Formation of Wave Packets in the Peyrard-Bishop Model with Solvent Interaction

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Abstract

Within the framework of the Peyrard-Bishop model for DNA, we show that the phenomenon of modulational instability in the DNA with solvent interaction gives rise to coherent spatial structures of localized excitations as well as energy localization. Theoretical studies, based on the multiple scale analysis for boundary value problems, leads to a general physical model with application to DNA dynamics. Numerical simulations show the validity of the analytical approach with the generation of wave packets provided that the wave numbers fall in the instability domain. We show the effect of the solvent interaction on the dynamics of the system. Energy localization via MI is studied.


1 Introduction

DNA (Deoxyribonucleic acid) is the fundamental information storage medium which contains the genetic information of most organisms. As a replicating information unit, DNA has fascinated not just biologists, but also physicists, biophysicists and chemists. The basic structure of DNA is fairly well understood since the discovery of Crick and Watson [1], where the molecule were presented as a static structure, but it is becoming increasingly apparent that structure alone does not explain its complex functionality sufficiently [2].

One of the earliest research works on the nonlinear physics of DNA was done by Englander et al. [3], who introduced the nonlinear conformational excitations. Assuming a mobile open unit diffusing along the double helix, Englander et al. [3] concluded from the data of kinetic and thermodynamic experiments that these open configurations can consist of mobile segments on the order of 10 base pairs in length. As a model for open configuration of the double-helical polynucleotide chains, they proposed two parallel rods on which pendula are attached and suggested that the open state is consistently described as a solitary excitation. Thereafter, many approaches have been followed to probe the existence of nonlinear localized excitations in DNA. Among them one can name, the one proposed by Yakushevich [4] and improved by Gaeta [5], and the second proposed by Peyrard and Bishop (PB) [6], which concentrates on transversal openings of base pairs. In fact, the PB model is one of the simplest models that investigates DNA at the scale of a base pair [6, 7]. The complex double-stranded molecule is described by postulating some simple effective interaction among bases within a pair and along strands.

The PB model has been successfully applied to a variety of situations, such as DNA transcription initiation [8] and denaturation of hairpins [9]. Recently, this model has been applied to study sharp transition for DNA melting [10] as well as for evaluating the thermal equivalence of short DNA probes [11]. Furthermore, the PB model allows to easily include the effect of heterogeneities [12] yielding a sharp staircase structure of the melting curve (number of open base pairs as a function of the temperature T) [13]. 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 [14, 15].

In what follows, we will focus on studying the creation process of soliton-like structures and energy localization induced by MI by adding a solvent interaction term to the harmonic PB Hamiltonian [6]. Particular attention will be paid on the impact of the solvent interaction term in the process of energy localization. The paper is organized as follows. In section 2, we give a brief review of the PB-like DNA model. In section 3, the discrete multiple-scale analysis is briefly presented and allows us to obtain the equation that governs the amplitude of waves in the form of the discrete nonlinear Schrödinger. In section 4, we derive the MI condition. We study the dynamics of the nonsoliton initial amplitude in the PB model by numerical simulations. We show the creation and evolution of solitary waves which are found to be in excellent agreement
with analytical predictions. Finally, this paper is summarized and concluding remarks are made in section 5.

2 Model and mathematical background

According to the PB model [6], DNA is made of two strands, \(S_1\) and \(S_2\), linked by nearest-neighbor harmonic interaction along the chain. Only the transversal displacements of 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 nucleotides in a strand, and the same coupling constant \(k\) along each strand is assumed. The Hamiltonian of the discrete system is then written as follows [6, 16]:

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

The intrapair potential is given by

\[
V(y_n - z_n) = D \left( e^{-a(y_n - z_n)} - 1 \right)^2 - f_s D \left( \tanh \left( \frac{y_n - z_n}{\lambda_s} \right) - 1 \right). \tag{2}
\]

The first term is the Morse potential which describes interactions between hydrogen bonds within the bases. The second term stands for the solvent interaction potential [10, 17], which mimics the formation of hydrogen bonds between the base pairs and the solvent molecules once the interbase hydrogen bonds are stretched by more than a value \(\lambda_s\) from their equilibrium values. In fact, the base pairs are pulled away from each other for \(y_n - z_n < \lambda_s\) until the hydrogen bonds with the solvent are established. The bases are then linked to freely moving solvent molecules, through hydrogen bond, and are no more allowed to move in any particular direction as soon as \(y_n - z_n > \lambda_s\). The solvent potential and the Morse potential form a single barrier of height and width of the orders of \(f_s D\) and \(\lambda_s\), respectively. This potential is presented in Fig. 1. The solid line refers to the unmodified Morse potential, while the dotted-dashed line takes into account the combination of Morse and solvent potentials.

