United Nations Educational, Scientific and Cultural Organization
and
International Atomic Energy Agency
THE ABDUS SALAM INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

MODULATIONAL INSTABILITY AND EXACT SOLITONLIKE SOLUTION IN DNA DOUBLE HELIX

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MIRAMARE – TRIESTE
August 2008

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Abstract

We report on properties of modulational instability (MI) and the generation of solitonlike excitations in DNA nucleotide. Taking the Peyrard-Bishop-Dauxois (PBD) model of DNA dynamics as an example, we show that the original difference differential equation for the DNA dynamics can be reduced to the Ablowitz-Ladik (AL) equation. We derive the modulational instability criterion in this case. The effect of the anharmonic stacking term on the domain of instability/stability has been pointed out. 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. The impact of the anharmonic stacking interactions is investigated and gives rise to a spectrum of behaviors which corroborates experimental facts. One finds that the presence of the anharmonic stacking term is responsible for the bearing of localized solutions.
1 Introduction

Although an understanding of the chemical changes involved in transcription and replication of DNA and RNA rests on fairly secure footing, the dynamics of these processes are still being examined. Doubled-stranded DNA (dsDNA, the DNA double helix) is the genetic memory element of all cells. Two copies of the genetic information are encoded into the two complementary-sequence strands that are base paired together through most of cell cycle. However, the two strands must be completely separated during DNA replication, and partially separated during DNA transcription. In cell, the separation of DNA strands occurs via forces applied by DNA-processing machinery. Force-driven dsDNA "unzipping" is therefore of direct biological relevance.

Several theoretical models have been proposed for describing nonlinear molecule excitations in the DNA double helix. These theoretical models are based on longitudinal and transverse motions, as well as being stretching and rotational [1]. Among the different motions, the rotational motion of base in DNA is found to contribute more towards the opening of base pairs. The first contribution towards the nonlinear dynamics of DNA was made by Englander and his co-worker [2] who studied the dynamics of DNA open states taking into account only the rotational motion of nitrogenous base, which made the main contribution towards the formation of open states. Yomosa [3] developing this idea further proposed a dynamic plane-base rotator model which is a generalization version of the Frenkel-Kontrova [4] model that was at the same time improved by Takeno and Homma [5] in which attention was paid to the degree of freedom characterizing base rotations in plane perpendicular to the helical axis around the backbone structure. In the above, the DNA dynamics was governed by the completely integrable sine-Gordon model admitting kink-type solitons. Christiansen and his colleagues [6], using the Toda lattice model in which two types of internal motions, namely, transverse motion along the hydrogen bond direction and longitudinal motion along the backbone direction, were found to contribute to the DNA denaturation process in terms of travelling solitary waves and standing waves. Then Peyrard and Bishop [7] studied the process of denaturation in which only the transverse motion of bases along the hydrogen bond was taken into account. The improved version, which we call the Peyrard-Bishop-Dauxois (PBD) [8], takes helicosity into consideration.

Helicoidal structure of the DNA chain is such that neighboring nucleotide from different strands are close enough so that they interact in terms of filaments of solvent. This means that the nucleotide at the site n of one strand interacts with both the (n+h)th and (n-h)th nucleotides of the other strand. Assuming a mobile open unit [9] diffusing along the double helix, Englander et al. [10] suggested that the open state in DNA may be described as a solitary excitation. Also, Yomosa has proposed a soliton theory in order to give a theoretical explanation of the open states in DNA duplexes [11]. But the most standard mechanism through which bright solitons and solitary wave structures appear is through the activation of the MI of plane waves.

In recent times, the study of wave propagation, especially solitons through inhomogeneous or
disordered media, has attracted a lot of interest [12, 13]. For instance, kink-impurity interaction and its scattering in the sine-Gordon model was studied in detail by Zhang et al. [12, 13]. So, our aim in this work is to investigate the MI conditions and derive some exact new type of solitons solution for the PBD model. Attention is paid to the impact of the anharmonic stacking constant on the MI criterion as well as on the existence of solitonlike solution. The paper is organized as follows. In section 2, we briefly present the PBD model of DNA dynamics. The DNA dynamics is shown to be governed by an Ablowitz-Ladik (AL) equation. In section 3, we derive the condition for obtaining a train of pulses in the DNA. Numerical simulations are also performed and reveal some additional features of MI such as energy localization. Since the MI phenomenon is deeply related to soliton creation, we therefore find solutions of the AL equation through the Ricatti method [14] in Section 4. The last section is devoted to the conclusion.

