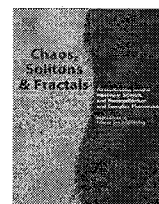




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Semi-discrete DNA breather in Peyrard–Bishop–Dauxois model with fifth-order-approximation Morse potential

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ABSTRACT

We discuss the existence of DNA breather in helicoidal Peyrard–Bishop–Dauxois model with fifth-order-approximation Morse potential based on semi-discrete approximation. This approximation handles the cases which are not admitted in the previous model with fourth-order-approximation Morse potential. It is found that the associated DNA breather is governed by Quintic Nonlinear Schrödinger equation with restricted parameter set. We give an example to explain its existence and dynamics, and confirm it by numerical integration of the discrete equation of motion with full Morse potential. Collision dynamics between the two contra-propagating Quintic DNA breathers is also discussed.

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1. Introduction

The discovery of Deoxyribonucleic Acid (DNA) double helix structure is undoubtedly one of the most important findings in the history of science. DNA is basically a complex structure consisting of two strands of linear polymers of nucleotides [1], where each strand is made up from sugars, purine [adenine (A) and guanine (G)] and pyrimidine [thymine (T) and cytosine (C)] bases, and phosphates. These two strands are connected by relatively weak hydrogen bonds between A(G) bases in one strand and T(C) bases in the other strand.

The dynamics of base pair opening or denaturation process due to energy propagation in a DNA has attracted many attentions because of its important roles in the biological processes of DNA. The internal longitudinal, transversal and torsional motions of DNA determine its biological functionalities in transcription and translation, replication, and DNA–protein recognition [2]. Attempts to study this process theoretically on the basis of mechanical point of view have led to several approximate models e.g Refs. [3–11].

The first attempt was done by Englander et al. [3] and modified later by many authors [4–8] with increasing

accuracy. In those models, the torsional motion of the DNA is considered to be dominantly responsible for the opening process. A comprehensive discussion regarding those models can be found in Ref. [9]. On the other hand, Peyrard and Bishop [10] have developed a simple model which is mainly concern on the propagation of the localized base pair opening known as denaturation bubble, that occur due to transversal motion (stretching) of each strand in the direction of hydrogen bond. Later on, Dauxois [11] inserted the helicoidal coupling between each strand into the model. This helicoidal Peyrard–Bishop–Dauxois (PBD) model (which for short we will call it as PBD model) was basically developed by neglecting the effect of torsional motion and based on an assumption that each hydrogen bond connection 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 strand due to DNA helicoidal structure are assumed to be harmonic forces.

By means of multiple scale expansion method [12] and assumption of relatively small opening amplitude, it was shown that for the semi-discrete approximation and Taylor expansion of Morse potential up to fourth order, the PBD model revealed the possibility of local disturbance that stretches the hydrogen bond to propagate in the form of DNA breather excitation, which is related to a single hump solitonic envelope [11]. It was demonstrated that the prop-

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agation of the corresponding DNA breather is governed by Cubic Nonlinear Schrödinger Equation (CNLSE). The possible experiment to test the existence and dynamical propagation of this Cubic DNA breather has been proposed by Zdravković et al. in Refs. [13,14]. In the mean time, its dynamical characteristics due to the impact of viscosity of surrounding medium have been reported in Refs. [15,16]. It was demonstrated that the effect of viscosity leads to the decay of breather envelope velocity to its group velocity.

As pointed out above, all studies in Refs. [11,13–16] were conducted under assumption that the associated base pair opening amplitude is deviated relatively not far from the bottom of the associated Morse potential where its Taylor expansion was taken only up to fourth order. Therefore, it is obvious that to study the dynamics of larger opening amplitude one has to investigate the effect of higher order expansion terms. To our knowledge, the existence of DNA breather with the associated Taylor expansion order of Morse potential larger than four has never been investigated, even for the next Taylor expansion term. Based on this fact, the present report discusses its existence by taking into account the fifth order term to the related Taylor expansion and shows that the associated governing equation is remarkably given by the Quintic Nonlinear Schrödinger Equation (QNLSE). It is found that the corresponding DNA breather is related to a specific set of parameters which could not be handled by the CNLSE of previous approximate PBD model. By performing numerical integration to the associated full equation of motion, we confirm its existence and simulate the collision dynamics between two contra-propagating breathers.

We organize this report as follows. In Section 2, the approximate PBD model with fifth order Taylor expansion will be considered and the derivation of the associated QNLSE based on semi-discrete approximation is discussed. In Section 3, we present the corresponding DNA breather and its numerical confirmation. Finally, a summary is presented in Section 4. It has to be noted that in this report, we use the Cubic and Quintic DNA breather nomenclatures for the particular semi-discrete breather solutions which governed by the CNLSE and QNLSE, respectively.

