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Soliton dynamics in a modified Yakushevich model

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Abstract. We study a modified Yakushevich model with different disc diameters representing different bases and find two new in-phase solitonic solutions. We also discuss here the effect of helical structure which acts as perturbation on soliton centre of mass.

Keywords. Solitons; DNA dynamics; Fourier series; non-linear coupled equations.

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1. Introduction

For nearly two decades the role of soliton in DNA dynamics has been stressed by various researchers. In modeling double DNA strands, coupled non-linear equations were first used by Yomosa in 1983 [1,2] and then by Takeno and Homma [3] in which the base was depicted as an arrow and complementary base pairs were described by conjugate arrows directed inward. He obtained in the continuum limit, coupled sine-Gordon equations in order to describe the motion of rotation of the bases. In some particular cases soliton-like solutions were found and Yomosa estimated the velocity to be 8.3×10^3 cm/s and width nine times the distance between two bases. He also calculated number density of these excitations as well as average number of bases in open states. Takeno and Homma [3] modified this plane base rotator model by including discreteness of the structure. In a particular case the differential difference equations can be decoupled into double sine-Gordon equations (DsG). Though DsG equation is not a completely integrable system it has solitonic solutions with richer dynamics than the sG model utilized by Yomosa. Zhang [4] in 1987, considered interstrand interactions through hydrogen bonds and also took into account the prominent dipole interaction and the dispersion interaction between two bases in a complementary base pair. The dynamics of the rotations of the bases was described by a set of coupled DsG equations with solitonic solutions. Yakushevich in 1989 [5] introduced two non-linear coupled equations to discuss the torsion dynamics of DNA structure. The bases were considered as hard discs whose position along DNA double helix is fixed in space. The collective changes in DNA molecule in space were neglected. This model consists of two chains of discs connected with each other by longitudinal and transverse springs. The longitudinal potential which represents interaction through sugar phosphate backbone structure is taken harmonic whereas the non-linearity was introduced via intrastrand potential. In some special cases this model decoupled into sine-Gordon (sG) and double sine-Gordon (DsG) equations. In this way the dynamics was described by sG kinks as well as solitonic excitations of DsG equation. But they could not find out general solutions when the equations do not decouple. One of the purposes of this paper is to apply the method of mixing exponentials in order to examine whether the solutions exist in decoupling limit only or general coupled solutions in functional form are possible. This mixing exponential method has now been applied to numerous non-linear equations; single, coupled, discrete as well as partial differential cases [6–10]. Recently by the application of this method to two-coupled field equations, some solutions not obtained by other methods are reported [10]. These new solutions also include collapsible shock states which accompany all the solitonic solutions of those coupled equations. For the present coupled equations modeling DNA, we investigate these possibilities. Again Yakushevich has considered the diameters of the discs representing different base pairs to be equal and also neglected the influence of helical structure in the dynamics. In the present work, we have taken different diameters for different bases and also we include a weak interaction due to helical structure of the chains. In §2 we take into account modified Yakushevich Hamiltonian with different disc diameters and apply mixing exponential method to the equations of motion. Section 3 deals with the effect of helicity and §4 contains the discussions of results and conclusions.

2. Model equations

Yakushevich model is an important step in the study of structure and dynamics of biopolymers. The non-linear dynamics envisaged in the model is designed to study the phenomena in nanosecond range. Since the non-linear dynamics is a part of general complex dynamics of DNA chains, it possesses a close link with more accurate structural models. In that sense the model has strong analogy with Barkley and Zimm's [11] computer simulated structure. Now-a-days fairly large amount of information are available on the structure of DNA molecules and the long chain. It is becoming comparatively easier to form non-linear models to explain experimental results of microwave absorption, neutron scattering, transcription and replication. It should be clearly kept in mind that Yakushevich model consisting of rods and discs are designed to study the phenomena associated with nanosecond range only, where interaction between chains can be considered as elastic forces between hydrogen molecules and along the chain it may be imagined as long rods capable of twist motion. However, the rods cannot be straight and small interaction must be of importance due to helicity. Though Yakushevich has neglected this effect it can later be included, once the appropriate solitonic excitations are identified. To understand these excitations, Yakushevich has extracted from the model two coupled equations [4] by considering equal diameters for the discs representing bases. However, when two strands are considered the diameters of different bases will be unequal. Hence, we propose the following simplified coupled equations to model DNA dynamics.

$$u_{1xt} = -\lambda \sin u_1 + \eta \sin(u_1 + u_2), \tag{1}$$

$$u_{2xt} = -\lambda \sin u_2 + \eta \sin(u_1 + u_2), \tag{2}$$

where u is the field variable and η, λ are parameters and subscripts represent partial derivatives. The form of eq. (1) and (2) are chosen with general parameters η, λ so that it can be used to study a general modified model where diameters of the discs representing bases are different. When $\lambda = 2\eta$, the model will reduce to Yakushevich equations with discs of equal diameters.

