

Bubble Formation in Helicoidal DNA Molecules

Conrad Bertrand Tabi^{1,2*}

¹Laboratory of Biophysics, Department of Physics, Faculty of Science, University of Yaoundé I, PO Box 812, Yaoundé, Cameroon

²Department of Physics and Astronomy, Botswana International University of Science and Technology, Private Mail Bag 16, Palapye, Botswana

Abstract

Wave interaction is addressed the framework of the helicoidal Peyrard-Bishop model of DNA. The model is first reduced to a set of coupled nonlinear Schrodinger equations via the multiple scale expansion. Modulational instability analysis shows that multi-breather trains exist in large regions of instability, while trains of one-humped breathers are observed for the single excitation mode. Analytical solutions are proposed, where single modes are proposed to described DNA respiration and coupled waves rather describe the bubbles observed in experiments. These bubbles are shown to be more effective under weak helicoidal coupling. The process of strand separation is also discussed. PACS number(s): 87.14.E-, 87.15.H-, 05.45.Yv, 05.45.-a

Keywords: DNA; Solitons; Transcription; Bubble formation; Base pairs

Introduction

The fundamental role and effects of enzymes in the key processes of DNA replication and transcription have been deeply addressed during the last ten years. In fact, it is well established nowadays that the initiation of DNA transcription is tributary to the synthesis of the polymerase-RNA which is known as the main factor contributing to break the strong hydrogen bonds linking bases in pairs, for the genetic code to be exposed out of the stack. Unlocking the complexity of such a phenomenon has then been shown to mainly depend on the DNA complex structure, as it requires, among the numerous involved degrees of freedom, the unwinding of the double helix. That complexity mainly comes from its structure which is primarily made of random distributions of four types of bases, adenine (A), thymine (T), cytosine (C) and Guanine (G). Besides, the pairing of the bases respects a universal complementarity where A can bind only to T and C to G. The bases are put together by hydrogen bonds, and the AT pair contains two H-bonds while the GC pair contains three of them. Among the models introduced to describe the dynamics of such a complex molecule, the Peyrard-Bishop (PB) model [1,2] has been extensively used in the last ten years because of its capability of predicting the occurrence of denaturation bubbles as widely observed in experiments where the so-called first-order phase transition emerges [2,3]. Furthermore, many studies have been carried out, showing that it support solitonic structures and is rather suitable to observe the localization of the energy which drives the key dynamical processes known as replication and transcription. Over the years, the PB model has been improved to take into account other features such the helicoidal structure of DNA [4,5], the cooperativity among adjacent base pairs [6,7] and the roto-torsional behaviours of the molecule [8-11]. For example, modifications brought to the PB model have shown new features in the way the base pairs oscillate and its modulational instability has been extensively studied as well [5]. Analytical solutions of the helicoidal PB model have been studied [12], but no relationship has been established, to our knowledge, between fluctuating bubbles and soliton emergence in DNA nonlinear models. The main objective of the present work is therefore to show that wave mixing can has some features of fluctuating bubbles and can be used to explain the opening of the DNA double helix. For this purpose, we use the so-called asymptotic expansion to derive the amplitude equations of the interacting waves. In fact, we assume that the RNA-polymerase which breaks H-bonds behaves as a wave which interacts with breathing modes so that the transcription

bubble emerges. The helicoidal PB model we consider in this work is described by the Hamiltonian [4,10].

$$H = \sum_{n=1}^N \left\{ \frac{m}{2} (\dot{u}_n^2 + \dot{v}_n^2) + \frac{s}{2} [(u_n - u_{n-1})^2 + (v_n - v_{n-1})^2] + \frac{s}{2} [(u_n - v_{n+h})^2 + (u_n - v_{n-h})^2] + V(u_n - v_n) \right\} \quad (1)$$

While the first term of Eq. (1) represents the kinetic energy, the second one stands for the nearest-neighbour stacking energy with coupling parameter s . In the helicoidal configuration of the DNA chain, nucleotides from different strands and close enough to interact via filaments of solvent. Otherwise, the nucleotide n of one strand interacts with the nucleotides $(n - h)$ and $(n + h)$ of the other strand. This is given by the third term in Hamiltonian (1). Also, the helicoidal pitch of DNA being 11 per turn, we consider $h=5$. S is the helicoidal coupling parameter and the on-site potential is the Morse potential $V(u_n - v_n) = D[e^{-\alpha(u_n - v_n)} - 1]^2$, where D is the dissociation energy and 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 u_n and v_n . Furthermore, by using the center-of-mass coordinates representing the in-phase and the out-of-phase transversal motions, i.e.,

$$X_n = (u_n + v_n)/\sqrt{2}, \quad Y_n = (u_n - v_n)/\sqrt{2} \quad (2)$$

it is possible to decouple the two variables u_n and v_n as follows

$$m\ddot{X}_n - s(X_{n+1} + X_{n-1} - 2X_n) - S(X_{n+h} + X_{n-h} - 2X_n) = 0 \quad (3a)$$

$$m\ddot{Y}_n - s(Y_{n+1} + Y_{n-1} - 2Y_n) - S(Y_{n+h} + Y_{n-h} - 2Y_n) - 2\sqrt{2}aDe^{-\alpha\sqrt{2}Y_n}(e^{-\alpha\sqrt{2}Y_n} - 1) = 0 \quad (3b)$$

The first equation admits plane wave solutions and does not really interests us as the second one which support localized structures.

