NEW CLASSES OF STABLE EXACT SOLUTIONS FOR A NONLINEAR ROTATIONAL DNA MODEL*

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We consider a system of two coupled nonlinear partial differential equations for describing the rotational motions of bases in both polynucleotide chains of the DNA molecule. The model was proposed by L.V. Yakushevich and it is well known that the model supports, for some operating regimes, traveling wave solutions as kink–(antikink) soliton solutions. We have tried to make some progress by performing an analysis of the classical symmetries of this model. Our study shows that the model does not have enough symmetries as to reduce the equations to ordinary differential equations. Nevertheless, the known symmetries have been useful for finding several classes of exact solutions, by imposing adequate Ansätze. Some of them are kink–(antikink) like solutions, but other ones are not traveling wave solutions. For some of the new solutions, we have carried out a qualitative study and analyzed some stability properties. We think that they could be significant for the description of the DNA molecule as well as for some other applications.

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1. Introduction

Nonlinear physics of DNA is a part of nonlinear science which has attained an enormous development since the beginning of the last eighties. It is generally accepted that it started in 1980 with the article by Englander

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et al. [1] entitled *Nature of the Open State in Long Polynucleotide Double Helices: Possibility of Soliton Excitations*, where they proposed the first nonlinear Hamiltonian model of DNA.

The DNA molecule is a discrete system consisting of many atoms having a quasi-one-dimensional structure. There exist different kinds of interactions between the main atomic groups. One of them is the stacking interaction between neighboring bases along the DNA axis, these are short-range forces which stabilize the DNA structure and hold one base over the next one forming a stack of bases. The DNA can be considered as a complex dynamical system because DNA interacts with its environment in the cell, as many kind of proteins and thermal fluctuations can impose different functioning regimes.

A first approximation to a theoretical description of DNA begins by ignoring all the external influences and assuming that the amplitudes of the internal motions in DNA are small. This gives rise to the linear theory of DNA which is based on linear mathematical models. But without this last assumption, necessarily, the mathematical models are nonlinear, the mathematical difficulties increase and much more interesting phenomena appear. There are many experimental data and theoretical results published about the nonlinear properties of DNA (for a review see, *e.g.*, [2]). Many authors have contributed to the nonlinear theory of DNA by proposing improved Hamiltonian models and also working in the study of possible solutions to the dynamical equations. Among them, it is worth remarking the Peyrard–Bishop model [3] introduced for the study of DNA thermal denaturation. This model describes the motions of the displacements of the bases from their equilibrium positions along the direction of the hydrogen bonds that connect the two bases in a pair. Other approaches describe the rotational motions of bases in both polynucleotide chains of the DNA molecule. The Yakushevich model (Y-model) [4] belongs to this type of models and in a certain sense can be considered as an improved version of the Englander model, it is the continuous limit of a discrete model describing two chain of disks connected with one another by lengthwise and transverse springs. It consists in a system of two coupled nonlinear partial differential equations and at present nobody has succeeded in finding the general solution of this nonlinear system. However, after some assumptions the model can be reduced to the well known sine-Gordon equation or to the double sine-Gordon equation. In this context, kink soliton solutions have been found by Newton's method and by Hereman's method [5]. The sine-Gordon equation also appears in many branches of physics, where the known solutions have been applied, although to our knowledge some of them have not been related to the physics of DNA.

A method for finding some families of particular solutions is based on the introduction of some specific Ansätze that yield to a reduction of the system to a a well known partial differential equation or to ordinary differential equations. Sometimes, the Ansätze are suggested by particular functional regimes of the DNA molecule, as when it is imposed to some external constrains. Fortunately, there exists a method for obtaining a diversity of Ansätze which is based on the invariance properties of the system under Lie groups of transformations [7,8]. Following this procedure we have been able to find new classes of particular solutions some of which are not traveling waves and we have analyzed some stability properties.

This paper is organized as follows: Section 2 introduces the Y-model, and we perform a symmetry group analysis of this model obtaining the classical symmetries. In Section 3 we show that it is possible to obtain two classes of similarity solutions. One of them is constituted by traveling wave solutions, some of them can be obtained explicitly, but other ones are implicitly determined by integrals. The other class of solutions are not traveling waves solutions and we have carried out a qualitative study and analyzed some stability properties. Finally, a summary and some conclusions are presented in Section 4.

2. Symmetry properties of the Yakushevich model

The Y-model is a continuous model describing the dynamics of the DNA molecule, it takes into account the rotational motions of bases in both polynucleotide chains of DNA. As stressed by Yakushevich, it should be seen as the first step in a hierarchy of more and more realistic models, but its study deserves attention just due to its simplicity, opening the possibility of discovering some essential features of DNA torsion dynamics without unessential complications due to more realistic modeling. The Y-model is defined by the following two coupled nonlinear partial differential equations:

$$
\begin{aligned}
\alpha(\varphi_1)_{tt} &= \beta(\varphi_1)_{zz} + \delta(2\sin(\varphi_1) - \sin(\varphi_1 + \varphi_2)), \\
\alpha(\varphi_2)_{tt} &= \gamma(\varphi_2)_{zz} + \delta(2\sin(\varphi_2) - \sin(\varphi_1 + \varphi_2)),
\end{aligned}
\tag{1}
$$

where $\varphi_1(z,t)$ and $\varphi_2(z,t)$ represent the angles of rotation at the point z and time t of the polynucleotide chains 1 and 2, respectively, and $\alpha, \beta, \delta, \gamma$ are constant parameters.

