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BIOMECHANICS OF DNA: ROTATIONAL OSCILLATIONS OF BASES

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In the present paper we investigate the rotational oscillations of the nitrous bases that form a central base pair in a short DNA fragment consisting of three base pairs. For this purpose we use a simple mechanical model of the DNA fragment where the bases are imitated by pendulums, and the interactions between the bases are imitated by springs. It is suggested that the pendulums of the central pair oscillate, and the pendulums of neighboring pairs located at the edges of the fragment are immovable. The model takes into account the hydrogen bonds between the bases in pairs, the stacking interactions between neighboring base pairs and the helicity of the DNA structure. We derived the Lagrangian of the model system and the nonlinear equations of motions. Parameters of the equations were considered in details. We found solutions of the equations in the homogeneous case when the fragment contained only identical base pairs: Adenine-Thymine (AT) or Guanine-Cytosine (GC). The trajectories of the model system in the configuration space were also constructed in this approximation.

Keywords: DNA; mechanical model; two coupled pendulum oscillations.

1. Introduction

It is widely accepted that the DNA molecule is a complex dynamical system consisting of many different oscillating structural elements: atoms, atomic groups (sugars, phosphate groups, bases) and small fragments of polynucleotide chains. Among them rotational oscillations of bases around the sugar-phosphate chains are of special interest. These oscillations are directly connected with the process of opening of individual base pairs [6] and with the formation of so-called open states that contain several neighboring base pairs [1] with broken hydrogen bonds connecting complementary bases inside these pairs (Fig. 1). Usually the DNA molecule contains some amount of open base pairs. This phenomenon is known as “the breathing of DNA”. It is widely accepted that “the breathing” is an important element of the DNA functioning.

In most of theoretical studies of rotational oscillations of bases and their role in the opening of base pairs, the methods of molecular dynamics are used [3, 5, 8, 12, 15]. However,

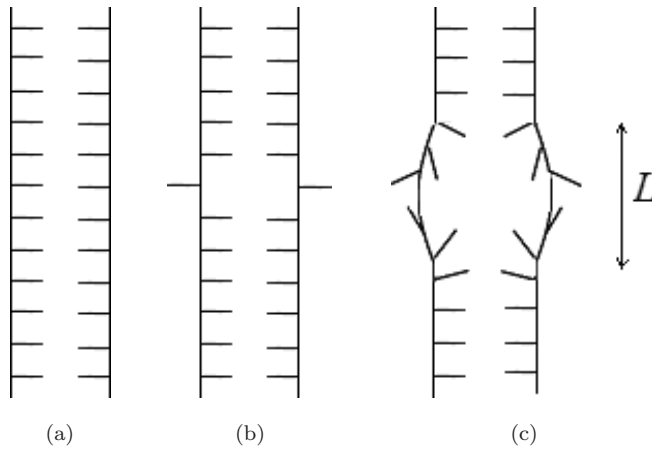


Fig. 1. Aschematic picture of different states of the double DNA chains: (a) closed state, (b) individual base pair opening, (c) open state containing several open base pairs. L is the length of the open state. The helicity of the DNA structure is not shown.

these methods are too cumbersome. A more simple approach has been proposed in the work of Englander and co-authors [1], who suggested to use a mechanical analog of DNA where the DNA bases were replaced with pendulums and the interactions between the bases were replaced with springs. This approach was developed later in the works of Yomosa [14], Takeno and Homma [9], Zhang [23]. The theme was continued in the works of Salerno [13], Cuenda and Sanchez [4], Gaeta [2], Yakushevich [16, 19, 20, 22], who improved the mechanical model by taking into account effects of asymmetry, helicity, dissipation and inhomogeneity of the molecule. These models were successfully applied to study the dynamics of open states in infinitely long double DNA chains.

In this paper, we apply the approach of Englander and co-authors [1] to study rotational oscillations of the bases forming a central pair in a short ($L = 3$ b.p.) DNA fragment. In the next section, we present the detailed description of corresponding mechanical analog, the model Lagrangian and the nonlinear equations of motions. In the Sec. 3, the parameters of the equations are considered in details. Transformation of the model equation to a more convenient form is shortly described in the Sec. 4. Results obtained in the frameworks of the mechanical model are presented in the Secs. 5–7. Discussion of the results and possible perspectives are presented in the final Sec. 8.

2. Model

Let us take a fragment of the DNA molecule (Fig. 2(a)) containing three base pairs. In accordance with the idea of Englander and co-authors [1], let us model the bases by pendulums and the interactions between the bases by springs (Fig. 2(b)). We suggest that the bases of the central (n -th) pair oscillate and the bases of two neighboring pairs ($(n-1)$ -th and $(n+1)$ -th) are immovable. To simplify calculations, it is suggested also that the bases of the central pair oscillate in the horizontal plane that is perpendicular to the main axis (z) of the molecule. To take into account the helicity of the DNA molecule, each of the three planes shown in Fig. 2(b) is turned by the angle $\varphi_0 = (2\pi/10)$.

