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MODULATIONAL INSTABILITY AND PATTERN FORMATION  
IN THE MODEL OF DNA DYNAMICS  

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Abstract

We report on the analytical and numerical investigation of modulational instability in discrete nonlinear chains, taking the Peyrard-Bishop model of DNA dynamics as an example. It is shown that the original difference differential equation for the DNA dynamics can be reduced to the discrete complex Ginzburg-Landau equation. We derive the modulational instability criterion in this case. Numerical simulations show the validity of the analytical approach with the generation of wave packets provided that the wave number falls in the instability domain. We also show that, modulational instability leads to spontaneous localization of energy in DNA molecule.
I. Introduction

The interest in the dynamics of discrete systems comes from the diversity of their numerous applications in physical and biological sciences. For example, the dynamics of desoxyribonucleic acid (DNA) is one of the most fascinating problems of modern biophysics because it is at the basis of life. Its double helical structure undergoes a very complex dynamics and knowledge of that dynamics provides insights into various related biological phenomena such as transcription, translation, mutation and energy-localization. The key problem in DNA biophysics is how to relate functional properties of DNA with its structural and physical dynamical characteristics. The possibility that nonlinear effects might focus the vibration energy of DNA into localized soliton-like excitation was first contemplated by Englander et al. [1]. Indeed, Englander et al. [1] were the first to suggest a theory of soliton excitations as an explanation of the open states of DNA. Later, Yomosa [2] proposed another soliton theory using a plane base-rotator model that was further refined by Takeno and Homma [3], who introduced a model allowing some discreteness effects to be taken into account, and by Zhang [4], who improved the model for base coupling.

As a mechanism leading to the formation of solitons, one can name the modulational instability (MI). MI is the result of the interplay between the nonlinear and dispersive effects. This phenomenon appears in continuum as well as in discrete models. It has been recently suggested that it could be responsible for energy-localization mechanisms leading to the formation of large-amplitude nonlinear excitations in hydrogen-bonded crystals or DNA molecules [5,6]. In nonlinear lattices, discreteness effects can give rise to intrinsic localized vibrational states [7-9] that would not exist in a continuum system and may be considered as a discrete version of soliton excitations in nonintegrable models [10,11]. Recently, Efremidis and Christodoulides have shown that discrete solitons are possible in complex Ginzburg-Landau lattices [12].

Although many studies have been undertaken in various systems showing that the dynamics of nonlinear excitations are governed by the complex Ginzburg-Landau (CGL), to our knowledge, no work using the DNA molecule has been reported which shows that the nonlinear excitations are modeled by the discrete complex Ginzburg-Landau (DCGL) equation.

In the this work, we present theoretical and numerical results concerning the properties of nonlinear modulated waves on the Peyrard-Bishop (PB) model of DNA dynamics [5,13,14]. We discuss MI in lattice models, taking the PB models as an example. We derive a discrete complex Ginzburg-Landau equation for the amplitude of the carrier wave and analyze the stability condition of the carrier wave in the lattice. In particular, we show that, above a given threshold in the wave amplitude, a carrier wave at small wave number is unstable to all possible modulation. The validity of this analysis is then checked by numerical simulations that reveal some additional features of MI as energy localization.
II. The model

The PB model has been used to model the processes of transcription and replication, particularly the action and the motion of the transcription bubble. This model only considers short-range interactions due to the stacking of base pairs. The strands are coupled to one another through hydrogen bonds, which are supposed to be responsible for the lateral displacements of nucleotides. The lattice then has the following Hamiltonian:

\[ H = \sum_n \frac{1}{2} my_n^2 + V(y_n) + W(y_n, y_{n-1}) \]  

where \( y_n \) is a scalar variable introduced for the \( n \)th base pair. It measures the stretching of the hydrogen bonds that connect the bases. The stacking interactions of the bases along the molecules are given by \( W(y_n, y_{n+1}) \), which can be simply taken as harmonic \( W(y_n, y_{n-1}) = \frac{1}{2} k (y_n - y_{n-1})^2 \). The quantity \( k \) is the coupling stacking constant. The on-site potential \( V(y_n) \) describes the interactions between two bases in a pair, including several contributions such as the hydrogen bonds linking the two bases and the repulsion of the charged phosphate groups belonging to the backbone. We use for \( V(y_n) \) a Morse potential: \( V(y_n) = D(e^{-\alpha y_n} - 1)^2 \), where \( D \) represents the dissociation energy and \( \alpha \) the parameter homogeneous to the inverse of a length, which sets the spatial scale of the potential.

