimentally studied by dynamic light scattering [24]. We assume that the segments of polymers interact with each other through the long-range hydrodynamic interaction, which is described by the Oseen tensor $H_{mn}$. We define the dynamic structure factor of a polymer by

$$g(q) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle \exp(i \mathbf{k} \cdot (\mathbf{r}_i(t) - \mathbf{r}_j(0))) \rangle.$$  (31)

Here, the symbol $\mathbf{r}_i(t)$ denotes the position vector of the $i\text{th}$ segment at time $t$. Then, the dynamic structure factor $g(k, t)$ in the regime $k R_G \ll 1$ decays as

$$g(k, t) = \exp\left(-\frac{1}{\Gamma_{k}^{(0)}} k t\right)$$  (32)

where the initial decay rate $\Gamma_{k}^{(0)}$ is given by

$$\frac{\Gamma_{k}^{(0)}}{k} = \frac{k_B T}{N^2} \sum_{m,n} \langle H_{mn} : \mathbf{k} \mathbf{k} \rangle.$$  (33)

We define the diffusion constant $D_{G,L}$ through the initial decay rate by

$$\frac{\Gamma_{k}^{(0)}}{k} = D_{G,L} k^2.$$  (34)

Then the diffusion coefficient $D_{G,L}$ is equivalent to the diffusion coefficient $D_{G,L}^{(K)}$ derived by Kirkwood’s method.

The diffusion coefficient $D_{G,L}$ is given by the sum of the ensemble average of the inverse distance between two points of SAP over all pairs of segments:

$$D_{G,L} = \frac{k_B T}{6\pi \eta s N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left\{ \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \right\}.$$  (35)

Here $\eta_s$ denotes the solvent viscosity. We then evaluate the ensemble average of the inverse distance in terms of the probability distribution function, as follows:

$$D_{G,L} = \frac{k_B T}{6\pi \eta s N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \int_{0}^{\infty} \frac{1}{r} p(r; i, j; N) 4\pi r^2 \, dr$$

$$= 4N \int_{0}^{\infty} \mu \int_{0}^{1/(1+2\mu)} \lambda \, d\lambda \int_{0}^{\infty} \frac{1}{r} p(r; i, j; N) 4\pi r^2 \, dr.$$  (36)

4. Scaling behavior of intrachain correlation of SAP

4.1. Mean-square radius of gyration for SAP of cylindrical segments under a topological constraint

Let us now show the data of the mean-square radius of gyration for cylindrical SAP under a topological constraint of type $K$. We denote it by $R_{G,K}^2$, briefly. Here we recall that SAP consists of $N$ cylindrical segments with radius $r_{ex}$ of unit length. In figure 11 the mean-square radius of gyration of cylindrical SAP under no topological constraint, $R_{G,All}^2$, is plotted for several different values of radius $r_{ex}$ with several numbers $N$ of segments up to $N = 3000$. The
Figure 11. Double-logarithmic plot of the mean-square radius of gyration of SAP consisting of $N$ cylindrical segments with radius $r_{ex}$ of unit length under no topological constraint $\langle R_{g}^2 \rangle_{All}$. For the cases of $r_{ex} = 0.0, 0.05, 0.01, 0.02, 0.03, 0.05$ and $0.1$ the data points are plotted with purple filled circles, red filled squares, yellow filled triangles, green crosses, light blue stars, dark blue triangles and purple filled diamonds, respectively.

Table 3. Best estimates of the fitting formula: $R_{g}^2 = AN^{2\nu} (1 + B/N)$ for the mean-square radius of gyration for SAP consisting of $N$ cylindrical segments with radius $r_{ex}$ of unit length under no topological constraint $\langle R_{g}^2 \rangle_{All}$.

| $r_{ex}$ | $A$       | $\nu$       | $B$       | $\chi^2$/datum |
|---------|-----------|-------------|-----------|-----------------|
| 0       | 0.0833 ± 0.0004 | 0.5000 ± 0.0003 | 1.2 ± 0.2 | 1.04            |
| 0.005   | 0.0584 ± 0.0006 | 0.5379 ± 0.0008 | 8.0 ± 0.6 | 7.93            |
| 0.01    | 0.0529 ± 0.0006 | 0.5528 ± 0.0007 | 9.0 ± 0.6 | 7.59            |
| 0.02    | 0.0504 ± 0.0005 | 0.5667 ± 0.0006 | 8.5 ± 0.5 | 7.99            |
| 0.05    | 0.0538 ± 0.0003 | 0.5798 ± 0.0003 | 5.3 ± 0.3 | 2.57            |
| 0.1     | 0.0623 ± 0.0003 | 0.5862 ± 0.0004 | 2.7 ± 0.5 | 0.421           |