System (1) is rather involved and only special classes of solutions are known. Most of the known solutions have been obtained after some assumptions are made, which are suggested by special regimes of the DNA dynamics, and by introducing some simple specific Ansätze. In most cases, only some specific classes of solutions of the reduced equations have been considered as applied to DNA.

It is expected that the most probable conformational distortions in DNA resulting in an open state configuration are obtained through an evolution with $\varphi_1 = -\varphi_2 = \varphi$ or with $\varphi_1 = \varphi_2 = \varphi$. Both assumptions make possible the reduction of the two-field model (1) to a one-field equation. The first assumption gives rise to the well known sine-Gordon equation and has been considered by many authors (see [2]). The second assumption gives rise to a double sine-Gordon equation. Nevertheless, to our knowledge nobody has connected sufficiently the richness of the solutions of both equations with the physics of DNA, and in particular with this rotational model.

If, for instance, we suppose that $\varphi_1 = -\varphi_2 = \varphi$, system (1) reduces to

$$(\gamma - \beta)\varphi_{zz} = 0\,,$$
$$2\alpha\varphi_{tt} - (\beta + \gamma)\varphi_{zz} - 4\delta\sin(\varphi) = 0\,. \tag{2}$$

This equation describes the torsion dynamics when the two DNA strands move out of phase by π.

If in addition we suppose $\beta = \gamma$, system (2) reduces to

$$\varphi_{tt} = a\varphi_{zz} + b\sin(\varphi)\,, \tag{3}$$

where $a = \frac{\beta}{\alpha}$ and $b = 2\frac{\delta}{\alpha}$.

Equation (3) is the sine-Gordon equation and, in the context of the Y-model, kink–(antikink) soliton solutions have been found following Newton's Method and Hereman's Method (see [2]). This equation also appears in relativistic field theory, condensed matter physics and in a number of other physical applications, as dislocations in crystals or the propagation of fluxons in Josephson junctions.

In this section we investigate the symmetry properties of system (1) under Lie groups of transformations [7, 8]. The knowledge of the invariance properties usually permits some reductions of the system and to obtain the so-called similarity solutions.

Since, nowadays, this is a standard method in the study of ordinary and partial differential equations, we omit the intermediate details and directly give the relevant reductions that the symmetry groups generate.

We denote by Z, T, U, V the infinitesimals corresponding to the variables $z, t, \varphi_1, \varphi_2$, respectively. The classical symmetries of system (1) can be obtained imposing the invariance conditions. The procedure leads to a complicated system of equations, from which we obtain the corresponding Lie group. Two cases appear, depending of the values of the parameters β and γ:

1. In the general case ($\beta \neq \gamma$), we obtain a 2-parameter Lie group given by

$$Z = c_1\,, \qquad T = c_2\,, \qquad U = 0\,, \qquad V = 0\,.$$

The infinitesimal generators of this group are

$$\boldsymbol{v}_1 = \frac{\partial}{\partial z}, \qquad \boldsymbol{v}_2 = \frac{\partial}{\partial t}. \tag{4}$$

2. In the special case of $\beta = \gamma$ we obtain a 3-parameter Lie group given by

$$Z = c_3 \beta t + c_1, \qquad T = c_3 \alpha z + c_2, \qquad U = 0, \qquad V = 0. \tag{5}$$

The generators of this group are $\boldsymbol{v}_1$, $\boldsymbol{v}_2$ and $\boldsymbol{v}_3 = \beta t \frac{\partial}{\partial z} + \alpha z \frac{\partial}{\partial t}$.

The commutator table is

	$\boldsymbol{v}_1$	$\boldsymbol{v}_2$	$\boldsymbol{v}_3$
$\boldsymbol{v}_1$	0	0	$\alpha \boldsymbol{v}_2$
$\boldsymbol{v}_2$	0	0	$\beta \boldsymbol{v}_1$
$\boldsymbol{v}_3$	$-\alpha \boldsymbol{v}_2$	$-\beta \boldsymbol{v}_1$	0

$$\tag{6}$$

As we can observe, for both cases the model lacks nontrivial symmetries. Nevertheless, the known symmetries are useful for finding new classes of stable exact solutions. We dedicate the next section to obtain the similarity solutions. Some of them are also kink–(antikink) soliton solutions, which are obtainable either explicitly or implicitly, and other ones are not traveling waves.

