New Traveling Waves for DNA's Vibrational Dynamics

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Abstract—In this paper, we focus on studying traveling waves for the nonlinear vibrational dynamics modeling DNA, which is modified from the Yakushevich model. The Yakushevich model of DNA torsion dynamics supports soliton solutions, which are supposed to be of special interest for DNA transcription. In the discussion of the model, we will use the traveling wave and a direct integral method, in special, take the integral constant to be some special value and a special change of variable to conclude some new explicit forms of traveling waves are given including smooth solitary waves, solitary waves with blow-up points, rational solutions with decay, periodic waves and polynomial solutions. While nonlocalized ones included periodic waves and polynomial solutions. At the same time, we give the figure of the smooth solitary, solitary waves with blow-up points, rational solution with decay and periodic waves. Those obtained new waves might show some special phenomena in transporting energy.

Keywords-component; DNA dynamics; Traveling waves; Smooth solitary waves

I. INTRODUCTION

The investigation of DNA dynamics via continuous and discrete models has successfully predicted the appearance of important nonlinear structures. It has also been shown that nonlinearity is responsible for forming localized waves. These localized waves are extremely interesting because they have the capability to transport energy without any dissipation [1-8].

Recently, there are several works about DNA dynamics. In [9] Cadoni M, De Leo R and Gaeta G propose and investigate, both analytically and numerically, a "composite" version of the Y model, in which the sugar-phosphate group and the base are described by separate degrees of freedom. Peng XF focused on The properties of bio-energy transport and influence of structure nonuniformity and temperature of systems on energy transport along polypeptide chains [10]. J. D. Bashford [11]did some research for the sequence-dependent behaviour of localised excitations in a toy, nonlinear model of DNA base-pair opening originally proposed by Salerno. Specifically for whether “breather” solitons could play a role in the facilitated location of promoters by RNA polymerase (RNAP). For the inhomogeneous, DNA double helical molecular chain with flexible strands is investigated by studying its internal dynamics in [12] For the study, a generalized model which takes into account the energies involved in stacking and hydrogen bonds along with inhomogeneity, helicity, and phonons coupled to the stacking and hydrogen bonds is proposed. By using Riccati parameterized factorization method, W.Alka, Amit Goyal, C.Nagaraja. Kumar[13] studied the nonlinear dynamics of DNA, for longitudinal and transverse motions, in the framework of the microscopic model of Peyrard and Bishop, which consists of two long elastic homogeneous strands connected with each other by an elastic membrane. The improved Dauxoi–Peyrard–Bishop model for DNA as the simplest one for describing the appearance of nonlinear structures was analyzed by A Aguero and Jose Pecina in [14], and obtained new nonclassical traveling wave solutions i.e. anti-cuspon and peakon for specific restricted parametric values of the model. What about the propagation of a soliton-like excitation in a DNA was investigated through numerical integration of the motion equations[15], it showed that discreteness can completely change the soliton shape and the impact of viscosity as well as elasticity on DNA dynamic is also presented.

In [16], Daniel M,Vanitha M studied the internal nonlinear dynamics of an inhomogeneous short lattice DNA model, which is expressed in terms of open-state configurations represented by kink and antikink solitons with fluctuations, by solving numerically the governing discrete perturbed sine-Gordon equations under the limits of a uniform and a nonuniform angular rotation of bases.

What about the Perturbed soliton excitations of the nonlinear dynamics of the inhomogeneous DNA double-helical chain was studied in [17], by using the dynamic plane–base rotator model by considering angular rotation of bases in a plane normal to the helical axis. And inspired by [17], V Vasumathi and M Daniel obtained the conclusions about perturbed solution-like molecular excitations in a deformed DNA chain in [18] .By an analysis of a multiple scale soliton perturbation, it solved the perturbed sine-Gordon equation and the resultant perturbed kink and antikink solitons represent open state configuration with small fluctuation. The perturbation due to periodic deformation of the lattice changes the velocity of the soliton, but the width remains unchanged. Slobodan Zdravkovic and Miljko V. Sataric studied a possible solitary wave solution of the nonlinear Schrödinger equation (NLSE) and DNA dynamics in [19] ,in which it was shown that the wave can be both modulated and nonmodulated depending on a ratio of the envelope and the carrier wave velocities.

In order to study some important aspects of DNA at the scale of base pairs, the oscillator-chain PB model proposed by Peyrard and Bishop has successfully predicted the appearance of solitonic structures [7]. Taking into consideration the inharmonic potential, Aguero et al. gave and studied the modified PB model [1] formed asThe paper is to be written in two-column format and be right and left justified. The column width should be 85 mm (3.35 inches). The gap between the two columns should be 5 mm (0.2 inches).

