Modeling B – A Transformations of the DNA Double Helix

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Abstract. An approach to the description of DNA conformational transformations of B – A type is presented. Due to the consideration of joint motions of DNA structural elements the model for DNA transformation is constructed in the two-component form. One component is the degree of freedom of the elastic rod, and another component – the effective coordinate of the conformational transformation. In the model the internal and external components are interrelated, as it is characteristic for DNA B – A rearrangements. It is demonstrated that kinetic energy of the double helix transformations of heterogeneous DNA can be put in homogeneous form. In the frame of the developed approach the possible localized excitations in a static state are found to compare with the experiments on DNA B – A deformability. The comparison shows good qualitative agreement between theory and experiment. The conclusion is made that the found excitations in the DNA structure may be classified as static conformational solitons, and that such localized excitations may play the key role in the mechanisms of DNA intrinsic bending.

Key words: DNA, conformational transformations, localized excitations, deformability

1. Introduction

The DNA macromolecule is a polymorphic structure with a variety of helix conformations which vary depending on nucleotide content and sequence, conditions of the solution, and interaction with proteins or ligands [1]. The variations in helix geometry play the role of conformational information for the regulatory proteins and ferments [2–4]. That is why the study of the conformational transformations of the DNA double helix is an approach to understanding the mechanisms of many genetic processes.

The experimental study of the DNA double helix transformations meets with the obstacles connected with complex structure of macromolecule and dynamical character of conformational rearrangements. The detailed analysis of DNA transformations is possible mainly for short fragments in a static state. On the other hand, the theoretical studies have also some restrictions. The use of the computational approach based on quantum mechanical consideration of the interactions of all atoms in the macromolecule is restricted by DNA fragments of a few base pairs [5]. In the case of using of atom-atom potential functions the computations may be

fulfilled for greater DNA fragments, about 20 base pairs [6, 7]. But, the atom-atom potential parameters are sorted out for description of ground state of the system, and therefore these results cannot be considered as so correct for macromolecule metastable or excited configurations.

One productive way to understand the conformational resources of DNA double helix is the use of the phenomenological model approach. Under successful model construction the phenomenological approach allows one to describe the structural transformations in macromolecules of real size and taking account of surrounding factors. It is also important that the phenomenological approach make clear the physical nature of the processes under consideration, and then may be amplified by the precise calculations in some principal points.

In the present work it is shown that the phenomenological approach allows us to construct a model which can predict the conformational state and the shape of the chain for DNA macromolecules. Using the phenomenological approach the DNA *B*–*A* transitions are modelled, and the conformational transformations that may take place in the macromolecule are found. The obtained results are compared with the experimental data on DNA deformability.

2. Model Construction

The DNA molecule consists of two strands which are formed by the linked phosphate groups and deoxyribose (or sugar) rings. The nucleic bases are attached to the sugar rings. The DNA bases have different content of atoms, so the primary structure of the macromolecule is heterogeneous and may be used for writing the genetic information.

Under natural conditions, in an ion-hydrate environment, the DNA strands form a double helix – DNA secondary structure. The organization of the DNA secondary structure is conditioned by two types of subsystems. The first one is formed by complementary pairs of hydrogen-bonded nucleic bases A·T and G·C, which disposed in the center of the double helix [1]. This subsystem is supported by the van der Waals (stacking) interactions along the chain. The second subsystem is the backbone of the macromolecule: the chains of the phosphate groups and sugar rings. The DNA backbone is stabilized mainly by the electrostatic interactions. Both subsystems coordinate mutually their conformations through the flexible sugar rings [1, 2, 8, 9]. So, in modeling the transformations of the DNA double helix it is important to use the components for the description of internal conformational rearrangements and external transformation of macromolecule shape.

To describe the DNA transformations we use the four-mass model approach developed earlier [10–12] for description of DNA conformational vibrations. The achieved agreement with experiment on DNA low-frequency spectra shows the accordance of the four-mass model to the double helix transformations on small scales. It would appear reasonable to generalized the four-mass model approach to the study of DNA large-scale transformations.