To analyze the motion of the two strands, it is convenient to introduce the following dependent variables,

\[
r_n = (y_n + z_n)/\sqrt{2}, \quad u_n = (y_n - z_n)/\sqrt{2}. \tag{3}
\]

We then have, with the above consideration, from (1), equations in \(r_n\) and \(u_n\)

\[
M \ddot{r}_n = k(r_{n+1} + r_{n-1} - 2r_n), \tag{4a}
\]

\[
M \ddot{u}_n = k(u_{n+1} + u_{n-1} - 2u_n) + 2\sqrt{2}aDe^{-a\sqrt{2}u_n} \left( e^{-a\sqrt{2}u_n} - 1 \right) - f_s D \frac{\sqrt{2}}{\lambda_s} \text{sech}^2 \left( \frac{u_n \sqrt{2}}{\lambda_s} \right). \tag{4b}
\]
The variables $r_n$ and $u_n$ represent the in-phase and out-of-phase motion, respectively. Equation (4a) is a linear differential-difference equation with the usual plane wave solutions. On the other hand, Eq. (4b) contains nonlinear terms. It will be interesting to relate our model to nonlinear excitation. Furthermore, we use the parameter values $D = 0.04 \text{eV}$, $a = 4.45 \text{Å}^{-1}$, $M = 300 \text{a.m.u}$, $d = 3.4 \text{Å}$, the distance between adjacent base pairs at equilibrium, and the coupling parameter $k = 0.04 \text{eV/Å}^2$, which are known in DNA-like model [18] and $f_s = 0.1$ [10]. The system of units (a.m.u, Å, eV) defines a time unit (t.u.) equal to $1.021 \times 10^{-14} \text{s}$ [15].

3 The multiple scales analysis

3.1 Discrete multiple scaling

Equation (4b) forms a system of nonlinear ODEs which cannot be solved exactly. Thus, there exist several techniques to convert it into more integrable systems [19, 20, 21, 22]. In this frame, we apply the method developed by Leon and Manna [21] known as the multiple scale analysis. The reductive perturbation method (or multiple scales analysis) allows the deduction of simplified equation from a basic model without losing its characteristic features. The method consists essentially in an asymptotic analysis of a perturbation series, based on the existence of different scales. More specially, the method generates a hierarchy of (small) scales for the space and time variations of the envelopes of a fundamental (linear) plane wave and all the overtones. Moreover, the scale is directly related to the small amplitude of the wave itself. The scaling of variables is performed via a Taylor expansion of the frequency $\omega(q_0)$ in powers of a small deviation of the wave number $q_0$. This deviation from the linear dispersion relation is, of course, generated by the nonlinearity. There are actually three different approaches to multiple scales analysis for a discrete evolution. The first is obviously to go to the continuous limit right in the starting system, for which discreteness effects are wiped out. The second is the semi-discrete approach which consists in having a discrete carrier wave modulated by a continuous envelope. In the latter case, some discreteness aspects are preserved, in particular, the resulting MI may depend on the carrier frequency. The third stems from the adiabatic approximation, but the approach requires one to use the rotating wave approximation to artificially eliminate the overtones. The price to pay is that the predictions, for example the MI, are not trustworthy for large time [22].

