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Nonlinear mechanics of DNA doule strand: existence of the compact-envelope bright solitary wave

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Abstract— **We study the nonlinear dynamics of a homogeneous DNA chain which is based on site-dependent finite stacking and pairing enthalpies. We introduce an extended nonlinear Schrödinger equation describing the dynamics of modulated wave in DNA model. We obtain envelope bright solitary waves with compact support as a solution. Analytical criteria of existence of this solution are derived. The stability of bright compactons is confirmed by numerical simulations of the exact equations of the lattice. The impact of the finite stacking energy is investigated and we show that some of these compact bright solitary waves are robust, while others decompose very quickly depending on the finite stacking parameters.**

I. INTRODUCTION

The dynamics of DNA has been extensively studied during the last decade. Particularly, the nonlinear field of sciences pays special attention to the process that takes place at the base pair scale [1]. The local opening of the DNA double helix at the transcription start site is a crucial step for the genetic code. This opening is driven by proteins but the intrinsic fluctuations of DNA itself probably play an important role. The dynamical properties of these bubbles and their relations to biological functions have therefore been the subject of many experimental and theoretical studies [2]. Note that the stacking interaction in the Dauxois-Peyrard-Bishop (DPB) [3] model is not harmonic, but it still differs fundamentally from that of statistical models because it does not make reference to any characteristic energy [4]. Since its introduction, this model was used to unravel several aspects of melting. Joyeux and Buyukdagli (JB) [5] proposed a few years ago a dynamical model for DNA, which is closer to the statistical ones than the DPB model, in the sense that it is based on site-specific stacking enthalpies and showed that the finiteness of the stacking interaction is, in itself, sufficient to ensure a sharp melting transition.

In the present work, we show that this finite stacking energy interaction model supports envelope bright solitary waves with compact support. To this end, the organization of the paper is as follows. In sec. II, we present the model and its equations. In sec. III, by means of the semi-discrete approximation, we derive the extended nonlinear Schrödinger equation governing modulated waves in the lattice. Exact analytical solution with compact support is obtained for this extended nonlinear Schrödinger equation in sec. IV. Numerical investigations are considered in order to verify the validity and the stability of analytical predictions and we draw our conclusions in sec. V.

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II. MODEL AND EQUATION OF MOTION

The general form of the model we are considering in this paper is

$$H=\sum_n \frac{1}{2m}P_n^2+W\left(y_n,y_{n-1}\right)+D\left(e^{(-\alpha y_n)}-1\right)^2, \quad (1)$$

where we chooce the (JB) model, i.e.

$$W\left(y_n,y_{n-1}\right)=\frac{\triangle H_n}{C}\left(1-e^{-b(y_n-y_{n-1})^2}\right)+K_b\left(y_n-y_{n-1}\right)^2, \quad (2)$$

$\Delta H_n/C$ is a Gaussian hole of depth and the backbone stiffness is taken as a harmonic potential of constant K_b. In this set of equations, m is the reduced mass of the bases, while y_n is the displacement that stretches the hydrogen bonds. The last term in Eq.(1) is the on-site Morse potential, where D denotes the dissociation energy while the parameter α, homogeneous to the inverse of a length, sets the special scale of the potential. This on-site Morse potential appears as a "substrate" potential in the model, which comes directly from the structure of DNA. In this work, numerical values of our parameters are those of Refs. [5], [6], that is, $m=300$ a.m.u, $D=0.04eV$, $\alpha=4.45\mathring{A}^{-1}$, $K_b=10^{-5}$ eV $\mathring{A}^{-2}$. Including Eq.(2) in (1) yields the corresponding equation of motion of the nth base pair.

$$\begin{aligned}\frac{d^2y_n}{dt^2}=&\frac{2K_b}{m}\left(y_{n+1}+y_{n-1}-2y_n\right)+\\&\frac{2\alpha D}{m}e^{(-\alpha y_n)}\left(e^{-\alpha y_n}-1\right)+\\&\left[\left(y_{n+1}-y_n\right)e^{-b(y_{n+1}-y_n)^2}-\left(y_n-y_{n-1}\right)e^{-b(y_n-y_{n-1})^2}\right]\times\\&\frac{2b\triangle H_n}{mC}.\end{aligned} \quad (3)$$

