On the Convergence of the Homotopy Analysis Method for Solving the Schrödinger Equation

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ABSTRACT

In this paper, solving the linear and nonlinear Schrödinger equations are considered by a new numerical approach based on the homotopy analysis method (HAM). For this purpose, at first the convergence theorems of the HAM are proved to ensure that the series solution obtained from this method is able to evaluate the exact solution of the linear or nonlinear Schrödinger equation. Then, an algorithm is applied to evaluate the components of the series solution in the HAM numerically in order to approximate the solution of the Schrödinger equation at a given point. Finally, two examples are solved to illustrate the efficiency of the proposed algorithm.

KEYWORDS: Homotopy analysis method (HAM), Schrödinger equation, Convergence.

1. INTRODUCTION

HAM is an efficient and considerable method in order to solve linear and nonlinear problems\textsuperscript{[1,2]}. This method was introduced by Liao\textsuperscript{[3-5]}. The Schrödinger equation is one of the important partial differential equation with many applications in hydrodynamics, optics, chemistry and physics. We consider the linear Schrödinger equation of the form,

\[ u_t + iu_{xx} = 0, \quad u(x, 0) = f(x), \quad i^2 = -1 \]  

(1)

and nonlinear Schrodinger equation of the form,

\[ iu_t + \frac{1}{2}u_{xx} + \gamma |u|^2u = 0, \quad u(x, 0) = f(x), \quad i^2 = -1, \]  

(2)

where \( \gamma \) is a real constant, \( t \geq 0 \) and \( u = u(x,t) \) is the complex unknown function.

In recent years, some analytical and numerical methods have been proposed in order to solve these equations. Some of these methods are, finite differences method\textsuperscript{[6]}, differential transform method\textsuperscript{[7]}, Adomian decomposition and homotopy perturbation methods\textsuperscript{[8-10]}, exp-function method\textsuperscript{[11]}, and variational iteration method\textsuperscript{[12]}. Alomari \textit{et al.}\textsuperscript{[13]} applied the homotopy analysis method (HAM) in order to solve the equations (1) and (2) analytically. They obtained the explicit series solutions for Schrödinger equation. The present work is another vision of this work to prove the convergence theorems of the HAM and to solve the equations (1) and (2) numerically.

The main purpose of this work is to answer the following questions:

1. Under what conditions the series solution obtained from the homotopy analysis method is convergent in order to solve a linear or nonlinear Schrödinger equation?

2. How one can estimate the value of the solution at a given point in convergence region for Schrödinger equation via a numerical algorithm?

In this work, we apply HAM in order to obtain the numerical solution of the equations (1) and (2) and propose an algorithm to evaluate the approximate solution at a given point. Also, we prove the theorems to illustrate the convergence of the method. At first, in section 2, we introduce the preliminaries of HAM, then in section 3, we use this method for solving the linear and nonlinear Schrodinger equations (1) and (2) and prove the convergence of this method. Finally, in section 4, we solve two numerical examples by using the proposed algorithm based on the HAM to illustrate the efficiency and accuracy of the HAM.

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2. Preliminaries
In order to describe the HAM, we consider the following differential equation:

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

(3)

where \( N \) is a nonlinear operator, \( x \) and \( t \) denote the independent variables and \( u \) is an unknown function. By means of the HAM, we construct the zeroth-order deformation equation

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

(4)

where \( q \in [0; 1] \) is the embedding parameter, \( h \neq 0 \) is an auxiliary parameter, \( L \) is an auxiliary linear operator and \( H(x, t) \) is an auxiliary function. \( \phi(x, t; q) \) is an unknown function and \( u_0(x, t) \) is an initial guess of \( u(x, t) \). It is obvious that when \( q = 0 \) and \( q = 1 \), we have:

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

respectively. Therefore, as \( q \) increases from 0 to 1, the solution \( \phi(x, t; q) \) varies from the \( u_0(x, t) \) to the exact solution \( u(x, t) \). By Taylor's theorem, we expand \( \phi(x, t; q) \) in a power series of the embedding parameter \( q \) as follows:

\[ \phi(x, t; q) = u_0(x, t) + \sum_{m=1}^{+\infty} u_m(x, t) q^m \]  