3. Similarity solutions

The known symmetries make it possible to obtain two classes of solutions, characterized by a different type of dependence with respect to the variables z, t.

3.1. Traveling wave solutions

The above results inform that, for both the cases $\beta \neq \gamma$ and $\beta = \gamma$, system (1) is invariant under the translations of $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$. This property leads us to look for traveling wave solutions.

These solutions are of the form

$$\varphi_1 = f_1(z + \lambda t), \qquad \varphi_2 = f_2(z + \lambda t). \tag{7}$$

Substituting, it can be seen that f_1 and f_2 must satisfy the following system of ordinary differential equations

$$\begin{aligned} a_1 f_1'' - 2\sin(f_1) + \sin(f_1 + f_2) &= 0, \\ a_2 f_2'' - 2\sin(f_2) + \sin(f_1 + f_2) &= 0, \end{aligned} \tag{8}$$

where $a_1 = \frac{\alpha \lambda^2 - \beta}{\delta}$; $a_2 = \frac{\alpha \lambda^2 - \gamma}{\delta}$ and the derivatives are with respect to the similarity variable $x = z + \lambda t$.

For obtaining similarity solutions of system (8) we have to determine its classical symmetries. However, we have investigated that system (8) lacks nontrivial symmetries. Therefore, Lie symmetries are of no help to reduce system (8) and the solutions, we are able to find, are consequence of some specific Ansätze.

Let us suppose that $f_2 = f_1 + 2k\pi$, being $k \in \mathbb{Z}$, and $a_1 = a_2$; in this case system (8) reduces to the equation

$$a_1 f_1'' - 2\sin(f_1) + \sin(2f_1) = 0. \tag{9}$$

With the appropriate change of the dependent variable, this equation can be written in a rational form or in a non transcendent form.

- Rational form:

  It can be achieved by making a change of the dependent variable in the form $f_1 = 2p \arctan(h)$, where p is a non null integer number. For each different value of p, a different ordinary differential equation for h is obtained. In the following, we consider the cases corresponding to $p = 1, 2, 3$. For any positive integer p, the corresponding possible values of the angle φ_1 are in the interval $(-p\pi, p\pi)$.

  1. Taking $p = 1$, the change of the dependent variable is $f_1 = 2\arctan(h)$, equation (9) becomes

  $$a_1 \left(1 + h^2\right) h'' - 2h \left(2h^2 + a_1 \left(h'\right)^2\right) = 0. \tag{10}$$

  We have found several families of solutions of this equation that determine the following solutions of (9) in terms of the Jacobi elliptic functions [9]:

  $$f_1 = \pm 2\arctan\left(\sqrt{\frac{-1-m}{2}} sn\left(\frac{2}{m-1}\sqrt{\frac{m+1}{a_1}}(x+c_1), m\right)\right),$$

  $$f_1 = \pm 2\arctan\left(\sqrt{\frac{-1-m}{2m}} sn^{-1}\left(\frac{2}{m-1}\sqrt{\frac{m+1}{a_1}}(x+c_1), m\right)\right),$$

  $$f_1 = \pm 2\arctan\left(\sqrt{\frac{1-2m}{2(m-1)}} cn\left(2\sqrt{\frac{1-2m}{a_1}}(x+c_1), m\right)\right),$$

  $$f_1 = \pm 2\arctan\left(\sqrt{\frac{2-m}{2(m-1)}} dn\left(\frac{2\sqrt{m-2}}{m\sqrt{a_1}}(x+c_1), m\right)\right),$$

  $$f_1 = \pm 2\arctan\left(\sqrt{\frac{m-2}{2}} dn^{-1}\left(\frac{2\sqrt{m-2}}{m\sqrt{a_1}}(x+c_1), m\right)\right),$$

  $$f_1 = \pm 2\arctan\left(\sqrt{m-\frac{1}{2}} sd\left(2\sqrt{\frac{1-2m}{a_1}}(x+c_1), m\right)\right). \tag{11}$$

All the functions appearing in these solutions are bounded.

As an example, we represent in Fig. 1 the profile and the graphic of the first traveling wave solution in (11), for the parameters $a_1 = -1$, $m = c_1 = 0$.
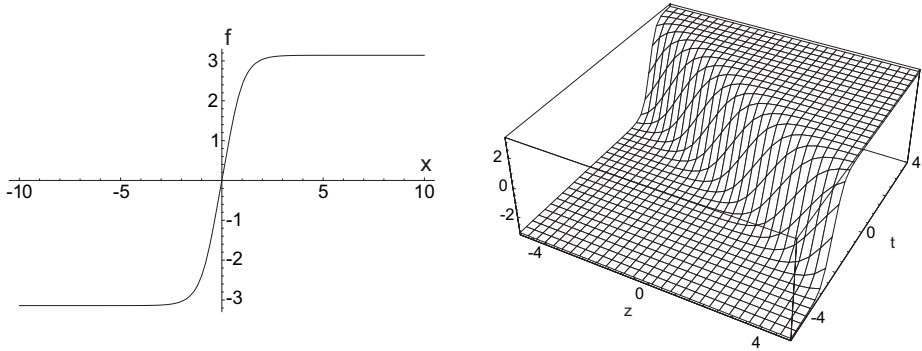

Fig. 1. Representation of the profile and the graphic of the first solution in (11) that corresponds to $m = 0$, $c_1 = 0$ and $a_1 = -1$. The ranges of the dependent variables are $x = z + 2t \in [-5, 5]$ (left), $z \in [-5, 5]$ and $t \in [-5, 4]$ (right).