It is convenient for the analytical and numerical calculations to transform these equations into a dimensionless form [7] by defining the dimensionless variables

$$Y_n=\alpha y_n, \qquad \tau=(\sqrt{D\alpha^2/m})t, \quad (4)$$

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which transforms Eq.(4) in:

$$\frac{d^2Y_n}{d\tau^2} = C_l\left(Y_{n+1}+Y_{n-1}-2Y_n\right) + C_{nl}\left[\left(Y_{n+1}-Y_n\right)^3-\left(Y_n-Y_{n-1}\right)^3\right] - \omega_g^2\left(Y_n-\frac{3}{2}Y_n^2+\frac{7}{6}Y_n^3\right), \quad (5)$$

where $\omega_g^2=2$, $C_l=\frac{2}{D\alpha^2}(K_b+\frac{b\triangle H_n}{C})$ and $C_{nl}=-\frac{2}{D\alpha^4}\frac{b^2\triangle H_n}{C}$. Note that the control parameters b and $\Delta H_n/C$ allow to fix independently C_l and C_{nl} For finite amplitude of wave, nonlinearities of the system give rise to the generation of higher harmonics. However, we are using the so-called "rotating-wave" approximation which consists essentially in neglecting harmonics by substituting in the equation of motion, the solution [8], [9]

$$Y_n(\tau) = B(X,T)e^{i\theta_n}+B^*(X,T)e^{-i\theta_n}, \quad (6)$$

where the asterisk denotes complex conjugation. The above expression of $Y_n(\tau)$ includes the fast local oscillation through the dependence of the phase $\theta_n = kn-\omega\tau$, and then preserves the discrete character of the system [10], while the dependence of the envelope part is described by the slow amplitude variation of the function $B(X,T)$ with respect to the slow variables $T=\varepsilon^2\tau$ and $X=\varepsilon(n-v_g\tau)$, ε being a small dimensionless parameter. Here the lattice spacing has been taken as equal to unity. The parameter $v_g=\frac{d\omega}{dk}$ is the group velocity associated to the wave packet. The linear oscillation frequency of the base pairs, and wave number, are related by the dispersion equation

$$\omega^2 = \omega_g^2+4C_l\sin^2(k/2). \quad (7)$$

As shown by Eq.(7), the linear equation has a gap ω_g and is limited by the cutoff frequency $\omega_m=\sqrt{\omega_g^2+4C_l}$ due to the discreteness whereas $v_g=\frac{C_l\sin(k)}{\omega}$. Instead of applying the standard reductive perturbation method in the semi-discrete limit to Eq.(6), which forbids to appreciate the role of the nonlinear dispersion in Eq.(6), we substitute Eq.(6) into Eq.(6), and neglect all terms in ε^5 or more [8], [11].

Assuming that $B(X,T)$ and all its derivative converge to zero sufficiently rapidly as $X\longrightarrow\pm\infty$, The Hamiltonian $H=\int\hat{H}dX$ corresponds to invariance under translations in X, where the Hamiltonian density is

$$\hat{H} = \hat{H}_1+\hat{H}_2+\hat{H}_2^*, \quad (8)$$

with

$$\hat{H}_1 = -P|B_X|^2+\frac{Q}{2}|B|^4+\frac{3l_7C_{nl}}{2\omega}|B_X|^4-l_5\left[|B|^2|B_X|^2\right], \quad (9)$$

$$\hat{H}_2 = \frac{C_{nl}}{\omega}\{\frac{il_1}{2}\left[|B|^2BB_X^*\right]+\frac{il_2}{4}\left[B^*|B_X|^2B_X\right] + \frac{il_3}{2}\left[|B_X|^2B_X^*\right]+\frac{3l_4}{4}\left[B^2B_X^{*2}\right]+2l_6\left[B^{*2}B_X^2\right]\}. \quad (10)$$

