Chromatin Fiber Model: Structure and Behaviour Under Torsion

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Chromatin is a key assembly in eucariotic cell nuclei. Despite the efforts to elucidate chromatin fiber structure, the detail of its organization remains still unknown. There are two principal classes of competing models of the fiber: the solenoid models and the zig-zag or crossed-linker models [1]. The solenoid model involves first neighboring nucleosome interaction and strong bending of the DNA linker. On the other hand, crossed-linker model involves straight linkers connecting nucleosomes located on opposite sides of the fiber, resulting in a three- dimensional zig-zag-like pattern of the linker. At the present it is impossible to resolve experimentally which model describes better the fiber structure under physiological conditions. However, certain observable features in the fiber organization are generally accepted, namely: (1) the nucleosomes are peripherally situated in the fiber and at low ionic strength form a zig-zag chain, (2) DNA linker is situated in the interior of the fiber, and (3) nucleosome-nucleosome interactions play an active role in condensation-decondensation processes. In addition, experimental evidence shows that DNA linker is responsible only on second-order effects over the fiber structure [2].

Theoretical analysis helps to elucidate which conformations are most plausibles for the fiber geometry. One of the ways to approach the problem is look for the minimal energy structure the fiber can adopt, regarding its mechanical, electrostatic and geometrical characteristics. To achive it, is necessary to identify robust parameters of the DNA-protein assembly on the smaller scale controling the conformation of the fiber on the bigger scale. Here, we propose a simple model based on the interactions between nucleosomes. The type of interaction proposed has allowed us previously to describe with success the condensed phases in acqueous solutions of nucleosomes with digested linker DNA, both in physiological conditions and in a wide range of monovalent salt concentration [3]. Taking into account the polar and chiral nature of nucleosomes, we perform detailed group theory analysis to construct the free energy of the system. The minimization process reveals the two-start helix geometry as the minimum energy structure of the fiber.

The effects of mechanical torsion applied over the fiber are also studied. We show that the two-start helix unwinding takes place in two steps: a) formation of the linear zig-zag structure for rather small torsional moment applied; b) zig-zag destruction and bead-on-a-string structure formation for moments higer than the threshold value. Such a scenario, known since many years, had no simple explanation in previous theoretical works.

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