Conformational Transition of Artificial Chromatins

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真核生物のDNAは塩基性のヒストンタンパク質と複合体を形成し、クロマチンとして核内にコンパクトに収納されている。最近、私達はクロマチンの折り畳み様式解明に向けて、荷電高分子とナノサイズの粒子とからなる実空間モデルを構築し研究を行っている。本発表では、そこで見られる多様な折り畳み様式について、数値実験の結果を中心に報告する。

1 Background

Unveiling the mechanism of gene expression in living organisms would be one of the main goals in modern biology. To this end, there have been many attempts to investigate the structure and dynamics of DNA-proteins ("histone") complexes known as "chromatin"; a common phasis in all eukaryotes.

The compaction of eucaryotic DNA involves several hierarchical steps (starting from the "nucleosome" formation, i.e., DNA wrapping around a histone, to highest-ordered chromosome in mitotic phase), but unfortunately, almost entire section of chromatin structure is not known yet. Although it is widely recognized that chromatins function by utilizing various specific mechanisms, one also approves of the imperative impact of general (most importantly electrostatic) interactions. Given the current poor understanding on chromatin behaviours, then, it would be a natural strategy to focus on a simple model system by constructing chromatin analogues governed by general interactions only, whose properties are controllable with comparative ease. Such an approach is also expected to provide useful insights on the application in gene therapy.

2 Folding of "Artificial Chromatin"

Our system of "artificial chromatin" consists of a long semiflexible polyelectrolyte (PE) and oppositely charged nanosized particles (NPs). They interact via steric and electrostatic (modelled by Debye-Hückel type potential) forces. This simple model exhibits a rich variety of behaviours. We first identify three distinct interaction modes between PE and NP; 1) random adsorption, 2) regular wrapping and 3) collection. These modes are shown to be highly correlated to the manner of the PE folding.

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In suitable conditions with regular wrapping mode, structures reminiscent of real chromatins are obtained. The manner of PE folding induced by the addition of NPs is markedly influenced by the salt concentration. We will argue the mechanism of the chromatin folding by analyzing real as well as numerical experiments.

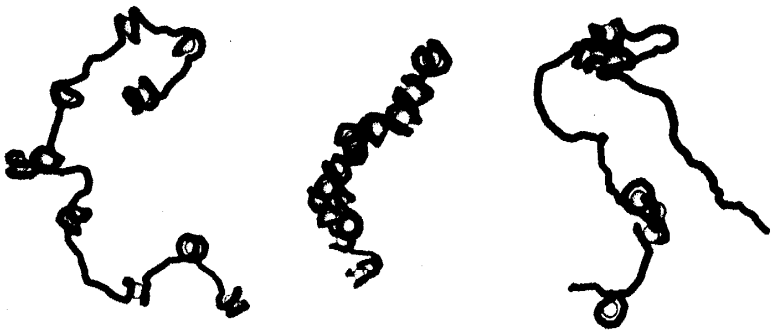

Figure 1: Typical structures of "artificial chromatin" obtained in numerical experiments. [Left] κ^{-1} (Debye length) $= 1$, N_p (number of NPs) $= 10$, [Middle] $\kappa^{-1} = 1$, $N_p = 15$, [Right] $\kappa^{-1} = 0.3$, $N_p = 10$, where the unit length is the diameter of chain monomers.

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References

1) A. Zinchenko et. al., Phys. Rev. Lett. **95** (2005), 228101.