2.1 *Application of mixing exponential method*

We now consider two transformations, namely, inverse and direct transformations.

(1) *Inverse transformation*

This transformation is identified by

$$u_1 = 2\tan^{-1}\left(\frac{1}{\psi_1}\right),$$
$$u_2 = 2\tan^{-1}\left(\frac{1}{\psi_2}\right). \tag{3}$$

Using these transformations, eqs (1) and (2) can be rewritten as

$$\psi_{1xt} + \psi_{1xt}\psi_1^2 + \psi_{1xt}\psi_2^2 + \psi_{1xt}\psi_1^2\psi_2^2 - 2\psi_{1x}\psi_{1t}\psi_1\psi_2^2 - 2\psi_{1x}\psi_{1t}\psi_1$$
$$= \psi_1(\eta + \lambda) + \eta\psi_2 + (\eta + \lambda)\psi_1^3 - (\eta - \lambda)\psi_1\psi_2^2 - (\eta - \lambda)\psi_1^3\psi_2^2 - \eta\psi_2\psi_1^4 \tag{4}$$

and

$$\psi_{2xt} + \psi_{2xt}\psi_2^2 + \psi_{2xt}\psi_1^2 + \psi_{2xt}\psi_1^2\psi_2^2 - 2\psi_{2x}\psi_{2t}\psi_2 - 2\psi_{2x}\psi_{2t}\psi_2\psi_1^2$$
$$= \psi_2(\eta + \lambda) + \eta\psi_1 + (\eta + \lambda)\psi_2^3 - (\eta - \lambda)\psi_2\psi_1^2 - (\eta - \lambda)\psi_2^3\psi_1^2 - \eta\psi_1\psi_2^4. \tag{5}$$

In the most general case the solutions of eqs (4) and (5) can be written as

$$\psi_1 = C + \hat{\psi}_1, \tag{6}$$

$$\psi_2 = C + \hat{\psi}_2. \tag{7}$$

Substitution of expressions (6) and (7) in relations (4) and (5) yield equations containing $\hat{\psi}_1\hat{\psi}_2$, linear part of which will have exponential solutions, $\exp[\pm K(v)z]$ provided

$$C[(2\eta+\lambda)+C^2(2\lambda)-C^4(2\eta-\lambda)]=0. \tag{8}$$

Solving the above equation we get

$$C=0 \quad \text{or} \quad C=\pm\sqrt{\frac{2\eta+\lambda}{2\eta-\lambda}}. \tag{9}$$

Now with $C=0$

Let us take a scaling,

$$\begin{aligned}\hat{\psi}_1 &= \pm\sqrt{\frac{2\eta+\lambda}{2\eta-\lambda}}\tilde{\psi}_1,\\ \hat{\psi}_2 &= \pm\sqrt{\frac{2\eta+\lambda}{2\eta-\lambda}}\tilde{\psi}_2.\end{aligned} \tag{10}$$

Here we choose exponential series expansions as

$$\begin{aligned}\psi_1 &= \sum_{n=1}^{\infty} a_n g^n,\\ \psi_2 &= \sum_{n=1}^{\infty} b_n g^n\end{aligned} \tag{11}$$

with

$$g(z)=\mathrm{e}^{-Kz} \quad \text{and} \quad z=x-\nu t. \tag{12}$$

Using eqs (10) and (11) in eqs (4) and (5) and considering the linear part we have

$$\begin{aligned}&\text{(a)} \qquad K^2=-\frac{(\lambda+2\eta)}{V}\\ &\text{(b)} \qquad K^2=-\frac{\lambda}{V}.\end{aligned} \tag{13}$$

