Adomian's decomposition method for solving one dimensional Schrödinger equation

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Abstract

In this paper, the Adomian decomposition method for solving the Schrödinger equation is implemented with appropriate initial conditions. In comparison with existing techniques and exact solution, the decomposition method is highly effective in terms of accuracy and rapid convergence.

Keywords: Adomian's decomposition method, Schrödinger equation

1. Introduction

In this work, we want to apply Adomian's decomposition method (ADM) to obtain an approximate solution for one-dimensional Schrödinger equation. The ADM was introduced by Adomian in the 1980s for solving linear and nonlinear ordinary and partial differential equation [1,5,7] . This method avoids artificial boundary conditions, linearization and yields an efficient numerical solution with a high accuracy.

We consider the Schrödinger equation

$$i\frac{\partial U(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(a(x,t)\frac{\partial U(x,t)}{\partial x}\right) \qquad a(x,t) > 0, \qquad 0 \leq x \leq 1, \quad 0 \leq t \leq T \quad (1)$$

with an initial and boundary conditions,

$$U(x,0) = f(x), \qquad 0 \leq x \leq 1 \tag{2}$$

$$U(0,t) = g_1(x), \qquad U(1,t) = g_2(x), \quad 0 \leq t \leq T \tag{3}$$

Several numerical methods have been proposed to solve (1)-(3) approximately. Many of them are explicit difference scheme [2,3] and Adomian method applied to differential equations [1,4]. Recently, the Adomian decomposition method has emerged as an alternative method for solving a wide range of problems whose mathematical models involve algebraic, differential, Integral differential and partial differential equations. In this paper, various test of Schrödinger equations were handled easily, quickly and elegantly by implementing the ADM. Moreover it's compare to the FDM [2] and available exact solution. The presentation of the current paper is as follows: In section 2 , we give an analysis of ADM for the problem, in section 3, we give an application of ADM and in the last section we give some conclusions.

2. The Adomian decomposition method

In this section we sketch the ADM for equation (1) in operator form

$$L_t U = \frac{1}{i}[\frac{\partial}{\partial x}a(x,t)L_x + a(x,t)L_{xx}]U \tag{4}$$

where $L_t = \frac{\partial}{\partial t}, L_x = \frac{\partial}{\partial x}$ and $L_{xx} = \frac{\partial^2}{\partial x^2}$ are the linear differential operators.

Assuming that the inverse of the operator L_t^{-1} exists and can conveniently be taken as the one-fold definite integral with respect to **t** from **0** to **t**. That is

$$L_t^{-1}(.) = \int_0^t (.)\,dt \tag{5}$$

Application of the inverse operator L_t^{-1} to equation (4) yields

$$U(x,t) = U(x,0) + \frac{1}{i}L_t^{-1}[\frac{\partial}{\partial x}a(x,t)L_x U + a(x,t)L_{xx}U] \qquad (6)$$

We obtain the zero-th component as

$$U_0(x,t) = U(x,0) \qquad (7)$$

Which is defined by a term that arises from the initial condition. The unknown function $U_n(x,t)$, $n \geq 1$, is decomposed into a sum of components defined by the decomposition series

$$U(x,t) = \sum_{n=1}^{\infty} U_n(x,t) \qquad (8)$$

With the zeroth component as defined above the remaining components $U_n(x,t)$, $n \geq 1$, can be completely determined in such a way that each term is computed by using the previous term since U_0 is known,

$$U_1(x,t) = \frac{1}{i}L_t^{-1}[\frac{\partial}{\partial x}a(x,t)L_x U_0 + a(x,t)L_{xx}U_0]$$

$$U_2(x,t) = \frac{1}{i}L_t^{-1}[\frac{\partial}{\partial x}a(x,t)L_x U_1 + a(x,t)L_{xx}U_1] \qquad (9)$$

$$\vdots$$

$$U_{n+1}(x,t) = \frac{1}{i}L_t^{-1}[\frac{\partial}{\partial x}a(x,t)L_x U_n + a(x,t)L_{xx}U_n], \quad n \geq 0.$$

The convergence of ADM is studied presently by many researchers such as [4,6].

3. Applications

To give a clear overview of our study and to illustrate the above discussed technique, we use the following examples.