(5)

where

\[ u_m(x, t) = \frac{1}{m!} \frac{\partial^m \phi(x, t; q)}{\partial q^m} \Big|_{q=0}. \]  

(6)

Let the initial guess \( u_0(x, t) \), the auxiliary linear operator \( L \), the nonzero auxiliary parameter \( h \) and the auxiliary function \( H(x, t) \) be properly chosen so that the power series (5) converges at \( q = 1 \), then, we have:

\[ u(x, t) = u_0(x, t) + \sum_{m=1}^{+\infty} u_m(x, t), \]  

(7)

which must be the solution of the original nonlinear equation. Now, we define the following set of vectors:

\[ \bar{u}_m = \{ u_0(x, t), u_1(x, t), \ldots, u_m(x, t) \}. \]  

(8)

By differentiating the zeroth order deformation (4) \( m \) times with respect to the embedding parameter \( q \) and then setting \( q = 0 \) and finally dividing by \( m! \), we get the following \( m \)th order deformation equation:

\[ L[u_m(x, t) - \chi_m u_{m-1}(x, t)] = h H(x, t) R_m(\bar{u}_{m-1}), \]  

(9)

where

\[ R_m(\bar{u}_{m-1}) = \frac{1}{(m-1)!} \frac{\partial^{m-1} N[\phi(x, t; q)]}{\partial q^{m-1}} \Big|_{q=0}, \]  

(10)

and

\[ \chi_m = \begin{cases} 0, & m \leq 1, \\ 1, & m > 1. \end{cases} \]  

(11)

It should be emphasized that \( u_m(x, t) \) for \( m \geq 1 \) is governed by the linear equation (9) with linear boundary conditions that come from the original problem. For more details about HAM, we refer the reader to [1-5].
3. Convergence of the HAM

In this section, we consider both linear and nonlinear Schrödinger equations and prove the convergence of the series solution obtained from the HAM to the exact solution of the equation. In [14], the existence of the series solution for Schrödinger equation was proved.

3.1 Linear form

In order to solve (1), let the initial approximation:

\[ u_0(x, t) = f(x) \]

nonlinear operator

\[ N[\phi(x, t; q)] = \frac{\partial \phi(x, t; q)}{\partial t} + i \frac{\partial^2 \phi(x, t; q)}{\partial x^2} \]

and the linear operator

\[ L[\phi(x, t; q)] = \frac{\partial \phi(x, t; q)}{\partial t} \]

with the property

\[ L[c_1(x)] = 0 \]

where \( c_1(x) \) is the integration constant [13]. Applying (9) under the initial condition \( u_m(x, t) = 0 \) where

\[ R_m(\vec{u}_{m-1}) = \frac{\partial \phi(x, t; q)}{\partial t} + i \frac{\partial^2 \phi(x, t; q)}{\partial x^2}. \] (12)

The solution of the \( m \)-th order deformation equation (9) for \( m \geq 1 \) becomes

\[ u_m(x, t) = \chi_m u_{m-1}(x, t) + h L^{-1}[H(x, t) R_m(\vec{u}_{m-1})]. \] (13)

Then the series solution is

\[ u(x, t) = u_0(x, t) + u_1(x, t) + u_2(x, t) + \cdots \] (14)

**Theorem 3.1.** If the series solution (14) of equation (1) obtained from the HAM is convergent then it converges to the exact solution of the equation (1).

**Proof.** Let the series

\[ \sum_{m=0}^{+\infty} u_m(x, t) \]

be convergent. We assume:

\[ u(x, t) = \sum_{m=0}^{+\infty} u_m(x, t) \]

where

\[ \lim_{m \to +\infty} u_m(x, t) = 0. \] (15)

We have

\[ \sum_{m=1}^{+\infty} [u_m(x, t) - \chi_m u_{m-1}(x, t)] = u_1 + (u_2 - u_1) + (u_3 - u_2) + \cdots + (u_n - u_{n-1}) = u(x, t). \]

By using (15),

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\[
\sum_{m=1}^{+\infty} [u_m(x, t) - \chi_m u_{m-1}(x, t)] = \lim_{n \to +\infty} u_n(x, t) = 0.
\]