Theoretical curves given by the formula $R_{g}^2 = AN^{2\nu} (1 + B/N)$ are shown in figure 11 together with the data points obtained by simulation. The $\chi^2$ values per datum are shown in table 3. The $\chi^2$ values are small in the cases of $r_{ex} = 0.0$ (i.e., the ideal case) and $r_{ex} = 0.10$. Here, in the latter case the excluded volume has the largest value.

In the case of $r_{ex} = 0.10$, the estimate of exponent $\nu$ is numerically close to the exponent of SAW, as shown in table 3. We suggest that only for the case of $r_{ex} = 0.10$, the SAP is long enough so that the excluded volume is fully effective. We shall also confirm it through fitting curves to the distribution functions of the distance between two points in subsection 4.2.

In figure 12, the ratio of the mean-square radius of gyration of the cylindrical SAP with the trivial knot (0), $R_{g,0}^2$, to that of under no topological constraint (All), $R_{g,All}^2$, is plotted against the number of nodes $N$ for several different values of cylindrical radius $r_{ex}$. The ratio is always larger than 1.0 except for the case of $r_{ex} = 0.1$. Furthermore, the ratio decreases as the cylindrical radius increases. Here we remark that the values of $R_{g,All}^2$ for the different values of cylindrical radius $r_{ex}$ are given in figure 11.

The ratio of the mean-square radius of gyration of the cylindrical SAP with the trefoil knot (3), $R_{g,3}^2$, to that of under no topological constraint, $R_{g,All}^2$, is plotted in figure 13 against the number of nodes $N$ for different values of cylindrical radius $r_{ex}$. The ratio is larger than 1.0 for the cases of small values of $r_{ex}$ and large $N$. It decreases as the cylindrical radius increases.

We thus observe topological swelling in figures 12 and 13 [17]. In the cases when the cylindrical radius $r_{ex}$ is small, the mean-square radius of gyration of cylindrical SAP with a
fixed knot type becomes larger than that of no topological constraint for large enough $N$; i.e., the ratio $\frac{R_{g,K}^2}{R_{g,All}^2}$ becomes larger than 1.0 if $N$ is large enough. Here $K$ denotes a knot type. We consider that topological swelling occurs since entropic repulsive forces appear effectively among segments of the SAP under a topological constraint of a fixed knot [17, 40]. Here we remark that the ratios of the mean-square radii of gyration of $N$-noded cylindrical SAP under a topological constraint, $\frac{R_{g,K}^2}{R_{g,All}^2}$, were evaluated for the trivial and trefoil knots in [17], although the number of $N$ was limited up to $N = 1000$.

We also observe in figure 13 that the ratio $\frac{R_{g,31}^2}{R_{g,All}^2}$ is smaller than 1.0 for any value of radius $r_{ex}$ if $N$ is smaller than 200. It is due to the finite-size effect: the polymer chain is short so that the size of the polymer making the trefoil knot is rather small. However, if the chain is long enough, the necessary number of segments to make the trefoil knot becomes much smaller than the total number of segments $N$, and the rest of the chain becomes as large as SAP of the trivial knot. Therefore, the ratio $\frac{\langle R_{g,31}^2 \rangle}{\langle R_{g,All}^2 \rangle}$ becomes larger than 1.0 for large $N$. 

---

**Figure 12.** Double-logarithmic plot of the ratio of the mean-square radius of gyration for the $N$-noded SAP with trivial knot (01) to that of no topological constraint (including all knots) against the number of nodes $N$ for various different values of cylindrical radius $r_{ex}$. Error bars are not shown in the figure.