***Corresponding author:** Conrad Bertrand Tabi, Laboratory of Biophysics, Department of Physics, Faculty of Science, University of Yaoundé I, PO Box 812, Yaoundé, Cameroon, Tel: +23778873550; E-mail: conrad@aims.ac.za (or) tabic@biust.ac.bw

Received October 17, 2016; **Accepted** October 26, 2016; **Published** November 06, 2016

Citation: Tabi CB (2016) Bubble Formation in Helicoidal DNA Molecules. J Phys Chem Biophys 6: 230. doi: 10.4172/2161-0398.1000230

Copyright: © 2016 Tabi CB. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

We will therefore work with Eq. (3b). The rest of the paper is then organized as follows. In section 2, we first use the multiple scaling expansion to show that interacting waves can be described via a set of coupled nonlinear Schrodinger (NLS) equations and we study their modulational instability (MI). We show that the coupling mode enlarges the instability domain and therefore brings about new features in the bearing of modulated trains of waves in the helicoidal PB model. In section 3, we derive solitonic solutions for both for the single and coupled modes and we show that the coupled mode gives rise to fluctuating bubbles at their interaction point. Concluding remarks end the paper.

Amplitude Equations and MI

Amplitude equations

In order to use the multiple-scaling method, we first expand the terms in exponential up to the third order, and reduce Eq. (3b) to

$$\ddot{Y}_n - k(Y_{n+1} + Y_{n-1} - 2Y_n) + K(Y_{n+h} + Y_{n-h} + 2Y_n) + \omega_g^2(Y_n + \alpha Y_n^2 + \beta Y_n^3) = 0 \quad (4)$$

$$k = \frac{s}{m}, K = \frac{S}{m}, \omega_g^2 = \frac{4a^2 D}{m}, \alpha = \frac{3a}{\sqrt{2}}, \beta = \frac{7a^2}{3}$$

Investigating the effects of nonlinearity and discreteness through the asymptotic expansion imposes us to assume the following quasi-discreteness approximation [13-15].

$$Y_n = \epsilon Y_{n,n}^{(1)} + \epsilon^2 Y_{n,n}^{(2)} + \epsilon^3 Y_{n,n}^{(3)} + \dots = \sum_{\nu=1}^{\infty} \epsilon^{\nu} Y_{n,n}^{(\nu)} \quad (5)$$

where ϵ is a small, but finite, parameter which stands for the relative amplitude of the excitations. In its general form, $Y_{n,n}^{(\nu)} = Y_{n,n}^{(\nu)}(\xi_n, \tau, \theta_n^+(t), \theta_n^-(t))$ where the first and second subscripts n represent the variables ξ_n and $\theta_n^{\pm}(t)$ respectively. Along the same line, the slow variables $\xi_n = \epsilon(nl - \mu t)$ and $\tau = \epsilon^2 t$ are also known as the multiple scale variables. μ is a small variable which will be determined by a solvability condition. The fast variables $\theta_n^+(t)$ and $\theta_n^-(t)$ represent the phases of two carrier, but counter-propagating, waves. Considering the derivative expansion

$$\frac{d}{dt} = \frac{\partial}{\partial t} - \epsilon \mu \frac{\partial}{\partial \xi_n} + \epsilon^2 \frac{\partial}{\partial \tau} \quad (6)$$

and taking into account all the above hypotheses, and using the Taylor's expansions

$$Y_{n\pm 1}(t) = \epsilon Y_{n,n\pm 1}^{(1)} + \epsilon^2 \left[Y_{n,n\pm 1}^{(2)} \pm l \frac{\partial Y_{n,n\pm 1}^{(1)}}{\partial \xi_n} \right] + \epsilon^3 \left[Y_{n,n\pm 1}^{(3)} \pm l \frac{\partial Y_{n,n\pm 1}^{(2)}}{\partial \xi_n} + l^2 \frac{\partial^2 Y_{n,n\pm 1}^{(1)}}{\partial \xi_n^2} \right] + \dots$$

$$Y_{n\pm h}(t) = \epsilon Y_{n,n\pm h}^{(1)} + \epsilon^2 \left[Y_{n,n\pm h}^{(2)} \pm lh \frac{\partial Y_{n,n\pm h}^{(1)}}{\partial \xi_n} \right] + \epsilon^3 \left[Y_{n,n\pm h}^{(3)} \pm lh \frac{\partial Y_{n,n\pm h}^{(2)}}{\partial \xi_n} + \frac{(lh)^2}{2} \frac{\partial^2 Y_{n,n\pm h}^{(1)}}{\partial \xi_n^2} \right] + \dots \quad (7)$$

the problem to solve reduces to the following set of equations

$$M_{n,n}^{(0)} = \left(\frac{\partial^2}{\partial \tau^2} + \omega_1^2 \right) Y_{n,n}^{(0)} - k \left(Y_{n,n+1}^{(0)} + Y_{n,n-1}^{(0)} \right) + K \left(Y_{n,n+h}^{(0)} + Y_{n,n-h}^{(0)} \right) \quad (8)$$

With

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

$$M_{n,n}^{(2)} = 2\mu \frac{\partial^2 Y_{n,n}^{(1)}}{\partial \tau \partial \xi_n} + kl \frac{\partial}{\partial \xi_n} \left(Y_{n,n+1}^{(1)} - Y_{n,n-1}^{(1)} \right) - Klh \frac{\partial}{\partial \xi_n} \left(Y_{n,n+h}^{(1)} - Y_{n,n-h}^{(1)} \right) - \alpha \omega_g^2 \left(Y_{n,n}^{(1)} \right)^2$$

$$M_{n,n}^{(3)} = 2\mu \frac{\partial^2 Y_{n,n}^{(2)}}{\partial \tau \partial \xi_n} - \mu^2 \frac{\partial^2 Y_{n,n}^{(1)}}{\partial \xi_n^2} - 2 \frac{\partial^2 Y_{n,n}^{(1)}}{\partial \tau \partial \tau} + \frac{1}{2} kl^2 \frac{\partial^2}{\partial \xi_n^2} \left(Y_{n,n+1}^{(1)} + Y_{n,n-1}^{(1)} \right) + kl \frac{\partial}{\partial \xi_n} \left(Y_{n,n+1}^{(2)} - Y_{n,n-1}^{(2)} \right)$$

$$- \frac{1}{2} kl^2 h^2 \frac{\partial^2}{\partial \xi_n^2} \left(Y_{n,n+h}^{(1)} + Y_{n,n-h}^{(1)} \right) - Klh \frac{\partial}{\partial \xi_n} \left(Y_{n,n+h}^{(2)} - Y_{n,n-h}^{(2)} \right) - \omega_g^2 \beta \left(Y_{n,n}^{(1)} \right)^3 - 2\alpha \omega_g^2 Y_{n,n}^{(1)} Y_{n,n}^{(2)} \quad (9)$$

