

SOLITON-LIKE EXCITATION IN A NONLINEAR MODEL OF DNA DYNAMICS WITH VISCOSITY

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ABSTRACT. The study of solitary wave solutions is of prime significance for nonlinear physical systems. The Peyrard-Bishop model for DNA dynamics is generalized specifically to include the difference among bases pairs and viscosity. The small amplitude dynamics of the model is studied analytically and reduced to a discrete complex Ginzburg-Landau (DCGL) equation. Exact solutions of the obtained wave equation are obtained by the mean of the extended Jacobian elliptic function approach. These amplitude solutions are made of bubble solitons. The propagation of a soliton-like excitation in a DNA is then investigated through numerical integration of the motion equations. We show that discreteness can drastically change the soliton shape. The impact of viscosity as well as elasticity on DNA dynamic is also presented. The profile of solitary wave structures as well as the energy which is initially evenly distributed over the lattice are displayed for some fixed parameters.

1. Introduction. The local opening of DNA is an intriguing phenomenon from a statistical-physics point of view, but is also essential for its biological function. For instance, the transcription and replication of our genetic code cannot take place without the unwinding of the DNA double helix. Although these biological processes are driven by protein, there might well be a relation between these biological opening processes and the spontaneous bubble formation. The key problem in DNA biophysics is how to relate functional properties of DNA with its structural and physical dynamical characteristics. The local openings can be analytically described as breather-like objects of small amplitude, which nevertheless have interesting properties: as long as their amplitude is small enough, they can move along the chain, collect energy and grow [1]. They can also be trapped by some

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local dishomogeneities [2], which suggests that the properties of breathers could allow the formation of the transcription bubble after the interaction with the bound RNA-polymerase.

However, biological macromolecules undergo a complex dynamics, and the knowledge of their motions provides insight into biological phenomena. Englander et al. [3] suggested the presence and the functional role of solitonic excitation in the DNA double chain. Discrete solitons in nonlinear lattices have been the focus of considerable attention in diverse branches of science [4]. Discrete solitons are possible in several physics fields, such as biological systems [5], atomic chains [6], solid state physics [7], electrical lattices [8], Bose-Einstein condensate [9], and DNA molecules [10]. Recently, attention has been focused on the dynamics of large amplitudes of localized excitation in DNA, in which the double helix fluctuates between an open state and its equilibrium structure. These oscillatory states, also called the breathing mode [11] or fluctuational opening, are expected to be precursor states for the local denaturation observed during DNA transcription or thermal denaturation.

Usually, the dynamic of such systems is modelled by the nonlinear Schrödinger (NLS) equation or the complex Ginzburg-Landau (CGL) equation [12]. Hence, their exact solution can be checked through different methods, such as the Darboux transformation [13], various Tanh methods [14-16], the inverse scattering method [17], the homogeneous balance method [18], the Painlevé truncation expansion [19], and the Jacobian elliptic functions approach [20, 21].

In this paper, we investigate nonlinear (NL) wave modulation as well as possible stationary states in the form of localized structures of the PB model of DNA dynamics with viscosity. The paper is organized in the following fashion. In Section 2, we show that the modulation of the NL wave is described by DCGL equation. Possible exact travelling solutions of the model under study are obtained through the Jacobian elliptic function approach in Section 3. The profile of different nonlinear excitations and energy are graphically exhibited in Section 4. A summary and discussion of our work is contained in Section 5.

2. Modulated waves in the Peyrard-Bishop model of DNA dynamics.

2.1. Description of the Model. We consider a simplified geometry for the DNA chain. The asymmetry of the base pairs is neglected, and each strand is represented by an array of point masses which correspond to nucleotides. The chain consists of two strands, S_1 and S_2 . We focus our attention only on transverse motions. The displacement from equilibrium of the n th nucleotide in strand S_1 is denoted by y_n , and in strand S_2 it is denoted by z_n . The longitudinal displacements are not considered, because their typical amplitudes are significantly smaller than the amplitudes of the transverse ones. Two neighboring nucleotides on the same strand are assumed to interact through a harmonic potential, because the displacements due to the bubbles change only gradually from one site to the next. On the other hand, the bonds connecting the two bases belonging to different strands are extremely stretched when the double helix opens locally. The Morse potential is used to describe not only the hydrogen bonds but the repulsive interaction between the phosphate and surrounding solvent action. The Hamiltonian for the model is

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

The first term is the kinetic energy of the transverse vibrations, and the second and third terms are respectively the potential energies of the transverse and longitudinal connections. The on-site potential, announced to be the Morse, takes the form $\mathbf{V}(\mathbf{y}_n - \mathbf{z}_n) = \mathbf{D}[\mathbf{e}^{-\mathbf{a}(\mathbf{y}_n - \mathbf{z}_n)} - \mathbf{1}]^2$, where \mathbf{D} is the dissociation energy and \mathbf{a} a parameter homogeneous to the inverse of a length, which sets the spatial scale of the potential.