According to the definition of the operator \( L \), we can write

\[
\sum_{m=1}^{+\infty} L[u_m(x, t) - \chi_m u_{m-1}(x, t)] = L \sum_{m=1}^{+\infty} [u_m(x, t) - \chi_m u_{m-1}(x, t)] = 0.
\]

From above expression and equation (13), we obtain

\[
\sum_{m=1}^{+\infty} L[u_m(x, t) - \chi_m u_{m-1}(x, t)] = hH(x, t) \sum_{m=0}^{+\infty} [R_m(\bar{u}_{m-1})].
\]

Since \( h \neq 0 \) and \( H(x, t) \neq 0 \), we have

\[
\sum_{m=0}^{+\infty} [R_m(\bar{u}_{m-1})] = 0 \tag{16}
\]

From (12), it holds

\[
\sum_{m=1}^{+\infty} [R_m(\bar{u}_{m-1})] = \sum_{m=1}^{+\infty} \frac{\partial u_{m-1}}{\partial t} + i \sum_{m=1}^{+\infty} \frac{\partial^2 u_{m-1}}{\partial x^2} = \sum_{m=0}^{+\infty} \frac{\partial u_m}{\partial t} + i \sum_{m=0}^{+\infty} \frac{\partial^2 u_m}{\partial x^2} + \frac{\partial^2 u_m}{\partial x^2}. \tag{17}
\]

From (16) and (17), we have

\[
u_t + i u_{xx} = 0.\]

### 3.2 Nonlinear form

In order to solve (2), let

\[
L[\phi(x,t;q)] = i \frac{\partial \phi(x,t;q)}{\partial t},
\]

with the property

\[
L[c_1(x)] = 0,
\]

Where \( c_2(x) \) is the integration constant. The nonlinear operator is taken as

\[
N[\phi(x,t;q)] = i \phi_t(x,t;q) + \frac{1}{2} \phi_{xx}(x,t;q) + \gamma |\phi(x,t;q)|^2 \phi(x,t;q). \tag{18}
\]

Therefore

\[
\sum_{m=1}^{+\infty} \frac{\partial u_m}{\partial t} + hL^{-1}[H(x,t)R_m(\bar{u}_{m-1})],
\]

then

\[
u_m(x,t) = \chi_m u_{m-1}(x,t) - i h \int h(x,t) R_m(\bar{u}_{m-1}) dt + c_1(x), \tag{19}
\]

where \( c_1(x) \) is determined by the initial condition. Based on the relation \(|u|^2 u = \bar{u} u^2\), we can write:

\[
R_m(\bar{u}_{m-1}) = i \frac{\partial u_{m-1}}{\partial t} + \frac{1}{2} \frac{\partial^2 u_{m-1}}{\partial x^2} + \gamma \sum_{i=0}^{m-1} \sum_{k=0}^{m-1-i} u_i u_k \bar{u}_{m-k-i-1}. \tag{20}
\]

**Theorem 3.2.** If the series solution (14) of equation (2) obtained from the HAM is convergent then it converges to the exact solution of the equation (2).

**Proof.** If the series

\[6079\]
From above expression and equation (9), we obtain

$$u(x,t) = \sum_{m=0}^{+\infty} u_m(x,t)$$

where

$$\lim_{m \to +\infty} u_m(x,t) = 0.$$ \hspace{1cm} (21)

We write

$$\sum_{m=1}^{+\infty} [u_m(x,t) - \chi_m u_{m-1}(x,t)] = u_1 + (u_2 - u_1) + (u_3 - u_2) + \cdots + (u_n - u_{n-1}) = u(x,t).$$

By using (21), we have

$$\sum_{m=1}^{+\infty} [u_m(x,t) - \chi_m u_{m-1}(x,t)] = \lim_{n \to +\infty} u_n(x,t) = 0.$$

According to the definition of the operator $L$, we can write

$$\sum_{m=1}^{+\infty} L[u_m(x,t) - \chi_m u_{m-1}(x,t)] = L \sum_{m=1}^{+\infty} [u_m(x,t) - \chi_m u_{m-1}(x,t)] = 0.$$

From above expression and equation (9), we obtain

$$\sum_{m=1}^{+\infty} L[u_m(x,t) - \chi_m u_{m-1}(x,t)] = h H(x,t) \sum_{m=0}^{+\infty} [R_m(\tilde{u}_{m-1})].$$