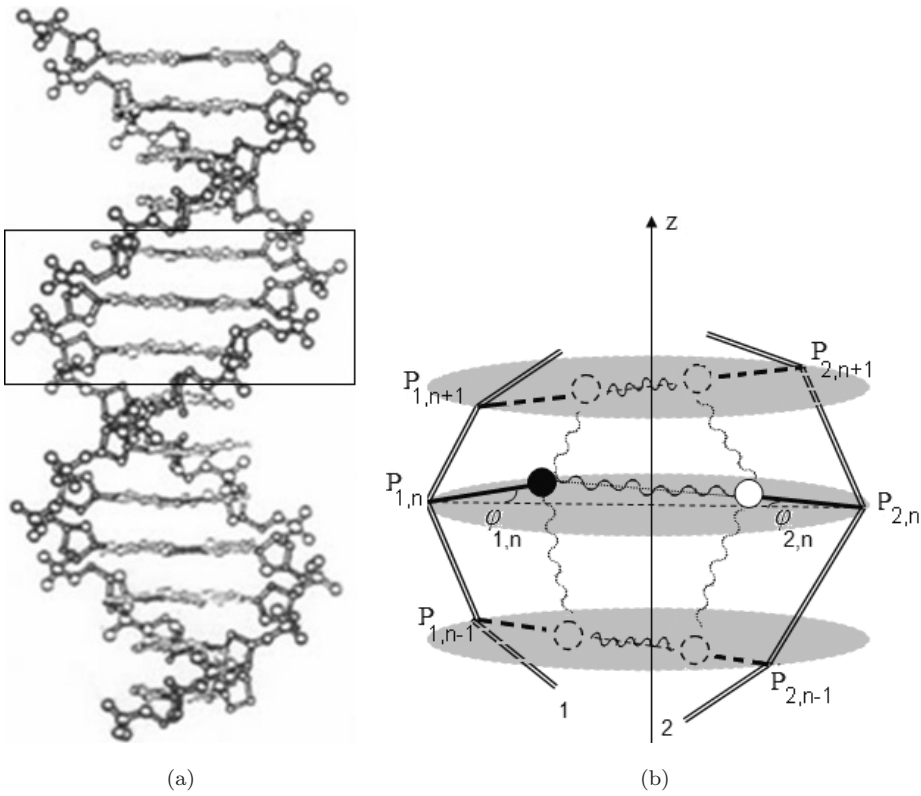


Fig. 2. Schematic picture of (a) the DNA double helix; (b) the mechanical model of the three coupled pairs of pendulums: one central (n -th) pair and two neighboring pairs ($(n - 1)$ -th and $(n + 1)$ -th).

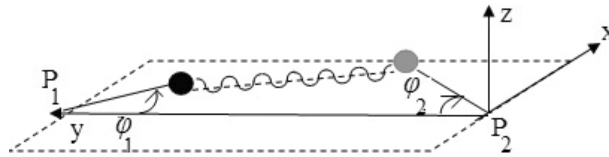


Fig. 3. Schematic picture of two coupled pendulums.

To obtain the function of Lagrange, let us begin with a simpler mechanical model consisting of one pair of nonidentical pendulums shown in Fig. 3. The function of Lagrange of this system has the form [18]

$$L_{\text{single pair}} = (1/2)[I_1(d\varphi_1/dt)^2 + I_2(d\varphi_2/dt)^2] - K_{1-2}[r_1(r_1 + r_2 + a)(1 - \cos(\varphi_1)) + r_2(r_1 + r_2 + a)(1 - \cos(\varphi_2)) - r_1r_2(1 - \cos(\varphi_1 + \varphi_2)) + (a^2/2)]. \quad (2.1)$$

Here functions $\varphi_1(t)$ and $\varphi_2(t)$ are the angles of inclination of the 1-st and 2-nd pendulums; I_1 and I_2 are their moments of inertia; K_{1-2} is the rigidity of the horizontal spring coupling the pendulums; r_1 and r_2 are the lengths the pendulums; a is the distance between masses of the pendulums when they are in the equilibrium state ($\varphi_1 = \varphi_2 = 0$).

Let us generalize formula (2.1) to pass to the case of three coupled pendulums shown in Fig. 2(b). For the purpose, let us (1) introduce two indexes, first index denoting the number of the chain, the other — the number of pair, and (2) add additional terms describing vertical interactions between pairs. We should note here that in the general case, vertical interactions between neighboring base pairs should include both stacking interactions and covalent interactions through the sugar-phosphate backbone. However, we can leave in the model only stacking interactions because covalent interactions are more rigid (see, for example, Chap. 1 in [17]), and in the first approximation the sugar-phosphate backbone can be considered as an absolutely rigid (nonmoveable) skeleton which only fixes the points $P_{1,n}$, $P_{1,n-1}$, $P_{1,n+1}$, $P_{2,n}$, $P_{2,n-1}$ and $P_{2,n+1}$ shown in Fig. 2(b). So, the generalized formula for Lagrangian takes the form

$$L = T - V \tag{2.2}$$

with kinetic energy

$$T = \sum_{i=1}^2 \sum_{j=n-1}^{n+1} (1/2)I_{i,j}(\text{d}\varphi_{i,j}/\text{d}t)^2 \tag{2.3}$$

and potential energy

$$V = U_{\text{horizontal}} + U_{\text{vertical}}, \tag{2.4}$$

where

$$\begin{aligned} U_{\text{horizontal}} &= \sum_{j=n-1}^{n+1} \{U_{1,j}(1 - \cos(\varphi_{1,j})) + U_{2,j}(1 - \cos(\varphi_{2,j})) \\ &\quad - U_{1-2,j}(1 - \cos(\varphi_{1,j} + \varphi_{2,j}))U_{0,j}\}, \\ U_{\text{vertical}} &= S_{1;n,n-1}[(\varphi_{1,n} + \varphi_0) - \varphi_{1,n-1}]^2/2 + S_{1;n,n+1}[(\varphi_{1,n+1} + \varphi_0) - \varphi_{1,n}]^2/2 \\ &\quad + S_{2;n,n-1}[(\varphi_{2,n} + \varphi_0) - \varphi_{2,n-1}]^2/2 + S_{2;n,n+1}[(\varphi_{2,n+1} + \varphi_0) - \varphi_{2,n}]^2/2. \end{aligned}$$

Here $\varphi_{i,j}(t)$ is the angular amplitude of the (i, j) -th pendulum; $I_{i,j}$ is the moment of inertia of the pendulum; $U_{1,j} = K_{1-2,j}r_{1,j}(r_{1,j} + r_{2,j} + a_j)$; $U_{2,j} = K_{1-2,j}r_{2,j}(r_{1,j} + r_{2,j} + a_j)$; $U_{1-2,j} = K_{1-2,j}r_{1,j}r_{2,j}$; $U_{0,j} = (K_{1-2,j}a_j^2/2)$; $r_{i,j}$ is the length of the (i, j) -th pendulum; $K_{1-2,j}$ is the rigidity of the horizontal spring imitating interaction between the pendulums; a_j is the distance between masses of the pendulums at the equilibrium state ($\varphi_{i,j} = 0$); $S_{1;n,n\pm 1} = Q_{1;n,n\pm 1}(r_{1,n})^2$, $S_{2;n,n\pm 1} = Q_{2;n,n\pm 1}(r_{2,n})^2$. $Q_{i;n,n\pm 1}$ is the coefficient of the rigidity of vertical springs connecting (i, n) -th and $(i, n \pm 1)$ -th pendulums; $i = 1, 2$.