The Hamiltonian (1) gives the equations of motion for y_n and z_n .

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

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

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

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

We have then,

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

$$m\ddot{x}_n = k(x_{n+1} + x_{n-1} - 2x_n) + 2\sqrt{2}aDe^{-a\sqrt{2}x_n}(e^{-a\sqrt{2}x_n} - 1). \quad (6)$$

The variables r_n and x_n represent the in-phase and out-of-phase motion respectively. Equation (5) is a linear differential-difference equation with the usual plane wave solutions. On the other hand, equation (6) contains nonlinear terms. It is interesting to relate our model to nonlinear excitations.

To deal with a more realistic description of DNA dynamics, which takes into account the impact of the medium, surrounding a DNA molecule we would consider the viscosity [22,23]. Recently, Peyrard [24] stressed the importance of hydrating water for the biochemical activities of proteins and DNA. Since water molecules are highly polar, they form an ordered network on the surface of a protein along which protons can be transferred. The formation of this network with long-range connecting has been detected as a percolation when the water content approaches 0.5 g per gram of protein [25]. The helicoidal spring constant may be suggested to reflect the mediating role of the water molecules. Moreover, the helicoidal structure itself arises as the result of optimization of the interplay between hydrogen bonding, hydrophobicity and long-range connectivity. On the other hand, we must take into account the fact that the solvating water does act as a viscous medium that damps out DNA dynamic, favoring energy expenditure. It appears that a viscous force proportional to the velocity of nucleotide oscillations does not affect the out-of-phase base pair dynamics, so we took into consideration a viscous force of the Newtonian kind, proportional to the square of the velocity. Here we start from a probably more realistic and favorable approach, that viscous force can be taken into consideration to express the effect of the medium [22,23]. Therefore the viscous forces exerted on the bases within a pair n are $-\alpha\dot{y}_n$, and $-\alpha\dot{z}_n$. It leads to the effective damping force acting on the out-of-phase base pair motion as follows: $\mathbf{F}_v = -\alpha\dot{\mathbf{x}}_n$. Now, the perturbed equation of motion can be written as follows

$$m\ddot{x}_n + \alpha\dot{x}_n = k(x_{n+1} + x_{n-1} - 2x_n) + 2\sqrt{2}aDe^{-a\sqrt{2}x_n}(e^{-a\sqrt{2}x_n} - 1), \quad (7)$$

which becomes, in the dimensionless form

$$\ddot{u}_n + \gamma\dot{u}_n = K_1(u_{n+1} + u_{n-1} - 2u_n) - e^{-u_n} + e^{-2u_n}, \quad (8)$$

where the dimensionless parameters are $\mathbf{u}_n = \mathbf{a}\sqrt{2}\mathbf{x}_n$, $\mathbf{t} = \omega_0\mathbf{t}$, $\mathbf{K}_1 = \frac{\Omega}{\omega_0}$, $\Omega = \sqrt{\frac{k}{m}}$ and $\gamma = \frac{\alpha}{m\omega_0}$ with $\omega_0^2 = \frac{4a^2D}{m}$. Since we need to perform analytical calculation, it is important to expand the terms exponentially until the third order, and we get

$$\ddot{u} + \gamma\dot{u} = K_1(u_{n+1} + u_{n-1} - 2u_n) - u_n + \frac{3}{2}u_n^2 - \frac{7}{6}u_n^3. \quad (9)$$

Numerical experiment would be performed on equation(8).