**Figure 13.** Double-logarithmic plot of the ratio of the mean-square radius of gyration for the $N$-noded SAP with the trefoil knot (31) to that of no topological constraint (including all knots) against the number of nodes $N$ for various different values of cylindrical radius $r_{ex}$. Error bars are not shown in the figure.
Distance $r(\lambda)$ between the $i$th and $j$th vertices of a long SAP of $N$ steps, where $1 \leq i < j \leq N$ and $N \gg 1$. In terms of the parameter $\lambda$ we express the difference $|i - j|$ as $|i - j| = \lambda N$ for $0 \leq \lambda \leq 1/2$.

We may consider physical backgrounds of topological swelling as follows [17]. If we assign a topological constraint on a ring polymer in solution, possible configurations of the polymer reduces very much in number. In fact, any bond crossing is prohibited in the time evolution of the ring polymer, which can be physically interpreted as effective repulsive interactions acting among segments of the ring polymer, as first pointed out by des Cloizeaux [31]. The effective repulsive forces make the average size of the ring polymer enhance if the number of segments $N$ is large enough. If $N$ is small, the average size of a knotted polymer should be smaller than that of a ring polymer with no topological constraint, since it is self-entangled. Here we should also remark that it is not clear whether the effective repulsive forces are as strong as those of the excluded volume effect or not.

Topological swelling occurs only if the excluded volume is small [17]. For $r_{ex} = 0.05$, the ratio $\langle R_{i,j}^2 \rangle_{K}/\langle R_{i,j}^2 \rangle_{All}$ becomes larger than 1.0 only at $N = 3000$, as shown in figure 13. We may therefore consider that the excluded volume effect is not compatible with the topological entropic repulsions among segments of SAP under a topological constraint.

### 4.2. Probability distribution functions of the distance between two nodes of SAP

Let us consider the probability distribution function of the distance between two nodes $i$ and $j$ of SAP with knot type $K$ consisting of $N$ cylindrical segments with radius $r_{ex}$ and of unit length. We define it by

$$p_K(r; i, j; N) = \langle \delta(r - (R_j - R_i)) \rangle_K.$$  \hspace{1cm} (37)

Here the symbol $\langle \cdot \rangle$ denotes the average over all possible configurations of cylindrical SAP of $N$ nodes having knot type $K$. For the case of no topological constraint, we denote $K$ as All, which suggests that all knots are included.

Due to the cyclic symmetry, the distribution function $p_K(r; i, j; N)$ depends only on the distance $|i - j|$. Let us introduce the parameter $\lambda$ for SAP by

$$\lambda = |j - i|/N.$$  \hspace{1cm} (38)

We thus express the probability distribution function of the distance between two points $i$ and $j$ of SAP, as $p_K(r; \lambda, N)$.

Let us denote by $R_{i,j,K}(\lambda)$ the root-mean-square distance between $i$ and $j$ of $N$-noded SAP with knot type $K$ where $i$ and $j$ are separated by $\lambda N$ steps. Here, the distance $r(\lambda)$ between $i$ and $j$ is illustrated in figure 14. It is given by the following:
By 0.02. The curves. Thus, we conclude that the fitting curves are good.

For the distance between the two nodes $i$ and $j$, $r_{i,j}$, we introduce the normalized distance $x_{i,j}$ by

$$x_{i,j} = r_{i,j}/R_{N,K} (\lambda).$$

(40)

We denote by $f_K(x; \lambda, N)$ the distribution function of normalized distance $x$ between two nodes $i$ and $j$ of $N$-noded SAP with knot $K$ consisting of cylindrical segments with radius $r_N$, where $i$ and $j$ are separated by $\lambda N$ steps. It is expressed in terms of the probability distribution function $p_K(r; \lambda, N)$ as follows:

$$f_K(x; \lambda, N) = 4\pi R_{N,K}^3 (\lambda) p_K (x R_{N,K}; \lambda, N).$$

(41)

Here we recall $|i - j| = \lambda N$.

