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TWO-COMPONENT LOCALIZED SOLUTIONS IN A NONLINEAR DNA MODEL

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1. One of the most important and interesting problems in contemporary molecular biophysics is to find a mechanism of excitation transmission along molecular chains of proteins [1] and nucleic acids (DNA and RNA) (see, e.g., reviews [2,3]). In order to explain an experimental fact of transmission of excitation of the given form through a large distance without noticeable deformation the hypothesis is successfully used that solitons (solitary waves) can be excitation carriers [1-9,13-15]. Solitary waves have been studied in papers cited above within various nonlinear DNA models, permitting to describe nonstationary wave processes of energy, momentum and information transmission through hundreds or even thousands of elementary structure units (e.g., nucleotide pairs of DNA double helix [16]). However, one-component ($N = 1$) nonlinear DNA models were predominantly considered, which describe localized excitations of only one degree of freedom of molecular chain (e.g., torsional oscillations of DNA bases) [1-9,13-15].

On the other hand, the detailed analysis of conformational oscillation spectrum has been accomplished by using linear approximation within 2- and 3- component DNA models taking into account (i) torsion oscillations of nucleosides, attached to sugar-phosphate backbone in "suspension points", (ii) transverse displacements of suspension points and (iii) conformational sugar rings deformations [10-12].

Then solitary wave solutions describing the transmission of nonlinear excitations which are weakly sensitive to heterogeneity of chain DNA macromolecule, have been studied (see [13] and references cited therein) and it was shown that such solitons can propagate along the deformed (i.e., being in elastically stressed state) macromolecule chain only. Hence the possibility of the localized multi-component excitations to propagate along the nondeformed DNA molecule needs a further investigation. We shall not restrict ourselves to studying the nonlinear oscillations modes, which are weakly sensitive to the DNA heterogeneity (in particular, to mass difference of bases, being constituents of nucleosides) and consider DNA models, with masses and other nucleoside characteristics not depending on their numbers (or coordinates along the chain). In order to describe nonlinear oscillation attenuation due to the DNA heterogeneity, one should research a more general model, in which energy pumping and damping are considered.
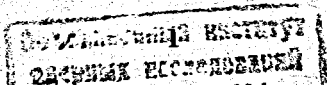
Specific nonlinear terms in DNA models can be defined by taking into consideration the intrinsic nonlinearity of one or several of the N interacting components (transverse backbone displacements, torsional nucleoside oscillations, variations of furanose sugar ring geometry ("sugar puckering") and glycoside bond angle [16]). It is worth mentioning here (i) paper [14], in which soliton solutions to three-component dynamic DNA model have been found (in this model nonlinearity appears when conformational deformations of sugar rings are described by using a double-well potential, $V(P) = (P^2 - 1)^2$, P is pseudorotational angle [16]) and (ii) paper [15], in which a nonlinear two-component RNA model is considered; in this model linear torsion base displacements are interacting with nonlinear conformational deformations of sugar rings.

2. Following [10], we take into consideration excitations of two degrees of freedom of each DNA monomer, namely: (i) transverse "suspension points" displacements and (ii) transverse motions of nucleosides considered to be rigid bodies. However contrary to the model studied in [10] we describe torsion oscillations using equations which are nonlinear in angular displacements, in the same way as has been done when considering solitons in one-component ($N = 1$) dynamic DNA model (see, e.g., [4-9]). We model hydrogen bonds connecting bases in pairs within DNA double helix by using harmonic approximation for energy, $U(\delta r) = \alpha(\delta r)^2$, here δr is a distance between bases within pair, assuming linear dependence of δr on angular and transverse displacements [10]. It should be noted that in such approximation only small angular and transverse displacements can be considered in a general case; nevertheless if angular and transverse oscillations have almost opposite phases, then, δr can be small even at moderate values of $\Theta's$ and $X's$ (see relationship (4) below). Hamiltonian and Lagrangian densities of the dynamic system under consideration are as follows (see [10] for details):