2.2. The discrete complex Ginzburg-Landau equation to describe DNA dynamics. Several methods for the study of the NL wave modulation have been put forward in the past, following the general direction of distinguishing fast and slow evolution scales in space and time. A priori, they all suggest a certain approximation, which might limit both the region of their validity and the accuracy of the corresponding results. A common element in all of them is that they lead to some equation which describes the evolution of the modulated amplitude of the NL wave considered. Very often, the equation in question can take the form of the NLS equation or the CGL equation. Two interesting aspects of the latter are (a) that it exhibits the interesting phenomenon of modulational instability i.e., the possibility of a plane wave's bursting into a series of localized pulses (already widely studied in optical fibers, for example); and (b) that it accepts solitary wave solutions. The nonlinearity in the dynamics of the lattice might be imposed either by the anharmonicity of the interaction between the atoms or by the existence of an on-site potential. In the first case, it has been shown in a general manner that a constant term (a non-oscillating NL wave) appears in the same order as the small amplitude phonon considered (first order perturbation) and hints have been made that its existence might influence the stability of the modulated envelope soliton [26]. However, in the second case, the first constant contribution usually appears in the second order in perturbation, together with a second harmonic term. Among the methods developed to study the NLS wave modulation one can name: the method developed by Newell et al., which consists in studying the continuum limit, making no hypothesis for the form of the solutions. Another way to derive the NLS equation is by studying the NL (amplitude dependent) dispersion relation obtained by considering a phonon in the first order of perturbation, in the discrete (or continuum) equation of motion. The next method consists of considering the continuum limit only for the (slowly varying, anyway) amplitude, but treating the phase exactly. To do so, however, one must suppose a specific form for the solution [11,12]. Recently, Kivshar and Peyrard [27] have developed an interesting approach, deriving the NLS equation in a Klein-Gordon chain. Along the same line, Ndzana et al. [28] obtained the discrete complex Ginzburg-Landau (DCGL) equation in the nonlinear electrical transmission line. Hence, we consider that the small-amplitude solutions \mathbf{u}_n of the above expanded equation can be written in the form a Fourier series as

$$u_n(t) = \sum_{p=-\infty}^{+\infty} a_p^{(p)} e^{ip\omega_b t}. \quad (10)$$

Introducing equation(10) into equation(9) yields

$$\begin{aligned}
\sum_p \left[\frac{d^2 a_n^{(p)}}{dt^2} + 2ip\omega_b \frac{da_n^{(p)}}{dt} - p^2 \omega_b^2 a_n^{(p)} \right] e^{ip\omega_b t} &= -[\gamma \sum_p \left(\frac{da_n^{(p)}}{dt} + ip\omega_b a_n^{(p)} \right)] e^{ip\omega_b t} \\
&+ \sum_p [K_1(a_{n+1}^{(p)} + a_{n-1}^{(p)} - 2a_n^{(p)}) - a_n^{(p)}] e^{ip\omega_b t} \\
&+ \frac{3}{2} \left(\sum_p a_n^{(p)} e^{ip\omega_b t} \right)^2 - \frac{7}{6} \left(\sum_p a_n^{(p)} e^{ip\omega_b t} \right)^3 + \vartheta(\epsilon^5).
\end{aligned} \tag{11}$$

We then consider the first harmonic $\mathbf{p} = \mathbf{1}$, which leads us to DCGL equation

$$\begin{aligned}
2i\omega_b \frac{da_n^{(1)}}{dt} - \omega_b^2 a_n^{(1)} &= -\gamma \left[\frac{da_n^{(1)}}{dt} + i\omega_b a_n^{(1)} \right] + K_1(a_{n+1}^{(1)} + a_{n-1}^{(1)} - 2a_n^{(1)}) \\
&- a_n^{(1)} - \frac{7}{6} |a_n^{(1)}|^2 a_n^{(1)}.
\end{aligned} \tag{12}$$

Rescaling the coefficients, the time-dependent amplitude can then be written in the form

$$a_n^{(1)}(t) = \sqrt{\frac{4\omega_b}{7}} \psi_n e^{i \frac{1-\omega_b^2+2K_1}{2\omega_b} t}. \tag{13}$$

Introducing equation(13) into equation(12), we finally get the following DCGL equation

$$i \frac{d\psi_n}{dt} + p(\psi_{n+1} + \psi_{n-1}) + q|\psi_n|^2 \psi_n = i\delta \psi_n, \tag{14}$$

where \mathbf{p} , \mathbf{q} , and δ are complex parameters; i.e, $\mathbf{p} = \mathbf{p}_1 + i\mathbf{p}_2$, $\mathbf{q} = \mathbf{q}_1 + i\mathbf{q}_2$ and $\delta = \delta_1 + i\delta_2$ with

$$\begin{aligned}
p_1 &= -\frac{2\omega_b K_1}{4\omega_b^2 + \gamma^2}, & p_2 &= -\frac{\gamma K_1}{4\omega_b^2 + \gamma^2}, \\
q_1 &= \frac{4\omega_b}{3(4\omega_b^2 + \gamma^2)}, & q_2 &= \frac{2\gamma}{3(4\omega_b^2 + \gamma^2)}, \\
\delta_1 &= -\frac{\gamma(1 + \omega_b^2 + 2K_1)}{4\omega_b^2 + \gamma^2}, & \delta_2 &= -\frac{\gamma^2(1 + \omega_b^2 + 2K_1)}{2\omega_b(4\omega_b^2 + \gamma^2)}.
\end{aligned} \tag{15}$$

