Araştırma Makalesi **BAUN Fen Bil. Enst. Dergisi, 27(1), 94-109, (2025)**

DOI:10.25092/baunfbed. 1470617 **J. BAUN Inst. Sci. Technol., 27(1), 94-109, (2025)**

Some efficient schemes of variational iteration method for handling Schrödinger equations in quantum mechanics

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Geliş Tarihi (Received Date): 19.04.2024
Kabul Tarihi (Accepted Date): 03.10.2024

Abstract

At the atomic level, one of the fundamental differential equations that describe the universe and everyday life is the Schrödinger equation in quantum mechanics. Solutions of Schrödinger equations have attracted the attention of researchers. In this study, the variational iteration method is used to handle three dimensional linear and nonlinear time dependent Schrödinger equations. Different iteration formulas have been constructed with the Lagrange multipliers. The accuracy of the approximate solutions obtained by using different iteration formulas of the variational iteration method is given with numerical examples. Comparisons of approximate solutions and exact solutions are shown with graphs. In addition, absolute error tables are included for these comparison results. As a result, it is seen that the variational iteration method gives approximations that converge to the exact solution more rapidly thanks to different iteration formulas.

Keywords: *Analytical solution, variational iteration method, Schrödinger equation*

Kuantum mekaniğinde Schrödinger denklemlerini ele almak için varyasyonel iterasyon yönteminin bazı etkili şemaları

Öz

Atomik düzeyde evreni ve günlük yaşamı tanımlayan temel diferansiyel denklemlerden biri kuantum mekaniğindeki Schrödinger denklemidir. Schrödinger denklemlerinin çözümleri araştırmacıların ilgisini çekmiştir. Bu çalışmada, üç boyutlu lineer ve lineer olmayan zamana bağlı Schrödinger denklemlerini ele almak için varyasyonel iterasyon yöntemi kullanılmıştır. Lagrange çarpanları ile farklı iterasyon formülleri

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oluşturulmuştur. Varyasyonel iterasyon yönteminin farklı iterasyon formülleri kullanılarak elde edilen yaklaşık çözümlerin doğruluğu sayısal örneklerle verilmiştir. Yaklaşık çözümlerin ve tam çözümlerin karşılaştırmaları grafiklerle gösterilmiştir. Ayrıca bu karşılaştırma sonuçları için mutlak hata tablolarına da yer verilmiştir. Sonuç olarak, varyasyonel iterasyon yönteminin farklı iterasyon formülleri sayesinde tam çözüme daha hızlı yakınsayan yaklaşımlar verdiği görülmektedir.

Anahtar kelimeler: *Analitik çözüm, varyasyonel iterasyon yöntemi, Schrödinger denklemi*

1. Introduction

In physics, engineering, and many applied sciences, differential equations are used in mathematical modeling of the behavior of systems. In order to better analyze the behavior of systems, the search for solutions to differential equations has always been a focus of interest [1-5]. One of these differential equations is the Schrödinger equation, the fundamental physics equation used to calculate quantum mechanical states. The solution function of the Schrödinger equation describes how a particle will move through a quantum mechanical system. This function gives the probability of finding a particle at a particular time and location. Motivated by the importance of the solution functions of the Schrödinger equations in describing a quantum mechanical system, we search the solution functions of the time dependent Schrödinger equations. In this work, we focus on the linear time dependent Schrödinger equation (LTSE)

$$\left(i\frac{\partial}{\partial t}+\nabla^2-\mathcal{V}(\mathbf{r})\right)\varphi(\mathbf{r},t)=0,\ t>0,\ \mathbf{r}\in\mathbb{R}^3 \tag{1}$$

and the nonlinear time dependent Schrödinger equation (NLTSE)

$$\left(i\frac{\partial}{\partial t}+\nabla^2-\mathcal{V}(\mathbf{r})-\kappa|\varphi(\mathbf{r},t)|^2\right)\varphi(\mathbf{r},t)=0,\ t>0,\ \mathbf{r}\in\mathbb{R}^3 \tag{2}$$

[6, 7]. Here, $i=\sqrt{-1}$, $\mathbf{r}=(x,y,z)$, $\nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$ is the Laplace operator, $\mathcal{V}$ is the arbitrary potential function, κ is the real parameter and φ is the solution function, $|\varphi(\mathbf{r},t)|^2=\varphi(\mathbf{r},t)\varphi^*(\mathbf{r},t)$, and φ^* is the complex conjugate of φ.