Example 1

we consider the following pure Schrödinger equation

$$iU_t + U_{xx} = 0 \qquad 0 \leq x \leq 1, \qquad 0 \leq t \leq T$$

with initial and boundary conditions

$$U(x,0) = e^x$$
$$U(0,t) = e^{it} \qquad (10)$$
$$U(1,t) = e^{it+1}$$

It has an exact solution $U(x,t) = e^{it+x}$

By using (9) the terms of Adomian polynomial can be derived as follows

$$U_1 = -\frac{1}{i}te^x, \qquad U_2 = -\frac{t^2}{2}e^x$$

$$U_3 = \frac{t^3}{6i}e^x, \qquad U_4 = \frac{t^4}{24}e^x$$

$$U_5 = -\frac{t^5}{120i}e^x \cdots \cdots \qquad (11)$$

Comparison of the ADM and exact solution is given in Table (1), for t=0.2 and h=0.1 with various values of x. As seen in this table the numerical solutions we get are very close to the exact ones with small error. Also these results are shown in Figs.(1) and (2).

Table 1: Numerical results of example 1 at t=0.2 and h=0.1

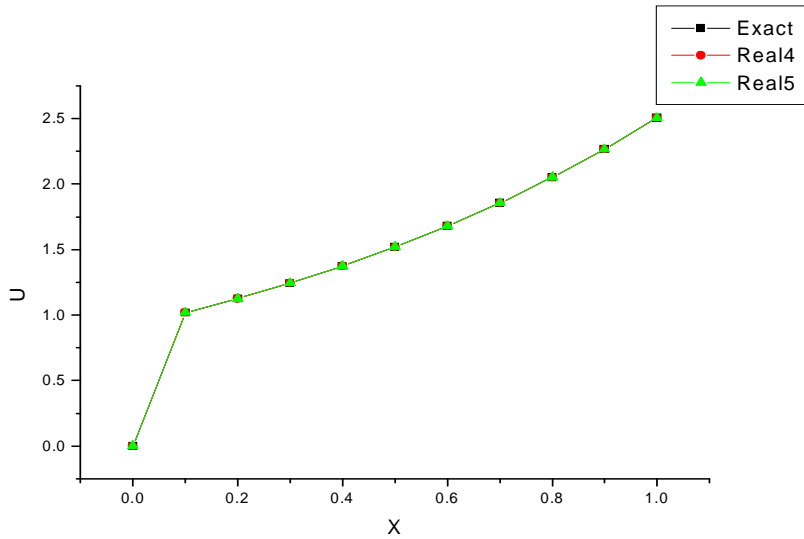| x	Exact solution		Numerical solution		Absolute error	
	Real	Imaginary	Real	Imaginary	Real	Imaginary
0.0	0	0	0	0	0	0
0.1	1.01793	0.43037	1.01794	0.43037	6.19888E-6	3.27826E-7
0.2	1.12499	0.47564	1.12499	0.47564	6.91414E-6	3.57628E-7
0.3	1.2433	0.52566	1.24331	0.52566	7.62939E-6	4.17233E-7
0.4	1.37406	0.58094	1.37407	0.58094	8.46386E-6	4.17233E-7
0.5	1.51857	0.64204	1.51858	0.64204	9.29832E-6	5.36442E-7
0.6	1.67828	0.70957	1.67829	0.70957	1.0252E-5	5.36442E-7
0.7	1.85479	0.78419	1.8548	0.78419	1.14441E-5	5.96046E-7
0.8	2.04986	0.86667	2.04987	0.86667	1.26362E-5	7.15256E-7
0.9	2.26544	0.95781	2.26546	0.95781	1.38283E-5	7.7486E-7
1	2.5037	1.05855	2.50372	1.05855	1.52588E-5	8.34465E-7

Figure (1): Comparison between exact solution, and numerical solution of real part for 4th and 5th iterations
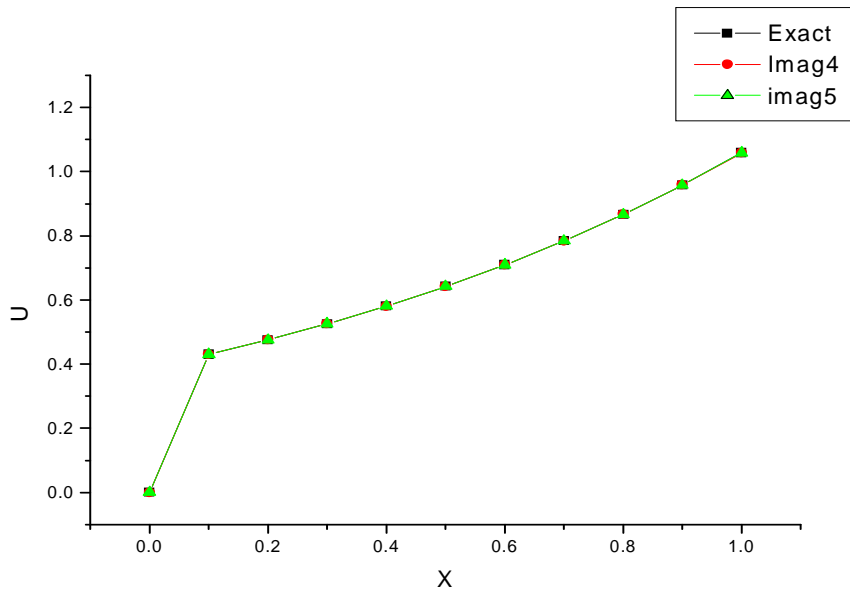