Equation (14) is the so-called discrete cubic complex Ginzburg-Landau (DCGL) equation. This equation is known to play a ubiquitous role in science. DGL models have also been considered in the literatures [12,28-34]. These DGL lattices are quite often used to describe a number of physical systems, such as Taylor and frustrated vortices in hydrodynamics [29,30] and semiconductor laser arrays in optics [31-34]. In these latter studies, the DGL model has been predominantly used in connection with spatiotemporal chaos, instabilities, and turbulence [29,30]. Soto-Crespo et al. [33] studied a discrete CGL equation having several exact solutions. However, by a numerical study, they found that the solitons are unstable in the model where the highest nonlinearity is cubic. Efremidis and Christodoulides [34] also studied another DCGL equation with all local nonlinear terms. They found that discrete solitons of the DCGL equation have several features that have no counterparts in either continuous limit or other conservative discrete models. The interest in the dynamics of discrete systems comes from the diversity of their applications in physical and biological sciences. The present study is also relevant because the DCGL equation is recovered in the PB models of DNA dynamics.

2.3. The soliton-solution of the DCGL equation. Several powerful methods have been proposed to solve differential-difference equations and to obtain exact solutions to nonlinear partial differential equation. One can think of the inverse scattering method [17], the tanh method [14-16], the Jacobian elliptic function method [20,21], the multilinear variable separation and so on. To obtain some exact solutions of equation (14), we use the Jacobian elliptic function approach. First, we make the transformations

$$\psi_n = e^{i\theta_n} \varphi_n(\xi_n), \quad \theta_n = pn + qt + \zeta, \quad \xi_n = kn + ct + \chi, \quad (16)$$

replacing ψ_n in equation(9), and, separating the real from the imaginary part, we get the following set of equations:

$$-q\varphi_n + p_1(\varphi_{n+1} + \varphi_{n-1})\cos(p) - p_2(\varphi_{n+1} - \varphi_{n-1})\sin(p) + q_1\varphi_n^3 + \delta_2\varphi_n = 0 \quad (17)$$

$$c\varphi_n' + p_2(\varphi_{n+1} + \varphi_{n-1})\cos(p) + p_1(\varphi_{n+1} - \varphi_{n-1})\sin(p) + q_2\varphi_n^3 - \delta_1\varphi_n = 0. \quad (18)$$

With the properties of Jacobian elliptic function [20,21], it is possible to expand and balance the linear term of the highest order with the highest nonlinear terms in equations (17) and (18); i.e,

$$\varphi_n(\xi_n) = a_0 + a_1 sn(\xi_n) \quad (19)$$

$$\varphi_{n+1}(\xi_n) = a_0 + a_1 \frac{sn(\xi_n)cn(k)dn(k) + sn(k)cn(\xi_n)dn(\xi_n)}{1 - m^2 sn^2(\xi_n)sn^2(k)} \quad (20)$$

$$\varphi_{n-1}(\xi_n) = a_0 + a_1 \frac{sn(\xi_n)cn(k)dn(k) - sn(k)cn(\xi_n)dn(\xi_n)}{1 - m^2 sn^2(\xi_n)sn^2(k)} \quad (21)$$

Now, we substitute the above equations into equations(18) and (20). This leads us to a set of algebraic equations with \mathbf{a}_0 , \mathbf{a}_1 , \mathbf{c} , and \mathbf{q} to be determined. We then find after some calculations

$$\begin{aligned} a_0 &= 0, & a_1 &= \pm m \sqrt{-\frac{2p_1}{q_1} cn(k)\cos(p)dn(k)sn(k)} \\ c &= -2p_1 sn(k)\sin(p), & q &= \delta_2 + 2p_1 cn(k)dn(k)\cos(p) \end{aligned} \quad (22)$$