(1) $$y_{tt} - [C_1 + 3C_2 y_x^2] y_{xx} - 2\alpha D e^{-\alpha y}(e^{-\alpha y} - 1) = 0$$

where C_1, C_2, D and α are constants. By a direct integral method, taking the integral constant to be some special value and a special change of variable, Aguero et al. obtained some nonclassical solution.

It is clear that the results in [1] are incomplete for the modified PB model. The purpose of this paper lies in a more complete study of the explicit traveling wave solutions. In this paper, by considering integral constants different from [1], we fortunately obtain some new explicit
traveling wave solutions, including localized waves and nonlocalized ones.

This paper is organized as follows. In Section 2, some new explicit forms of traveling waves are given by a direct integral method. Last section is the conclusion.

II. NEW TRAVELING WAVES

For a traveling wave $S = X - V_t$, Eq.(1) takes the form after integrating once

(2)
$$\frac{V^2 - C_1}{2} y_s^2 - \frac{3}{4} C_2 y_s^4 + D e^{-\alpha y}(e^{-\alpha y} - 2) + C = 0$$

where C is an arbitrary integration constant. In order to simplify Eq.(2), we need to redefine the variables as follows

(3) $$\phi = e^{-\alpha y}$$

Clearly, the fuction ϕ is positive. Hence we have $y = -\frac{1}{\alpha}\ln\phi$ and $y_s = -\frac{\phi_s}{\alpha\phi}$ .Substituting y and y_s into (2), we obtain

(4) $$A\phi_s^4 - B\phi_s^2\phi^2 - D\phi^5(\phi - 2) - C\phi^4 = 0,$$

where $A = \frac{3}{4\alpha^4} C_2$ and $B = \frac{V^2 - C_1}{2\alpha^2}$.

Simplifying (4) lets to

(5) $$\phi_s^2 = \frac{\phi^2}{2}(a + k\sqrt{4b(\phi - 1)^2 + a^2 - 4b + 4c})$$

where $k = \pm 1, \alpha = \frac{B}{A}, b = \frac{D}{A}$ and $c = \frac{C}{A}$

Letting $a^2 - 4b + 4c = 0$, that is, taking an integral constant $D = \frac{B^2}{4A} + C$ which is not the same as [1], then (5) becomes

(6) $$\phi_s^2 = \phi^2(\frac{a}{2} - k\sqrt{b} + k\sqrt{b}\phi)$$

By considering the different values of a, b, k and noting the fact that ϕ is positive, we can obtain a series of fundamental solutions of Eq.(6) as follows.

If $b = 0$, we have $\phi = \lambda \exp[\pm\sqrt{\frac{a}{2}}(s - s_0)]$, where $\lambda > 0$.

If $\frac{a}{2} - k\sqrt{b} > 0$ and $b > 0$, we have $$\phi = \frac{a}{2\sqrt{b}} + 1 + \sec h^2[\frac{1}{2}\sqrt{\frac{a}{2} + \sqrt{b}}(s - s_0)].$$

If $\frac{a}{2} - k\sqrt{b} > 0$ and $b > 0$, we can also obtain $$\phi = \frac{a}{2\sqrt{b}} - 1 + \csc h^2[\frac{1}{2}\sqrt{\frac{a}{2} - \sqrt{b}}(s - s_0)].$$

If $\frac{a}{2} - k\sqrt{b} = 0$ and $b > 0$,we have $$\phi = \sqrt{\frac{\alpha}{8}}(s - s_0)^{-2}.$$

If $\frac{a}{2} - k\sqrt{b} < 0$ and $b > 0$, we have $$\phi = -\frac{a}{2\sqrt{b}} + 1 + \sec^2[\frac{1}{2}\sqrt{\sqrt{b} - \frac{a}{2}}(s - s_0)].$$

By Eq.(3) and the above analysis, we find that Eq. (1) possesses some new traveling waves, which are classified as follows.

- Case A

If $D=0$, Eq.(1) possesses the polynomial solutions

$$y=-\frac{\mu}{\alpha}\pm\frac{1}{\alpha}\sqrt{\frac{B}{2A}}(s-s_0)$$

where μ is an arbitrary constant.

- Case B

If $\frac{B}{2A}+\sqrt{\frac{D}{A}}>0$ and $D>0$, Eq. (1) admits the smooth solitary waves

$$y=-\frac{1}{\alpha}\ln\{\frac{B}{2\sqrt{AD}}+1+\sec h^2[\frac{1}{2}\sqrt{\frac{B}{2A}+\sqrt{\frac{D}{A}}}(s-s_0)]\}$$

Its 2-dimension graph when $t=0$ is shown in Fig.1 with $B=\alpha=A=D=1, s_0=0$.