1(a)

$$K^2=-\frac{(\lambda+2\eta)}{V} \text{ implies } a_1=b_1.$$

The recursion relation becomes

$$\begin{aligned}&[(2\eta+\lambda)n^2-(\eta+\lambda)]a_n-\eta b_n\\ &\quad=\sum_{m=2}^{n-1}\sum_{l=1}^{m-1} a_1 a_{m-1} a_{n-m}\left[2lmA-3Al^2+\left(\frac{\eta+\lambda}{2\eta+\lambda}\right)A\right]\end{aligned}$$

$$
\begin{aligned}
&+\sum_{m=2}^{n-1}\sum_{l=1}^{m-1} a_1 b_{m-1} b_{n-m}\left[-Al^2-\left(\frac{\eta-\lambda}{2\eta+\lambda}\right)A\right]\\
&+\sum_{q=4}^{n-1}\sum_{p=3}^{q-1}\sum_{m=2}^{p-1}\sum_{l=1}^{m-1} a_1 a_{m-1} a_{p-m} b_{q-p} b_{n-q}\\
&\times\left[\frac{2(2\eta+\lambda)}{2\eta-\lambda}Alm-3\frac{(2\eta+\lambda)}{2\eta-\lambda}Al^2-\frac{(\eta-\lambda)}{2\eta-\lambda}A\right]\\
&-\eta\frac{(A)}{2\eta-\lambda}\sum_{q=4}^{n-1}\sum_{p=3}^{q-1}\sum_{m=2}^{p-1}\sum_{l=1}^{m-1} b_1 a_{m-1} a_{p-m} a_{q-p} a_{n-q}
\end{aligned}
\tag{14}
$$

and

$$
\begin{aligned}
&[(2\eta+\lambda)n^2-(\eta+\lambda)]b_n-\eta a_n\\
&=\sum_{m=2}^{n-1}\sum_{l=1}^{m-1} b_1 b_{m-1} b_{n-m}\left[2lmA-3Al^2+\frac{(\eta+\lambda)}{(2\eta+\lambda)}A\right]\\
&+\sum_{m=2}^{n-1}\sum_{l=1}^{m-1} b_1 a_{m-1} a_{n-m}\left[-Al^2-\frac{(\eta-\lambda)}{(2\eta+\lambda)}A\right]\\
&+\sum_{q=4}^{n-1}\sum_{p=3}^{q-1}\sum_{m=2}^{p-1}\sum_{l=1}^{m-1} b_1 b_{m-1} b_{p-m} a_{q-p} a_{n-q}\\
&\times\left[\frac{2(2\eta+\lambda)}{2\eta-\lambda}Alm-3\frac{(2\eta+\lambda)}{2\eta-\lambda}Al^2-\frac{(\eta-\lambda)}{2\eta-\lambda}A\right]\\
&-\eta\frac{(A)}{2\eta-\lambda}\sum_{q=4}^{n-1}\sum_{p=3}^{q-1}\sum_{m=2}^{p-1}\sum_{l=1}^{m-1} a_1 b_{m-1} b_{p-m} b_{q-p} b_{n-q},\quad \text{for } n\geq 3
\end{aligned}
$$

and

$$
A=\frac{(2\eta+\lambda)^2}{2\eta-\lambda}.
$$

By solving the above recursion relation with a_1 arbitrary and positive,

$$
\begin{aligned}
a_3&=\left(\frac{\lambda}{4(2\eta-\lambda)}\right)a_1^3=b_3,\quad a_2=b_2=0\\
a_5&=\left(\frac{\lambda}{4(2\eta-\lambda)}\right)^2\cdot a_1^5=b_5,\quad a_4=b_4=0\\
a_7&=\left(\frac{\lambda}{4(2\eta-\lambda)}\right)^3\cdot a_1^7=b_7,\quad a_6=b_6=0.
\end{aligned}
$$

Thus $a_{2n}=b_{2n}=0$ and

$$
a_{2n+1}=2\sqrt{\frac{2\eta-\lambda}{\lambda}}a^{2n+1}=b_{2n+1},
$$

where

$$a = \sqrt{\frac{\lambda}{4(2\eta - \lambda)}} \cdot a_1. \tag{15}$$

$$\tilde{\psi}_1 = \sum_{n=0}^{\infty} a_{2n+1} g^{2n+1} = 2\sqrt{\frac{2\eta - \lambda}{\lambda}} \sum_{n=0}^{\infty} (ag)^{2n+1} = \sqrt{\frac{2\eta - \lambda}{\lambda}} \operatorname{cosech} x,$$

where

$$ag = \mathrm{e}^{-x} = e - (Kz + \delta) \quad \text{and} \quad x = (Kz + \delta)$$

$$\psi_1 = \hat{\psi}_1 = \pm\sqrt{\frac{2\eta + \lambda}{\lambda}} \operatorname{cosech} x.$$