When $\mathbf{m} \rightarrow \mathbf{1}$, the parameters take the form

$$\begin{aligned} a_0 &= 0 \\ a_1 &= \pm m \sqrt{-\frac{2p_1}{q_1} \operatorname{sech}^2(k)\cos(p) \tanh(k)} \\ c &= -2p_1 \tanh(k)\sin(p) \\ q &= \delta_2 + 2p_1 \operatorname{sech}^2(k)\cos(p) \\ \theta_n &= p n + (\delta_2 + 2p_1 \operatorname{sech}^2(k)\cos(p))t + \zeta \\ \xi_n &= k n - (2p_1 \tanh(k)\sin(p))t + \varsigma, \end{aligned} \quad (23)$$

and the function

$$\begin{aligned}
\varphi_n &= \pm m \sqrt{-\frac{2p_1}{q_1} \operatorname{sech}^2(k) \cos(p) \tanh(k) \tanh(kn - (2p_1 \tanh(k) \sin(p))t + \varsigma)} \\
\psi_n &= \pm m \sqrt{-\frac{2p_1}{q_1} \operatorname{sech}^2(k) \cos(p) \tanh(k) \tanh(kn - (2p_1 \tanh(k) \sin(p))t + \varsigma)} \\
&\quad \times \exp(i(pn + (\delta_2 + 2p_1 \operatorname{sech}^2(k) \cos(p))t + \zeta))
\end{aligned} \tag{24}$$

$\mathbf{a}_n^{(1)}$ can then be written, taking the + sign, as

$$\begin{aligned}
a_n^{(1)}(t) &= m \sqrt{\frac{4\omega_b}{7}} \sqrt{-\frac{2p_1}{q_1} \operatorname{sech}^2(k) \cos(p)} \\
&\quad \times \tanh(k) \tanh(kn - (2p_1 \tanh(k) \sin(p))t + \varsigma) \\
&\quad \times \exp(i(pn + [\frac{1 - \omega_b^2 + 2K_1}{2\omega_b} + \delta_2 + 2p_1 \operatorname{sech}^2(k) \cos(p)]t + \zeta)).
\end{aligned} \tag{25}$$

The general solution of equation (8), giving the displacement of the base pairs; i.e, \mathbf{u}_n , therefore take the form:

$$\begin{aligned}
u_n(t) &= m \sqrt{-\frac{8p_1\omega_b}{7q_1} \operatorname{sech}^2(k) \cos(p)} \\
&\quad \times \tanh(k) \tanh(kn - (2p_1 \tanh(k) \sin(p))t + \varsigma) \\
&\quad \times \exp(i(pn + [\frac{1 + \omega_b^2 + 2K_1}{2\omega_b} + \delta_2 + 2p_1 \operatorname{sech}^2(k) \cos(p)]t + \zeta)).
\end{aligned} \tag{26}$$

Solution (26) is a dark soliton as displayed by figure 1. The static dark solitons of the NLS equation can be classified under two broad classes. Bubbles are one-, two-, and three-dimensional nontopological solitons arising typically in models with competing interactions [35-37]. The second class includes topological solitons of the Gross-Pitayevski equation and their one-dimensional counterparts, kinks. The static bubbles are always unstable [35-39], and this property endows them with a transparent physical interpretation as nuclei of the first-order transition [40]. The above classification (topological vs. nontopological) is difficult to extend to traveling dark solitons, which always have some topological properties (the phase approaches different values at different spatial infinities). One-dimensional traveling dark solitons have been experimentally observed in optical fibers [41,42]; it was noticed that dark solitons are less influenced by noise, and their interaction is weaker than that of bright solitons. These facts suggest the feasibility of the use of dark solitons in optical communications [42]. In optics, much attention has been devoted to spatial dark solitons. Here, we also find that dark solitons are possible in DNA dynamics.

3. Numerical results. Direct numerical simulations were run to determine the outcome of the evolution of the exact solution derived in the previous section through the system. We have integrated equation (8) using the fourth-order Runge-Kutta scheme with a time step equal to 0.055. Most of simulations are made with a set of 300-molecule base pairs with periodic boundary conditions. The initial condition is the solution of (26):