Now let us take into account that only the bases of the central (n -th) pair oscillate and the bases of the two neighboring pairs ($(n - 1)$ -th and $(n + 1)$ -th) are “frozen” ($\varphi_{1,n-1} = \varphi_{1,n+1} = \varphi_{2,n-1} = \varphi_{2,n+1} = 0$). Then instead of Eqs. (2.2)–(2.4) we obtain the following Lagrangian and equations of motions

$$\begin{aligned} L_{\text{central pair}} &= (1/2)[I_1(\text{d}\varphi_1/\text{d}t)^2 + I_2(\text{d}\varphi_2/\text{d}t)^2] - [U_1(1 - \cos(\varphi_1)) + U_2(1 - \cos(\varphi_2)) \\ &\quad - U_{1-2}(1 - \cos(\varphi_1 + \varphi_2)) + U_0 + U_0^{(+)} + U_0^{(-)} + S_1^{(-)}(\varphi_1 + \varphi_0)^2/2 \\ &\quad + S_1^{(+)}(\varphi_1 - \varphi_0)^2/2 + S_2^{(-)}(\varphi_2 + \varphi_0)^2/2 + S_2^{(+)}(\varphi_2 - \varphi_0)^2/2], \end{aligned} \tag{2.5}$$

$$I_1(d^2\varphi_1/dt^2) = -U_1 \sin(\varphi_1) + U_{1-2} \sin(\varphi_1 + \varphi_2) - (S_1^{(-)} + S_1^{(+)})(\varphi_1) - \beta_1(d\varphi_1/dt), \quad (2.6)$$

$$I_2(d^2\varphi_2/dt^2) = -U_2 \sin(\varphi_2) + U_{1-2} \sin(\varphi_1 + \varphi_2) - (S_2^{(-)} + S_2^{(+)})(\varphi_2) - \beta_2(d\varphi_2/dt). \quad (2.7)$$

For convenience, we omitted here repeating index “ n ”. At the same time we introduced indexes “ $(+)$ ” and “ $(-)$ ” to denote $(n + 1)$ -th and $(n - 1)$ -th neighbors: $U_0^{(+)} = U_{0,n+1}$, $U_0^{(-)} = U_{0,n-1}$, $S_1^{(+)} = S_{1;n,n+1}$, $S_2^{(+)} = S_{2;n,n+1}$, $S_1^{(-)} = S_{1;n,n-1}$, $S_2^{(-)} = S_{2;n,n-1}$. To take into account effects of dissipation, we added terms, proportional to angular velocities $(d\varphi_1/dt)$, $(d\varphi_2/dt)$. Coefficients of dissipation β_1 and β_2 are suggested to be constants.

3. Parameters of the Model

Parameters of Eqs. (2.5)–(2.7) can be divided into two groups. First group consists of parameters I_1 , I_2 , U_1 , U_2 , U_{1-2} , U_0 , β_1 and β_2 , which do not depend on the sequence of bases in the DNA fragment considered. The other group consists of parameters $S_1^{(-)}$, $S_1^{(+)}$, $S_2^{(-)}$ and $S_2^{(+)}$, which depend on the sequence.

Let us consider the first group. The values of parameters I_1 , I_2 , β_1 and β_2 are known [21]. We present them in Table 1.

To estimate parameters U_1 , U_2 , U_{1-2} and U_0 , let us take into account that at the equilibrium point ($\varphi_1 = \varphi_2 = 0$) the energy of interaction between Adenine and Thymine is equal to $U_{0,AT} = 10 \text{ kcal/mole} = 6,95 \times 10^{-20} \text{ J}$ and the energy of interaction between Guanine and Cytosine is equal to $U_{0,GC} = 15 \text{ kcal/mole} = 10,42 \times 10^{-20} \text{ J}$. Taking into account that $K_{AT} = U_{0,AT}/a_{AT}^2 = 0,25 \text{ (J/m}^2\text{)}$ and $K_{GC} = U_{0,GC}/a_{GC}^2 = 0,36 \text{ (J/m}^2\text{)}$, we find that for AT pair

$$\begin{aligned} U_1 &= K_{AT} r_A(r_A + r_T + a_{AT}) = 26,49 \times 10^{-20} \text{ (J)}, \\ U_2 &= K_{AT} r_T(r_A + r_T + a_{AT}) = 21,92 \times 10^{-20} \text{ (J)}, \\ U_{1-2} &= K_{AT}, \quad r_A r_T = 7,06 \times 10^{-20} \text{ (J)}, \end{aligned}$$

and for GC pair

$$\begin{aligned} U_1 &= K_{GC} r_G(r_G + r_C + a_{GC}) = 37,03 \times 10^{-20} \text{ (J)}, \\ U_2 &= K_{GC} r_C(r_G + r_C + a_{GC}) = 30,53 \times 10^{-20} \text{ (J)}, \\ U_{12} &= K_{GC} r_G r_C = 9,67 \times 10^{-20} \text{ (J)}. \end{aligned}$$

Now let us estimate the other group of parameters ($S_1^{(-)}$, $S_1^{(+)}$, $S_2^{(-)}$ and $S_2^{(+)}$). Because the values of the parameters depend on the sequence of the bases in the DNA fragment

Table 1. Parameters of Eqs. (2.5)–(2.7).

Central base pair	I_1 [$10^{-44} \text{ kg} \cdot \text{m}^2$]	I_2 [$10^{-44} \text{ kg} \cdot \text{m}^2$]	U_1 [10^{-20} J]	U_2 [10^{-20} J]	U_{1-2} [10^{-20} J]	U_0 [10^{-20} J]	β_1 [10^{-34} Js]	β_2 [10^{-34} Js]
AT	7.610	4.86	26.49	21.92	7.06	6.95	4.25	3.52
GC	8.22	4.11	37.03	30.53	9.67	10.42	4.18	3.45

considered we need to choose some sequence. As an example, let us consider two simple cases when all pairs are identical

$$\begin{aligned} &| - A = T - | \\ &| - A = T - | \\ &| - A = T - | \end{aligned} \tag{3.1}$$

and

$$\begin{aligned} &| - G \equiv C - | \\ &| - G \equiv C - | \\ &| - G \equiv C - | \end{aligned} \tag{3.2}$$

In both cases, we have $S_1^{(-)} = S_1^{(+)}$, $S_2^{(-)} = S_2^{(+)}$. Taking into account that the values of stacking energy between the base pairs are equal to [11]

$$E_{\text{stack}} \begin{pmatrix} A & T \\ A & T \end{pmatrix} = 3.73 \times 10^{-20}(\text{J}) \quad \text{and} \quad E_{\text{stack}} \begin{pmatrix} G & C \\ G & C \end{pmatrix} = 5.74 \times 10^{-20}(\text{J})$$

we easily find

$$(S_1^{(-)} + S_2^{(-)})_{\text{AT}} = (S_1^{(+)} + S_2^{(+)})_{\text{AT}} = 2E_{\text{stack}} \begin{pmatrix} A & T \\ A & T \end{pmatrix} (2\pi/10)^{-2} = 18,92 \times 10^{-20}(\text{J}),$$

$$(S_1^{(-)} + S_2^{(-)})_{\text{GC}} = (S_1^{(+)} + S_2^{(+)})_{\text{GC}} = 2E_{\text{stack}} \begin{pmatrix} G & C \\ G & C \end{pmatrix} (2\pi/10)^{-2} = 29,10 \times 10^{-20}(\text{J}),$$

and hence the coefficients of rigidity of vertical springs are equal to

$$\underline{K}_{\text{AT}} = 0,33 (\text{J}/\text{m}^2), \quad \underline{K}_{\text{GC}} = 0,53 (\text{J}/\text{m}^2).$$

