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Parameter selection in a Peyrard–Bishop–Dauxois model for DNA dynamics

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ABSTRACT

In this Letter we study possible intervals for some parameters existing in the Peyrard–Bishop–Dauxois (PBD) model for the DNA dynamics. These parameters describe longitudinal and helicoidal interactions between nucleotides and a Morse potential approximating transverse interactions. We also estimate a possible interval for a wave number of a carrier component of a modulated solitonic wave. Finally, we compare our statements with experimental value of solitonic velocity in DNA.

1. Introduction

To study DNA dynamics we very often need to guess values of some still unknown parameters. The purpose of this Letter is to give possible intervals for these parameters. This will certainly allow better and easier estimations and calculations related to future DNA research.

In this Letter we rely on the Peyrard–Bishop–Dauxois (PBD) model for the DNA dynamics [1]. This model, taking helicoidal structure into consideration, represents an extended version of a former Peyrard–Bishop (PB) model [2]. We assume that readers are familiar with this model. Hence, in Section 2, we only give some basic features of the model.

Sections 3 and 4 are primarily devoted to a ratio of the harmonic constants of the longitudinal and helicoidal springs. Possible values of this ratio are estimated according to two criteria.

According to the PBD model, DNA dynamics is described by a solitonic wave, which is a localized modulated wave called breather. To calculate a solitonic width, an amplitude, etc., we should know the wavelength of the carrier component. The value of this parameter is estimated in Sections 4 and 5.

Finally, in Section 6, we use the basic characteristics of the solitonic wave to show how the upper limits of the very troublesome parameters of the longitudinal and the helicoidal springs can be determined.

One can find a variety of the values of these parameters in literature. This is why we did our best to be systematic as much as possible. We use different procedures to estimate the values of these parameters. For example, in Sections 3 and 4 our estimates are based on satisfying some constraints of the model. In Section 5 we estimate the upper limit of the solitonic carrier wave width following physical arguments only. Finally, in Section 6 we deal with four parameters. For two of them we rely on experimental results while for the remaining two we suggest a procedure for their estimations based on the very basic physical principle of nonlinear DNA dynamics.

We close this Letter with the summary and concluding remarks in Section 7.

2. The PBD model

In this section we very briefly describe the basic features of the PBD model. The model assumes that DNA molecule is a homogeneous and periodic structure with a period $l = 0.34$ nm [1,3,4]. Only transversal motions of nucleotides are taken into consideration. If u_n and v_n are the transversal displacements of the nucleotides of different strands at the site n from their equilibrium positions then a Hamiltonian for DNA molecule is

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$$H=\sum\left\{\frac{m}{2}\left(\dot u_n^2+\dot v_n^2\right)+\frac{k}{2}\left[(u_n-u_{n-1})^2+(v_n-v_{n-1})^2\right]\right.$$
$$+\frac{K}{2}\left[(u_n-v_{n+h})^2+(u_n-v_{n-h})^2\right]$$
$$\left.+D\left[e^{-a(u_n-v_n)}-1\right]^2\right\} \tag{1}$$

where $m=5.1\times10^{-25}$ kg is the nucleotide mass and k and K are harmonic constants of the longitudinal and the helicoidal springs, respectively. The important helicoidal structure is taken into account through the harmonic interaction of the nucleotides having the coordinates u_n and $v_{n\pm h}$ [1]. As the helix has a corresponding pitch of about 10 nucleotide pairs per turn, we assume $h=5$. The last term in Eq. (1) is a Morse potential representing the transverse interaction of the nucleotides at the same site where D and a are the depth and the inverse width of the Morse potential well, respectively. Note that, for $K=0$, we obtain the Hamiltonian for the PB model.

As DNA is assumed to be homogeneous the values for all these parameters as well as the nucleotide masses are equal along the chain. The value for m, mentioned above, is the average of the four possible values.

Using coordinates x_n and y_n, describing the in-phase and the out-of-phase transversal motions, defined through

$$x_n=(u_n+v_n)/\sqrt{2},\qquad y_n=(u_n-v_n)/\sqrt{2}, \tag{2}$$

we can obtain decoupled dynamical equations of motions [1,3,4]

$$m\ddot x_n=k(x_{n+1}+x_{n-1}-2x_n)+K(x_{n+h}+x_{n-h}-2x_n) \tag{3}$$

and

$$m\ddot y_n=k(y_{n+1}+y_{n-1}-2y_n)-K(y_{n+h}+y_{n-h}+2y_n)$$
$$+2\sqrt{2}aD\left(e^{-a\sqrt{2}y_n}-1\right)e^{-a\sqrt{2}y_n}. \tag{4}$$

Of course, these equations are derived from the Hamiltonian (1). All derivations and explanations can be found in Ref. [5].