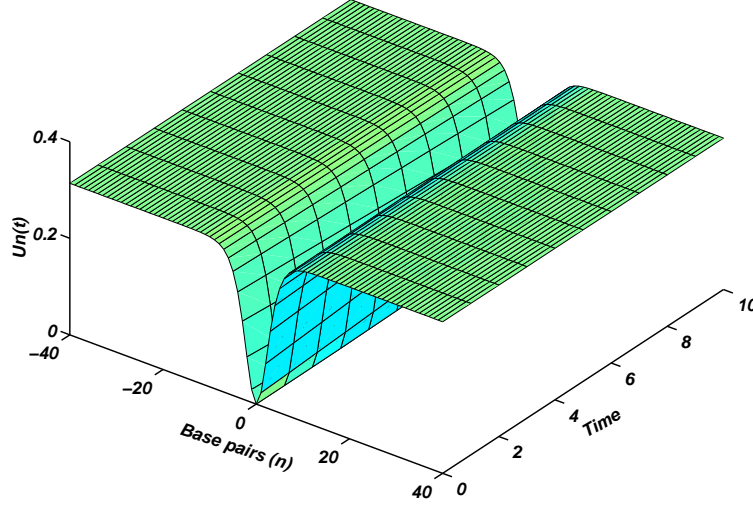


FIGURE 1. Profile of the exact bubble soliton solution for the parameters $\delta = 0.5$, $K_1 = 0.002$, $p = 0.06$, $k = 0.3$, $m = 0.95$.

$$u_n(t=0) = m \sqrt{-\frac{8p_1\omega_b}{7q_1} \text{sech}^2(k) \cos(p) \tanh(k) \tanh(kn + \varsigma) \exp(i(pn + \zeta))}. \quad (27)$$

Now we launch solution (27) through the system. As a first remark, we note that during the propagation, the initial bubble soliton solution is transformed in pulse solitons. For the parameters $\delta = 0.5$, $K_1 = 0.02$, $p = 0.001$, $k = 0.3$, and $m = 0.95$, we observe in figure 2(a) a train of pulse with an ultrashort width propagating in the DNA chain. From the previous parameters, we increase the value of the wavenumber p which is now equal to $p = 0.008$. Figure 2 (b) depicts this case. The amplitude of the pulse has increased as well as its width. As we continue to increase the value of p ($p = 0.02$, $p = 0.04$, and $p = 0.06$), one sees respectively, in figure 2(c) through figure 2 (e), that the number of pulses in the chain drastically decreases. As the number of pulses in the chain decreases, the width of these pulses increases. But, the amplitude of the pulse fluctuates (the amplitude increases figure 2(b), decreases figure 2(c), then increases figure 2(d) and again decreases). Because of the discrete nature of the lattice, the difference in the shape of the pulse propagating through the lattice strongly depends on the range of the values of the wavenumber p .

Many physical phenomena involve some localization of energy in space. Formation of vortices in hydrodynamics, self-focusing in optics or plasma, the formation of dislocations in solids under stress, and self-trapping of energy in proteins are well known examples. Hence, since Benjamin and Feir [43] discovered the modulational instability of Stokes waves in fluids, nonlinear energy localization in continuous media has been extensively investigated but very little has been done in lattices although it would be of wide interest for solids or macromolecules. Also, following the original work by Anderson [44], disorder-induced localization has been widely