As a result we find that

$$\begin{aligned} (S_1^{(-)})_{\text{AT}} &= (S_1^{(+)})_{\text{AT}} = \underline{K}_{\text{AT}}(r_A)^2 = 11,23 \times 10^{-20}(\text{J}), \\ (S_2^{(-)})_{\text{AT}} &= (S_2^{(+)})_{\text{AT}} = \underline{K}_{\text{AT}}(r_T)^2 = 7,69 \times 10^{-20}(\text{J}), \\ (S_1^{(-)})_{\text{GC}} &= (S_1^{(+)})_{\text{GC}} = \underline{K}_{\text{GC}}(r_G)^2 = 17,32 \times 10^{-20}(\text{J}), \\ (S_2^{(-)})_{\text{GC}} &= (S_2^{(+)})_{\text{GC}} = \underline{K}_{\text{GC}}(r_C)^2 = 11,78 \times 10^{-20}(\text{J}). \end{aligned}$$

4. Transformation

To simplify further calculations, let us make transformation

$$t = \eta\tau, \quad \eta = 10^{-12}. \tag{4.1}$$

Then Eqs. (2.6)–(2.7) take the form

$$\underline{I}_1(d^2\varphi_1/d\tau^2) = -\underline{U}_1 \sin(\varphi_1) + \underline{U}_{1-2} \sin(\varphi_1 + \varphi_2) - (\underline{S}_1^{(-)} + \underline{S}_1^{(+)})(\varphi_1) - \underline{\beta}_1(d\varphi_1/d\tau), \tag{4.2}$$

$$\underline{I}_2(d^2\varphi_2/d\tau^2) = -\underline{U}_2 \sin(\varphi_2) + \underline{U}_{1-2} \sin(\varphi_1 + \varphi_2) - (\underline{S}_2^{(-)} + \underline{S}_2^{(+)})(\varphi_2) - \underline{\beta}_2(d\varphi_2/d\tau). \tag{4.3}$$

Table 2. Parameters of Eqs. (4.2)–(4.3).

Central base pair	$\underline{I}_{1,n}$ [kg · m ²]	$\underline{I}_{2,n}$ [kg · m ²]	$\underline{U}_{1,n}$ [J]	$\underline{U}_{2,n}$ [J]	$\underline{U}_{1-2,n}$ [J]	$\underline{U}_{0,n}$ [J]	$\underline{\beta}_{2,n}$ [Js]	$\underline{\beta}_{1,n}$ [Js]	$\underline{\beta}_{1,n}$ [J]	$\underline{S}_{2,n}$ [J]
AT	7.60700	4.8623	26.4863	21.9197	7.0630	6.9477	0.0425	0.0352	11.2290	7.6916
GC	8.2174	4.1069	37.0283	30.5321	9.6685	10.4216	0.0418	0.0345	17.3237	11.7799

Recalculated parameters of model Eqs. (4.2)–(4.3) are presented in Table 2.

5. Potential Energy Surface

According to (2.5) potential energy of the model system is equal to

$$\begin{aligned}
 V_{\text{central pair}} = & U_1(1 - \cos(\varphi_1)) + U_2(1 - \cos(\varphi_2)) - U_{1-2}(1 - \cos(\varphi_1 + \varphi_2)) \\
 & + U_0 + U_0^{(+)} + U_0^{(-)} + S_1^{(-)}(\varphi_1 + \varphi_0)^2/2 + S_1^{(+)}(\varphi_1 - \varphi_0)^2/2 \\
 & + S_2^{(-)}(\varphi_2 + \varphi_0)^2/2 + S_2^{(+)}(\varphi_2 - \varphi_0)^2/2.
 \end{aligned} \tag{5.1}$$

After transformation (4.1) formula (5.1) takes the form

$$V_{\text{central pair}}(\varphi_1, \varphi_2) = \underline{V}(\varphi_1, \varphi_2) \times 10^{-20}, \tag{5.2}$$

where

$$\begin{aligned}
 \underline{V}(\varphi_1, \varphi_2) = & \underline{U}_1(1 - \cos(\varphi_1)) + \underline{U}_2(1 - \cos(\varphi_2)) - \underline{U}_{1-2}(1 - \cos(\varphi_1 + \varphi_2)) \\
 & + \underline{U}_0 + \underline{U}_0^{(+)} + \underline{U}_0^{(-)} + \underline{S}_1^{(-)}(\varphi_1 + \varphi_0)^2/2 + \underline{S}_1^{(+)}(\varphi_1 - \varphi_0)^2/2 \\
 & + \underline{S}_2^{(-)}(\varphi_2 + \varphi_0)^2/2 + \underline{S}_2^{(+)}(\varphi_2 - \varphi_0)^2/2.
 \end{aligned} \tag{5.3}$$

Results of calculations of the function $\underline{V}(\varphi_1, \varphi_2)$ obtained with the help of the Program MAPLE and parameters presented in Table 2 are shown in Fig. 4.

The surfaces have minimum in the vicinity of the equilibrium point $\{\varphi_1 = 0; \varphi_2 = 0\}$, the white surface being deeper than the gray one. This means that it is easier to activate oscillations in the fragment with sequence (3.1) than with sequence (3.2).