Let us introduce the formula for fitting curves to the data of the probability distribution function of the normalized distance between two segments separated by $\lambda N$ steps, $f(x; \lambda, N)$, as follows:

$$f_K(x; \lambda, N) = C_K (\lambda) e^{\delta x (\lambda)} \exp (-D_K x^\nu)$$

(42)

where $\delta = 1/(1 - \nu)$. The constants $D$ and $C$ are given by

$$D_K = \frac{\Gamma((5 + \theta_K)/\delta K)}{\Gamma((3 + \theta_K)/\delta K)}, \quad C_K = \frac{\delta}{\Gamma((3 + \theta_K)/\delta K)} \left( \frac{\Gamma((3 + \theta_K)/\delta K)}{\Gamma((3 + \theta_K)/\delta K)} \right)^{(3 + \theta_K)/2}.$$

(43)

Here we recall that $x$ denotes the normalized distance: $x = r/R_{N,K} (\lambda)$, where $R_{N,K} (\lambda) = \sqrt{A_K (\lambda N)^3}$.

We have evaluated exponent $\nu_K (\lambda)$ of the $N$-noded cylindrical SAP with topological condition $K$ of radius $r_N$ for various values of $r_N$ such as $r_N = 0, 0.005, 0.01, 0.02, 0.05$ and 0.1, and various numbers of $N$ such as $N = 400, 800, 1600, 2000, 3000$. We have applied formula (42) to the data of the distribution function of the normalized distance between two nodes of the cylindrical SAP, and obtained the best estimates of exponents $\delta_K (\lambda)$ for each value of $\lambda$ from the fitting curves to the data. We then calculated $\nu_K (\lambda)$ from the estimates of $\delta_K (\lambda)$. Here, we have considered the three topological conditions, the trivial knot (01), the trefoil knot (31) and no topological constraint (‘IAL’), and for 25 values of $\lambda$ from 0.02 to 0.5 by 0.02. The $\chi^2$ values per datum are given by less than or equal to 1.0 or 2.0 for all the fitting curves. Thus, we conclude that the fitting curves are good.

For an illustration, in figure 15, the estimates of $\nu_{IAL} (\lambda)$ with no topological constraint (i.e. $K = IAL$) are plotted against $\lambda$ for the three cases: the thick case of $r_N = 0.10$ and $N = 3000$ (filled red circles), the thin case of $r_N = 0.005$ and $N = 1600$ (downward orange triangles) and the ideal case of $r_N = 0.0$ and $N = 1600$ (filled dark-blue diamonds). Here we plot the ideal case for reference.

In the thick case ($r_N = 0.10$ and $N = 3000$), the value of $\nu_{IAL} (\lambda)$ is almost consistent with the exponent of SAW, $\nu_{SAW} = 0.588$, over all range of $\lambda$. However, in the thin case ($r_N = 0.005$ and $N = 1600$), the value of $\nu_{IAL} (\lambda)$ is rather smaller than the exponent of SAW, $\nu_{SAW}$. Moreover, in the ideal case ($r_N = 0.0$ and $N = 1600$), the estimates of $\nu_{IAL} (\lambda)$ are almost equal to 0.5 for all values of $\lambda$.

Thus, as far as the excluded volume effect of SAP is concerned, we conclude that for $r_N = 0.10$, SAW of $N = 3000$ is large enough to see the effect of excluded volume, while for $r_N = 0.005$ and $N = 1600$, SAW of $N = 1600$ is not large enough to see it.
Figure 15. Estimates of the exponent $\nu(\lambda)$ evaluated by applying formula (42) to the distribution function of the distance between two vertices of SAP with $N$ cylindrical segments of radius $r_{ex}$ under no topological constraint.

Figure 16. Data points and fitting curves of the distribution functions $f_{K}(x; \lambda, N)$ of normalized distance $x$ between two nodes of cylindrical SAP of $N = 3000$ with radius $r_{ex} = 0.1$ (thick cylinders) at $\lambda = 0.3$ for three topological conditions: the trivial knot (01), the trefoil knot (31) and no topological constraint (All).

4.3. Exponents $\theta_{K}(\lambda)$ of short-distance correlation of SAP with knot $K$

4.3.1. The case of thick cylindrical SAP. We plotted in figure 16 the data points of distribution functions $f_{K}(x; \lambda, N)$ of normalized distance $x$ between two nodes of cylindrical SAP of $N = 3000$ consisting of cylindrical segments of radius $r_{ex} = 0.1$ of unit length (thick cylinders). Here, the two nodes are separated by $\lambda N$ steps with $\lambda = 0.3$. We consider three topological conditions: the trivial knot (01), the trefoil knot (31) and no topological constraint (All). We recall that the fitting curves are given by formula (42) with two parameters $\theta_{K}$ and $\delta_{K}$.