Since $h \neq 0$ and $H(x,t) \neq 0$, we have

$$\sum_{m=0}^{+\infty} [R_m(\tilde{u}_{m-1})] = 0.$$ \hspace{1cm} (22)

From (20), it holds

$$i \sum_{m=0}^{+\infty} [R_m(\tilde{u}_{m-1})] = i \sum_{m=0}^{+\infty} \frac{\partial u_{m-1}}{\partial t} + \frac{1}{2} \sum_{m=0}^{+\infty} \frac{\partial^2 u_{m-1}}{\partial x^2} + \gamma \sum_{i=0}^{+\infty} \sum_{m=i+1}^{+\infty} \sum_{k=0}^{m-i-1} u_i u_k \tilde{u}_{m-k-i-1} =$$

$$i \sum_{m=0}^{+\infty} \frac{\partial u_m}{\partial t} + \frac{1}{2} \sum_{m=0}^{+\infty} \frac{\partial^2 u_m}{\partial x^2} + \gamma \sum_{i=0}^{+\infty} \sum_{m=i+1}^{+\infty} \sum_{k=0}^{m-i-1} u_i \tilde{u}_{m-k-i-1} =$$

$$i \sum_{m=0}^{+\infty} \frac{\partial u_m}{\partial t} + \frac{1}{2} \sum_{m=0}^{+\infty} \frac{\partial^2 u_m}{\partial x^2} + \gamma \sum_{i=0}^{+\infty} \sum_{m=i+1}^{+\infty} \sum_{k=0}^{m-i-1} u_k \tilde{u}_{m-k-i-1} =$$

$$i \sum_{m=0}^{+\infty} \frac{\partial u_m}{\partial t} + \frac{1}{2} \sum_{m=0}^{+\infty} \frac{\partial^2 u_m}{\partial x^2} + \gamma \sum_{i=0}^{+\infty} \sum_{m=i+1}^{+\infty} \sum_{k=0}^{m-i-1} u_k \tilde{u}_{m-k-i-1} =$$

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Consider the linear Schrödinger equation (1) with initial condition

\[ i \sum_{m=0}^{+\infty} \frac{\partial u_m}{\partial t} + \frac{1}{2} \sum_{m=0}^{+\infty} \frac{\partial^2 u_m}{\partial x^2} + \gamma \sum_{i=0}^{+\infty} u_i \sum_{k=0}^{+\infty} u_k \bar{u}_m = 0, \]

under the initial condition $u(x,0) = f(x)$.

Example 4.2. Consider the nonlinear Schrödinger equation (2) as follows \[^{[13]}\]

\[ iu_t = -\frac{1}{2} u_{xx} + |u|^2 u, \quad t \geq 0 \]

under the initial condition $u(x,0) = e^{ix}$.

4 Numerical examples

In this section, we solve a linear and a nonlinear Schrödinger equation via the HAM numerically by applying the following algorithm where $\text{sum}$ is the approximate value of the solution for equation (1) or (2) at the given point $(x,t)$. The programs have been provided by Maple.

Algorithm 1.

1) Read $n, x \in \mathbb{R}, t \in [0, T]$ and $f(x)$,
2) Put $\text{sum} = 0$ and $u(x,0) = f(x)$,
3) For $m = 1(1)n$ do
   3.a) Evaluate $u_m(x,t)$ via (13) for equation (1) or via (19) for equation (2),
   3.b) Set $\text{sum} = \text{sum} + u_m(x,t)$,
4) write $n$ and $\text{sum}$.

Example 4.1. Consider the linear Schrödinger equation (1) with initial condition $u(x,0) = 1 + \cosh(2x)$ \[^{[13]}\]. We assume $h = -1$ and $H(x, t) = 1$. The exact solution is $u(x,t) = 1 + \cosh(2x)e^{-4it}$. Table 1 shows the results of the algorithm at the points $(x_1, t_1) = \left(\frac{\pi}{2}, 0.25\right)$ and $(x_2, t_2) = \left(\frac{3\pi}{2}, 0.75\right)$ for $n = 2, 4, 8, 16$ and 20. The value of the exact solution at these points are:

\[ u(x_1, t_1) = 1 + \cosh \pi \cos 1 - \cosh \pi \sin 1 \approx 7.26315908428001271301 - 9.7542923386002156321i, \]
\[ u(x_2, t_2) = \cosh 3\pi \cos 3 - \cosh 3\pi \sin 3 \approx -6132.8192151224027047 + 874.354152495827845679i. \]