In order to deal with a more realistic description of a DNA dynamics, which takes into account the influence of the medium surrounding the DNA molecule, we consider the viscosity. The importance of hydrating water is well-known for the biochemical activities of proteins and especially in DNA. We must take into consideration the fact that the solvating water does act as a viscous medium that damps out DNA dynamics then favoring energy expenditure. Thus, we start from probably more realistic and favorable approach that viscous force has features of small perturbation. The viscous forces exerted on the bases within a pair \( n \) are \( -\alpha \dot{x}_n \). This leads to the effective damping force acting on the out of phase base pair motion as follows: \( F_v = -\alpha \dot{x}_n \). Now, starting from the perturbed equation of motion

\[ m \ddot{x}_n + \alpha \dot{x}_n - k(x_{n+1} + x_{n-1} - 2x_n) + 2aD(e^{-ax_n} - e^{-ax_{n-1}}) = 0 \]  

and performing the expansion of the above equation, one finds

\[ u_n = -\gamma \dot{u}_n + s(u_{n+1} + u_{n-1} - 2u_n) - u_n + \frac{3}{2} u_n^2 - \frac{7}{6} u_n^3 \]  

where

\[ u_n = ax_n , \quad \tau = \omega_0 t , \quad S = \Omega / \omega_0 , \quad \Omega = (\kappa / m)^{1/2} , \quad \gamma = \alpha / m \omega_0 \]  

(4)
are all dimensionless parameters. In order to study dynamical processes in this model, we look for a solution in the form

\[ u_n = \phi_n \exp(-it) + \phi_n^* \exp(it) \]  

(5)

Inserting Eq. (5) in Eq. (3), the coefficients of \( \exp(-it) \) lead to the one-dimensional discrete complex Ginzburg-Landau (DCGL) equation

\[ i\phi_n + \frac{s(2 - i\gamma)}{4 + \gamma^2}(\phi_{n+1} + \phi_{n-1} - 2\phi_n) - \frac{7(2 - i\gamma)}{2(4 + \gamma^2)}|\phi_n|^2 \phi_n = i\frac{\gamma(-2 + i\gamma)}{4 + \gamma^2} \phi_n \]  

(6)

The CGL equation is known to play a ubiquitous role in science. This equation is encountered in several diverse branches of physics and describes modulated amplitude waves [15], spatio-temporal dynamics and spontaneous development of coherent structures in a variety of nonlinear dissipative systems [16,17]. Example include pulse generation by passively model-locked solitons laser [18], signal transmission in all optical communication lines [19], traveling waves in binary fluid mixtures [20], and also pattern formation in many other physical systems [21]. In addition to the well-studied continuous CGL equation, DCGL models have also been considered in the literature [12,22,23]. These DGL lattices are quite often used to describe a number of physical systems such as Taylor and frustrated vortices in hydrodynamics [22] and semiconductor laser in optics [12,23]. Recently, the CGL equation has been used in one space dimension as a test case for space-extended control/synchronization schemes [24,25]. The authors of [24,25] focused on different chaotic regimes. Equation (6) shows that the DCGL equation may also be derived in DNA dynamics.

III. Linear stability analysis

We begin our analysis by considering the linear dispersion properties of the DCGL equation. To do so, we write \( \phi_n = \phi_0 \exp[i(qn - \omega t)] \), where the wave number \( q \), the angular frequency \( \omega \) and the amplitude \( \phi_0 \) satisfy the dispersion relation:

\[ \omega = \frac{1}{4 + \gamma^2} \left[ 8S \sin^2 \left( \frac{q}{2} \right) + 7|\phi_0|^2 - \gamma^2 \right], \]  

(7)

and

\[ |\phi_0|^2 = \frac{2}{7} \left[ 2 + 4S \sin^2 \left( \frac{q}{2} \right) \right]. \]  