For all the three topological conditions, the $\chi^2$ values per datum are small. We thus find that the fitting curves to the distribution functions are good. The fitting parameters are listed in table 4. Here we recall that we have observed in figure 11 that the excluded volume effect appears clearly for SAP with $N = 3000$ segments in the case of $r_{ex} = 0.1$, i.e., the thick cylindrical SAP.
Figure 17. Estimates of $\theta_K(\lambda)$ against parameter $\lambda$ for cylindrical SAP with radius $r_{ex} = 0.1$ of $N = 3000$. Here $K$ is given by the trivial knot (01), the trefoil knot (31) and no topological constraint (All).

Figure 18. Estimates of $\nu_K(\lambda)$ against parameter $\lambda$ for cylindrical SAP with radius $r_{ex} = 0.1$ of $N = 3000$. Here $K$ is given by the trivial knot (01), the trefoil knot (31) and no topological constraint (All).

Table 4. Estimates of fitting parameters and the $\chi^2$ value per datum for the fitting curves in figure 16: $r_{ex} = 0.1$, $\lambda = 0.3$ and $N = 3000$.

| $K$         | No constraint (All) | Trivial knot (0) | Trefoil knot (31) |
|-------------|---------------------|------------------|-------------------|
| $\theta_K$ | 0.664 ± 0.004       | 0.679 ± 0.004    | 0.623 ± 0.009     |
| $\nu_K$    | 0.583 ± 0.001       | 0.583 ± 0.001    | 0.581 ± 0.002     |
| $\chi^2$/datum | 1.19             | 1.07             | 1.24              |

For the thick cylindrical SAP we plotted in figure 17 the estimates of exponent $\theta_K(\lambda)$ against $\lambda$ with 25 values of parameter $\lambda$ for three topological conditions: the trivial knot (01), the trefoil knot (31) and no topological constraint (All). All the estimates of exponent $\theta_K(\lambda)$ are roughly the same such as $\theta(\lambda) \approx 0.7$. In each topological condition $K$ the estimate of $\theta_K(\lambda)$ is almost constant with respect to parameter $\lambda$. Furthermore, they do not depend on topological conditions $K$. The exponents for the trivial knot and the trefoil knot are rather close to each other, while that of the trefoil knot is smaller than others: $\theta_0 \approx \theta_{All} > \theta_3$.

For the thick cylindrical SAP we also plotted in figure 18 the estimates of exponent $\nu_K(\lambda)$ against $\lambda$ with 25 values of parameter $\lambda$ for three topological conditions: the trivial knot (01),
Figure 19. Data points and fitting curves of the distribution functions $f_K(x; \lambda, N)$ of normalized distance $x$ between two nodes of cylindrical SAP of $N = 1600$ with radius $r = 0.005$ (thin cylinders) for topological conditions, such as the trivial knot (01), the trefoil knot (31) and no topological constraint (All) (thin cylinders).

Table 5. Estimates of fitting parameters and the $\chi^2$ value per datum for the fitting curves in figure 19: $r_{ex} = 0.005, \lambda = 0.3$ and $N = 1600$.

| $K$     | No constraint (All) | Trivial knot (0) | Trefoil knot (31) |
|---------|---------------------|------------------|-------------------|
| $\theta_K$ | 0.161 ±0.005 | 0.26 ±0.02 | 0.33 ±0.02 |
| $\nu_K$   | 0.538 ±0.001 | 0.582 ±0.004 | 0.551 ±0.004 |
| $\chi^2$/datum | 3.32   | 0.492 | 1.26 |

the trefoil knot (31) and no topological constraint (All). All of them are numerically close to the value of exponent of SAW, $\nu_{SAW} = 0.588$. The estimates of the exponent $\nu_K(\lambda)$ are independent of topological conditions. We observe that the exponent of 31, $\nu_{31}$, is a little smaller than the other two cases. As a function of the parameter $\lambda$, the estimate of the exponent $\nu_K(\lambda)$ is almost constant for each of the three topological conditions $K$.