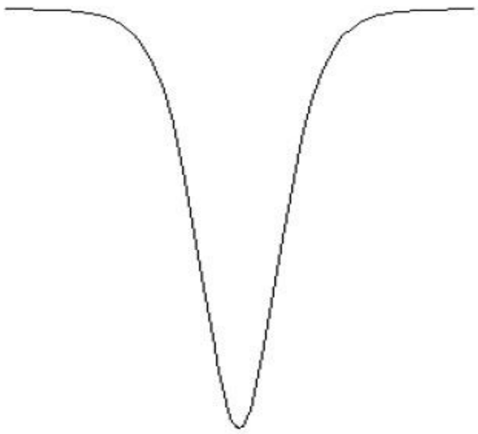

Figure 1. Smooth solitary waves

- Case C

If $\frac{B}{2A}-\sqrt{\frac{D}{A}}>0$ and $D>0$, Eq. (1) admits the solitary waves with blow-up points

$$y=-\frac{1}{\alpha}\ln\{\frac{B}{2\sqrt{AD}}-1+\csc h^2[\frac{1}{2}\sqrt{\frac{B}{2A}-\sqrt{\frac{D}{A}}}(s-s_0)]\}$$

Its 2-dimension graph when $t=0$ is shown in Fig.2 with $B=3, \alpha=A=D=1, s_0=0$

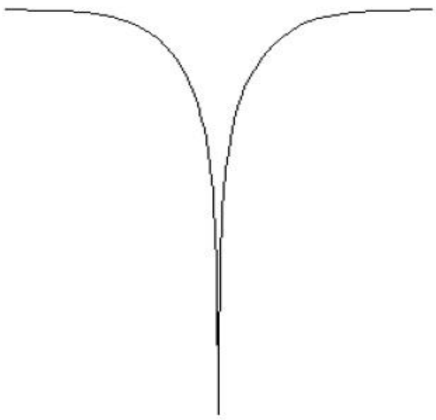

Figure 2. Solitary waves with blow-up points

- Case D

If $\frac{B}{2A}-\sqrt{\frac{D}{A}}=0$ and $D>0$,Eq. (1) admits the rational solutions with decay,

$$y=\sqrt{\frac{\alpha}{8}}(s-s_0)^{-2}$$

Its 2-dimension graph when $t=0$ is shown in Fig.3 with $\alpha=1, s_0=0$.

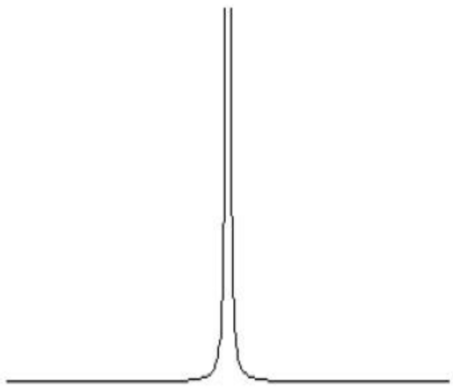

Figure 3.Rational solutions with decay

- Case E

If $\frac{B}{2A}+\sqrt{\frac{D}{A}}<0$ and $D>0$, Eq. (1) admits the periodic waves

$$y=-\frac{1}{\alpha}\ln\{\frac{B}{2\sqrt{AD}}+1+\sec^2[\frac{1}{2}\sqrt{-\frac{B}{2A}+\sqrt{\frac{D}{A}}}(s-s_0)]\}$$

Its 2-dimension graph when $t=0$ is shown in Fig.4 with $B=-3, \alpha=A=D=1, s_0=0$

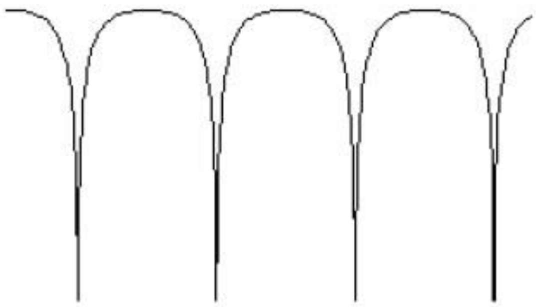

Figure 4.periodic waves

III. CONCLUSIONS

By a direct integral method, some localized traveling waves and nonlocalized traveling waves for the modified PB model were determined. Those localized waves included smooth solitary waves, solitary waves with blow-up points and rational solutions with decay. While nonlocalized ones included periodic waves and polynomial solutions. Those obtained new waves might show some special phenomena in transporting energy.

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