2. PBD model with fifth-order-approximation Morse potential and QNLSE

Let us first discuss the Hamiltonian of PBD model and for the sake of continuous discussion with the previous studies we consider the same form and notations as used in Refs. [11,13–16] as follows:

$$H = \sum_N \left\{ \frac{m}{2} (\dot{u}_n^2 + \dot{v}_n^2) + \frac{k}{2} [(u_n - u_{n-1})^2 + (v_n - v_{n-1})^2] + \frac{K}{2} [(u_n - v_{n+h})^2 + (u_n - v_{n-h})^2] + D [e^{-a(u_n - v_n)} - 1]^2 \right\}. \quad (1)$$

Here, the time dependent functions $u_n(t)$ and $v_n(t)$ represent the position of the n th nucleotide in the two strands, while the dot indicates the time derivative. The Hamiltonian (1) is related to the transversal motion of N -nucleotides of DNA where each of them is assumed to have

mass m . The n th and $(n-1)$ th nucleotides in the same strand are assumed to be connected by uniform longitudinal harmonic forces with spring constant $k > 0$. Similarly, the connection between two nearest nucleotides due to helicoidal structure, namely the n th and $(n+h)$ th, and n th and $(n-h)$ th of different strand are represented by the spring constant $K > 0$ of corresponding helicoidal harmonic forces, while $2h$ is the number of nucleotides in one helical turn. Meanwhile, the depth and inverse width of Morse potential related hydrogen bond are determined by the constants D and a , respectively [11].

For a convenient discussion, it is useful to define the in-phase and out-phase center-of-mass coordinates namely: $x_n = (u_n + v_n)/\sqrt{2}$ and $y_n = (u_n - v_n)/\sqrt{2}$, respectively. In these coordinates, the associated equations of motion are in a decoupled form of the linear and nonlinear motions as given respectively as follows:

$$m\ddot{x}_n = k(x_{n+1} - 2x_n + x_{n-1}) + K(x_{n+h} - 2x_n + x_{n-h}), \quad (2a)$$

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

Next, we focus our discussion only to the nonlinear motion described by Eq. (2b), where y_n clearly represents the stretching motion of each base pair.

By assuming that the oscillation of y_n [given in Eq. (2b)] around the bottom of Morse potential at $y_n = 0$ is relatively small but larger than the previous studies [11,13–16], we therefore consider it to be in the following form:

$$y_n = \varepsilon^{1/2} \Phi_n, \quad (3)$$

where the scaling factor $\varepsilon \ll 1$, such that it allows us to expand the Morse potential of the associated Hamiltonian up to fifth order Taylor expansion, which leads to the following equation of motion for Φ_n :

$$\ddot{\Phi}_n = \frac{k}{m} (\Phi_{n+1} - 2\Phi_n + \Phi_{n-1}) - \frac{K}{m} (\Phi_{n+h} + 2\Phi_n + \Phi_{n-h}) - \omega_g^2 \left(\Phi_n + \alpha \varepsilon^{1/2} \Phi_n^2 + \beta \varepsilon \Phi_n^3 + \gamma \varepsilon^{3/2} \Phi_n^4 \right), \quad (4)$$

with

$$\omega_g^2 = \frac{4a^2D}{m}, \quad \alpha = \frac{-3a}{\sqrt{2}}, \quad \beta = \frac{7a^2}{3}, \quad \gamma = \frac{-5a^3}{2\sqrt{2}}. \quad (5)$$

It is worth to note that $y_n = \varepsilon \Phi_n$ was taken in the previous studies [11].

We assume that the approximate semi-discrete solution of Φ_n is given as follows:

$$\Phi_n = F_1(\varepsilon n l, \varepsilon t) e^{i\theta_n} + c \cdot c + \varepsilon^{1/2} [F_0(\varepsilon n l, \varepsilon t) + F_2(\varepsilon n l, \varepsilon t) e^{2i\theta_n} + c \cdot c] + O(\varepsilon), \quad (6)$$

where the assumed order of $\varepsilon^{1/2}$ in the right hand side of Eq. (6) is a bit different than that was originally considered in Refs. [10,11] where it was taken to be ε^1 . Here, $\theta_n = nql - \omega t$, with the parameters l , ω and $q = 2\pi/\lambda$ denote the distance between two adjacent nucleotides in the same strand, the vibrational frequency and its corresponding wave number, respectively, while λ is the related wavelength. It is important to note that the gentle variation of F_i functions ($i = 0, 1, 2$) in Eq. (6) with respect to the space

variable is retained to be still in order of ϵ^1 . In other words, in contrast to the previous approximation [10–12], where the smallness of the opening base amplitude and the gentleness of wave variation in space–time were taken to be of the same order, here we consider it to be different. It will be shown later that this difference leads to the inclusion in the governing equation of DNA breather the effect of fifth order term of associated Taylor expansion.

For the semi-discrete approximation, we assume $nl \rightarrow z$ for the F_i functions, such that in general:

$$F_i[\epsilon(n \pm h)l, \epsilon t] \rightarrow F_i(Z, T) \pm \epsilon h l \frac{\partial F_i}{\partial Z} + \frac{1}{2} \epsilon^2 h^2 l^2 \frac{\partial^2 F_i}{\partial Z^2}, \quad i=0, 1, 2, \tag{7}$$

where the continuous variables z and t have been substituted by $z = Z/\epsilon$ and $t = T/\epsilon$, respectively. Substituting Eq. (6) into Eq.(4) and collecting the $\exp(i0)$ terms one find from the $\epsilon^{1/2}$ order the relation:

$$F_0 = \mu |F_1|^2, \tag{8}$$

with

$$\mu = \frac{-2\alpha}{1 + 4K/m\omega_g^2}. \tag{9}$$

On the other hand, from the $\exp(2i\theta_n)$ harmonic terms we can derive out of order ϵ^0 the following relation for F_2 :

$$F_2 = \delta F_1^2, \tag{10}$$

where

$$\delta = \frac{m\omega_g^2 \alpha}{2[k(\cos 2ql - 1) - K(\cos 2qlh + 1)] + m(4\omega^2 - \omega_g^2)}. \tag{11}$$

