# Diffusion of supercoiled DNA and the effect of base-flipping by Brownian dynamics

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Abstract: We have evaluated the diffusion constant of a ladder-like model of supercoiled DNA (see figure) in solution through Brownian dynamics with both hydrodynamic and excluded volume effects. After
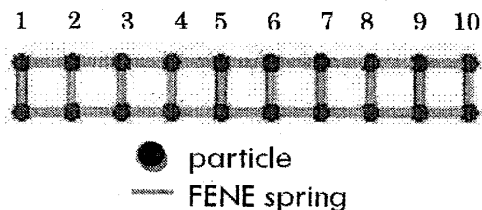
twisting the ladder we connect the ends so that its linking number L_k is conserved. We found that the diffusion constant is a linear function of L_k. In order to study the effect of base-flipping we disconnect the FENE spring potential that connects one of the pairs. The diffusion constant of the model with base-flipping becomes smaller especially when we take into account the angle potential.

Supercoiled DNA は、2本の環状鎖が絡み合っている link とみなせる。その絡み目数(linking number L_k)は、熱揺らぎのもとで保存する。我々ははしご型のモデルを作り、絡み目数と拡散の関係を調べた。はしごを何度かねじった後に右端と左端のビーズを FENE バネでつなぐことにより、絡み目数を保存する。その結果、拡散定数は絡み目数の線形関数であることが分かった。さらに我々は base-flipping の拡散に与える影響を調べるため、FENE バネでつながれたペアの1つを切り離した。その結果拡散は、base-flipping を考慮しないモデルに比較して遅くなることが分かった。この傾向は角度ポテンシャルを考慮する時、より顕著となった。

1. Introduction

We make a ladder-like model (see above figure) of supercoiled DNA. We connect the ends of the ladder after twisting it. The linking number L_k is conserved for the model. With the model, we investigate the relation between the diffusion constant and the linking number. We have evaluated the diffusion constants of the model in solution by Brownian dynamics with both hydrodynamic and excluded volume effects. We found that the diffusion is a linear function of L_k. Randall et al suggest that one of the hydrogen bond that connects the base-pairs may disappear in all atom simulations of underwound DNA. It is called "base-flipping". We examine the effect of base-flipping on diffusion. We disconnect the FENE spring potential that connects one of the pairs. The diffusion constant becomes smaller when we assume base-flipping. The diffusion constant becomes much smaller when we employ the angle potential.

2. Results

Figs 1 and 2 show the graphs of the diffusion constant and the squared gyration radius versus linking number L_k fitted with $a+b*L_k$ where a and b are fitting parameters. We found that the diffusion constant and the squared gyration radius are linear functions of L_k. The diffusion constant should be small for the model with large squared gyration radius.
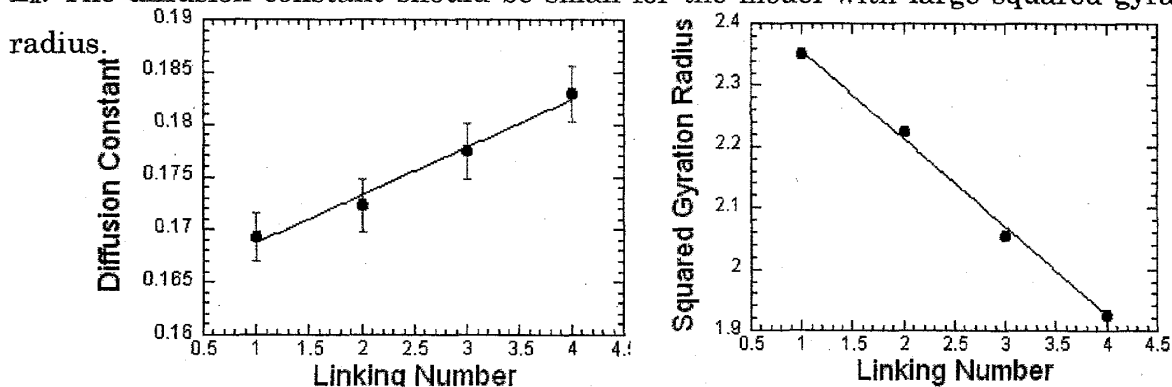
We evaluated the diffusion and squared gyration radius when we disconnect the FENE spring potential that connects one of base-pairs (we call the model bf=1). We call the model with no base-flipping "nbf". The diffusion constant and squared gyration radius of bf=1 model become smaller than those of the nbf model. Figs 3 and 4 show the diffusion constant and the squared gyration radius versus the L_k under the angle potential. The squared gyration radii of both models are almost the same. The difference of diffusion constants between the two models becomes larger than that of the model with no angle potential.
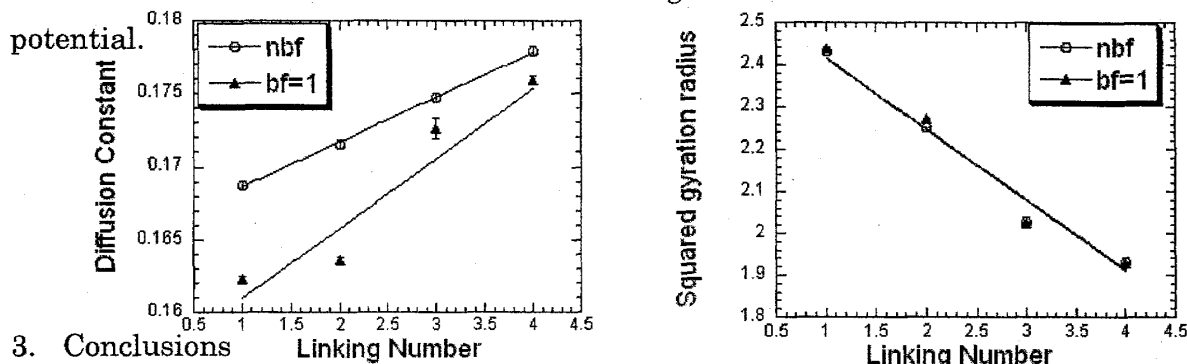
3. Conclusions

We make the ladder-like model where the linking number is conserved. We evaluated the diffusion constant against linking number L_k. We examined the effect of base-flipping and found that the diffusion constant becomes smaller for the model with base-flipping.

References [1] Randall, G.L., Zechiedrich, L. and Pettitt, B.M. DNA relieves torsional stress with localized, sequence-dependent structural failure to preserve B-form. submitted [2] Fogg, J.M., Catanese, D.J., Randall, G.L., Swick, M.C., and Zechiedrich, L. Differences between positively and negatively supercoiled DNA that topoisomerases may distinguish. *Proc. Institute Math. App. in press.*

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