2. Taking $p = 2$, the change of the dependent variable is $f_1 = 4\arctan(h)$, equation (9) becomes

$$a_1 h'' \left(1 + h^2\right)^3 - 2a_1 h \left(h'\right)^2 \left(1 + h^2\right)^2 + 16h^3 \left(-1 + h^2\right) = 0 \,. \quad (12)$$

This equation admits a family of solutions that is implicitly given by

$$x + c_2 = \pm \int^h \frac{\xi^2 + 1}{\sqrt{\frac{8}{a_1}\xi^4 + c_1 \left(1 + \xi^2\right)^4}} \, d\xi \,, \quad (13)$$

where c_1 and c_2 are arbitrary constants.

The existence domains of the functions h, implicitly determined by equation (13), are given by the convergence of the integral in the right-hand side of (13). A solution with domain $(-\infty, \infty)$ requires the divergence of the integral. For $c_1 \neq 0$ the integrals are convergent, as improper integrals, at $\pm\infty$. If the radicand have only complex roots, the solution h is defined in a bounded interval. If the radicand have only simple real roots a_i, it changes the sign at a_i and the integrand behaves as $(\xi - a_i)^{-1/2}$ when $\xi \to a_i^+$; in this case the improper integral is convergent and

the solution is only defined in a finite interval. Therefore, to obtain solutions defined for all x, the radicand must have real roots of multiplicity greater or equal than 2; this happens when the radicand and its derivative have common roots. Two cases appear:

A. When $c_1 = 0$, the right member of (13) is an improper integral at $h = 0$ and $h = +\infty$. In this case it is easy to calculate the integral and we get the solution

$$f_1 = \pm 4 \arctan\left(\frac{\sqrt{2}(x + c_2) \pm \sqrt{a_1 + 2(x + c_2)^2}}{\sqrt{a_1}}\right). \quad (14)$$

In Fig. 2 we show the profile and the graphic of the kink soliton solution corresponding to $\lambda = -4$, $a_1 = 1$ and $c_2 = 0$, *i.e.*

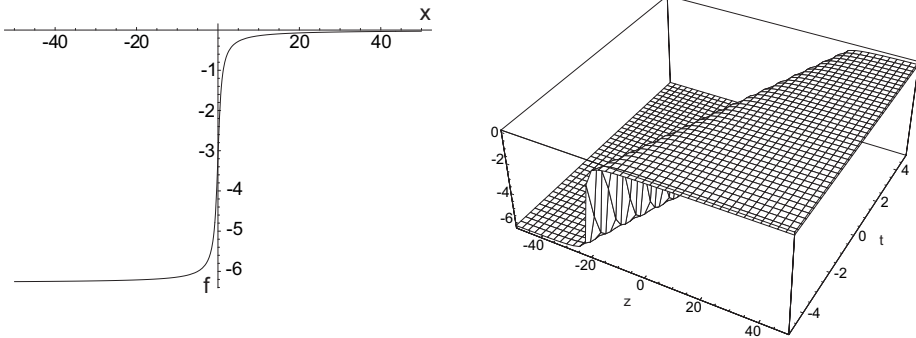$$f_1 = 4 \arctan\left(\frac{\sqrt{2}(z - 4t) - \sqrt{1 + 2(z - 4t)^2}}{A}\right). \quad (15)$$

Fig. 2. Representation of the profile and the graphic of the solution (15), $\lambda = -4$, $a_1 = 1$ and $c_2 = 0$, $x = z - 4t \in [-50, 50]$, $z \in [-50, 50]$ and $t \in [-5, 5]$.

B. When $c_1 = -\frac{1}{2a_1}$ the radicand in (13) has the double roots $\xi = -1$ and $\xi = +1$. The corresponding integral is divergent at $\xi = \pm 1$ and it is convergent at $\xi = \pm\infty$. The branch that corresponds to the interval $(-1, 1)$ is defined for $x \in \boldsymbol{R}$. Therefore, the solution f_1 of (9) determined by h is implicitly given by the equation

$$x + c_2 = \pm \frac{1}{\sqrt{-2a_1}} \int\limits_{0}^{\tan(f_1/4)} \frac{\xi^2 + 1}{\sqrt{\xi^8 + 6\xi^4 + 1}} d\xi, \quad (16)$$

where $a_1 < 0$ and c_2 are arbitrary constants. The class of solutions given by (16) corresponds to a kink soliton solution of (9). In Fig. 3 we exhibit the profile of one of these solutions.
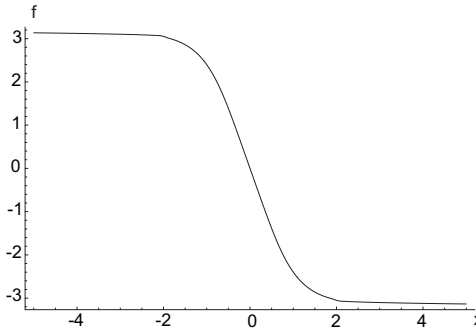

