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Traveling Wave Solutions of DNA-Torsional Model of Fractional Order

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Abstract: Our attentions here is to show that (DNA-torsional model is reduced to the sine-Gordon SG and double sine-Gordon (DSG) equations. The fractional order equations of the SG and (DSG), based on the Caputo derivative is considered. One of the main results found here is to show that these equations of the fractional-order are reduced to partial differential equations (PDEs). Exact explicit formulas of some solitary and periodic traveling wave solutions are obtained. The effects exhibited in the later case are illustrated. The effects exhibited in the latter case are illustrated. While the fractional space derivative leads the formation of " parabolic" wave in the transition state.

Keywords: DNA, Fraction, traveling wave solutions (TWS), Sin-Gordan (SG) equation, double Sin-Gordan (DSG) equation.

1 Introduction

In recent years, it is presently realized that the understanding of the dynamics of DNA may be one of the most challenging problems posed to the human knowledge. This fascinating suggestion attracted the attention of many researchers, particularly that ones in theoretical physics and nonlinear dynamics and also triggered the formulation of several simple models of nonlinear DNA dynamics.

From the theoretical point of view, DNA is usually considered so far as three-dynamical motions, namely s torsional, transverse and longitudinal motions. On the important DNA- model is that one which describes the rotational motion of DNA (torsion models of DNA). See also the (Y-model) where it is introduced by Yakushevich) [1,2,3]. In this model each nucleotide (sugar-phosphate-backbone) is described by two degrees of freedom with a single angular variable (i.e. microscopic models) [4].

In this context, we study the case in the homogeneous medium. That is both strands have the same mass density and the interactions between bases at different sites are equal). It describes the angle of rotation of bases about the backbone (or between the atom-bridge Hydrogen H-bond and the backbone) are considered [5,6].

The discrete torsion model of DNA is follows as:

$$I\,\ddot{\psi}_n = k_s(\psi_{n+1}+\psi_{n-1}-2\psi_n) - k_p r^2(\sin\psi_n\cos\chi_n)\,,$$
$$I\,\ddot{\chi}_n = k_s(\chi_{n+1}+\chi_{n-1}-2\chi_n) - k_p r^2(\sin\chi_n(\cos\psi_n-\cos\chi_n))\,, \tag{1}$$

where ψ_n and χ_n are the angles referring to the out of phase (center of basses mass) for each chain. I is the moment of inertia of the bridge between two bases and k_s, k_p are the dimensional coupling constants [4].

To get the continuum version for the equation (1), we write $\psi_n(t) \simeq \psi(\delta n,t)$, $\chi_n(t) \simeq \chi(\delta n,t)$, with $\delta n = x$, where δ is the distance between successive n sites along the axis of the double helix ($\delta = 3.4\mathring{A}$)in B-DNA) [7,8]. We get the equations

$$\begin{aligned}\psi_{tt} &= K_s\psi_{xx} - K_p\sin\psi\cos\chi\,,\\ \chi_{tt} &= K_s\chi_{xx} - K_p\sin\chi(\cos\psi-\cos\chi)\,.\end{aligned} \tag{2}$$

For symmetric angle between the bases ($\chi = 0$) and equation (2) reduces to the sine-Gordan SG equation

$$\psi_{tt} = K_s\psi_{xx} - K_p\sin\psi\,, \tag{3}$$

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For antisymmetric angles ($\psi = 0$), the equation (2), tends to the double sine-Gordon (DSG) equation

$$\chi_{tt} = K_s \chi_{xx} - K_p \sin\chi(1-\cos\chi), \qquad (4)$$

where $K_s = \frac{k_s \delta^2}{I}$, $K_p = \frac{k_p r^2}{I}$. Indeed $K_s = C_0^2$, C_0 is the speed of linear wave.

2 The second order fractional Caputo derivative

The fractional order have recently proved to be valuable tools to the modeling of many physical phenomena [9, 10-12] and here we use the right-Caputo-derivative for nonlinear evolution equations (NLEs) [13, 14-16]

$$D_t^{\beta_1} f(x,t) - D_x^{\beta_2} f(x,t) = k(x,t), \qquad (5)$$

where

$$D_t^{\beta_1} f(x,t) = \frac{1}{\Gamma(2-\beta_1)} \int_0^t (t-t_1)^{1-\beta_1} \frac{\partial^2}{\partial t_1^2} f(x,t_1) dt_1,$$