$$E = T + \Pi, \qquad L = T - \Pi, \tag{1}$$

$$T = \frac{1}{2} \sum_{n,i} [M \dot{X}_{in}^2 + m(l^2 \dot{\Theta}_{in}^2 + 2 l_a \dot{\Theta}_{in} \dot{X}_{in})], \tag{2}$$

$$\dot{X} = \frac{\partial X}{\partial \tau}, \qquad \dot{\Theta} = \frac{\partial \Theta}{\partial \tau},$$

$$\Pi = \frac{1}{2} \sum_{n,i} [\alpha(\delta r_n)^2 + 2V(\Theta_{in}) + f(\Theta_{in} - \Theta_{i,n-1})^2 + g(X_{in} - X_{i,n-1})^2], \tag{3}$$

$$\delta r_n \approx l_a(\Theta_{1n} + \Theta_{2n}) + X_{1n} + X_{2n}. \tag{4}$$

Here the summation over DNA chain numbers $i = 1, 2$ and nucleoside numbers n is executed. We consider (cf. [4-9])

$$V(\Theta_i) = \beta(1 - \cos \Theta_i). \tag{5}$$

To accomplish the analytic investigation, it is useful to perform the transition from the lattice model (1)-(5) to the continuous one. Using notations [10]

$$\alpha_0 = \frac{2\alpha}{M}, \quad \beta_0 = \frac{\beta}{ml^2}, \quad s^2 = \frac{fh^2}{ml^2}, \quad s_0^2 = \frac{gh^2}{M} \tag{6}$$

(here h is the distance between adjacent nucleosides along the double helix axis), substituting the variables

$$\varphi = \Theta_1 + \Theta_2, \qquad X = X_1 + X_2, \tag{7}$$

$$\psi = \Theta_1 - \Theta_2, \qquad x = x_1 - x_2, \tag{8}$$

and using an equality

$$\frac{\partial V(\Theta_1)}{\partial \Theta_1} + \frac{\partial V(\Theta_2)}{\partial \Theta_2} = 2\beta \sin \varphi \cdot \cos \psi, \tag{9}$$

we find the following equation set for variables φ and X (cf. with (8) at $G = 0$ in [10]):

$$\varphi_{\tau\tau} + \frac{l_a}{l^2} X_{\tau\tau} - s^2 \varphi_{zz} + 2\beta \sin \varphi \cos \psi + \alpha_0 \frac{M}{m} \frac{l_a}{l^2}(l_a \varphi + X) = 0, \tag{10}$$

$$X_{\tau\tau} + \frac{ml_a}{M} \varphi_{\tau\tau} - s_0^2 X_{zz} + \alpha_0(l_a \varphi + X) = 0. \tag{11}$$

Here z is the continuous coordinate along the double helix axis. This set describes the relative oscillations (variables φ and X) in the double helix, i.e., "breathing" of the DNA macromolecule. Similar equations for x and ψ variables, which describe the motion of the DNA helix as a unit (bending and torsion), admit a zero solution: $x = 0, \psi = 0$. Substituting it into the set (10), (11), introducing new variables u, v by $u = \varphi/2$, $v = X/2$ and denoting

$$\mu = \frac{m}{M}, \quad \rho = \frac{l_a}{l} = \sin \Theta_0, \quad k^2 = \frac{s_0^2}{s^2} = \mu \frac{g}{f}, \tag{12}$$

in dimensionless variables t, x defined by relations

$$\tau = t \cdot \alpha_0^{1/2}, \quad x = z \cdot \frac{\alpha_0^{1/2}}{s}, \tag{13}$$

we arrive at the following nonlinear set of equations for u and v

$$u_{tt} - u_{zz} + \rho v_{tt} + \mu^{-1} \rho(v + \rho u) + \beta \sin u = 0, \tag{14}$$

$$v_{tt} - k^2 v_{xx} + \mu \rho u_{tt} + (v + \rho u) = 0. \tag{15}$$

Lagrangian and Hamiltonian densities of the dynamic system described by Eqs. (14), (15) are as follows:

$$\mathcal{L} = \frac{1}{2}[u_t^2 - u_x^2 + \mu^{-1}(v_t^2 - k^2 v_x^2) + 2\rho u_t v_t - \mu^{-1}(v + \rho u)^2 - 2\beta(1 - \cos u)], \tag{16}$$

$$\mathcal{H} = \frac{1}{2}[u_t^2 + u_x^2 + \mu^{-1}(v_t^2 + k^2 v_x^2) + 2\rho u_t v_t + \mu^{-1}(v + \rho u)^2 + 2\beta(1 - \cos u)]. \tag{17}$$

