High-order nonlinear excitations in the Joyeux-Buyukdagli model of DNA

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Abstract By means of the semidiscrete multiple-scale method, we study the existence and properties of high-order envelope solitons and discrete breathers in a homogeneous DNA chain model that is based on pairing enthalpies and site-dependent finite stacking. We obtain the analytical solutions for an envelope soliton, and find that at the Brillouin zone center, discrete breather solutions can appear below the bottom of the phonon band. The behavior of two solitons in collisions and the stability of discrete breathers are confirmed by numerical simulations of the exact equations of the system.

Keywords High-order solution · Envelope solitons · Discrete breathers · DNA models

1 Introduction

Nonlinear mathematics and physics are well known as rapidly developing areas of natural science with numerous interesting applications, such as deoxyribonucleic acid (DNA) science [1–10]. DNA plays a vital role in all living organisms since it is the key molecule responsible for duplication, storage, and realization of genetic information [11]. DNA is basically a complex structure containing two strands of linear polymers of residues (nucleotides), where each strand is made up of sugars, purine [adenine (A) and guanine (G)] and pyrimidine [cytosine (C) and thymine (T)] bases, and phosphates [12]. The two strands are linked by relatively weak hydrogen bonds

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between A(G) bases in one strand and T(C) bases in the other strand. The most important sections are genes, parts of DNA which carry information about the sequence of amino acids in proteins. The double helix structure of DNA was initially discovered by Watson and Crick, which is indubitably one of the most important findings in the history of life science [13].

To study the nonlinear dynamics and statistical mechanics of DNA, some theoretical models have been proposed over the years, focusing on different aspects of the DNA molecule and on different biological, chemical, and physical processes in which DNA is included. In 1989, Peyrard and Bishop presented a model where DNA is viewed as a pair of harmonic chains coupled by a nonlinear potential (Morse potential) [14]. This model describes, by a simplified approach, the hydrogen bond and has been applied successfully to many applications such as energy localization [15] and calculation of solitonic speed [16]. In this model, the double strand corresponds to a Klein–Gordon chain, the variable parameters are the distances between nucleotides within each base pair, and only short-range interactions are considered because of the stacking coupling [17]. It is well known that the Peyrard–Bishop (PB) model can produce solitons due to the balanced competition between dispersion and nonlinear effects [18–20]. For example, in the continuum limit, nonlinear equations of motion for the system reduce to a pair of sine-Gordon-type equations, which have kink soliton solutions [21]. Later on, Dauxois [22] inserted the helicoidal structure between each strand into the model, and proposed a helicoidal DNA model, which is called the Peyrard–Bishop–Dauxois (PBD) model. This model was basically developed by ignoring the effect of torsional motion and based on an assumption that each hydrogen bond link is represented by a Morse potential with exponential form, while the coupling between two neighboring nucleotides in the same strand, and two nearest nucleotides in different strands, are assumed to be harmonic forces due to DNA's helicoidal structure. The PBD model was also confirmed to be consistent with the formation of temporary sequence-dependent openings observed by S1 nuclease cleavage experiments and with a multistep melting envisaged by experiments in heterogeneous DNA [23]. Some works have shown that the PBD model supports nonlinear local excitations [11, 12, 24–26]. A few years ago, Joyeux and Buyukdagli [27] proposed a new dynamical model (JB model) for DNA, which is closer to the statistical ones than the PBD model. This model is based on site-specific stacking enthalpies and showed that the finiteness of the stacking interaction is sufficient to guarantee a sharp melting transition.

In this paper, we investigate high-order envelope solitons and discrete breathers in the JB model by making use of the semidiscrete multiple-scale method. In general, envelope solitons can move, while discrete breathers are static. The excitation of discrete breathers is a very interesting local phenomenon, the former being spatially localized and temporally periodic in nonlinear lattices with translational invariance due to the interplay between discreteness and nonlinearity [28]. Some experimental works have shown that the existence and spontaneous generation of discrete breathers have significant ramifications for cellular gene expression [29, 30]. In the present work, we obtain an analytical solution for high-order envelope solitons and discrete breathers. By using molecular dynamics simulation, moreover, we find that two high-order solitons pass through each other without losing their identity in the collision, and high-order discrete breathers are quite long-lived. Details are shown in the following text.