Figure 1. The four-mass model for the DNA monomer link, showing the masses' displacements in the plane of XOY ; OZ is the helix axis; * – positions of the base pair's centers of mass in B- and A-forms.

2.1. GENERALIZED FOUR-MASS MODEL

According to the four-mass model approach [1–12] the basic conformational degrees of freedom for the DNA monomer link are the following. First, displacements of the nucleosides (nucleic bases together with sugar rings) as pendulums “suspended” to the backbone chain. Secondly, intranucleoside transformations, i.e. the displacements of nucleic bases under the changes in the sugar rings conformation. The third type is displacements of the nucleotide (nucleic base + sugar + phosphate group) whole. In terms of the approach [10–12] two masses of the pendulum-nucleosides (m_i) and two masses of the backbone atom groups (m_0) (Figure 1) are used. The masses of nucleosides are different according to the kind of the nucleic base. The backbone masses (m_0) consist of the group of atoms $PO_2 + 2O + C_{5'}$, and are identical along the chain.

In order to consider the possibility of using the four-mass model for the description of non-small transformations of the DNA double helix we will write the expression for the energy in the generalized four-mass model without envisaging the smallness of displacements:

$$E = \sum_{i,n} \left\{ \frac{m_0}{2} \dot{\mathbf{R}}_{i,n}^2 + \frac{m_i}{2} \dot{\mathbf{r}}_{i,n}^2 + U(\mathbf{r}_{i,n}; \mathbf{R}_{i,n}) \right\}. \quad (1)$$

In expression (1) the summation is over all monomer links (n) of the double chain ($i = 1, 2$). The radius-vectors $\mathbf{R}_{i,n}(t)$ and $\mathbf{r}_{i,n}(t)$ describe the displacements of the mass centers of the backbone groups and nucleosides in each strand.

The first two terms in expression (1) describe the kinetic energy of the system ($\dot{\mathbf{R}}$ and $\dot{\mathbf{r}}$ denote the time derivatives). The function U is the potential energy of conformational transformations.

Taking into account the structural organization of a macromolecule, the potential energy of the n -th monomer link would be presented as:

$$U(n) = U^{(1)}(n) + U^{(2)}(n, n-1) + U^{(3)}(n; n \pm 1). \quad (2)$$

The first term in the sum (2) describes the energy of internal rearrangements in the n -th monomer of the macromolecule. The term $U^{(2)}$ describes the energy of the interaction between structural elements along the macromolecule chain. The term $U^{(3)}$ describes the energy of the interrelation between the intermonomer conformational rearrangements and the displacements of the monomer link with respect to $n-1$ and $n+1$ neighbor links of the macromolecule. Writing the potential energy of the system in the form (2) supposes the use of nearest-neighbors approximation. This approximation is traditionally used to describe the interactions along the monomer chain, and in special cases may be supplemented with other terms provided that related force constants are known.

In the terms of the four-mass model, the energy $U^{(1)}$ may be written as

$$U^{(1)} = U_1^{(1)}[\mathbf{R}_1 - \mathbf{r}_1] + U_2^{(1)}[\mathbf{R}_2 - \mathbf{r}_2] + U_3^{(1)}[\mathbf{r}_1 - \mathbf{r}_2] + U_4^{(1)}[\mathbf{R}_1 - \mathbf{R}_2], \quad (3)$$

where $U_1^{(1)}$ and $U_2^{(1)}$ are the energies of the nucleoside displacements with respect to the backbone group in each strand, $U_3^{(1)}$ is the energy of the H-bond stretching in the base pairs, and $U_4^{(1)}$ is the energy of the interaction of the backbone groups of different helix chains.