2 Hamiltonian and equation of motion

The PBD model [8, 15, 16] reduces the myriad degrees of freedom of DNA to a one-dimensional chain of effective atom compounds describing the relative base-pair separations from the ground-state positions [8, 17]. An important essence of the PBD model is the nonlinear stacking interaction which reproduces the experimental measured sharp phase transition of long homopolymers [17]. Moreover, the model, parameterized for heterogeneous DNA chains, has given accurate results for denaturation curves of short heterogeneous DNA sequences [18]. Although the PBD model is a very strong simplification of the actual DNA molecule in solution, the qualitative and even quantitative agreement with numerous experimental findings have given confidence to this model. The Hamiltonian of the PBD model takes the form [8, 16, 19]

\[ H = \sum_{n=1}^{N} \left\{ \frac{1}{2} m u_n^2 + \frac{1}{2} S[1 + \rho e^{-b(u_{n+1} + u_n)}] (u_{n+1} - u_n)^2 + D(e^{-a u_n} - 1)^2 \right\}, \]  

(1)

where \( u_n \) represents the transverse stretching of the hydrogen bonds connecting two bases at the site \( n \). The Morse potential describes chemical interactions between the hydrogen bonds contained in a pair. It is wellknown that, an AT base has two hydrogen bonds while a GC pair has three hydrogen bonds. In this frame, \( D \) is the dissociation energy and \( a \) stands for a parameter homogeneous to the inverse of a length, which sets the spatial scale of the potential. The second term in Eq.(1) represents the modified stacking interaction potential. As soon as one of the two interacting base pairs is open (and not necessarily both simultaneously), the effective coupling constant drops from \( S(1+\rho) \) to \( S \). This has been shown to bring a very big qualitative improvement that leads to a sharp transition when realistic parameters are used [8, 17, 19]. For this reason, the parameters used in this work are those derived from the study of bubble formation in DNA [17, 20, 21]: \( m = 300 \) amu, \( S = 0.025 \) eV/Å\(^2\), \( D = 0.05 \) eV, \( a = 4.2 \) Å\(^{-1}\), \( \rho = 2 \) and \( b = 0.35\)Å\(^{-1}\), and which are specific to AT pairs. A system of units (amu, Å, eV) defines a time unit (t.u.) equal to 0.01021 ps.
From Hamiltonian (1), the equation governing the stretching of the base pairs is written as:

\[
m\ddot{u}_n = S(u_{n+1} + u_{n-1} - 2u_n) + \frac{1}{2}S[2 + b\rho(u_{n+1} - u_n)](u_{n+1} - u_n) e^{-b(u_{n+1} + u_n)} - \frac{1}{2}S[2 - b\rho(u_n - u_{n-1})](u_n - u_{n-1}) e^{-b(u_n + u_{n-1})} - 2aD(e^{-a\rho} - e^{-2a\rho}).
\] (2)

Expanding the terms in exponential \(e^{-b((u_{n+1} + u_n))}, e^{-b((u_n + u_{n-1}))}\) and \(e^{-a\rho}\), respectively, until the second and third orders, we obtain the following equation of motion

\[
m\ddot{u}_n = K_1(u_{n+1} + u_{n-1} - 2u_n) + \frac{bS\rho}{2}[(u_n - u_{n-1})^2 - (u_{n+1} - u_n)^2] - bS\rho[(u_{n+1} - u_n)(u_{n+1} + u_n) - (u_n - u_{n-1})(u_n + u_{n-1})] - \frac{b^2S\rho}{2}[(u_{n+1} - u_n)^2(u_{n+1} + u_n) - (u_n - u_{n-1})^2(u_n + u_{n-1})] + \frac{b^2S\rho}{2}[(u_{n+1} - u_n)(u_{n+1} + u_n)^2 - (u_n - u_{n-1})(u_n + u_{n-1})^2] - 2aD(u_n + \alpha u_n^2 + \beta u_n^3),
\] (3)

where \(K_1 = S(1 + \rho)\).