Where $\omega_1^2 = 2k + 2K + \omega_g^2$ Solving the above system (8) will be performed step by step. For $j=1$,

one can easily get the solution

$$Y_{n,n}^{(1)} = A(\xi_n, \tau) e^{i\theta_n^+(t)} + B(\xi_n, \tau) e^{i\theta_n^-(t)} + c.c., \quad (10)$$

Where $A(\xi_n, \tau)$ and $B(\xi_n, \tau)$ are envelope functions to be determined later, with $\theta_n^+ = qnl - \omega t$ and $\theta_n^- = -qnl - \omega t$, with ω being the carrier wave frequency, related to the carrier wavenumber q via

the dispersion relation

$$\omega^2 = \omega_g^2 + 4k \sin^2 \left(\frac{ql}{2} \right) + 4K \cos^2 \left(\frac{qlh}{2} \right) \quad (11)$$

For $j=2$, the solvability condition

$$\mu = v_g = \frac{\partial \omega}{\partial q} = \frac{kl \sin(ql) - Klh \sin(qlh)}{\omega} \quad (12)$$

is found and the terms in $Y_{n,n}^{(2)}$ is given by

$$Y_{n,n}^{(2)} = f_0 |A|^2 + f_1 A^2 e^{2i\theta_n^+} + f_3 |B|^2 + f_4 B^2 e^{2i\theta_n^-} + c.c., \quad (13)$$

Where

$$f_4 = f_1 = \frac{-\alpha \omega_g^2}{-4\omega^2 + \omega_1^2 - 2k \cos(2ql) + 2K \cos(2qlh)}, f_3 = f_0 = \frac{-2\alpha \omega_g^2}{\omega_1^2 - 2k + 2K}$$

For $j=3$, the solvability condition leads us to the set of coupled equations for the amplitudes A and B as follows

$$i \frac{\partial A}{\partial \tau} + P_1 \frac{\partial^2 A}{\partial \xi_n^2} + \left(\eta_{11} |A|^2 + \eta_{12} |B|^2 \right) A = 0 \quad (14a)$$

$$i \frac{\partial B}{\partial \tau} + P_2 \frac{\partial^2 B}{\partial \xi_n^2} + \left(\eta_{21} |A|^2 + \eta_{22} |B|^2 \right) B = 0, \quad (14b)$$

Coming back to original variables, $\tau = \epsilon^2 t$ and $\xi_n = \epsilon(nl - \mu t) = \epsilon x$, imposes us to set $(\psi_1, \psi_2) = \epsilon(A, B)$, and the set of equations (14) becomes

$$i \frac{\partial \psi_1}{\partial \tau} + P_1 \frac{\partial^2 \psi_1}{\partial x^2} + \left(\eta_{11} |\psi_1|^2 + \eta_{12} |\psi_2|^2 \right) \psi_1 = 0 \quad (15a)$$

$$i \frac{\partial \psi_2}{\partial \tau} + P_2 \frac{\partial^2 \psi_2}{\partial x^2} + \left(\eta_{21} |\psi_1|^2 + \eta_{22} |\psi_2|^2 \right) \psi_2 = 0, \quad (15b)$$

Where

$$P_1 = P_2 = \frac{1}{2\omega} \left[-\mu^2 + kl^2 \cos(ql) - Kl^2 h^2 \cos(qlh) \right]$$

$$\eta_{11} = \eta_{22} = -\frac{\omega_g^2}{\omega} (2\alpha(f_0 + f_1) + 3\beta), \eta_{12} = \eta_{21} = -\frac{\alpha \omega_g^2}{\omega} \quad (16)$$

The set of equation (15) describes the possibility of wave mixing in the helicoidal model of DNA. We should however stress that it is nowadays well introduced in the DNA dynamics as clearly discussed by Tabi et al. [15,16]. Besides, it also appears in a broad range of physical settings such electrical lattices [17], Bose-Einstein condensates [18], plasma physics [19], just to cite a few. In electrical transmission lines, for example, it has been shown to bring about modulated turbulent patterns [20]. In the case of the Peyrard-Bishop model, coupled NLS equations have been shown to bring about kink-breather solitonic structures with interesting biological implications for the processes of DNA breathing [15]. In the meantime, the process of wave mixing has not yet been addressed in DNA and could give rise to new features in the process of bubble emergence

Modulational instability

The most direct way solitonic structures emerge in nonlinear systems is through MI. In order to investigate the possibility of wave mixing in the set of Eq. (15), we assume that it admits the plane waves

$\psi = \psi_{j0} e^{i\omega_j t}$ as solutions, where the real constants $\omega_j (j=1,2)$, and the complex amplitudes ψ_{j0} are related by the equations.

$$\omega_j = \eta_{jj} |\varphi_{j0}|^2 + \eta_{jk} |\varphi_{k0}|^2, \quad j, k = 1, 2, \text{ with } k \neq j. \quad (17)$$

