Computer Science Department of The University of Auckland
CITR at Tamaki Campus (http://www.citr.auckland.ac.nz)

CITR-TR-67 September 2000

Decomposition Method for the Linear Schrödinger Equation

Tiangong Wei[1] and Reinhard Klette[1]

Abstract

The Schrödinger equation is solved by using the decomposition method. A rapidly convergent series solution is achieved. The accuracy of the results obtained indicates the superiority of the decomposition methods over the existing numerical methods that were applied to this equation.

[1] The University of Auckland, Tamaki Campus, Centre for Image Technology and Robotics, Computer Vision Unit, Auckland, New Zealand

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CITR, University of Auckland, Tamaki Campus, Building 731
Auckland, New Zealand

Abstract. The Schrödinger equation is solved by using the decomposition method. A rapidly convergent series solution is achieved. The accuracy of the results obtained indicates the superiority of the decomposition methods over the existing numerical methods that were applied to this equation.

Keywords: Schrödinger equation, decomposition method, series solution, numerical approximation

1 Introduction

It is well known that the Schrödinger equations are of great importance in physics and can be used to describe extensive physical phenomena. So a great deal of interest has been focused on the numerical approximation of the Schrödinger equations. Most of these studies employ mainly finite difference method [1]–[3]. In [1] a class of explicit schemes which are conditionally stable is obtained by adding dissipative terms to the standard forward Euler scheme. However, adding dissipative terms may mean that the problem being solved is no longer a proper representation of the physical problem whose solution is desired. Thus the result may not be physically realistic.

The Adomian's decomposition method has been applied to a wide class of linear and nonlinear equations [4]– [9]. The solution obtained by using this method is expressed as an infinite series which converges very fast to accurate solutions. The series developed yields an accurate approximate solution by considering a truncated number of terms.

In this paper, the Adomian's decomposition method is used for solving the linear Schrödinger equation. In Section 2, the outline of the decomposition method for the linear Schrödinger equation is given. The solution is presented in terms of an infinite series, while in Section 3 we discuss some examples to illustrate the effectiveness and the performance of the method. Comparing this scheme with finite difference methods shows that the present approach is highly accurate. The conclusion and extension of the approach are given in Section 4.

2 Outline of the method

In this paper, we consider the linear Schrödinger equation in its standard form [3]

$$i\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(a(x,t)\frac{\partial u}{\partial x}\right), -\infty < x < +\infty, t > 0, \tag{1}$$

with initial condition

$$u(x,0) = f(x), -\infty < x < +\infty. \tag{2}$$

Here $u(x,t)$ and $f(x)$ are complex valued functions, $a(x,t)$ is a real function, and $i = \sqrt{-1}$. For simplicity, the equation (1) can be written in the form

$$\frac{\partial u}{\partial t} = -i\frac{\partial}{\partial x}\left(a\frac{\partial u}{\partial x}\right), \tag{3}$$

where $a = a(x,t)$. To apply the decomposition method, we write (3) in the operator form

$$L_t u = -iL_x(aL_x u), \tag{4}$$

where L_t and L_x are the linear differential operators defined by $L_t = \frac{\partial}{\partial t}$ and $L_x = \frac{\partial}{\partial x}$, respectively. It is obvious that L_t^{-1} is a definite integral from 0 to t, i.e., $L_t^{-1}(\cdot) = \int_0^t (\cdot)dt$. Applying the operator L_t^{-1} to both sides of (4) yields

$$L_t^{-1}L_t u = -iL_t^{-1}L_x(aL_x u),$$

and using the initial condition (2) leads to

$$u(x,t) = f(x) - iL_t^{-1}L_x(aL_x u). \tag{5}$$

Following the decomposition method [4], we assume that the solution u can be decomposed into the form

$$u = \sum_{n=0}^{\infty} u_n, \tag{6}$$

where the first term u_0 is given by $u_0 = f(x)$. Substituting (6) into (5) determines all components of u by

$$u_0 = f(x), \tag{7}$$

and

$$u_{n+1} = -iL_t^{-1}L_x(aL_x u_n), n \geq 0. \tag{8}$$

Hence the complete solution $u(x,t)$ in (6) can be formally established. The decomposition scheme outlined above leads always to a computable, accurate and rapidly convergent series solution, i.e., the sum $\sum_{n=0}^{\infty} u_n$ converges [4] [10], generally quite rapidly to u.

For a numerical computation, we denote the n-term approximation to the solution $u(x,t)$ by $\phi_n = \sum_{i=0}^{n-1} u_i$. Since the series converges ($\lim_{n\to\infty} \phi_n = u$) and does so very rapidly, the n-term approximation ϕ_n can serve as a practical solution. In many problems, the n-term approximation ϕ_n is accurate for low values of n.

3 Examples

To illustrate the introduced technique, we have chosen the following two examples.

