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**WAVE PROPAGATION OF COUPLED MODES
IN THE DNA DOUBLE HELIX**

Conrad B. Tabi¹

*Laboratory of Biophysics, Department of Physics, Faculty of Science,
University of Yaoundé I, P.O. Box 812, Yaoundé, Cameroon*

and

The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy,

Alidou Mohamadou

*Condensed Matter Laboratory, Department of Physics, Faculty of Science,
University of Douala, P.O. Box 24157, Douala, Cameroon*

and

*Laboratory of Mechanics, Department of Physics, Faculty of Science,
University of Yaoundé I, P.O. Box 812, Yaoundé, Cameroon*

and

Timoleon C. Kofané

*Laboratory of Mechanics, Department of Physics, Faculty of Science,
University of Yaoundé I, P.O. Box 812, Yaoundé, Cameroon.*

MIRAMARE – TRIESTE

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¹contab408@hotmail.com

Abstract

The dynamics of waves propagating along the DNA molecule is described by the coupled nonlinear Schrödinger equations. We consider both the single and the coupled nonlinear excitation modes, and we discuss their biological implications. Furthermore, the characteristics of the coupled mode solution are discussed and we show that such a solution can describe the local opening observed within the transcription and the replication phenomena.

1 Introduction

DNA (Deoxyribonucleic acid) is the fundamental information storage medium which contains the genetic information of most organisms. Contained in every cell, it reaches lengths of several meters per cell and its complementary strands are made of a long sequence of four different nucleotides (Adenine, Guanine, cytosine and thymine) attached to a phosphate-sugar backbone. The complementarity of the strands is guaranteed by hydrogen bonds [1] and the typical helical structure is induced by the stacking interactions between subsequent base pairs. As a replicating information unit, DNA has fascinated not just biologists, but also physicists, biophysicists and chemists and, even nowadays, it remains difficult to fully understand, from a physical point of view, all the dynamical processes (transcription and replication processes are the main) involved and the influence of the related factors. Nevertheless, the interest in the nonlinear dynamics of DNA started when Englander et al. [2] suggested that the existence of solitons propagating along the DNA molecule may be important in DNA transcription, where a specialized enzyme (RNA-Polymerase) binds to a specific site of the DNA double helix and unwinds it in a local region of 15-20 base pairs, thus creating a transcription bubble; the RNA-polymerase and the bubble then travel along the DNA, copying its sequence and producing a RNA-Messenger to be later used to express genes or replicate the local sequence. In the last decade, several models were proposed in order to substantiate this idea in quantitative terms but there are two important models, the one proposed by Yakushevich [3] and improved by Gaeta [4], and the second proposed by Peyrard and Bishop (PB) [5] which concentrates on transversal openings of base pairs. In fact, the PB model is one of the simplest models that investigate DNA at the scale of a base pair [5]. The complex double-stranded molecule is described by postulating some simple effective interaction among the bases within a pair and along the strands. The model has been successfully applied to analyze experiments on the melting of short DNA chains [6]. Furthermore, it allows to easily include the effect of heterogeneities [7] yielding a sharp staircase structure of the melting curve (number of opened base pairs as a function of the temperature T) [8]. Beyond its original motivation to explain the denaturation, the PB model has an intrinsic theoretical interest as one of the simplest one-dimensional systems displaying a genuine phase transition [9, 10].

The nonlinear effects might focus on the vibrational energy of DNA into localized soliton-like excitations [3, 11, 12, 13]. Soliton-like objects arise in various physical settings and, are due to the interplay between dispersion and nonlinearity. They are mostly present in optical materials (where there exist a lower and an upper cut-off modes). As it is well-known, the nonlinear localized excitations related to the lower and upper continuous wave spectrum have been considered separately [14] in discrete lattices. Consequently, with an attempt to describe DNA dynamics in a more realistic way, it could be interesting to consider the nonlinear coupling between the various available modes in discrete lattices and in DNA, which naturally leads to more complicated and rich dynamical behaviors. It is the main purpose of this paper to relate

DNA dynamics to the strong coupling of such modes, with a focus on strong interactions between different cut-off modes of the continuous wave spectrum in the framework of the PB model of DNA dynamics.