Various numerical methods have been extended and developed for Schrödinger equations. In this paper, our aim is to extend the variational iteration method (VIM) to three dimensional LTSE and NLTSE. The reason for choosing VIM is that it preserves the physical properties of the equation at each step while iteratively approaching the solution function of the Schrödinger equation, providing analytical and faster approximate solutions. VIM was developed to solve nonlinear differential equations by J. H. He [8]. This method has been applied to ordinary and partial differential equations and gives successive approximate solutions that converge rapidly to the exact solution. Many researchers have used VIM for various equations, such as Burger's equation [9], Boussinesq equation [10], fractional differential equations [11, 12], wave equation [13, 14], telegraph equations [15], delay differential-algebraic equations [16], Schrödinger equations [17-19], optimal control problems [20], Korteweg-De-Vries equation, Benjamin equation, Airy equation [21].

The organization of this paper is in the following way. In Section 2, VIM is reviewed. We extend VIM to LTSE (NLTSE) in Section 3 (Section 4) and form different iteration formulas. Some numerical examples are displayed to support the accuracy and applicability of the proposed iteration formulas in Section 5. In Section 6, the results and discussion for the research are presented. A brief conclusion is given in Section 7.

2. Variational iteration method

J. H. He presented VIM to solve differential equation

$$(\mathcal{L}+\mathcal{N})\omega(t)=u(t), \tag{3}$$

where ω is unknown solution function, u is known analytical function [8]. $\mathcal{L}$, $\mathcal{N}$ are linear, nonlinear operators, respectively. For equation (3), correction functional is expressed as

$$\omega_{n+1}(t)=\omega_n(t)+\int_0^t \lambda(\varepsilon)\big(\mathcal{L}\omega_n(\varepsilon)+\mathcal{N}\widetilde{\omega_n}(\varepsilon)-u(\varepsilon)\big)d\varepsilon, \tag{4}$$

$n=0,\ 1,\ 2,\ ...$ [8], where ω_n is nth approximate solution, λ is Lagrange multiplier and $\widetilde{\omega_n}$ is restricted variation, i. e. $\delta\widetilde{\omega_n}=0$. λ is determined optimally using variational theory. Then substituting λ into correction functional (4) gives an iteration formula. The approximations $\widetilde{\omega_n}$ are obtained by using selective function ω_0 and the iteration formula. The solution is

$$\omega(t)=\lim_{n\to\infty}\omega_n(t).$$

3. VIM for LTSE

For a linear time dependent Schrödinger equation, faster convergent approximations to its exact solution can simply be obtained if some of the linear terms are considered as restricted variations. Depending on which linear terms are considered as restricted variations, different Lagrange multipliers are identified. To specify the linear terms considered as restricted variations, equation (1) is rewritten as follows

$$(\mathcal{P}+\mathcal{R}+\mathcal{S}+\mathcal{T}-\mathcal{U})\varphi(\mathbf{r},t)=0, t>0, \mathbf{r}\in\mathbb{R}^3, \tag{5}$$

where $\mathcal{P}=i\frac{\partial}{\partial t}$, $\mathcal{R}=\frac{\partial^2}{\partial x^2}$, $\mathcal{S}=\frac{\partial^2}{\partial y^2}$, $\mathcal{T}=\frac{\partial^2}{\partial z^2}$ are linear operators and $\mathcal{U}\varphi(\mathbf{r},t)=\mathcal{V}(\mathbf{r})\varphi(\mathbf{r},t)$ is linear term. For equation (5), we give two different correction functionals are constructed as follows

$$\begin{aligned}\varphi_{j+1}(\mathbf{r},t)&=\varphi_j(\mathbf{r},t)+\int_0^t\lambda_1(\eta)\Big(\mathcal{P}\varphi_j(\mathbf{r},\eta)+(\mathcal{R}+\mathcal{S}+\mathcal{T}-\mathcal{U})\widetilde{\varphi_j}(\mathbf{r},\eta)\Big)d\eta\\&=\varphi_j(\mathbf{r},t)+\int_0^t\lambda_1(\eta)\left(i\frac{\partial\varphi_j(\mathbf{r},\eta)}{\partial\eta}+\big(\nabla^2-\mathcal{V}(\mathbf{r})\big)\widetilde{\varphi_j}(\mathbf{r},\eta)\right)d\eta\end{aligned} \tag{6}$$

