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Frequency dependence of amplitude of nonlinear transverse waves in DNA molecule

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In this article the frequency dependence of the amplitude nonlinear transverse waves in DNA molecule is considered with take into account additionally the frequency dependence from the wave number. Also in this article we have considered both driven and free oscillations.

Keywords: DNA molecule, Peyrard-Bishop model, Galerkin method, resonance curves

1. Introduction

The problem of local opening of the DNA chain in a process of m-RNA transcription is very interesting and important.

In this strongly nonlinear case the optical frequency depends on the amplitude excitation. Some frequency, which is eigenfrequency at small amplitudes is not eigenfrequency at big amplitudes.

The frequency dependence of amplitude of nonlinear transverse waves in DNA molecule is obtained by means of Galerkin method on bases of the nonlinear Peyrard-Bishop model that is describing the transversal oscillations of nucleotides.

2. The Model

The model include two types of internal motions, namely, the displacements (u_n and v_n) of the bases from their equilibrium positions along the direction of the hydrogen bonds that connect the two bases in a pair (fig. 1).

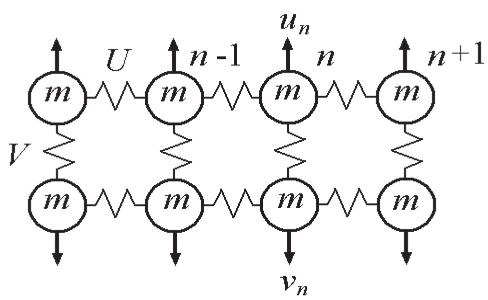

FIG. 1. The Peyrard-Bishop model.

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The potential energy for the hydrogen bonds connecting AT or CG base pair is modeled by a Morse potential

$$V = D\left[\mathrm{e}^{(-a(u_n - v_n))} - 1\right]^2, \tag{1}$$

where D and a are the depth and the inverse width of the Morse potential well, respectively.

This is shown in fig. 2.

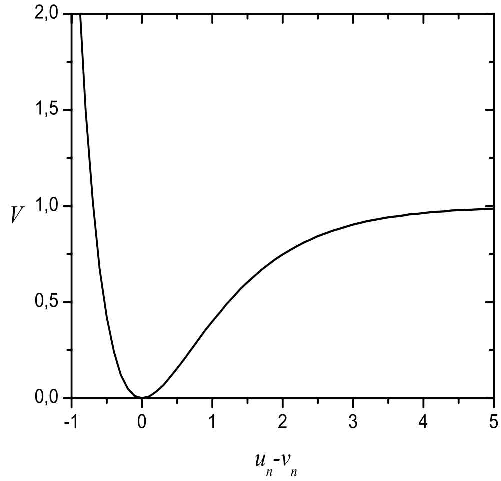

FIG. 2. The Morse potential.

The Hamiltonian for the model is

$$\begin{aligned} H = \sum \tfrac{m}{2}\left(\dot{u}_n^2 + \dot{v}_n^2\right) + \tfrac{c}{2}\Big[(u_n - u_{n-1})^2 + \\ + (v_n - v_{n-1})^2 + D\left(e^{-a(u_n - v_n)} - 1\right)^2\Big], \end{aligned} \tag{2}$$

where m is mass of base pair; c is the harmonic constant of the longitudinal spring.

It is convenient to introduce the new coordinates

$$\begin{aligned} x_n &= (u_n + v_n)/\sqrt{2}, \\ y_n &= (u_n - v_n)/\sqrt{2}. \end{aligned} \tag{3}$$

The equations for the transversal oscillation of nucleotides are

$$m\ddot{x}_n = c\left(x_{n+1} + x_{n-1} - 2x_n\right), \tag{4}$$

$$\begin{aligned} m\ddot{y}_n = c\left(y_{n+1} + y_{n-1} - 2y_n\right) + \\ +2\sqrt{2}aD\left(\mathrm{e}^{-a\sqrt{2}y_n} - 1\right)\left(\mathrm{e}^{-a\sqrt{2}y_n}\right). \end{aligned} \tag{5}$$

The first equation describes the usual linear waves (phonons). The second one describes the nonlinear waves (breathers). Hence, we restrict our attention on the second nonlinear equation.

The traditional solution of equation (5) is

$$y = \varepsilon, (\varepsilon \ll 1),$$

$$\begin{gathered} {}_n(t) = F_1(\varepsilon nh, \varepsilon t) e^{i\theta_n} + \\ +\varepsilon \left[F_0(\varepsilon nh, \varepsilon t) + F_2(\varepsilon nh, \varepsilon t) e^{i2\theta_n} \right] + \\ +cc + O(\varepsilon^2), \end{gathered}$$

$$\theta_n = nkh - \omega t.$$

Here ω is frequency, k is wave number, h is distance between neighboring nucleotides of same strand.

The function and can be expressed through the function [1, 2], which is a solution of the nonlinear Schrödinger equation.

In our paper we shall be used the solution of the equation (5) in form of traveling wave [3]

$$y_n = A \cos(\omega t - knh) = A \cos x, \tag{6}$$

where ω is frequency, which dependent from the amplitude A.