2 The DNA model Hamiltonian and equation of motion

The general form of the Hamiltonian for the model that we consider is as follows:

$$H = \sum_j \left[\frac{p_j^2}{2m} + U(q_j, q_{j-1}) + D(e^{-aq_j} - 1)^2 \right], \quad (1)$$

where m is the reduced mass of the bases, and q_j 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, and the parameter a , homogeneous to the inverse of a length, sets the special scale of the potential. In our work, we choose the JB model. Thus, the stacking interaction potential U has the following form

$$U(q_j, q_{j-1}) = \frac{\Delta H_j}{C} \left[1 - e^{-b(q_j - q_{j-1})^2} \right] + K_b (q_j - q_{j-1})^2, \quad (2)$$

where $\Delta H_j/C$ is the depth of the Gaussian hole and the backbone stiffness is taken as a harmonic potential of constant K_b . In this work, we consider that $\Delta H_1 = \Delta H_2 = \dots = \Delta H$. From the Hamiltonian in Eq. (1), we can obtain the Hamiltonian canonical equations,

$$\dot{q}_n = \partial H / \partial p_n = \frac{p_n}{m}, \quad (3)$$

$$\begin{aligned} \dot{p}_n = -\partial H / \partial x_n &= \frac{2K_b}{m} (q_{n+1} + q_{n-1} - 2q_n) + \frac{2b\Delta H}{mC} [(q_{n+1} - q_n) \\ &\times e^{-b(q_{n+1} - q_n)^2} - (q_n - q_{n-1})e^{-b(q_n - q_{n-1})^2}] + \frac{2\alpha D}{m} e^{-\alpha q_n} (e^{-\alpha q_n} - 1). \end{aligned} \quad (4)$$

Substituting Eq. (4) into Eq. (3) yields the equation of equation of the n th base pair:

$$\begin{aligned} \frac{d^2 q_n}{d\tau^2} &= \frac{2K_b}{m} (q_{n+1} + q_{n-1} - 2q_n) + \frac{2b\Delta H}{mC} [(q_{n+1} - q_n) \\ &\times e^{-b(q_{n+1} - q_n)^2} - (q_n - q_{n-1})e^{-b(q_n - q_{n-1})^2}] + \frac{2\alpha D}{m} e^{-\alpha q_n} (e^{-\alpha q_n} - 1). \end{aligned} \quad (5)$$

From Ref. [31], it is assumed that the oscillations of bases are large enough so as to be anharmonic, but still insufficient to break the bond because the plateau of the Morse potential is not reached. Under the assumption, the base nucleotides should oscillate around the bottom of the Morse potential. Hence, one can expand the exponential function up to the third-order approximation. Thus, Eq. (5) can be written as

$$\begin{aligned} \frac{d^2 q_n}{d\tau^2} &= \left(\frac{2K_b}{m} + \frac{2b\Delta H}{mC} \right) (q_{n+1} + q_{n-1} - 2q_n) - \frac{2b^2\Delta H}{mC} [(q_{n+1} - q_n)^3 - (q_n - q_{n-1})^3] \\ &\quad - \frac{2\alpha^2 D}{m} \left(q_n - \frac{3}{2}\alpha q_n^2 + \frac{7}{6}\alpha^2 q_n^3 \right). \end{aligned} \quad (6)$$

For the sake of a dimensionless description, we shall rescale the variables by introducing the dimensionless parameters

$$\begin{aligned} x_n &= \alpha q_n, t = \left(\sqrt{D\alpha^2/m\tau} \right), \\ K_l &= \frac{2}{D\alpha^2} \left(K_b + \frac{b\Delta H}{C} \right), K'_l = -\frac{2}{D\alpha^4} \frac{b^2\Delta H}{C}. \end{aligned} \quad (7)$$

Using Eq. (7), the equation of motion Eq. (6) can be rewritten in the form

$$\begin{aligned} \frac{d^2 x_n}{dt^2} &= K_l(x_{n+1} + x_{n-1} - 2x_n) + K'_l \left[(x_{n+1} - x_n)^3 \right. \\ &\quad \left. - (x_n - x_{n-1})^3 \right] - \Omega_0^2 \left(x_n - \frac{3}{2}x_n^2 + \frac{7}{6}x_n^3 \right), \end{aligned} \quad (8)$$

where $\Omega_0^2=2$. Note that the control parameters b and $\Delta H/C$ allow us to fix independently K_l and K'_l .