Linearizing Eq.(3) yields plane wave solutions with wave number \(q\) and frequency \(\omega(q)\) given by the dispersion relation \(\omega^2(q) = \frac{1}{m}[K_1 + 2a^2D\sin^2(\frac{q}{2})]\). For the nonlinear equation (3), we look for small-amplitude time-periodic solutions as \([16, 22]\)

\[u_n(t) = \sum_{p=-\infty}^{+\infty} a_n^{(p)} e^{ip\omega_b t},\] (4)

where \(\omega_b\) is close to some linear oscillation frequency and the Fourier coefficients are slowly depending on time, \(a_n^{(p)}(e^{2t})\). Due to exponential decay of the Fourier coefficients in \(p\), they must satisfy \(a_n^{(p)} \sim \varepsilon^p\) for \(p > 0\), while \(a_n^{(0)} \sim \varepsilon^2\). Moreover \(a_n^{(p)} = a_n^{(-p)^*}\) since \(u_n\) is real.

This allows, for a slow time dependence of the Fourier coefficients \(a_n^{(p)}\), a DNLS equation for the dominating coefficient \(a_n^{(1)}\) describing the leading-order nonlinear effects [22]. Defining \(a_n^{(1)}\) as

\[a_n^{(1)}(t) = (-1)^n(\frac{2\omega_b}{3\beta\omega_g^2 + 6\eta})^{1/2}\psi_n e^\frac{\omega_b^2 - \omega_g^2 + 2K}{2\omega_b} t,\] (5)

the AL equation of the DNA model reads

\[i\frac{d\psi_n}{dt} + (P_1 + Q_1|\psi_{n+1}|^2)(\psi_{n+1} + \psi_{n-1}) + Q_2|\psi_n|^2\psi_n = 0,\] (6)

where

\[P_1 = \frac{K}{2\omega_b}, \quad Q_1 = \frac{\eta}{3\beta\omega_g^2 + 6\eta}, \quad Q_3 = \frac{\eta + \beta\omega_g^2}{3\beta\omega_g^2 + 6\eta},\] (7)

with \(\omega_g^2 = \frac{2a^2D}{m}, \quad \eta = \frac{b^2S\rho}{m}\) and \(K = \frac{K_1}{m}\).

The AL system has N-soliton solution and a rich mathematical structure [23]. The DNLS equation interpolates between the integrable AL and discrete self-trapping models [24]. Intrinsics
 localized states as well as solitons of the AL equation have been studied by many authors (see [25] to cite a few). One can see that, for $\rho = 0$, Eq. (6) reduces to the DNLS equation, for which MI has been studied in [26]. Kivshar and Salerno [27] explained the physical meaning of an almost similar equation and proposed that, its application may be found in nonlinear optics, where the DNLS equation describes the interactions of partial Transverse Electric modes in an array of (focussing or defocussing) waveguides. Here, we have also shown that the dynamics of the DNA double helix give rise to an AL equation, from which we will study the behaviors.

3 Modulational instability analysis

3.1 The linear stability analysis

Equation (6) has an exact plane-wave exact $\psi_n(t) = \psi_0 e^{i(qn-\omega_0 t)}$. The wavenumber $q$, the angular frequency $\omega_0$ and the amplitude $\psi_0$ satisfy the dispersion relation:

$$\omega_0 = 4(P_1 + Q_1 \psi_0^2) \sin^2 \frac{q}{2} - [2P_1 + (2Q_1 + Q_2) \psi_0^2],$$

(8)

To examine the linear stability of the initial plane waves, we look for a solution of the form:

$$\psi_n(t) = \psi_0 [1 + B_n(t)] e^{i(qn-\omega_0 t)},$$

where the perturbation amplitude $B_n(t)$ is assumed to be small in comparison with the carrier wave amplitude $\psi_0$. Then, one obtains an equation describing the evolution of the perturbation $B_n(t)$. Furthermore, assuming a general solution of the above-mentioned system of the form:

$$B_n(t) = B_1 e^{i(Qn-\Omega t)} + B_2^* e^{-i(Qn-\Omega^* t)},$$

where the asterisk denotes complex conjugation, $Q$ and $\Omega$ represent, respectively, the wavenumber and the angular frequency of the perturbation amplitude, $B_1$ and $B_2$ are complex constant amplitudes. Inserting this modulated solution into the equation describing the evolution of the perturbation and after linearization around the unperturbed plane wave, we obtain the linear homogeneous system for $B_1$ and $B_2$:

$$
\begin{pmatrix}
  a_{11} - \Omega & a_{12} \\
  a_{21} & a_{22} + \Omega
\end{pmatrix}
\begin{pmatrix}
  B_1 \\
  B_2
\end{pmatrix} =
\begin{pmatrix}
  0 \\
  0
\end{pmatrix},
$$

(9)