In order to study MI on the PB-solvent system, we perform multiple scale analysis of the discrete evolution equation (4b). The physical problem we are concerned with is the following: the first particle of the chain (say $n = 0$) is given oscillation (or submitted to an external force) at frequency $\Omega$. In a linear chain, this oscillation would propagate without distortion as the plane wave $\exp[i(\Omega t + qnd)]$, where $d$ is the lattice spacing. However, the nonlinearity induces some deviations from the value $\Omega$, namely, the wave propagates with actual frequency $\omega$ and wave number $q_0$ that defined as [21]
\[ \omega = \Omega + \epsilon \lambda, \quad q_0 = q + \epsilon \frac{\lambda}{v_g} + \epsilon^2 c_g \lambda^2 + \ldots \]  \hspace{1cm} (5) 

where \( \frac{1}{v_g} = \frac{\partial \Omega}{\partial q} \) is the group velocity and \( 2c_g = \frac{\partial^2 q}{\partial \Omega^2} \) is the group velocity dispersion.

For notation simplicity, we shall assume here that \( c_g = 1 \), which does not reduce the generality of our task. Let us consider the wave packet given by the Fourier transform

\[ u_n(t) = \int d\omega \hat{u}(\omega)e^{i(\omega t + q_0 dn)} \]  \hspace{1cm} (6) 

With the use of Eqs.(16), Eq.(17) can be expanded as

\[ u_n(t) = e^{i(\Omega t + q_0 d)} \left( \epsilon \int d\lambda \hat{u}(\lambda)e^{i\lambda(\epsilon t + \frac{\epsilon}{v_g} n \epsilon^2)}e^{i\lambda^2dn} \right) \]  \hspace{1cm} (7) 

By means of the following change of independent variables

\[ \tau_n = \epsilon(t + nd/v_g), \quad \xi_n = \epsilon^2 n \]  \hspace{1cm} (8) 

we obtain the following expression for the wave packet:

\[ u_n(t) = A(n, t)\psi(\xi_n, \tau_n) \]  \hspace{1cm} (9) 

where

\[ A(n, t) = e^{i(q_0 d + \Omega t)}, \quad \psi(\xi_n, \tau_n) = \epsilon \int d\lambda \hat{u}(\lambda)e^{i(\lambda\tau_n + \lambda^2d\xi_n)} \]  \hspace{1cm} (10) 

Eq.(10) has a clear physical meaning: one considers long distance (\( \epsilon^{-2} \)) effects in the retarded time to give the input disturbance enough time to reach the observed lattice point. In such a situation, the lattice is excited at one end. This corresponds, in other words, to a boundary value problem. The quantity \( \psi(\xi_n, \tau_n) \) defines the slow modulation.

In order to keep discreteness in space variable for the envelope \( \psi(\xi_n, \tau_n) \), one fixes the small parameters as

\[ \epsilon^2 = 1/N \]  \hspace{1cm} (11) 

and, for any given \( n \), we shall consider only the set of points \( ..., n - N, n, n + N, ... \) of a large grid indexed by the slow variable \( m \), that is,

\[ ... (n - N) \to (m - 1), n \to m, (n + N) \to (m + 1) ... \]  \hspace{1cm} (12) 

As a consequence, we can index the variable \( \xi_n \) by \( m \) in the new grid; we can call \( m \) a given point \( n \) and \( m + j \) the points \( n + jN \) for all \( j \). To simplify the notation, we shall be using everywhere

\[ \psi(\xi_j, \tau_j) = \tilde{\psi}_j, \quad \psi(\xi_j, \tau_n) = \psi_j \]  \hspace{1cm} (13) 

for a given \( n \) and all \( j \) (note that \( \tilde{\psi}_n = \psi_n \)). Hence, we are interested in expressing everything in terms of \( \psi_n(\psi(m, \tau) \) defined as
\[ \psi_{n-N} = \psi_{m-1}, \quad \psi_n = \psi_m, \quad \psi_{n+N} = \psi_{m+1}. \]  

(14)

The problem is now to express the various different operators occurring in nonlinear evolutions for the product \( A(n,t)\psi_m \) in terms of different operators for \( \psi_m \). The traditional approach to multiple scaling for continuous media originates from water waves theory for which the physical problem is usually that of the evolution of an initial disturbance (e.g. of the surface). In this case, the observer has to follow the deformation at the (linear) group velocity. This operation corresponds to making, in the general Fourier transform solution, the expansion of \( \omega(q_0) \) around small deviations of \( q_0 \) from the linear dispersion law.