In order to investigate the stability of the plane wave solutions, we perturb slightly their amplitude as $\psi_j = (\psi_{j0} + \epsilon \psi_j) e^{i\omega_j t}$, where $\psi_j = u_j + i v_j$ and $\psi_{j0} = a_j + i b_j (j=1,2)$. After linearizing around the unperturbed waves and separating the real from the imaginary, from the previous assumption, we assume $u_j = u_{j0} e^{i(\lambda x - \Omega t)} + \text{c.c.}$ and $v_j = v_{j0} e^{i(\lambda x - \Omega t)} + \text{c.c.}$, where λ and Ω are the perturbation wave number and perturbation, respectively. We therefore obtain an homogeneous system for u_{j0} and v_{j0} as follows

$$\begin{bmatrix} -i\Omega + m_{11} & m_{12} & m_{13} & m_{14} \\ m_{21} & i\Omega + m_{11} & m_{23} & m_{24} \\ m_{31} & m_{32} & -i\Omega + m_{33} & m_{34} \\ m_{41} & m_{42} & m_{43} & i\Omega + m_{33} \end{bmatrix} \begin{bmatrix} u_{10} \\ v_{10} \\ u_{20} \\ v_{20} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad (18)$$

Where

$$\begin{aligned} m_{11} &= 2\eta_{11} a_1 a_2, & m_{12} &= -P_1 \lambda^2 + 2\eta_{11} a_2^2, & m_{13} &= 2\eta_{11} a_2 b_1 \\ m_{14} &= 2\eta_{12} a_2 b_2, & m_{21} &= -P_1 \lambda^2 + 2\eta_{11} a_1^2, & m_{23} &= 2\eta_{12} a_1 b_1 \\ m_{24} &= 2\eta_{12} a_1 b_2, & m_{31} &= 2\eta_{21} a_1 b_2, & m_{32} &= 2\eta_{21} a_2 b_2, & m_{33} &= 2\eta_{22} b_1 b_2, \\ m_{34} &= -P_2 \lambda^2 + 2\eta_{22} b_2^2, & m_{41} &= 2\eta_{21} a_1 b_1, & m_{42} &= 2\eta_{21} a_2 b_1, \\ m_{43} &= -P_2 \lambda^2 + 2\eta_{22} b_1^2 \end{aligned} \quad (19)$$

The condition for the above system to have nontrivial solutions is obtained by setting its determinant to zero, which leads us to the following nonlinear dispersion relation:

$$\Omega^4 - P \Omega^2 + Q = 0, \quad (20)$$

Where

$$\begin{aligned} P &= (P_1^2 + P_2^2) \lambda^4 - 2(P_1 \eta_{11} |\varphi_{10}|^2 + P_2 \eta_{22} |\varphi_{20}|^2) \lambda^2 \\ Q &= P_1^2 P_2^2 \lambda^8 - 2P_1 P_2 (P_2 \eta_{11} |\varphi_{10}|^2 + P_1 \eta_{22} |\varphi_{20}|^2) \lambda^6 + 4P_1 P_2 |\varphi_{10}|^2 |\varphi_{20}|^2 (\eta_{11} \eta_{22} - \eta_{12} \eta_{21}). \end{aligned} \quad (21)$$

Solutions for Eq. (20) can easily be found as

$$\Omega_{\pm}^2 = \frac{1}{2} \left[P + \sqrt{P^2 - 4Q} \right], \quad \Omega_{\pm}^2 = \frac{1}{2} \left[P - \sqrt{P^2 - 4Q} \right], \quad (22)$$

therefore, for the plane wave solutions to be stable under modulation, the conditions $P > 0$, $Q > 0$ and $\Delta = P^2 - 4Q > 0$ should be simultaneously fulfilled. In other words, when this is effective, the plane waves will be expected to spread in the molecule without any change. On the other hand, solutions (22) could also be complex and this may deeply depend on the sign of the discriminant Δ . On this background, the instability is a purely growing mode for $\Delta > 0$ and the growth rate of instability Δ can be obtained as $\sqrt{-\Omega^2}$. This growth rate will then be positive if $P < 0$, i.e., $(P_1^2 + P_2^2) \lambda^4 - 2(P_1 \eta_{11} |\varphi_{10}|^2 + P_2 \eta_{22} |\varphi_{20}|^2) \lambda^2 < 0$ leading to the condition $P_1 \eta_{11} + P_2 \eta_{22} > 0$ for σ to remain positive, with $|\varphi_{10}| = |\varphi_{20}|$. Accordingly, the condition $\Delta > 0$ implies $Q > 0$, i.e.,

$$P_1^2 P_2^2 \lambda^8 - 2P_1 P_2 (P_2 \eta_{11} |\varphi_{10}|^2 + P_1 \eta_{22} |\varphi_{20}|^2) \lambda^6 + 4P_1 P_2 |\varphi_{10}|^2 |\varphi_{20}|^2 (\eta_{11} \eta_{22} - \eta_{12} \eta_{21}) > 0$$

Since $P_1 = P_2$, the plane wave solutions will be stable if $\eta_{11} \eta_{22} - \eta_{12} \eta_{21} > 0$ and unstable if the later is not satisfied. Otherwise, for $\Delta < 0$, the growth rate of instability is given by $\sigma = \pm \sqrt{|\Delta|} / 2$. σ is represented in Figure 1, both for the single and coupled modes, versus the perturbation wavenumber λ . For the single mode, the region of instability is situated in the interval $0 < \lambda < 0.35\pi$, while for the coupled mode, unstable wave patterns are expected to take place in the region $0 < \lambda < 0.65\pi$. To remind, the single