The present paper is therefore organized as follows. In section 2, we recall the PB model of DNA dynamics, and we show that, using the asymptotic expansion, it reduces to a set of CNLS equations. In section 3, after solving the single and coupled mode equations, we perform numerical simulations on the PB model with realistic values of parameters. We also show that the coupled-mode configuration can be used to simulate the shape of the bubbles usually observed in DNA transcription and replication. The last section is devoted to concluding remarks.

2 Model and mathematical background

2.1 The Peyrard-Bishop model

The PB model is one of the models describing the dynamics of large-amplitude localized excitations in DNA molecule [5]. The B-form DNA of the Watson and Crick model is a double helix, which consists of two strands, S_1 and S_2 , linked by nearest-neighbor harmonic interaction along the chain. The strands are coupled to each other through hydrogen bonds, which are supposed to be responsible for transverse displacements of nucleotides. Only the transversal displacements of the bases denoted by y_n and z_n from their equilibrium positions along the direction of the hydrogen bonds are considered. The molecule consists of the following elements: a common mass m is used for all the nucleotides in a strand, and the same coupling constant c along each strand is assumed. With the above notation, the Hamiltonian of the discrete system is written as follows [5]

$$H = \sum_{n=1}^N \left[\frac{1}{2}m(\dot{y}_n^2 + \dot{z}_n^2) + V(y_n - z_n) + \frac{1}{2}c(y_n - y_{n-1})^2 + \frac{1}{2}c(z_n - z_{n-1})^2 \right]. \quad (1)$$

The intrapair potential is the Morse potential $V(y_n - z_n) = D[e^{-a(y_n - z_n)} - 1]^2$, where D is the dissociation energy and a a parameter homogeneous to the inverse of a length, which sets the spatial scale of the potential. The Hamiltonian (1) gives the equations of motion for y_n and z_n .

$$m\ddot{y}_n = c(y_{n+1} + y_{n-1} - 2y_n) + 2aD\{e^{-a(y_n - z_n)} - 1\}e^{-a(y_n - z_n)} \quad (2)$$

$$m\ddot{z}_n = c(z_{n+1} + z_{n-1} - 2z_n) - 2aD\{e^{-a(y_n - z_n)} - 1\}e^{-a(y_n - z_n)}. \quad (3)$$

To analyze the motions of the two strands, it is convenient to introduce the following independent variables,

$$r_n = (y_n + z_n)/\sqrt{2}, \quad u_n = (y_n - z_n)/\sqrt{2}. \quad (4)$$

We then have

$$m\ddot{r}_n = c(r_{n+1} + r_{n-1} - 2r_n) \quad (5)$$

$$m\ddot{u}_n = c(u_{n+1} + u_{n-1} - 2u_n) + 2\sqrt{2}aDe^{-a\sqrt{2}u_n}(e^{-a\sqrt{2}u_n} - 1). \quad (6)$$

The variables r_n and u_n represent the in-phase and out-of-phase motions, respectively. Equation (5) is a linear differential-difference equation with the usual plane wave solution. On the other hand, Eq. (6) contains nonlinear terms. It is interesting to relate this analysis to nonlinear excitations and then, the equation of the out-of-phase motion is written, after expanding the terms in exponential, as

$$\ddot{u}_n = C(u_{n+1} + u_{n-1} - 2u_n) - \omega_g^2 (u_n + \alpha u_n^2 + \beta u_n^3) \quad (7)$$

where $C = \frac{c}{m}$, $\omega_g^2 = \frac{4a^2D}{m}$, $\alpha = -\frac{3a}{\sqrt{2}}$ and $\beta = \frac{7a^2}{3}$.

We use the parameter values $D = 0.35\text{eV}$, $a = 4.45\text{\AA}^{-1}$, $m = 300$ a.m.u, $l = 3.4\text{\AA}$, and the coupling parameter $c = 0.104\text{eV}/\text{\AA}^2$, which are known in DNA-like models [5].