We now have to obtain the analogous relations for the product \( u_n(t) = A(n,t)\psi(\xi_n,\tau_n) = A_n\psi_n \), appearing in definition (8). The quantity \( u_{n+1} + u_{n-1} - 2u_n \) is factorized as follows [21]

\[ u_{n+1} + u_{n-1} - 2u_n = [A_{n+1} - 2A_n + A_{n-1}]\psi_m + \epsilon[A_{n+1} - A_{n-1}]{\left( \frac{d}{v_g} \right)}\frac{\partial\psi_m}{\partial\tau} + \epsilon^2\left[ A_{n+1} + 2[A_{n+1} - A_{n-1}]\left[ \psi_{m+1} - \psi_{m-1} \right] + \theta(\epsilon^3) \right] \]

(15)

The formula (15) constitutes our basic tool for deriving reduced models in the following.

3.2 Evolution of the envelope

As we have defined above, we seek a solution of Eq.(4b) in the form of a Fourier expansion in harmonics of the fundamental \( A(n,t) = \exp[i(\Omega t + qnd)] \), where the Fourier components are developed in a Taylor series in powers of the small parameters \( \epsilon \) measuring the amplitude of the initial wave

\[ u_n(t) = \sum_{p=1}^{\infty} \epsilon^p \sum_{l=-p}^{p} A^{(l)}(n,t)\psi_p^{(l)}(m,\tau), \quad \text{with} \quad A^{(l)}(n,t) = \exp(i\epsilon(l\Omega t + qnd)) \quad \text{and} \quad \psi_p^{(-l)} = \left( \psi_p^{(l)} \right)^* \]

(16)

the asterisk denoting complex conjugation.

By substituting Eq.(16) into Eq.(4b), we obtain the following equation describing the evolution
of the envelope:

\[
\sum_{p=1}^{\infty} \epsilon^p \sum_{l=-p}^{p} \left[ e^{2\partial_{\tau} \psi_p^{(l)}(m, \tau)} + 2i\epsilon l \omega \partial_{\tau} \psi_p^{(l)}(m, \tau) - (\epsilon \omega)^2 \psi_p^{(l)}(m, \tau) \right] A^{(l)}(n, t) - K \sum_{p=1}^{\infty} \epsilon^p \sum_{l=-p}^{p} \left[ (e^{ilqd} + e^{-ilqd} - 2) \psi_p^{(l)}(m, \tau) + \epsilon \left( \frac{d}{\nu_g} \right) (e^{ilqd} - e^{-ilqd}) \partial_{\tau} \psi_p^{(l)}(m, \tau) \right] + \frac{\epsilon^2}{2} \left( e^{ilqd} + e^{-ilqd} \right) \left( \frac{d}{\nu_g} \right)^2 \partial_{\tau} \psi_p^{(l)}(m, \tau) + \frac{\epsilon^2}{2} (e^{ilqd} - e^{-ilqd}) \left( \psi_p^{(l)}(m + 1, \tau) - \psi_p^{(l)}(m - 1, \tau) \right) \right] A^{(l)}(n, t) - \frac{2\sqrt{2}aD}{M} \exp[-a\sqrt{2} \sum_{p=1}^{\infty} \epsilon^p \sum_{l=-p}^{p} A^{(l)}(n, t) \psi_p^{(l)}(m, \tau)] \exp[-a\sqrt{2} \sum_{p=1}^{\infty} \epsilon^p \sum_{l=-p}^{p} A^{(l)}(n, t) \psi_p^{(l)}(m, \tau)] - 1\]

\[
+ \frac{f_s \sqrt{2}}{M \lambda_s \text{sech}^2} \sum_{p=1}^{\infty} \epsilon^p \sum_{l=-p}^{p} \sqrt{2} \frac{\lambda_s}{\lambda_s} A^{(l)}(n, t) \psi_p^{(l)}(m, \tau) = 0.
\]

Equation (17) can be rewritten as

\[
\epsilon : \psi_1^{(0)} = 0;
\]

\[
\epsilon^2 : \psi_2^{(0)} = 2 \left( \frac{3a}{\sqrt{2}} + \frac{f_s \sqrt{2}}{2a^2 \lambda^2} \right) |\psi_1^{(1)}|^2 = -2a |\psi_1^{(1)}|^2
\]

\[
\epsilon^3 : \psi_3^{(0)} = 0.
\]