All these relations (8)–(11) have been derived in the previous study [11]. Based on relations (8) and (10), we find the following consistency condition derived from the $\exp(i0)$ term with $\epsilon^{3/2}$ order:

$$\alpha(\mu^2 + 2\delta^2) + 6\beta(\mu + \delta) + 6\gamma = 0. \tag{12}$$

Finally, by focusing our self only to the $\exp(i\theta_n)$ harmonic term and neglecting the effects of the other higher harmonic terms [12], we arrive at the following equation:

$$\begin{aligned} \epsilon^2 \frac{\partial^2 F_1}{\partial T^2} - 2i\epsilon\omega \frac{\partial F_1}{\partial T} - \omega^2 F_1 &= \frac{k}{m} \left[2F_1(\cos ql - 1) + 2i\epsilon l \frac{\partial F_1}{\partial Z} \sin ql + \epsilon^2 l^2 \frac{\partial^2 F_1}{\partial Z^2} \cos ql \right] \\ &- \frac{K}{m} \left[2F_1(\cos qlh + 1) + 2i\epsilon l h \frac{\partial F_1}{\partial Z} \sin qlh + \epsilon^2 l^2 h^2 \frac{\partial^2 F_1}{\partial Z^2} \cos qlh \right] \\ &- \omega_g^2 \{ F_1 + \epsilon[2\alpha(\mu + \delta) + 3\beta] |F_1|^2 F_1 \\ &+ \epsilon^2 [3\beta(\mu^2 + 2\mu\delta + 2\delta^2) + 4\gamma(3\mu + 4\delta)] |F_1|^4 F_1 \}. \end{aligned} \tag{13}$$

Clearly, by equating the terms of ϵ^0 order in Eq. (13), we can find the dispersion relation as follows:

$$\omega^2 = \frac{2}{m} [k(1 - \cos ql) + K(1 + \cos qlh)] + \omega_g^2. \tag{14}$$

Next, we define the co-moving coordinates: $S = Z - V_g T$ and $\tau = \epsilon T$, such that Eq. (13) transforms into:

$$\begin{aligned} \left[V_g - \frac{l}{m\omega} (k \sin ql - Kh \sin qlh) \right] \frac{\partial F_1}{\partial S} \\ = i \frac{\omega_g^2}{2\omega} [2\alpha(\mu + \delta) + 3\beta] |F_1|^2 F_1 \end{aligned} \tag{15}$$

for the ϵ order, while for the ϵ^2 order is given by:

$$\begin{aligned} \frac{1}{2\omega} \left[V_g^2 - \frac{l^2}{m} (k \cos ql - Kh^2 \cos qlh) \right] \frac{\partial^2 F_1}{\partial S^2} - i \frac{\partial F_1}{\partial \tau} \\ = - \frac{\omega_g^2}{2\omega} [3\beta(\mu^2 + 2\mu\delta + 2\delta^2) + 4\gamma(3\mu + 4\delta)] |F_1|^4 F_1. \end{aligned} \tag{16}$$

From the dispersion relation given by Eq. (14), we can find the related group velocity defined by $V_g = d\omega/dq$, which gives:

$$V_g = \frac{l}{m\omega} (k \sin ql - Kh \sin qlh). \tag{17}$$

It is easy to see that the group velocity (17) makes the left hand side of Eq. (15) to vanish. As a consequence, in addition to Eq. (12), we get the second consistency condition:

$$2\alpha(\mu + \delta) + 3\beta = 0. \tag{18}$$

It is interesting to note that the left hand side of Eq. (18) is proportional to the “ Q ” coefficient of CNLSE cubic term discussed in Ref. [11]. The consequence of this fact will be considered later. Solving simultaneously the consistency conditions (12) and (18) for μ and δ yields:

$$\mu = \frac{-\beta \pm \sqrt{10\beta^2 - 8\alpha\gamma}}{2\alpha}, \tag{19a}$$

$$\delta = \frac{-2\beta \mp \sqrt{10\beta^2 - 8\alpha\gamma}}{2\alpha}, \tag{19b}$$

respectively, where α, β and γ are given by Eq. (5). It is easy to prove that the Eq. (19) are always real since $10\beta^2 - 8\alpha\gamma = 220a^2/9 > 0$.

By equating Eq. (19) with Eqs. (9) and (11), respectively, and considering the dispersion relation (14), we can determine the spring constants k and K for a given ql, a, D, h and m parameters through the relations:

$$K = -\frac{1}{4} m\omega_g^2 (1 + 2\alpha/\mu), \tag{20a}$$

$$k = \frac{m\omega_g^2 (\alpha/\delta - 3) + 4K[\cos^2 qlh - 2(\cos qlh + 1)]}{4(\cos ql - 1)^2}, \tag{20b}$$

which restrict their values. Clearly from Eq. (20b) that k goes to infinity for $ql \rightarrow 0, 2\pi$. It should be realized that the spring constants k and K are the internal properties of the related DNA structure, while the wave number q determines the oscillation characteristic of the corresponding breather. Therefore, Eq. (20) indicate that the existence of the related DNA breather is restricted since the possible values of k and K are uniquely determined by those ql, a, D, h and m parameters.