4.3.2. The case of thin cylindrical SAP. In the case of thin cylindrical SAP with radius $r_{ex} = 0.005$ we plotted in figure 19 the data points of distribution functions $f_K(x; \lambda, N)$ of normalized distance $x$ between two nodes of cylindrical SAP of $N = 1600$ with parameter $\lambda = 0.3$. Here we recall that the two nodes of SAP are separated by $\lambda N$ steps along the chain. We consider the three topological conditions: the trivial knot (01), the trefoil knot (31) and no topological constraint (All). The fitting curves given by formula (42) are also plotted in figure 19, which are determined with two fitting parameters $\theta_K$ and $\delta_K$.

Also for the thin cylindrical SAP the $\chi^2$ values per datum are small for all the three topological conditions. We find that the fitting curves to the distribution functions are good. The fitting parameters are listed in table 5.

The estimates of exponent $\theta_K$ in the thin case are much smaller than the case of thick SAP. For instance, we have $\theta_{All} = 0.2$. It is maybe due to the fact that the excluded volume effect is not strong, yet. Here we recall that we have observed in figure 11 that the excluded volume effect does not clearly appear for SAP of $N = 1600$ segments in the case of $r_{ex} = 0.005$.  

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4.4. Correlation functions through exponents $\theta(\lambda)$

We now discuss that the distribution function of the distance between two points of SAP with knot type $K$, $p_K(r; i, j; N)$, is useful for constructing various important quantities of knotted ring polymers in solution. Let us assume that the two points are separated by $\lambda N$ steps along the chain of the SAP. Due to the translational symmetry among the vertices of SAP along the chain, the expressions of the physical quantities are much simpler than those of SAW. Here we remark that the structure factor of dilute ring polymers have been studied numerically [39].

The pair correlation function of SAP with knot $K$ is given by

$$g_K(r) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} p_K(r; i, j; N)$$

$$= \sum_{j=1}^{N} p_K(r; 0, j; N). \quad (44)$$

In terms of parameter $\lambda$, we express it as a single integral as follows:

$$g_K(r) = N \int_{0}^{1} d\lambda p_K(r; \lambda; N). \quad (45)$$

5. Diffusion constants of knotted SAP

We now evaluate the diffusion coefficient of $N$-noded cylindrical SAP with a knot type $K$ in solution by Kirkwood’s approximation:

$$D_{G,K} = \frac{k_B T}{6\pi \eta_s N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left\langle \frac{1}{|R_i - R_j|} \right\rangle_K.$$  \quad (46)

Here we recall that $\eta_s$ denotes the solvent viscosity and $\left\langle \cdot \right\rangle_K$ denotes the average over all configurations of SAP with a given knot type $K$.

The estimates of the diffusion coefficient $D_{G,K}$ of cylindrical SAP with radius $r_{ex} = 0.1$ are plotted against the number $N$ of nodes for no topological constraint denoted by $0_1$ and the trivial knot denote by $0_1$ in figure 20 in double-logarithmic scales. Here, we evaluated the ensemble average $\left\langle \frac{1}{|R_i - R_j|} \right\rangle_K$ by taking the sum over all the configurations of SAP with knot type $K$.

For the two topological conditions, $K = All$ and $K = 0_1$, the diffusion coefficients coincide with each other. Furthermore, they are well fitted by a straight line in the double-logarithmic scale. For the thick cylinder case, the topology of the majority of SAPs is given by the trivial knot, and hence $D_{G,All}$ and $D_{G,0_1}$ have the same value.

The ratio of diffusion coefficients $D_{G,K}/D_{G,0_1}$ is plotted against the number of segments $N$ in figure 21. Here we recall that the diffusion coefficient of SAP under no topological constraint and that of the trivial knot coincides numerically very well.

We observe in figure 21 that the ratio gradually decreases with respect to the number of $N$. We suggest that it reaches an asymptotically constant value at some large value of $N$. Following RG arguments we expect that the ratio should be universal and independent of details of models. It would be interesting to compare the ratio with experimental data in future.

The diffusion coefficient of the figure-eight knot has large error bars because the number of SAPs with the knot type is very small for the thick case with cylindrical radius $r_{ex} = 0.1$. 