The condition for the existence of non trivial solutions of this linear homogenous system is given by a second order equation for the frequency $\Omega$, that is

$$(a_{11} - \Omega)(a_{22} + \Omega) - a_{12}a_{21} = 0,$$

(10)

with

$$a_{11} = -2P_1 [\sin(Q) \sin(q) - \cos(Q) - \cos(q)]$$

$$- 2Q_1 |\psi_0|^2 [\sin(Q) \sin(q) - \cos(Q) \cos(q)] + Q_2 |\psi_0|^2,$$

$$a_{12} = a_{21} = (2Q_1 \cos(q) + Q_2) |\psi_0|^2,$$

$$a_{22} = 2P_1 [\sin(Q) \sin(q) + (\cos(Q) - 1) \cos(q)]$$

$$+ 2Q_1 |\psi_0|^2 [\sin(Q) \sin(q) - \cos(Q) \cos(q)] + Q_2 |\psi_0|^2.$$
Equation (10) can be rewritten as:

\[
(\Omega_1)^2 = \left| \Omega + 2P_1 \sin(Q) \sin(q) + 2Q_1 |\psi_0|^2 \sin(Q) \sin(q) \right|^2 \\
= 16(P_1 + Q_1 |\psi_0|^2) \sin^2\left(\frac{Q}{2}\cos(q)\right)\left|(P_1 + Q_1 |\psi_0|^2) \sin^2\left(\frac{Q}{2}\cos(q)\right) - (Q_1 + Q_2) |\psi_0|^2 \right|^2.
\]

(11)

If \((\Omega_1)^2\) is negative, two complex numbers are solutions of the above equation and the exponential growth for \(q = 0\) takes place with rate [26]

\[
\sigma(Q) = 4\sin\left(\frac{Q}{2}\right) \sqrt{(P_1 + Q_1 |\psi_0|^2)\left|(Q_1 + Q_2) |\psi_0|^2 - (P_1 + Q_1 |\psi_0|^2) \sin^2\left(\frac{Q}{2}\cos(q)\right)\right|^2}.
\]

(12)

This is possible if the initial amplitude \(|\psi_0|\) exceeds the threshold amplitude \(|\psi_{0,cr}|\) defined as follows

\[
|\psi_0|^2 \geq |\psi_{0,cr}|^2 = \frac{2P_1 \sin^2\left(\frac{Q}{2}\cos(q)\right)}{Q_1 + Q_2 - 2Q_1 \sin^2\left(\frac{Q}{2}\cos(q)\right)}.
\]

(13)

The above threshold amplitude is shown in Fig. 1. In Fig. 1(a), the threshold amplitude has been plotted for the parameter values given in the previous section. In Fig. 1(b), we obtain that the dimensionless parameter \(\rho\) influences the magnitude of the threshold amplitude (we have set \(q = 0\)). One can conclude that the increasing of the parameter \(\rho\) increases the threshold amplitude.

Also, the stability/instability diagrams plotted in Fig. 2 show that, the stacking potential has an impact on the stability/instability region (region (1) represents zone of stability, while region (2) stands for zone of instability). The same phenomenon has been obtained when one depicts the growth rate versus the perturbation wavenumber. It is shown that the instability growth rate may be dramatically affected by the PBD stacking potential. It is clear, once more, that, for the PB model (i.e., \(\rho = 0\)), the dynamics of the system presents a large zone of instability [see the first panel of Fig. 3] while, in the case of the PBD model \((\rho = 1\) or \(\rho = 2\)), the instability growth rate is considerably reduced by the anharmonicity of the stacking energy [see the second and third panels of Fig. 3]. For all those cases, the growth rate is maximum in general, for \(Q_{cr} = 2 \arcsin \sqrt{\frac{(Q_1 + Q_2)|\psi_0|^2}{2(P_1 + Q_1 |\psi_0|^2) \cos(q)}}\).