The appropriate linear dispersion relation, which is optical in the present case, is given by

$$\omega^2 = \omega_g^2 + 4C \sin^2\left(\frac{ql}{2}\right) \quad (8)$$

with q being the wave length and l , the base pairs spacing. $\omega_0 = \omega_g$ is the lower cut-off frequency, while $\omega_{max} = \sqrt{\omega_g^2 + 4C}$ is the upper cut-off frequency. Furthermore, we assume $\omega_g^2 \gg 4C$ because of the discreteness of the DNA lattice.

Eq.(7) is a nonlinear differential-difference which cannot be solved exactly. Thus, there exist several techniques to convert them into more integrable systems [14, 15, 16]. In the next section, we therefore use the asymptotic expansion [14] to derive the CNLS equations that describe DNA dynamics by coupling the upper and lower cut-off modes.

2.2 The CNLS equations

We investigate the effects of nonlinearity and discreteness in DNA and we use the following asymptotic expansion

$$u_n = \epsilon u_{n,n}^{(1)} + \epsilon^2 u_{n,n}^{(2)} + \epsilon^3 u_{n,n}^{(3)} + \dots = \sum_{\nu=1}^{\infty} \epsilon^\nu u_{n,n}^{(\nu)}, \quad (9)$$

with $u_{n,n}^{(\nu)} = u_{n,n}^{(\nu)}(\xi_n, T, \theta_{0,n}(t), \theta_{max,n}(t))$, where ϵ is a small parameter denoting the amplitude of the excitation, $\xi_n = \epsilon(nl - \eta t)$ and $T = \epsilon^2 t$, which are the multiple scale variables. η is a small variable which will be determined by a solvability condition. The fast variables $\theta_{0,n}(t)$ and $\theta_{max,n}(t)$ represent the phases of two carrier waves. Considering the derivative expansion

$$\frac{d}{dt} = \frac{\partial}{\partial t} - \epsilon\eta \frac{\partial}{\partial \xi_n} + \epsilon^2 \frac{\partial}{\partial T}, \quad (10)$$

the problem of solving Eq.(7) reduces to the following equations

$$\left(\frac{\partial}{\partial t^2} + \omega_1^2\right) u_{n,n}^{(j)} - C \left(u_{n,n+1}^{(j)} + u_{n,n-1}^{(j)}\right) = M_{n,n}^{(j)}, \quad (11)$$

with

$$M_{n,n}^{(1)} = 0, \quad (12)$$

$$M_{n,n}^{(2)} = Cl \frac{\partial}{\partial \xi_n} (u_{n,n+1}^{(1)} + u_{n,n-1}^{(1)}) + 2\eta \frac{\partial}{\partial t} \left(\frac{\partial u_{n,n}^{(1)}}{\partial \xi_n} \right) - \alpha \omega_g^2 [u_{n,n}^{(1)}]^2, \quad (13)$$

$$M_{n,n}^{(3)} = \frac{Cl^2}{2} \frac{\partial}{\partial \xi_n^2} (u_{n,n+1}^{(1)} + u_{n,n-1}^{(1)}) + Cl \frac{\partial}{\partial \xi_n} (u_{n,n+1}^{(2)} + u_{n,n-1}^{(2)}) + 2\eta \frac{\partial}{\partial t} \left(\frac{\partial u_{n,n}^{(2)}}{\partial \xi_n} \right) - \eta^2 \frac{\partial u_{n,n}^{(1)}}{\partial \xi_n^2} - 2 \frac{\partial}{\partial t} \left(\frac{\partial u_{n,n}^{(1)}}{\partial T} \right) - 2\alpha \omega_g^2 u_{n,n}^{(1)} u_{n,n}^{(2)} - \alpha \omega_g^2 [u_{n,n}^{(1)}]^3 \quad (14)$$

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where $\omega_1^2 = \omega_g^2 + 2C$

Eq.(7) is solved step by step, where, for $j = 1$ we set

$$u_{n,n}^{(1)} = A_1(T, \xi_n) e^{i\theta_{0,n}(t)} + A_2(T, \xi_n) e^{i\theta_{max,n}(t)} + c.c., \quad (15)$$

where c.c. stands for complex conjugates. A_1 and A_2 are two undetermined envelope functions. For both cut-off modes, we have $\theta_{0,n}(t) = \omega(q=0)t = \omega_g t$ and $\theta_{max,n}(t) = \pi n - \omega(q = \frac{\pi}{l})t = \pi n - \omega_{max} t$, and $u_{n,n}^{(1)}$ becomes

$$u_{n,n}^{(1)} = A_1(T, \xi_n) e^{-i\omega_g t} + (-1)^n A_2(T, \xi_n) e^{-i\omega_{max} t} + c.c. \quad (16)$$

