The homotopy analysis method for solving discontinued problems arising in nanotechnology

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Abstract—This paper applies the homotopy analysis method to a nonlinear differential-difference equation arising in nanotechnology. Continuum hypothesis on nanoscales is invalid, and a differential-difference model is considered as an alternative approach to describing discontinued problems. Comparison of the approximate solution with the exact one reveals that the method is very effective.

Keywords—homotopy analysis method, differential-difference, nanotechnology

I. INTRODUCTION

In 1992, Liao [15] employed the basic ideas of the homotopy in topology to propose a general analytic method for nonlinear problems, namely homotopy analysis method (HAM), [16], [17], [18], [19]. Based on homotopy of topology, the validity of the HAM is independent of whether or not there exist small parameters in the considered equation. Therefore, the HAM can overcome the foregoing restrictions and limitations of perturbation techniques. This method has been successfully applied to solve many types of nonlinear problems [1], [2], [11].

The HAM contains a certain auxiliary parameter h which provides us with a simple way to adjust and control the convergence region and rate of convergence of the series solution. Moreover, by means of the so-called h-curves, it is easy to determine the valid regions of h to gain a convergent series solution.

The HAM offers certain advantages over routine numerical methods. Numerical methods use discretization which gives rise to rounding off errors causing loss of accuracy, and requires large computer memory and time. This computational method yields analytical solutions and has certain advantages over standard numerical methods. The HAM method is better since it does not involve discretization of the variables and hence is free from rounding off errors and does not require large computer memory or time.

According to E-infinity theory [6], [7], [8], 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 [9], [21], [3]. On nanoscales, He et al. [4] 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 [5] 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:

\[
\frac{du_n}{dt} = (u_{n+1} - u_{n-1}) + \sum_{k=1}^{m} (\alpha_k + \beta_k (u_n)^k)
\]

where \(\alpha_k\) and \(\beta_k\) are constants. Physical interpretation is given in Ref. [5]. Eq. (1) includes the well-known discretized mKdV lattice equation:

\[
\frac{du_n}{dt} = (a - u_n^2)(u_{n+1} - u_{n-1})
\]

where the subscript n in Eq. (1) represents the nth lattice. The aim of this paper is to directly extend the HAM to consider the explicit analytic solution of the Eq. (2). Previously such equations were solved by the exp-function method [10], [12], [13] and the homotopy perturbation method [14].

II. BASIC IDEA OF HAM

In this section we employ the homotopy analysis method [15] to the discussed problem.

To describe the basic ideas of the HAM, we consider the following differential equation

\[
N[u(x,t)] = 0,
\]

where \(N\) is a nonlinear operator, \(x, t\) denotes independent variables, \(u(x,t)\) is an unknown function, respectively. For simplicity, we ignore all boundary or initial conditions, which can be treated in the similar way. By means of generalizing the traditional homotopy method, Liao [15] constructs the so-called zero-order deformation equation

\[
(1 - q)L[\phi(x,t;q) - u_0(x,t)] = q h H(x,t)N[\phi(x,t;q)],
\]

where \(q \in [0, 1]\) is the embedding parameter, \(h \neq 0\) is a non-zero auxiliary parameter, \(H(x,t) \neq 0\) is an auxiliary function, \(L\) is an auxiliary linear operator, \(u_0(x,t)\) is an initial guess of \(u(x,t)\), \(u(x,t;q)\) is a unknown function, respectively. It is important, that one has freedom to choose auxiliary things in HAM. Obviously, when \(q = 0\) and \(q = 1\), it holds

\[
\phi(x,t;0) = u_0(x,t), \phi(x,t;1) = u(x,t),
\]

respectively. Thus, as \(q\) increases from 0 to 1, the solution \(u(x,t;q)\) varies from the initial guess \(u_0(x,t)\) to the solution \(u(x,t)\). Expanding \(u(x,t;q)\) in Taylor series with respect to \(q\), we have

\[
\phi(x,t; q) = u_0(x,t) + \sum_{m=1}^{\infty} u_m(x,t)q^m,
\]
where
\[ u_m(x, t) = \frac{1}{m!} \frac{\partial^m \phi(x, t; q)}{\partial q^m} |_{q=0}. \] (7)