$$D_x^{\beta_2} f(x,t) = \frac{1}{\Gamma(2-\beta_2)} \int_0^x (x-x_1)^{1-\beta_2} \frac{\partial^2}{\partial x_1^2} f(x_1,t) dx_1,$$

$$1 < \beta_i < 2,\ i = 1,2. \qquad (6)$$

It is worthy to mention that the time-fraction derivative expresses the effects of the distributed time delay on the evolution of the dynamical system. While the space-fractional derivative exhibits the behavior of the system in the transition from a state to another one's. As an example, the second equation in (6) shows the behavior of the system in transition from the transnational to the diffusion states. We put $\frac{\partial}{\partial t_1} f(x,t_1) = g(x,,t_1)$ and $\frac{\partial}{\partial x_1} f(x_1,t) = h(x_1,t)$, Thus, we get respectively

$$D_t^{\beta_1} g(x,t_1) = \frac{1}{\Gamma(2-\beta_1)} \int_0^t (t-t_1)^{1-\beta_1} \frac{\partial}{\partial t_1} g(x,t_1) dt_1,$$
$$D_x^{\beta_2} h(x_1,t) = \frac{1}{\Gamma(2-\beta_2)} \int_0^x (x-x_1)^{1-\beta_2} \frac{\partial}{\partial x_1} h(x_1,t) dx_1 \qquad (7)$$

we write $\alpha_i = \beta_i - 1$, $t \to t_1$, $t_1 \to t_2$, $x \to x_1$, $x_1 \to x_2$ and by integrating both sides on $[0,t]$ and $[0,x]$ respectively, we have

$$\int_0^t D_t^{\alpha_1} g(x,t_2)\, dt_2 = \frac{1}{\Gamma(1-\alpha_1)} \int_0^t \int_0^{t_1} (t_1-t_2)^{-\alpha_1} \frac{\partial}{\partial t_2} g(x,t_2) dt_2 dt_1,$$

$$\int_0^x D_x^{\alpha_2} h(x_2,t)\, dx_2 = \frac{1}{\Gamma(1-\alpha_2)} \int_0^x \int_{0_1}^{x_1} (x_1-x_2)^{-\alpha_2} \frac{\partial}{\partial x_2} h(x_2,t) dx_2 dx_1, \qquad (8)$$

by changing the limits of the internal integrals and by permuting the inner with outer ones, so that the integral on t_1 is carried first and we get

$$\int_0^t D_t^{\alpha_1} g(x,t_2)\, dt_2 = \int_0^t \frac{-\alpha_1}{\Gamma(2-\alpha_1)} \frac{\partial}{\partial(t-t_2)} g(x,,t_2,\tau).dt_2, \qquad (9)$$
$$\tau = (T-t)^{\alpha_1}\ 0 \le t \le T.$$

The equation (9) holds when

$$D_t^{\alpha_1} g(x,t_2) = \frac{-\alpha_1}{\Gamma(2-\alpha_1)} \frac{\partial}{\partial \pi} g(x,t_2,\tau). \qquad (10)$$

In the equation (10) t and t_2 are replaced by and T and t respectively. For convenience we may write the equation (10) in the form

$$D_t^{\alpha_1} g(x,t) = \frac{\alpha_1}{\Gamma(2-\alpha_1)} \frac{\partial}{\partial \pi} g(x,t,\tau), \qquad (11)$$
$$\tau = T^{\alpha_1} - (T-t)^{\alpha_1}\ 0 \le t \le T.$$

By bearing $g(x,t,\tau) = \frac{\partial}{\partial t} f(x,t,\tau)$. A result similar to (10) holds for the second equation in (8), namely

$$D_x^{\alpha_2} g(x,t,X) = -\frac{\alpha_2}{\Gamma(2-\alpha_2)} \frac{\partial}{\partial X} g(x,t,X), \qquad (12)$$
$$X = (M-x)^{\alpha_2},\ 0 \le x \le M.$$

3 Solutions of the fractional models

Here we are interested to consider the equations (3)and (4) with space-time- fractional derivatives.

