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THREE-DIMENSIONAL CONFORMATIONS OF LOOPED DNA IN AN ELASTOMECHANICAL APPROXIMATION

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ABSTRACT The equilibrium shapes of a closed DNA are investigated by employing an elastic model. An approach is developed that allows to compute space conformations for various values of parameters.

I. INTRODUCTION

The duplex DNA molecule exists in either linear or circular form. The looped DNA can wind in space to form a superhelix of a higher order, in which case it is said to be supercoiled. A large proportion of DNAs take a supercoiling form at least once in their life cycles.

Adequate understanding of how the DNA works is impossible without complete investigation of its largescale, tertiary structure, of which the mechanical properties of the molecule are known to be important determinants.

II. MODEL AND EQUATIONS

The DNA molecule can be modeled as a symmetric, homogeneous, isotropic, elastic, slender rod[1]. It is characterized by its torsional (A) and bending (C) stiffnesses (see [3] for their numerical values).

An equilibrium configuration of such an initially straight and twisted rod, submitted to external forces and to couples at its ends only, is described by the equations that are formally analogous to those governing the rotation of a symmetric gyrostat spinning about a fixed point in a gravitational field[1]. Their exact solution may be expressed in Jacobi elliptic functions and elliptic integrals.

To represent the equilibrium of the looped DNA, the model rod must be smoothly closed into a circle. Without loss of generality, its length may be put 1. The corresponding BVP results in the system of four nonlinear equations, which should be solved with respect to h, l, p and d:

$$\sqrt{p(\gamma_3-\gamma_1)} = 4m_0\boldsymbol{K}(k), \qquad m_0 = 1,2,\cdots, \tag{1}$$

$$\frac{l(d^2-l^2+h)-pd}{d^2-l^2+h-p\gamma_1}\boldsymbol{\Pi}(n,k) = (l-4\pi m_1)\boldsymbol{K}(k), \quad m_1 = 0,\pm1,\pm2,\cdots, \tag{2}$$

$$\gamma_3\boldsymbol{K}(k) = (\gamma_3-\gamma_1)\boldsymbol{E}(k) \tag{3}$$

$$\omega_1^0 = \Phi(d) - \sigma d \tag{4}$$

where $0 \le k^2 = \dfrac{\gamma_2-\gamma_1}{\gamma_3-\gamma_1} \le 1$; $n = \dfrac{p(\gamma_2-\gamma_1)}{d^2-l^2+h-p\gamma_1}$; $\boldsymbol{K}$, $\boldsymbol{E}$, $\boldsymbol{\Pi}$ are the complete elliptic integrals of the I, II and III kind, respectively, $-1 \le \gamma_1 \le \gamma_2 \le 1 < \gamma_3$ are the roots of the

cubic polynomial $f(\gamma) = (h - p\gamma)(1 - \gamma^2) - (l - d\gamma)^2$;

$$\Phi(d) = \frac{1}{2\boldsymbol{K}(k)}\left[\frac{l-d}{1-\gamma}\boldsymbol{\Pi}(n_1,k) - \frac{l+d}{1+\gamma_1}\boldsymbol{\Pi}(n_2,k)\right] + 2\pi m_2, \quad m_2 = 0, \pm 1, \pm 2, \cdots,$$

$$n_1 = \frac{\gamma_1 - \gamma_2}{\gamma_1 - 1}, \quad n_2 = \frac{\gamma_1^1 - \gamma_2}{\gamma_1 + 1}$$

The sense of the four unknown parameters is as follows:

1) $h = (2H - A\omega_1^{*2})/C$, H is the analogue of the energy in the rigid body motion;

2) $p = -2P/C$, P is the end force value;

3) $l = L/C$, L is the end torque value;

4) $d = (\omega_1^* - \omega_1^0)/(\sigma + 1)$, $\sigma = C/A - 1$ is the Poisson ratio of the rod, ω_1^0 and ω_1^* are the molecule twist rates in the relaxed and stressed state, respectively.

Eqs. (1)–(3) determine the shape of the central axis of the molecule (hence, the writhing number[2]), while Eq. (4) corresponds to the proper closure of the chains of complementary nucleotides (hence, its solutions correlate with the twisting number).

III. SOLUTIONS

In [3] two exact solutions are found that describe circular and 8-figure plane shapes. In order to obtain nonplanar solutions of the system (1)–(4), a parameter continuation approach is proposed. The plane ring may be considered as a generating solution. It can be shown by perturbation analysis that periodic solutions are born, when

$$\begin{aligned} &l = 2\pi m_1, \ m_1 = 0, \pm 1, \pm 2, \cdots, \ d = \pm 2\pi\sqrt{(m_0^2 - m_1^2)}, \ m_0 \geq m_1 \\ &h = l^2, \ p = 2ld \end{aligned} \tag{5}$$

Having chosen a set of the integers m_0, m_1 and m_2, the value of d is made slightly different and the system (1)–(3) is solved by the Newton iteration process with respect to h, l, p. The function $\Phi(d)$ may also be evaluated and the initial twist ω_1^0 may then be found from (4). The cycle repeats after that.

In Figs. 1–4 the computed functions $\Phi(d)$, $h(d)$, $l(d)$, and $p(d)$ are shown for closed conformations. The curves are marked (m_0, m_1); $m_2 = 0$ — these values correspond to non-perturbed solutions.