and

$$\begin{aligned}\varphi_{j+1}(\mathbf{r},t)=\varphi_j(\mathbf{r},t)+\int_0^x\lambda_2(\gamma)\big(\mathcal{R}\varphi_j(\gamma,y,z,t)+(\mathcal{P}+\mathcal{S}+\mathcal{T}\\-\mathcal{U})\widetilde{\varphi_j}(\gamma,y,z,t)\big)d\gamma\end{aligned}$$

$$= \varphi_j(\mathbf{r},t) + \int_0^x \lambda_2(\gamma) \Big(\frac{\partial^2 \varphi_j(\gamma,y,z,t)}{\partial \gamma^2} + \left(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \mathcal{V}(\gamma,y,z) \right) \widetilde{\varphi_j}(\gamma,y,z,t) \Big) d\gamma \tag{7}$$

$j = 0, 1, 2, \ldots$, where λ_1 and λ_2 are Lagrange multipliers, $\widetilde{\varphi_j}$ is restricted variation. With known $\delta\varphi_j = 0$, the stationary conditions are as follows

$$1 + i\,\lambda_1(\eta)\Big|_{\eta=t} = 0, \frac{d\lambda_1(\eta)}{d\eta} = 0,$$
$$\lambda_2(\gamma)\Big|_{\gamma=x} = 0, 1 - \frac{d\lambda_2(\gamma)}{d\gamma}\Big|_{\gamma=x} = 0, \frac{d^2\lambda_2(\gamma)}{d\gamma^2} = 0.$$

Hence,

$$\lambda_1(\eta) = i, \lambda_2(\gamma) = \gamma - x. \tag{8}$$

If we substitute the values (8) into functionals (6)-(7), we get the following different iteration formulas

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + i\int_0^t \left(i\frac{\partial}{\partial \eta} + \nabla^2 - \mathcal{V}(\mathbf{r}) \right) \varphi_j(\mathbf{r},\eta)d\eta, \tag{9}$$

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + \int_0^x (\gamma - x)\Big(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial \gamma^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \mathcal{V}(\gamma,y,z)\Big)\varphi_j(\gamma,y,z,t)d\gamma, \tag{10}$$

$j = 0, 1, 2, \ldots$. Following the above iteration process, if $\mathcal{S}\varphi(\mathbf{r},t)$ is the only term in equation (5) that is not considered as a restricted variation, the iteration formula

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + \int_0^y (\beta - y)\Big(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial \beta^2} + \frac{\partial^2}{\partial z^2} - \mathcal{V}(x,\beta,z)\Big)\varphi_j(x,\beta,z,t)d\beta, \tag{11}$$

$j = 0, 1, 2, \ldots$, is obtained, which is different from the iteration formulas (9) and (10). Similarly, if $\mathcal{T}\varphi(\mathbf{r},t)$ is the only term in equation (5) that is not considered as a restricted variation, we obtain the following iteration formula

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + \int_0^z (\alpha - z)\Big(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial \alpha^2} - \mathcal{V}(x,y,\alpha)\Big)\varphi_j(x,y,\alpha,t)d\alpha, \tag{12}$$

$j = 0, 1, 2, \ldots$. The solution is

$$\varphi(\mathbf{r},t) = \lim_{j\to\infty} \varphi_j(\mathbf{r},t).$$

4. VIM for NLTSE

In nonlinear time dependent Schrödinger equation, applying restricted variations to the nonlinear term and some of the linear terms simply provides faster convergent approximations to its exact solution. Different Lagrange multipliers are identified depending on which terms are considered as restricted variations. Equation (2) is rewritten as follows to specify the linear terms that are considered as restricted variations

$$(\mathcal{P}+\mathcal{R}+\mathcal{S}+\mathcal{T}-\mathcal{U}-\mathcal{N})\varphi(\mathbf{r},t)=0, t>0, \mathbf{r}\in\mathbb{R}^3, \tag{13}$$

where $\mathcal{P}=i\frac{\partial}{\partial t}$, $\mathcal{R}=\frac{\partial^2}{\partial x^2}$, $\mathcal{S}=\frac{\partial^2}{\partial y^2}$, $\mathcal{T}=\frac{\partial^2}{\partial z^2}$ are linear operators, $\mathcal{U}\varphi(\mathbf{r},t)=\mathcal{V}(\mathbf{r})\varphi(\mathbf{r},t)$ is linear term and $\mathcal{N}\varphi(\mathbf{r},t)=\kappa|\varphi(\mathbf{r},t)|^2\varphi(\mathbf{r},t)$ is nonlinear term. For equation (13), we construct the following two different correction functionals

