Diffusion of circular DNA in solution by Brownian Dynamics

Naoko Kanaeda[1] and Tetsuo Deguchi[2], Department of Physics,
Graduate School of Humanities and Sciences, Ochanomizu University,
Ohtsuka 2-1-1, Bunkyo-ku, Tokyo 112-8610, Japan .

Abstract: We have evaluated the ratio of diffusion constant of a ring to that of a linear polymer in solution by the Brownian dynamics with both hydrodynamic and excluded-volume effects. The ratio is called the C-factor. It is given by about 1.1 when we use the bead-spring model where beads are connected by the finite extensible non-linear elongational (FENE) potential[1]. The value 1.1 is consistent with the experiments of synthesized ring polymers. However, it is different from the C-factor ～1.3 for the experiments of circular DNA. However, we found that the C-factor becomes about 1.3 when we employ the strong angle potential. It agrees well with the experimental results of circular DNA. We also suggest the strong angle potential should describe the effect of a kink, which is a sharp-bending part in a DNA.

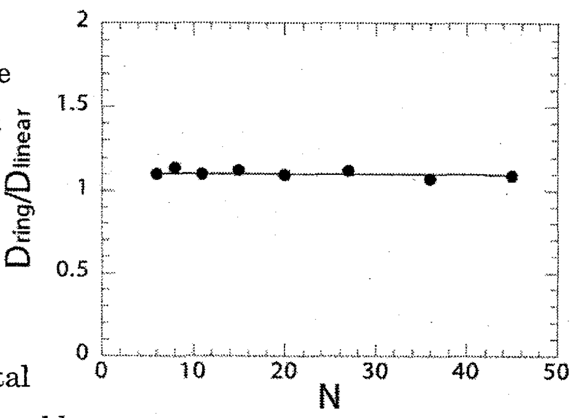
我々は環状鎖と線形鎖の拡散定数の比（C 因子）を、Brownian dynamics により排除体積効果および流体力学的相互作用を考慮して計算した。その目的は環状鎖のモデルの妥当性を、実験と比較することにより検討することである。FENE バネでつながれたバネビーズ模型では、C 因子は 1.1 であった。これは合成環状高分子の実験結果と一致する。その一方この結果は、環状 DNA による実験結果 C～1.3 と合わない。しかし強い角度ポテンシャルを与えた場合、C 因子はおよそ 1.3 になることが分かった。この強い角度ポテンシャルは、kink と呼ばれる DNA 分子内部の鋭く曲がった構造を表しているのかもしれない。

1. Introduction

In this work, we have evaluated the ratio of the diffusion constant of a ring polymer to that of a linear polymer in solution through the Brownian dynamics with hydrodynamic and excluded volume effects. The ratio is called the C-factor. In recent development of experiments, the C-factor has been measured in experiments of circular DNA quite accurately[2]. In the experiments of synthesized ring polymers, the C-factor is given by about 1.1. In the experiments of circular DNA, the C-factor is given by about 1.3. In the context of the renormalization group theories, the C-factor should be independent of the details of a polymer model. In simulation we have evaluated the C-factor of the bead-spring model whose beads are connected by the FENE potential. We then found that the C-factor is given about 1.1. However, we also found that the C-factor becomes about 1.3 when we employ the strong angle potential.

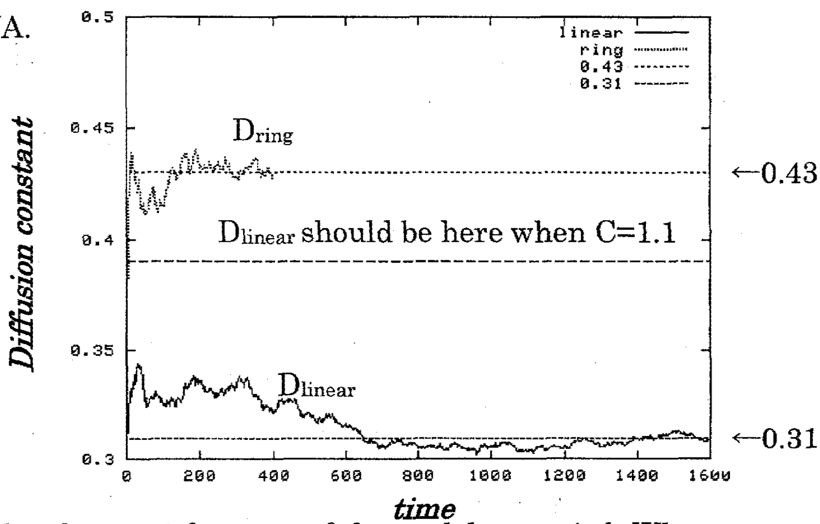
2. Result

Fig. 1 shows the N-dependence of the C-factor D_{ring}/D_{linear} from N=6 to N=45 in the case of the bead-spring model. The data is completely flat with respect to N. The data is fitted with $C=C^{\infty}(1+aN^{-\Delta})$ here $C^{\infty}=1.14$. The result is consistent with the experimental results of synthesized ring polymers. However, the estimate is not consistent with the experimental results of circular DNA. We suggest that we should employ a more complicated model in which we might have other potentials of DNA.



The C-factor is always given by about 1.1 for the most models we have tried. When we take into account the angle (whose coefficient is 10.0) and dihedral potential, C is given by about 1.1. Considering the coulomb potential, C is also given by about 1.1. Even when we use the double stranded model, C is given by about 1.1.

The C-factor is given by about 1.3 when we employ the strong angle potential with coefficient 50.0. Fig2. shows the diffusion constant of a ring and that of a linear polymer where the x axis denotes the time steps times the time interval. $D_{ring}=0.43\pm0.01$ and $D_{linear}=0.31\pm0.01$ so that $C=1.41\pm0.07$. A strong angle potential should describe the effect of a kink in DNA.



3. Conclusion

The C factor is given by about 1.1 for most of the models we tried. When we employ the strong angle potential, however, the C-factor becomes about 1.3. We suggest the strong angle potential should describe the effect of a kink, i.e. a sharp bending part of DNA.

References

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1 kanaeda@degway.phys.ocha.ac.jp 2 deguchi@phys.ocha.ac.jp