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Numerical solution for discontinued problems arising in nanotechnology using HAM

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Abstract: This article is devoted to consider homotopy analysis method (HAM) for discontinued problems arising in nanotechnology. Continuum hypothesis on nanoscales is invalid, and a nonlinear differential-difference model is considered as an alternative approach to describing discontinued problems. This procedure is powerful tool for solving large amount of problems. Using this method, it is possible to find the exact solution or an approximate solution of the problem. This technique provide a series of functions which may converges to the exact solution of the problem. The comparison of the approximate solution with the exact solution and the Adomian decomposition method reveals that the proposed method is an attractive method in solving the differential-difference equations.

Keyword: Discretized mKdV lattice equation; Nonlinear differential-difference equations. Homotopy analysis method; Adomian decomposition method.

1. Introduction

Many different analytical methods have recently introduced to solve nonlinear problems, such as, HAM ([14]-[16]), Adomian decomposition method (ADM) ([3], [7], [20], [22]), and variational iteration method ([9], [17], [21], [23], [24]) and others. The HAM which devised by Shi-Jun Liao in 1992, is strongly and simply capable for solving a large class of linear or nonlinear differential equations without the tangible restriction of sensitivity to the degree of the nonlinear term and also it reduces the size of calculations besides, its interactions are direct and straightforward. This method has been successfully applied to solve many types of nonlinear problems in science and engineering by many authors ([1], [2], [8], [13]), and references therein.

We aim in this work to effectively employ HAM to establish the analytical solutions for the nonlinear differential-difference equations arising in nanotechnology. By the presented method, numerical results can be obtained with using a few iterations [14]. Moreover, HAM contains the auxiliary parameter $\hbar$, which provides us with a simple way to adjust and control the convergence region of solution series [15]. Therefore, HAM handles linear and nonlinear problems without any assumption and restriction. On the other side, many authors considered the proposed problem, for example, Mokhtari [17], used the variational iteration method to solve the nonlinear differential-difference equations, Shun and et. al. [18], used the homotopy perturbation method [10] to solve the discontinued problems arising in nanotechnology.

According to E-infinity theory ([4]-[6]), space at the quantum scale is not a continuum, and it is clear that nanotechnology possesses a considerable richness which bridges the gap between the discrete and the continuum [5]. On nanoscales, He et al. [11] found experimentally an uncertainty phenomenon similar to Heisenberg's uncertainty principle in quantum mechanics. Continuum hypothesis on the nanoscales becomes, therefore, invalid. He and Zhu [12] suggested some differential-difference models describing fascinating phenomena arising in heat/electron conduction and flow in carbon nanotubes, among which we will study the following model:

$$\frac{du_n}{dt} = (u_{n+1} - u_{n-1}) \sum_{i=1}^{m} \left(a_i + b_i (u_n)^i\right), \tag{1}$$

Where ai and bi are constants. Physical interpretation is given in [12]. Eq.(1) includes the well- known discretized mKdV lattice equation [19]:

$$\frac{du_n}{dt} = (\alpha - u_n^2)(u_{n+1} - u_{n-1}), \tag{2}$$

Where the subscript n in Eq.(1) represents the nth lattice. Previously such equations were solved by the exp-function method [25] and the variational iteration method [17].

The main aim of this work is effectively study analytically using the homotopy analysis method to establish the approximate solution of a nonlinear differential-difference equation arising in nan- otechnology (2). Also, comparison our results with those obtained using Adomian decomposition method is given.

2. HAM for differential-difference equations

We apply HAM ([14]-[16]) to the problem (2) equations. In this section we extent Liao's basis idea to the nonlinear differential-difference equation of the form:

$$\boldsymbol{DN}[u_n(t), u_{n+1}(t), u_{n-1}(t)] = 0, \tag{3}$$

Where DN is a nonlinear differential operator for the proposed problem, t and n denote independent variables, un(t) is an unknown function. For simplicity, we ignore all boundary and initial conditions, which can be treated in the similar way.