Similarly

$$\psi_2 = \pm\sqrt{\frac{2\eta + \lambda}{\lambda}} \operatorname{cosech} x.$$

The solutions of eqs (1) and (2) can be written as

$$u_1 = 2\tan^{-1}\left(\frac{1}{\psi_1}\right) = 2\tan^{-1}\left[\pm\sqrt{\frac{\lambda}{2\eta + \lambda}} \sinh x\right]$$

and

$$u_2 = 2\tan^{-1}\left(\frac{1}{\psi_2}\right) = 2\tan^{-1}\left[\pm\sqrt{\frac{\lambda}{2\eta + \lambda}} \sinh x\right]. \tag{16}$$

Choosing negative values of a_1

$$a_{2n+1} = (-1)^n \cdot 2\sqrt{\frac{\lambda - 2\eta}{\lambda}} a^{2n+1} = b_{2n+1} \quad \text{and} \quad a_{2n} = b_{2n} = 0$$

$$\tilde{\psi}_1 = \sum_{n=0}^{\infty} a_{2n+1} g^{2n+1} = \sqrt{\frac{\lambda - 2\eta}{\lambda}} \operatorname{sech} x$$

$$\psi_1 = \hat{\psi}_1 = \pm\sqrt{\frac{-(\lambda + 2\eta)}{\lambda}} \operatorname{sech} x.$$

Similarly

$$\psi_2 = \pm\sqrt{\frac{-(\lambda + 2\eta)}{\lambda}} \operatorname{sech} x.$$

The solutions of eqs (1) and (2) can be written as

$$u_1 = 2\tan^{-1}\left[\pm\sqrt{\frac{-\lambda}{2\eta+\lambda}}\cosh x\right]$$

and

$$u_2 = 2\tan^{-1}\left[\pm\sqrt{\frac{-\lambda}{\lambda+2\eta}}\cosh x\right]. \tag{17}$$

The coefficients λ, η and v are so chosen that the expression under radicals are positive.

1(b)

$$\begin{aligned}
&K^2 = -\frac{\lambda}{V} \quad \text{implies } a_1 = -b_1\\
&a_{2n} = 0 = -b_{2n}\\
&a_{2n+1} = \frac{2}{C}\cdot a^{2n+1} \quad \text{where } a = \frac{C}{2}a_1\\
&\psi_1 = \pm\sqrt{\frac{2\eta+\lambda}{2\eta-\lambda}}\tilde{\psi}_1 = \operatorname{cosech} x; \quad \psi_2 = -\operatorname{cosech} x.
\end{aligned}$$

The solutions of eqs (1) and (2) can be written as

$$u_1 = 2\tan^{-1}\left(\frac{1}{\psi_1}\right) = 2\tan^{-1}\sinh x$$

and

$$u_2 = 2\tan^{-1}\left(\frac{1}{\psi_2}\right) = -2\tan^{-1}\sinh x. \tag{18}$$

(2) *Direct transformation*

The direct transformation can be written as

$$u_1 = 2\tan^{-1}\psi_1 \quad \text{and} \quad u_2 = 2\tan^{-1}\psi_2. \tag{19}$$

Now using eq. (19) in eqs (1) and (2) we obtain

$$\begin{aligned}
&\psi_{1xt} + \psi_{1xt}\psi_1^2 + \psi_{1xt}\psi_2^2 + \psi_{1xt}\psi_1^2\psi_2^2 - 2\psi_{1x}\psi_{1t}\psi_1 - 2\psi_{1x}\psi_{1t}\psi_2^2\\
&= \psi_1(\eta-\lambda) + \eta\psi_2 + \psi_1^3(\eta-\lambda) - (\eta+\lambda)\psi_1\psi_2^2\\
&\quad - (\eta+\lambda)\psi_1^3\psi_2^2 - \eta\psi_1^4\psi_2
\end{aligned} \tag{20}$$

and

$$\begin{aligned}
&\psi_{2xt} + \psi_{2xt}\psi_2^2 + \psi_{2xt}\psi_1^2 + \psi_{2xt}\psi_2^2\psi_1^2 - 2\psi_{2x}\psi_{2t}\psi_2 - 2\psi_{2x}\psi_{2t}\psi_2\psi_1^2\\
&= \psi_2(\eta-\lambda) + \eta(\psi_1) + \psi_2^3(\eta-\lambda) - (\eta+\lambda)\psi_2\psi_1^2\\
&\quad - (\eta+\lambda)\psi_2^3\psi_1^2 - \eta\psi_2^4\psi_1.
\end{aligned} \tag{21}$$