It should be noted at once that the term $U_4^{(1)}$ in expression (3) may be omitted because interaction between backbone groups in a monomer link is much weaker than the similar interaction along the macromolecule chain (the corresponding distances for some conformations differ by a factor greater than two [1]). The interactions along the backbone chains will be taken into account in the potential terms $U^{(2)}$ and $U^{(3)}$. The form of these terms will be specified later, after going to generalized coordinates of the conformational rearrangements.

Notice that the energy expressions (1–3) are rather complicated for direct use. Firstly the vector character of the displacements requires the construction of the corresponding force field for the macromolecule. Secondly the heterogeneity of the energy terms makes the analytical study practically impossible.

However, it is known [1, 2, 6, 8, 9, 13] that under rearrangements of DNA structure in the frame of the double helix the DNA structural elements move jointly along some conformational pathways. Taking this fact into account, the expression of the energy of the considered system would be essentially simplified. Let us consider the applicability of such an approach for constructing a model to describe the B – A transformations in the DNA double helix.

2.2. B–A TRANSFORMATIONS

To model the DNA conformational transformations, we introduce the displacements of the center of mass of the pair of nucleosides ($\mathbf{r}_p$) and the mass center of the backbone groups ($\mathbf{r}_q$)

$$\begin{aligned}\mathbf{r}_p &= \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_p}, \quad m_p = m_1 + m_2 \\ \mathbf{r}_q &= \frac{1}{2}(\mathbf{R}_1 + \mathbf{R}_2), \quad m_q = 2m_0\end{aligned}\quad (4)$$

as well as the displacements of the nucleosides with respect to each other in the monomer link (δ), and the same for the backbone masses (Δ):

$$\begin{aligned}\delta &= \mathbf{r}_1 - \mathbf{r}_2, \quad \mu_p = m_1 \cdot m_2 / m_p \\ \Delta &= \mathbf{R}_1 - \mathbf{R}_2, \quad \mu_q = m_0/2.\end{aligned}\quad (5)$$

where m_p , m_q , μ_p and μ_q are the corresponding masses.

In the designations (4) and (5) the expression for the n -th item of the kinetic energy of the system is given by:

$$K(n) = \frac{1}{2} \{ m_p \dot{\mathbf{r}}_p^2 + m_q \dot{\mathbf{r}}_q^2 + \mu_p \dot{\delta}^2 + \mu_q \dot{\Delta}^2 \}.\quad (6)$$

Next, it is useful to express the displacements of the center of mass of a monomer link ($\mathbf{R}$) and displacements of the mass center of a pair with respect to the backbone masses ($\mathbf{r}$):

$$\begin{aligned}\mathbf{R} &= \frac{m_p \mathbf{r}_p + m_q \mathbf{r}_q}{M}, \quad M = m_1 + m_2 + 2m_0 \\ \mathbf{r} &= \mathbf{r}_p - \mathbf{r}_q, \quad m = m_p \cdot m_q / M.\end{aligned}\quad (7)$$

Here M and m are the mass and the reduced mass of a monomer link, respectively. In terms of (7) the expression for the kinetic energy reduces to the following form:

$$K = \frac{1}{2} \sum_n \{ M \dot{\mathbf{R}}_n^2 + m \dot{\mathbf{r}}_n^2 + \mu_p \dot{\delta}_n^2 \}.\quad (8)$$

In the expression (8), the term with coordinate Δ is omitted. The potential energy associated with it is very small ($U_4^{(1)} \sim 0$ in expression(3)), as was mentioned above. From the point of classical mechanics Δ is a cyclic coordinate, and it may be ignored here.

Notice that after passing to description of the joint motions along the conformational pathway, the masses in the kinetic energy become independent of the

Table I. The mass values for modeling the conformational transitions in DNA

Nucleoside	m_i^a (a.u.m.)	Base pairs	M (a.u.m.)	m (a.u.m.)	μ_p (a.u.m.)
Ade	203(134)	A·T	615	140.7	99.2
Thy	194(125)				
Gua	219(150)	G·C	616	140.8	98.5
Cyt	179(110)				

^aThe masses of nucleic bases are given in parentheses.

heterogeneity of the monomer content of DNA macromolecule. The calculated values of the masses are shown in the Table I for A·T and G·C pairs.