Zeroth-order deformation equation

Liao [14], construct the so-called zeroth-order deformation equation:

$$(1-q)\pounds\left[\Psi_n(t;q) - u_{n,0}(t)\right] = q\hbar H_n(t)\boldsymbol{DN}\left[\Psi_n(t;q), \Psi_{n+1}(t;q), \Psi_{n-1}(t;q)\right], \tag{4}$$

Where £ is an auxiliary linear operator, un;0(t) is an initial guess of un(t), ħ ≠ 0 is an auxiliary parameter and q ϵ [0;1] is the embedding parameter, Ψn(t;q) is the unknown function on independent variables n; t. Obviously, when q = 0 and q = 1, it holds respectively:

$$\Psi_n(t;0) = u_{n,0}(t), \qquad \Psi_n(t;1) = u_n(t). \tag{5}$$

Thus, as q increasing from 0 to 1, the solution Ψn (t;q) various from un;0(t) to un(t). Expanding Ψn (t;q) in Taylor series with respect to the embedding parameter q, one has:

$$\Psi_n(t;q) = u_{n,0}(t) + \sum_{m=1}^{\infty} u_{n,m}(t) q^m, \tag{6}$$

where

$$u_{n,m}(t) = \frac{1}{m!} \frac{\partial^m \Psi_n(t;q)}{\partial q^m}\Big|_{q=0}, \qquad n, m \in N. \tag{7}$$

Assume that the auxiliary linear operator, the initial guess, the auxiliary function Hn(t) and the auxiliary parameter ħ are selected such that the series (6) is convergent at q = 1, then at q = 1, and by (5), the series (6) becomes:

$$u_n(t) = u_{n,0}(t) + \sum_{m=1}^{\infty} u_{n,m}(t). \tag{8}$$

3. The mth-order deformation equation

Define the vector

$$\vec{u}_{n,m}(t) = [u_{n,0}(t), u_{n,1}(t), ..., u_{n,m}(t)], \qquad n, m \in N. \tag{9}$$

Differentiating Eq.(4) m times with respect to the embedding parameter q, then setting q = 0 and dividing them by m!, finally using (7), we have the so-called mth-order deformation equations:

$$\pounds[u_{n,m}(t) - \delta_{n,m} u_{n,m-1}(t)] = \hbar\, H_n(t)\, \boldsymbol{D}\Re_{n,m}(\vec{u}_{n,m-1}, \vec{u}_{n+1,m-1}, \vec{u}_{n-1,m-1}), \tag{10}$$

where

$$\begin{aligned} &\boldsymbol{D}\Re_{n,m}(\vec{u}_{n,m-1}, \vec{u}_{n+1,m-1}, \vec{u}_{n-1,m-1}) \\ &= \frac{1}{(m-1)!} \frac{\partial^{m-1} \boldsymbol{DN}[\Psi_n(t;q), \Psi_{n+1}(t;q), \Psi_{n-1}(t;q)]}{\partial q^{m-1}}\Big|_{q=0}, \end{aligned} \tag{11}$$

and

$$\delta_{n,m} = \begin{cases} 0, & m \le 1\,,\ n \in N; \\ 1, & m > 1\,,\ n \in N. \end{cases} \tag{12}$$

4. Application to the proposed problem

We apply HAM to the proposed problem (2) to illustrate the strength of the method and to establish approximate solutions for this problem. We choose the linear operator:

$$\pounds[\Psi_n(t;q)] = \frac{\partial \Psi_n(t;q)}{\partial t}, \tag{13}$$

With the property £[c1] = 0; where c1 is an integral constant to be determined by initial condition.

We now define a nonlinear operator as:

$$\boldsymbol{DN}[\Psi_n(t;q), \Psi_{n+1}(t;q), \Psi_{n-1}(t;q)] = \frac{\partial \Psi_n(t;q)}{\partial t} - (\alpha - (\Psi_n(t;q))^2)(\Psi_{n+1}(t;q) - \Psi_{n-1}(t;q)). \tag{14}$$

Using above definition, we construct the zeroth-order deformation equation:

$$(1-q)\pounds[\Psi_n(t;q) - u_{n,0}(t)] = q\hbar\, H_n(t)\, \boldsymbol{DN}[\Psi_n(t;q), \Psi_{n+1}(t;q), \Psi_{n-1}(t;q)]. \tag{15}$$

For q = 0 and q = 1, we can write:

$$\Psi_n(t;0) = u_{n,0}(t), \qquad \Psi_n(t;1) = u_n(t). \tag{16}$$

Thus, we obtain the mth-order deformation equations

$$\pounds[u_{n,m}(t) - \delta_{n,m} u_{n,m-1}(t)] = \hbar\, H_n(t)\, \boldsymbol{D}\Re_m(\vec{u}_{n,m-1}, \vec{u}_{n+1,m-1}, \vec{u}_{n-1,m-1}), \tag{17}$$

