“Average Structure” of a Ring Polymer with the Trefoil Knot

Dept. of Physics, Keio Univ. Shinya Saka[1] and Hiroshi Takano

本研究では、結び目部分の局在の鎖長依存性を理解するために、ブラウン動力学シミュレーションを行い、“平均構造”を解析した。“平均構造”は、シミュレーションで得られた個々の構造を“平均構造”からの二乗変位が最小となるように並進・回転操作をさせた後、それらを平均した構造として反復法で得られる。鎖長の異なる三葉結び目の“平均構造”を求めた結果、環状高分子の構造は鎖長が長くなるにしたがい、結び目部分が高分子全体に広がった状態（一様状態）から結び目部分が局在した状態（相分離状態）へと変化することがわかった。

1 Introduction

The “average structures” of a single ring polymer with the trefoil knot is studied by Brownian dynamics simulations. In the previous study of knotted ring polymers, the dependences of various physical quantities on polymer length suggest that the localization of knotted parts of the ring polymer occurs for long polymer length.[1, 2] This localization-delocalization transition is considered to correspond to the change of the structure of the ring polymer from a “uniform” state for short polymer length, where the knotted parts is expanded widely along the ring polymer, to a “phase segregated” state for long polymer length, where the knotted parts is localized to a parts of the ring polymer and the rest of the ring polymer behaves like a ring polymer with the trivial knot (Figure 1). The purpose of this study is to confirm this localization of the knotted parts by the analysis of the “average structure.”

2 Model & “Average Structures”

Brownian dynamics simulations of a bead-spring model of a single ring polymer with the excluded volume chain interaction are performed. In the following, $\mathbf{R}_i$ denotes the position of the ith segment relative to the center of mass of a ring polymer with N segments. The “average structure” (AS) is obtained self-consistently by averaging many structures obtained from simulations, which are translated and rotated to be matched to the “average structure.”[3] We use three kinds of the matching operations for mth structure $\mathbf{R}_i^m$ ($m = 0, \cdots, M$), where M is the number of the structures obtained from the simulations. (1) Find a translational and rotational transformation $\mathcal{R}_m$ which minimizes $\sum_{i=1}^{N}(\mathcal{R}_m(\mathbf{R}_i^m) - \mathbf{R}_i^{\mathrm{AS}})^2$, where $\mathcal{R}_m(\mathbf{R}_i^m)$ denotes the position of the ith segment transformed by $\mathcal{R}_m$ and $\mathbf{R}_i^{\mathrm{AS}}$ represents the position of the ith segment in the average structure. (2) Find $\mathcal{R}_m$ and a shift number n_m ($= 0, 1, \cdots, N-1$) which minimize $\sum_{i=1}^{N}(\mathcal{R}_m(\mathbf{R}_{i+n_m}) - \mathbf{R}_i^{\mathrm{AS}})^2$. (3) Find $\mathcal{R}_m$, n_m and a direction sign σ_m ($= \pm 1$) which

[1]E-mail: ssaka@rk.phys.keio.ac.jp

minimize $\sum_{i=1}^{N}(\mathcal{R}_m(\mathbf{R}_{\sigma_m i+n_m}) - \mathbf{R}_i^{\mathrm{AS}})^2$. Note that the segment number i in $\mathbf{R}_i$ is considered modulo N.

3 Results & Discussion

The average structure for operation (1) changes from a double loop structure for small N to a single loop structure for large N. The double loop structure orbits the center of mass twice and the single loop orbits one onece. This transition corresponds to the localization-delocalization transition mentioned above. In this case, the average structure does not preserve the topology of the original structure. On the other hand, the average structures for operations (2) and (3) preserve the topology of the original one. Therefore, the average structures are considered to represent the most probable state of the ring polymer with the trefoil knot. The structure of the trefoil knot can be regarded as a structure consisting of three leaves. For the operation (2), one leaf becomes larger and the others become smaller. For the operation (3), Leaves change as if the largest leaf absorbs the smallest one.

The localization of knotted parts is clealy comfirmed by the average structure analysis.

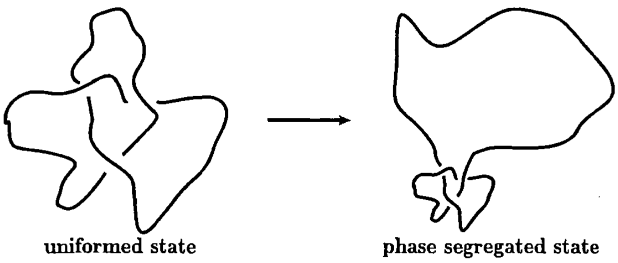

Figure 1: Localization of knotted parts

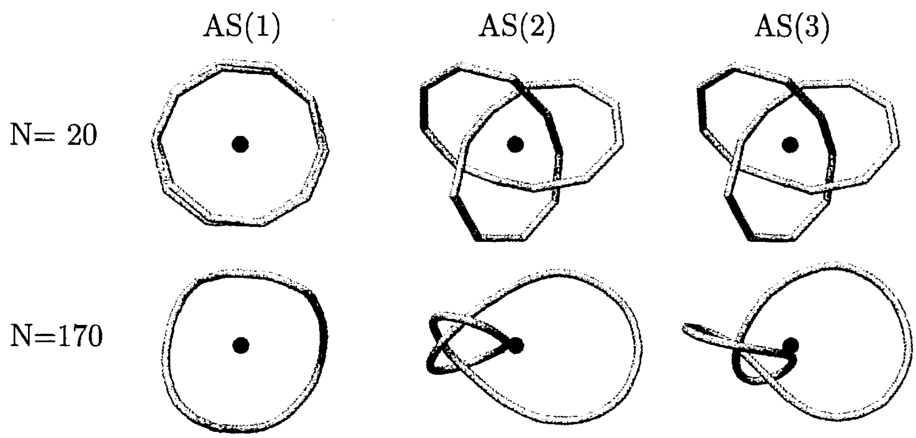

Figure 2: Average structuers of a ring polmer with the trefoil knot

References

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