Substituting eqs (6) and (7) in eqs (20) and (21) yield equations containing $\hat{\psi}_1$, the linear part of which will have exponential solutions $\exp[\pm K(v)z]$, provided

(a) $C = 0$,

(b) $C = \pm\sqrt{\dfrac{(2\eta-\lambda)}{(2\eta+\eta)}}$.

2(a)

When $C = 0$,

$$K^2 = \frac{\lambda - 2\eta}{V} \quad \text{or} \quad K^2 = \left(\frac{\lambda}{V}\right).$$

(i) For $K^2 = (\lambda - 2\eta)/V$, the recursion relation becomes

$$\begin{aligned}
&[(2\eta-\lambda)n^2 - (\eta-\lambda)]a_n - \eta b_n \\
&= \sum_{m=2}^{n-1}\sum_{l=1}^{m-1} a_1 a_{m-1} a_{n-m}[(2\eta-\lambda)(-3l^2+2lm) + (\eta-\lambda)] \\
&\quad + \sum_{m=2}^{n-1}\sum_{l=1}^{m-1} a_1 b_{m-1} b_{n-m}[(2\eta-\lambda)(-l^2) - (\eta+\lambda)] \\
&\quad + \sum_{q=4}^{n-1}\sum_{p=3}^{q-1}\sum_{m=2}^{p-1}\sum_{l=1}^{m-1} a_1 a_{m-1} a_{p-m} b_{q-p} b_{n-q}[(2\eta-\lambda)(-3l^2+2lm) - (\eta+\lambda)] \\
&\quad - \eta \sum_{q=4}^{n-1}\sum_{p=3}^{q-1}\sum_{m=2}^{p-1}\sum_{l=1}^{m-1} b_1 a_{m-1} a_{p-m} a_{q-p} a_{n-q}.
\end{aligned} \tag{22}$$

and

$$\begin{aligned}
&[(2\eta-\lambda)n^2 - (\eta-\lambda)]b_n - \eta a_n \\
&= \sum_{m=2}^{n-1}\sum_{l=1}^{m-1} b_1 b_{m-1} b_{n-m}[(2\eta-\lambda)(-3l^2+2lm) + (\eta-\lambda)] \\
&\quad + \sum_{m=2}^{n-1}\sum_{l=1}^{m-1} b_1 a_{m-1} a_{n-m}[(2\eta-\lambda)(-l^2) - (\eta+\lambda)] \\
&\quad + \sum_{q=4}^{n-1}\sum_{p=3}^{q-1}\sum_{m=3}^{p-1}\sum_{l=1}^{m-1} b_1 b_{m-1} b_{p-m} a_{q-p} a_{n-q}[(2\eta-\lambda)(-3l^2+2lm) - (\eta+\lambda)] \\
&\quad - \eta \sum_{q=4}^{n-1}\sum_{p=3}^{q-1}\sum_{m=2}^{p-1}\sum_{l=1}^{m-1} a_1 b_{m-1} b_{p-m} b_{q-p} b_{n-q}.
\end{aligned} \tag{23}$$

Solving the above recursion relations we get the solutions as

$$u_1 = 2\tan^{-1}\sqrt{\frac{(2\eta-\lambda)}{\lambda}}\operatorname{sech} x,$$
$$u_2 = 2\tan^{-1}\sqrt{\frac{(2\eta-\lambda)}{\lambda}}\operatorname{sech} x, \tag{24}$$

where $x = (Kz+\delta)$ and for

$$K = \sqrt{\frac{(\lambda-2\eta)}{V}},$$
$$u_1 = 2\tan^{-1}\sqrt{\frac{(\lambda-2\eta)}{\lambda}}\operatorname{cosech} x,$$
$$u_2 = 2\tan^{-1}\sqrt{\frac{(\lambda-2\eta)}{\lambda}}\operatorname{cosech} x. \tag{25}$$

λ, η and V are so chosen that the expression under radicals are positive.