Subject to initial condition

$$u_{n,m}(0) = \begin{cases} n, & m \le 1\ ,\ \ n \in N; \\ 0, & m > 1\ ,\ \ n \in N, \end{cases} \tag{18}$$

where

$$\begin{aligned} &\boldsymbol{D}\Re_m(\vec{u}_{n,m-1}, \vec{u}_{n+1,m-1}, \vec{u}_{n-1,m-1}) \\ &\quad = \frac{\partial u_{n,m-1}(t)}{\partial t} - \alpha(u_{n+1,m-1}(t;q) - u_{n-1,m-1}(t;q)) - \alpha \sum_{j=0}^{m-1} u_{n,j}(t) u_{n+1,m-1-j}(t) \\ &\quad\ - \alpha \sum_{j=0}^{m-1} u_{n,j}(t) u_{n-1,m-1-j}(t). \end{aligned} \tag{19}$$

Now the solution of the mth-order deformation equations (17) for the corresponding auxiliary function Hn(t) = 1, m ≥1 become:

$$u_{n,m}(t) = \delta_m u_{n,m-1}(t) + \hbar\, \pounds^{-1}[\boldsymbol{D}\Re_m(\vec{u}_{n,m-1}, \vec{u}_{n+1,m-1}, \vec{u}_{n-1,m-1})]. \tag{20}$$

In order to illustrate the effectiveness of the method, we consider the following initial condition:

$$u_{n,0}(t) = \sqrt{\alpha}\tanh(d)\tanh(dn),$$

Where d is an arbitrary constant. Now, Eq.(20) gives the first few components of the approximate solution:

$$u_{n,0}(t) = \sqrt{\alpha}\tanh(d)\tanh(dn),$$
$$u_{n,1}(t) = \hbar\left[t\left(\alpha - \alpha\tanh^2(d)\tanh^2(dn)\right)\left(-\sqrt{\alpha}\tanh(d)\tanh(d(n-1)) + \sqrt{\alpha}\tanh(d)\tanh(d(1+n))\right)\right], \ldots$$

Other components of the approximate solution can obtain in the same manner.

Numerical results of our proposed method (HAM) at different the solution using HAM and the exact solution is presented in Figure 3. We note that there is a complete agreement between computed results by present algorithm and the exact solution. From these results we can see that the presented approach is more efficient than the different methods, regarding HAM which takes three components only of the solution.

It is noted that our approximate solutions converges at (_2 $\leq \hbar \leq$ _2) (see Figures 1-2). The explicit, analytic expression given by Eq.(20) contains the auxiliary parameter $\hbar$, which gives the convergence region and rate of approximation for HAM. However, the errors can be further be reduced by calculating higher order approximations. This proves that HAM is a very useful method to get accurate analytic solutions to linear and strongly nonlinear differential-difference equations. It must be noted that HAM used here gives the possibility of obtaining an analytical satisfactory solution for which the other techniques of calculation are more laborious and the results contain a great complexity.

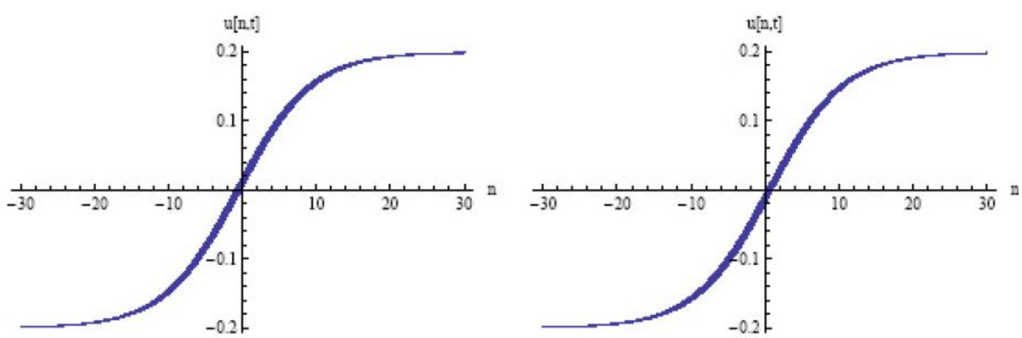

Figure 1. The HAM solution at:
$\hbar = -1.2, -1.4, -1.6, -1.8, -2.0$ (Left) and $\hbar = 1.2, 1.4, 1.6, 1.8, 2.0$ (Right).