Then, let us take into account that under such structural transformations as transitions between the *B*- and *A*-forms of the double helix, the nucleic bases in the pair displace together without significant mutual shifts and remain in the configuration of complementary pairs both in the initial and in the final helix forms [1, 2, 8, 9, 13]. So, we assume that when modeling the DNA conformational transitions one may put: $\delta \approx \hat{\delta} \approx 0$. Therefore, the expression for the model kinetic energy in the description of conformational transitions is given by:

$$K_{tr} = \frac{1}{2} \sum_n \{M\dot{\mathbf{R}}_n^2 + m\dot{\mathbf{r}}_n^2\}. \quad (9)$$

The kinetic energy in the form (9) still remains rather complicated for the modeling. As the next step in the model construction, let us take into account that in the conformational transformations of the macromolecule the masses M and m have displacements in the primary directions. In fact, under the conformational transitions of *B*–*A* type the mass center of DNA monomer link has the largest displacement in the plane which is orthogonal to the helix axis [1, 2, 8, 9, 13]. Thus, for the degree of freedom of the monomer center of mass it is convenient to express the displacements in the plane *XOY* (we put the helix axis along *OZ*, Figure 1). In this case $M\dot{\mathbf{R}}^2 = M\dot{R}^2 + I\dot{\varphi}^2$, where R and φ are the displacement and the angle of rotation of the link in the plane *XOY*, $I = I_{0Z}$ is the moment of inertia of the monomer link with respect to the helix axis. These degrees of freedom of the monomer link describe the bending and torsion of the double helix.

Note that the need to take into account the double helix bending and torsion simultaneously is associated with specific conditions of the transition. Both types of helix deformation are observed in the experimental studies [1–4]. Introducing both degrees of freedom in the model does not cause difficulties, but for purposes of the present study it is sufficient to include one of them to denote this type of the transformation. We will use the coordinate R – bending.

Besides, it is also known [1, 2, 8, 9, 13], that under conformational transitions the base pairs displace transversely to the helix axis, along the axis *O*X (Figure 1). Thus, for the component *r* it is expedient to express the displacement along the trajectory of the mass center motion: *r* → *r*.

Thus the expression for the kinetic energy of the *B*–*A* transition may be written in terms of *R* and *r* coordinates in the scalar form:

$$K_{tr} = \frac{1}{2} \sum_n \{M \dot{R}_n^2 + m \dot{r}_n^2\}. \quad (10)$$

Let us consider the form of the potential energy for the *B*–*A* transformation in the chosen coordinates. In this case according to the expression (2) the energy term $U^{(1)}$ reduces to the energy of the pair displacement (coordinate *r*) relative to the backbone. The displacements of base pair in the monomer link occur due to the conformation changes in both sugar rings [1, 2, 8, 9, 13]. The energy of such joint transformations of both sugars in the monomer link ($U_1^{(1)} + U_2^{(1)}$ in expression (3)) brings a contribution to the potential energy which we will denote $\Phi[r]$.

The function $\Phi[r]$ describes the potential energy of the internal subsystem on the pathway of a conformational transformation from one stable state to another. Hence, it must have the shape of a double well (Figure 2). Under the conditions when one helix form is more stable (for example, under physiological conditions the most stable is *B*-form of the double helix [1]) the function $\Phi[r]$ will be asymmetric with two non-equivalent stable states: ground and metastable (Figure 2a). If the conformational transition takes place under equilibrium between the states (for example in the interval of *B*–*A* equilibrium), the function $\Phi[r]$ must be symmetric with two equivalent states (Figure 2b).