3. Investigate steady-state solutions to the set (14),(15)

$$u(x,t) = u(\xi), \quad v(x,t) = v(\xi), \quad \xi = x - Mt, \quad M = const.$$

For such solutions the set (14), (15) takes the form

$$(M^2 - 1)u_{\xi\xi} + \rho M^2 v_{\xi\xi} + \mu^{-1}\rho(v + \rho u) + \beta \sin u = 0, \tag{18}$$

$$(M^2 - k^2)v_{\xi\xi} + \mu\rho M^2 u_{\xi\xi} + (v + \rho u) = 0. \tag{19}$$

We seek solutions of this set assuming that

$$v + \rho u = 0, \tag{20}$$

and consequently $v_{\xi\xi} = -\rho u_{\xi\xi}$. Then it follows from (19) that for the nonzero solution $v(\xi) = -\rho u(\xi)$ to exist, the relation must be fulfilled

$$M^2 = k^2(1 - \mu)^{-1}, \tag{21}$$

which defines the velocity of localized excitation transmission; note that its value proves to be uniquely fixed by parameters k and μ. Using (20), (21) and boundary conditions $u_\xi(\pm\infty) = 0$, $v_\xi(\pm\infty) = 0$ $(u(+\infty) = 2\pi n, \quad u(-\infty) = 2\pi(n \pm 1))$, by integrating Eq. (18) we find localized

(soliton) solution to the set (18), (19) with the $u(\xi)$ and $v(\xi)$ functions having the form of kink (antikink):

$$u(\xi) = 4\arctan[\exp(\pm\delta^{1/2}\xi)], \quad v(\xi) = -\rho u(\xi), \tag{22}$$

$$\delta = \frac{\beta}{1 + M^2(\rho^2 - 1)} = \frac{\beta(1 - \mu)}{1 - \mu + k^2(\rho^2 - 1)}, \tag{23}$$

here we assume that $\delta > 0$, i.e.

$$1 + k^2(\rho^2 - 1)(1 - \mu)^{-1} > 0. \tag{24}$$

It is natural to call the solution (22),(23) a two-component kink (antikink), or a two-component topological soliton (antisoliton).

The case $k^2 = 0$, $\mu = 1$ needs special consideration. For such parameter values Eq.(15) takes the form

$$(v + \rho u)_{tt} + v + \rho u = 0, \tag{25}$$

it has obviously particular solution (20). By using (20), one gets from (14) an equation

$$(1 - \rho^2)u_{tt} - u_{xx} + \beta \sin u = 0, \tag{26}$$

which can be transformed by using the linear substitution $t = (1 - \rho^2)^{1/2}\tau$ into the sine-Gordon equation having well-known soliton and breather solutions. It is easily seen that the velocities M of these localized solutions to Eq.(26) obey the inequality $M^2 < (1 - \rho^2)^{-1}$. Thus the set of Eqs.(14),(15) at $k^2 = 0$, $\mu = 1$ has exact nonstationary solutions which describe (i) completely elastic interaction of N two-component solitons and (ii) nonradiating two-component breathers (bions, soliton bound states) having u amplitudes in the interval $(0, 2\pi)$. Hence one may conjecture that Eqs.(14), (15) at $k^2 = 0$, $\mu = 1$ describe completely integrable dynamic system.

It should be noted that in general case of (14), (15) the solution (22), (23) describes the angular displacements of a large value, and therefore the relationship (4) should be superseded by a more complicated exact relation.