3.1 Solution of sine-Gordon SG equation

By using the results for the equations (5)-(12), the fractional SG equation (3) is

$$\rho_1 \frac{\partial^2 \psi}{\partial t\, \partial \tau} - \rho_2 \frac{\partial^2 \psi}{\partial x\, \partial X} + K_p \sin\psi = 0,$$

$$\rho_1 = \frac{\alpha_1}{\Gamma(2-\alpha_1)},\ \rho_2 = \frac{\alpha_2 C_0^2}{\Gamma(2-\alpha_2)},\ \alpha_i = \beta_i - 1, \qquad (13)$$

$$0 < \alpha_i < 1,\ i = 1, 2.$$

We aim to solve the equation (13). To this end, we use the transformation $\psi(x,X,t,\tau) = u(z)$, $z = \kappa x + \eta X + \omega t + \nu\tau$. The equation (13) becomes

$$\lambda u'' + K_p \sin u = 0, \qquad (14)$$
$$\lambda = \rho_1 \omega \nu - \rho_2 \kappa \eta,$$

where ω, υ, $\kappa\,\eta$ arbitrary constants.

The traveling wave solutions (TWS) of equation (14) are given in the following three cases:

Case – I

By integrating (14), and in terms of the original variable the solution is

$$\psi(x,t) = 4\tan^{-1}\left(\exp\left(\sqrt{-\frac{k_p}{\lambda_1}}\left(-\eta(M-x)^{\beta_2-1} - \nu(T-t)^{\beta_1-1} - t\omega - \kappa x\right)\right)\right)$$

$$\lambda_1 = -\lambda. \qquad (15)$$

Case – II

By taking the transformations $u(z) = 2\arctan(v(z))$ [17, 18-20], the equation (14) is

$$\lambda(v'' - \frac{2vv'^2}{1+v^2}) + K_p v = 0\,, \tag{16}$$

the first integral of the equation (16) is

$$v'^2(z) = \sqrt{\frac{1}{\lambda}(K_p(1+v^2) + A_0(1+v^2)^2}\,. \tag{17}$$

In terms of the original variables the solution of equation (13) is

$$\psi(x,t) = 4\cot^{-1}\left(e^{-\frac{\sqrt{\mathrm{Kp}}(\eta(M-x)^{\beta_2-1}+\nu(T-t)^{\beta_1-1}+t\,\omega+\kappa x)}{\sqrt{\lambda}}}\right), \quad A_0 = \mathrm{Kp} \tag{18}$$

Case − III

By using the transformations [21,22,23];

$$v(z) = \exp(i\tfrac{u(z)}{2}),\ u(z) = -i\ln v^2(z) \qquad \cos u = \tfrac{v^2+v^{-2}}{2},\ \sin u = \tfrac{v^2-v^{-2}}{2i}\,. \tag{19}$$

From the equation (19) into equation (14), we have

$$4\lambda(vv'' - 2v'^2) + K_p(v^4 - 1) = 0\,. \tag{20}$$

Here we use the unified method UM [24,25], to find the solution of equation (20).

Where the solution is taken to be polynomial with an auxiliary function φ that satisfies an auxiliary equation:

$$u(z) = \textstyle\sum_{i=0}^{n} a_i \varphi^i(z), \tag{21}$$

$$\varphi'(z) = \textstyle\sum_{j=0}^{kp} c_j \varphi^j(z),\ p = 1, 2$$

where a_i, c_j are unknown parameters.

In the cases, when $p = 1$and 2, the solution of the auxiliary equation gives rise to elementary or elliptic (explicit or implicit) solutions respectively. In the equation (21) the balance equation for n and k is determined from the leading analysis between the higher derivative and nonlinearity terms in the equation (20) $(n = k-1)$.

(i) When $p = 1$. In this case, exact solutions are found as elementary functions and $k = 2, 3$.

(i_1) When $p = 1$, $k = 2$, We now suppose that equation (21) has the solution in the form

$$v(z) = a_1\varphi(z) + a_0, \qquad \varphi'(z) = c_2\varphi^2(z) + c_1\varphi(z) + c_0 \tag{22}$$

By substituting equation (22) into (20) with a computer algebraic system, or otherwise we find

$$v(z) = -\frac{i\left(H\tanh\left(\frac{H(4c_2B_0\lambda+z)}{2\sqrt{\lambda}}\right)+c_1\sqrt{\lambda}\right)}{\sqrt{k_p}}, \quad H = \sqrt{c_1^2\lambda - k_p} \tag{23}$$

and the solution of equation (13) is

$$\psi(x,t) = \cos^{-1}[\tfrac{1}{2}(-\frac{(H\tanh(Q+c_1\sqrt{\lambda})^2}{k_p} - \frac{k_p}{(H\tanh Q+c_1\sqrt{\lambda})^2})], \quad Q = \left(\frac{H\left(4B_0c_2\lambda+\eta(M-x)^{\beta_2-1}+t\,\omega+\nu(T-t)^{\beta_1-1}+\kappa x\right)}{2\sqrt{\lambda}}\right) \tag{24}$$

where c_1, c_2, and $B_0$are arbitrary constants.

