Linking Probabilities of Self-Avoiding Polygons

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We have numerically investigated the probability \( P_L(r) \) for a pair of self-avoiding random polygons (SAPs) being link \( L \) such that each of them have the trivial knot type and they have no overlaps among the segments where they are placed with a distance \( r \) between the centers of mass. We call it the linking probability of link \( L \). We propose the following fitting formula:

\[
P_L(r) = \exp(-\alpha r^\nu) - C \exp(-\beta r^\mu),
\]

where \( \alpha, \nu, C, \beta \) and \( \mu \) are parameters. For example, \( P_{02}(r) \) denotes the probability of the trivial link. We apply the formula also to the data of \( P_{\text{link}}(r) \), where it is given by

\[
P_{\text{link}}(r) = 1 - P_{02}(r).
\]

With respect to the \( \chi^2 \) values, the formula gives good fitting curves to the values of \( P_{\text{link}/L}(r) \) versus \( r \) obtained by simulation for \( r_d \leq 0.20 \). In the simulation we generate SAPs consisting of \( N \) spherical segments of radius \( r_d \), where the bond length, i.e. the distance between adjacent segments, is fixed to 1. We have numerically obtained \( P_{\text{link}/L}(r) \) for the cases of \( N = 32, 64, 128 \) and 256 for \( r_d = 0.00, 0.05, \ldots, 0.30 \).

1 Introduction

Recently, a number of experimental techniques have been developed and ring polymers and catenanes have been synthesized by various researchers (see [1], for instance). In the systems of ring polymers conservation of the topology plays an important role in the statistical and dynamical properties. The linking probability should be fundamental to understand the entropic behavior of topologically restricted polymers such as ring polymers.

Suppose that we have a pair of SAPs that have no overlaps among the segments when the centers of mass are separated by a distance \( r \), and also that each of the SAPs has the trivial knot type. We define the linking probability \( P_L(r) \) by the probability that such a pair of SAPs has link type \( L \). Here, \( r \) is normalized by the root-mean-square radius of gyration of the SAP. We denote by \( P_{02} \) the probability of the trivial link. We also define the linking probability \( P_{\text{link}}(r) \) by the probability that two such SAPs make a non-trivial link. In other words, we have

\[
P_{\text{link}} = \sum_{L \neq 02} P_L = 1 - P_{02}.
\]

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Although various formulas of $P_{\text{link/}L}$ as functions of $r$ have been suggested (see [2] and [3], for instance), they do not give good fitting curves to the simulation results of $P_{\text{link/}L}(r)$ with sufficiently small $\chi^2$ values. In this paper, we propose a new formula:

$$P_{\text{link/}L}(r) = \exp(-\alpha r^\nu) - C \exp(-\beta r^\mu), \quad \alpha, \nu, C, \beta \text{ and } \mu: \text{fitting parameters.} \quad (1)$$

We also show numerically how linking probability $P_{\text{link/}L}(r)$ depends on the excluded-volume.

In Section 2, we explain numerical methods of the present work in detail. The validity of the formula is confirmed in Section 3. Finally, the main results and conclusions are summarized in Section 4.

2 Procedure of simulations

We generate SAPs using the crank-shaft algorithm. It is similar to the pivot algorithm on a lattice [4]. The procedure is given as follows. Let us begin with a regular polygon of $N$ nodes. In the polygon, the beads of radius $r_d$ are located at all nodes and the bond length is given by 1. Under the self-avoiding conditions, the beads are not allowed to overlap with each other. First, we randomly choose two nodes of the polygon. Next, we rotate a sub-chain between the two nodes around the axis through them. Here the rotation angle is given by a random number. We then check all nodes whether they overlap or not. If the nodes have no overlaps, the conformation is accepted as a new one. On the other hand, if a pair of the nodes has an overlap, we return the polygon to the state before the deformation. We repeat the procedure many times. Finally, we employ the polygon as a member of an ensemble of SAP when it has an effectively independent conformation from the initial one. We should comment that an independent conformation can be practically obtained if successful deformation is repeated about $N$ times. In the present work, we perform such deformation $2N$ times to generate a SAP.

We define a self-avoiding random link by such a pair of two SAPs that have no overlaps and are put at a normalized distance $r$ between the centers of mass. Here, we assume that the two SAPs have the same $N$ and $r_d$ and both of them have the trivial knot type. They are randomly chosen from an ensemble of such SAPs. We produce $10^5$ self-avoiding random links to estimate $P_L(r)$.

The linking probability $P_L(r)$ with link type $L$ is calculated by

$$P_L(r) = \frac{M_L}{M} \quad (2)$$

where $M_L$ is the number of self-avoiding random links with link type $L$ and $M$ is the total number of all self-avoiding links, which is given by $10^5$ in our simulation.