By letting $j = 2$, the solvability condition imposes $\eta = 0$ and $\xi_n = \epsilon n l$, and we have the second order approximation equation

$$\left(\frac{\partial}{\partial t^2} + \omega_1^2 \right) u_{n,n}^{(2)} - C (u_{n,n+1}^{(2)} + u_{n,n-1}^{(2)}) = -\alpha \omega_g^2 \times (A_1^2 e^{-2i\omega_g t} + A_2^2 e^{-2i\omega_{max} t} + 2|A_1|^2 + 2|A_2|^2), \quad (17)$$

Solving (17), we obtain

$$u_{n,n}^{(2)} = c_0 |A_1|^2 + c_1 |A_2|^2 + c_2 A_1^2 e^{-2i\omega_g t} + c_3 A_2^2 e^{-2i\omega_{max} t} + c.c., \quad (18)$$

with $c_0 = c_1 = -\frac{2\alpha\omega_g^2}{\omega_g^2 - 2C}$, $c_2 = \frac{\alpha}{3}$ and $c_3 = -\frac{\alpha\omega_g^2}{4\omega_{max}^2 - \omega_g^2}$.

When $j = 3$, we have, from the solvability conditions, the CNLS equations for A_1 and A_2

$$4i\omega_g \frac{\partial A_1}{\partial T} + Cl^2 \frac{\partial^2 A_1}{\partial \xi_n^2} - [2\alpha\omega_g^2(c_0 + c_1) + 3\beta\omega_g^2] |A_1|^2 A_1 - 2\alpha\omega_g^2 c_1 |A_2|^2 A_1 = 0, \quad (19)$$

$$4i\omega_{max} \frac{\partial A_2}{\partial T} - Cl^2 \frac{\partial^2 A_2}{\partial \xi_n^2} - [2\alpha\omega_g^2(c_1 + c_3) + 3\beta\omega_g^2] |A_2|^2 A_2 - 2\alpha\omega_g^2 c_0 |A_1|^2 A_2 = 0.$$

In comparison with the single mode [5], there exist in Eq.(19), cross-phase terms $|A_1|^2 A_2$ and $|A_2|^2 A_1$ that will have important consequences in the characteristics of the localized excitations. It is then possible to return to original variables by setting $(\psi_1, \psi_2) = \epsilon(A_1, A_2)$ and by considering the slow variables $T = \epsilon^2 t$ and $\xi_n = \epsilon n l$. We can rewrite the set of Eq.(19) as

$$i \frac{\partial \psi_1}{\partial t} + P_1 \frac{\partial^2 \psi_1}{\partial x^2} + [V_{11} |\psi_1|^2 + V_{12} |\psi_2|^2] \psi_1 = 0, \quad (20)$$

$$i \frac{\partial \psi_2}{\partial t} - P_2 \frac{\partial^2 \psi_2}{\partial x^2} + [V_{21} |\psi_1|^2 + V_{22} |\psi_2|^2] \psi_2 = 0,$$

with

$$\begin{aligned} P_1 &= \frac{Cl^2}{4\omega_g}, & P_2 &= \frac{Cl^2}{4\omega_{max}}, & V_{11} &= -\frac{2\alpha^2\omega_g(c_0 + c_1) + 3\beta\omega_g}{4}, \\ V_{12} &= -\frac{\alpha\omega_g c_1}{2}, & V_{21} &= -\frac{\alpha\omega_g^2 c_0}{2\omega_{max}}, & V_{22} &= -\frac{2\alpha^2\omega_g^2(c_1 + c_3) + 3\beta\omega_g^2}{4\omega_{max}}, \end{aligned} \quad (21)$$

being the coefficients of the CNLS equations and $x = nl$.