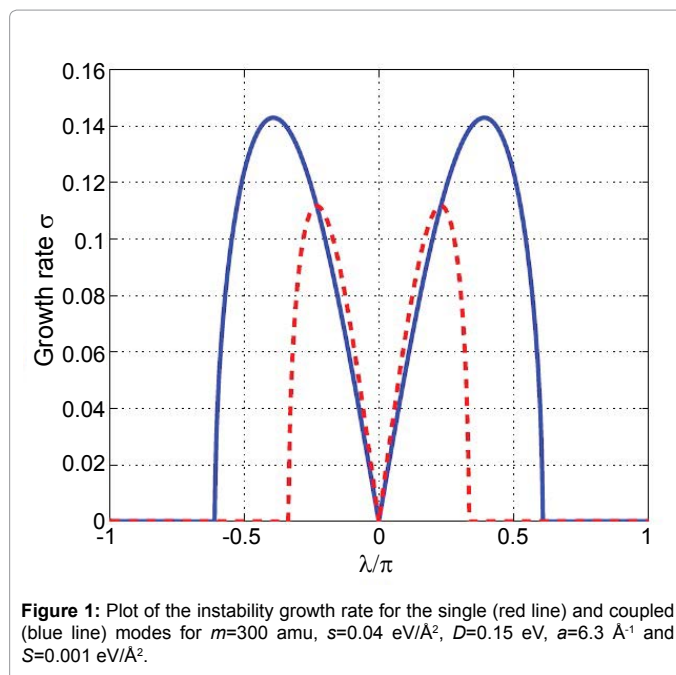


Figure 1: Plot of the instability growth rate for the single (red line) and coupled (blue line) modes for $m=300$ amu, $s=0.04$ eV/Å², $D=0.15$ eV, $a=6.3$ Å⁻¹ and $S=0.001$ eV/Å².

mode is obtained for $\eta_{12} = \eta_{21} = 0$. Uncoupled identical NLS equations are then obtained, with the same stability/instability features. On the other hand, the coupled mode implies $\eta_{12} \neq 0$ and $\eta_{21} \neq 0$, and takes account of the nonlinear coupling between the two NLS equations. Comparing qualitatively these two cases, one sees that coupled modes expand the regions of instability and even cover the unstable region for the single mode. Also, the growth rate of instability is high for the coupled modes. On this basis, we also suspect the unstable modes from these two cases to be different. However, this can be verified through direct numerical simulations on the generic equation (3b). This has been done using the fourth-order Runge-Kutta computation scheme on a chain of 350 base pairs with periodic boundary conditions and time-step $\Delta t = 10^{-3}$ tu. The wavenumber have been fixed as $q l = 0.28 \pi$ and $\lambda = 0.15 \pi$, values which fall well inside the instability regions of the two modes. The corresponding results are given in Figure 2, where panel (a) shows the MI features of the single mode and panel (b) displays nonlinear oscillations of the coupled mode. In both cases, trains of soliton-like structures, with breaching features, are observed. Their importance in collecting the energy necessary for the initiation of the key precesses of replication and transcription has been discussed in many DNA nonlinear models, with suitable biological implications [7,10,12]. Indeed, the breaking of the hydrogen bonds starts with slight oscillations of the bases and then grow progressively in amplitude under the action of RNA-polymerase till the breaking of the hydrogen bond, condition for the genetic information to be collected by the messenger-RNA. This suggest the presence of many modes that contribute to collect such an energy, leading to some modification of the way DNA strands breathe [21-23]. For example, the single mode here displays one-humped oscillatory structures (Figure 2a), while trains of multi-breather elements correspond to the coupled mode (Figure 2b). Also, one can notice that the structures that emerge in the second case are highly localized in comparison to the single mode. It is the clear that coupled modes could bring about new features in the way hydrogen bonds oscillate and therefore need to be regarded in the cases of highly localized structures and bubbles.

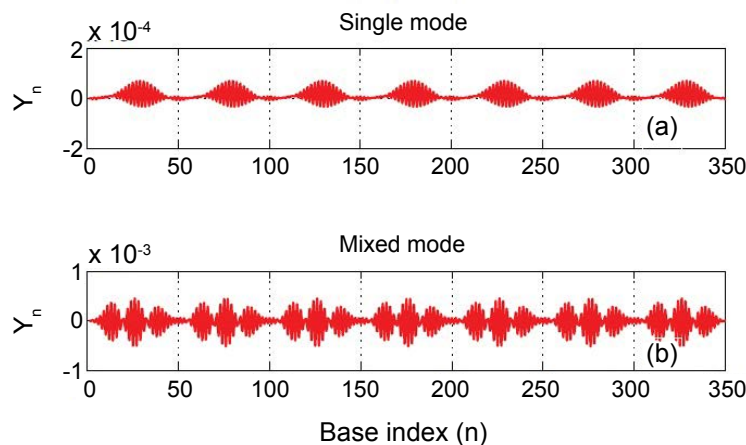


Figure 2: The panels show development of MI in the (a) single (b) coupled modes. The parameters are $m=300$ amu, $s=0.04$ eV/Å², $D=0.15$ eV, $a=6.3$ Å⁻¹ and $S=0.006$ eV/Å².