The term $U_3^{(1)}$ in the expression (3) which describes the energy of the *H*-bonds stretching in the base pairs should be omitted because DNA transformations of *B*–*A* type, as was mentioned above, occur without significant change of the distance between the nucleosides' centers of mass ($\delta \approx 0$).

The potential energy of the interaction along the macromolecule chain (term $U^{(2)}$ in the expression (2)) includes the energy along component *R*, which should

Figure 2. A sample view of the potential functions $\Phi(r)$ and $F(r)$: (a) the typical case for the physiological conditions: the double well with non-equivalent stable conformations; (b) the case of the equilibrium of the macromolecule conformations.

be similar to the bending energy of the elastic rod, and the energy along component r , that describes the change of pair stacking interactions. Both these terms will be written using the nearest neighbors approximations.

Therefore, the expression of the potential energy for the conformational transitions of the DNA macromolecule is given by

$$U_{tr} = \sum_n \left\{ \frac{k_R}{2} [R_n - R_{n-1}]^2 + \frac{k_r}{2} [r_n - r_{n-1}]^2 + \Phi[r_n] + \chi F[r_n][R_{n+1} - R_{n-1}] \right\}. \quad (11)$$

In the expression (11), k_R and k_r are the elastic constants of the interactions along the macromolecular chain for double helix bending and pair displacement components, respectively.

The term with the coefficient χ describes the interrelation between the intramonomer transformation and the displacement of the monomer with respect to the nearest neighbors (term $U^{(3)}$ in the expression (2)). The potential function $F(r)$ reflects the change in the interrelation energy under the transition of the internal component from one stable state to another. By its physical meaning, $F(r)$ is the function that increases from the ground state of the system and decreases near another stable state. In the case of a transition between the equilibrium states this function must be of a symmetric form in accordance with the physical equivalence of the states. A sample form of this potential function is shown in Figure 2.

It should be noted that the $B \rightarrow A$ transformation of DNA may be described in the terms of a continuum approximation. As known, the $B \rightarrow A$ transition in DNA is a cooperative transformation [8, 9]. In such transformations of the double helix the base pair stacking is well preserved [1, 14, 15] and interactions between the monomers along the chain are sufficiently large in comparison with the intramonomer transformation energies. In the continuum approximation the expression for the energy (10–11) may be written as:

$$\mathbf{E} = \int \frac{dz}{h} \left[\frac{M}{2} (\dot{R}^2 + s_R^2 R'^2) + \frac{m}{2} (\dot{r}^2 + s_r^2 r'^2) + \Phi(r) + 2\chi h F(r) R' \right]. \quad (12)$$

In the expression (12) $R = R(z, t)$ and $r = r(z, t)$, R' and r' are the derivatives with respect to z , $s_R^2 = k_R h^2 / M$ and $s_r^2 = k_r h^2 / m$.

In a set of works [16–19] it was shown that the two-component model of type (12) for potential $\Phi(r)$ with non-equivalent bistable states has the solution in the form of a dynamical solitonic wave – a conformational soliton. The soliton has a bell shape, and moves along the chain with the velocity $s_R > v > s_r$. In [16, 17, 20] this solution was used to describe the dynamics of local $B \rightarrow A$ transition in the DNA chain and to explain the effects of long-range action in stressed DNA. Notice that the observed conformational soliton in DNA has a dynamical character and

cannot be observed in experiment directly. There is only some indirect evidence of the existence of conformational solitons in the DNA structure.

3. Localized Excitations in a Static State

For comparison of the theoretical results with available experimental data on DNA transformations, let us study the static localized excitations of the system (12). These excitations can be observed in real conditions, using a set of X-ray data on localized *B*–*A* transformations in DNA fragments [21]. In the experiments the observed DNA deformations caused by the proteins attached to both (or one of the) ends of the macromolecule fragments, and have to be considered as intrinsically produced transformations of the DNA double helix with certain boundary conditions. It is important that the experimental data is analyzed in the terms of two components: deformation of the DNA chain and conformation state of the macromolecule fragment [21]. So, these X-ray data may be used for direct comparison with the results of the present modeling and can serve as an indication of the intrinsic localized excitations existence in DNA structure in a static state.