Continuous change of d may be interpreted either as the natural twist variation for the DNA in solution, or as the variation of the elastic properties of the molecule (hence, the coefficient α). Both cases are experimentally accessible.

In the model considered, the molecule is treated as self-penetrating.

IV. EXAMPLE

As an example, discuss the transition between the circle and the 8-figure conformations. The initial one is the plane ring: $d = 2\pi\sqrt{3}$, $l = 2\pi$, $h = 4\pi^2$, $p = 8\pi^2\sqrt{3}$ $(m_0 = 1, \ m_1 = 1)$, for which $\Phi(d) = d + 2\pi m_2$. As d decreases, the molecule begins to writhe until it forms the 8-figure at $d = 0$. After that, the self-intersection occurs and the linking number[2] changes by 2 (to compensate this, the twisting number, i.e. m_2, is changed by the same value). In

what follows, all the events take place in the reverse order and eventually the plane ring is obtained at $d = -2\pi\sqrt{3}$, $l = -2\pi$, $h = 4\pi^2$, $p = 8\pi^2\sqrt{3}$.

All these transformations can readily be demonstrated by using the model made of a rubber hose.

The developed approach and its computer program implementation permit to compute three-dimensional closed conformations of the DNA starting with an arbitrary plane ring (5).

The example stereopair of the closed molecule model is presented in Fig.5 for $d = 8.6665$, $l = 2.1132$, $h = 221.68$, $p = 310.16$, $m_0 = 3$, $m_1 = 1$, $m_2 = 25$. The linking number is $Lk = 25$, the writhing $Wr = 1.08$, and the twisting $Tw = 23.92$.

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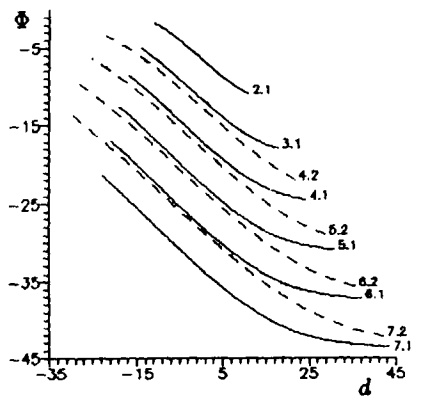

Fig.1

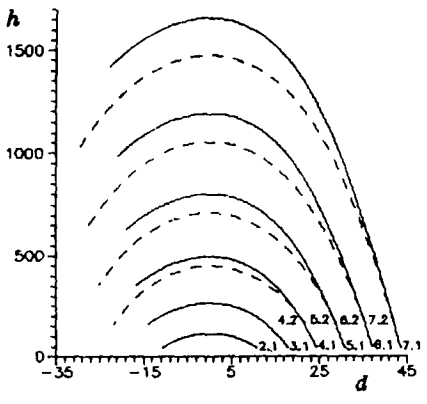

Fig.2

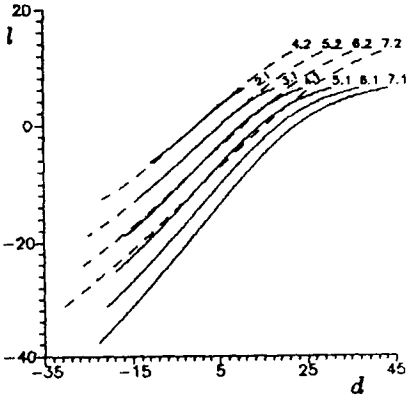

Fig.3

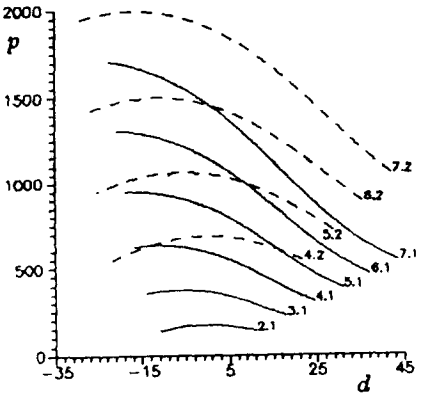

Fig.4

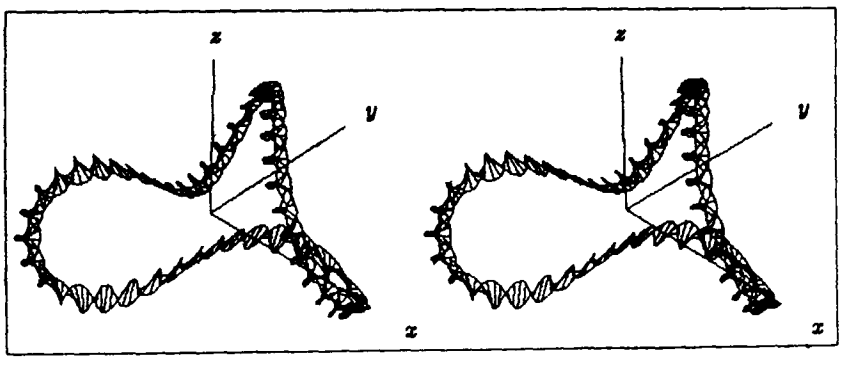

Fig.5