<table>
<thead>
<tr>
<th>$n$</th>
<th>$(\pi/2, 0.25)$</th>
<th>$(3\pi/2, 0.75)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n=2$</td>
<td>6.7959766377067063-11.59159532755215206i</td>
<td>-21684.383805079376-18587.4718329241i</td>
</tr>
<tr>
<td>$n=4$</td>
<td>7.2789746909074903-9.6599610629346005i</td>
<td>-773.477993085313-9293.735916462161i</td>
</tr>
<tr>
<td>$n=8$</td>
<td>7.2631622546437581-9.75426068283467638i</td>
<td>-6038.545349264264-564.62534977852i</td>
</tr>
<tr>
<td>$n=16$</td>
<td>7.2631590842800124-9.7542923386001831i</td>
<td>-6132.81889810180+874.352533796956i</td>
</tr>
<tr>
<td>$n=20$</td>
<td>7.2631590842800127-9.754292336002156i</td>
<td>-6132.81219492262-874.354572371974i</td>
</tr>
</tbody>
</table>

As we observe in table 1, the number of significant digits common between the approximate and exact solutions in both real and imaginary parts increase when $n$ increases such that for $n=20$ the absolute error (the modulus of error in complex number) at the point $(\pi/2, 0.25)$ is less than $10^{-16}$ and at the point $(3\pi/2, 0.75)$ is about $0.125787 \times 10^{-7}$ which decreases for larger $n$.

Example 4.2. Consider the nonlinear Schrödinger equation (2) as follows \[^{[13]}\],

\[ iu_t = -\frac{1}{2} u_{xx} + |u|^2 u, \quad t \geq 0 \]

under the initial condition $u(x,0) = e^{ix}$. 

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We assume \( h = -1 \) and \( H(x, t) \equiv 1 \), the exact solution of (24) is \( u(x, t) = e^{i(x+\frac{t}{2})} \). Table 2 shows the results of the algorithm at the points \((x_1, t_1) = (\frac{\pi}{4}, 0.25)\), \((x_2, t_2) = (\frac{\pi}{2}, 0.75)\) for \( n = 2, 4, 6, 8 \) and 10. In this table, the values \(|u_n - u|\) are the absolute error of \( u_n \) (which is the modulus of error in complex numbers) obtained from the algorithm by applying the HAM. One can see the value of error at the given points decreases as \( n \) increases. Also, the rate of convergence is fast such that we can achieve a satisfactory estimate for the solution at the point \((x,t)\) with a few number of iterations in the HAM.

| \( n \) | \( u_n \left( \frac{\pi}{4}, 0.25 \right) \) | \( |u_n - u| \) | \( u_n \left( \frac{\pi}{2}, 0.75 \right) \) | \( |u_n - u| \) |
|---|---|---|---|---|
| 2 | -0.125000000000000000000000000000 | 0.000325 | 0.375000000000000000000000000000 | 0.008766 |
| 4 | -0.992187500000000000000000000000 | 0.25427×10^{-4} | -0.929687500000000000000000000000 | 0.000062 |
| 6 | -0.9921976722526041666670i | 0.94602×10^{-10} | -0.930511474609375000000000000000 | 0.20674×10^{-8} |
| 8 | -0.99219767227851020000i | 0.20530×10^{-15} | -0.93050761222839355470 | 0.40390×10^{-7} |
| 10 | -0.99219767229329309800i | 0.29104×10^{-17} | -0.93050762191229815960 | 0.51643×10^{-12} |

Conclusion

In this paper, the convergence of the homotopy analysis method for solving the linear and nonlinear Schrodinger equation was discussed. For this purpose, we proved two theorems to illustrate the convergence of the series solution obtained from HAM. By solving two examples, we showed the accuracy of the numerical solution stems from the proposed algorithm and fast convergence of the HAM to evaluate the approximate solution of the equation at a given point. Consequently, one can apply the HAM via a numerical scheme to solve the Schrodinger equation in any cases and can guarantee the validation and accuracy of the results.

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