$$\begin{aligned}\varphi_{j+1}(\mathbf{r},t)&=\varphi_j(\mathbf{r},t)+\int_0^t\mu_1(\eta)\left(\mathcal{P}\varphi_j(\mathbf{r},\eta)+(\mathcal{R}+\mathcal{S}+\mathcal{T}-\mathcal{U}-\mathcal{N})\widetilde{\varphi_j}(\mathbf{r},\eta)\right)d\eta\\&=\varphi_j(\mathbf{r},t)+\int_0^t\mu_1(\eta)\left(i\frac{\partial\varphi_j(\mathbf{r},\eta)}{\partial\eta}+(\nabla^2-\mathcal{V}(\mathbf{r})\right.\\&\qquad\left.-\kappa\left|\widetilde{\varphi_j}(\mathbf{r},\eta)\right|^2\right)\widetilde{\varphi_j}(\mathbf{r},\eta)\Big)d\eta,\end{aligned} \tag{14}$$

$$\begin{aligned}\varphi_{j+1}(\mathbf{r},t)&=\varphi_j(\mathbf{r},t)+\int_0^x\mu_2(\gamma)\big(\mathcal{R}\varphi_j(\gamma,y,z,t)+(\mathcal{P}+\mathcal{S}+\mathcal{T}\\&\qquad-\mathcal{U}-\mathcal{N})\widetilde{\varphi_j}(\gamma,y,z,t)\big)d\gamma\\&=\varphi_j(\mathbf{r},t)+\int_0^x\mu_2(\gamma)\left(\frac{\partial^2\varphi_j(\gamma,y,z,t)}{\partial\gamma^2}+\left(i\frac{\partial}{\partial t}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right.\right.\\&\qquad\left.\left.-\mathcal{V}(\gamma,y,z)-\kappa\left|\widetilde{\varphi_j}(\gamma,y,z,t)\right|^2\right)\widetilde{\varphi_j}(\gamma,y,z,t)\right)d\gamma,\end{aligned} \tag{15}$$

$j=0, 1, 2, \ldots$, where μ_1 and μ_2 are Lagrange multipliers, $\widetilde{\varphi_j}$ is restricted variation. $\left|\widetilde{\varphi_j}(\gamma,y,z,t)\right|^2=\widetilde{\varphi_j}(\gamma,y,z,t)\widetilde{\varphi_j}^*(\gamma,y,z,t)$, and $\widetilde{\varphi_j}^*$ is the complex conjugate of $\widetilde{\varphi_j}$. With known $\delta\varphi_j=0$, the Lagrange multipliers are identificated as

$$\mu_1(\eta)=i, \mu_2(\gamma)=\gamma-x. \tag{16}$$

Substituting the values (16) into functionals (14)-(15), we obtain the following different iteration formulas

$$\varphi_{j+1}(\mathbf{r},t)=\varphi_j(\mathbf{r},t)+i\int_0^t\left(i\frac{\partial}{\partial\eta}+\nabla^2-\mathcal{V}(\mathbf{r})-\kappa\left|\varphi_j(\mathbf{r},\eta)\right|^2\right)\varphi_j(\mathbf{r},\eta)d\eta, \tag{17}$$

$$\begin{aligned}\varphi_{j+1}(\mathbf{r},t)&=\varphi_j(\mathbf{r},t)+\int_0^x(\gamma-x)\left(i\frac{\partial}{\partial t}+\frac{\partial^2}{\partial\gamma^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right.\\&\qquad\left.-\mathcal{V}(\gamma,y,z)-\kappa\left|\varphi_j(\gamma,y,z,t)\right|^2\right)\varphi_j(\gamma,y,z,t)d\gamma,\end{aligned} \tag{18}$$

$j=0, 1, 2, \ldots$. By applying the above iteration process in a similar manner, if $\mathcal{S}\varphi(\mathbf{r},t)$ is the only term in equation (13) that is not considered as a restricted variation, then we get the iteration formula as follows

