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**CONSIDERING VIBRATIONS OF THE DOUBLE DNA  
MAIN CHAINS BY USING TWO MODELS:  
HEREDITARY AND FRACTIONAL ORDER MODEL**

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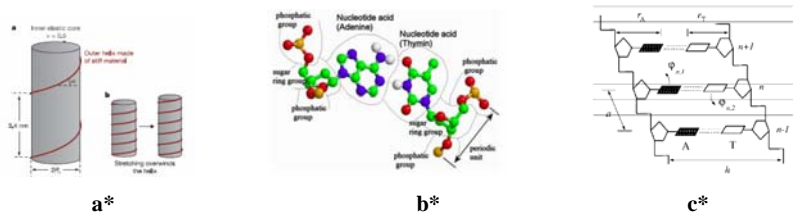
*Abstract:* Using a basic approach to DNA mathematical models published by N.Kovaleva, L.Manevich in 2005 and 2007, and investigated corresponding linearized model, we consider the double DNA (dDNA) as a system with elements with hereditary properties as well as a fractional order system to obtain main chain subsystems of the double DNA. Analytical expressions of the eigen circular frequencies for the homogeneous linerized model of the dDNA chain helix are used to obtain corresponding eigen fractional order creep vibration modes. We identified two sets of eigen normal coordinates of the DNA fractional order chain helix for separation of the system into two uncoupled fractional order chains. The visualization of the eigen fractional order creep vibration modes of the DNA fractional order chain helix is presented. The results open possibilities for different approach to explaining the behavior of the double chain DNA and of transfer of oscillatory signals trough the chains. Under certain sequences it is possible that oscillatory signal is transferred only through one chain. This may correspond to base pair order and translation process in complementary fractional order chains of DNA double helix in a living cell.

*Key words:* DNA, double chain system, eigen main chains, eigen modes, hereditary vibration modes, fractional order vibration modes, DNA models by N. Kovaleva and L. Manevich, viscoelastic properties, creep properties.

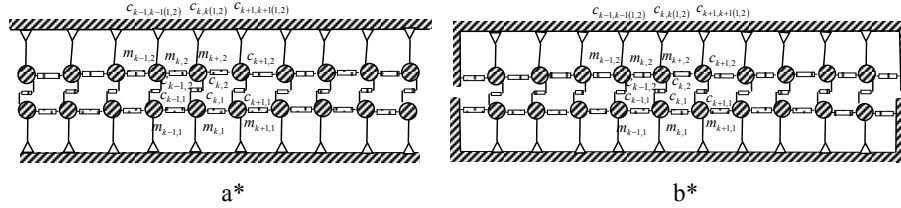
## **1. Introduction**

A number of mechanical models of the DNA double helix have been proposed till today (see Fig. 1 and Refs. [1-6], [15-16], [17-10], [22-23]). Different models are focusing on different aspects of the DNA molecule (biological, physical and chemical processes in which DNA is involved). In a double DNA helix a localized excitation (breather) can exist which corresponds to predominant rotation of one chain and small perturbation of second chain using coarse-grained model of DNA double helix. In this model, each nucleotide is represented by three beads with interaction sites corresponding to a phosphate group, the group of sugar ring, and the base (see Ref. [16]).

N. Kovaleva and L. Manevich [15] point out that solitons and breathers play a functional role in DNA chains. In a model, the DNA backbone is reduced to the polymeric structure and the base is covalently linked to the center of sugar ring group, thus a DNA molecule with  $N$  nucleotides corresponds to  $3N$  interaction centers. Starting from a coarse-grained off-lattice model of DNA and using cylindrical coordinates, authors derive simplified continuum equations corresponding to vicinities of gap frequencies in the spectrum of linearized equations of motion. It is shown that obtained nonlinear continuum equations describing modulations of normal modes, admit spatially localized solitons, which can be identified with breathers. Authors formulated conditions of the breathers existence and estimate their characteristic parameters. The relationship between derived model and more simple and widely used models is discussed. The analytical results are compared with the data of a numerical study of discrete equations of motion (See Figure 1.b\*).