We will find the possible static excitations for two cases. First, when the DNA macromolecule is in the ground state (*B*-form) and *A*-form is a metastable state. Second, when the macromolecule is in the conditions of equilibrium between *B* and *A* states.

For a more general character of the consideration we will study the static states of the system without definition of explicit forms for the potential functions. In accordance with the shape of the potential functions we assume that the potential energy of the system has three extrema: two minima (r_0, r_2) and one maximum (r_1) between them. In the ground state $r = r_0$ (DNA *B*-form) we assume that $\Phi(r_0) = F(r_0) = 0$. In the metastable state ($r = r_2$) $\Phi(r_2) \neq 0, F(r_2) \neq 0$ (Figure 2a). For the conditions when the macromolecule has two equivalent stable states (Figure 2b) for state r_2 we assume $\Phi(r_2) = F(r_2) = 0$.

Let us find the static excitations of the macromolecule. We will assume: $r = r(z)$ and $R = R(z)$. The equations for the static excitations have the form:

$$R'' + \chi_R \frac{dF}{dr} r' = 0; \quad (13)$$

$$r'' - \frac{\sigma_r}{2} \frac{d\Phi}{dr} - \chi_r \frac{dF}{dr} R' = 0. \quad (14)$$

In the equations (13, 14) $r = r(z)$ and $R = R(z)$, $\chi_R = 2\chi/k_R h$, $\chi_r = 2\chi/k_r h$ and $\sigma_r = 2/k_r h^2$.

After one time integration of the equation (13) for the external component we have:

$$R' + \chi_R F(r) = 0, \quad (15)$$

where the integration constant is put to zero according to the initial conditions for the stable state.

For determination of the macromolecule deformation we will coin the value:

$$\tau = hR'(z) = -\frac{\chi}{k_R}F(r). \quad (16)$$

Having substituted the expression for R' (15) in the equation (14) and performed one time integration we obtain the equation for the internal component, i.e.,

$$r'^2 - \sigma_r \Phi(r) + \chi_r \chi_r F^2(r) = C,$$

which may be rewritten in the form

$$r'^2 + Q(r) = 0. \quad (17)$$

The equation (17) has the form of the energy of the mechanical system with the potential energy

$$Q(r) = -\sigma_r \left[\Phi(r) - \frac{2\chi^2}{k_R} F^2(r) \right] - C, \quad (18)$$

where C is the integration constant.

The solution of equation (17) may be found as the conversion of the integral

$$\int_{r(0)}^{r(z)} \frac{du}{\sqrt{-Q(u)}} = z. \quad (19)$$

This solution depends completely on the form of $Q(r)$ and specified forms of the potential functions Φ and F . Considering the bistability of the system we assume that $\Phi(r) > 2\chi^2 F^2(r)/k_R$, and the effective potential $Q(r)$ (19) has the form of a double hump.

3.1. STATIC EXCITATION IN THE MACROMOLECULE WITH GROUND AND METASTABLE STATES

Let us consider the possible solutions of the equation (17) for the case when the DNA macromolecule has a ground state and a metastable state. We will find the excitations with a restricted trajectory and the asymptote of one of the stable states of the system because such excitations are the most stable under real conditions. For the potential $Q(r)$ (which in this case has the form of two non-equivalent humps) we will search the excitation with the asymptote of the metastable state r_2 (Figure 3a). In this case it is convenient to present the polynomial $Q(r)$ in the form:

$$Q(r) = -Q_m^2(r_2 - r)^2(r - \eta_1)(r - \eta_2). \quad (20)$$

Figure 3. Static excitation of the macromolecule chain in the case of non-equivalent stable states for DNA monomer link: (a) the view of the effective potential Q ; (b) the form of the excitation, for internal component; (c) the same for external component; (d) the molecular image of DNA B-A transformation induced by protein (the central part of the DNA fragment is free)[21].