Example 1. We first consider a linear Schrödinger equation

$$i\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\left(1+(1+t)x^2\right)\frac{\partial u}{\partial x}\right), -\infty < x < +\infty, t > 0, \tag{9}$$

and

$$u(x,0) = x\exp(-i), -\infty < x < +\infty. \tag{10}$$

This model has been investigated numerically by the finite difference method [3]. The equation (9) can be rewritten in the form

$$L_t u = -iL_x\left(\left(1+(1+t)x^2\right)L_x u\right).$$

To determine the components of the solution $u(x,t)$, we use (7) and (8) to obtain

$$u_0 = x\exp(-i), \tag{11}$$

and

$$u_{n+1} = -iL_t^{-1}L_x\left(\left(1+(1+t)x^2\right)L_x u_n\right), n \geq 0. \tag{12}$$

It follows that

$$\begin{aligned}
u_1 &= -iL_t^{-1}L_x\left(\left(1+(1+t)x^2\right)L_x u_0\right)\\
&= -iL_t^{-1}\left(2(1+t)x\exp(-i)\right)\\
&= -ix\exp(-i)\left(2t+t^2\right),\\
u_2 &= -iL_t^{-1}L_x\left(\left(1+(1+t)x^2\right)L_x u_1\right)\\
&= -iL_t^{-1}\left(-2i\exp(-i)\left(2t+3t^2+t^3\right)x\right)\\
&= -\frac{1}{2!}x\exp(-i)\left(2t+t^2\right)^2,\\
u_3 &= -iL_t^{-1}L_x\left(\left(1+(1+t)x^2\right)L_x u_2\right)\\
&= -iL_t^{-1}\left(-4\exp(-i)\left(t^2+2t^3+\frac{5}{4}t^4+\frac{1}{4}t^5\right)x\right)\\
&= -i\frac{1}{3!}x\exp(-i)\left(2t+t^2\right)^3,\\
u_4 &= -iL_t^{-1}L_x\left(\left(1+(1+t)x^2\right)L_x u_3\right)\\
&= -iL_t^{-1}\left(2i\frac{1}{3!}x\exp(-i)(1+t)\left(2t+t^2\right)^3\right)\\
&= \frac{1}{4!}x\exp(-i)\left(2t+t^2\right)^4,\\
u_5 &= -i\frac{1}{5!}x\exp(-i)\left(2t+t^2\right)^5,
\end{aligned}$$

and so on. Consequently, we obtain

$$\begin{aligned} u(x,t) &= \sum_{n=0}^{\infty} u_n \\ &= x\exp(-i)\left(1 - \frac{1}{2!}\left(2t+t^2\right)^2 + \frac{1}{4!}\left(2t+t^2\right)^4 - ...\right) \\ &\quad -ix\exp(-i)\left(\left(2t+t^2\right) - \frac{1}{3!}\left(2t+t^2\right)^3 + \frac{1}{5!}\left(2t+t^2\right)^5 - ...\right). \end{aligned}$$

which is the approximate solution.

If we denote the approximation to n-terms by ϕ_n, we have improved approximations

$$\begin{aligned} \phi_1 &= x\exp(-i), \\ \phi_2 &= x\exp(-i)[1 - i(2t+t^2)], \\ \phi_3 &= x\exp(-i)\left[\left(1 - \frac{1}{2!}\left(2t+t^2\right)^2\right) - i\left(2t+t^2\right)\right], \\ \phi_4 &= x\exp(-i)\left[\left(1 - \frac{1}{2!}\left(2t+t^2\right)^2\right) - i\left(\left(2t+t^2\right) - \frac{1}{3!}\left(2t+t^2\right)^3\right)\right]. \end{aligned}$$

Hence,

$$\begin{aligned} u(x,t) &= \lim_{n\to\infty} \phi_n \\ &= x\exp(-i)\left(\cos\left(2t+t^2\right) - i\sin\left(2t+t^2\right)\right) \\ &= x\exp(-i)\cdot\exp\left(-i\left(2t+t^2\right)\right) \\ &= x\exp\left(-i(1+t)^2\right) \end{aligned}$$

is the analytic solution which clearly satisfies the Schrödinger equation(9) and the initial condition (10).

Table 1 shows the absolute errors obtained by using the approximation ϕ_6, i.e., 6 terms only. An improved approximation is easy to achieve if 10 terms of the decomposition are used.

x	Exact solution	Approximate solution	Absolute error
0.0	(0.000 000, 0.000 000)	(0.000 000, 0.000 000)	0.00E+0
0.2	(-0.075 890, -0.185 042)	(-0.075 799, -0.185 238)	0.21E-3
0.4	(-0.151 781, -0.370 085)	(-0.151 599, -0.370 047)	0.43E-3
0.6	(-0.227 671, -0.555 127)	(-0.227 399, -0.555 715)	0.64E-3
0.8	(-0.303 561, -0.740 169)	(-0.303 198, -0.740 953)	0.86E-3
1.0	(-0.379 452, -0.925 212)	(-0.378 998, -0.926 191)	0.10E-2