**Figure 2.** **a\*** “Toy mechanical” model of DNA [6] by Jeff Gore, Zev Bryant, Marcelo (2006) **b\*** The model scheme of a double helix on six coarse-grained particles [11]; **c\*** Fragment of the DNA double chain consisting of three AT base pairs.



**Figure 2.** Double DNK fractional order (or/and hereditary) chain helix in the form of multipendulum model with free(a\*) and fixed (b\*) ends

Ref. [16] by N.Kovaleva, L.Manevich (2005)) presented at DSTA'05, presented the simplest model describing opening of DNA double helix. Corresponding differential equations are solved analytically using multiple-scale expansions after transition to complex variables. Obtained solution corresponds to localized torsional nonlinear excitation – breather. Stability of breather is also investigated. In the Reference [12] authors listed a choice of different models of two coupled homogeneous DNA chain vibrations proposed in the literature. By using as a basis the approach to

DNA mathematical models published by N. Kovaleva, L. Manevich in 2005 and 2007, authors consider the linearized model to obtain main chain subsystems of the double DNA helix. Analytical expressions of the eigen circular frequencies for the homogeneous model of the double DNA chain helix are obtained, as well as corresponding eigen vibration modes and possibilities of the appearance of resonant regimes, as well as dynamical absorption under the external forced excitations are considered. Two sets of eigen normal coordinates of the double DNA chain helix for separation of the system into two uncoupled chains are identified. This may correspond to base pair order in complementary chains of DNA double helix in a living cell. Expressions for the kinetic and potential energy as well as energy interaction between chains in the double DNA chain helix are obtained and analyzed for a linearized model [14]. By obtained expressions we concluded that there is no energy interaction between eigen main chains of the double DNA chain helix. Using a basic approach to DNA mathematical models published by N.Kovaleva, L.Manevich in 2005 and 2007, and investigated corresponding linearized model [12], we consider the fractional order model to obtain main chain subsystems of the double DNA fractional order chain helix [13]. Analytical expressions of the eigen circular frequencies for the homogeneous linerized model of the double DNA chain helix are used to obtain corresponding eigen fractional order creep vibration modes. Two sets of eigen normal coordinates of the double DNA fractional order chain helix for separation of the system into two uncoupled fractional order chains are identified. The visualization of the eigen fractional order creep vibration modes of the double DNA fractional order chain helix is presented. The results open the possibilities for different approach to explaining the behavior of the double chain DNA and of transfer of oscillatory signals trough the chains. Under certain sequences it is possible that oscillatory signal is transferred only through one chain. This may correspond to base pair order in complementary fractional order chains of DNA double helix in a living cell. These data contribute to better understanding of biomechanical events of DNA transcription that occur parallel with biochemical processes.

## 2. Linearized model and sets of the eigen main chains of the double DNA chain helix

Authors deal with the planar DNA model in which the chains of the macromolecule form two parallel straight lines placed at a distance  $h$  from each other, and the bases can make only rotation motions around their own chain, being all the time perpendicular to it. Authors accepted as generalized (independent) coordinates  $\varphi_{k,1}$  that are the angular displacement of the  $k$ -th base of the first chain, and as generalized (independent) coordinates  $\varphi_{k,2}$  is the angular displacement of the  $k$ -th base of the second chain. Here  $J_{k,1}$  is the axial moment of mass inertia of the  $k$ -th base of the first

chain;  $\mathbf{J}_{k,2}$  is the axial moment of mass inertia of the  $k$ -th base of the second chains (for detail see Refs.[15-16]). Parameter  $K_{k,i}$ ,  $i = 1,2$  characterizes the potential energy of interaction of the  $k$ -th base with the  $(k+1)$ -th one along the  $i$ -th chain. There are different estimations of rigidity. For the calculation we use the most appropriate value that is close to  $K_{k,i} = K = 6 \times 10^3 [kJ/mol]$ . By using the following notations (see Refs. [12-14]):

$$\kappa = \frac{K_{\alpha\beta}}{2K} \left( 1 - \frac{\omega_{\alpha\beta 2}}{\omega_{\alpha\beta 1}} \right) (r_\alpha - r_\beta)^2, \quad \mu = \frac{K_{\alpha\beta} r_\alpha (r_\alpha - r_\beta)}{K}, \quad u = \frac{\mathbf{J}}{K} \omega^2 \quad (1)$$