3 High-order envelope solitons and discrete breathers

Since Eq. (8) is a discrete nonlinear equation, it is extremely hard to seek its exact solution. Here, we employ the semidiscrete multiple-scale method [32] to get the soliton solution. In this method, we must first make a scale transformation

$$x_n = \varepsilon \varphi_n, \quad (9)$$

where ε is a small but finite parameter. After substituting Eq. (9) into Eq. (8), one has

$$\begin{aligned} \frac{d^2 \varphi_n}{dt^2} &= K_l(\varphi_{n+1} + \varphi_{n-1} - 2\varphi_n) + \varepsilon^2 K'_l \left[(\varphi_{n+1} - \varphi_n)^3 \right. \\ &\quad \left. - (\varphi_n - \varphi_{n-1})^3 \right] - \Omega_0^2 \left(\varphi_n - \varepsilon \frac{3}{2} \varphi_n^2 + \varepsilon^2 \frac{7}{6} \varphi_n^3 \right). \end{aligned} \quad (10)$$

Now, we look for the following modulated wave solutions of the form

$$\varphi = F_1^n(x_1, t_1)e^{i\theta_n} + c.c. + \varepsilon[F_0^n(x_1, t_1) + F_2^n(x_1, t_1)e^{2i\theta_n} + c.c.], \quad (11)$$

which contains a first-harmonic term and also a c.c and second-harmonic term. Since Eq. (10) includes an even power of φ , the c.c and second-harmonic terms in Eq. (11) are necessary. Physically, c.c represents the non-oscillating component. Here, $t_1=\varepsilon t$ and $x_1=\varepsilon na$ are the introduced multiple-scale variables, $\theta_n=kna-\omega t$ denotes the phase of the carrier wave. From the basic of semidiscrete approximation, it is assumed that

envelope function F_β ($\beta=0, 1, 2$) is as a continuum variable, while the phase θ is discrete variable. Therefore, we need to use the continuum approximation for F_β :

$$\begin{aligned} F_\beta^n(x_1, t_1) &= F_\beta(x_1, t_1), \quad (\beta = 0, 1, 2) \\ F_0^{n\pm 1} &= F_0 \pm \varepsilon \frac{\partial F_0}{\partial x_1} + \frac{\varepsilon^2}{2} \frac{\partial^2 F_0}{\partial x_1^2} + \dots, \\ F_1^{n\pm 1} &= F_1 \pm \varepsilon \frac{\partial F_1}{\partial x_1} + \frac{\varepsilon^2}{2} \frac{\partial^2 F_1}{\partial x_1^2} + \dots, \\ F_2^{n\pm 1} &= F_2 \pm \varepsilon \frac{\partial F_2}{\partial x_1} + \frac{\varepsilon^2}{2} \frac{\partial^2 F_2}{\partial x_1^2} + \dots \end{aligned} \quad (12)$$

Inserting Eq. (11) into Eq. (10) and using Eq. (12), one has

$$\omega^2 = \Omega_0^2 + 2K_I(1 - \cos k), \quad (13)$$

$$F_0 = 3|F_1|^2, \quad (14)$$

$$F_2 = \frac{3\Omega_0^2}{2[\Omega_0^2 + 2K_I(1 - \cos 2k)]} F_1^2, \quad (15)$$

$$\begin{aligned} 2i\varepsilon \left(\omega \frac{\partial F_1}{\partial t_1} + K_I \sin k \frac{\partial F_1}{\partial x_1} \right) - \varepsilon^2 \frac{\partial^2 F_1}{\partial t_1^2} + K_I \varepsilon^2 \cos k \frac{\partial^2 F_1}{\partial x_1^2} \\ - 48\varepsilon^2 K_I' \sin^2 \left(\frac{k}{2} \right) |F_1|^2 F_1 + 3\varepsilon^2 \Omega_0^2 F_1 F_0 + 3\varepsilon^2 \Omega_0^2 F_1^* F_2 - \frac{7}{2} \varepsilon^2 \Omega_0^2 |F_1|^2 F_1 = 0. \end{aligned} \quad (16)$$

Obviously, Eq. (13) is the dispersion relation. Using it, one can obtain the group velocity, namely,

$$V_g = \frac{d\omega}{dk} = \frac{K_I \sin k}{\omega}. \quad (17)$$

Then, we introduce new scales z and s , which are defined as

$$z = x_1 - V_g t_1, s = \varepsilon t_1. \quad (18)$$

Finally, from Eq. (16), one can obtain the cubic nonlinear Schrödinger (NLS) equation

$$i \frac{\partial F_1}{\partial s} + P \frac{\partial^2 F_1}{\partial z^2} + Q |F_1|^2 F_1 = 0 \quad (19)$$

with

$$P = \frac{(K_I \cos k - V_g^2)}{2\omega} \quad (20)$$

and

$$Q = \frac{1}{2\omega} \left[\frac{9\Omega_0^2}{2} \frac{3\Omega_0^2 + 4K_I(1 - \cos 2k)}{[\Omega_0^2 + 2K_I(1 - \cos 2k)]} - \frac{7}{2} \Omega_0^2 - 48K_I' \sin^4 \left(\frac{k}{2} \right) \right]. \quad (21)$$