III. Bright solitons with compact support solution

The existence of compact wave has been rigorously proven by Saccomandi and Sgura [12] for Hamiltonian systems, provided that an anharmonicity condition is fulfilled. To proceed with the integration of the extended nonlinear Schrödinger equation, we first separate the complex envelope function and the phase shift [8] $\xi(X,T)$ according to

$$B(X,T) = \phi(X,T)\exp\left[-i\xi(X,T)\right]. \quad (11)$$

where ϕ and ξ are real functions of X and T. From the analysis of the coefficients l_k with $k=1,2,3,..7$, it appears that $8l_6=2l_5-l_4$. Let us look for travelling wave solutions in the form $\phi(X,T)=\phi(z)$ with $z=(X-v_eT)$ and linear phase shift $\xi(X,T)=\gamma\left(X-v_\phi T\right)$, where v_e and v_ϕ are the envelope and phase velocities, respectively. We can consider the following equations

$$\phi_T = -v_e\phi_z \;\; \phi_X=\phi_z, \quad (12)$$

By using the drop boundary conditions

$$\phi\to 0,\;\; \phi_z\to 0 \;\; at \;\; z\to\pm\infty, \quad (13)$$

we obtain

$$v_e = 2P\gamma. \quad (14)$$

The integration yields the following solution in the compact support:

$$\phi(z) = B_0\cos\mu(z-z_0),\;\; if \;\; |(z-z_0)|\le\pi/2\mu, \quad (15)$$

while in the non compact domain, $\phi(z)=0$. The parameter μ may serve as a measure of the importance of discreteness effect in the system. This solution indicates that the compact bright solitary wave is characterized by amplitude B_0 and a strictly limited width $L=\pi/\mu$. Moreover, z_0 locates the center of mass of the solution.

Note that Gaeta et al. [13] combine two (or more) kink solutions to obtain a multi-kink solution, which is a special type of multi-compacton solutions by considering a periodic on-site potential leading to an arbitrary sequence of kinks and anti-kinks.

The existence condition of compact bright solitary wave is

$$-r<C_{nl}<0, \quad (16)$$

with

$$r=\frac{(7/6)\omega_g^2}{12\sin^4(k/2)-(1/8)(l_1\gamma+8l_6\gamma^2+(l_2-2l_3)\gamma^3-3l_7\gamma^4)}. \quad (17)$$

We remark that this criterion is independent of the G.V.D. in the formation of this compact bright solitary wave.

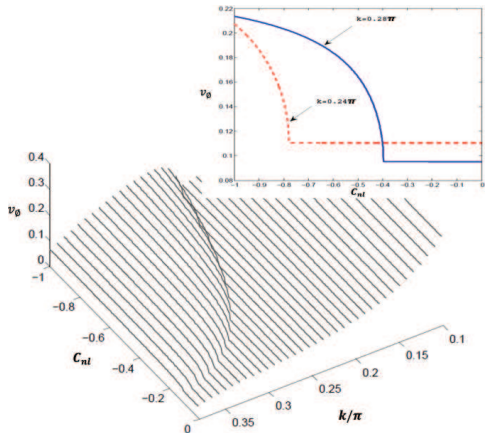

Fig. 1. Variation of phase velocity versus negative anharmonicity parameter C_{nl} and wavenumber k. In insert, two values of wavenumber are chosen: $k = 0.28\pi$ (solid line), $k = 0.24\pi$ (dashed line).

IV. Direct numerical analysis

In order to check if the above analytic continuum bright soliton with compact support can survive in the discrete lattice, different numerical simulations of the equation (4) have been performed, using the following initial condition

$$Y_n(t=0) = A_0 \cos\mu(n-n_0)\exp[i(k-\gamma)n] \qquad (18)$$
$$|(n-n_0)| \le \pi/2\mu$$
$$Y_n(t=0) = 0 \quad otherwise,$$

obtained from the equations (6). The system has been integrated with a fourth-order Runge-Kutta scheme with a timestep chosen to conserve the energy to an accuracy better than 10^{-6} over a complete run. The number of base pairs is fixed at $N = 600$ in order to avoid any wave reflection at the end of the molecule that can affect the creation process and the dynamics of the localized structures.