Table 1. solutions to (9) at $t = 0.4$

Example 2. Consider the following problems described by

$$\frac{\partial u}{\partial t} = i\frac{\partial^2 u}{\partial x^2}, \tag{13}$$

and

$$u(x,0) = \exp(ikx). \tag{14}$$

This linear Schrödinger equation provides a model for the propagation of *dispersive* waves with the wave number of k. In [1] a class of explicit schemes for (13) is obtained by adding dissipative terms to the standard forward Euler scheme. It is worth while to mention that the decomposition technique does not require adding dissipative terms. We can show that this linear problem may be handed more easily, quickly and elegantly by applying the above outlined decomposition method. Using (7) and (8) we find

$$\begin{aligned} u_0 &= \exp(ikx), \\ u_{n+1} &= iL_t^{-1}L_x u_n, \, n \geq 0, \end{aligned}$$

where $L_x = \partial^2/\partial x^2$. Proceeding as before, we obtain the following components:

$$\begin{aligned} u_1 &= iL_t^{-1}L_x u_0 = -i\exp(ikx)k^2t, \\ u_2 &= iL_t^{-1}L_x u_1 = -\exp(ikx)\frac{(k^2t)^2}{2!}, \\ u_3 &= iL_t^{-1}L_x u_2 = i\exp(ikx)\frac{(k^2t)^3}{3!}, \\ u_4 &= iL_t^{-1}L_x u_3 = \exp(ikx)\frac{(k^2t)^2}{2!}, \\ u_5 &= iL_t^{-1}L_x u_4 = -i\exp(ikx)\frac{(k^2t)^5}{5!}, \end{aligned}$$

and so on. Thus the approximate solution is

$$\begin{aligned} u(x,t) &= \sum_{n=0}^{\infty} u_n \\ &= \exp(ikx)\left(1 - \frac{(k^2t)^2}{2!} + \frac{(k^2t)^4}{4!} - \dots\right) \\ &\quad -i\exp(ikx)\left(k^2t - \frac{(k^2t)^3}{3!} + \frac{(k^2t)^5}{5!} - \dots\right). \end{aligned}$$

It immediately follows that

$$\begin{aligned} u(x,t) &= \exp(ikx)\left(\cos(k^2t) - i\sin(k^2t)\right) \\ &= \exp(ikx).\exp(-ik^2t) \\ &= \exp\left(i(kx - k^2t)\right), \end{aligned}$$

which is the analytic solution of (13)and (14).

If a numerical computation is needed, we can use the n-term approximation ϕ_n:

$$\phi_1 = \exp(ikx),$$
$$\phi_2 = \exp(ikx)\left(1 - ik^2t\right),$$
$$\phi_3 = \exp(ikx)\left(\left(1 - \frac{(k^2t)^2}{2!}\right) - ik^2t\right),$$
$$\phi_4 = \exp(ikx)\left(\left(1 - \frac{(k^2t)^2}{2!}\right) - i\left(k^2t - \frac{(k^2t)^3}{3!}\right)\right).$$

Table 2 shows the absolute errors if 6 terms are used. It is evident that the overall errors can be made smaller by adding new terms of the decomposition.

x	Exact solution	Approximate solution	Absolute error
0.0	(0.921 061, -0.389 418)	(0.921 067, -0.389 419)	0.57E-5
0.2	(0.980 067, -0.198 669)	(0.980 072, -0.198 669)	0.57E-5
0.4	(1.000 000, 0.000 000)	(1.000 010, 0.000 001)	0.57E-5
0.6	(0.980 067, 0.198 669)	(0.980 071, 0.198 672)	0.57E-5
0.8	(0.921 061, 0.389 418)	(0.921 065, 0.389 422)	0.57E-5
1.0	(0.825 336, 0.564 642)	(0.825 339, 0.564 647)	0.57E-5

Table 2. solutions to (13) at $t = 0.4, k = 1$

4 Conclusion and Discussion

The decomposition method provides series solutions which converge very rapidly in general. The method makes unnecessary the massive computations of discretization methods for solving partial differential equations, and it is a general analytic technique with clear advantages over the methods that require many restrictive assumptions in mathematics.

Numerical approximations show a high degree of accuracy and in most cases, the n-term approximation ϕ_n is accurate for quite low values of n for quite low values of n. The numerical results we obtained confirm the superiority of the method over the existing techniques. Tables 1 and 2 clearly indicate how the decomposition methodology yields reliable results much closer to the exact solutions.

It is clear that the extension to the more general equation:

$$u_t = ia(x,t)u_{xx} + b(x,t)u_x c(x,t)u + f(x,t)$$

is straightforward. Here the functions $b(x,t), c(x,t)$ and $f(x,t)$ may be complex valued functions and $a(x,t)$ is a real valued function. Using the techniques in [5] we can easily obtain the series solution to the following nonlinear Schrödinger equation:

$$i\,u_t + u_{xx} + q|u|^2 u = 0, -\infty < x < \infty, t \geq 0;$$
$$u(x,0) = g(x), -\infty < x < \infty.$$

where u is a complex valued function, q a real parameter and $i^2 = -1$. In fact, nonlinear term $N(u) = |u|^2 u$ can be written as an infinite sum of the Adomian's polynomials A_n by $N(u) = \sum_{n=0}^{\infty} A_n$, where A_n depends only on $u_0, u_1, \cdots, u_n$. For boundary value problems, evaluating the constants of integration must be done at each level of ϕ_n.

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