6. Particular Case: Analytical Solutions in the Linear (Harmonic) Approximation

Let us suggest that the angular amplitudes $\varphi_1(t), \varphi_2(t)$ are small. Then Eqs. (4.2)–(4.3) can be linearized

$$\underline{I}_1(d^2\varphi_1/d\tau^2) = -[\underline{U}_1 + 2(\underline{S}_1^{(-)} + \underline{S}_1^{(+)})](\varphi_1) + \underline{U}_{12}(\varphi_1 + \varphi_2) - \underline{\beta}_1(d\varphi_1/d\tau), \tag{6.1}$$

$$\underline{I}_2(d^2\varphi_2/d\tau^2) = -[\underline{U}_2 + 2(\underline{S}_2^{(-)} + \underline{S}_2^{(+)})](\varphi_2) + \underline{U}_{12}(\varphi_1 + \varphi_2) - \underline{\beta}_2(d\varphi_2/d\tau). \tag{6.2}$$

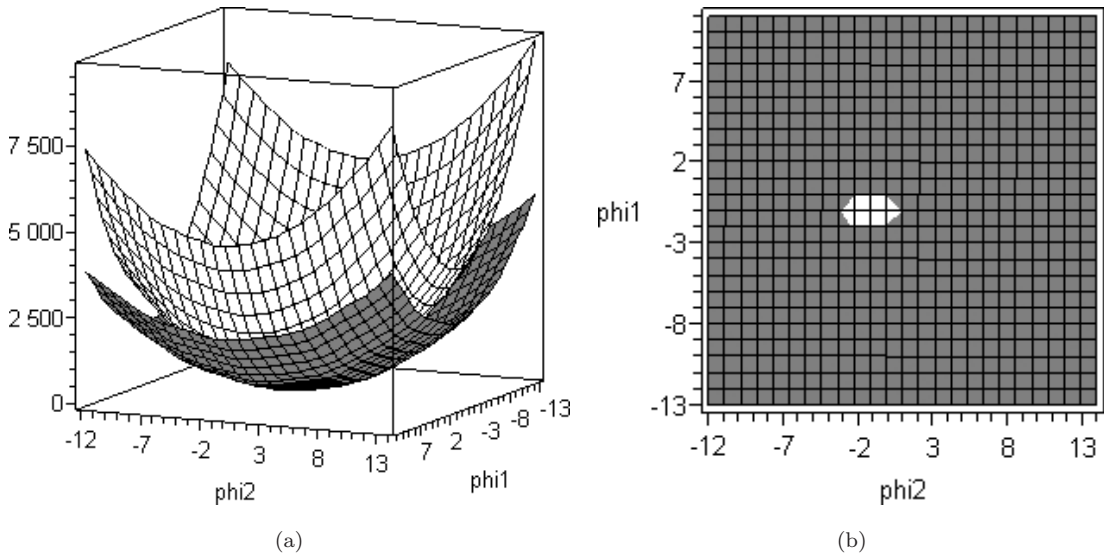


Fig. 4. Two potential energy surfaces: white surface corresponds to AT oscillating central pair and gray surface — to GC oscillating central pair. View from the side (a), and view from below (b).

Analytical solutions of Eqs. (6.1)–(6.2) can be easily found with the help of standard theory of oscillations [10]. The results of calculations can be written as

$$\begin{aligned}
 \varphi_1(\eta\tau) &= A_{(-)}\underline{I}_1^{-1/2}\exp(-\underline{\delta}_1\tau)\cos(\underline{w}_{(-)}\tau - \underline{\alpha}_{(-)}) \\
 &\quad + A_{(+)}\underline{I}_1^{-1/2}\exp(-\underline{\delta}_1\tau)\cos(\underline{w}_{(+)}\tau - \underline{\alpha}_{(+)}), \\
 \varphi_2(\eta\tau) &= A_{(-)}\underline{I}_2^{-1/2}p^{(-)}\exp(-\underline{\delta}_2\tau)\cos(\underline{w}_{(-)}\tau - \underline{\alpha}_{(-)}) \\
 &\quad + A_{(+)}\underline{I}_2^{-1/2}p^{(+)}\exp(-\underline{\delta}_2\tau)\cos(\underline{w}_{(+)}\tau - \underline{\alpha}_{(+)}),
 \end{aligned}
 \tag{6.3}$$

where $\underline{\delta}_1 = \underline{\beta}_1/2\underline{I}_1$; $\underline{\delta}_2 = \underline{\beta}_2/2\underline{I}_2$; $p^{(-)} = (\underline{w}_{(-)}^2 - \underline{a}_{(1)})/\underline{c}$; $p^{(+)} = (\underline{w}_{(+)}^2 - \underline{a}_{(2)})/\underline{c}$; $\underline{a}_{(1)} = \underline{A}_1 - \underline{\delta}_1^2$; $\underline{a}_{(2)} = \underline{A}_2 - \underline{\delta}_2^2$; $\underline{A}_1 = [\underline{U}_1 + 2(\underline{S}_1^{(-)} + \underline{S}_1^{(+)}) - \underline{U}_{1-2}]/\underline{I}_1$; $\underline{A}_2 = [\underline{U}_2 + 2(\underline{S}_2^{(-)} + \underline{S}_2^{(+)}) - \underline{U}_{1-2}]/\underline{I}_2$; $\underline{c} = -\underline{U}_{1-2}/(\underline{I}_1\underline{I}_2)^{1/2}$; the amplitudes $A_{(-)}$, $A_{(+)}$ and phases $\alpha_{(-)}$, $\alpha_{(+)}$ are constants that are determined by initial conditions, whereas the frequencies $\underline{w}_{(-)}$, $\underline{w}_{(+)}$ are determined by formula

$$\underline{w}_{(\pm)} = \{(\underline{a}_{(1)} + \underline{a}_{(2)})/2 \pm [(1/4)(\underline{a}_{(1)} - \underline{a}_{(2)})^2 + \underline{c}^2]^{1/2}\}^{1/2}.
 \tag{6.4}$$

The data presented in Tables 3–5 show that the including of the stacking interactions into the model leads to the substantial increasing of the values of the frequencies. At the same time, the including of the helicity does not change the frequencies.

Table 3. Frequencies calculated in the general case.

General case	$\underline{w}_{(+)}$	$\underline{w}_{(-)}$
AT	3.00	2.98
GC	3.77	3.76

Table 4. Frequencies calculated without stacking.

Without stacking	$\underline{w}_{(+)}$	$\underline{w}_{(-)}$
AT	1.69	1.66
GC	2.06	2.04

Table 5. Frequencies calculated without stacking and helicity.