the corresponding analytical expressions of the square of  $\omega$  - eigen circular frequencies of vibration modes of separate main chains of linearized double DNA chain helix model, obtained by trigonometric method (see Refs. [20], [8], [10-14]) are:

$$\omega_{\xi,s}^2 = \frac{K}{J} \left[ 2 \sin^2 \frac{\varphi_s}{2} + (\mu - \kappa) \right] \quad \text{and} \quad \omega_{\eta,r}^2 = \frac{K}{J} \left[ 2 \sin^2 \frac{\vartheta_r}{2} + \mu \right] \quad (2)$$

where  $\varphi_s$  and  $\vartheta_r$ ,  $s, r = 1, 2, 3, \dots, n$  depend of the boundary chain conditions.

### 3. Standard light fractional order creep and hereditary element

**Light standard coupling element** of negligible mass in the form of axially stressed rod without bending, and which has the ability to resist deformation under static and dynamic conditions. **Light standard fractional order creep element** for which the constitutive stress-strain relation for the restitution force as the function of element elongation is given by fractional order derivatives in the form

$$P(t) = -\{c_0 x(t) + c_\sigma \mathfrak{D}_t^\sigma [x(t)]\} \quad (3)$$

where  $\mathfrak{D}_t^\sigma[\bullet]$  is operator of the  $\sigma^{th}$  derivative with respect to time  $t$  in the following form:

$$\mathfrak{D}_t^\sigma [x(t)] = \frac{d^\sigma x(t)}{dt^\alpha} = x^{(\sigma)}(t) = \frac{1}{\Gamma(1-\sigma)} \frac{d}{dt} \int_0^t \frac{x(\tau)}{(t-\tau)^\sigma} d\tau \quad (4)$$

where  $c, c_\alpha$  are rigidity coefficients – momentary and prolonged one, and  $\alpha$  a rational number between 0 and 1,  $0 < \sigma < 1$ ;  $P$  is the force appearing in the element;  $x$  is a rheological coordinate, usually presented as deformation or relative displacement. **Light standard hereditary element** for which the constitutive stress-strain relation for the restitution force as the function of element elongation is given by integral member in the form

$$P(t) = -c_0 \left[ x(t) - \int_0^t \mathcal{H}(t-\tau) x(\tau) d\tau \right] = -c_0 [x(t) - \mathfrak{F}[x(t)]] \quad (5)$$

where  $\mathcal{H}(t-\tau) = \frac{c_\sigma - c_0}{nc_\sigma} e^{-\frac{1}{n}(t-\tau)}$  is relaxation kernel,  $\beta = \frac{1}{n}$  is coefficient of the element relaxation

(for detail see Monograph [7] and Ref. [8]) and

$$\mathfrak{F}[x(t)] = \left[ \int_0^t \mathcal{H}(t-\tau) x(\tau) d\tau \right] = \left( \int_0^t \mathcal{H}(t-\tau) \bullet(\tau) d\tau \right) x(t) \quad (6)$$

integral operator.

### 3. The double DNA fractional order chain helix model on the basis of the Kovaleva-Manevich's DNA model

For the double DNA fractional order chain model on the basis of the linearized Kovaleva-Manevich's DNA model (see Refs. [16], [12], [13], [14]), we accept the two chains as they are presented in Figure 2. in the form of the double chain fractional order system containing two coupled multi pendulum subsystems, with corresponding material particles of the corresponding multipendulum chains, that are each two inter coupled by one standard light fractional order element (see Refs. [8], [9] and [13]).