Back to Eq. (16), it is obvious that the equation is nothing but the QNLSE which can be written in the simple form:

$$i \frac{\partial F_1}{\partial \tau} + P \frac{\partial^2 F_1}{\partial S^2} + R |F_1|^4 F_1 = 0, \tag{21}$$

with

$$P = \frac{1}{2\omega} \left[\frac{f^2}{m} (k \cos ql - Kh^2 \cos qlh) - V_g^2 \right], \tag{22a}$$

$$R = -\frac{\omega_g^2}{2\omega} \left[3\beta(\mu^2 + 2\mu\delta + 2\delta^2) + 4\gamma(3\mu + 4\delta) \right]. \tag{22b}$$

At this point, it is useful to rewrite the following associated CNLSE found previously in Ref. [11]:

$$i \frac{\partial F_1}{\partial \tau} + P \frac{\partial^2 F_1}{\partial S^2} + Q |F_1|^2 F_1 = 0, \tag{23}$$

with P is given by Eq. (23a), while

$$Q = -\frac{\omega_g^2}{2\omega} [2\alpha(\mu + \delta) + 3\beta]. \tag{24}$$

It is readily seen that the coefficient Q of cubic term in the CNLSE given by Eq. (23) is proportional to the left hand side expression of consistency condition given by Eq. (18), such that $Q = 0$ for the chosen parameters, especially k, K and ql . Therefore, it is reasonable to consider that the QNLSE (21) with restricted parameters is actually related to a specific set of parameters which can not be handled by the CNLSE of the related approximate PBD model. Similar with CNLSE (23), the QNLSE (21) also admits solitonic solutions. However, their dynamical characteristics might be different. In the next section, we discuss the existence and dynamics of the corresponding DNA breather solution.

3. Semi-discrete quintic DNA breather and its example

Theoretically, it was assumed that the finite speed propagation of denaturation bubble along a DNA can be described approximately by Eq. (6) [11]. Therefore, similar to Ref. [11,13–16], we seek for a traveling solution of Eq. (21) in the form of:

$$F_1(S, \tau) = f(S - u_e \tau) \exp[i\sigma(S - u_e \tau)], \tag{25}$$

where f is a real function, while σ is a real parameter to be determined. The parameters u_e and u_c represent the envelope and carrier wave velocities, respectively. Substituting Eq. (25) into Eq. (21) we find from the imaginary part the relation:

$$\sigma = \frac{u_e}{2P}, \tag{26}$$

while the real part resulting in the following ordinary differential equations:

$$f'' - Af + Bf^5 = 0, \tag{27}$$

with

$$A = \frac{u_e^2 - 2u_e u_c}{4P^2}, \quad B = \frac{R}{P}. \tag{28}$$

Here, the prime denotes the derivative with respect to the $(S - u_e \tau)$ co-moving coordinate. Multiplying Eq. (27) with f yields its first integral:

$$(f')^2 - Af^2 + \frac{B}{3} f^6 = C_0, \tag{29}$$

with C_0 is a constant. Since we are interested in a denaturation bubble process, this constant should be set to $C_0 = 0$. By introducing $w = f^2$, we can transform the Eq. (29) into the following integral form:

$$\int \frac{dw}{w \sqrt{1 - Bw^2/3A}} = 2\sqrt{A}(S - u_e \tau + C_1), \tag{30}$$

with C_1 is an integration constant. Let us consider the left hand side of Eq. (30), it is easy to prove that the corresponding integral can be written in the form of $\int dg/g$ with:

$$g = \frac{w}{18 \left(1 + \sqrt{1 - Bw^2/3A} \right)}, \tag{31}$$

such that the Eq. (31) becomes:

$$\ln \left[\frac{w}{18 \left(1 + \sqrt{1 - Bw^2/3A} \right)} \right] = 2\sqrt{A}(S - u_e \tau) + C_1. \tag{32}$$

Solving the above Eq. (32) for w we find:

$$w = \frac{36A \exp \left[2\sqrt{A}(S - u_e \tau) + C_1 \right]}{108B \exp \left[4\sqrt{A}(S - u_e \tau) + 2C_1 \right] + A}. \tag{33}$$

To determine the constant C_1 , we calculate $w' = 0$ at $S - u_e \tau = 0$ and find:

$$C_1 = \ln \sqrt{\frac{A}{108B}} \tag{34}$$

From all these results we find for Eq. (27) a simple solution

$$f(S - u_e \tau) = \left(\frac{3A}{B} \right)^{1/4} \operatorname{sech}^{1/2} \left[2\sqrt{A}(S - u_e \tau) \right]. \tag{35}$$