The analytical solution style of the NLS equation depends on the sign of P and Q [33]. In the case of $\text{sign}(PQ) > 0$, i.e., both P and Q are positive or negative, the NLS

equation has an envelope soliton solution, the amplitude of which disappears at $|z| \rightarrow \infty$. Since it corresponds to a pulse of light, the envelope soliton is known as a bright soliton. In contrast, for $\text{sign}(PQ) < 0$, the solution of the NLS equation is a hole soliton, which has a hole in the amplitude function. In the context of optics, the hole soliton corresponds to a hole in the continuous light wave, namely, the portion where light is absent. Hence, the hole soliton is also called a dark soliton.

Here, we must consider the small-amplitude soliton due to the use of the third-order approximation for equation of motion. Hence, we only study the case of $\text{sign}(PQ) > 0$. In this case, the NLS equation has the following envelope soliton solution [33]

$$F^1(s, z) = A_0 \text{sech} \left[\sqrt{\frac{Q}{2P}} A_0 (z - z_0) \right] \exp \left(\frac{iQA_0^2 s}{2} \right), \quad (22)$$

where A_0 is the amplitude of the soliton and z_0 denotes the initial position.

Then, it is not too difficult to get the following solution for equation motion (8)

$$\begin{aligned} x_n(t) = & 2 \varepsilon A_0 \text{sech} \left[\varepsilon \sqrt{C} A_0 (n - n_0 - V_g t) \right] \cos(kna - \Omega t) \\ & + \varepsilon^2 \left\{ 3A_0^2 \text{sech}^2 \left[\varepsilon \sqrt{C} A_0 (n - n_0 - V_g t) \right] \right. \\ & \left. + 3A_0^2 \text{sech}^2 \left[\varepsilon \sqrt{C} A_0 (n - n_0 - V_g t) \right] \cos[2(kna - \Omega t)] \right\}, \end{aligned} \quad (23)$$

where $\Omega = \omega - \varepsilon^2 Q A_0^2 / 2$ is the mode frequency of the soliton vibration. Since DNA is a dispersive system, the group velocity V_g is determined by the dispersion relation $\omega = \omega(k)$. Obviously, Eq. (23) is a high-order envelop soliton solution in the present system.

At the Brillouin zone center $k=0$, we have

$$\omega(k=0) = \omega_{\min} = \Omega_0, \quad (24)$$

$$V_g(k=0) = 0, \quad (25)$$

$$P(k=0) = P_0 = \frac{K_l}{2\omega_{\min}} > 0, \quad (26)$$

$$Q(k=0) = Q_0 = \frac{5\Omega_0^2}{2\omega_{\min}} > 0. \quad (27)$$

From Eq. (25), we find that the velocity of the envelope soliton solution is equal to zero. In principle, stationary envelope solitons can be viewed as discrete breathers. Thus, we can obtain the high-order discrete breather solution, which is given by

$$\begin{aligned} x_n(t) = & 2 \varepsilon A_0 \text{sech} \left[\varepsilon \sqrt{C_0} A_0 (n - n_0) \right] \cos(\Omega_b t) \\ & + \varepsilon^2 \left\{ 3A_0^2 \text{sech}^2 \left[\varepsilon \sqrt{C_0} A_0 (n - n_0) \right] \right. \\ & \left. + 3A_0^2 \text{sech}^2 \left[\varepsilon \sqrt{C_0} A_0 (n - n_0) \right] \cos(2\Omega_b t) \right\}, \end{aligned} \quad (28)$$

where $C_0 = Q_0 / 2P_0$ and Ω_b is the eigen frequency of the discrete breather. The central position of the localized mode is at site $n = n_0$, which is determined by the initial exciting condition of the lattice system. Owing to translational symmetry of the lattice, these high-order discrete breathers can be excited at any lattice site.