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + \int_0^{y} (\beta - y)\left(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial \beta^2} + \frac{\partial^2}{\partial z^2}\right.$$
$$\left. -\mathcal{V}(x,\beta,z) - \kappa\left|\varphi_j(x,\beta,z,t)\right|^2\right)\varphi_j(x,\beta,z,t)d\beta, \quad (19)$$

$j = 0, 1, 2, \ldots$, which is different from the iteration formulas (17) and (18). Similarly, if $\mathcal{T}\varphi(\mathbf{r},t)$ is the only term in equation (13) that is not considered as a restricted variation, then the iteration formula

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + \int_0^{z} (\alpha - z)\left(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial \alpha^2}\right.$$
$$\left. -\mathcal{V}(x,y,\alpha) - \kappa\left|\varphi_j(x,y,\alpha,t)\right|^2\right)\varphi_j(x,y,\alpha,t)d\alpha, \quad (20)$$

$j = 0, 1, 2, \ldots$ is obtained. The solution is

$$\varphi(\mathbf{r},t) = \lim_{j\to\infty} \varphi_j(\mathbf{r},t).$$

5. Numerical examples

Some examples are given to demonstrate the accuracy and reliability of the VIM for solving three dimensional LTSE and NLTSE. Depending on the choice of the iteration formulas given in Eqs. (9)-(12) formed for LTSE and the iteration formulas given in Eqs. (17)-(20) formed for NLTSE, four cases arise for each of LTSE and NLTSE. Here, two cases are examined depending on the choice of iteration formulas given in Eqs. (9)-(10) for LTSE and iteration formulas given in Eqs. (17)-(18) for NLTSE.

Example 5.1.
Consider the following problem for LTSE

$$\left(i\frac{\partial}{\partial t} + \nabla^2\right)\varphi(\mathbf{r},t) = 0,\ t > 0,\ \mathbf{r} \in \mathbb{R}^3,$$

with the initial condition

$$\varphi(\mathbf{r},0) = e^{i(x+y+z)}$$

and boundary conditions

$$\varphi(0,y,z,t) = e^{i(y+z-3t)},\ \left.\frac{\partial\varphi(\mathbf{r},t)}{\partial x}\right|_{x=0} = ie^{i(y+z-3t)},$$
$$\varphi(x,0,z,t) = e^{i(x+z-3t)},\ \left.\frac{\partial\varphi(\mathbf{r},t)}{\partial y}\right|_{y=0} = ie^{i(x+z-3t)},$$
$$\varphi(x,y,0,t) = e^{i(x+y-3t)},\ \left.\frac{\partial\varphi(\mathbf{r},t)}{\partial z}\right|_{z=0} = ie^{i(x+y-3t)}.$$

The exact solution of this problem is

$$\varphi_e(\mathbf{r},t) = e^{i(x+y+z-3t)}. \quad (21)$$

Case 5.1.1. [iteration formula (9)]
From the iteration formula (**9**), we have

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + i\int_0^t \left(i\frac{\partial}{\partial\eta} + \nabla^2\right)\varphi_j(\mathbf{r},\eta)d\eta, \tag{22}$$

$j = 0, 1, 2, \dots$. Starting with $\varphi_0(\mathbf{r},t) = \varphi(\mathbf{r},0)$ and using (22), we get

$$\begin{aligned}\varphi_1(\mathbf{r},t) &= \varphi_0(\mathbf{r},t) + i\int_0^t \left(i\frac{\partial}{\partial\eta} + \nabla^2\right)\varphi_0(\mathbf{r},\eta)d\eta \\ &= (1-3it)\varphi_0(\mathbf{r},t),\end{aligned}$$

$$\varphi_2(\mathbf{r},t) = \left(1 - 3it - \tfrac{9t^2}{2!}\right)\varphi_0(\mathbf{r},t),$$
$$\vdots$$
$$\varphi_j(\mathbf{r},t) = \left(1 - 3it - \tfrac{9t^2}{2!} + \cdots + \tfrac{(-3it)^j}{j!}\right)\varphi_0(\mathbf{r},t). \tag{23}$$

The solution is

$$\varphi(\mathbf{r},t) = \lim_{j\to\infty}\varphi_j(\mathbf{r},t) = \varphi_e(\mathbf{r},t).$$

Case 5.1.2. [iteration formula (10)]
The formula (**10**) becomes

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + \int_0^x (\gamma - x)\left(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial\gamma^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\varphi_j(\gamma,y,z,t)d\gamma, \tag{24}$$