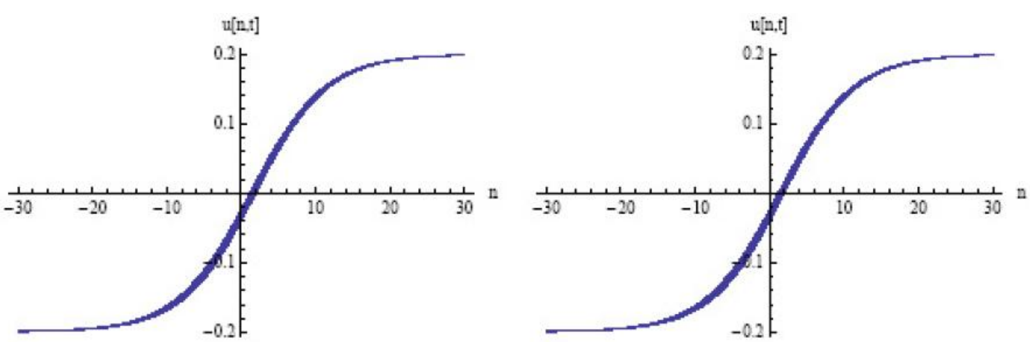

Figure 2. The HAM solution at:
$\hbar = -0.2, -0.4, -0.6, -0.8, -1.0$ (Left) and $\hbar = 0.2, 0.4, 0.6, 0.8, 1.0$ (Right).

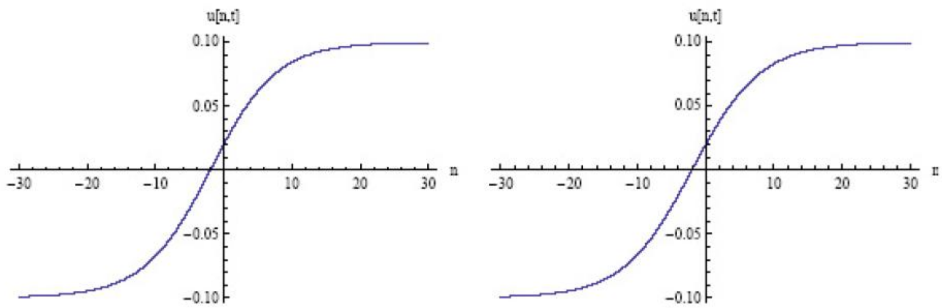

Figure 3. The behavior of the solution using HAM (Left) and the exact solution (Right).

5. Solution procedure using ADM

In this section, we implement ADM to solve the proposed problem (2). For this, we rewrite Eq.(2) in the following operator form:

$$L\, u_n(t) = \alpha\,(u_{n+1} - u_{n-1}) - \alpha\,\mathbf{N}(u_n, u_{n-1}, u_{n+1}), \tag{21}$$

Where $L = \frac{d}{dt}$ is an invertible differential operator, N(un, un -1, un +1), presents the nonlinear term and defined by:

$$\mathbf{N}(u_n, u_{n-1}, u_{n+1}) = u_n^2\,(u_{n+1} - u_{n-1}). \tag{22}$$

Applying the inverse operator L-1 to the both sides of (21) and using the given conditions we obtain:

$$u_n(t) = \varphi(t) + \alpha\, L^{-1}[u_{n+1} - u_{n-1}] - \alpha\, L^{-1}[\mathbf{N}(u_n, u_{n-1}, u_{n+1})], \tag{23}$$

Where the function ρ(t) presents the solution of the homogeneous differential equation Lun = 0, using the given conditions. The ADM defines the solution un(t) by the series in the following form:

$$u_n(t) = \sum_{m=0}^{\infty} u_{n,\,m}(t), \tag{24}$$

and the nonlinear operator N(un, un -1, un +1) represented by an infinite series of the so-called Adomian's polynomials:

$$\mathbf{N}(u_n, u_{n-1}, u_{n+1}) = \sum_{m=0}^{\infty} A_{n,\,m}, \tag{25}$$

where un;m(t); m ≥ 0 are the components of un(t) that will be elegantly determined and An;m are called Adomian's polynomials and defined by:

$$A_{n,m} = \frac{1}{m!}\Big[\frac{d^m}{d\lambda^m}\mathbf{N}\Big(\sum_{i=0}^{\infty}\lambda^i u_{n,i}\Big)\Big]_{\lambda=0}, \qquad m \geq 0. \tag{26}$$

From the above considerations, the decomposition method defines the components un;m(t) for m ≥ 0, by the following recursive relationship:

$$u_{n,0}(t) = \varphi(t), \qquad u_{n,m+1}(t) = \alpha\, L^{-1}[u_{n+1,m} - u_{n-1,m}] - \alpha\, L^{-1}[A_{n,m}], \qquad m \geq 0. \tag{27}$$