Then we can use a system of coupled linear differential equations (see Refs. [16], [12], [13], [14]) extended by members containing fractional order differential operators in the form (3)-(4). Then we can write a corresponding system of the fractional order differential coupled equations for the homogeneous double DNA fractional order chain helix in the form:

$$\begin{aligned} & \frac{2\mathbf{J}}{K} \ddot{\varphi}_{k,1} - [(\varphi_{k+1,1} - \varphi_{k,1}) - (\varphi_{k,1} - \varphi_{k-1,1})] - \kappa_\sigma \mathfrak{D}_t^\sigma [(\varphi_{k+1,1} - \varphi_{k,1}) - (\varphi_{k,1} - \varphi_{k-1,1})] + \\ & + 2\mu\varphi_{k,1} - \kappa(\varphi_{k,1} - \varphi_{k,2}) - \kappa\kappa_\sigma \mathfrak{D}_t^\sigma [(\varphi_{k,1} - \varphi_{k,2})] = 0 \\ & \frac{2\mathbf{J}_{k,2}}{K_{k,2}} \ddot{\varphi}_{k,2} - [(\varphi_{k+1,2} - \varphi_{k,2}) - (\varphi_{k,2} - \varphi_{k-1,2})] - \kappa_\sigma \mathfrak{D}_t^\sigma [(\varphi_{k+1,2} - \varphi_{k,2}) - (\varphi_{k,2} - \varphi_{k-1,2})] + \\ & + 2\mu\varphi_{k,2} + \kappa(\varphi_{k,1} - \varphi_{k,2}) + \kappa\kappa_\sigma \mathfrak{D}_t^\sigma [(\varphi_{k,1} - \varphi_{k,2})] = 0 \end{aligned} \quad (6)$$

as our intention is to use previous double DNA fractional order chain model for the case of the homogeneous system parameters we take into account that:  $K_{k,1,\sigma} = K_{k,2,\sigma} = K$ . and  $K_{\alpha\beta,\sigma} =$

$K_{\alpha\beta,\sigma}$ , where  $\kappa_\sigma = \frac{K_{\alpha\beta,\sigma}}{K}$ . By using change of the generalized coordinates  $\varphi_{k,1}$  and  $\varphi_{k,2}$  for

$k$ -th bases of both chains in the DNA model into following new  $\xi_k$  and  $\eta_k$  by the following

dependence:  $\xi_k = \varphi_{k,1} - \varphi_{k,2}$  and  $\eta_k = \varphi_{k,1} + \varphi_{k,2}$ , previous system of differential equations (6) obtains the following form:

$$\frac{2J}{K} \ddot{\xi}_k - \xi_{k-1} + 2\xi_k - \xi_{k+1} + \kappa_\sigma \mathfrak{D}_t^\sigma [-\xi_{k-1} + 2\xi_k - \xi_{k+1}] + 2\mu\xi_k - 2\kappa\xi_k - 2\kappa\kappa_\sigma \mathfrak{D}_t^\sigma [\xi_k] = 0 \quad (7)$$

$$\frac{2J}{K} \ddot{\eta}_k - \eta_{k-1} + 2\eta_k - \eta_{k+1} + \kappa_\sigma \mathfrak{D}_t^\sigma [-\eta_{k-1} + 2\eta_k - \eta_{k+1}] + 2\mu\eta_k = 0, k = 1, 2, 3, \dots, n \quad (8)$$

First series (7) of the previous system of fractional order differential equations are decoupled and independent with relations of the second series (8) of the fractional order differential equations. *Then we can conclude that new coordinates of  $\xi_k$  and  $\eta_k$  are main coordinates of double DNA fractional order chains and that we obtain two fictive decoupled independent eigen fractional order, different, chains of the double DNA fractional order chain helix model. This is the first fundamental conclusion as an important property of the fractional order homogeneous model of vibrations in a double DNA fractional order homogeneous helix.*

Systems of differential equations (7)-(8) contains two separate subsystems of fractional order differential equations expressed by *coordinates of  $\xi_k$  and  $\eta_k$  which are main coordinates of the eigen main chains of a double DNA fractional order chain helix and separate DNA fractional order model into two independent fractional order chains.*

#### 4. The double DNA hereditary chain helix model on the basis of the Kovaleva-Manevich's DNA model

For the double DNA hereditary chain model on the basis of the linearized Kovaleva-Manevich's DNA model (see Refs. [16], [12], [13], [14]), we accept the two chains as they are presented in Figure 2. in the form of the double chain fractional order system containing two coupled multi pendulum subsystem, in with corresponding material particles of the corresponding multipendulum chains are each two inter coupled by one standard light hereditary element (see Refs. [7] and [8]).