3.2 Numerical analysis of MI

According to the above analytical results based on linear stability analysis, the stability condition of an extended plane wave has been determined for the AL equation (6) which is only an approximate description of the initial Eq.(2) of the PBD model. The linear stability analysis cannot tell us the long-time evolution of a modulated extended nonlinear wave. Therefore, in order to check the validity of our analytical approach and to determine the evolution of the system under the instability zone, we have performed numerical simulations of the equation of motion (2) with a given initial condition. They are integrated with a fourth-order Runge-Kutta scheme with a time step chosen to conserve the energy to an accuracy better than 0.005. Most of the simulations are performed with a molecule of 300 base pairs with periodic boundary conditions; this is why the wave-numbers \(q\) and \(Q\) necessarily have the forms \(q = 2\pi l/N\) (rad) and \(Q = 2\pi L/N\) (rad),
where \( l \) and \( L \) are integers lower than \( N/2 \). We chose as an initial condition a linear wave with a slightly modulated amplitude \([26]\)

\[
\begin{aligned}
\psi_n(t = 0) &= \psi_0[1 + 0.01\cos(Qn)]\cos(qn), \\
\dot{\psi}_n(t = 0) &= \psi_0[1 + 0.01\cos(Qn)]\omega\sin(qn).
\end{aligned}
\]

(14)

Our aim in this numerical analysis is to bring out the impact of the anharmonic stacking term on the occurrence of soliton-like objects induced by MI. For a first case, we set \( \rho = 0 \) (the system becomes the PB mode). As a first case, let us take for the wavenumbers: \( q = 0.45\pi \text{ rad} \) and \( Q = 0.98\pi \text{ rad} \) (the corresponding point lies in an instability region of Fig.2(a)). We observe in Fig.4(a) that the initial condition tends to disintegrate during the propagation, leading to breakup of wave into wave trains of patterns. Each element in this figure has the shape of soliton-like object and their amplitude during propagation remains constant. This confirms the fact that, MI is the most standard mechanism through which bright soliton or solitary structure can appear in physical system. Dauxois et al. \([8, 26, 28]\) have suggested that, such localized oscillations can be precursors of bubbles that appear in the thermal denaturation of DNA. In this frame, they can be good candidates in transporting energy and charge in discrete lattices in general and in DNA, in particular. As a second case, we take into account the anharmonic potential \( (\rho = 2) \) and, as one can see, with the use of the same set of wave numbers \( (q, Q) \), the amplitude of the patterns increases progressively with the time \([\text{see Fig.4(a)}]\). This probably reinforces the conclusion from the thermal denaturation of DNA double helix on the PBD model \([8, 29, 30]\). In comparison to the PB model, the anharmonic stacking interaction term is responsible for the sharp transition in the PBD model. The recent work Kapri et al. \([31]\) was based on the study of force induced first-order transition in the DNA lattice model. They have analyzed a randomly forced DNA and concluded that fluctuating force unzips DNA by a gradual increase of bubble size. Of course, in the present work, we do not take thermal fluctuations into consideration but our results corroborate, to some extent, those assumptions. Furthermore, in reality, in the initiation of the leading phenomena of replication and transcription, there is an input of energy that the PB and PBD neglect even if there is energy localization induced by MI as shown in Fig.5 (in this way, energy localization is known to be a robust phenomenon in the PB and PBD models as explained in Ref. \([32]\]). This energy, which is constant in the case \( \rho = 0 \) \([\text{see Fig.5(a)}]\) and increases with the time for \( \rho = 2 \) \([\text{see Fig.5(b)}]\), comes from the surrounding which means that this surrounding should be understood as the external force.

The m-RNA polymerase presence around DNA sequence seems to highly enhance the efficiency of opening respective nucleotides pairs. Its role, in the framework of such a biological structure, could then be to progressively collect the thermal energy available in the molecule.

To conclude this analysis, one should keep in mind that the features displayed by the PBD model under modulation includes a gradual increasing of both the bubbles amplitude and the energy involved in the various processes that take place in DNA. While comparing such results
with known experimental facts, there appear some similarities, namely the sharp opening of the bases due to the sharp increase of the energy density.

4 Solutions of the DNA double helix

Since the disintegration on waves train typically occurs in the same parameters region where bright solitons are observed, MI is considered, to some extend, a precursor to soliton formation. So, in this section, we will find some exact solutions of the model understudy. In this frame, there are many approaches for finding exact soliton solutions of the nonlinear partial differential equations. These methods include: the inverse scattering method [33], the Jacobian elliptic function method [16, 22, 34], Backlund transformation method and the exp-function method [35], the Ricarti method [14] just to cite a few. In order to obtain some exact solutions of Eq.(10), we use the Ricarti method [14]. We set $T_n = t - n\varsigma$, where $n$ is the number of base pairs in the DNA molecule, $\varsigma$ is the lateness time due the neighbor pairs and $t$ is the real time of propagation in absence of the neighboring effects. Equation (6) then becomes

$$i\frac{d\psi_n}{dT_n} + (P_1 + Q_1|\psi_n|^2)(\psi_{n+1} + \psi_{n-1}) + Q_2|\psi_n|^2\psi_n = 0. \quad (15)$$