Without stacking and helicity	$\underline{w}_{(+)}$	$\underline{w}_{(-)}$
AT	1.69	1.66
GC	2.06	2.04

7. General Case: Numerical Solutions and Trajectories in the Configuration Space

To find solutions in the general (nonlinear) case, it is convenient to rewrite the initial two partial differential equations as the following four ordinary differential equations

$$\begin{aligned}
 d\varphi_1/d\tau &= \gamma_1, \\
 d\varphi_2/d\tau &= \gamma_2, \\
 d\gamma_1/d\tau &= -\underline{a}_1 \sin \varphi_1 + \underline{d}_1 \sin(\varphi_2 + \varphi_1) - \underline{s}_1(\varphi_1) - \underline{b}_1\gamma_1, \\
 d\gamma_2/d\tau &= -\underline{a}_2 \sin \varphi_2 + \underline{d}_2 \sin(\varphi_2 + \varphi_1) - \underline{s}_2(\varphi_2) - \underline{b}_2\gamma_2,
 \end{aligned}
 \tag{7.1}$$

and then to solve them numerically [7]. Here $\underline{a}_1 = (\underline{U}_1/\underline{I}_i)$; $\underline{a}_2 = (\underline{U}_2/\underline{I}_2)$; $\underline{d}_1 = (\underline{U}_{1-2}/\underline{I}_i)$; $\underline{d}_2 = (\underline{U}_{1-2}/\underline{I}_2)$; $\underline{b}_1 = (\underline{\beta}_1/\underline{I}_1)$; $\underline{b}_2 = (\underline{\beta}_2/\underline{I}_2)$; $\underline{s}_1 = 2(\underline{S}_1^{(-)} + \underline{S}_1^{(+)})/\underline{I}_1$; $\underline{s}_2 = 2(\underline{S}_2^{(-)} + \underline{S}_2^{(+)})/\underline{I}_2$. Reestimated coefficients of Eqs. (7.1) are presented in Table 6.

The graphs of the solutions of Eqs. (7.1) calculated with the Program Maple are shown in Fig. 5. Trajectories in configuration space are shown in Fig. 6. In both cases, initial conditions are suggested to be $\varphi_1(0) = 0, 1; \varphi_2(0) = 0; \gamma_1(0) = \gamma_2(0) = 0$.

Note that the forms of the solutions and of the trajectories calculated for two different homogeneous sequences ((3.1) and (3.2)) differ from one another. So, we can state that the dynamics of the model proposed is really sensitive to the sequence of bases.

To understand the role of stacking interactions, we present Figs. 7 and 8 with solutions and the trajectories calculated in the absence of stacking interactions.

Comparison of the graphs calculated with and without stacking interactions shows that the solutions and the trajectories obtained in these two cases are quite different. So, this confirms once more that the including into the model of the stacking interactions is necessary and important.

Table 6. Coefficients of Eqs. (7.1).

Central base pair	\underline{a}_1	\underline{a}_2	\underline{d}_1	\underline{d}_2	\underline{b}_1	\underline{b}_2	\underline{s}_1	\underline{s}_2
AT	3,48	4,51	0,93	1,45	0,0056	0,0072	5,90	6,33
GC	4,51	7,43	1,18	2,35	0,0051	0,0084	8,43	17,3

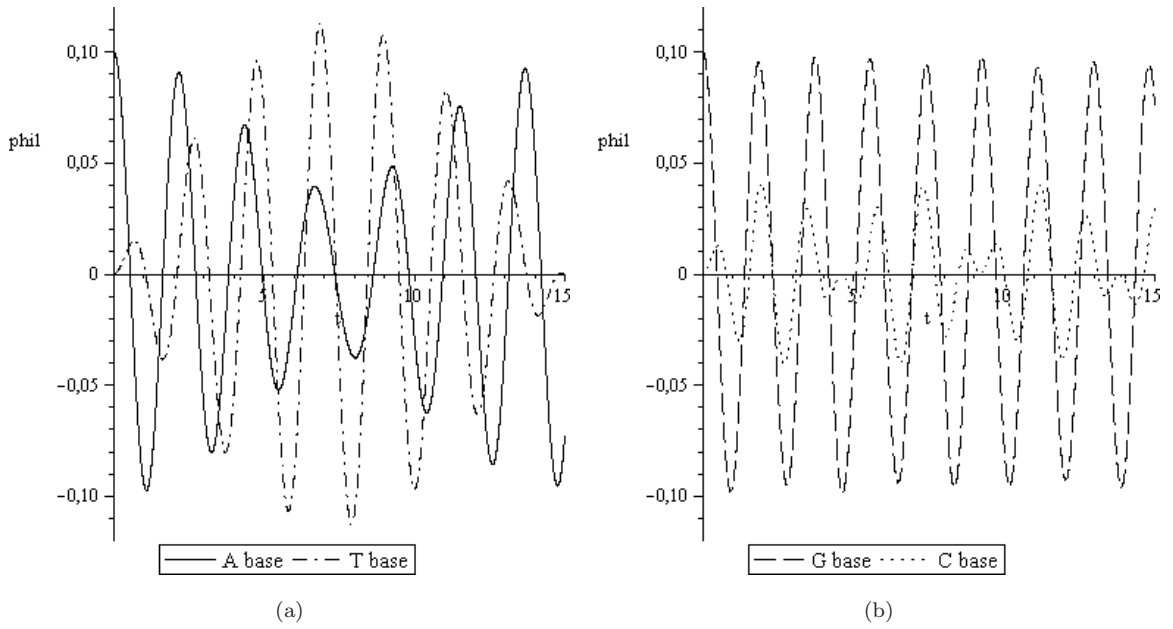


Fig. 5. Solutions of Eqs. (7.1) obtained for (a) AT and (b) GC central pairs. Solid line is used to show oscillations of Adenine, dash-dotted — Thymine, dashed — Guanine, dotted — Cytosine.