4 Numerical simulations

The results obtained in the previous section are only approximated ones because they are obtained not from the initial equations of motion (Eq. 5) but from the extended NLS Eq. (8) derived after some hypothesis. In order to test the above analytic high-order soliton and discrete breather obtained, different numerical simulations of Eq. (5) will be performed. Now, let us discuss briefly the numerical technique. Taking the analytical solutions as initial conditions, we investigate the evolution of the system by integrating numerically the equation of motion Eq. (5), making use of the fourth-order Runge–Kutta scheme. In numerical simulations, we consider the system with N base pair and adopt periodic boundary conditions (i.e., $x_{N+1}=x_1$ and $x_0=x_N$). From Ref. [14], the values of the system parameters are set to $m=300$ amu, $D=0.04$ eV, $\alpha=4.45$ Å⁻¹, $K_b=10^{-5}$ eVÅ⁻², and $b=8$ Å⁻². For the purpose of convenience of numerical calculations, we use the dimensionless lengths x_n and times t , which are defined by Eq. (7). All computations are carried out to double precision. The time step is set to 10^{-3} so as to ensure enough high accuracy. Numerical results are shown by classifying into two cases: (1) two solitons collision; (2) the long-time evolution of discrete breathers.

It is well known that solitons remain intact after collision, which is an important characteristic of the soliton. In order to examine this characteristic of our solitons, we now study the behavior of two solitons in collisions. In simulation, we set $N=1000$. The parameter values of solitons are $\varepsilon=0.05$, $A_0=0.2$, $k_1=\pi/3$, $k_2=-\pi/3$, $n_1=250$, and $n_2=750$. According to parameters that we choose, the two solitons have identical speeds, but are moving in opposite directions. In Fig. 1, we show the collisional process of two high-order solitons in the lattice system. We can see clearly that two solitons slowly approach each other with the same speed, but from opposite directions. When two solitons overlap, due to their interaction, amplitude will increase. After the collision, note that the waveform of two solitons during recovery is similar to the shape before the collision. In other words, two solitons pass through each other without losing their identity in the collision.

Next, we calculate the long-time evolution of the discrete breather. In this simulation, we set $N=800$. The parameter values of the breather are $\varepsilon=0.05$ and $A_0=0.15$. In Fig. 2, we plot the long-time evolution of the n th base pair displacements x_n for the high-order discrete

Fig. 1 Time evolution of base pair displacements x_n for the collision of two high-order solitons

breather. Here, considering that the amount of data is large, we only show the data during four time intervals. The time intervals are all 20 dimensionless time units. Figure 2a shows that the vibration localizes in part of the sites and the envelope evolves periodically. From Fig. 2b–d, it is clearly seen that the spatially localized and the time-periodic feature remains after long-time evolution. The high-order discrete breather can last for at least 2000 time periods. This means that our high-order discrete breathers are quite long-lived. The lifetime of the discrete breather solutions determined above is an important parameter since only long-lived excitations can be detected experimentally. Because the long lifetime of our discrete breathers is quite long, it is easy to find them in experiments.

5 Conclusions

In conclusion, we have investigated high-order envelope solitons and discrete breathers in the JB model. By making use of the semidiscrete multiple-scale method, the equation of motion has been reduced to the cubic nonlinear Schrödinger equation. We found that the system can produce the high-order envelope solitons, and at the Brillouin zone center those envelope solitons with zero group velocity can be viewed as the high-order discrete breathers. In order to check our analytical solutions, we have carried out numerical experiments by employing the fourth-order Runge-Kutta

Fig. 2 Long-time evolution of the high-order discrete breather in different time domains: **a** $t \in [0, 20]$; **b** $t \in [1000, 1020]$; **c** $t \in [5000, 5020]$; **d** $t \in [10000, 10020]$

scheme. Our results showed that two high-order solitons pass through each other without losing their identity in the collision. In addition, it was found that the long lifetime of our high-order discrete breathers is quite long. Such breathers can last for at least 2000 time periods.

In this work, we focus on the small-amplitude nonlinear waves. In order to simplify the problem, we have therefore used the third-order approximation for the Morse potential. Due to technical difficulties, it is extremely hard to consider the effect of the temperature in theoretical works on nonlinear waves in DNA. Theoretical works can suggest interesting experiments to improve the physical knowledge of nonlinear waves in DNA. Here, it should be pointed out that applications of these theoretical results in biology must be done with prudence since the stability and lifetime of such nonlinear localized solutions are very sensitive to thermal fluctuations [34, 35]. The DNA is in contact with a thermal reservoir in the cell [36]. Hence, it is worthwhile to explore the role of the thermal noise in the process of formation of these nonlinear localized excitations to investigate the creation and dynamics of localized structures in the DNA in a cell environment [31].

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