If the auxiliary linear operator, the initial guess, the auxiliary parameter \( h \), and the auxiliary function are properly chosen, the series (6) converges at \( q = 1 \), then we have
\[ u(x, t) = u_0(x, t) + \sum_{m=1}^{\infty} u_m(x, t), \] (8)
which must be one of solutions of original nonlinear equation, as proved by Liao [16]. As \( h = -1 \) and \( H(x, t) = 1 \), Eq. (4) becomes
\[ (1 - q)L[\phi(x, t; q) - u_0(x, t)] + qN[\phi(x, t; q)] = 0, \] (9)
which is used mostly in the homotopy perturbation method [3], where as the solution obtained directly, without using Taylor series. According to the definition (7), the governing equation can be deduced from the zero-order deformation equation (4). Define the vector
\[ \vec{u}_m = \{ u_0(x, t), u_1(x, t), \ldots, u_n(x, t) \}. \]
Differentiating equation (4) \( m \) times with respect to the embedding parameter \( q \) and then setting \( q = 0 \) and finally dividing them by \( m! \), we have the so-called \( m \)th-order deformation equation
\[ L[u_m(x, t) - \chi_m u_{m-1}(x, t)] = h H(x, t) R_m(\vec{u}_{m-1}), \] (10)
where
\[ R_m(\vec{u}_{m-1}) = \frac{1}{(m-1)!} \frac{\partial^{m-1} N[\phi(x, t; q)]}{\partial q^{m-1}} |_{q=0}. \] (11)
and
\[ \chi_m = \begin{cases} 0, & m < 1, \\ 1, & m > 1. \end{cases} \] (12)
It should be emphasized that \( u_m(x, t) \) for \( m \geq 1 \) is governed by the linear equation (10) under the linear boundary conditions that come from original problem, which can be easily solved by symbolic computation software such as Matlab. For the convergence of the above method we refer the reader to Liao’s work. If Eq. (3) admits unique solution, then this method will produce the unique solution. If equation (3) does not possess unique solution, the HAM will give a solution among many other (possible) solutions.

**Remark 3.1.**
Liao [16] proved that, as long as a series solution given by the homotopy analysis method converges, it must be one of exact solutions. So, it is important to ensure that the solution series (8) is convergent. Note that the solution series (8) contain the auxiliary parameter \( h \), which we can choose properly by plotting the so-called \( h \) -curves to ensure solution series converge. As suggested by Liao [16], the appropriate region for \( h \) is a horizontal line segment.