This will enable us to determine the components un;m(t) recurrently. However, in many cases the exact solution in a closed form may be obtained. The first An;m Adomian's polynomials that represent the nonlinear term N(un, un - 1, un +1) are given by:

$$A_{n,0} = u_{n,0}^2(u_{n+1,0} - u_{n-1,0}),$$

$$A_{n,1} = u_{n,0}^2(u_{n+1,1} - u_{n-1,1}) + 2u_{n,1}u_{n,0}(u_{n+1,0} - u_{n-1,0}), \ldots .$$

Also, from the recurrence relation (27), we can obtain the components of the solution un(t) as follows:

$$u_{n,0}(t) = \sqrt{\alpha}\tanh(d)\tanh(dn),$$

$$u_{n,1}(t) = t\,(\alpha - \alpha\tanh^2(d)\tanh^2(dn))(-\sqrt{\alpha}\tanh(d)\tanh(d(n-1))$$

$$+\sqrt{\alpha}\tanh(d)\tanh(d(1+n))), \ldots$$

For numerical comparisons purpose, we construct the solution un(t) such that:

$$\lim_{m\to\infty} U_{n,m}(t) = u_n(t), \quad \text{where} \quad U_{n,m}(t) = \sum_{i=0}^{m-1} u_{n,i}(t), \qquad m \geq 0. \tag{28}$$

For more details about ADM and its convergence see ([3], [20]).

Figure 4. presents a comparison between the solution using ADM and the solution obtained from HAM at ħ = -1: From this figure we can see that the solution of ADM is excellent agreement with the solution of HAM, this ensure that the ADM is a special case of HAM at the value of ħ = -1: Also, the obtained results in [17] using variational iteration method and [18] using homotopy perturbation method are excellent agreement with the solution of HAM, this ensure that the variational iteration method and homotopy perturbation method are special cases of HAM at the value of ħ = -1:

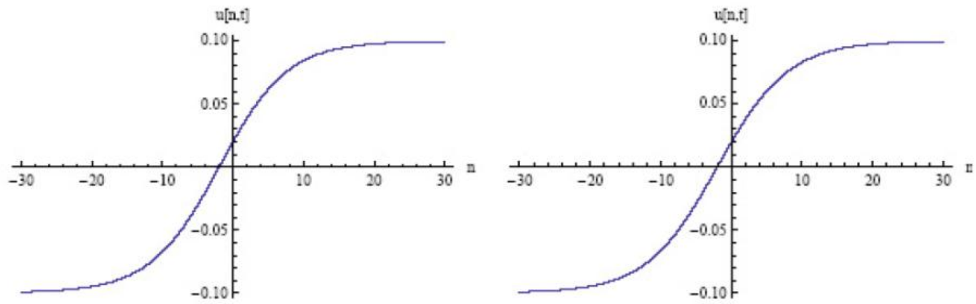

Figure 4. Comparison between ADM solution (Left) and HAM solution (Right), $\hbar = -1$.

Conclusions

In this Letter, the homotopy analysis method and Adomian decomposition method have been successfully applied to find the solution of nonlinear differential-difference model, which arising in nanotechnology. The presented numerical results show that the results of the proposed method are in excellent agreement with those of ADM. It is noted that our approximate solutions converges at _2 ≤ ħ ≤_2 (see Figures 1 and 2). The explicit, analytic expression given by Eq.(20) contains the auxiliary parameter ħ, which gives the convergence region and rate of approximation for HAM. However, the errors can be further be reduced by calculating higher order approximations. This proves that HAM is a very useful analytic method to get accurate analytic solutions to linear and strongly nonlinear problems. The numerical results showed that the proposed method has very accuracy and reductions of the size of calculations compared with the VIM [17] and the homotopy perturbation method [18]. In addition, we see that the homotopy perturbation method, variational iteration method and Adomian decomposition method are special cases of HAM for ħ = _1. It may be concluded that this methodology is very powerful and efficient technique in finding exact solutions for wide classes of problems. It is also worth noting to point out that the advantage of this methodology shows a fast convergence of the solutions by means of the auxiliary parameter, ħ = _1 (see Figs.1-4). HAM is very easy applied to both differential equations and nonlinear differential-difference equations. The advantage of the method is that it does not need a small parameter in the system, leading to wide application in nonlinear problems. In our work, we use the Mathematica Package.

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