4. However, there are localized excitations, described by the nonlinear set (14), (15), for which the using of relation (4) is allowable. We mean self-localized oscillating two-component excitations with rather a small

amplitude, that can be interpreted as bound states of a two-component kink and an antikink (22),(23). To investigate them, we applied the Bogolubov-Mitropolsky method, i.e., the expansion of solution under investigation in asymptotic series; previously, similar self-localized solutions have been investigated with this technique in one-component nonlinear dynamic models described by the nonlinear Klein-Gordon PDEs, at first in one-dimensional (x,t) geometry [17], and then in spherically symmetric (r,t) models [18]. We search for small-amplitude ($u, v \ll 1$) self-localized oscillating solutions to Eqs. (14), (15) in the form:

$$u = A(x)\cos\omega t + B(x)\cos 3\omega t + \ldots, \quad B(x) \ll A(x), \quad (27)$$

$$v = a(x)\cos\omega t + b(x)\cos 3\omega t + \ldots, \quad b(x) \ll a(x). \quad (28)$$

Substituting (27), (28) into (14), (15), using relation $\sin u \simeq u - \frac{1}{6}u^3$ and equating coefficients at $\cos\omega t$ and $\cos 3\omega t$ to zero, we get from (14), (15)

$$A_{xx} - (\beta + \mu^{-1}\rho^2 - \omega^2)A + \frac{\beta}{8}A^3 + (\omega^2 - \mu^{-1})\rho a = 0, \quad (29)$$

$$B_{xx} - (\beta + \mu^{-1}\rho^2 - 9\omega^2)B + \frac{\beta}{24}A^3 + (9\omega^2 - \mu^{-1})\rho b = 0, \quad (30)$$

$$k^2 a_{xx} + (\omega^2 - 1)a + (\mu\omega^2 - 1)\rho A = 0, \quad (31)$$

$$k^2 b_{xx} + (9\omega^2 - 1)b + (9\mu\omega^2 - 1)\rho B = 0. \quad (32)$$

First consider for simplicity the case $k^2 = 0$. From (31) and (32) we get

$$a(x) = -\frac{\rho(\mu\omega^2 - 1)}{\omega^2 - 1}A(x), \quad (33)$$

$$b(x) = -\frac{\rho(9\mu\omega^2 - 1)}{9\omega^2 - 1}B(x). \quad (34)$$

In view of (33) we get from (29) an equation for $A(x)$

$$A_{xx} - \frac{(\beta + \mu^{-1}\rho^2 - \omega^2)(\omega^2 - 1) + \mu^{-1}\rho^2(\mu\omega^2 - 1)^2}{(\omega^2 - 1)}A + \frac{\beta}{8}A^3 = 0, \quad (35)$$

which may be transformed, by using relations obtained when investigating the linear two-component set [10], to the form:

$$A_{xx} + \frac{(1-\eta)(\omega^2 - \omega_1^2)(\omega^2 - \omega_2^2)}{(\omega^2 - 1)}A + \frac{\beta}{8}A^3 = 0, \quad (36)$$

where

$$\omega_1^2 \approx p(1-\eta)^{-1}, \quad \omega_2^2 \approx \frac{\beta}{1-\eta}, \quad \eta = \mu\rho^2, \quad p = 1 - \rho^2(2 - \mu^{-1}). \quad (37)$$

For $\beta \ll 1$ an equality $\omega_2^2 \ll \omega_1^2$ holds. To make numerical estimations, one can use the following values: $\rho = 1/2$, $\mu = 2/3$ (cf. experimental data cited in [10]).

Consider self-localized oscillations having frequency $\omega \lesssim \omega_2$; neglecting ω^2 value in comparison with $\omega_1^2 \approx 1$, one gets from (36):

$$A_{xx} + p(\omega^2 - \omega_2^2)A + \frac{\beta A^3}{8} = 0. \quad (38)$$

Introducing dimensionless variables

$$y = x\omega_2 p^{1/2}, \quad \gamma = \beta(8p\omega_2^2)^{-1}, \quad \Omega = \omega/\omega_2, \quad (39)$$

we transform (38) into

$$A_{yy} - (1 - \Omega^2)A + \gamma A^3 = 0. \quad (40)$$

The localized solution to (40)

$$A(y) = (2\gamma^{-1})^{1/2}\varepsilon\frac{1}{\cosh(\varepsilon y)}, \quad \varepsilon = (1 - \Omega^2)^{1/2}, \quad (41)$$

in initial x variable has the form

$$A(x) = 4\omega_2(p\beta^{-1})^{1/2}\varepsilon\frac{1}{\cosh(\varepsilon\omega_2 p^{1/2}x)}, \quad \varepsilon = [1 - (\frac{\omega}{\omega_2})^2]^{1/2}. \quad (42)$$