(8)
According to the concept of MI, the perturbation is mainly formed from two satellite waves at 
$q \pm Q$ plus additional waves generated via wave-mixing processes. In the linear stability analysis, we neglect combination waves and seek trial solutions of the following form:

$$\phi_n = \phi_0 [1 + B_n(t)] \exp[i(qn - \omega t)]$$  \hspace{1cm} (9)

where the perturbation amplitude $B_n(t)$ is assumed to be small in comparison with the carrier wave amplitude $\phi_0$. The perturbation amplitude has the following form:

$$B_n = B_1 \exp[i(Qn + \Omega t)] + B_2^* \exp[-i(Qn + \Omega^* t)]$$  \hspace{1cm} (10)

where the asterisk denotes complex conjugation, $Q$ and $\Omega$ represent, respectively the wave number and the angular frequency of the perturbation amplitude, $B_1$ and $B_2$ are complex constant amplitudes. Inserting Eq. (10) into the DCGL equation and using the standard procedure of linear stability analysis, i.e., linearization around the unperturbed plane wave, we obtain the linear homogeneous system for $B_1$ and $B_2$. The condition for the existence of non trivial solutions of this linear homogeneous system is given by a second order equation for the frequency $\Omega$, that is

$$\Omega^2 + i(a_{11} + a_{22})\Omega + a_{11}a_{22} - a_{12}a_{21} = 0$$  \hspace{1cm} (11)

The discriminant of Eq.(11) is $\Delta = X + iY$, where $X$ and $Y$ are defined in appendix. The solutions of Eq. (11) are given by

$$\Omega_1 = (f + h_1) + i(g - h_2)$$ \hspace{1cm} (12.a)
$$\Omega_2 = (f - h_1) + i(g + h_2)$$ \hspace{1cm} (12.b)

where $f$ and $g$ are defined respectively, by $f = -c_{qr}(\cos(Q) - 1)\cos(q) + c_{ir} |\phi_0|^2$, $g = -c_{qr} \sin(Q) \sin(q)$. The roots of $\Delta$ are defined by: $h_1 = \sqrt{\frac{1}{2} \left( X + \sqrt{X^2 + Y^2} \right)}$ and $h_2 = \sqrt{\frac{1}{2} \left( -X + \sqrt{X^2 + Y^2} \right)}$. Equation (12.a) and (12.b) are established for the case $Y < 0$. In the other case ($Y > 0$), the roots of Eq. (11) lead to solutions which have the same asymptotic behavior as those of Eq. (12). Because $\Omega_1$ and $\Omega_2$ are complex, it is not possible to precise their sign. Nevertheless, their imaginary part contributes to add effects of perturbations in the system. Introduction of Eq. (12.a) into Eq. (10) helps in understanding the behavior of Eq.
(10). Since \( h_2 \) is always positive, \( g - h_2 < g + h_2 \) holds and then this behavior depends on the sign of the quantity \( g - h_2 \), which corresponds to the imaginary part of \( \Omega_i \). Indeed, this operation gives from Eq. (10)

\[
B_1 e^{im\theta} = B_1 e^{i(f + h_1)t} \times e^{-(g - h_2)t}
\]  

(13)

The asymptotic behavior of Eq. (10) is related to the sign of the constant \( g - h_2 \). If \( g < 0 \), then \( h_2 - g \) is always positive and the solution (10) increases exponentially when \( t \) tends to infinity. The system remains unstable under modulation. If \( g > 0 \), then the asymptotic behavior of Eq. (10) will depend on the sign of \( h_2 - g \). We shall distinguish two cases:

(i) When \( h_2 - g > 0 \) i.e., \( g - h_2 < 0 \) i.e., \( \text{Im}(\Omega_i) < 0 \), the solution (10) diverges without limit as \( t \) increases and the corresponding solution is said to be modulationally unstable. In this case, the explicit form of the difference \( g - h_2 \) is:

\[
g - h_2 = g - \left\{ \frac{1}{2} \left[ -4c_0^2 \sin^2(Q) \sin^2(q) + 2 \phi_0^2 \left( c_{0r}c_{1r} + c_{0l}c_{1l} \right) \sin(Q) \sin(q) \right] \cdot \right. \left. \left( \cos(Q) - 1 \right)^2 \cos^2(q) + r_0 \right\}^{1/2}
\]  

(14)

where \( r_0 \) which is defined in appendix, is a positive constant. After removing the positive terms in Eq. (14), the following inequality is obtained:

\[
g - h_2 \leq -\frac{1}{2} \left[ 4c_0^2 \sin^2(Q) \sin^2(q) + 2 \phi_0^2 \left( c_{0r}c_{1r} + c_{0l}c_{1l} \right) \sin(Q) \sin(q) - \left( c_{0r}^2 + c_{0l}^2 \right) \left( \cos(Q) - 1 \right)^2 \cos^2(q) \right]^{1/2}
\]  

(15)