Fig. 3. Representation of the profile h of the solution f_1 that corresponds to (16), $c_2 = 0$, $a_1 = -1/2$, $x \in [-5, 5]$, $f_1 \in (-\pi, \pi)$.

3. Finally, taking $p = 3$, the change of the dependent variable is $f_1 = 6 \arctan(h)$, equation (9) becomes

$$-4h^3 \left(h^2 - 3\right)^3 \left(3h^2 - 1\right) + 3a_1 \left(h^2 + 1\right)^4 \left(h''(h^2 + 1) - 2hh'^2\right) = 0 \,. \tag{17}$$

This equation admits solutions that can be given implicitly by

$$x + c_2 = \pm \int^h \frac{-3a_1(\xi^2 + 1)^2}{\sqrt{-2a_1(2\xi^6 - 3\xi^4 + 12\xi^2 + 1)(3\xi^2 - 1)^2 + 9c_1\, a_1^2(1 + \xi^2)^6}} d\xi \,. \tag{18}$$

This case is similar to the former one. The radicand has double roots when $c_1 = 0$ and $c_1 = 2/(9a_1)$. For $c_1 = 0$ the double roots are $\xi = \pm 1/\sqrt{3}$; in this case there is a solution that is defined for $x \in \mathbf{R}$. When $c_1 = 2/(9a_1)$ the double roots are $\xi = 0$ and $\xi = \pm\sqrt{3}$; in this case there are two solutions that are defined for $x \in \mathbf{R}$; these solutions correspond to the intervals $(-\sqrt{3}, 0)$ and $(0, \sqrt{3})$.

- Non transcendent form:

The change of the dependent variable $f_1 = (2p + 1)\arctan(h)$, where p is an integer number, allows us to write equation (9) in a non transcendent form.

1. By setting $f_1 = \arctan(h)$, equation (9) becomes

$$2h\left(1+h^2\right)^2 - \sqrt{1+h^2}\left(2h\left(1+h^2\right) + a_1\left(\left(1+h^2\right)h'' - 2hh'^2\right)\right) = 0. \tag{19}$$

This equation admits solutions implicitly given by

$$x + c_2 = \pm\int^{h}\sqrt{\frac{a_1}{\left(1+\xi^2\right)\left(c_1 a_1\left(\xi^2+1\right) - 4\sqrt{1+\xi^2} + 2\right)}}\, d\xi. \tag{20}$$

The radicand in (20) has real roots if, and only if, $c_1 a_1 \leq 2$. For $c_1 a_1 < 2$ these roots are simple and the integral is convergent at these points. If $c_1 a_1 = 2$ the radicand has a double root at $\xi = 0$, but the integral is divergent at $\xi = 0$. There are no solutions of this class that are defined for $x \in \mathbf{R}$.

2. With the change $f_1 = 3\arctan(h)$, equation (9) becomes

$$2h\left(1+h^2\right)^3\left(h^2-3\right) + \sqrt{1+h^2}\left(2h\left(3-7h^2-7h^4+3h^6\right)\right.$$
$$\left. +3a_1\left(1+h^2\right)^2\left((1+h^2)h'' - 2hh'^2\right)\right) = 0. \tag{21}$$

This equation has solutions implicitly given by

$$x + c_2 = \pm3\int^{h}\sqrt{\frac{a_1\left(\xi^2+1\right)}{9c_1 a_1\left(1+\xi^2\right)^3 + 2\left(3\xi^2-1\right)\left(3\xi^2-1+2\left(1+\xi^2\right)^{3/2}\right)}}\, d\xi. \tag{22}$$

3.2. Non traveling wave solutions

When $\beta = \gamma$, the symmetry algebra of (1) is three-dimensional. The use of the symmetry v_3 leads to search similarity solutions of the form $f_j = g_j(w)$, where the similarity variable is $w = z^2 - \frac{\beta}{\alpha}t^2$. The reduced system is

$$4\beta\alpha(wg_1'' + g_1') + \delta(-2\sin(g_1) + \sin(g_1+g_2)) = 0,$$
$$4\beta\alpha(wg_2'' + g_2') + \delta(-2\sin(g_2) + \sin(g_1+g_2)) = 0. \tag{23}$$