Wave Mixing and Bubbles in DNA

The single mode

For the single mode, we assume $\eta_{12}=\eta_{21}=0$ and the system reduces to two identical and uncoupled NLS equations. The equation for ψ_1 is for example given by

$$i \frac{\partial \psi_1}{\partial \tau} + P_1 \frac{\partial^2 \psi_1}{\partial x^2} + \eta_{11} |\psi_1|^2 \psi_1 = 0 \tag{23}$$

and admits the solution [15,24]

$$\psi_1(x, t) = b \sqrt{\frac{2P_1}{\eta_{11}}} \operatorname{sech} [b(x - u_e t)] e^{i(L_1 x - \Omega_1 t)} + c.c., \tag{24}$$

which is the same for the NLS equation in ψ_2 . The general solution for DNA dynamics is then written as

$$Y_n(t) = 2A_1 [\cos(L_1 n l - (\Omega_1 + L_1 v_g) t + \theta_1^*)] \operatorname{sech} [b(nl - (u_e + v_g) t)] + [f_0 A_1^2 + 2f_1 A_1^2 \cos(2L_1 n l - 2(\Omega_1 + L_1 v_g) t + 2\theta_1^*)] \operatorname{sech}^2 [b(nl - (u_e + v_g) t)], \tag{25}$$

where u_e stands for the velocity of the envelope. The corresponding solution is represented in Figure 3a, and clearly displays a breather solution. The same class of solution has already been obtained numerically in the previous section, and are found to be robust in DNA nonlinear models. Two classes of such waves have been discussed already, the ones describing the so-called DNA respiration and those related to the eye-like configuration usually observed in thermal denaturation experiments [12,25].

The mixed solutions

Solving the set of equations (15) depends on the sign of the coefficients [15,26,27]

$$\Delta_1 = \frac{P_1 \eta_{22} - P_2 \eta_{12}}{\eta_{11} \eta_{22} - \eta_{21} \eta_{12}}, \text{ and } \Delta_2 = \frac{P_2 \eta_{11} - P_1 \eta_{21}}{\eta_{11} \eta_{22} - \eta_{21} \eta_{12}}. \tag{26}$$

In relation (26), one can notice the presence of the term $\eta_{11} \eta_{22} - \eta_{21} \eta_{12} > 0$, which bring together the coupled solution and the MI analysis performed in the previous section. Breathing solutions for this model are found for $\Delta_1 > 0$ and $\Delta_2 > 0$, and is explicitly given by

$$Y_n(t) = 2A_1 [\cos(L_1 n l - (\Omega_1 + L_1 v_g) t + \theta_1^*)] + A_2 [\cos(L_2 n l - (\Omega_2 + L_2 v_g) t + \theta_2^*)] \operatorname{sech} [b(nl - (u_e + v_g) t)] + [f_0 (A_1^2 + A_2^2) + 2f_1 A_1^2 \cos(2L_1 n l - 2(\Omega_1 + L_1 v_g) t + 2\theta_1^*) + 2f_2 A_2^2 \cos(2L_2 n l - 2(\Omega_2 + L_2 v_g) t + 2\theta_2^*)] \operatorname{sech}^2 [b(nl - (u_e + v_g) t)], \tag{27}$$

where

$$A_1^2 = \frac{2b^2 (P_1 \eta_{22} - P_2 \eta_{12})}{\eta_{11} \eta_{22} - \eta_{21} \eta_{12}}, L_1 = \frac{u_e}{2P_1}, \Omega_1 = \frac{u_e^2}{4P_1} - P_1 b^2 \tag{28}$$

$$A_2^2 = \frac{2b^2 (P_2 \eta_{11} - P_1 \eta_{21})}{\eta_{11} \eta_{22} - \eta_{21} \eta_{12}}, L_2 = \frac{u_e}{2P_2}, \Omega_2 = \frac{u_e^2}{4P_2} - P_2 b^2$$

The corresponding solution is plotted in Figure 3b. In comparison to the single mode case, the mixing of the counter propagating waves rather gives rise to a perturbed breather-like solution which seems to be more localized with noisy-like envelope. Of course, the reader should notice that from the beginning we did not include any noise to the model, rather these fluctuations in the breather solution are due to wave collision, i.e., at the point where the two counter-propagating waves mix. However, the features of that solution are expected to change for different values of the helicoidal coupling parameters S . This may be evident as the unwinding of the double helix implies a decrease of S . It was in fact shown that the resonant mode, the one supporting highly localized bubbles, is possible only when the helicoidal effects are weak [12,25]. Therefore, in the rest of the present work, the effect of small helicoidal coupling on the mixed solution is discussed. For $S=0.002$ eV/Å², we have the solution of Figure 4a and for $S=0.001$ eV/Å², the patterns of Figure 4b are obtained. When the value of S decreases, the compression of the hydrogen bonds reduces while the oscillations tend to become positive as shown in Figure 4b. We therefore have in mind to describe the fluctuating opening of the DNA double helix using the found mixed solution whose the features are described above. Under the action of RNA-polymerase, the hydrogen bonds linking bases in pairs are broken progressively to make the codon readable. The hydrolysis of ATP brings about energy that enhances the action of RNA-polymerase and therefore contribute to separate the two strands of DNA. In so doing, the effect of temperature is no more to be ignored through the action of ATP. We have simulated the opening of the molecule using solution (27), mainly at the point where the two counter-propagating waves collide, in order to picture the way environmental factors enhance DNA breathing. One of the waves describes the breathing of the double-stranded molecule, while the other stands for the biological factors that create and enhance bubbles in DNA. The subsequent bubbles are not different from those observed through DNA melting experiments. This shows and reinforces the fact that different waves are present in the process of DNA dynamics, and some are brought by the presence of enzymes around the coding sequences of DNA [28]. We