Finally, by combining Eqs. (6), (25), (26), (28) and (35), and returning $Z \rightarrow \epsilon nl$, we can write down the corresponding semi-discrete Quintic DNA breather as follows:

$$y_n(t) = 2\epsilon^{1/2} A \operatorname{sech}^{1/2} \left[2\epsilon \sqrt{A}(nl - V_e t) \right] \times \left\{ \cos(\Theta nl - \Omega t) + A\epsilon^{1/2} \operatorname{sech}^{1/2} \left[2\epsilon \sqrt{A}(nl - V_e t) \right] \times (\mu/2 + \delta \cos[2(\Theta nl - \Omega t)]) \right\} + O(\epsilon^{3/2}), \tag{36}$$

with

$$A = \left[\frac{3(u_e^2 - 2u_e u_c)}{4PR} \right]^{1/4}, \tag{37a}$$

$$V_e = V_g + \epsilon u_e, \tag{37b}$$

$$\Theta = q + \frac{\epsilon u_e}{2P}, \tag{37c}$$

$$\Omega = \omega + \frac{\epsilon u_e}{2P} (V_g + \epsilon u_e). \tag{37d}$$

It is readily seen from Eqs. (28) and (37a), respectively that the existence of the breather solution should satisfies reality conditions:

$$u_e^2 - 2u_e u_c > 0, \tag{38a}$$

$$PR > 0, \tag{38b}$$

with P and R are given by Eq. (22). It is obvious that the reality condition (38b) leads to the restriction of ql . In addition to this reality condition, it has been discussed in Ref. [15] that the relation of $ql = 2\pi/\lambda$ should also be physically accepted, where the wavelength λ must be determined by the multiple integer of l .

Let us discuss an example of the related Quintic DNA breather based on the following chosen parameter values [14]:

$$l = 3.4 \times 10^{-10} \text{ m}, \quad m = 5.1 \times 10^{-25} \text{ kg}, \quad h = 5, \\ a = 0.9 \times 10^{10} \text{ m}^{-1}, \quad D = 9.6 \times 10^{-21} \text{ J}. \quad (39)$$

Inserting these parameters into Eq. (20a) yield one $K > 0$, namely $K = 1.146 \text{ N/m}$. For this K value, the Eq. (20b) gives the possible values of k as a function of $ql = 0$ to 2π rad as depicted in Fig. 1, drawn only for $k \leq 50 \text{ N/m}$. It is found numerically that the lowest value of k is given by $k_{\min} = 5.370 \text{ N/m}$ at $ql = 0.8515\pi$ and 1.1485π rad. Although the proper choice of the model parameters are still questionable [13,14,17], however, we expect that the chosen values of $5.370 \leq k \leq 50 \text{ N/m}$, which correspond to $0.377\pi \leq ql \leq 1.623\pi$ rad, and $K = 1.146 \text{ N/m}$ are reason-

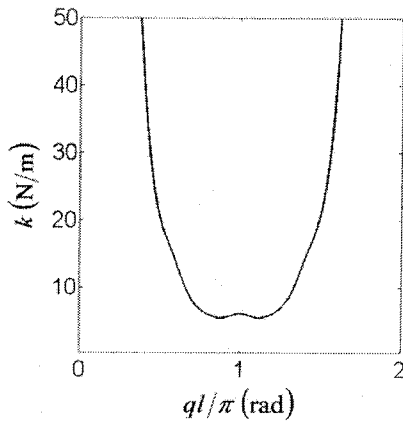


Fig. 1. Longitudinal spring constant k as a function of ql .

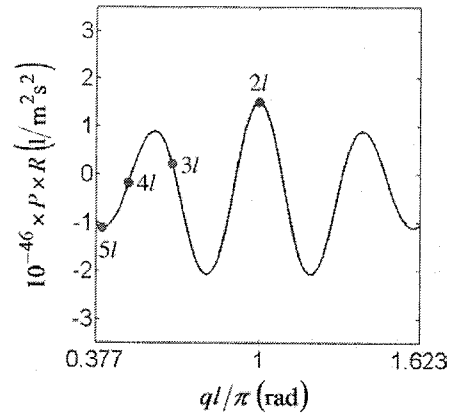


Fig. 2. (Color online) Product of P and R parameters as a function of ql . Red solid circles indicate the values of ql that of related to $\lambda = 5l, 4l, 3l$ and $2l$, as discussed in the text.

able enough to describe the dynamical propagation of the considered DNA denaturation bubble.

In the chosen range of ql , there are four wavelengths that satisfy the physical condition namely $\lambda = 5l, 4l, 3l$

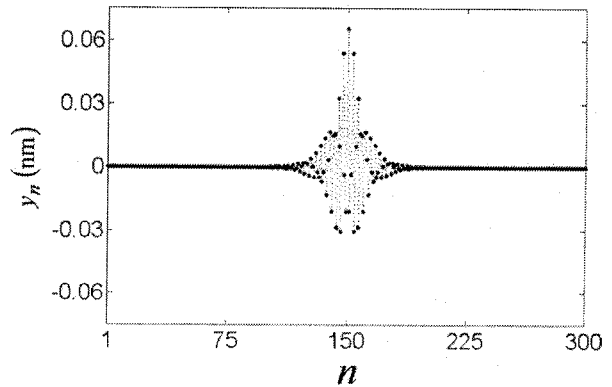


Fig. 3. Profile of Quintic DNA breather given by Eq. (36) at $t = 0$ ps.