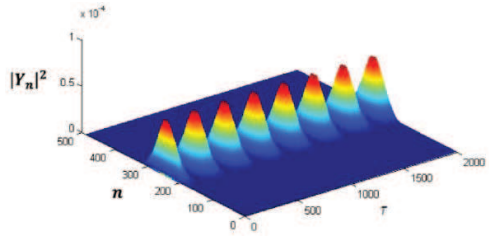

Fig. 2. Temporal behavior of compacton (initial speed equal zero) spacial profil. Magnitude $A_0 = 0.015$, width L=50, and central cite located at $n_0 = N/2$. The solution is stable.

A. Stability of the compact static wave

To check the stability of the solutions over time, the solution is evolved over a very long time. First, the initial velocity is taken to be zero. Fig.2 shows the stability of the lattice profile of the bright soliton with compact envelope over the time $\tau = 2000$ $(4,2\times10^{-12}s)$ which is much greater than the typical time scale of the transversal movements in DNA $(10^{-14}s)$. The initial width and amplitude of compactons

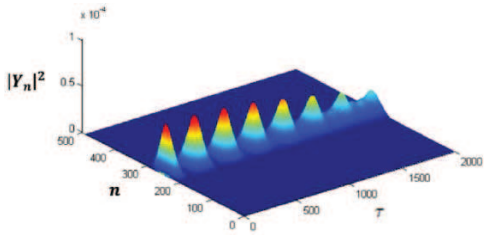

Fig. 3. Same as in Fig.2 but the initial envelop width is now $L = 22$. The initial compacton loses its shape.

are chosen to be respectively $L = \pi/\mu = 50$ times the lattice spacing, and $A_0 = 2B_0 = 0.015$ where B_0 and μ are respectively obtained analytically. As can be seen from this figure, the initial analytic continuum compact envelope solutions of Eq.(15) remains stable even after a very long time in the discrete lattice. We have also considered the compact envelope solution with width $L = 22$. In this case, the results of the numerical simulations show that although the solutions remain stable after 500 time units, it loses its compact support and develops some structures near its edge after a larger time 1000 time units (it starts developing a tail near the edge of the compacton, thereby destroying the compact nature of the solutions, see Fig.3). It is clear that the stability of the compacton solutions with initial speed equal to zero, in a discrete lattice, depends crucially on its width which measures the discreteness effects in the system.

B. Stability of the compact propagating wave

Fig.4 demonstrates that the initial compact wave can be stable for a long time, moving slowly rightwards along the strand in the chain. Here the initial wave is given via (19) with a fixed width $L = 50$ and amplitude $A = 0.012$.

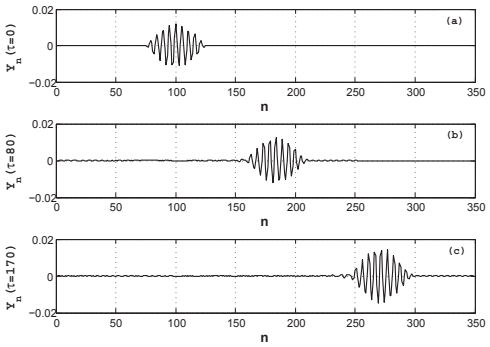

Fig. 4. Time behavior of propagating compact bright solitary wave in DNA for $C_{nl} = -0.4$, i.e. $\Delta H_n/C = 0.2eV$ and $b = 4\mathring{A}^{-2}$ (a) The initial wave is the compact envelope bright solitary wave located at site $n_0 = 100$ with amplitude $A_0 = 1.2\times10^{-2}$, width $L = 50$ and wave number $k = 0.26\pi$. (b) and (c) show the wave at given times of propagation: 15000 and 30000, respectively. The wave experiences are uniform, and the propagation is stable along the DNA lattice with a low speed.