The coefficients of \( A^{(1)} \), at different order of \( \epsilon \), give:

\[
\epsilon : \Omega^2 = \omega_g^2 + 4K \sin^2 \left( \frac{qd}{2} \right)
\]

\[
\epsilon^2 : \nu_g = \frac{dK \sin(qd)}{\Omega};
\]

\[
\epsilon^3 : \left( 1 - K \left( \frac{d}{\nu_g} \right)^2 \cos(qd) \right) \frac{\partial^2 \psi_1^{(1)}}{\partial \tau^2} - iK \sin(qd) \left( \psi_1^{(1)}(m + 1) - \psi_1^{(1)}(m - 1) \right) + \omega_g^2 \left( 2a \left( \psi_2^{(1)} \psi_1^{(1)} - \psi_2^{(0)} \psi_1^{(1)} \right) \right) - \left( \Omega^2 - \omega_g^2 - 4K \sin^2 \left( \frac{qd}{2} \right) \right) \psi_3^{(1)} = 0.
\]

Equation (19) can be rewritten as

\[
\left( 1 - K \left( \frac{d}{\nu_g} \right)^2 \cos(qd) \right) \frac{\partial^2 \psi_1^{(1)}}{\partial \tau^2} - iK \sin(qd) \left( \psi_1^{(1)}(m + 1) - \psi_1^{(1)}(m - 1) \right) + \omega_g^2 \left( 2a \left( \psi_2^{(1)} \psi_1^{(1)} - \psi_2^{(0)} \psi_1^{(1)} \right) \right) = 0,
\]

where \( \omega_g^2 = \frac{4a^2 D}{M} \), \( \alpha = - \left( \frac{3a}{\sqrt{2}} + \frac{f_s \sqrt{2}}{2a^2 \lambda^2} \right) \) and \( \beta = \frac{7a^2}{3} \).

The coefficients of \( A^{(2)} \), at order \( \epsilon^2 \), give:

\[
\psi_2^{(2)} = \frac{\alpha \omega_g^2}{4 \Omega^2 - \omega_g^2 - 4K \sin^2(qd)} \left( \psi_1^{(1)} \right)^2 = \mu \left( \psi_1^{(1)} \right)^2.
\]
With the expression of $\psi^{(0)}$ and $\psi^{(2)}_2$, Eq. (20) becomes

$$P\frac{\partial^2 \eta_m}{\partial \tau^2} + i(\eta_{m+1} - \eta_{m-1}) - Q|\eta_m|^2 \eta_m = 0,$$

(22)

with

$$P = \frac{K}{\sin(qd)} \left( \frac{d^2}{v_g^2} \right) \cos(qd) - 1, \quad Q = \frac{\omega_g^2[2\alpha(\mu - 2\alpha) + 3\beta]}{K\sin(qd)}, \quad \text{and} \quad \eta_m(\tau) = \psi^{(1)}_1(m, \tau).$$

(23)

From (16) and expressions of $\psi^{(l)}_p(m, \tau)$, we have

$$u_n(t) = \epsilon \eta_m e^{i(qnd - \Omega t)} + O(\epsilon^2)$$

(24)

It should mainly be pointed out that, the higher order corrections to $u_n(t)$ are either explicitly expressed in terms of $\eta$ through expressions $\psi^{(l)}_p(m, \tau)$ or by linear inhomogeneous differential equations. This means that, the theory is self-consistent and, in particular, that the overtones are by no means neglected.

4 Modulational instability

Equation (22) has been recovered in the limit of large detuning and the high-frequency limit waves in the special cases of microscopic model [23]. Its continuous version has also been studied in boundary value problems in optical fibers [24] and in the case of initial value problems in unstable media to describe, for instance, Rayleigh-Taylor instability. It, thus, has stationary solutions in the form

$$\eta_m = B e^{i(\lambda m - \nu \tau)},$$

(25)

and obeys the dispersion relation

$$\nu^2 = -\frac{2}{P} \left( \sin(\lambda) + \frac{Q}{2} |B|^2 \right).$$

(26)

Here, $\nu$ and $B$ are the frequency and the amplitude of the modulation, respectively. The sign of the constant $Q$ determines properties of instability. According to Eq. (23), $Q$ vanishes at $q = q_{cr}$.