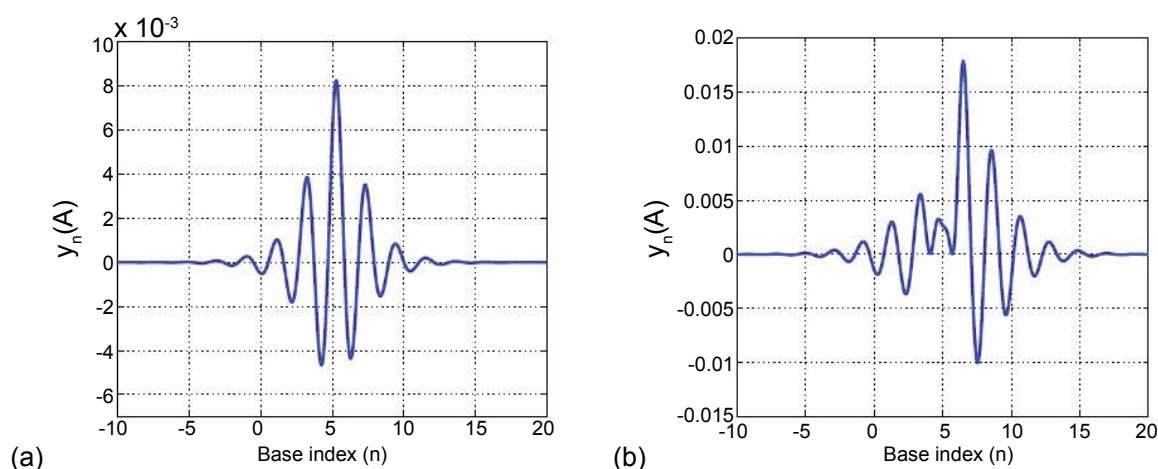


Figure 3: The panels show breather-like solitons in DNA for both the single (a), and mixed modes (b). The values of parameters are $m=300$ amu, $s=0.04$ eV/Å², $D=0.15$ eV, $a=6.3$ Å⁻¹ and $S=0.006$ eV/Å².

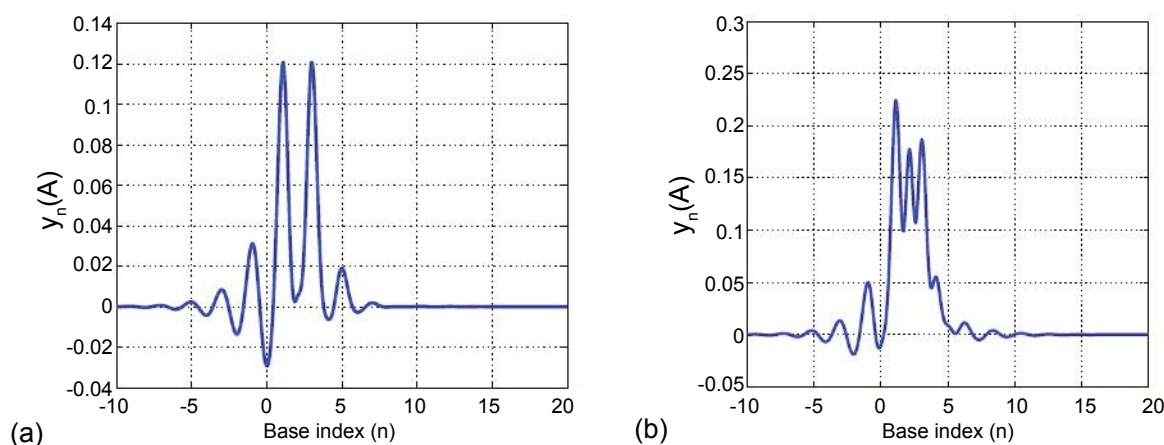


Figure 4: The panels show plots of DNA strands oscillations under weak helicoidal coupling for (a) $S=0.002$ eV/Å² and (b) $S=0.001$ eV/Å². Values of parameters are $m=300$ amu, $s=0.04$ eV/Å², $D=0.05$ eV and $a=6.3$ Å⁻¹.

therefore see how the bubble grows with decreasing S , in a fluctuating way, while hydrogen bonds are broken progressively as depicted in Figure 5. In Figure 5a, bubbles are created through wave mixing for $S=0.002$ eV/Å². Progressively, as transcription factors modify the value of ξ the hydrogen bonds are broken and finally lead to the fluctuating transcription eyelike structure observed in Figure 5b for $S=0.001$ eV/Å². The action of RNA-polymerase through this work can therefore be seen as a wave that surfs the DNA helix and mixes with DNA breathing waves, a collision which yields fluctuating breather-like structures for the genetic code to be read.

Conclusion

Wave interaction in the helicoidal PB model has been addressed in this work. Using the multiple scaling expansion, we have shown that the dynamics of counter-propagating waves can fully be described via a set of coupled NLS equations. MI has been studied with emphasis on the features of single and mixed modes. In that context, the coupled

mode has been found to expand the instability region, and numerical simulations have displayed trains of one-humped breathers for the single mode, and multi-breather trains for the coupled mode. Exact solutions have also been investigated for the two cases. Breather-like solutions have been found for the single mode, while highly localized fluctuating breather solutions have been derived for the mixed mode. We have further argued that the release of energy by ATP and the effect of RNA-polymerase could be assimilated to waves that collide with the weak DNA breathing in order for the molecule to be opened. However, recent developments have shown that when the hydrogen bond stretching is effective, the solvent molecules present in the DNA environment stabilize the molecule in the opened configuration [21,29,30] in order to prevent the molecule from re-closing. We should therefore modify the present model by taking accounts of these effects which could enrich our investigations on the most realistic profile of transcription and replication eye-like structures. In the meantime, the present work brings about the possible importance of multi-wave flowing in DNA double helix.