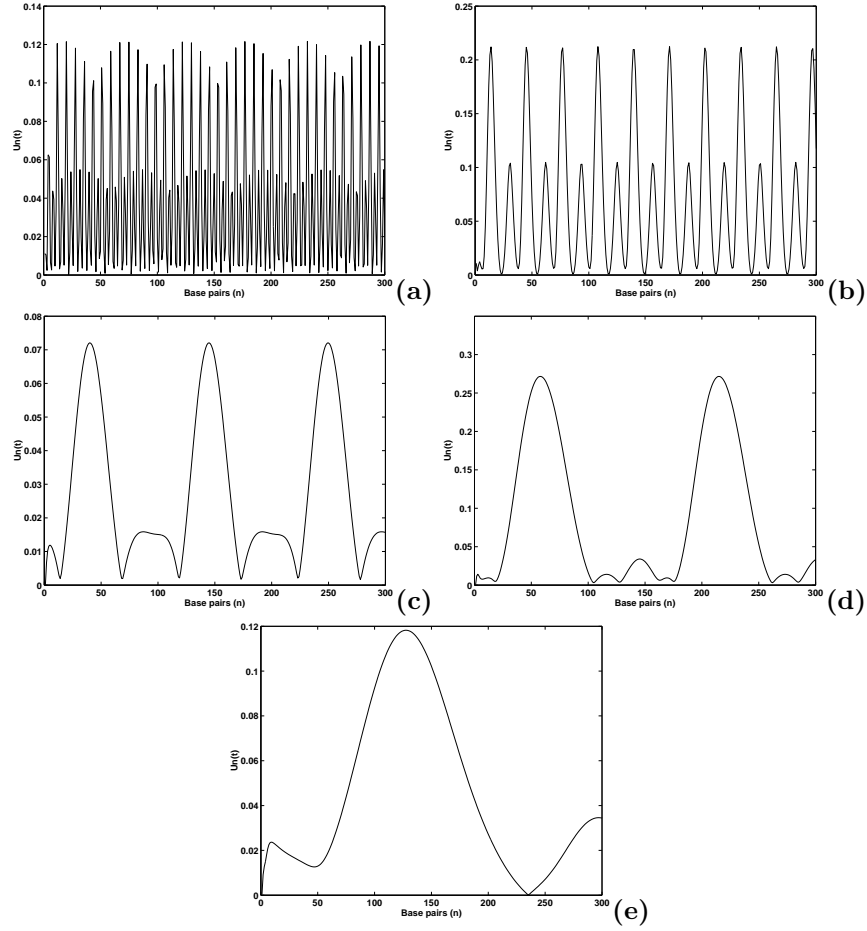


FIGURE 2. Propagation of the initial solution in the chain for different value of the wavenumber p changes (a) $\delta = 0.5$, $K_1 = 0.02$, $p = 0.001$, $k = 0.3$, $m = 0.95$ (b) $\delta = 0.5$, $K_1 = 0.02$, $p = 0.008$, $k = 0.3$, $m = 0.95$ (c) $\delta = 0.5$, $K_1 = 0.02$, $p = 0.02$, $k = 0.3$, $m = 0.95$ (d) $\delta = 0.5$, $K_1 = 0.02$, $p = 0.04$, $k = 0.3$, $m = 0.95$ (e) $\delta = 0.5$, $K_1 = 0.02$, $p = 0.06$, $k = 0.3$, $m = 0.95$

studied, but, more recently, attention has turned to the possibility of localized energy in a homogeneous system due to nonlinear effects. We have monitored the energy along the DNA chain,

$$E_n = \frac{1}{2} \left(\frac{du_n}{dt} \right)^2 + W(u_n, u_{n+1}) + W(u_{n-1}, u_n) + V(u_n). \quad (28)$$

For the parameters $\delta = 0.5$, $p = 0.04$, $k = 0.3$, and $m = 0.95$, we plot in figure 3 the shape of the soliton solution as well as the energy of the system. As the elasticity coefficient K_1 increases, the amplitude of the pulse also increases (See Figures 3(a) for $K_1 = 0.1$ and figures 3(c) for $K_1 = 0.4$, respectively). The elastic coupling constant \mathbf{K}_1 also influences the energy barrier of the DNA chain as plotted in Fig. 3(b) for $K_1 = 0.1$ and in Fig. 3(d) for $K_1 = 0.4$. Figures 3(b) and 3(d) show that energy is localized in our system. Many studies have pointed out that the