To detect the link types of the $10^5$ self-avoiding random links, we use two link invariants: the linking number and the Alexander polynomial. By the invariants, we have practically classified the link types such as $0_1^2$, $2_1^2$, $4_1^2$ and $5_1^2$ (Fig 1).

Figure 1: Some link types
3 Results

The simulation results of $P_{\text{link/L}}(r)$ as a function of $r$ are plotted in Fig. 2 for the case of $N = 256$ for $r_d = 0.0, 0.1, 0.2$ and 0.3. The solid lines are fitting curves given by formula (1). Fig. 2 shows that formula (1) is consistent with the data.

![Graphs showing linking probabilities](image)

Figure 2: Linking probabilities $P_{\text{link/L}}(r)$ with $N = 256$. Data points of "all non-trivial links" denote those of linking probability $P_{\text{link}}(r)$. $P_{21}(r)$, $P_{41}(r)$ and $P_{51}(r)$ are the probabilities of link types $2^1_1$, $4^1_1$ and $5^1_1$. And $P_{\text{other types}}(r)$ denotes the probability that a given self-avoiding random link is equivalent to a non-trivial link other than $2^1_1$, $4^1_1$ and $5^1_1$.

The $\chi^2$ values are listed in Table 1. Note that there are 31 points on each curve. The $\chi^2$ values are sufficiently small for all the cases of $r_d \leq 0.20$. Furthermore, simulation results for the cases of $N = 32, 64$ and 128 are also approximated by the formula (1) with small $\chi^2$ values. From the results, we conclude that formula (1) gives good fitting curves to the estimates of $P_{\text{link/L}}(r)$ as a function of $r$ with respect to the $\chi^2$ values for $r_d \leq 0.20$. 

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Table 1: $\chi^2$ values of $P_{\text{link/L}}(r)$ for $N = 256$

<table>
<thead>
<tr>
<th>$L$</th>
<th>$rd = 0.00$</th>
<th>$rd = 0.05$</th>
<th>$rd = 0.10$</th>
<th>$rd = 0.15$</th>
<th>$rd = 0.20$</th>
<th>$rd = 0.25$</th>
<th>$rd = 0.30$</th>
</tr>
</thead>
<tbody>
<tr>
<td>link</td>
<td>43.4</td>
<td>33.3</td>
<td>13.0</td>
<td>12.2</td>
<td>51.3</td>
<td>143.</td>
<td>267.</td>
</tr>
<tr>
<td>$2_1^2$</td>
<td>16.7</td>
<td>17.4</td>
<td>10.1</td>
<td>13.4</td>
<td>37.1</td>
<td>153.</td>
<td>233.</td>
</tr>
<tr>
<td>$4_2^2$</td>
<td>8.00</td>
<td>9.20</td>
<td>33.5</td>
<td>42.6</td>
<td>21.8</td>
<td>15.5</td>
<td>7.80</td>
</tr>
<tr>
<td>$5_2^2$</td>
<td>12.2</td>
<td>9.20</td>
<td>13.8</td>
<td>8.60</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

From the fitting curves of $P_{\text{link/L}}(r)$ given by formula (1), we obtain the $\chi^2$ values for the case of $N = 256$ for $rd = 0.00, 0.05, \ldots$, and 0.30. It was not possible to evaluate the $\chi^2$ values for the case of $L = 5_2^2$ for $rd = 0.25$ and 0.30 because the numerical values of $P_{5_2^2}(r)$ are almost 0.

We have investigated the excluded-volume dependence of $P_{\text{link/L}}(r)$. In Fig. 2, we found that $P_L(r)$ of $L = 4_2^2, 5_2^2$ and other types decrease quickly for all values of $r$ when $rd$ increases for $rd \geq 0.20$. However, only $P_{2_2^2}(r)$ does not vanish when $rd$ is large such as $rd = 0.30$. That is, almost all the self-avoiding random links of non-trivial link types have the link type $2_2^2$ for $rd \geq 0.30$.

Furthermore, we found that the graph of $P_{2_2^2}(r)$ has a peak for all values of $rd$, and also that the peak position approaches $r \approx 0.5$ as $rd$ increases for $rd \geq 0.20$.

4 Conclusions

We proposed formula (1) to express linking probabilities $P_{\text{link}}$ and $P_L$ as a functions of $r$ for some link types such as $L = 2_1^2, 4_2^2$ and $5_2^2$. With respect to the $\chi^2$ values, formula (1) is consistent with the simulation data at least in the case of $rd \leq 0.20$.

We found that when the excluded-volume is very large, probabilities $P_L$ of non-trivial links $L$ vanish except for $P_{2_1^2}$. Moreover, the value of $P_{2_1^2}$ remains constant when $rd$ increases for $rd \geq 0.20$.

References