In the expression (20), Q_m^2 is the combination of the model parameters, r_2 , η_1 , and η_2 ($\eta_1 < \eta_2 < r_2$) are the zeros of the polynomial $Q(r)$ with the constant $C = -\sigma_r \Phi(r_2) + \chi_R \chi_r F^2(r_2)$ for the boundary conditions of the metastable state ($r = r_2$ and $r' = 0$).

For the polynomial $Q(r)$ in the form (20) the integral equation (19) gives the solution for internal component $r(z)$ of the static excitation in the form:

$$r(z) = r_2 - r_{\text{ex}}(z), \quad r_{\text{ex}}(z) = \frac{a}{\text{ch}(q_m z) + b}. \quad (21)$$

Here: $a = 2(r_2 - \eta_2)(r_2 - \eta_1)/(\eta_2 - \eta_1)$, $b = (2r_2 - \eta_1 - \eta_2)/(\eta_2 - \eta_1)$, and $q_m = \pm Q_m \sqrt{(r_2 - \eta_2)(r_2 - \eta_1)}$.

As seen from expression (21), for $z \rightarrow 0$ (the middle point of the excitation) $r_{\text{ex}} \rightarrow r_2 - \eta_2$ and $r(z) \rightarrow \eta_2$. For $z \rightarrow \infty$, $r_{\text{ex}} \rightarrow 0$ and $r(z) \rightarrow r_2$ (Figure 3b).

The deformation of the external component of the excitation according to equation (16), is given by

$$\tau_{\text{ex}}(z) = -\chi_1 h F[r_2 - r_{\text{ex}}(z)] \quad (22)$$

for $z \rightarrow \infty$, $r_{\text{ex}} \rightarrow 0$, $\tau_{\text{ex}} \rightarrow \tau_2$, and for $z \rightarrow 0$, $r_{\text{ex}} \rightarrow r_2 - \eta_2$, $\tau_{\text{ex}} \rightarrow \tau_\eta = -\chi_1 h F[\eta_2]$, where $0 > \tau_\eta > \tau_2$.

Thus, if the system has ground and metastable states, it follows from equations (21, 22) that the static excitation has the shape of a bell of width proportional to $|q_m^{-1}| \sim [(r_2 - \eta_1)(r_2 - \eta_2)]^{-\frac{1}{2}}$, and height $(r_2 - \eta_2)$. At the middle point of the excitation both components have the values close to those for the ground state

(Figure 3c) and the deformation of the macromolecule fragment is minimal. On the edges of the excitation, the components have the values of the metastable state with the definite deformation, larger than in the center.

The results obtained may be compared with the observed static deformation of the DNA fragments. So, in the work [22] the atoms coordinates are found for the DNA-protein complex, where the protein interacts with the ends of the DNA fragment, and the central part of the fragment is free from interaction with protein. By its nucleotide content and sequence the DNA fragment has the *B*-form as a ground state.

The reconstruction of the DNA structure in this complex show that the attached protein has induced *B*→*A* transition in DNA and the DNA fragment is bent, and looks like a bell [21] (Figure 3d). The conformation of the double helix in the center of DNA fragment is close to the ground state (*B*-form), and on the edges, close to the *A*-form. As seen, the solution (21, 22) for static excitation is in complete agreement with the observed form of DNA deformation and conformational state of the DNA fragment presented in [21, 22].

3.2. STATIC EXCITATION IN THE MACROMOLECULE WITH EQUIVALENT STATES IN THE MONOMER LINK

Let us consider the static excitations of the macromolecule with equivalent states in the monomer link (Figure 2b). Similarly to previous case, the form of the excitation for internal and external components is determined by equations (16, 17). For the equivalent states in the monomer link the effective potential $Q(r)$ has the shape of the double hump with equal humps (Figure 3a). We will find the solution of equation (17) for the boundary conditions of the stable states ($r \rightarrow r_0$ or r_2 and $r' \rightarrow 0$). For these conditions the constant c in the polynomial $Q(r)$ is equal to 0. In this case it is convenient to write the potential $Q(r)$ in the form:

$$Q(r) = -Q_e^2(r_2 - r)^2(r - r_0)^2, \quad (23)$$

where Q_e^2 is the combination of the model parameters.