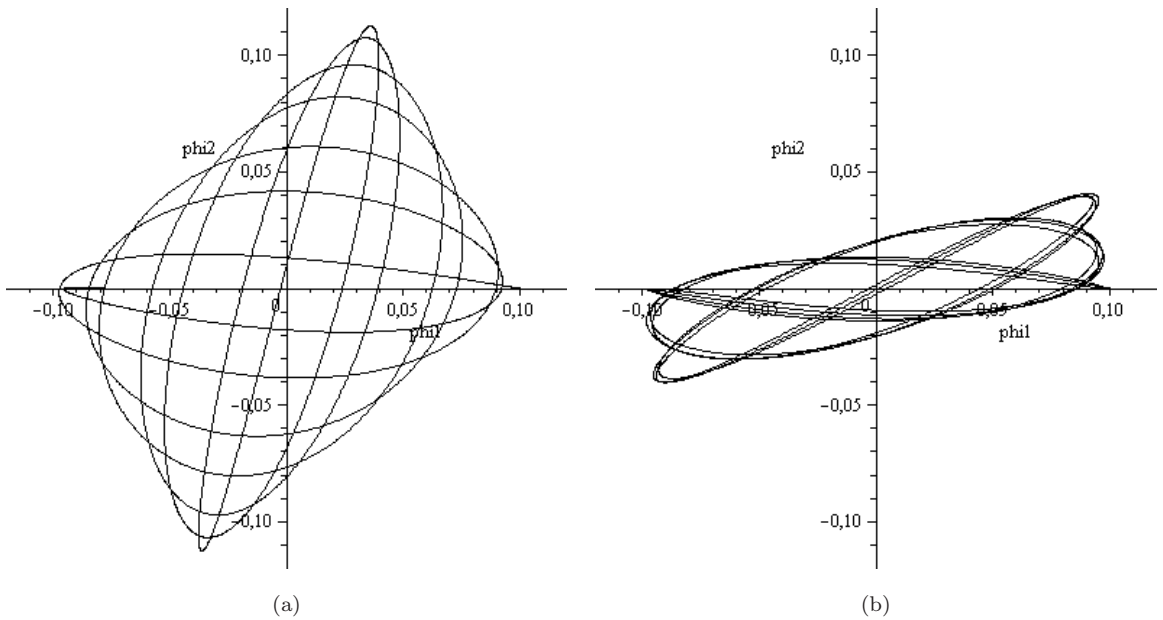


Fig. 6. Trajectories in configuration space $\{\varphi_1(t), \varphi_2(t)\}$ obtained for (a) AT and (b) GC central pairs.

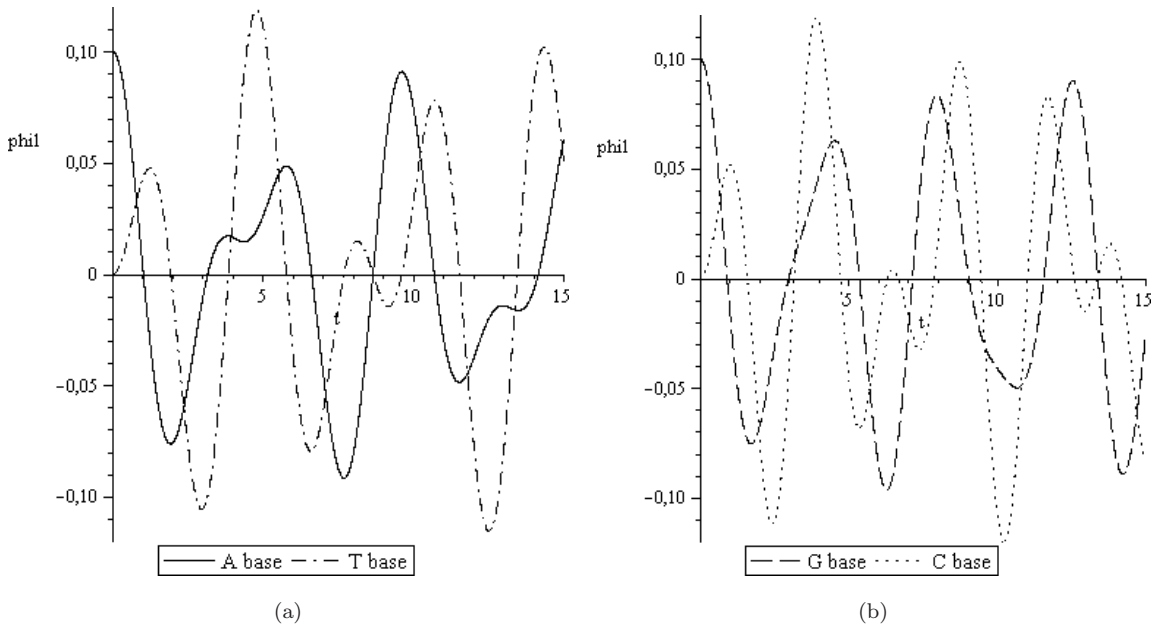


Fig. 7. Solutions of Eqs. (7.1) obtained under condition $S_1^{(-)} = S_1^{(+)} = S_2^{(-)} = S_2^{(+)} = 0$ for (a) AT and (b) GC central pairs. Solid line is used to show oscillations of Adenine, dash-dotted — Thymine, dashed — Guanine, dotted — Cytosine.

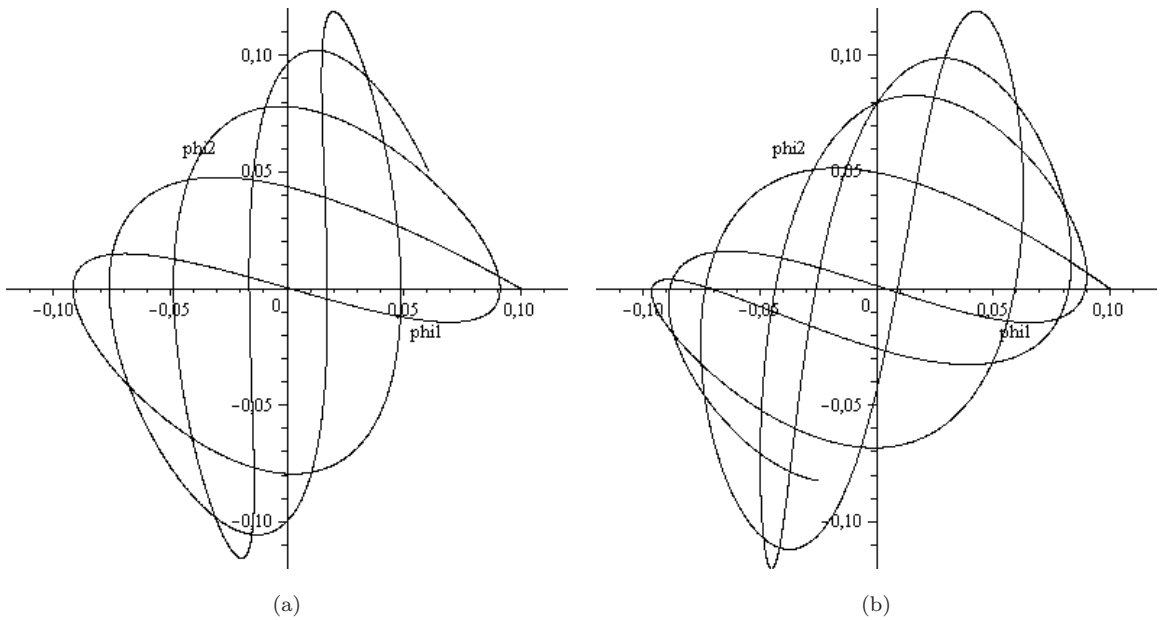


Fig. 8. Trajectories in configuration space $\{\varphi_1(t), \varphi_2(t)\}$ obtained under condition $S_1^{(-)} = S_1^{(+)} = S_2^{(-)} = S_2^{(+)} = 0$ for (a) AT and (b) GC central pairs.