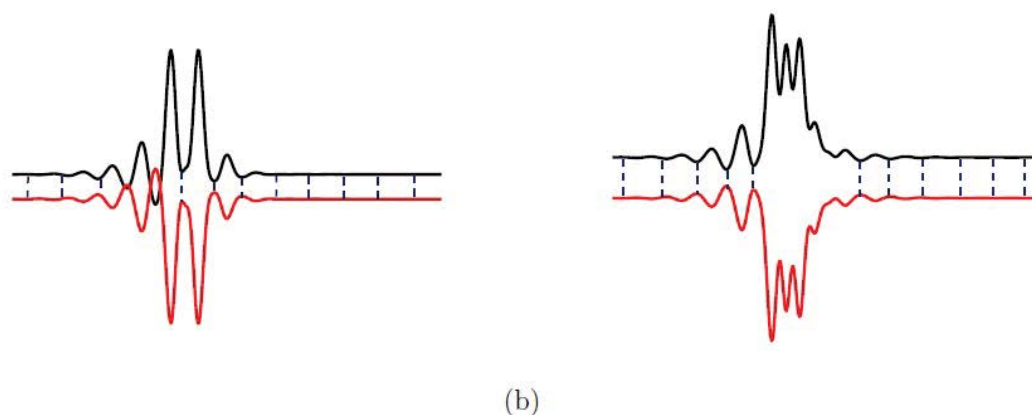


Figure 5: The panels display bubbles formation in DNA due to wave mixing (a) $S=0.002 \text{ eV/\AA}^2$ and (b) $S=0.001 \text{ eV/\AA}^2$. Values of parameters are $m=300 \text{ amu}$, $s=0.04 \text{ eV/\AA}^2$, $D=0.05 \text{ eV}$ and $a=6.3 \text{ \AA}^{-1}$.

References

- Reiss C (1994) Nonlinear Excitations in Biomolecules. Peyrard M (ed.). Les Houches School, Springer.
- Peyrard M, Bishop AR (1989) Statistical mechanics of a nonlinear model for DNA denaturation. Phys Rev Lett 62: 2755.
- Dauxois T, Peyrard M (1993) Energy localization in nonlinear lattices. Phys Rev E 70: 3935.
- Dauxois T (1991) Dynamics of breather modes in a nonlinear "helicoidal" model of DNA. Phys Lett A 159: 390-395.
- Tabi CB, Mohamadou A, Kofane TC (2008) Formation of localized structures in the Peyrard-Bishop-Dauxois model. J Phys Cond Matter 20: 415104.
- Dauxois T, Peyrard M, Bishop AR (1993) Phys Rev E 47: R44.15.
- Tabi CB, Mohamadou A, Kofane TC (2010) Modulational instability in the anharmonic Peyrard-Bishop model of DNA. Eur Phys J B 74: 151-158.
- Barbi M, Cocco S, Peyrard M (1999) Helicoidal model for DNA opening. Phys Lett A 253: 358-369.
- Barbi M, Cocco S, Peyrard M, Theodorakopoulos N (2003) Thermal denaturation of a helicoidal DNA model. Phys Rev E 68: 061909.
- Tabi CB, Mohamadou A, Kofane TC (2009) Modulational instability and exact soliton solutions for a twist-opening model of DNA dynamics. Phys Lett A 373: 2476-2483.
- Tabi CB (2010) Energy localization in an anharmonic twist-opening model of DNA dynamics. J Phys Condens Matter 22: 414107.
- Tabi CB, Mohamadou A, Kofane TC (2008) Wave propagation of nonlinear modes and formation of bubble in a two-component helicoidal lattice. Eur Phys J D 50: 307-316.
- Huang G (1995) Soliton excitations in one-dimensional diatomic lattices. Phys Rev B 51: 12347.
- Huang G, Hu B (1998) Asymmetric gap soliton modes in diatomic lattices with cubic and quartic nonlinearity. Phys Rev B 57: 5746.
- Tabi CB, Ekobena HPF, Mohamadou A, Kofane TC (2011) Wave propagation of coupled modes in the DNA double helix. Phys Scr 83: 035802.
- Ekobena HPF, Tabi CB, Zdravkovic S, Kofane TC (2012) Helicity and Wave Switching in a Nonlinear Model of DNA Dynamics. J Phys Chem Biophys S4: 001.
- Yemélé D, Kofané TC (2006) Suppression of the fast and slow modulated waves mixing in the coupled nonlinear discrete LC transmission lines. J Phys D Appl Phys 39: 4504.
- Li L, Malomed BA, Mihalache D, Liu WM (2006) Phys Rev E Scr 73: 066610.
- Kourakis I, Shoukla PK (2004) Nonlinear theory of solitary waves associated with longitudinal particle motion in lattices. Eur Phys J D 29: 247-263.
- Tan B, Liu S (1995) Collision interactions of solitons in a baroclinic atmosphere. J Atmos Sci 52: 1501-1512.
- Tabi CB, Bineli G, Mohamadou A (2015) Energy patterns in twist-opening models of DNA with solvent interactions. J Biol Phys 41: 391-408.
- Toko D, Tabi CB, Mohamadou A, Kofane TC (2011) Coherent Modes and Parameter Selection in DNA Models with Finite Stacking Enthalpy. J Comput Theor Nanosci 9: 97-101.
- Mohamadou A, Toko D, Alim D, Tabi CB, Kofane TC (2015) Modulational instability and energy localization of twisted DNA with solvent interaction. Int J Mod Phys B 29: 1550049.
- Remoissenet M (1999) Waves Called Solitons - Concepts and Experiments. Springer-Verlag, Berlin.
- Zdravkovic S, Sataric MV (2007) High amplitude mode and DNA opening. Europhys Lett 78: 38004.
- Bhakta JC (1987) A pair of coupled equations for high frequency Langmuir and dispersive ion-acoustic waves with collisional damping. Plasma Phys Control Fusion 29: 245.
- Kofane TC, Zebaze M, Zibi AA (1991) J Phys D Appl Phys 23: 764.
- Tabi CB (2014) J Phys Chem Biophys 4: 161.
- Weber G (2006) Sharp DNA denaturation due to solvent interaction. Europhys Lett 73: 806.
- Tabi CB, Mohamadou A, Kofane TC (2009) Modulated Waves in the DNA Double Helix with Finite Stacking Enthalpy Interaction. J Bionanosci 3: 110-117.