The study of physical and mathematical aspects of the CNLS equations and its different forms is of considerable current interest, as these equations arise in diverse areas of science. They are encountered in optical communications, in biophysics, in Bose-Einstein condensates and in plasma physics [17, 18, 19].

3 Nonlinear mode excitations in the PB model

3.1 The single mode excitation

In the single mode excitation, we decouple the two CNLS equations by setting one of the components to zero. Thus, the system is described by just one NLS equation.

Taking $\psi_2 = 0$ leads us to the following single NLS equation

$$i\frac{\partial\psi_1}{\partial t} + P_1\frac{\partial^2\psi_1}{\partial x^2} + V_{11}|\psi_1|^2\psi_1 = 0, \quad (22)$$

which admits the soliton solution [16]

$$\psi_1(x, t) = K\sqrt{\frac{2P_1}{V_{11}}}\operatorname{sech}(Kx + 2P_1K K_1 t)e^{i[K_1x - P_1(K_1^2 - K^2)t]}, \quad (23)$$

where K and K_1 are two free parameters.

The stretching of the base pairs is, therefore, given by

$$\begin{aligned} u_n(t) &= 2K\sqrt{\frac{2P_1}{V_{11}}}\operatorname{sech}(Knl + 2P_1K K_1 t) \\ &\quad \times \cos[K_1nl - (\omega_g + P_1(K_1^2 - K^2))t]. \end{aligned} \quad (24)$$

Next, by setting $\psi_1 = 0$, we obtain the NLS equation bounded to the upper cut-off frequency,

$$i\frac{\partial\psi_2}{\partial t} - P_2\frac{\partial^2\psi_2}{\partial x^2} + V_{22}|\psi_2|^2\psi_2 = 0. \quad (25)$$

According to the sign of its parameters, it admits the kink type solution [16]

$$\psi_2(x, t) = K\sqrt{-\frac{2P_2}{V_{22}}}\tanh(Kx - 2P_2K K_2 t)e^{i[K_2x - P_2(K_2^2 + 2K^2)t]}, \quad (26)$$

where K and K_2 are two free parameters.

The configuration of the molecule can be described by the solution

$$\begin{aligned} u_n(t) &= 2(-1)^n K\sqrt{-\frac{2P_2}{V_{22}}}\tanh(Knl - 2P_2K K_2 t) \\ &\quad \times \cos[K_2nl - (\omega_{max} + P_2(K_2^2 + 2K^2))t]. \end{aligned} \quad (27)$$

In order to carry out the behaviors of the system, taking solutions (24) and (27) as initial conditions, we have integrated Eq.(6), numerically, using the Runge-Kutta computational scheme, and we have considered absorbing boundary condition by assuming two imaginary base pairs at each end of the molecule. The time step has been taken equal to 5×10^{-3} , and the same values of the PB parameters have been used for the different cases.

In Fig. 1(a), we represent the time evolution of the single lower cut-off breather-like soliton [14, 20] and in Fig. 1(b), we represent the time evolution of the single upper cut-off kink-like soliton [14, 20]. In both cases the solutions are very stable. Breather solitons are known to play various roles in biomolecules and in DNA. They specifically describe the binding of specific enzymes to DNA and the thermal evolution of enzyme-created bubbles [21]; the displacement of the bubble from the promoter to the coding region [3]; the process of energy collection in the active regions under the enzyme action [22, 23, 24, 25]; the opening of bubbles in the start sites of transcription. They have also been found to be responsible for the so-called *breathing modes* in DNA. On the other hand, the effect of bending and twisting to modify the elasticity of DNA has been considered by Barkley and Zimm [26]. Salerno [27] studied the dynamical properties of a DNA promoter with particular interest in kink soliton. This can account for the resonant kink obtained in Fig. 1(b).

Beyond the above biological implications of the single excitation modes, there is a particular interest to study the coupled mode excitation.