8. Discussion and Conclusions

In this paper, rotational oscillations of the nitrous bases forming a central base pair in a short ($L = 3$ b.p.) DNA fragment have been investigated. For this purpose, the mechanical model has been constructed. The model takes into account (1) hydrogen interactions between bases in pairs, (2) stacking interactions between neighboring base pairs, and (3) helicity of the DNA. At the same time, the model does not take into account oscillations of the bases in the base pairs located at the edges of the DNA fragment.

We applied the mechanical model to obtain the function of Lagrange, to derive equations of motions, to find analytical solutions in the harmonic approximation and numerical solutions in the general (nonlinear) case, to construct the potential energy surface and to obtain the trajectories of the dynamical system in configuration space.

We compared the solutions and trajectories calculated for two particular cases:

- (1) for the model fragment consists of only AT base pairs and
- (2) for the model fragment consists of only GC base pairs.

We found that the solutions and trajectories noticeably differ. This result confirms quantitatively that the rotational dynamics of the DNA bases does depend on the composition of the DNA fragment.

From the analysis of the potential energy surfaces obtained for these two particular cases we can conclude that it is easier to activate rotational oscillations of the bases in the DNA fragment consisting of AT base pairs than in the DNA fragment consisting of only GC base pairs.

Comparing the graphs that we obtained from calculations made with and without stacking interactions, shows a noticeable difference. So, we confirm quantitatively that the stacking interactions play an important role in the rotational dynamics of bases, and they should be included into mechanical model of DNA.

At the same time, comparing the results that we obtained with and without helicity, shows that the helicity does not play an important role and can be omitted. Maybe situation will be different in the case of nonidentical base pairs.

The approach proposed has good perspectives. It can be applied to study rotational oscillations of the bases in the DNA fragments consisting of more than three base pairs. Moreover, the approach can be generalized to apply to DNA fragments with nonidentical base pairs. One can expect that comparing the dynamical properties of the DNA fragments having different sequences of bases will permit to find the relations between rotational base dynamics and functional properties of the DNA fragments.

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References

- [1] S. W. Englander, N. R. Kallenbach, A. J. Heeger, J. A. Krumhansl and A. Litwin, Nature of the open state in long polynucleotide double helices: Possibility of soliton excitations, *Proc. Natl. Acad. Sci.* **77** (1980) 7222–7226.

- [2] G. Gaeta, Solitons in planar and helicoidal Yakushevich model of DNA dynamics, *Phys. Lett. A* **168** (1992) 383–390.
- [3] E. Giudice, P. Várnai and R. Lavery, Base pair opening within B-DNA: Free energy pathways for GC and AT pairs from umbrella sampling simulations, *Nucleic Acids Res.* **31** (2003) 1434–1443.
- [4] S. Cuenda and A. Sánchez, Disorder and fluctuations in nonlinear excitations in DNA, *Fluctuation and Noise Letters* **4** (2004) L491–L504.
- [5] M. Guéron, M. Kochoyan and J.-L. Leroy, A single mode of DNA base-pair opening drives imino proton exchange, *Nature* **328** (1987) 89–92.
- [6] A. Krueger, E. Protozanova and M. Frank-Kamenetskii, Sequence-dependent base pair opening in DNA double helix, *Biophys. J.* **90** (2006) 3091–3099.
- [7] A. P. Kuznetsov, S. P. Kuznetsov and N. M. Ryskin, *Nonlinear Oscillations* (Fizmatgiz, Moscow, 2002, in Russian).
- [8] A. Lebrun and R. Lavery, Modeling the mechanics of a DNA oligomer, *J. Biomol. Struct. Dynam.* **16** (1998) 593–604.
- [9] S. Homma and S. Takeno, A coupled base-rotator model for structure and dynamics of DNA, *Prog. Theor. Phys.* **72** (1984) 679–693.
- [10] K. U. Ingard, *Fundamentals of Waves and Oscillations* (Cambridge University Press, Cambridge, 1988).
- [11] R. L. Ornstein, R. Rein, D. L. Breen and R. D. Macelroy, An optimized potential function for the calculation of nucleic acid interaction energies I. Base stacking, *Biopolymers* **17** (1978) 2341–2360.
- [12] C. Prévost, M. Takahashi and R. Lavery, Deforming DNA: From physics to biology, *Chem. Phys. Chem.* **13** (2009) 1399–1404.
- [13] M. Salerno, Discrete Model for DNA-Promoter Dynamics, *Phys. Rev. A* **44** (1991) 5292–5297.
- [14] S. Yomosa, Soliton excitations in deoxyribonucleic acid (DNA) double helices, *Phys. Rev. A* **27** (1983) 2120–2125.
- [15] P. Varnai and R. Lavery, Modeling DNA deformation, in *Computational Studies of DNA and RNA*, eds. F. Lankas and J. Sponer (Springer-Verlag, 2006), pp. 169–210.
- [16] L. V. Yakushevich, Theoretical physics of DNA: New ideas and tendencies in the modeling of the DNA nonlinear dynamics, *EJTP* **4** (2007) 97–114.
- [17] L. V. Yakushevich, *Nonlinear Physics of DNA* (Wiley, Weinheim, 2004).
- [18] L. V. Yakushevich, S. Gapa and J. Awrejcewicz, Mechanical analog of the DNA base pair oscillations, in *Dynamical Systems — Theory and Applications*, eds. J. Awrejcewicz, M. Kazmierczak, P. Olejnik and J. Mrozowski (Left Grupa, Lodz, 2009), pp. 879–886.
- [19] L. V. Yakushevich and L. A. Krasnobaeva, Effects of dissipation and external field on the dynamics of local conformational distortions in DNA, *Biophysics* (Russian Journal) **52** (2007) 237–243.
- [20] L. V. Yakushevich and L. A. Krasnobaeva, Peculiarities of the kink dynamics in inhomogeneous DNA, *Biophysics* **53** (2008) 36–41.
- [21] L. V. Yakushevich and L. A. Krasnobaeva, A. V. Shapovalov and N. Quintero, One- and two-soliton solutions of the sine-Gordon equation applied to DNA, *Biophysics* (Russian Journal) **50** (2005) 450–455.
- [22] L. V. Yakushevich, A. V. Savin and L. I. Manevitch, On the internal dynamics of topological solitons in DNA, *Phys. Rev. E* **66** (2002) 016614.
- [23] Ch.-T. Zhang, Soliton excitations in deoxyribonucleic acid (DNA) double helices, *Phys. Rev. A* **35** (1987) 886–891.