Here, we remark that relation: \( \text{Im}(\Omega_i) < 0 \) is verified as soon as we have

\[
g - \frac{1}{2} \left[ 4c_0^2 \sin^2(Q) \sin^2(q) + 2 \phi_0^2 \left( c_{0r}c_{1r} + c_{0l}c_{1l} \right) \sin(Q) \sin(q) - \left( c_{0r}^2 + c_{0l}^2 \right) \left( \cos(Q) - 1 \right)^2 \cos^2(q) \right]^{1/2} < 0
\]  

(16)

and since \( g \) is positive, the inequality (16) leads to

\[
2 \left| \phi_0 \right|^2 \left( c_{0r}c_{1r} + c_{0l}c_{1l} \right) \sin(Q) \sin(q) > 0.
\]  

(17)

Relation (17) represents the MI criterion for plane waves in the DNA model which is modeled by the DCGL equation. The criterion (17) depends on the elasticity parameter \( S \) and the viscosity parameter \( \gamma \), of the DNA model. In so doing, when \( \gamma \) and \( S \), respectively take the
values 0.005 and 0.008, we plot on Fig. 1, regions of MI (black regions) on the (Q,q) plane. Analytical result shows us that, MI is only possible for wave number taken in one of the three black regions of Fig 1.

(ii) On the other hand, we deduce from the above calculations, that the condition \( g - \frac{h_2}{2} > 0 \) (i.e., \( \text{Im}(\Omega) > 0 \)) leads to \( 2|\phi_0|^2(c_{n,0}c_{-n,0} + c_{n,0}c_{-n,0})\sin(Q)\sin(q) < 0 \). In this case, the solution (10) introduced in the system remains bounded as \( t \to +\infty \). Then, (10) is said to be stable under modulation.

IV Formation of soliton trains in model of DNA dynamics

According to analytical results discussed in the previous section, the stability of a plane wave with wave-number q modulated by a small amplitude wave of wave number Q is determined by the instability criterion (17). When this relation is fulfilled, we expect that the system exhibits an instability that leads to the self-induced modulation of an input plane wave with the subsequent generation of localized pulses [26]. Well known as MI, this phenomenon is responsible for various physical interesting phenomena such as the formation of envelope solitons in electrical transmission lines [27], nonlinear optical fibres [28], dielectric media [29], cavitons in plasma as well as the filamentation of laser beams [30] and the breakup of monochromatic waves. Thus, it becomes of interest to examine the nature of different wave pattern formation that may arise by the MI process in the PB model of DNA during the evolution of the wave in the system. However, the linear stability analysis has been obtained through the DCGL equation, which is only an approximate description of the equation of motion (3). 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 (3) 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 0.001. Most of the simulations are performed with a molecule of 300 base pairs with periodic boundary conditions; this is why the wave-number q and Q necessarily have the forms \( q = \frac{2\pi p}{N} \) and \( Q = \frac{2\pi P}{N} \), where p and P are integers lower than \( \frac{N}{2} \).

We chose as initial condition a linear wave with a slightly modulated amplitude

\[ u_n(t = 0) = \phi_0(1 + 0.01\cos(Qn))\cos(qn) \tag{18} \]