By grouping the constants, this system can be written in the form

$$a_1(wg_1'' + g_1') - 2\sin(g_1) + \sin(g_1+g_2) = 0,$$
$$a_1(wg_2'' + g_2') - 2\sin(g_2) + \sin(g_1+g_2) = 0. \tag{24}$$

We are able to find solutions of system (24) such that $g_2 = -g_1 + 2k\pi$, with $k \in \mathbf{Z}$. By setting $w = \frac{x}{a_1}$, the resulting equation can be converted into an equation of the form

$$xg'' + g' - 2\sin(g) = 0. \tag{25}$$

Now we analyze the qualitative behavior of the solutions of the initial value problem

$$\begin{cases} xg'' + g' = 2\sin(g), \\ g(x_0) = a_0, \\ g'(x_0) = b_0, \end{cases} \tag{26}$$

with $x_0 > 0$ and different values of a_0 and b_0. It is obvious that if g is a solution of (25) then $-g$ and $g + 2k\pi$ are also solutions of equation (25), for any $k \in \mathbb{Z}$. Also, the constant functions $g \equiv k\pi$, $k \in \mathbb{Z}$, are solutions of (25). These facts allow us to reduce the study of the problem (26) to the cases $a_0 \in [0, 2\pi)$ and b_0 arbitrary. A more detailed analysis reveals that it is sufficient to consider only the cases $a_0 \in [0, 2\pi)$ and $b_0 > 0$.

A complete study of the solutions of (25) is rather involved and it is not easy to obtain the classification of all the solutions of (26). Fig. 4 shows the graphic representation of the solutions of (26) corresponding to $x_0 = 1$, $a_0 = 0$ and five different values of b_0. All the solutions we have shown are such that $\lim_{x\to\infty} g(x) = (2k + 1)\pi$, for some $k \in \mathbb{Z}$, and $\lim_{x\to\infty} g'(x) = 0$. There are numerical evidences that all the solutions of (26) verify these two properties, although an analytical proof of this fact seems to be very difficult.
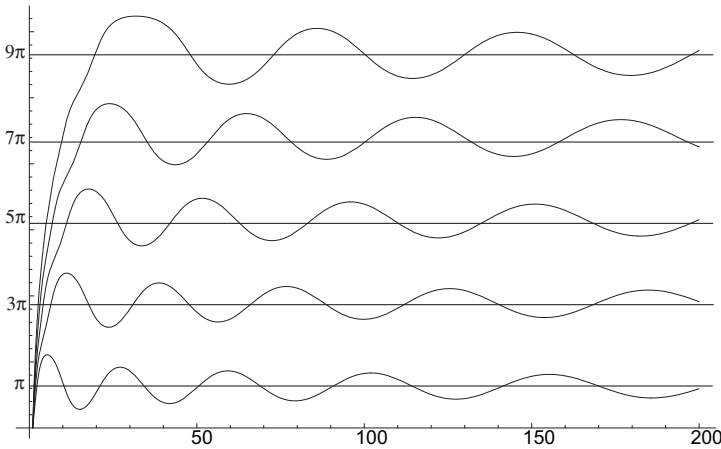

Fig. 4. Graphic representation of five solutions of (26) corresponding to $x_0 = 1$, $a_0 = 0$ and $b_0 = \pi$, 1.5π, 2π, 2.5π, 3π (from bottom to top).

Now, we demonstrate that the solutions $g(x) = (2k + 1)\pi$, $k \in \mathbb{Z}$ are stable and the solutions $g(x) \equiv 2k\pi$, $k \in \mathbb{Z}$ are unstable.

Suppose that g is a solution of (25). After the multiplication by $g'(x)$, equation (25) can be written in the form

$$\frac{d}{dx}\left(\tfrac{1}{2}x(g'(x))^2 + 2\cos g(x)\right) + \tfrac{1}{2}(g'(x))^2 = 0\,. \tag{27}$$

This implies that $\frac{d}{dx}\left(\tfrac{1}{2}x(g'(x))^2 + 2\cos g(x)\right) \leq 0$, then $h(x)$ defined by $h(x) = \tfrac{1}{2}x(g'(x))^2 + 2\cos g(x)$ is a decreasing function. Therefore,

$$0 \leq \tfrac{1}{2}\int_{x_0}^{x} g'(s)^2 ds = h(x_0) - h(x)\,, \qquad (x \geq x_0)\,. \tag{28}$$

Since $h(x) \geq -2$, (28) shows that $\int_{x_0}^{\infty} g'(s)^2 ds < +\infty$. Inequality (28) allows us to obtain several bounds for $g'(x)$ because

$$\tfrac{1}{2}x(g'(x))^2 \leq \tfrac{1}{2}z(g'(z))^2 + 2\cos g(z) - 2\cos g(x)\,, \qquad (x > z \geq x_0) \tag{29}$$

and

$$|g'(x)|^2 = (g'(x))^2 \leq \frac{1}{x}\left(zg'(z)^2 + 8\right)\,. \tag{30}$$

Therefore,

$$-\frac{\sqrt{zg'(z)^2 + 8}}{\sqrt{x}} \leq g'(x) \leq \frac{\sqrt{zg'(z)^2 + 8}}{\sqrt{x}}\,, \qquad (x \geq z \geq x_0)\,. \tag{31}$$