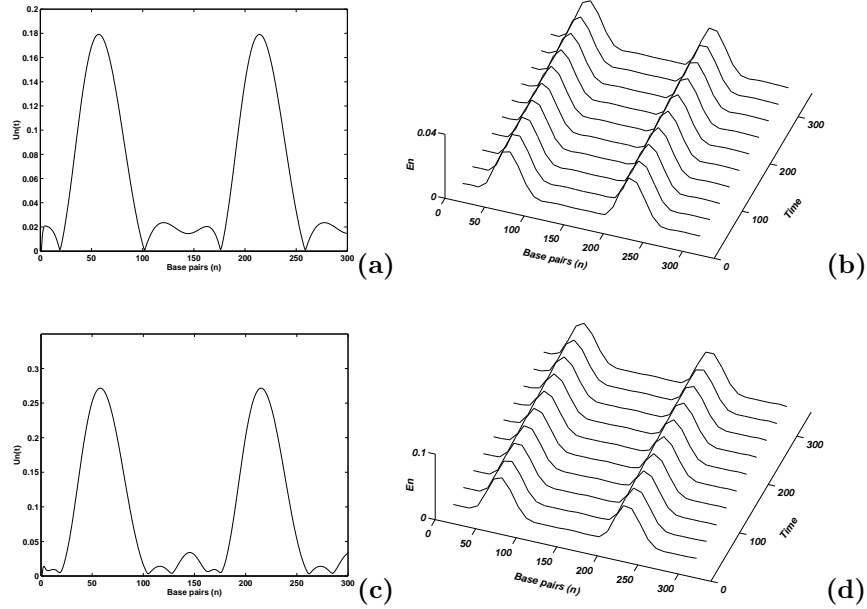


FIGURE 3. Pulse pattern generated during the propagation and time evolution of the density energy for the parameters $\delta = 0.5$, $p = 0.04$, $k = 0.3$, $m = 0.95$ (a) Profile of the exact solution for $K_1 = 0.1$ (b) The density energy for $K_1 = 0.1$ (c) Profile of the exact solution for $K_1 = 0.4$ (d) The density energy for $K_1 = 0.4$

energy initially concentrated in one mode will finally flow to all available modes in the Fourier space. Specifically, it has been demonstrated in computer simulation that modulational instability can be used to generate intrinsic localized vibrational modes in nonlinear lattices via optimal control scheme [45, 46]. Modulational instability is usually observed in the same parameters region where bright and dark solitons are observed. The previous results also confirm that localized excitation can be generated in the DNA chain, as the energy density is distributed in real space.

Next, for different value of the viscosity coefficient, we have plotted in figure 4 the energy density of the chain. figures 4 (a) and (b) represent the propagation of the pulse solution as well as the density energy of the system for the parameters $K_1 = 0.001$, $p = 0.02$, $k = 0.3$, $m = 0.95$ and $\delta = 0.05$. figures 4 (c) and (d) show the behavior of the system for $\delta = 0.09$. From figures 4 (b) and 4 (d), we see that the density energy is only localized in one mode. As the viscosity coefficient increases, we note that the amplitude of the exact solution decreases as can be viewed in figures 4(a) and 4(d).

4. Conclusion. Our results, using the nonlinear DNA chain as an example, point out the crucial role of discreteness on the DNA chain. First, the analytical approach as shown that the propagation of nonlinear waves in the DNA chain is reduced to the discrete complex Ginzburg-Landau equation. Using the elliptic function approach, we have derived the exact solution of this system made of bubble solitons. From

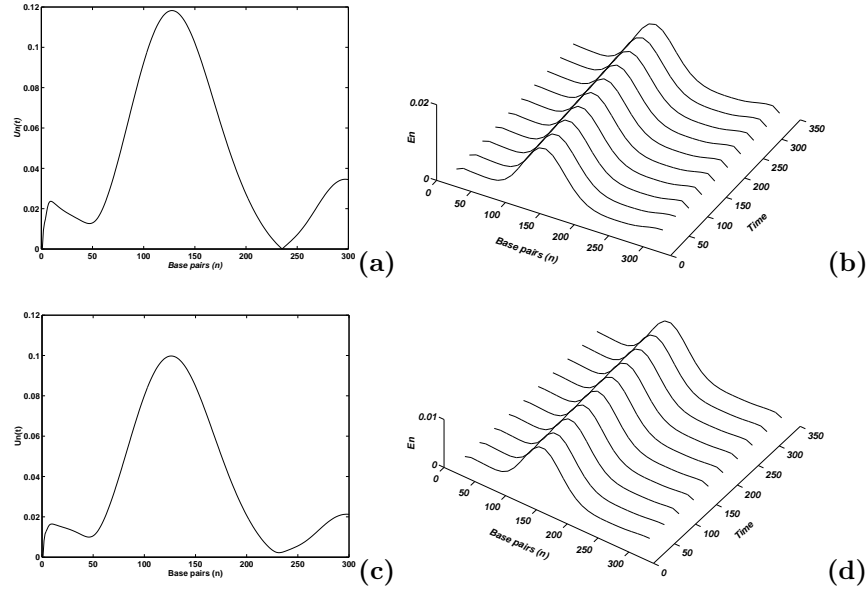


FIGURE 4. Pulse pattern generated during the propagation and time evolution of the density energy for the parameters $K_1 = 0.001$, $p = 0.02$, $k = 0.3$, $m = 0.95$ (a) Profile of the exact solution for $\delta = 0.05$ (b) density energy for $\delta = 0.05$ (c) Profile of the exact solution $\delta = 0.09$ (d) density energy for $\delta = 0.09$

numerical simulations, we have seen that the initial bubble soliton is transformed into pulse a soliton. The mechanism of discreteness-induced energy localization that appears in a large variety of physical systems has also been shown in the nonlinear model of DNA.

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