where the initial amplitude \( \phi_0 \) is derived from the dispersive relation (8). As a first example, let us consider the case \( q = 1.01\pi, Q = 0.98\pi, \gamma = 0.005 \) and \( S=0.0025 \). According to the instability diagram plotted in Fig. 1, the corresponding point lies in an instability region. We observe in Fig. 2(a) that the initial condition tends to disintegrate during the propagation, leading to break-up of wave into pulse train. Each element of the train has the shape of solitons like object. MI typically occurs in the same parameters region where another
universal phenomenon, soliton occurrence, is observed. Solitons are stationary localized wave packets that share many features with real particle. For example, their total energy and momentum are conserved even when they interact with one another [31]. Figure 2(a) depicts the fact that energy is localized in the system. Further, we increase the value of the coefficient of elasticity, which is now equal to 1.0. We realize that the waves are modulated in amplitude as it is shown in Fig. 2(c). The amplitude appears as an extended short wave moving with breather properties. Thus, the wave pattern displayed here is that of an extended wave that propagates with a breathing motion. Each element of the train has the shape of discrete breathers. Discrete breathers are periodic localized oscillations that arise in discrete nonlinear systems. These localized oscillations can be static, but, under certain conditions can move along the system. The existence of discrete breather in the PB model of DNA has been suggested by Dauxois et al. [32]. Afterwards, numerical simulations performed by Dauxois et al. [13,14,33] suggested that localized oscillations can be precursors of bubbles that appear in thermal denaturation of DNA. Even in this case, we also see that energy is localized through the system as depicted in Fig. 2(d). Let us now consider the case: \( q = 1.34\pi \), \( Q = 0.55\pi \), \( S = 0.0025 \), and \( \gamma = 0.005 \). It happens that the wave pattern displayed by wave motion exhibits an oscillating and breathing behaviour (see Fig. 3(a)). Figure 2(b) shows that energy is localized for these parameters. As a last example, we increase from the previous parameters, the value of the viscosity parameter which is now equal to \( \gamma = 0.9 \). We observe in Fig. 3(c) that, the amplitude of wave pattern displayed by wave motion is modulated into a train of double pulses. A soliton form when the localized wave packet induces a potential (via the nonlinearity) and “captures” itself in it, thus becoming a bound state in its own induced potential. The relation between MI and solitons is best manifested in the fact that the filaments (or the pulse train) that emerge from the MI process are actually trains of almost ideal solitons. Therefore, MI can be considered to be precursor to soliton formation. Hence, the energy initially concentrated in one mode finally flows to available modes in the Fourier space. However, the Fourier space alone does not tell us the complete process of energy redistribution. It is generally believed that the physical system will finally reach equipartition of energy in a sufficiently long time since the entropy should grow during the system’s time evolution. Otherwise, such a physical system should approach a state where the energy is evenly distributed not only among modes in Fourier space, but also on lattices sites in real space (Figs. 2(b), 2(d), 3(b), and 3(d)). This MI that induced energy localization has been proposed to be the mechanism responsible for the formation of intrinsic localization by many authors [33-35].

V. Conclusion

This paper presents the study of modulated wave trains in the PB model of DNA dynamics. We have established that the evolution of nonlinear excitations is governed by the
discrete complex Ginzburg-Landau equation. Making use of this equation, the MI criterion has been reviewed theoretically by performing the approach introduced by Stuart and Di Prima. Thus, we have shown that if \( 2 |\varphi_0|^2 (c_{o,r}c_{i,r} + c_{o,i}c_{i,i}) \sin(Q) \sin(q) < 0 \), a plane wave in the system is stable under the modulation and for \( 2 |\varphi_0|^2 (c_{o,r}c_{i,r} + c_{o,i}c_{i,i}) \sin(Q) \sin(q) > 0 \), it will be unstable under the modulation. We have observed from numerical simulations that, MI causes the propagation of wave trains which have the shape of discrete breather. A remarkably result of this study is that MI also leads to the creation of energy-localization.

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Appendix A. Linear stability analysis

\[ \begin{align*}
\dot{B}_n &= -s(y + 2i) \left( B_{n+1} + B_{n-1} - 2B_n \right) \cos(q) + \frac{S(2 - i\gamma)}{4 + \gamma^2} \left( B_{n+1} - B_{n-1} \right) \sin(q) + \frac{7(y + 2i)}{2(4 + \gamma^2)} \phi_0^2 \left( B_n + B_n^* \right) = 0 \\
\begin{pmatrix} a_{11} - i\Omega & a_{12} \\ a_{21} & a_{22} - i\Omega \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\end{align*} \]  
(A.1)

where

\[ a_{11} = (c_{i\gamma} + i\gamma) \phi_0^2 - (c_0 + i\gamma) \left[ \left( \cos(Q) - 1 \right) \cos(q) + \sin(Q) \sin(q) \right] \]  
(A.3)

\[ a_{12} = (c_{i\gamma} + i\gamma) \phi_0^2 \]  
(A.4)

\[ a_{21} = (c_{i\gamma} - i\gamma) \phi_0^2 \]  
(A.5)

\[ a_{22} = (c_{i\gamma} - i\gamma) \phi_0^2 - (c_0 - i\gamma) \left[ \left( \cos(Q) - 1 \right) \cos(q) - \sin(Q) \sin(q) \right] \]  
(A.6)

with

\[ c_{0\gamma} = \frac{2S\gamma}{4 + \gamma^2}, \quad c_{i\gamma} = -\frac{2S}{8 + 2\gamma^2}, \quad c_{i\gamma} = \frac{7\gamma}{4 + \gamma^2}, \quad c_{\gamma} = \frac{7}{4 + \gamma^2} \]  
(A.7)