3.2 The coupled mode excitations

The most interesting dynamics of our model could be described through the coupled mode, which is the main concern of this work. The coupled mode imposes $\psi_1 \neq 0$ and $\psi_2 \neq 0$. The CNLS equations then have exact solutions [28], depending on the sign of the coefficients

$$\frac{P_1 V_{22} + P_2 V_{12}}{V_{11} V_{22} - V_{12} V_{21}} \quad \text{and} \quad -\frac{P_2 V_{11} + P_1 V_{21}}{V_{11} V_{22} - V_{12} V_{21}} \quad (28)$$

The realistic parameters of DNA nonlinear dynamics allow us to get the following coupled kink and soliton solutions

$$\psi_1(x, t) = \psi_{01} \tanh(Kx + 2P_1 K K_1 t) e^{i(K_1 x - \Omega_1 t)}, \quad (29)$$

$$\psi_2(x, t) = \psi_{02} \operatorname{sech}(Kx + 2P_2 K K_2 t) e^{i(K_2 x - \Omega_2 t)}, \quad (30)$$

where

$$\begin{aligned} \psi_{01}^2 &= \frac{2K^2(P_2 V_{12} + P_1 V_{22})}{V_{11} V_{22} - V_{12} V_{21}} > 0, \\ \psi_{02}^2 &= \frac{2K^2(P_2 V_{11} + P_1 V_{21})}{V_{11} V_{22} - V_{12} V_{21}} > 0, \\ \Omega_1 &= -P_1(K^2 - K_1^2) - V_{12} \psi_{02}, \\ \Omega_2 &= -P_2(2K^2 + K_2^2) - V_{21} \psi_{01}, \quad K_2 = -\frac{P_1}{P_2} K_1. \end{aligned} \quad (31)$$

The stretching of the base pairs is fully described by

$$\begin{aligned}
u_n(t) = & 2\psi_{01} \tanh(Knl + 2P_1 K K_1 t) \cos[K_1 nl - (\omega_g + \Omega_1)t] \\
& + 2(-1)^n \psi_{02} \operatorname{sech}(Knl - 2P_2 K K_2 t) \cos[K_2 nl - (\omega_{max} + \Omega_2)t].
\end{aligned}
\tag{32}$$

As a first observation, the components of the above solution do not look like the solutions found in the single mode cases. The upper cut-off mode is a kink-like soliton and the lower cut-off mode is a breather-like soliton. Their features, through the DNA model, using realistic parameters, are studied in the rest of the paper.

In this frame, the time evolution of solution (32) is depicted in Fig. 1(c). As one can see, there is a coupling between the two modes, which leads to the opening of the base pairs. One of the modes (the lower cut-off soliton) can be seen as an energy carrier, while the other (the upper cut-off kink-type) describes the stretching of the base pairs in a given sequence. Furthermore, these nonlinearly coupled solutions are quite long lived, through the PB framework, and could be used in explaining more biological phenomena in DNA. Under such characteristics of the *kink-soliton* solution, one question arises: can this solution describe the open-state of the DNA double helix?

It has recently been shown that, by playing on the value of some parameters of the NLS equation [29, 30], it was possible to dissociate solutions related to the modulation and to the open-state of the molecule. In this frame, we carry out the impact of the inverse-width of the envelope K on the bubble configuration. This is depicted in Fig.2. Obviously, for small values of K , the solution is the kink-soliton solution [see Fig.2(a)]. Increasing progressively K reduces the modulation of the solution, leading, for $K = 1.5\text{\AA}^{-1}$, to the kink soliton [see Fig.2(d)]. Furthermore, the increase of K also induces the increase of the amplitude of the wave. Modulated waves have been shown recently to better contribute to information transfer in the DNA double helix. In the configuration shown in Fig.2(a), the oscillations of the strands enhance the fork of the kink which is usually observed in replication. On the other hand, the PB model does not consider all the factors involved in such a phenomenon and the action of the enzymes involved in replication and transcription can be modelled by the factor K . Then, increasing K can be seen as increasing the action of the messenger-RNA polymerase which breaks progressively the hydrogen bonds until the creation of the kink configuration observed in Fig.2(d). In the configuration that describes the total opening of the strands, there are no more oscillations and the messenger RNA can then be synthesized in order to copy the information stored in the genes.