After integration of equation (17) with polynomial (23) we have for the internal component

$$r(z) = r_1 + d \operatorname{th}(q_e z), \quad (24)$$

where $d = (r_2 - r_0)/2$ and $q_e = \pm d Q_e$.

As follows from equation (24) for $z \rightarrow \pm\infty$, $r(z) \rightarrow r_2$ or r_0 depending on the sine of q_e . For $z = 0$, $r(z) = r_1$ (Figure 4b).

For the external component given by equation (16) and the form of the potential function $F(r)$ in the case of equivalent states we have the following: when $z \rightarrow \pm\infty$, then $\tau \rightarrow 0$, and at $z = 0$ $\tau(0) = -\chi_1 h F[r_1]$ (Figure 3c). Thus, the form of the

Figure 4. Static excitation of the macromolecule chain in the case of equivalent stable states for DNA monomer link: (a) the view of the effective potential Q ; (b) the form of the excitation for internal component; (c) the same for external component; (d) the molecular image of DNA *B*–*A* junction induced by protein interacted with the *B*-part of the macromolecule fragment [21].

external component differs from that in the case of nonequivalent states. In the central part of the macromolecule fragment the deformation has the maximum value, and on the edges of the excitations the deformation is absent (Figure 4c).

These results may be compared with the data of molecular images of the *A*–*B* transformation in the DNA-protein complex [23]. In the complex the protein is attached to one part of the DNA fragment and another part is free. In the work [21] the structure of the DNA double helix in this complex is reconstructed, and the conformation of the helix is determined (Figure 4d). The DNA portion (that is in the complex with protein) is in the *B*-form, that is ground for this part of the fragment. Another, protein free, portion of DNA remains in the *A*-form (also ground for this portion because of its nucleotide content). This forms an example of equivalence of the conformations in one fragment. At the *A*–*B* junction, the DNA macromolecule curves sharply [21] (Figure 4d), and looks like a kink deformation of DNA [1].

The observed DNA transformations [21, 23] are in agreement with the results of the present modelling. As in experiment, in our theory the static excitation for the DNA with equivalent states has the form of a kink (24) – the transition between the conformations of the double helix and has maximum macromolecule deformation at the center of the *A*–*B* junction (Figure 4).

4. Conclusions

Thus, one constructs relatively simply a two-component model which describes the DNA *B*–*A* transformations in the frame of double-helical state. The model includes the external component which is the degree of freedom of the elastic rod, and the internal component which is the characteristic coordinate of the structural

transformation. As was shown, on the pathways of the conformational transformations the DNA macromolecule behaves as a homogeneous chain with identical masses in the monomer links. The two-component model of DNA conformational transformations is the basic construction that may be modified by including additional terms – the components of both types.

The comparison of the static excitations in the constructed model with observed deformations of the DNA fragments in *B*–*A* transformations show the qualitative agreement between the theory and experiment. From the correlation between the theory and experiment, it follows that the considered DNA transformations constitute intrinsically localized excitations – static conformational solitons by their nature. The results obtained may be regarded as the direct evidence of the existence of localized excitations in DNA macromolecule.

One should take into account the fact that the DNA intrinsic deformability may be caused by the formation of conformational solitons in the macromolecule. In this case the DNA deformability occurs in discrete portions in accordance with the number of excited solitons. Thus, the value of the macromolecule bending has to be proportional to the number of excitations. Such mechanism of macromolecule intrinsic bending differs from usual elastic deformation and may be tested experimentally.

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