Figure (2): Comparison between exact solution, and numerical solution of imaginary part for four and five iterations

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Example 2

we consider the following Schrödinger equation

$$i\frac{\partial U(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(((1+t)x^2 +1)\frac{\partial U(x,t)}{\partial x}\right) \qquad 0 \le x \le 1, \quad 0 \le t \le T \qquad (12)$$

with initial and boundary condition

$$U(x,0) = xe^{-i}, \qquad 0 \le x \le 1 \qquad (13)$$

$$U(0,t) = 0, \qquad U(1,t) = e^{-i(1+t)^2} \qquad (14)$$

this problem has an exact solution [2]

$$U(x,t) = xe^{-i(1+t)^2}$$

The first five polynomials approximating a solution to (12) satisfying the initial and boundary condition are given by

$$U_1(x,t) = \frac{1}{i}(2t + t^2)xe^{-i}$$

$$U_2(x,t) = -[2t^2 + 2t^3 + \frac{1}{2}t^4]xe^{-i}$$

$$U_3(x,t) = \frac{-1}{i}[\frac{4}{3}t^3 + 2t^4 + t^5 + \frac{1}{6}t^6]xe^{-i}$$

$$U_4(x,t) = [\frac{4}{3}t^4 + \frac{4}{3}t^5 + t^6 + \frac{1}{3}t^7 + \frac{1}{24}t^8]xe^{-i}$$

$$U_5(x,t) = \frac{1}{i}[\frac{4}{15}t^5 + \frac{2}{3}t^6 + \frac{2}{3}t^7 + \frac{1}{3}t^8 + \frac{1}{12}t^9 + \frac{1}{120}t^{10}]xe^{-i}$$

$$\vdots$$
$$\vdots$$

Comparison of the ADM and exact solution is given in Table (2), for t=0.4 and h=0.1 with various values of X . As seen in this table the numerical solutions we get are very close to the exact ones with smaller error. Also these results are shown in Figs.(3) and (4).