4 Conclusion

Studying nonlinear excitations in biopolymers still attracts deep interests. It contributes to describe biomolecular processes, such as the vibrational energy transport in proteins on the basis of 1D nonlinear lattices, the energy localization and the transcription and replication phenomena

in DNA. Many models have been proposed to account for these nonlinear phenomena but the one used in this work is the PB model. It is shown in this work that, while using the asymptotic expansion, the system reduces, under some considerations, to a set of CNLS equations. In the framework of the PB model, with realistic parameter values, we have investigated, both theoretically and analytically, the formation of nonlinear excitations. Attention has been paid to the existence of those localized structures by considering the single-mode as well as by coupling the lower and the upper cut-off frequencies of the optical mode. The obtained breather-like, kink-like and coupled solitons are quite stable through the model and could be used in explaining more phenomena in DNA. That is why we have studied some characteristics of that solution, playing on the increase of the inverse-width which could be a consequence of the action of the various enzymes involved in transcription and replication. We have shown that, the enzymes induce strand oscillations and progressively unwind the double helix which finally takes the configuration of the kink soliton, widely known in the literature [3, 4, 12]. It would therefore be of interest to introduce the helicoidal coupling in order to study the impact of helicity in such a model with an accent on the resonant mode [29, 30].

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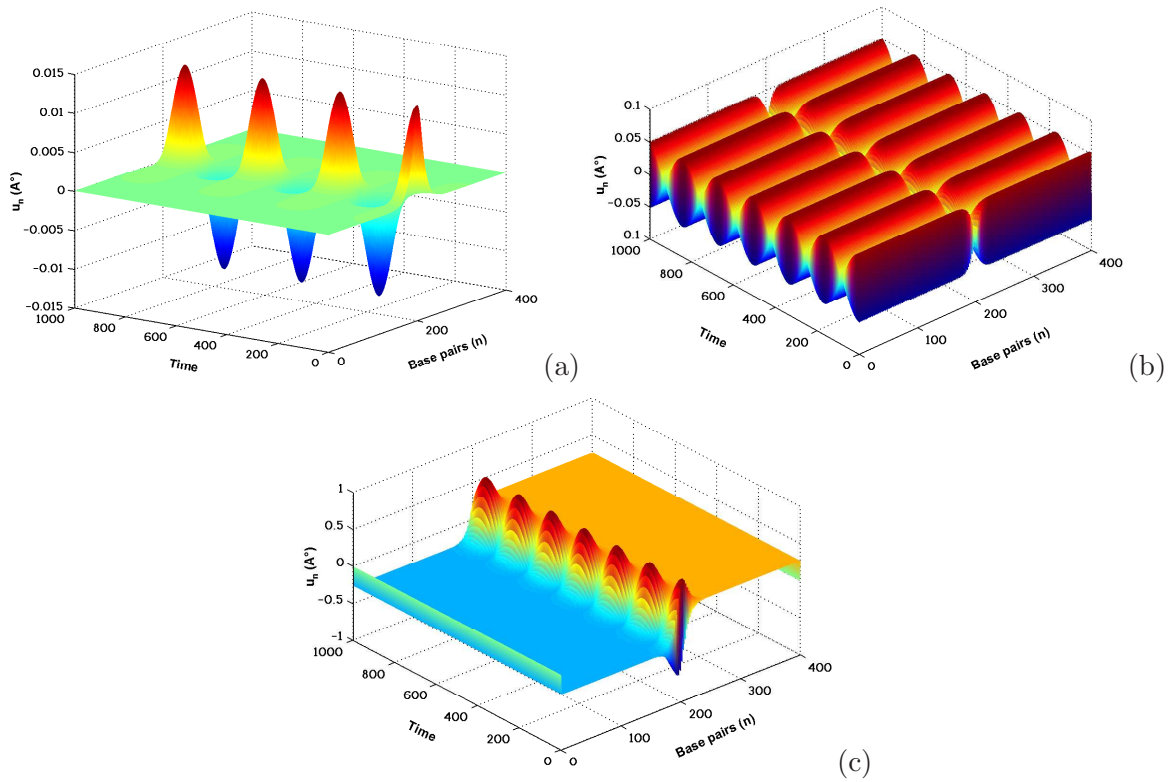


Figure 1: The panels show the space-time evolution of the single and coupled modes for $D = 0.35eV$, $a = 4.45\text{Å}^{-1}$, $m = 300$ a.m.u, $l = 3.4\text{Å}$, $c = 0.104eV/\text{Å}^2$, $K = 0.5\text{Å}^{-1}$, and $K_1 = K_2 = 0$.