Then we can use a system of coupled linear differential equations (see Refs. [16], [12], [13], [14]) extended by members containing integral operators in the form (5)-(6). Then we can write a corresponding system of coupled integro-differential equations for the homogeneous double DNA hereditary chain helix in the form:

$$\begin{aligned} \frac{2J}{K} \ddot{\varphi}_{k,1} - [(\varphi_{k+1,1} - \varphi_{k,1}) - (\varphi_{k,1} - \varphi_{k-1,1})] - \mathfrak{I}[(\varphi_{k+1,1} - \varphi_{k,1}) - (\varphi_{k,1} - \varphi_{k-1,1})] + \\ + 2\mu\varphi_{k,1} - \kappa(\varphi_{k,1} - \varphi_{k,2}) - \kappa\mathfrak{I}[(\varphi_{k,1} - \varphi_{k,2})] = 0 \end{aligned}$$

$$\begin{aligned} \frac{2J_{k,2}}{K_{k,2}} \ddot{\varphi}_{k,2} - [(\varphi_{k+1,2} - \varphi_{k,2}) - (\varphi_{k,2} - \varphi_{k-1,2})] - \mathfrak{F}[(\varphi_{k+1,2} - \varphi_{k,2}) - (\varphi_{k,2} - \varphi_{k-1,2})] + \\ + 2\mu\varphi_{k,2} + \kappa(\varphi_{k,1} - \varphi_{k,2}) + \kappa\mathfrak{F}[(\varphi_{k,1} - \varphi_{k,2})] = 0 \end{aligned} \quad (9)$$

as our intention is to use previous double DNA hereditary chain model for the case of the homogeneous system parameters we take into account that:  $K_{k,1,\sigma} = K_{k,2,\sigma} = K$ . By using change of the generalized coordinates  $\varphi_{k,1}$  and  $\varphi_{k,2}$  for  $k$ -th bases of both chains in the DNA model into following new  $\xi_k$  and  $\eta_k$  by the following dependence:  $\xi_k = \varphi_{k,1} - \varphi_{k,2}$  and  $\eta_k = \varphi_{k,1} + \varphi_{k,2}$ , previous system of differential equations (6) obtains the following form:

$$\frac{2J}{K} \ddot{\xi}_k - \xi_{k-1} + 2\xi_k - \xi_{k+1} + \mathfrak{F}[-\xi_{k-1} + 2\xi_k - \xi_{k+1}] + 2\mu\xi_k - 2\kappa\xi_k - 2\kappa\mathfrak{F}[\xi_k] = 0 \quad (10)$$

$$\frac{2J}{K} \ddot{\eta}_k - \eta_{k-1} + 2\eta_k - \eta_{k+1} + \mathfrak{F}[-\eta_{k-1} + 2\eta_k - \eta_{k+1}] + 2\mu\eta_k = 0, k = 1, 2, 3, \dots, n \quad (11)$$

First series (10) of the previous system of integro-differential equations is decoupled and independent in relation to the second series (11) of integro-differential equations. *Then we can conclude that new coordinates of  $\xi_k$  and  $\eta_k$  are main coordinates of double DNA hereditary chains and that we obtain two fictive decoupled eigen hereditary, different, chains of the double DNA hereditary chain helix model. This is the second fundamental conclusion as an important property of the hereditary order homogeneous model of vibrations in a double DNA hereditary homogeneous helix.*

Systems of integro-differential equations (10)-(11) contain two separate subsystems of integro-differential equations expressed by *coordinates of  $\xi_k$  and  $\eta_k$  which are main coordinates of eigen main chains of a double DNA fractional order chain helix and separate DNA hereditary model into two independent hereditary chains.*

We can see that there are full mathematical analogy and phenomenological mapping between two models: a double DNA fractional order chain helix model and a double DNA hereditary chain helix.