Looking for solution of Eq.(15) in the form

$$\psi_n = f(n,t)e^{i\theta_n} = f(T_n)e^{i\theta_n}, \quad (16)$$

we obtain

$$-f\frac{d\theta_n}{dT_n} + i\frac{df}{dT_n} + f(P_1 + Q_1f^2)[\cos(\theta_{n+1} - \theta_n) + \cos(\theta_n - \theta_{n-1})] + i\{f(P_1 + Q_1f^2)[\sin(\theta_{n+1} - \theta_n) + \sin(\theta_{n-1} - \theta_n)] + Q_2f^3\} = 0. \quad (17)$$

Separating the real and the imaginary parts of Eq.(17), we get

$$-f\frac{d\theta_n}{dT_n} + 2f(P_1 + Q_1f^2)\cos\left(\frac{\theta_{n+1} + \theta_{n-1} - 2\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1} - \theta_{n-1}}{2}\right) + Q_2f^3 = 0, \quad (18)$$

$$\frac{df}{dT_n} + 2f(P_1 + Q_1f^2)\sin\left(\frac{\theta_{n+1} + \theta_{n-1} - 2\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1} - \theta_{n-1}}{2}\right) = 0. \quad (19)$$

To obtain the majorant and minorant of Eqs.(18) and (19), we consider the limit values of $\cos\left(\frac{\theta_{n+1} + \theta_{n-1} - 2\theta_n}{2}\right)$, $\cos\left(\frac{\theta_{n+1} - \theta_{n-1}}{2}\right)$, $\sin\left(\frac{\theta_{n+1} + \theta_{n-1} - 2\theta_n}{2}\right)$, $\sin\left(\frac{\theta_{n+1} - \theta_{n-1}}{2}\right)$, $\cos(\theta_{n+1} + \theta_{n-1} - 2\theta_n)$ and $\sin(\theta_{n+1} + \theta_{n-1} - 2\theta_n)$.

Firstly, we consider the case where

$$|\cos\left(\frac{\theta_{n+1} + \theta_{n-1} - 2\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1} - \theta_{n-1}}{2}\right)| = 1, \quad (20)$$

which yields to

$$\theta_{n+1} + \theta_{n-1} - 2\theta_n = 2\pi n, \quad (21)$$

$$\theta_{n+1} - \theta_{n-1} = 2\pi n.$$
The set of equations (21) leads to the following recurrence relation between the terms of \((\theta_n)_{n \in \mathbb{N}}\)

\[
\theta_n(T_n) = \theta_0(T_n) + \pi n(n - 1).
\]  

(22)

Substituting Eq.(22) into Eqs.(18) and (19), we get the following reduced system

\[
\frac{d\theta_0}{dT_n} = 2(P_1 + Q_1f_0^2), \quad \frac{df}{dT_n} = 0.
\]  

(23)

We then get the solution

\[
f = f_0 = \text{const}, \\
\theta_0 = 2(P_1 + Q_1f_0^2)T_n + Q_2f_0^2T_n + \lambda_1, \\
\psi_n = f_0 \times \exp \{2(P_1 + Q_1f_0^2)T_n + Q_2f_0^2T_n + \pi n(n - 1) + \lambda_1\}. \]

(24)

The approximate solution of Eq.(2) can then be written in the form

\[
u_n(t) = (-1)^n \left( \frac{2\omega_b}{3\omega_b^2 + 6\eta} \right)^{1/2} f_0 \\
\times \exp \left\{2(P_1 + Q_1f_0^2) + Q_2f_0^2\right\}(t - n\varsigma) + \frac{\omega_b^2 + \omega_0^2 + 2K}{2\omega_b} t + \pi n(n - 1) + \lambda_1 \right}\}. \]

(25)

The above expression represents a plane wave solution, but we are interested by solitonlike solutions. It is also clear that, such a plane wave solution is also the only solution for the case \(\rho = 0\).