### III. Application
In this part, we apply the HAM to solve for the traveling wave solution of Eq. (2), subject to the initial conditions
\[ u_{n_0}(n, 0) = \sqrt{\tanh(d) \tanh(nd)}, \] (13)
where \( d \) is an arbitrary constant.
From Eq. (2), we define the nonlinear operator
\[ N[\phi(n, t; q)] = \frac{d\phi(n, t; q)}{dt} - (\alpha - \phi_0^2(n, t; q)) \left( \phi_{n+1}(n, t; q) - \phi_{n-1}(n, t; q) \right), \] (14)
According to the initial condition denoted by (13), it is natural to choose
\[ u_{n_0}(n, t) = \sqrt{\tanh(d) \tanh(nd)}, \] (15)
We choose the linear operator
\[ L[\phi(n, t; q)] = \frac{d\phi(n, t; q)}{dt}, \] (16)
with the property \( L[c] = 0 \), where \( c \) is coefficient.
To ensure this, let \( h \neq 0 \) denote an auxiliary parameter, \( q \in [0, 1] \) an embedding parameter. We have the zeroth-order deformation equation
\[ (1 - q)L[\phi_0(n, t; q) - u_{n_0}(n, t)] = qh H(n, t) N[\phi_0(n, t; q)], \] (17)
Obviously, when \( q=0 \) and \( q=1 \),
\[ \phi_0(n, t; 0) = u_{n_0}(n, t), \quad \phi_0(n, t; 1) = u_{n_0}(n, t), \] (18)
Thus, \( \phi_0(n, t; q) \) can be expanded in the Maclaurin series with respect to \( q \) in the form
\[ \phi_0(n, t; q) = u_{n_0}(n, t) + \sum_{m=1}^{\infty} u_{n_m}(n, t) q^m, \] (19)
where
\[ u_{n_0}(n, t) = \frac{1}{m!} \frac{\partial^m \phi_0(n, t; q)}{\partial q^m} |_{q=0}. \] (20)
Note that the zeroth-order deformation Eq.(17) contains the auxiliary parameter \( h \), so that \( \phi_0(n, t; q) \) is dependent on \( h \). Assuming that \( h \) is so properly chosen that the series Eq.(19) is convergent at \( q = 1 \), we obtain from Eq.(19) that
\[ u_n(n, t) = u_{n_0}(n, t) + \sum_{m=1}^{\infty} u_{n_m}(n, t), \]
Foe the sake of simplicity, introduce
\[ \vec{u}_{n_m} = \{ u_{n_1}, u_{n_2}, u_{n_3}, \ldots, u_{n_m} \}. \] (21)
We differentiate the zeroth-order deformation Eq.(17) \( m \) times with respect to \( q \), then set \( q = 0 \). Dividing the obtained equation by \( m! \), we get the so-called \( m \)th-order deformation equation:
\[ L[u_{n_m}(n, t) - \chi_m u_{n_m-1}(n, t)] = h H(n, t) R_m(\vec{u}_{n_m-1}), \] (22)
where
\[ R_m(\vec{u}_{n_m-1}) = \frac{du_{n_{m-1}}}{dt} - (\alpha - \sum_{k=0}^{m-1} u_{n_k} u_{n_{m-1-k}}) \left( u_{n+1_{m-1}} - u_{n-1_{m-1}} \right), \] (23)
We now successively obtain the solution to each high order deformation equation:

\[ u_{nm}(n,t) = x_m u_{m-1}(n,t) + L^{-1} \left[ hH(n,t)R_m \left( \alpha_{n-1} \right) \right], \quad m \geq 1, \quad (24) \]

We start with an initial approximation \( u_{n0}(n,t) \) and can obtain directly the other components as:

\[ u_{n1} = -h\left( \alpha - \delta \tanh(d) \right)^2 \left( \tanh((n + 1)d) - \tanh((n - 1)d) \right)/t, \]

\[ u_{n2} = -h\left( \alpha - \delta \tanh(d) \right)^2 \left( \tanh((n + 1)d) - \tanh((n - 1)d) \right)/t + \ldots \]

\[ : \]

IV. NUMERICAL RESULTS

In this case, we take \( \alpha = 1, \delta = 1, t = 1 \) as an example. In Table (1) we have presented approximate solution by 3rd-order HAM, and error of HAM. By HAM, it is easy to discover the valid region of \( h \), which corresponds to the line segments nearly parallel to the horizontal axis. To find the valid region of \( h \), the \( h \)-curve given by the 3rd-order HAM approximation is drawn in Fig. 1, which clearly indicates that the valid region of \( h \) is about \(-1.4 < h < -0.4 \). From Fig. 1, it is easily seen that \(-1 \) is a valid value of \( h \). Thus, The results of HAM in special case is similar to HPM results. In Fig. 2, one can also see the comparison between obtained results HAM with exact solution.

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Table 1

Fig. 1. The \( h \)-curve of \( u_n(3,1) \) based on the 3rd-order HAM.

Fig. 2. The comparison of the HAM(\( h=1 \)) and exact solution.

V. CONCLUSION

In this Letter, we have successfully developed HAM for solving discontinued problems arising in nanotechnology. It is apparently seen that HAM is a very powerful and efficient technique in finding analytical solutions for wide classes of linear problems. The results got from the performance of HAM over discontinued problems arising in nanotechnology, was specified that the solution of HAM is similar to HPM results.

Matlab has been used for computations in this paper.

REFERENCES


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