Note that the term B_{xx} in Eq.(30) is small in comparison with the others, $B_{xx} \sim \varepsilon^2 B$, and it may be neglected when $\varepsilon^2 \ll 1$. In view of (34) we find from (30)

$$B(x) = \frac{(9\omega^2 - 1)\beta A^3(x)}{24[(\beta + \mu^{-1}\rho^2 - 9\omega^2)(9\omega^2 - 1) + \mu^{-1}\rho^2(9\mu\omega^2 - 1)^2]}. \quad (43)$$

Relations (27), (28), (33), (34), (42), (43) describe two-component small-amplitude breather at rest ($M = 0$). Similar breather that moves in the laboratory frame of references at the velocity M, can be found as

the breather at rest in coordinates $\xi = x - Mt$, $\tau = t$ by searching for localized oscillating solution to the set:

$$M^2 u_{\xi\xi} - 2M u_{\tau\xi} + u_{\tau\tau} - u_{\xi\xi} + \rho(M^2 v_{\xi\xi} - 2M v_{\tau\xi} + v_{\tau\tau}) + \mu^{-1}\rho(v + \rho u) + \beta \sin u = 0, \quad (44)$$

$$M^2 v_{\xi\xi} - 2M v_{\tau\xi} + v_{\tau\tau} - k^2 v_{\xi\xi} + \mu\rho(M^2 u_{\xi\xi} - 2M u_{\tau\xi} + u_{\tau\tau}) + (v + \rho u) = 0. \quad (45)$$

In a class of one-field models described by the nonlinear Klein-Gordon Eqs. in (x,t) case the small-amplitude breathers are, as a rule, weakly radiating approximate solutions with rather a long lifetime [17,18] except the case of exactly solvable sine-Gordon equation; it is important to emphasize that these breathers are self-forming excitations [18]. Apparently the two-component small-amplitude breathers found in the present paper are self-forming long-lived excitations too. So we believe that N-component breathers should be considered as effective energy and information carriers in chain macromolecules (of proteins, DNA, RNA). Their role of carriers becomes especially important when the dynamic system under consideration does not possess stable solitons. As an example we recall that steady-state solitary waves (solitons) described by the Klein-Gordon equation

$$u_{tt} - u_{xx} + u - u^3 = 0 \qquad (46)$$

are unstable (see, e.g., review [19]); for the same Eq.(46) self-forming ("stable") long-lived breathers do exist [17,18] for all values of velocity M, such that $|M| < 1$.

The set of Eqs. (14), (15) possesses high-amplitude $(u_{max} \sim 2\pi)$ breathers too, but investigation of such breathers cannot be fulfilled by means of the Bogolubov-Mitropolsky technique (or other related methods based on expansion into a series in small amplitude). We have found high-amplitude breathers in computer experiments within the framework of Eqs. (14), (15) at $k^2 = 0.2$, $\mu = 2/3$, in which initial data have been specified as a two-component kink-antikink pair; evolution in time of this initial state leads to formation of weakly radiating high-amplitude breather which is an oscillating in time long-lived bound state of two-component kink and antikink (compare with the one-component case [20]). Formation of radiating breather and inelastic interaction of two-component solitons which we have seen in computer experiments within Eqs. (14), (15) at $k^2 = 0.2, \mu = 2/3$ mean that in a general case

$(k^2 \neq 0, \mu \neq 1)$ the system (14), (15) is not completely integrable unlike the special case $k^2 = 0, \mu = 1$. Detailed investigation of soliton interactions and breathers within the two-component DNA model considered in this paper will be published elsewhere.

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