On the other hand, for the case

\[
|\sin(\frac{\theta_{n+1} + \theta_{n-1} - 2\theta_n}{2})\cos(\frac{\theta_{n+1} - \theta_{n-1}}{2})| = 1,
\]  

(26)

we have the recurrence relation

\[
\theta_n(T_n) = \theta_0(T_n) + \frac{\pi}{2} \sum_{k=1}^{N} (4k - 3).
\]  

(27)

The set of equation for \(f\) and \(\theta_n\) become

\[
\frac{d\theta_0}{dT_n} = Q_2f_0^2, \quad \frac{df}{dT_n} = -2(P_1 + Q_1f_0^2). \]

(28)

The integration of the set of equations (28) gives us successively

\[
f(T_n) = \pm \sqrt{\frac{P_1 \text{sech}(P_1T_n)}{\sqrt{\lambda_1 P_1[\text{sech}(P_1T_n) + 2\tanh(P_1T_n)]^2 - Q_1 \text{sech}^2(P_1T_n)}}},
\]  

(29)

and

\[
\theta_0(T_n) = \frac{Q_2}{4Q_1} \text{Log} \left\{ \frac{\lambda_1 P_1[\text{sech}(P_1T_n) + 2\tanh(P_1T_n)]^2 - Q_1 \text{sech}^2(P_1T_n)}{\text{sech}^2(P_1T_n)} \right\} \\
- \frac{P_1Q_2}{Q_1} T_n + \lambda_2,
\]  

(30)
\( \lambda_1 \) and \( \lambda_2 \) are constants of integration. Setting \( T_n = t - n\zeta \), the full solution of Eq.(2) is then written as

\[
\begin{align*}
    u_n(t) &= \pm \frac{(-1)^n \sqrt{2\omega_0} P_1 sech(P_1(t - n\zeta))}{\sqrt{3\beta \omega_0^2 + 6\eta \sqrt{\lambda_1} P_1[sech(P_1(t - n\zeta)) + 2tanh(P_1(t - n\zeta))]^2 - Q_1 sech^2(P_1(t - n\zeta))}} \\
    &\times \exp \left[ \frac{iQ_2}{4Q_1} \log \left\{ \frac{\lambda_1 P_1[sech(P_1(t - n\zeta)) + 2tanh(P_1(t - n\zeta))]^2 - Q_1 sech^2(P_1(t - n\zeta))}{sech^2(P_1(t - n\zeta))} \right\} \\
    &\quad - \frac{P_1Q_2}{Q_1} (t - n\zeta) + \frac{\omega_0^2 + \omega_b^2 + 2K}{2\omega_0} t + \frac{\pi}{2} \sum_{k=1}^{N} (4k - 3) + \lambda_2 \right].
\end{align*}
\]

(31)

This solution, through its structure, represents a localized solution. As shown in Fig 6, one can see that it takes different shapes, depending on the values of parameters. In Fig. 6(a), we have a pulse soliton for \( \varsigma = 0.02 \) and \( \rho = 0.8 \). This solution is already known in the literature and represents the creation of a bubble (replication or transcription) within the lattice structure. By setting \( \varsigma = 0.5 \) and \( \rho = 2 \), we obtain the configuration shown in Fig. 6(b), which is kink soliton. Such a soliton solution has been widely discussed in Ref. [13], in the framework of the perturbed Sine-Gordon equation. The anharmonic term of the stacking interaction potential can thus be taken as the perturbation introduced by those authors.

Meanwhile, DNA, in nature, is a nonlinear structure and while modeling its dynamics, all the features related to nonlinearity should be taken into consideration. Of course, the on-site Morse potential already introduces a nonlinear term but it is not always sufficient to get a model capable of supporting nonlinear excitations in terms of solitary waves. This is possible for the continuous approximation but, results under discrete developments are very selective and should be taken with confidence. This can be illustrated by the fact that, with the Ricatti method, the reduced system \( (\rho = 0) \), does not support solitary waves solution while, for \( \rho \neq 0 \), we get a fully integrable system which brings about formation of open states which explain the functions such as replication and transcription.

### 5 Conclusion

In this work, we have investigated MI, in the DPB model. In this model, stacking interactions are modeled by an anharmonic potential. We have, in this frame, established that the dynamics nonlinear excitations is governed by the AL equation. Through the linear stability analysis, we have derived the MI criterion as well as the threshold amplitude. It has been observed that, when the anharmonic coupling constant \( \rho \) is equal to zero , the instability region is wider than for the case \( \rho \neq 0 \). This has been confirmed with the use of the instability growth rate, which is reduced for higher values of \( \rho \). In order to see to what extent the analytical predictions are valuable, numerical simulations, on the PBD model, have been carried out. It has been observed
that, the anharmonicity of stacking interactions leads to a gradual increase of the wave pattern created under modulation. This also has an influence on the localization of energy. The energy density increases gradually with time and is higher than in the case $\rho = 0$. It has also been shown that bubble amplitude is very sensitive to the presence of nonlinear stacking interactions. In so doing, the results obtained have been found to be in accordance with those relative to the thermal denaturation of DNA. In this context, the phase transition is sharp and bubbles are created at low temperatures.