\[ X = -4c_{i\gamma}^2 \sin^2(Q) \sin^2(q) + 4 \left[ c_{0\gamma} \phi_0^2 - c_0 \left( \cos(Q) - 1 \right) \cos(q) \right] ^2 - 2 \phi_0^2 \left( c_0 c_{i\gamma} + c_0 c_{\gamma} \right) \sin(Q) \sin(q) \]  
\[ - \left( c_{0\gamma} + c_0 \right) \left[ \left( \cos(Q) - 1 \right) \cos(q) - \sin^2(Q) \sin^2(q) \right] \]  
(A.8)

\[ Y = 8c_{i\gamma} \left[ c_{i\gamma} \phi_0^2 - c_{0\gamma} \left( \cos(Q) - 1 \right) \cos(q) \right] \sin(Q) \sin(q) - 2 \phi_0^2 \left( c_0 c_{i\gamma} - c_0 c_{\gamma} \right) \left( \cos(Q) - 1 \right) \cos(q) \]  
(A.9)

\[ f = -c_{0\gamma} \left( \cos(Q) - 1 \right) \cos(q) + c_{i\gamma} \phi_0^2 \]  
(A.10)

\[ g = -c_{0\gamma} \sin(Q) \sin(q) \]  
(A.11)

Considering the roots of \( \Delta \), that is, \( h_1 \) and \( h_2 \), solutions (22) can be written as

\[ \Omega_1 = (f + h_1) - i(g - h_2) \]  
(A.12)

\[ \Omega_2 = (f - h_1) + i(g + h_2) \]  
(A.13)

in which
\[ h_1 = \frac{1}{\sqrt{2}}(X + \sqrt{X^2 + Y^2}) \quad \text{and} \quad h_2 = \frac{1}{\sqrt{2}}(-X + \sqrt{X^2 + Y^2}) \] (A.14)

Expressions (A.12) and (A.13) are established for the case \( Y < 0 \). In the case \( Y > 0 \), the roots Eq. (11) take the forms:

\[ \Omega_1' = (f - h_1) + i(g - h_2) \] (A.15)
\[ \Omega_2' = (f + h_1) + i(g + h_2) \] (A.16)

and lead to the same asymptotic behavior as those obtained from (A.12) and (A.13).

\[ g - h_2 = g - \left\{ \frac{1}{2} - 4c_{10}^2 \sin^2(Q) \sin^2(q) + 4\left[ c_{1r} \left| h_0 \right|^2 - c_{10} \cos(Q) - c_{10} \cos(q) \right]^2 - 2 \left| h_0 \right|^2 \right\} \left( c_{10} c_{1r} + c_{10} c_{1r} \right) \sin(Q) \sin(q) \]
\[ - \left( c_{10}^2 + c_{1r}^2 \right) \cos(Q) - c_{10}^2 \sin^2(Q) \sin^2(q) \right) + \sqrt{X^2 + Y^2} \}^{1/2} \] (A.17)

\[ r_0 = (c_{10}^2 + c_{1r}^2) \sin^2(Q) \sin^2(q) + 4 \left[ c_{1r} \left| h_0 \right|^2 - c_{10} \cos(Q) - c_{10} \cos(q) \right]^2 + \sqrt{X^2 + Y^2} \] (A.18)

Appendix B. The energy of each particle

For the numerical calculation of the energy of each particle [see Figs.2(b) and 2(d) and Figs. 3(b) and 3(d)], we have derived the energy from

\[ H_n = \frac{1}{2} u_n^2 + \frac{1}{2} \left[ (u_n - u_{n-1})^2 + (u_{n+1} - u_n)^2 \right] + V(u_n) \] (B.1)

where \( V(u_n) \) is the dimensionless Morse potential
References

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Figure 1: Region of modulational instability/ stability on the (Q,q) plane for $\gamma=0.005$ and $S=0.0025$.

Figure 2: Propagation of wave train which has the shape of solitons like object in DNA molecule: (a) $\gamma=0.005$, $q=1.01\pi$, $Q=0.55\pi$, $t=200$, $S=0.0025$. (b) Localization of energy induced by MI. (c) $\gamma=0.005$, $q=1.01\pi$, $Q=0.55\pi$, $t=200$, $S=1$. (d) Localization of energy induced by MI.
Figure 3: Propagation wave train which has the shape of the discrete breather in DNA molecule: (a) $S=0.0025$, $q=1.34\pi$, $Q=0.55\pi$, $t=350$, $\gamma=0.005$. (b) Localization of energy induced by MI. (c) $S=0.0025$, $q=1.34\pi$, $Q=0.55\pi$, $t=350$, $\gamma=0.9$ (d) Localization of energy induced by MI.