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Figure 20. Double logarithmic plot of diffusion coefficient of \(N\)-noded cylindrical SAP under topological condition \(K\). The SAP consists of \(N\) thick cylindrical segments with radius \(r_{ex} = 0.1\) of unit length. Filled blue circle and filled red diamonds denote no topological constraint (All) and the trivial knot (0₁), respectively. The sum \(\sum_{i=1}^{N} \sum_{j=1}^{N} \langle \frac{1}{r_{ij}} \rangle_k\) is plotted.

In the method of Kirkwood’s approximation we can express diffusion coefficient \(D_{G,K}\) in terms of the probability distribution functions of the distance between two nodes of SAP. Here we take the sum over all pairs \(i\) and \(j\) of SAP as follows:

\[
D_{G,K} = \frac{k_B T}{6 \pi \eta s N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \int_0^\infty \frac{1}{r} p_K(r; i, j; N) 4\pi r^2.
\]  

(47)

Considering the cyclic symmetry of SAP we reduce the double sum into the single sum, as follows:

\[
\sum_{i=1}^{N} \sum_{j=1}^{N} \int_0^\infty \frac{1}{r} p_K(r; i, j; N) 4\pi r^2 = N \sum_{j=1}^{N} \int_0^\infty \frac{1}{r} p_K(r; 0, j; N) 4\pi r^2.
\]  

(48)

In terms of \(\lambda\) we have the following expression:

\[
D_{G,K} = \frac{k_B T}{6 \pi \eta s} \int_0^1 d\lambda \int_0^\infty \frac{1}{r} p_K(r; \lambda; N) 4\pi r^2.
\]  

(49)
6. Concluding remarks

We have shown that formula (16) gives good fitting curves to the data of the probability distribution functions of the distance between two points of SAW, \( f_0(x; N) \) and \( f_s(x; \lambda, N) \), for \( s = 1, 2 \), over a wide range of the normalized distance \( x \) such as from \( x = 0.05 \) to 1.95.

In the case of large \( x \), the distribution functions have the same asymptotic behavior: 
\[ f_s(x; \lambda, N) \propto \exp(-x^\delta) \]  
with \( \delta = 1/(1 - \nu) \) for many different values of \( \lambda \) such as from \( \lambda = 0.10 \) to 0.98. Thus, the exponent \( \delta \) does not change for \( s = 0, 1, 2 \) and for various values of \( \lambda \).

Moreover, exponent \( \delta \) does not change for any vertices \( i \) and \( j \) of \( N \)-step SAW.

We evaluated the exponents \( \theta_s \) which describe and characterize the short-distance behavior of \( f_s(x; \lambda, N) \), from the fitting curves to the data points from \( x = 0.05 \) to 1.95, which is almost the entire region of \( x \). The estimates of \( \theta_0(\lambda) \) are clearly smaller than the theoretical value \( \theta_0^{(\text{RG})} = 0.46 \) for \( 0.1 < \lambda < 0.8 \); The estimates of \( \theta_2(\lambda) \) are approximately equal to the theoretical value \( \theta_2^{(\text{RG})} = 0.71 \) for \( 0.1 < \lambda < 0.5 \).

We evaluated exponents \( \theta(i, j) \) which describe the short-distance intrachain correlation between vertices \( i \) and \( j \) of \( N \)-step SAW. They generalize des Cloizeaux’s three exponents \( \theta_s \) for \( s = 0, 1, 2 \). Expressing vertices \( i \) and \( j \) in terms of parameters \( \lambda \) and \( \mu \) we observed the crossover of exponents \( \theta(i, j) \): from \( \theta_2 \) to \( \theta_1 \) and from \( \theta_1 \) to \( \theta_0 \) as \( \lambda \) approaches 1; the exponent \( \theta(i, j) \) changes from \( \theta_2 \) to \( \theta_1 \) as the parameter \( \mu \) approaches 0.

We have shown that formula (42) gives good fitting curves to the data of the probability distribution functions of the distance between two points of cylindrical SAP. For the thick cylinder case of cylindrical radius \( r_\text{ex} = 0.1 \) the estimates of the exponent \( \theta(\lambda) \) for the short-distance correlation are a little smaller than the theoretical value \( \theta_0^{(\text{RG})} \) of SAW.