Integrating with respect to x we obtain the following bounds for $g(x)$

$$-2\sqrt{zg'(z)^2 + 8}(\sqrt{x} - \sqrt{x_0}) \leq g(x) - g(x_0) \leq 2\sqrt{zg'(z)^2 + 8}(\sqrt{x} - \sqrt{x_0})\,. \tag{32}$$

Equation (25) and inequality (31) allow us to write a bound for $g''(x)$

$$|g''(x)| \leq \frac{2}{x} + \frac{\sqrt{zg'(z)^2 + 8}}{x\sqrt{x}}\,, \qquad (x \geq z \geq x_0)\,. \tag{33}$$

Inequalities (31) and (33) show that both $g'(x)$ and $g''(x)$ tend to 0 as x tends to ∞. Notice that equation (25) can also be written as $(xg'(x))' = 2\sin g(x)$. If $a_0 \in [x_0, \pi)$ and $b_0 > 0$, $g(x) \in (0, \pi)$ for $x - x_0$ small enough. Let us suppose that $g(x) \in (0, \pi)$ for $x > x_0$; then $xg'(x) - x_0 g'(x_0) = 2\int_{x_0}^{x}\sin g(s)ds > 0$, $g'(x) > x_0 g'(x_0)\frac{1}{x}$ and, therefore, $g(x) > g(x_0) + x_0 g'(x_0)\ln\frac{x}{x_0}$ for $x > x_0$. This contradiction implies that there exists some $x_1 > 0$ such that $g(x_1) = \pi$. This implies that $g(x)$ attains the value π and that the constant solution $g \equiv 0$ cannot be stable.

The solution g verifies $g(x_1) = \pi$ and $g'(x_1) = b_1 > 0$. If b_1 is large enough it can be proved that $g(x)$ attains the value 2π. Let us analyze the case $\frac{1}{2}x_1 g'(x_1)^2 - 2 = \frac{1}{2}x_1 g'(x_1)^2 + 2\cos g(x_1) < 0$ (this happens if $\frac{1}{2}x_0 \beta^2 + 2\cos\alpha < 0$). Then, since $h(x)$ is a decreasing function,

$$0 \leq \tfrac{1}{2}x(g'(x))^2 < -2\cos g(x), \qquad (x \geq x_1). \qquad (34)$$

This proves that if $g(x_1) = \pi$ and $g'(x_1)^2$ is small enough (*i.e.* verifies $\frac{1}{2}x_1 g'(x_1)^2 < 2$), then $g(x) \in (\frac{\pi}{2}, \frac{3\pi}{2})$ for $x \geq x_0$. Now we prove that $g(x) \to \pi$ as $x \to \infty$. Since $b_1 > 0$, there exists a value $z_0 > x_1$, with $g'(z_0) = b_2 > 0$, such that $c_0 = \sin g(z_0) < 0$. It is not difficult to prove that $\sin g(x) > c_0$ for some $x > z_0$. If $\sin g(x) \leq \delta < 0$ for $x > z_0$ then

$$xg'(x) - z_0 g'(z_0) = 2\int_{z_0}^{x} \sin g(t)dt \leq 2\delta(x - z_0). \qquad (35)$$

By considering z_0, instead of z, in inequality (31), we also have

$$-\sqrt{z_0 g'(z_0)^2 + 8}\sqrt{x} - z_0 b_2 \leq xg'(x) - z_0 g'(z_0) \leq 2c_0(x - z_0), \qquad (x > z_0). \qquad (36)$$

This implies that $2(-c_0)(x - z_0) < \sqrt{z_0 g'(z_0)^2 + 8}\sqrt{x} + z_0 g'(z_0)$ for $x \geq z_0$. This is impossible because $-c_0 > 0$. Therefore, there exists a value $z_1' > z_0$ such that $\sin g(z_1') > \sin g(z_0)$. Bolzano's theorem implies that $\sin g(z_1) = \sin g(z_0)$ for some $z_1 \in [z_0, z_1']$. By the mean value theorem $0 = g(z_1) - g(z_0) = \cos g(\xi)g'(\xi)(z_1 - z_0) < 0$, for some $\xi \in (z_0, z_1) \subset (\frac{\pi}{2}, \frac{3\pi}{2})$. Since $\cos g(\xi)$ does not vanish because $g(x) \in (\frac{\pi}{2}, \frac{3\pi}{2})$, necessarily $g'(\xi) = 0$. We denote by ξ_1 the smallest point $\xi_1 > x_0$ such that $g'(\xi_1) = 0$. At this point we have $\xi_1 g''(\xi_1) + g'(\xi_1) = 2\sin g(\xi_1) \leq 0$. Therefore, $g''(\xi_1) < 0$ and there exists some $\xi_2 > \xi_1$ such that $g(\xi_2) > \pi$, $\sin g(\xi_2) < 0$, and $g'(\xi_2) < 0$. If $\sin g(x) < 0$ for $x > \xi_2$ then, as before, $xg'(x) - \xi_2 g'(\xi_2) = 2\int_{\xi_2}^{x} \sin g(\eta)d\eta < 0$ and $g'(x) < s_1 g'(\xi_2)\frac{1}{x}$. This implies that