$j = 0, 1, 2, \dots$. We begin with the zeroth approximation

$$\varphi_0(\mathbf{r},t) = (1+ix)e^{i(y+z-3t)}.$$

By using iteration formula (24), the following approximations are obtained

$$\begin{aligned}\varphi_1(\mathbf{r},t) &= \varphi_0(\mathbf{r},t) + \int_0^x (\gamma - x)\left(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial\gamma^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\varphi_0(\gamma,y,z,t)d\gamma \\ &= \left(1 + ix - \tfrac{x^2}{2!} - \tfrac{ix^3}{3!}\right)e^{i(y+z-3t)},\end{aligned}$$

$$\varphi_2(\mathbf{r},t) = \left(1 + ix - \tfrac{x^2}{2!} - \tfrac{ix^3}{3!} + \tfrac{x^4}{4!} + \tfrac{ix^5}{5!}\right)e^{i(y+z-3t)},$$
$$\vdots$$
$$\varphi_j(\mathbf{r},t) = \left(1 + ix - \tfrac{x^2}{2!} - \tfrac{ix^3}{3!} + \tfrac{x^4}{4!} + \tfrac{ix^5}{5!} + \cdots + \tfrac{(ix)^{2j+1}}{(2j+1)!}\right)e^{i(y+z-3t)}. \tag{25}$$

We get the solution $\varphi(\mathbf{r},t) = e^{i(x+y+z-3t)}$.

The solution φ_e considered in Figures 1-5, Tables 1-2 is the exact solution given in (21). Approximations $\varphi_{7(23)}$, $\varphi_{7(25)}$ are the solutions obtained from approximations φ_j given in equations (23) and (25) for $j = 7$, respectively. Keeping the variables y and z constant, $y = z = 0.25$ are taken in all figures and tables.

Taking different values of t and x, Table 1 (Table 2) presents the real (imaginary) parts of the solution φ_e, approximations $\varphi_{7(23)}$, $\varphi_{7(25)}$ and the absolute errors of approximations $\varphi_{7(23)}$, $\varphi_{7(25)}$ with respect to φ_e. Comparing the absolute errors, $\varphi_{7(25)}$ converges φ_e faster than $\varphi_{7(23)}$. Because of approximations $\varphi_{7(23)}$, $\varphi_{7(25)}$ consist of only a finite number of terms, the absolute error in Table 1 (Table 2) increases with increasing values of t and x. The number of terms in the approximate solutions obtained from equations (23) and (25) increases with the increase in the number j. The increase in the absolute error can be made smaller by using approximate solutions consisting of more terms obtained for larger number j.

Figures 1-3 show the graphs of the solution φ_e and approximations $\varphi_{7(23)}$, $\varphi_{7(25)}$, respectively. The real parts of the solutions are in (a), the imaginary parts are in (b). It is seen that the approximation $\varphi_{7(25)}$ is a closer solution to the φ_e solution than the approximation $\varphi_{7(23)}$.

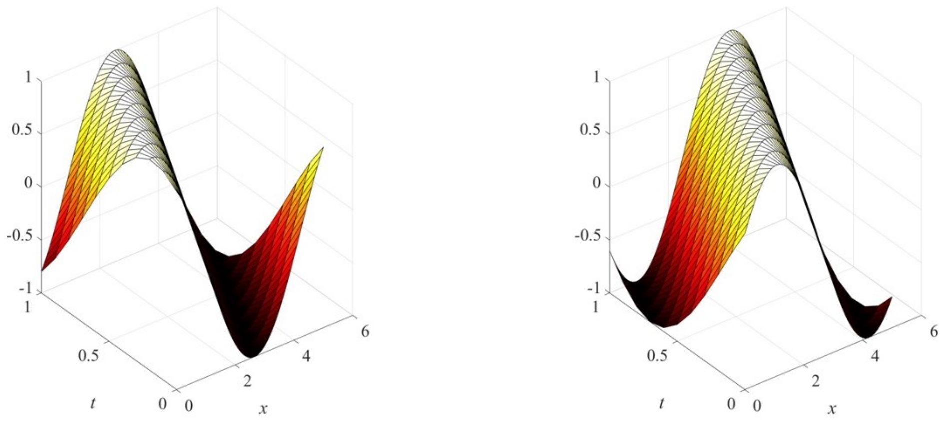
In Figures 4-5, the real parts of the absolute errors of the approximations $\varphi_{7(23)}$, $\varphi_{7(25)}$ with respect to the solution φ_e are given in (a), and the imaginary parts are given in (b), respectively. The graphs show that the error in the approximation $\varphi_{7(25)}$ is much smaller than the error in the approximation $\varphi_{7(23)}$.