(i_2) When $p = 1$, $k = 3$, we take

$$v(z) = a_2\varphi^2(z) + a_1\varphi(z) + a_0\,, \qquad \varphi'(z) = c_3\varphi^3(z) + c_2\varphi^2(z) + c_1\varphi(z) + c_0. \tag{25}$$

By substituting the equation (25) into equation (20) gives

$$v(z) = i\left(\frac{2}{2\exp\left(\frac{\sqrt{k_p}\left(6c_2B_1\lambda\left(2c_1\sqrt{\lambda}+\sqrt{k_p}\right)+z\right)}{\sqrt{\lambda}}\right)+1} - 1\right), \tag{26}$$

and the solution of equation (13) is

$$\psi(x,t) = \cos^{-1}\left(\frac{1}{2}\left(-\left(1-\frac{2}{2e^P+1}\right)^2 - \frac{1}{\left(1-\frac{2}{2e^P+1}\right)^2}\right)\right), \quad P = \frac{\sqrt{k_p}\left(6c_2B_1\lambda\left(2c_1\sqrt{\lambda}+\sqrt{k_p}\right)+\eta\,(M-x)^{\beta_2-1}+t\,\omega+\nu(T-t)^{\beta_1-1}+\kappa x\right)}{\sqrt{\lambda}}, \tag{27}$$

where B_1 is arbitrary constant.

(ii) In order to determine elliptic wave solutions when $(k = 2,\ p = 2)$, we write

$$(\varphi'(z))^2 = \sum_{j=0}^{j=4} c_j(t)\,\varphi^j(z)\,. \tag{28}$$

For particular values of c_j $j = 0, \ldots, 4$ we get different solutions in Jacobi elliptic functions and by using (according to the classification in [26,27]) namely:

$$c_0 = 1,\ c_2 = -1+m^2,\ c_4 = m^2\,, \quad c_1 = c_3 = 0\,, \tag{29}$$

$$\varphi(z) = \mathrm{sn}\left(z,\, m^2\right).$$

We have the elliptic solutions

$$v(z) = i\,m\,\mathrm{sn}\left(z,\, m^2\right),$$

$$\psi(x,t) = \cos^{-1}\left(\frac{-m^2\mathrm{sn}\left((M-x)^{\beta_2-1}\eta+x\,\kappa+(T-t)^{\beta_1-1}\nu+t\,\omega, m^2\right)^4-1}{2m\,\mathrm{sn}\left((M-x)^{\beta_2-1}\eta+x\kappa-(T-t)^{\beta_1-1}\nu+t\,\omega, m^2\right)^2}\right) \tag{30}$$

where $m\,(0 < m < 1)$ denotes the modulus of the Jacobi elliptic function.

The figures 1 (a) and (b) illustrate the delay of the time-fraction solution is slowing down due to the distributed time delay than classical (TWS) solution. While the parabolic wave is confirm for the space-fraction effect in the figures 2.

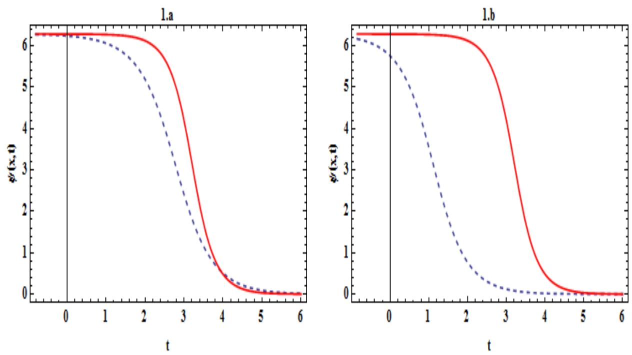

Fig. 1: Figs. 1 (a) and (b) The solution of equation (15) is displayed against $t-axis$ when the free parameters are K_p=1.5, C_0=1.2, T=M=10, ν= – 0.8, κ=0.5, η=0.4, ω=0.4 and$x = 1.5$ for the different values of $\beta_1$and β_2, namely $\beta_1 = 1.6$, $\beta_2 = 1.3$ (dashed curve) and for $\beta_1 = \beta_2 = 2$ (solid curve) in (1a). In (1b) the same values are taken, but $\beta_1 = 1.8$, $\beta_2 = 2$ (dashed curve).