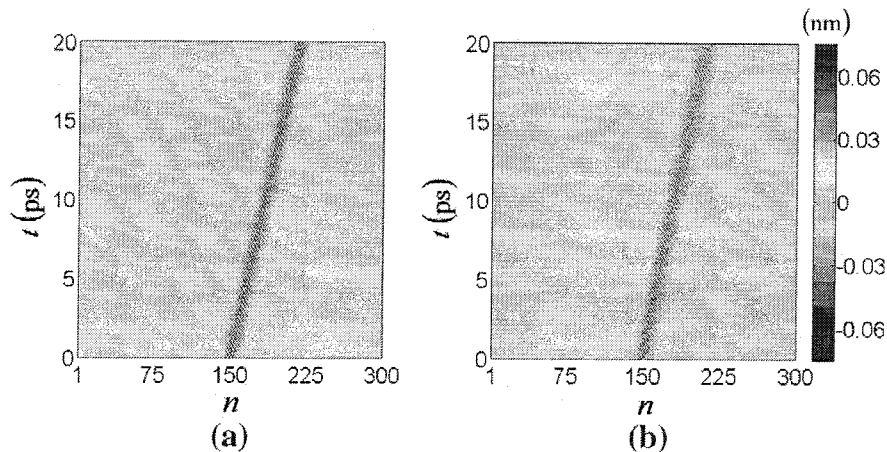


Fig. 4. (Color online) Contour of the dynamical propagation for semi-discrete Quintic DNA breather of (a) Eq. (36) and (b) numerical integration result.

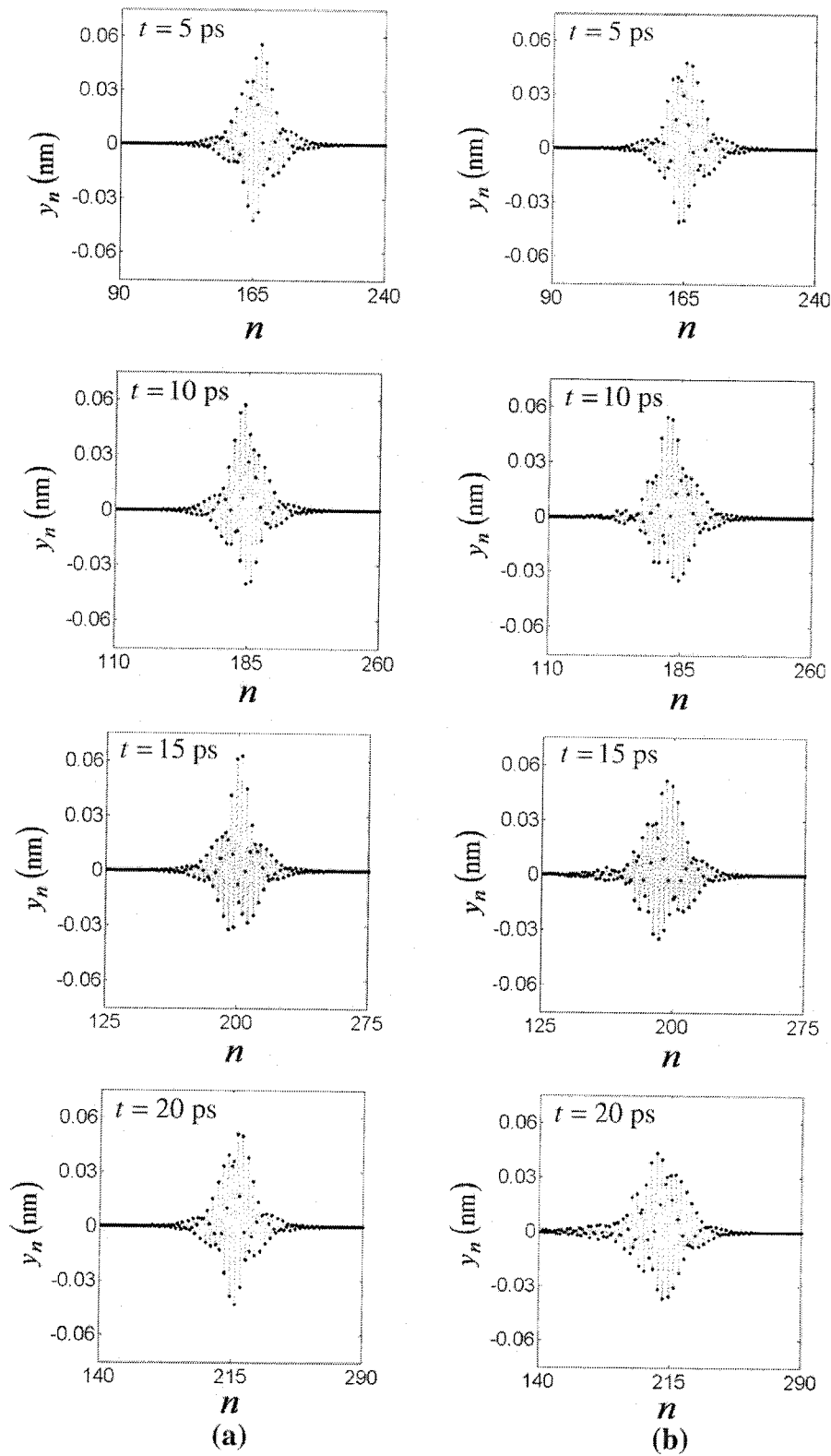


Fig. 5. Snapshots at particular times for semi-discrete Quintic DNA breather propagation of (a) Eq. (36) and (b) numerical integration result.

and $2l$. Next, by inserting these four particular wavelengths into Eq. (22b), as shown in Fig. 2, we found that $PR < 0$ for the case of $\lambda = 5l$ and $4l$, while for $\lambda = 3l$ and $2l$, $PR > 0$.