Table 2: Numerical results of example 2 at t=0.4 and h=0.1

x	Exact solution		Numerical solution		Absolute error	
	Real	Imaginary	Real	Imaginary	Real	Imaginary
0	0	0	0	0	0	0
0.1	-0.03795	-0.09252	-0.03802	-0.09269	6.9499E-5	1.7171E-4
0.2	-0.07589	-0.18504	-0.07603	-0.18539	1.3900E-4	3.4343E-4
0.3	-0.11384	-0.27756	-0.11404	-0.27808	2.0847E-4	5.1510E-4
0.4	-0.15178	-0.37008	-0.15206	-0.37077	2.7800E-4	6.8685E-4
0.5	-0.18973	-0.46261	-0.19007	-0.46346	3.4745E-4	8.5860E-4
0.6	-0.22767	-0.55513	-0.22809	-0.55616	4.1695E-4	0.00103
0.7	-0.26562	-0.64765	-0.2661	-0.64885	4.8643E-4	0.00120
0.8	-0.30356	-0.74017	-0.30412	-0.74154	5.5599E-4	0.00137
0.9	-0.34151	-0.83269	-0.34213	-0.83424	6.2543E-4	0.00155
1	-0.37945	-0.92521	-0.37945	-0.92521	0	0
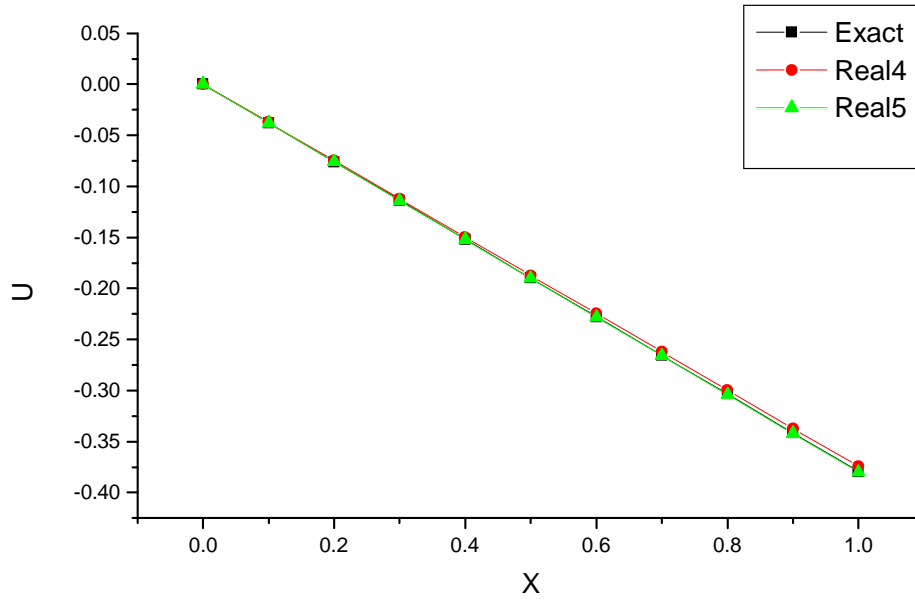
Figure(3): Comparison between exact solution, and numerical solution of real part for 4th and 5th iterations
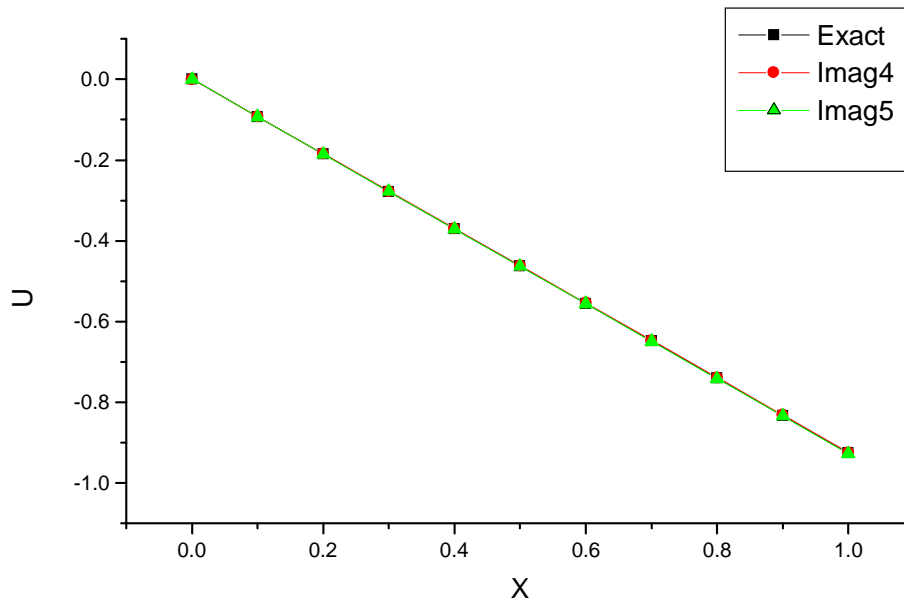

Figure (4) Comparison between exact solution, and numerical solution of imaginary part for 4th and 5th iterations

Table (3) shows comparison of the finite difference method (FDM)[2] and the ADM in absolute errors measurements. The numerical solution resulted from ADM is more accurate than the FDM. Moreover, the decomposition method is highly effective in rapid convergence

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Table 3: Comparison of errors of the DFM and the ADM at $t = 0.4$ & $h = 0.1$

x	FDM		ADM	
	Real	Imaginary	Real	Imaginary
0	0	0	0	0
0.1	0.00193122	0.00780821	6.9499E-5	1.7171E-4
0.2	0.00310273	0.01549867	1.3900E-4	3.4343E-4
0.3	0.00285988	0.02269095	2.0847E-4	5.1510E-4
0.4	0.00048757	0.02908629	2.7800E-4	6.8685E-4
0.5	0.00245094	0.03317088	3.4745E-4	8.5860E-4
0.6	0.00416866	0.03382456	4.1695E-4	0.00103
0.7	0.00462395	0.03099561	4.8643E-4	0.00120
0.8	0.00393724	0.02456307	5.5599E-4	0.00137
0.9	0.00232995	0.01432705	6.2543E-4	0.00155
1	0	0	0	0

4-Conclusions

The numerical solution showed that the ADM is a very convenient method , with this method it is possible to obtain more precise results than the traditional methods such as FDM [2], with less calculation and less time. As shown in the examples, the ADM is simples and easy to use.

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طريقة تحليل أدومين لحل معادلة شرودنكر ذات البعد الواحد

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المستخلص:

في هذا البحث تم استعمال طريقة تحليل أدومين لحل معادلة شرودنكر (Schrödinger) وبشروط ابتدائية مناسبة .

وبمقارنة نتائج هذه الطريقة مع نتائج طريقة الفروقات المحددة و الحل التحليلي للمعادلة وجدنا بان الطريقة ذات كفاءة ودقة عالية وأنها سريعة التقارب.