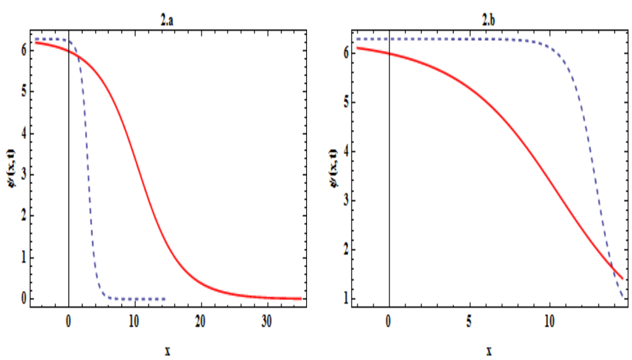

Fig. 2: Figs. 2 (a) and (b) are the solution of equation (15), is displayed against $x-axis$ when the free parameters are the same caption in figure1, but T=M=15, ν= – 0.5 and $t = 0.5$ for the different values of $\beta_1$and β_2. In (2a) to consider the same solution $\beta_1 = 1.6$, $\beta_2 = 1.3$ (dashed)$\beta_1 = \beta_2 = 2$ (solid). In fig (2b)$\beta_1 = 2$ and $\beta_2 = 1.5$ (dashed).

3.2 Solution of double sine-Gordon (DSG) equation

In this section, we consider the fractional solution of the (DSG) equation (4)

$$\frac{\partial^2\chi}{\partial t\,\partial\tau} - \frac{\partial^2\chi}{\partial x\,\partial X} - K_p(\sin\chi - \tfrac{1}{2}\sin 2\chi) = 0\,, \qquad (31)$$

and by using transformation $\chi(x,X,t,\tau) = w(z)$, $z = \kappa x + \eta X + \omega t + \nu\tau$. Thus we have

$$\lambda w''(z) - K_p(\sin w(z) - \frac{1}{2}\sin 2w(z)) = 0\,. \qquad (32)$$

Here , we use the transformation $w(z) = \exp(i\,\theta(z))$, and the equation (32) reduces to

$$4\lambda(\theta\,\theta'' - 2\theta'^2) + 2K_p\theta\,(\theta^2-1) - K_p(\theta^4-1) = 0. \quad (33)$$

The solutions of equations (33) are obtained by using the UM They are found as:

(I) When using $p = 1, k = 2$, into equation (21) the solutions of equation (31) is

$$\chi(x,t) = \arccos[\tfrac{1}{2}(1 - \frac{2\sqrt{\lambda}}{\sqrt{K_p}\left(4A_2\,c_2+\eta\,(M-x)^{\beta_2-1}+t\,\omega+\nu\,(T-t)^{\beta_1-1}+\kappa x\right)} + \frac{1}{1-\frac{2\sqrt{\lambda}}{\sqrt{K_p}\left(4A_2\,c_2+\eta\left((M-x)^{\beta_2-1}\right)+t\,\omega+\nu\left((T-t)^{\beta_1-1}\right)+\kappa x\right)}})]\,. \qquad (34)$$

(II) At $p = 1, k = 3$, we find

$$\chi(x,t) = \arccos[\tfrac{1}{2}(1 - \frac{2\sqrt{\lambda}}{\sqrt{K_p}\left(27A_3\,c_3^2+\eta\,(M-x)^{\beta_2-1}+t\,\omega+\nu\,(T-t)^{\beta_1-1}+\kappa x\right)} + \frac{1}{1-\frac{2\sqrt{\lambda}}{\sqrt{K_p}\left(27A_3\,c_3^2+\eta\left((M-x)^{\beta_2-1}\right)+t\,\omega+\nu\left((T-t)^{\beta_1-1}\right)+\kappa x\right)}})] \qquad (35)$$

where $A_2$and A_3 are integral constants.

4 Conclusions

In the present work, we have shown that the (PDEs) of any order of fractional orders can be reduced to retarded (PDEs). The time-fractional equation expresses for the distributed time delay. While space fractional equation describes the state of a dynamical system in transition from translate to the diffusion or from the later state to the dispersion state. In the present work as the solution is solitary, we have found the time-fractional solution leads to delay (TWS). While in the case of space fractional drive it leads to the formation of parabolic “ in the transition state. These results reveal new characteristics motivating further research on the dynamics of fractional equations in different branches of sciences.

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