Then, as $\sin(\lambda)$ is bounded, there is no real solution of Eq.(26) if

$$Q > 0, \quad |B|^2 > B_{cr}^2.$$  

(27)

That is possible only if $q > q_{cr}$. For $q < q_{cr}$, there is no real solution $\lambda$ if

$$Q < 0, \quad |B|^2 > |B_{cr}|^2,$$

(28)

where

$$B_{cr} = \sqrt{-\frac{\sin(qd)}{2a^2D} \left( 7a^2 - \left( \frac{6a^3\lambda_3^3 + 2f_s}{a^2\lambda_3^3\sqrt{2}} \right)^2 \frac{5a^2D}{2a^2D + 4k \sin^2 \left( \frac{qd}{2} \right) - k \sin^2(qd)} \right)^{-1}}$$

(29)
In summary, the waves are unstable for $q \in ]q_{cr}, \pi/d]$ and stable for $q \in ]0, q_{cr}]$ as shown in Fig. 2.

In order to check the validity of our analytical approach and to determine the evolution of the system beyond the instability point, we have performed numerical simulations of the equation of motion (4b) with a given initial condition. The system has been integrated using a fourth-order Runge-Kutta scheme with a time step $\Delta t = 5.5 \times 10^{-3}$ chosen to conserve the energy to an accuracy better than $10^{-6}$. The number of base pairs has been chosen equal to 600. The initial condition, in accordance with Eq. (24) is a modulated plane wave.

We study the impact of the solvent interaction factor $\lambda_s$ on the dynamics of the system. The parameters values $qd = 0.56\pi$, $\lambda = 0.99\pi$, and $f_s = 0.1$ have been chosen. With these values of parameters, one clearly observes, from Fig. 3 that the initial plane wave breaks into trains of breather-like excitations [see Fig. 3(a) and Fig. 3(b)]. In Fig. 3(a), oscillations of strands are shown for $\lambda_s = 1$Å and in Fig. 3(b), they are displayed for $\lambda_s = 3$Å. From these figures, increasing $\lambda_s$ leads to the gradual increase of the amplitude of the wave trains. For example, these oscillations become highly localized for $\lambda_s = 3$Å. MI is known to share the same parameter regions with solitons occurrence and has also been shown, by Daumont and co-workers [25] (look also at ref. [26] and references therein), to be responsible for energy localization in continuum and discrete media. In the present case, the density of energy is written as

$$E_n = \frac{1}{2} M \dot{u}_n^2 + \frac{1}{2} k (u_n - u_{n-1})^2 + \frac{1}{2} k (u_{n+1} - u_n)^2 + D \left( e^{-a\sqrt{2}u_n} - 1 \right) - f_s D \left( \tanh \left( \frac{u_n \sqrt{2}}{\lambda_s} \right) - 1 \right).$$

Thermal fluctuations which exist in the molecule due to the physiological temperature have been shown to be a pathway to energy localization and formation of localized structures. Furthermore, as shown in Figs. 4(a) and (b), such localized structures can emerge in our DNA model because of the robustness of energy localization in the PB and the Peyrard-Bishop-Dauxois (PBD) models [22]. Coming back to the spectrum of behaviors displayed by Figs. 4(a) and (b), one can easily see that, for $\lambda_s = 1$Å, yellow regions correspond to $E_n = 4.4 \times 10^{-6}$ eV (and black regions correspond to $E_n = 0$), while for $\lambda_s = 3$Å, yellow regions correspond to $E_n = 2.8 \times 10^{-4}$ eV. Therefore, increasing $\lambda_s$ makes possible a strong localization of energy in the Morse-solvent lattice. In consequence, the features displayed by Figs. 3 and 4 imply that the solvent interaction factor can be used as a theoretical tool to control the density of energy and the amplitude of oscillations of the hydrogen bonds. These oscillations have been shown to be a better way to transport information and charge in the double helical structure [22]. So, increasing $\lambda_s$ enhances their amplitude and information are better transmitted within the molecule. For the bases to oscillate, the strength of the hydrogen bonds linking them should be reduced and this is the importance of finding mechanisms that could lead to strongly localized patterns of energy. It is therefore obvious that the parameter $\lambda_s$ contributes to reduce the force between hydrogen bonds.
in order for the strands to undergo large oscillations and, hence, better transmission of localized structures which suggests that, the m-RNA polymerase plays a catalytic role resembling an enzyme. Its presence around DNA sequence seems to highly enhance the efficiency of oscillations of respective nucleotide pairs and could, if the energy involved is sufficient, cause the complete breaking of the hydrogen bonds linking the bases in pairs.