Therefore, the cases of $\lambda = 3l$ with $ql = 0.667\pi$ rad, and $\lambda = 2l$ with $ql = \pi$ rad, are the possible ones to exist, where the related longitudinal spring constants k for each case

is given by $k = 9.791 \text{ N/m}$ ($\approx 8.546K$) and $k = 6.009 \text{ N/m}$ ($\approx 5.244K$), respectively. However, it is readily seen from Eq. (17) that for the case of $\lambda = 2l$ we have $V_g = 0$.

To explain the dynamical propagation of Quintic DNA breather (36) we consider the case of $\lambda = 3l$ as an example, where the corresponding initial condition, as depicted in Fig. 3, is assumed to be launched from the middle of the DNA and involving around 100 base pairs. It is found that the maximum stretching is $y_{n,\text{max}} = 0.065 \times 10^{-9} \text{ m}$. Compared to the double helix diameter of DNA, which is $\geq 2 \times 10^{-9} \text{ m}$ [9], this maximum stretching seems still acceptable for a denaturation bubble to exist [18]. Next, we set the parameters u_e and u_c in Eq. (36) to $u_e = 10^5 \text{ m/s}$ and $u_c = 0$ [11], respectively, which satisfies the reality condition (38a). The scaling factor ε is chosen to be $\varepsilon^{1/2} = 2 \times 10^{-2}$. The group velocity V_g , dispersion coefficient P , nonlinear coefficient R and frequency ω in Eq. (36), are respectively given by $V_g = 1103.439 \text{ m/s}$, $P = 5.568 \times 10^{-8} \text{ m}^2/\text{s}$, $R = 3.807 \times 10^{52}/\text{m}^4 \text{ s}$ and $\omega = 8.120 \times 10^{12} \text{ rad/s}$, such that the other parameters in the equation are found to be in the following values: $V_e = 1143.439 \text{ m/s}$, $\Theta l = 0.705\pi \text{ rad}$ and $\Omega = 8.511 \times 10^{12} \text{ rad/s}$. To confirm this example, we integrate numerically the discrete equation of motion (2b) with full Morse potential based on finite difference scheme and use the same initial condition

given by Eq. (36) at $t = 0 \text{ ps}$, as shown in Fig. 3. Here, we choose the periodic boundary condition and to assure the numerical convergence, we check the conservation of total energy in each time step.

Depicted in Fig. 4 are the corresponding dynamics of Quintic DNA breather (36) and the result from numerical integration up to $t = 20 \text{ ps}$. Their snapshots at particular times are given in Fig. 5. It is observed from the figures that both results qualitatively show similar dynamics but with relatively visible discrepancy. It is readily seen that the numerical result exhibits slower propagation speed with $V_e \sim 969 \text{ m/s}$, which is $\sim 15\%$ lower than the envelope velocity given by Eq. (37b). In the mean time, we also observe the occurrence of dispersion which probably exists due to the effect of discrete harmonic parts of Eq. (2b) and we suspect this phenomenon is responsible for the slower speed.

To complete our investigation, we also study the collision of two contra-propagating Quintic DNA breathers by integrating Eq. (2b) with the following initial condition:

$$y_n(0) = y_{n-m}(0) + y_{n+m}(0). \tag{40}$$

Here, the initial conditions $y_{n-m}(0)$ and $y_{n+m}(0)$ are given by Eq. (36), and correspond to the right and left propagating DNA breathers, respectively, where $\dot{y}_{n-m}(0) = -\dot{y}_{n+m}(0) > 0$, while the subscripts $n \pm m$ are related to

