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Equilibrium configurations of a thin elastic rod with self-contacts

Spatial equilibria of a closed thin isotropic elastic rod are considered. The thin elastic rod is a classical model for the large-scale structure of relatively long DNA molecules. Particular attention is paid to the shapes with self-contacts which are assembled from the elementary loops.

1. Introduction

Since late 70-s, there has been a considerable interest in modelling the large-scale configurations of deoxyribonucleic acid (DNA) molecules by representing them as thin elastic rods [1, 7]. The radius of the double right-handed helix of DNA is about 1 nm and its length may achieve 1000 nm or even more. Approximately 10 base pairs correspond to one turn of the helix in the relaxed state. The specific conformations of DNA can facilitate or hinder various biochemical processes, including replication, transcription, and recombination.

The elastic model of DNA was elaborated on the basis of Kirchhoff's theory of linear elastic rods [6]. The elastic properties of the rod are characterized by three stiffness coefficients: two bending and one torsional. Their effective values for the DNA rod were determined experimentally [2].

2. Model and results

The DNA molecule is modeled as a symmetric rod that means equal bending stiffnesses in any direction orthogonal to the tangent to the centreline. The rod is assumed to be inextensible, unshearable, homogeneous and straight in the unstressed state, but it may be initially twisted. According to Kirchhoff's kinetic analogy, the equations of equilibrium governing a thin elastic rod under the forces and moments only acting at its ends, are formally analogous to the equations of motion of a gyrostat in a gravitational field. The symmetric case is an analog of the gyrostat with two equal moments of inertia. The problem of the heavy symmetric top was solved exactly by Lagrange in 1788. As first shown by Ilyukhin [3], the coordinates of the centreline are easily represented in a special cylindrical reference frame. Their explicit expressions as functions of the arc length include the elliptic integrals and the Jacobian elliptic functions. Although Kirchhoff's analogy is useful for solving the initial value problem of the rod in the stationary state, it does not solve the boundary value problem (BVP) where the spatial coordinates of the both end points of the rod are specified and the direction of the end force with respect to the rod is a priori unknown.

A sufficiently long segment of DNA is often in contact with the bending protein at both its ends that justifies the formulation of a BVP for a loop shape. It may be noted here that the loops are also common elements in the structure of the ribonucleic acid (RNA) [4]. In the simplest model, the both ends of the segment join together at one point. The tangents to the centreline may have different orientations at the ends. Such shapes are called simple loops here. In some particular case, this BVP is solved analytically and a one-parameter family of shapes is obtained. As the parameter varies, the simple loop evolves from the circle to the semi-"figure-8" configuration, which is achieved for the critical value of the elliptic modulus. The end force is orthogonal to the starting circle and lies in the same plane as the "figure-8".

Also interesting are circular DNAs because, on the one hand, the applied constraint may be efficiently controlled by varying the parameters of the DNA's double helix and, on the other hand, their spatial structure has been extensively studied by using various methods. The corresponding BVP was formulated for smoothly closed configurations and their solutions were obtained [8]. Two analytical solutions of the BVP have been known: the plane circle and the "figure-8" shape. With the change of the parameter (the effective twist density), the rod adopts the various conformations, when the centreline is drawn on a toroid. For every type of the toroid, there exists a critical value of the parameter when the centreline has one point of self-contact (the so-called multi-leafed roses [5]). The simple loop solution of the first mentioned BVP serves as a basic element of the multi-leafed roses. This means that a class of non-planar analytical solutions is obtained for the smoothly closed rod. There exists a countable set of such solutions, and, for each rational number, a propeller-like multi-leafed rose may be easily computed [9]. These solutions are natural generalizations of the classical "figure-8" configuration and they also have one self-intersection point but there is no self-contact force (it is assumed that the rod has zero thickness).

The further evolution of these symmetric shapes is calculated taking into account the additional contact force in the point of self-contact. This pointwise frictionless force is assumed to be orthogonal to the plane that is tangent to the two contacting fragments of the rod. An approach is proposed for the construction of the configurations with the self-contact force by assembling them from the known simple loop elements. The key part is played by the symmetry properties of the solutions and the arrangement of their proper orientations. The result delivers non-self-penetrating conformations of the rod.

Each shape consists of an integer number of identical simple loops, parameters of which satisfy certain conditions. In the general case, the simple loops constitute a number of surfaces in a 3D parameter space. Finding a solution of only one algebraic equation is needed to define the parameters of a particular loop instance. By solving an additional algebraic equation it is possible to compute a countable set of one-parameter families of symmetric solutions with self-contact. Bifurcation diagrams are obtained for the first branches of the configurations with two and three leaves.

The analysis of the symmetric self-interacted shapes serves the purpose of better understanding of the molecular conformations on the large scale. These shapes may be used as basic solutions by numerical computation of more complex configurations, described also by more elaborated models. The presented results may be readily applied to other mechanical objects that obey the theory of thin elastic rods. The approach may be easily generalized to regularly interwound solutions, to symmetric solutions with multiple self-contacts as well as to more complex symmetric and non-symmetric solutions of various kinds.

3. Conclusions

1. The special loop solutions widen the set of the known analytically described configurations of a closed rod.
2. A countable set of the two-parameter families of the general closed-loop solutions is investigated.
3. These loop solutions serve as building elements for the symmetric multi-leafed shapes of the rod with a self-interaction point.
4. A procedure of assembling the symmetric multi-leafed solutions with self-contact forces is proposed.
5. A countable set of the one-parameter families of the multi-leafed configurations is studied.

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4. References

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