$$g(x) - g(\xi_2) < \xi_2 g'(\xi_2)[\ln x - \ln \xi_2]. \qquad (37)$$

Since $g'(\xi_2) < 0$, the right member of (37) tends to $-\infty$ as $x \to \infty$. This cannot happen because $g(x) \in (\frac{\pi}{2}, \frac{3\pi}{2})$ for $x \geq x_0$. Consequently, there exists some $x_1' > x_0$ such that $\sin g(x_1') = 0$; *i.e.* $g(x_1') = \pi$. We denote by x_1 the smallest value $x_1 > \xi_1$ such that $g(x_1) = \pi$. For this value $g'(x_1) < 0$ and, since $x_1 g''(x_1) + g'(x_1) = 2\sin g(x_1) = 0$, $g''(x_1) > 0$. By following in this way, we could find an unbounded sequence of points $\{x_n\}$ such that $g(x_n) = \pi$ for $n \in \mathbb{N}$ and, by (30), $g'(x_n) \to 0$ as $n \to \infty$. Therefore, this solution oscillates around π with oscillations whose amplitudes tends to 0.

As we have mentioned above, if $g'(x_1)$ is large enough the values of $g(x)$ may leave the interval $[0, 2\pi)$ and there is a point z_1 such that $g(z_1) = 2\pi$. The study of this solution can be reduced to the former case by considering the solution $g_1(x) = g(x) - 2\pi$ which verifies $g_1(z_1) = 0$ and $g_1'(z_1) > 0$. Numerical evidence shows that *any* solution of (28) is bounded and that $g(x) \to (2k+1)\pi$ for some $k \in \mathbb{Z}$.

Fig. 5 shows a graphic representation of the particular solution g_1 of (23) that corresponds to the case $\frac{\beta}{\alpha} = -2$ with $a_0 = \frac{\pi}{2}$, $b_0 = 1/10$ in (26).
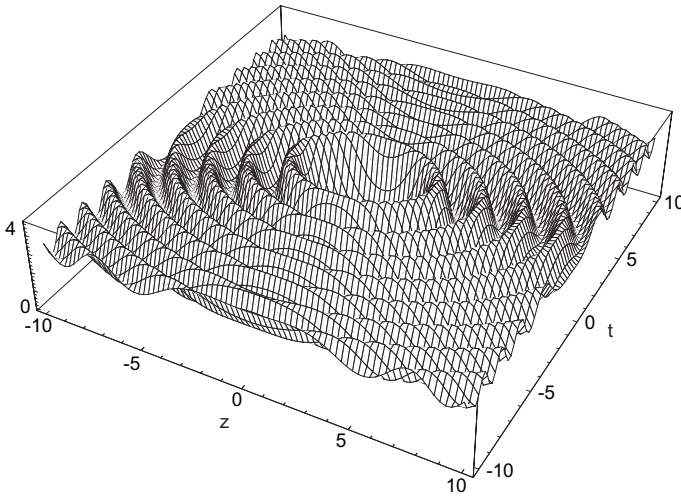

Fig. 5. Graphic representation of a solution g_1 corresponding to $\frac{\beta}{\alpha} = -2$ in equation (23).

We can also find solutions of (24) with $g_2 = g_1 + 2k\pi$. The resulting equation can be written as

$$a_1(wg_{ww} + g_w) - 2\sin(g) + \sin(2g) = 0. \qquad (38)$$

This equation can also be written as $a_1(wg')' - 2\sin(g) + \sin(2g) = 0$ and admits the constant solutions $g(x) = k\pi$, $k \in \mathbb{Z}$. This equation admits solutions whose qualitative behavior are similar to the solutions of (25).

4. Conclusions

We have considered the Yakushevich model of DNA torsion dynamics. The classical symmetries of the corresponding system of equations have been obtained imposing the invariance conditions. The procedure led to a complicated system of equations for obtaining the corresponding Lie groups of

transformations. Depending of the values of the parameters either a 2-parameter Lie group or a 3-parameter Lie group appear. Although the model does not have enough symmetries as to reduce the equations to ordinary differential equations, we have used existing symmetries to obtain several classes of solutions by imposing adequate Ansätze. Some classes of solutions we have obtained are traveling wave solutions, of the type kink soliton solutions, and other ones are non traveling wave solutions. The study must be continued introducing real parameter values and investigating which solutions can be really interpreted as describing observed phenomena in DNA. But even for the cases where the parameter values are not applicable to DNA, it is possible that they could be significant for the description of some other systems.

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