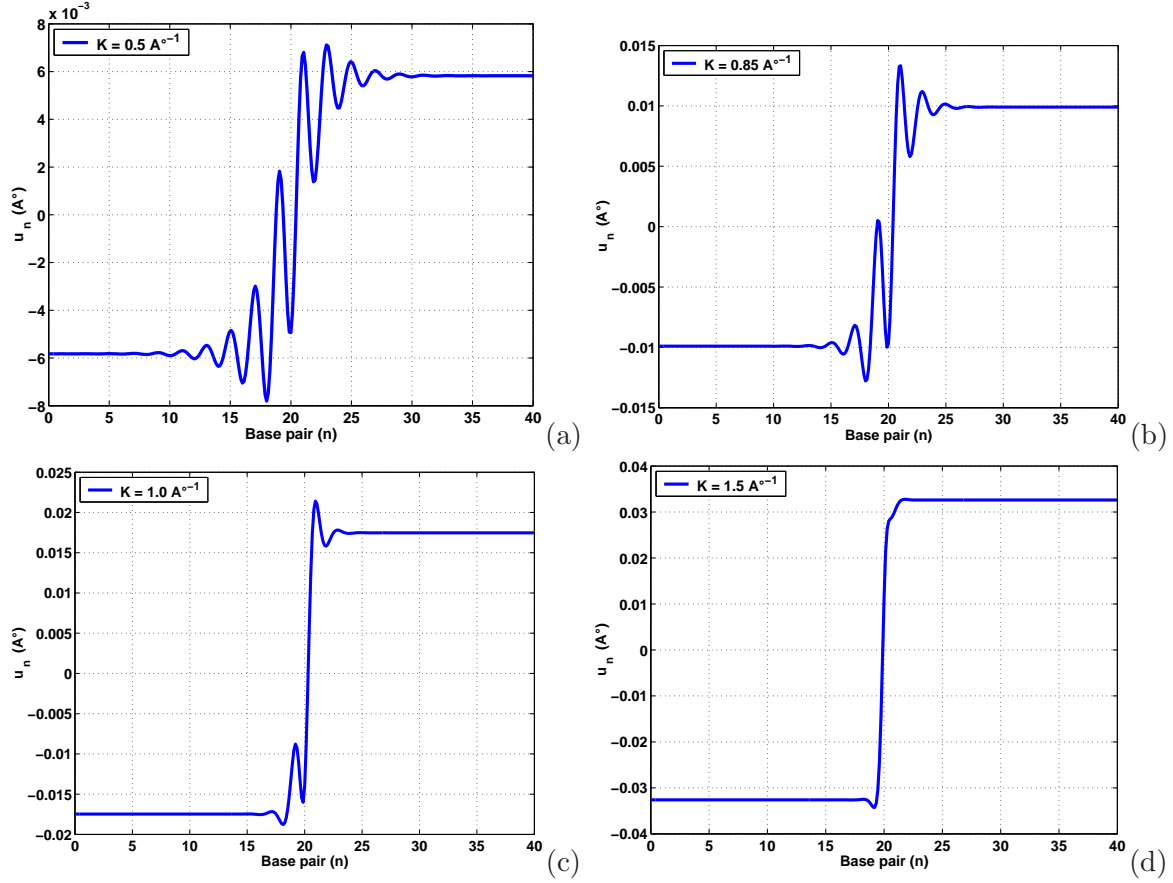


Figure 2: Elongation of the out-of-phase motion versus base pair number (n) for $D = 0.35eV$, $a = 4.45\text{\AA}^{-1}$, $m = 300$ a.m.u, $l = 3.4\text{\AA}$, $c = 0.104eV/\text{\AA}^2$, and (a) $K = 0.5\text{\AA}^{-1}$, (b) $K = 0.85\text{\AA}^{-1}$, (c) $K = 1.0\text{\AA}^{-1}$, and $K = 1.5\text{\AA}^{-1}$. Increasing K causes both the amplitude and the wave modulation to increase. The last panel materializes the effective opening of the strands as usually observed within replication and transcription.