As time goes on, the initial compact bright solitary wave propagates without changes of its initial profile and with the exact value of the velocity predicted by Eq.(14) as illustrated in Fig.4, where the evolution of the compact

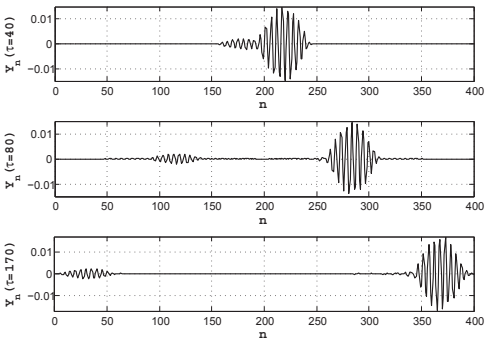

Fig. 5. The decomposition of an initial compacton for the parameter $Cnl = -0.9$ i.e. $\Delta H_n/C = 0.09eV$ and $b = 9\mathring{A}^{-2}$. An initial compact wave breaks into a string of compactons, each of them remaining stable after its birth.

solitary wave at $\tau = 0$, $\tau = 15000$ and $\tau = 30000$ are shown. This process may correspond to energy transfer in DNA molecules. This relative uniform and smooth envelope has compacton-like behavior. The energy is localized in a limited narrow region for biologically significant duration. This energy can propagate as the bright compacton and a large part of the energy is stored in the hydrogen bonds. For $-1 \leq C_{nl} \leq -0.4$, Fig.4 demonstrates the emergence of stable compactons out of more general initial data. The emerging compactons are stable and preserve their initial shape. For the original Rosenau and Hyman [14] compacton equations, numerical investigations showed some remarkable properties, namely whatever initial compact data were given, they eventually evolved into compactons. We show in Fig.5 that a relatively compact wave decomposes into a sequence of compactons whose number depends on the initial energy. Notably for larger energy, two emitted compactons appear and propagate to the left.

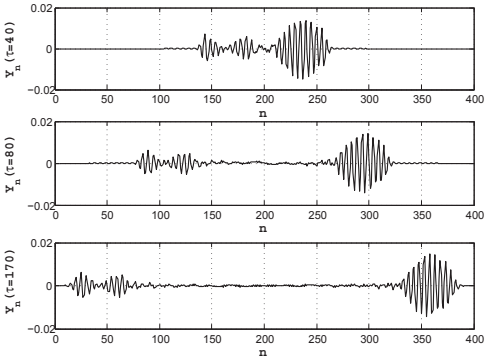

Fig. 6. Time evolution of the perturbated moving compact solitary wave, modulated at a wave number $q = 0.5\pi$. The amplitude and the width of the initial wave are respectively $A = 0.016$ and $L = 50$. The perturbated compact solitary wave appears to be stable during the displacement.

V. Conclusions

In this paper, we have derived an extended nonlinear Schrödinger equation governing the dynamics of modulated waves in DNA lattice with nonlinear dispersion. We have shown that this equation allows to successfully describe the propagation of envelope bright solitary wave with compact support. Numerical experiments have been carried out in order to confirm the analytical predictions. Compact initial data decompose into a train of stable compactons whose width depends on the number of emitted compactons.

For the physical point of our work, by showing the existence and the stability of compact bright solitary waves in DNA, we provide a possible physical mechanism for the effect of finite enthalpy stacking on DNA dynamics. This model with on site-dependent finite stacking is used here to show the existence of compact bright solitary wave in DNA double strands. We believe that this work shows a new vision on the concept of compactification of nonlinear waves in DNA and can also be exported in the study of many other physical systems. In the actual stage of the research on structures with compact support, it is true that the obtained results are still far away from practical applications. However a recent example gives an argument that a specific TeraHertz radiation exposure may significantly affect the natural dynamics of DNA: Alexandrov and al. [15] choose the compact wave to be an effective perturbation for the creation of a localized unbinding state at an arbitrary point.

It is necessary to explore the role of the thermal noise in the process of formation of these localized structures to study the creation and dynamics of localized structures in the (JB) model in a cell environment. On the other hand, such basic complex DNA functional processes as replication and transcription are controlled by means of the protein actions [16]. Therefore, to understand the DNA functioning, taking into account the internal interactions is necessary, but should be completed by studying the interplay between the internal motion, e.g., internal oscillations in the DNA, and the proteins involved in the processes.

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