Finally, we suggest that the results of this paper should be useful for studying the scaling behavior of intrachain correlation for topological polymers with more complex structures.

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Appendix A. The estimates of exponent \( \theta_0 \) for different chain lengths

Let us consider the discrepancy between the Monte Carlo estimate \( \theta_0^{(\text{MC})} = 0.23 \pm 0.02 \) and the theoretical value \( \theta_0^{(\text{RG})} = 0.273 \). We suggest that it is mainly due to the finite-size effect but partially due to the large errors in the data.

We have evaluated the exponent \( \theta_0 \) for eight values of \( N \) other than \( N = 8000 \) such as for \( N = 1000, 2000, 3000, 4000, 5000 \) and 6000, and also for \( N = 200, 500 \). For seven values out of the eight values of \( N \), the Monte Carlo estimate of \( \theta_0 \) is smaller than 0.23 which is the estimate for \( N = 8000 \). Here, the estimates are given in table A1. It is therefore likely that the estimate of \( \theta_0 \) is smaller than the RG value due to the finite-size effect even for \( N = 8000 \), and also that the estimate becomes larger than 0.23 if \( N > 8000 \). We suggest from figure A1 that the estimate \( \theta_0 \) increases with respect to the number of steps, \( N \), quite slowly.

However, the errors are not very small such as 0.02 even for \( N = 8000 \). Thus, we do not conclude that the discrepancy is only due to the finite-size effect. It is also possible that it is due to large errors, and that we had different values from 0.27 since the estimate can deviate from the true value sometimes by twice the error bar.
Figure A1. The best estimates of exponent $\theta_0$ versus the number of steps, $N$, for SAW with different values of $N$.

Table A1. The best estimates of exponents $\theta_0$ and $\nu$ for different values of the number of steps $N$ for SAW.

| $N$  | $\theta_0$ | $\Delta \theta_0$ | $\nu$ | $\Delta \nu$ | $\chi^2$/DF |
|------|------------|-------------------|-------|--------------|-------------|
| 200  | 0.21       | 0.06              | 0.61  | 0.01         | 4.51        |
| 500  | 0.15       | 0.02              | 0.606 | 0.005        | 0.988       |
| 1000 | 0.21       | 0.03              | 0.597 | 0.006        | 1.22        |
| 2000 | 0.21       | 0.04              | 0.592 | 0.007        | 2.09        |
| 3000 | 0.16       | 0.03              | 0.605 | 0.006        | 1.27        |
| 4000 | 0.14       | 0.03              | 0.605 | 0.005        | 1.35        |
| 5000 | 0.24       | 0.04              | 0.587 | 0.007        | 1.68        |
| 6000 | 0.18       | 0.02              | 0.599 | 0.004        | 0.694       |
| 8000 | 0.23       | 0.02              | 0.589 | 0.005        | 0.814       |

Appendix B. Auto-correlation plot of the position vectors relative to the center of mass of SAW

We define the autocorrelation function $C(t)$ between the position vectors of SAW relative to the center of mass at time $t$ and those of SAW at the initial time $t = 0$ by

$$C(t) = \frac{\sum_{i=1}^{N} (R_i(0) - R_G(0)) \cdot (R_i(t) - R_G(t))}{\sum_{i=1}^{N} (R_i(0) - R_G(0))^2}. \quad (B.1)$$

Here, the symbol $R_G(t)$ denotes the position vector of the center of mass at time $t$:

$$R_G(t) = \sum_{j=1}^{N} R_j(t). \quad (B.2)$$

Here, the symbol $t$ denotes the number of the Monte Carlo steps.

In figure B1 we observe that the autocorrelation function $C(t)$ decays exponentially with respect to the number of the Monte Carlo procedures, $t$. We took $10^5$ different initial states and applied the pivot moves up to $8N$ times such as $t = 800, 4000$ and $8000$ for $N = 100, 500$ and $1000$, respectively. However, the correlation $C(t)$ has become small even for $t = 10$ and $t = 20$ as shown in figure B1.
Figure B1. Correlogram: a semi-logarithmic plot of the autocorrelation function $C(t)$ versus the number of pivot moves. The average is taken over $10^3$ samples of $N$-step SAW for $N = 100, 500$ and $1000$.

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