After substitution (6) in (5) we find relation

$$\begin{gathered} m\omega^2 A \cos x = 2cA(1 - \cos kh) \cos x - \\ -2\sqrt{2} aD \left[\mathrm{e}^{-2a\sqrt{2} A \cos x} - \mathrm{e}^{-a\sqrt{2} A \cos x} \right]. \end{gathered} \tag{7}$$

According to Galerkin method we multiply (7) on $\cos x$ and then integrate over the x from -π to π.

3. Results

In result we obtain the equation for frequency ω as function the amplitude A and the wave number k

$$\begin{gathered} \frac{\omega}{\omega_0} = \left(2(1 - \cos kh) + \frac{4\sqrt{2} aD}{cA} \times \right. \\ \left. \times \left(I_1(2\sqrt{2} aA) - I_1(\sqrt{2} aA) \right) \right)^{\frac{1}{2}}. \end{gathered} \tag{8}$$

Here $\omega_0 = \sqrt{c/m}$, $I_1(x)$ is Bessel function of imaginary argument. The equation (8) given the sharp increase the amplitude at variation the frequency in bounded limits.

The relation (8) describes the nonlinear dependence of frequency from amplitudes for the optical modes in the case of the free vibrations (see fig. 3).

We may to support the assumption that local DNA denaturation is due to local strand separation.

Now we consider the forced oscillation or the DNA molecule due to external force which appear in result passing of the acoustic wave. Besides we ignore of the resistance of medium. As a result equation (5) takes the

$$\begin{gathered} m\ddot{y}_n = c\left(y_{n+1} + y_{n-1} - 2y_n\right) + \\ +2\sqrt{2} aD \left(\mathrm{e}^{-a\sqrt{2} y_n} - 1 \right) \left(\mathrm{e}^{-a\sqrt{2} y_n} \right) + \\ +S \cos(\omega t - knh) \end{gathered} \tag{9}$$

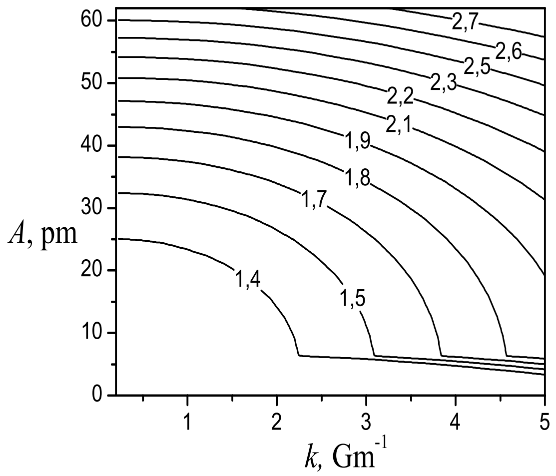

FIG. 3. The frequency dependence of amplitude of nonlinear transverse waves (curves $A(k)$ is corresponding relations $\frac{\omega}{\omega_0}$).

The second term in equation (9) describes the nonlinear forces and the last term takes in to account driving force with amplitude of S.

The solution the equation (9) present in the form (6). The result is

$$\begin{aligned} &\tfrac{\omega}{\omega_0} = (2(1-\cos kh)+ \\ &+\big(I_1(2\sqrt{2}aA) - I_1(\sqrt{2}aA)\big) + \\ &+\tfrac{4\sqrt{2}aD}{cA} + \tfrac{S}{m\omega_0 A}\Big)^{\frac{1}{2}}. \end{aligned} \tag{10}$$

Account must be taken of the next relation , besides (where b is amplitude the driving wave). In result we find

$$\begin{aligned} &\tfrac{\omega}{\omega_0} = (2(1-\cos kh) + \tfrac{4\sqrt{2}aD}{cA}\times \\ &\times \big(I_1(2\sqrt{2}aA) - I_1(\sqrt{2}aA)\big) + \tfrac{b}{A}\big)^{\frac{1}{2}} \end{aligned} \tag{11}$$

The dependence of the frequency from amplitude for the case of forcing oscillations is displayed in fig. 4.

In center of fig. 4 is skeleton curve by $S = 0$; at the left of skeleton curve is curve by $S = -0.8A$; at the right of skeleton curve is curve by $S = 0.8A$.

We hope that our description the large amplitude excitation will be useful for understanding of opening of DNA molecule.

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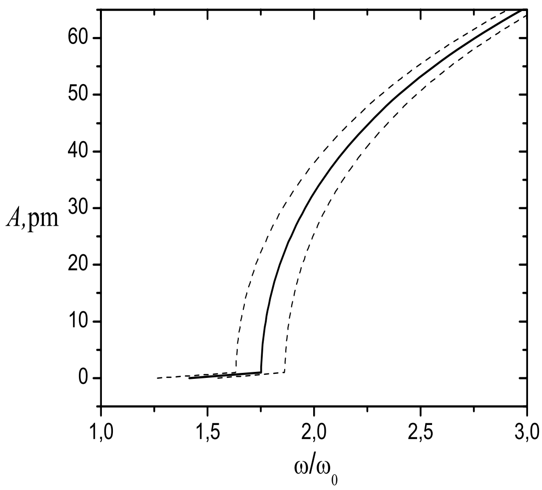

FIG. 4. The resonance curves for DNA molecule.

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