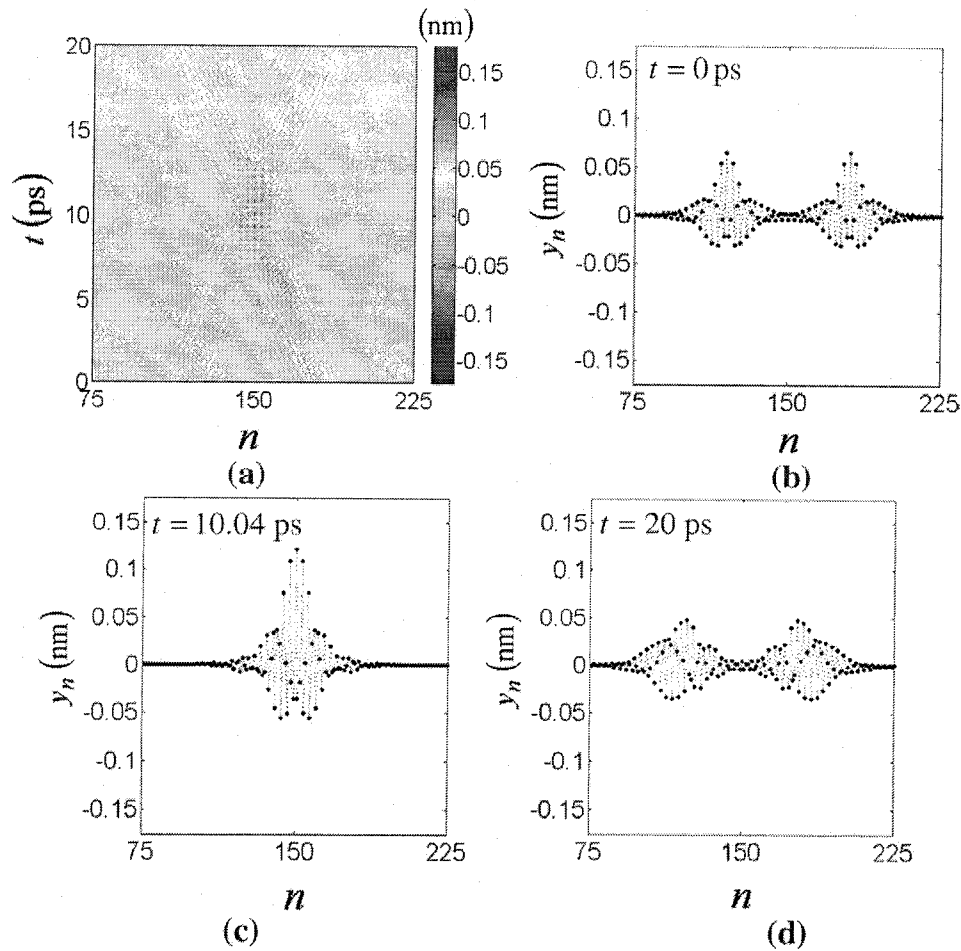


Fig. 6. (Color online) (a) Contour of a collision between two contra-propagating Quintic DNA breathers, along with its snapshots at (b) 0 ps, (c) 10.04 ps and (d) 20 ps.

the shifting of the corresponding profiles from the middle of DNA and we choose $m = 30$. The results are given in Fig. 6, showing an elastic collision between these breathers (see Fig. 6a), where the profile changes of both breathers after the collision are likely due to the aforementioned dispersion phenomenon. Therefore, this collision characteristic may indicate that the corresponding Quintic DNA breather have solitonic feature [19].

For the other case of $\lambda = 2l$, it is clear that the speed of the corresponding DNA breather is very small as indicated by its envelope velocity, $V_e = 40$ m/s, because $V_g = 0$. We found the maximum stretching for this case is $y_{n,\max} = 0.038 \times 10^{-9}$ m, and in general its characteristics are similar to the case of $\lambda = 3l$, except it has a wider and lower profile. Based on this fact, we do not discuss it in more detail.

It should be noted here that these two possible Quintic DNA breathers with different longitudinal spring constant k are related to relatively short wavelength modes. This is in contrast with the previous results that show the possible Cubic DNA breathers have longer wavelength modes, namely $\lambda \geq 6l$ [13–16]. Since the combination of the chosen k , K and ql parameters can not be handled by the CNLSE, then there is no direct comparison can be made to this result.

To this end, it is important to point it out that the stability of the Quintic DNA breather solution as well as its dynamics under the present of viscosity, damping and external force from the surrounding medium are worthy for further investigations. The later issue will be discussed elsewhere.

4. Summary

We have discussed the existence of DNA breather in the helicoidal Peyrard–Bishop–Dauxois model under assumption that its corresponding Morse potential is approximated up to fifth order Taylor expansion. Based on the semi-discrete approximation procedure, we find that the associated breather is governed by the QNLSE with

restricted parameter space. It is found that our approximation is related to the cases which are not admitted in the previously studied PBD model with fourth order approximation Morse potential. In our example, there are two possible longitudinal spring constants for a given set of parameters that allow this Quintic DNA breather to exist. It is also revealed that the associated wavelength modes of the Quintic DNA breathers are shorter than the Cubic DNA breathers. The given example is confirmed by numerical integration of discrete equation of motion with full Morse potential. From the collision dynamics, it is demonstrated that this semi-discrete breather possesses the well known solitonic feature namely the elastic collision.

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References

- [1] Watson JD, Crick FHC. Nature 1953;171:737.
- [2] Calladine CR, Drew HR, Luisi BF, Travers AA. Understanding DNA. Amsterdam: Elsevier; 1997.
- [3] Englander SW, Kalenbach NR, Heeger AJ, Krumhansl JA, Litwin S. Proc Natl Acad Sci 1980;77:7222.
- [4] Yomosa S. Phys Rev A 1984;30:474.
- [5] Yakushevich LV. Phys Lett A 1989;136:413.
- [6] Christiansen PL, Lomdahl PC, Muto V. Nonlinearity 1990;4:477.
- [7] Muto V, Lomdahl PS, Christiansen PL. Phys Rev A 1990;42:7452.
- [8] Daniel M, Vasumathi V. Phys Rev E 2009;79:012901.
- [9] Yakushevich LV. Nonlinear physics of DNA. New York: John Wiley; 1998.
- [10] Peyrard M, Bishop A. Phys Rev Lett 1989;62:2755.
- [11] Dauxois T. Phys Lett A 1991;159:390.
- [12] Remoissenet M. Phys Rev A 1986;33:2386.
- [13] Zdravković S, Satarić MV. Phys Rev E 2006;73:021905.
- [14] Zdravković S, Satarić MV. Phys Rev E 2008;77:031906.
- [15] Zdravković S, Satarić MV. Phys Scr 2001;64:612.
- [16] Zdravković S, Tuszyński JA, Satarić MV. J Comput Theor Nanosci 2005;2:263.
- [17] Van Zandt LL. Phys Rev A 1989;40:6143.
- [18] Lipniacki T. Phys Rev E 2001;64:051919.
- [19] Aossey DW, Skinner SR, Cooney JL, Williams JE, Gavin MT, Andersen DR, et al. Phys Rev A 1992;45:2606.