On the other hand, the presence of nonlinear stacking interactions leads to an integrable system under small modulations. We have then solved the AL equation using the Ricatti method and, it has been found that, for harmonic stacking interactions, i.e. $\rho = 0$, the system gives rise to plane wave solutions while for $\rho \neq 0$, there are two sets of solutions: the plane wave solution and localized solution. In the last family, depending on the values of $\varsigma$ and $\rho$, we have found the pulse soliton and the kink soliton.

Acknowledgments

This work was done within the framework of the Associateship Scheme of the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy. Mohamadou and Kofane thank the Condensed Matter and Statistical Physics Section of ICTP for the invitation, where this work was carried out. Tabi acknowledges fruitful discussions with Dr Nguyenang.

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Figure 1: The panels show the plot of the threshold amplitude for $\omega_b = 1$, $S = 0.025$ eV/Å$^2$ and $D = 0.05$ eV and $b = 0.35$ Å$^{-1}$. In panel (a), $|\psi_{0,cr}|^2$ has been plotted for $\rho = 2$. In panel (b), we compare the threshold amplitude of the PB model (solid blue line) with the threshold amplitude of the PBD model (dashed red line). It appears that, the amplitude is an increasing function of $\rho$.  

\begin{align*}
|\psi_{0,cr}|^2
\end{align*}
Figure 2: Panels (a) and (b) show the Stability/instability diagrams in the \((K,k)\) plane for \(\omega_b = 1\), \(S = 0.025 \text{ eV/Å}^2\) and \(D = 0.05 \text{ eV}\) and \(b = 0.35 \text{ Å}^{-1}\): (a) \(\rho = 0\); (b) \(\rho = 2\). One clearly sees that, the stability region (1) get larger for higher values of \(\rho\).
Figure 3: Growth rate versus the wavenumber of the perturbation $Q$ for $q = 0$, $\omega_b = 1$, $S = 0.025$ eV/A$^2$, $D = 0.05$ eV and $b = 0.35$Å$^{-1}$. It has been plotted for three values of the anharmonic stacking coupling constant $\rho$. It is obvious that, the increase of $\rho$ deeply reduces the region of instability as also shown in Fig. 2.
Figure 4: The panels show how the initial plane solution wave breaks into wave train which has the shape of soliton-like object in DNA molecule, as predicted by the analytical predictions, for $\omega_b = 1$, $S = 0.025 \text{ eV/Å}^2$, $D = 0.05 \text{ eV}$, $b = 0.35\text{Å}^{-1}$, $q = 0.45\pi$ and $Q = 0.98\pi$: (a) $\rho = 0$; (b) $\rho = 2$. In the first case, the waves propagates uniformly. The case depicted in (b) shows how the waves amplitude increases gradually. This could be a consequence of energy collection by an enzyme, the m-RNA polymerase. As predicted by Kapri et al. [31] the initiation of the leading phenomena of transcription and replication is based on a gradual increase of the created bubbles amplitude.
Figure 5: (Color online) Localization of energy induced by MI in the DNA model for $\omega_b = 1$, $S = 0.025$ eV/Å$^2$, $D = 0.05$ eV, $a = 4.2$ Å$^{-1}$, $b = 0.35$ Å$^{-1}$, $q = 0.45\pi$ and $Q = 0.98\pi$: (a) $\rho = 0$; (b) $\rho = 2$. In the case of (a), the energy density is constant while in panel (b), the energy density increases as time increases. This is fundamentally due to the presence of the anharmonic stacking interaction term.
Figure 6: The panels show the solution of the PBD model obtained through the Ricarti method for $\omega_h = 1$, $S = 0.025$ eV/Å^2, $D = 0.05$ eV, $a = 4.2$ Å$^{-1}$, $b = 0.35$Å$^{-1}$. The panel (a) represents the localized solution (31) for $\varsigma = 0.02$ and $\rho = 0.8$. The solution here is the well-known pulse excitation. The panel (b) shows the kink – pulse soliton for $\varsigma = 0.5$ and $\rho = 2$. 