## 5. The main partial fractional order/hereditary oscillator of a double DNA fractional order/hereditary chain helix model

By using system the (7)-(8) of uncoupled fractional order differential equations and analogous system (10)-(11) of uncoupled integro-differential equations as corresponding systems of eigen main chains of the corresponding models of double DNA fractional order/hereditary chain helix vibrations

can obtain corresponding main coordinates  $\zeta_{\xi,s}$  and  $\zeta_{\eta,r}, r, s = 1, 2, 3, \dots, n$  and corresponding double systems of the main partial fractional order oscillators described by the following uncoupled fractional order differential equations containing each only one normal coordinate  $\zeta_{\xi,s}$  and  $\zeta_{\eta,r}$ :

$$\ddot{\zeta}_{\xi,s} + \omega_{\xi,s}^2 \zeta_{\xi,s} + \omega_{\alpha\xi,s}^2 \mathfrak{D}_t^\alpha [\zeta_{\xi,s}] = 0, s = 1, 2, 3, 4, \dots, n \quad (12)$$

$$\ddot{\zeta}_{\eta,r} + \omega_{\eta,r}^2 \zeta_{\eta,r} + \omega_{\alpha\eta,r}^2 \mathfrak{D}_t^\alpha [\zeta_{\eta,r}] = 0, r = 1, 2, 3, \dots, n \quad (13)$$

and corresponding double systems of the main partial hereditary oscillators described by the following uncoupled integro-differential equations containing each only one normal coordinate  $\zeta_{\xi,s}$  and  $\zeta_{\eta,r}$ :

$$\ddot{\zeta}_{\xi,s} + \omega_{\xi,s}^2 \zeta_{\xi,s} + \omega_{\xi,s}^2 \mathfrak{I}[\zeta_{\xi,s}] = 0, s = 1, 2, 3, 4, \dots, n \quad (14)$$

$$\ddot{\zeta}_{\eta,r} + \omega_{\eta,r}^2 \zeta_{\eta,r} + \omega_{\eta,r}^2 \mathfrak{I}[\zeta_{\eta,r}] = 0, r = 1, 2, 3, \dots, n \quad (15)$$

In both of the previous systems \*12)-(13) and (13)-(14) square of the eigen frequencies,  $\omega_{\xi,s}^2$  and  $\omega_{\eta,r}^2$  of the linearized systems are defined by expression s (2) and it is easy to obtain corresponding expressions for the  $\omega_{\alpha\xi,s}^2$  and  $\omega_{\alpha\eta,r}^2$  in the following form:

#### 4. Concluding remarks

In the end, we can conclude that new coordinates of  $\xi_k$  and  $\eta_k$  composed by generalized coordinates in the way  $\xi_k = \varphi_{k,1} - \varphi_{k,2}$  and  $\eta_k = \varphi_{k,1} + \varphi_{k,2}$  are main coordinates eigen main chains of the double DNA fractional order/hereditary chain helix and that it is possible to obtain two fictive decoupled and separated eigen single fractional order chains of the double DNA fractional order/hereditary homogeneous chain helix model. This is the first fundamental conclusion and an important property of the fractional order/hereditary model of vibrations in a double DNA fractional order/hereditary helix. Considered as a fractional order/hereditary mechanical system, DNA molecule as a double fractional order/hereditary helix has its eigen fractional order/hereditary vibration modes and that is its characteristic. Mathematically, it is possible to decouple it into two chains with their eigen modes closest to the eigen modes of the linearized models of main chains with corresponding sets of the circular frequencies which are different. This may correspond to different chemical structure (the order of base pairs) of the complementary chains of DNA. We are free to propose that every specific set of base pair order has its eigen circular frequencies and it changes when DNA



chains are coupled in the system of double helix. DNA as a double helix in a living cell can be considered as nonlinear system but under certain condition its behavior can be describe by linear dynamics.

Then, analytical expressions of the square of  $\omega_{\xi,s}^2$  and  $\omega_{\eta,r}^2$  - *eigen circular frequencies of the vibration modes of the separate chains* of the homogeneous double DNA chain helix are obtained. By using these results it is easy to consider these values of the system  $\omega_{\xi,s}^2$  and  $\omega_{\eta,r}^2$  - *eigen circular frequencies of free vibrations as series of resonant frequencies under external multi frequencies excitations, and also possibilities for the appearance of dynamical absorbtion phenomena and find explanation with real processes in the homogeneous double DNA ideal-elastic/fractional order/ hereditary chain helix*. Next consideration is focused on the small nonlinearity in the double DNA chain helix vibrations and rare nonlinear phenomena such as resonant jumps and energy interactions between nonlinear modes.

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