(ii) Now $K^2 = \lambda/V$ implies $a_1 = -b_1$.

The solutions of eqs (1) and (2) become

$$u_1 = 2\tan^{-1}\psi_1 = 2\tan^{-1}\operatorname{cosech} x,$$
$$u_2 = 2\tan^{-1}\psi_2 = -2\tan^{-1}\operatorname{cosech} x, \tag{26}$$

2(b)

$$C = \pm\sqrt{\frac{(2\eta-\lambda)}{(2\eta+\lambda)}}.$$
$$K^2 = \frac{(2\eta-\lambda)(2\eta+\lambda)}{2\eta V} \quad \text{and} \quad a_1 = b_1.$$

The solutions of eqs (1) and (2) become

$$u_1 = 2\tan^{-1}\left[\pm\sqrt{\frac{(2\eta-\lambda)}{(2\eta+\lambda)}}\tanh\frac{x}{2}\right],$$
$$u_2 = 2\tan^{-1}\left[\pm\sqrt{\frac{(2\eta-\lambda)}{(2\eta+\lambda)}}\tanh\frac{x}{2}\right]. \tag{27}$$

Here the following choices are considered,

$$ag = \mathrm{e}^{-x},$$

where $a = a_1/2$ and a_1 is negative.

If the positive value of a_1 is taken, the solutions of eqs (1) and (2) become

$$u_1 = 2\tan^{-1}\left[\pm\sqrt{\frac{(2\eta-\lambda)}{(2\eta+\lambda)}}\coth\frac{x}{2}\right],$$

$$u_2 = 2\tan^{-1}\left[\pm\sqrt{\frac{(2\eta-\lambda)}{(2\eta+\lambda)}}\coth\frac{x}{2}\right]. \tag{28}$$

2.2 *Discussion of the result*

Modified Yakushevich model is essentially a coupled set of double sine-Gordon equations used to model DNA dynamics with different disc diameters. In the literature, solutions of double sine-Gordon model were elaborately studied by Condat *et al* [12] who obtained a variety of solitary wave solutions in the form of $\tan^{-1}$ (tanh), $\tan^{-1}$ (sech) and $\tan^{-1}$ (cosech). In our study of coupled DsG equation by mixing exponential method, we find two new solutions in the form of $\tan^{-1}$ (sinh) and $\tan^{-1}$ (cosh) besides the previously reported forms as in eqs (27), (28), (24) and (25). Again coupled non-linear equations involving NLS and KdV were studied by the present authors [8] using mixing exponential approach and some new solutions are reported, which includes shock structures that always accompany solitary waves in those coupled regime. Now, the coupled equations involving double sG equations do not exhibit this characteristic. No collapsible states in the form of diverging solutions appear in the present case. So blown up phenomena cannot be discussed by these models.

To summarize, the mixing exponential method shows that the only solutions in functional form possible in modified Yakushevich model are the in-phase solitons where $u_1 = u_2$ or out-of-phase solitons where $u_1 = -u_2$. Since solutions with other values of expansion coefficients in eq. (11) could not be found out, it suggests that other forms of solitonic solutions in functional form are not admissible for Yakushevich model. The in-phase solitons of double sG equation travel in both chains and the regime contains a richer dynamics because a variety of solutions exist as given in eqs (16), (17), (24), (25), (27) and (28). The solutions obtained in eqs (16), (17) have been reported here for the first time with the use of mixing exponential method. However, all these solutions are expected to represent enormous varieties of motions exhibited by a large number of degrees of freedom associated with the DNA molecule.

Further, the equations reduce to Yakushevich case when $\lambda = 2\eta$ and in that limit, solitons represented by eqs (28), (27), (25) and (24) vanish and the only solutions will be the new solutions found in eqs (16) and (17).

3. Helicity as perturbation

We consider here a helical perturbation in the form of the following function because it is very weak as the bases interact via water molecules due to proximity of 5 units on each side but not through direct bonding.

$$V = \varepsilon K_H d^2\{(u_1-u_2)^2 + \frac{\alpha}{2}(u_1-u_2)^4\},$$

with K_H as the interaction strength, ε represents the order of smallness of helicity, $d = 2kh$, with h representing distance among bases, d the distance in space among bases interacting through helicoidal potential, and $k = 5$.