The first of these decoupled equations describes usual linear waves (phonons) while the second one describes the nonlinear waves (breathers). Hence, we restrict our attention on Eq. (4) and look for the solution $y_n(t)$. To solve this problem we use a semi-discrete approximation [6]. This means that we assume small, but still nonlinear oscillations

$$y_n(t)=\varepsilon\Phi_n(t)\quad(\varepsilon\ll1) \tag{5}$$

and a series expansion [3–6]

$$\Phi_n(t)=F_1(\xi)e^{i\theta_n}+\varepsilon\left[F_0(\xi)+F_2(\xi)e^{i2\theta_n}\right]+cc+O\left(\varepsilon^2\right), \tag{6}$$
$$\xi=(\varepsilon nl,\varepsilon t),\qquad \theta_n=nql-\omega t, \tag{7}$$

where ω is the optical frequency of corresponding linear approximation, $q=2\pi/\lambda$ is the wave number of a carrier wave, F_0 is real and cc stands for complex-conjugate.

One can show that functions F_0 and F_2 can be expressed through F_1 as [1,3–5]

$$F_0=\mu|F_1|^2,\qquad F_2=\delta F_1^2 \tag{8}$$

where

$$\mu=-2\alpha\left(1+K/a^2D\right)^{-1}, \tag{9}$$
$$\delta=m\omega_g^2\alpha\left[4m\omega^2-2k\left(1-\cos(2ql)\right)\right.$$
$$\left.-2K\left(1+\cos(2hql)\right)-4a^2D\right]^{-1}, \tag{10}$$
$$\omega^2=(4/m)\left[a^2D+k\sin^2(ql/2)+K\cos^2(qhl/2)\right], \tag{11}$$

and

$$\omega_g^2=4a^2D/m,\qquad \alpha=-3a/\sqrt{2},\qquad \beta=7a^2/3. \tag{12}$$

The function F_1 is a solution of the nonlinear Schrödinger equation (NLSE):

$$iF_{1\tau}+PF_{1SS}+Q|F_1|^2F_1=0 \tag{13}$$

where τ and S are rescaled time and space variables [1,3–5]. P and Q are a dispersion and a nonlinear parameter, respectively:

$$P=\frac{1}{2\omega}\left\{\frac{l^2}{m}\left[k\cos(ql)-Kh^2\cos(qhl)\right]-V_g^2\right\}, \tag{14}$$

$$Q=-\frac{\omega_g^2}{2\omega}\left[2\alpha(\mu+\delta)+3\beta\right], \tag{15}$$

while the group velocity is

$$V_g\equiv\frac{d\omega}{dq}=\frac{l}{m\omega}\left[k\sin(ql)-Kh\sin(qhl)\right]. \tag{16}$$

A solution of Eq. (13), relevant for this Letter, exists if $PQ>0$. This can be found in aforementioned references. In this Letter we assume that both P and Q are positive [7]. All this brings about the following expression for the function $y_n(t)$ [1,3–5,7]:

$$y_n(t)=2\varepsilon A\,\mathrm{sech}\left(\frac{\varepsilon(nl-V_et)}{L_e}\right)\left\{\cos(\Theta nl-\Omega t)\right.$$
$$\left.+\varepsilon A\,\mathrm{sech}\left(\frac{\varepsilon(nl-V_et)}{L_e}\right)\left[\frac{\mu}{2}+\delta\cos\left(2(\Theta nl-\Omega t)\right)\right]\right\}$$
$$+O\left(\varepsilon^3\right) \tag{17}$$

where

$$V_e=V_g+\varepsilon u_e,\qquad \varepsilon A=\varepsilon\sqrt{\frac{u_e^2-2u_eu_c}{2PQ}}, \tag{18}$$

$$\Theta=q+\frac{\varepsilon u_e}{2P},\qquad \frac{L_e}{\varepsilon}=\frac{2P}{\varepsilon\sqrt{u_e^2-2u_eu_c}}, \tag{19}$$

and

$$\Omega=\omega+\frac{(V_g+\varepsilon u_c)\varepsilon u_e}{2P}. \tag{20}$$

We have already explained a source of the parameter ε in Eqs. (5)–(7). There are two more parameters coming from the mathematical procedure and these are u_e and u_c, the envelope and the carrier wave velocities of the function F_1, and there should be

$$u_e>2u_c. \tag{21}$$

If we look at all the formulas where these three parameters exist we can notice that all these expressions depend on two parameters only. These are εu_e and εu_c. Hence, there are two rather than three parameters coming from the mathematical procedure. It is convenient to introduce a new parameter η defined through

$$u_c=\eta u_e,\quad \eta\in[0,0.5). \tag{22}$$

According to Eq. (17) it is obvious that the envelope and the carrier wave velocities are V_e and Ω/Θ. In Refs. [8,9] we suggested a coherent mode meaning that these velocities are equal. This means that $y_n(t)$ is one phase function. From the equality of these two velocities one can express εu_e as a function of η [4,9]

$$z\equiv\varepsilon u_e=\frac{P}{1-\eta}\left[-q+q\sqrt{1+\frac{2(1-\eta)}{Pq^2}(\omega-qV_g)}\right]. \tag{23}$$