5 Conclusion

To summarize, the discrete multiscale analysis for boundary value problems has been applied to the PB model with solvent interactions. As a result a discrete nonlinear Schrödinger equation (with reversed spacetime) has been derived. We have studied MI as well as energy localization in the PB model with solvent interactions. The MI criterion has been presented. In order to complete and verify our analytical predictions, MI has been investigated numerically and, interesting phenomena have been found. As a result, the propagation of pulses train which have the shape of soliton-like structure has been shown. Breather solitons are known to play various roles in biomolecules and in DNA. They specifically described the binding of specific enzymes to DNA and the thermal evolution of enzyme-created bubbles [27]; the displacement of the bubble from the promoter to the coding region [26]; the process of energy collection in the active regions under the enzyme action [28]. With respect to the last point, the phenomenon of energy localization has been investigated. Solitary waves have been proposed as a possible precursor of the transcription process by the means of trapping this breather in extended regions of DNA where the coupling constant is weaker [29].

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Figure 1: Representation of the Morse-solvent potential. The solid line shows the evolution of the potential when solvent interactions are not taken into consideration while the dotted-dashed line correspond to the case where there are solvent interactions (we have chosen $\lambda_s = 10 \text{ Å}$).

Figure 2: The panel shows the threshold amplitude $B_{cr}$ versus the wave number $qd$. $M = 300$ amu, $\alpha = 4.45 \text{ Å}^{-1}$, $D = 0.04$ eV, $d = 3.4 \text{Å}$, $f_s = 0.1$, $k = 0.04 \text{ eV.Å}^{-2}$, and $\lambda_s = 10 \text{ Å}$. The waves are unstable for $q \in [q_{cr}, \pi/d]$ and stable for $q \in [0, q_{cr}]$. 
Figure 3: The panels illustrate the features of MI in the PB model for two values of the solvent interaction parameter $\lambda_s$ and for $M = 300$ amu, $a = 4.45$ Å$^{-1}$, $D = 0.04$ eV, $d = 3.4$ Å, $f_s = 0.1$, $k = 0.04$ eV.Å$^{-2}$, $qd = 0.56\pi$, $\lambda = 0.99\pi$, $B_{cr} = 0.14$ Å, and $\epsilon = \sqrt{1/N} \approx 0.04$. In panels (a) and (b), the oscillations of the base pairs are shown for $\lambda_s = 1$ Å and $\lambda_s = 3$ Å, respectively. It is obvious that, increasing $\lambda_s$ results in an increase of the wave trains which have the shape of discrete breather-like objects.
Figure 4: The panels show the evolution of the density of energy along the molecule for two values of the solvent interaction parameter $\lambda_s$ and for $M = 300$ amu, $a = 4.45 \text{ Å}^{-1}$, $D = 0.04$ eV, $d = 3.4\text{ Å}$, $f_s = 0.1$, $k = 0.04 \text{ eV.Å}^{-2}$, $qd = 0.56\pi$, $\lambda = 0.99\pi$, $B_{cr} = 0.14\text{ Å}$, and $\epsilon = \sqrt{1/N} \approx 0.04$. The horizontal axis indicates the position of the base pairs and the vertical axis corresponds to time (time is going upward and is expressed in t.u.). The energy density has been plotted for $\lambda_s = 1 \text{ Å}$[panel (a)] and for $\lambda_s = 3 \text{ Å}$[panel (b)]. In all the cases the black regions correspond to $E_n = 0$ and the yellow regions to $E_n = 4.4 \times 10^{-6}$ eV and $E_n = 2.8 \times 10^{-4}$ eV, respectively. By increasing the value of $\lambda_s$, energy increases and is much localized in the molecule.