This potential will contribute an extra term to eqs (1) and (2) so that

$$u_{1tt} - u_{1xx} + \lambda \sin u_1 - \eta \sin(u_1 + u_2)$$
$$= \varepsilon G\{(u_1 - u_2) + \alpha(u_1 - u_2)^3\},$$
$$u_{2tt} - u_{2xx} + \lambda \sin u_2 - \eta \sin(u_1 + u_2)$$
$$= \varepsilon G\{(u_2 - u_1) + \alpha(u_2 - u_1)^3\},$$

where $G = K_H d^2$.

Now for in-phase solitons, $u_1 = u_2$ and contribution from helicity is zero whereas the dynamics of out-of-phase solitons with $u_1 = -u_2$ can be described by the equations

$$u_{tt} - u_{xx} + \lambda \sin u = 2\varepsilon G u + 8\varepsilon\alpha G u^3. \tag{29}$$

We study this perturbed sine-Gordon equation using linear perturbation analysis [13–15]. In this method a convenient complete set of functions are identified where the only bound state Goldstone mode describes the dynamics and continuous scattering states represent small change in soliton form. To build this complete set when scattering states are integrated, they interact coherently to create a pseudo-translation mode which cancels the effect of translation mode. So one should be careful in applying this method. If the initial conditions are such that scattering states predominate and act coherently, soliton motion will be heavily dependent on initial conditions. This will induce strong soliton phonon interaction and copious radiations will make the dynamics sensitive to initial input. On the other hand, for small perturbation limit it is expected that the perturbative effect acts at the centre of solitons, large scale radiation will not be induced and dynamics will be governed by the translations mode. The scattering states will only contribute to small shape change of the solitons. These effects can be discussed either by introducing a characteristic time (t_0) at which effect of scattering states is zero [14] or by discussing different initial conditions [15]. For the present purpose we assume that helical perturbation is not so strong to induce copious radiation and dynamics will then be analysed by the translation mode. Introducing a perturbation function $\psi(x,t)$.

$$u = u_s + \varepsilon\psi(x,t),$$

where u_s is the out-of-phase kink soliton.

Now

$$\psi_{tt} - \psi_{xx} + (1 - 2\,\mathrm{sech}^2 x)\psi = 2Gu_s + 8G\alpha u_s^3.$$

Expand $\psi(x,t)$ in the complete set given by

$$f_b(x) = (1/\sqrt{2})\mathrm{sech}\, x \quad \text{and} \quad f_k(x) = \frac{1}{\sqrt{(2\pi)}}\frac{\mathrm{e}^{ikx}}{k^2+1}(k + i\tanh x),$$

$$\psi(x,t) = a_b(t) f_b(x) + \int_{-\infty}^{\infty} a_k(t) f_k(x)\mathrm{d}k.$$

Here $a_b(t)$ is the translation mode coefficient which represents soliton translation. Substitution in eq. (29) and adoption of the procedure of linear perturbation analysis [13–15] gives

$$a_{btt} = \sqrt{2}G\pi^2 + 8\sqrt{2}G\alpha\pi^4. \tag{30}$$

Hence, the out-of-phase solitons will move with an acceleration given by eq. (30) due to helical structure of DNA chain.

4. Conclusion

In this work with the application of mixing exponential method we find that solutions to modified Yakushevich model are possible when expansion coefficients of mixing exponential series $a_n = b_n$ or $a_n = -b_n$. These choices give rise to in-phase or out-of-phase solitons. Since, with other choices, recursion relations are not amenable to solution, it suggests that other types of interacting solitons in functional form may not be obtainable either for the present modified case or for the original Yakushevich model. However, considering the energy functional corresponding to our model, the existence of classical solution can be visualized. Of course one cannot expect explicit formula for the solution. Secondly, for in-phase regime the present method finds two new solutions in the form of $\tan^{-1}$ (sinh) and $\tan^{-1}$ (cosh) in addition to the previously known solutions which are intended to explain numerous varieties of DNA motions. Further, the role of helicity is described as a perturbing effect which shows that in-phase solitons are not affected by the helical structure whereas the out-of-phase solitons move with accelerations. Lastly, the modified model discussed in this paper with two parameters λ and η are quite general and are intended to account for other phenomena described by coupled double sine-Gordon chains also.

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