Table 1. The real parts of solution φ_e, approximations $\varphi_{7(23)}$, $\varphi_{7(25)}$ and absolute error of approximations in Ex. 5.1.

t	x	Exact solution	VIM solution		Absolute error	
		$\mathrm{Re}[\varphi_e]$	$\mathrm{Re}[\varphi_{7(23)}]$	$\mathrm{Re}[\varphi_{7(25)}]$	$\lvert\mathrm{Re}[\varphi_e-\varphi_{7(23)}]\rvert$	$\lvert\mathrm{Re}[\varphi_e-\varphi_{7(25)}]\rvert$
0.1	0.5	7.64842×10^{-1}	7.64842×10^{-1}	7.64842×10^{-1}	0	0
0.2	1.0	6.21610×10^{-1}	6.21610×10^{-1}	6.21610×10^{-1}	0	0
0.3	1.5	4.53596×10^{-1}	4.53600×10^{-1}	4.53596×10^{-1}	3.43960×10^{-6}	0
0.4	2.0	2.67499×10^{-1}	2.67575×10^{-1}	2.67499×10^{-1}	7.56843×10^{-5}	0
0.5	2.5	7.07372×10^{-2}	7.13364×10^{-2}	7.07371×10^{-2}	5.99161×10^{-4}	7.24400×10^{-8}
0.6	3.0	-1.28844×10^{-1}	-1.22619×10^{-1}	-1.28845×10^{-1}	2.65575×10^{-3}	8.75400×10^{-7}
0.7	3.5	-3.23290×10^{-1}	-3.15857×10^{-1}	-3.23294×10^{-1}	7.43290×10^{-3}	4.13390×10^{-6}
0.8	4.0	-5.04846×10^{-1}	-5.92687×10^{-1}	-5.04827×10^{-1}	1.21594×10^{-2}	1.93877×10^{-5}
0.9	4.5	-6.66276×10^{-1}	-6.65746×10^{-1}	-6.65804×10^{-1}	5.30100×10^{-4}	4.72466×10^{-4}
1.0	5.0	-8.01144×10^{-1}	-8.70366×10^{-1}	-7.96944×10^{-1}	6.92228×10^{-2}	4.19991×10^{-3}

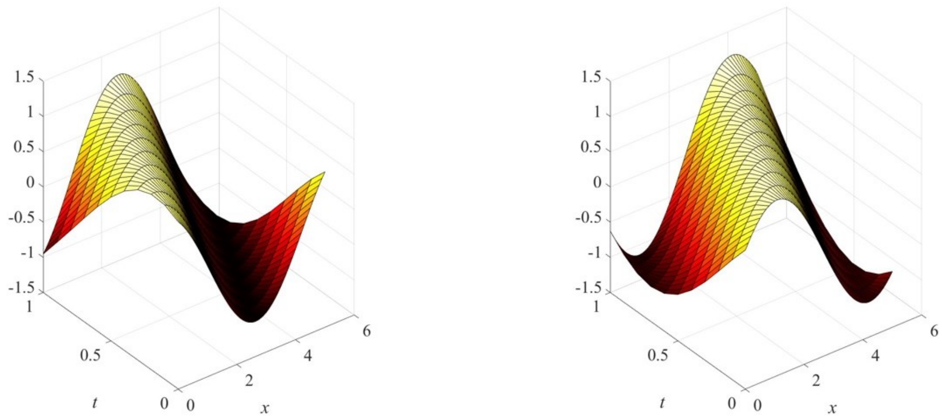
Table 2. The imaginary parts of solution φ_e, approximations $\varphi_{7(23)}$, $\varphi_{7(25)}$ and absolute error of approximations in Ex. 5.1.

t	x	Exact solution	VIM solution		Absolute error	
		$\mathrm{Im}[\varphi_e]$	$\mathrm{Im}[\varphi_{7(23)}]$	$\mathrm{Im}[\varphi_{7(25)}]$	$\lvert\mathrm{Im}[\varphi_e-\varphi_{7(23)}]\rvert$	$\lvert\mathrm{Im}[\varphi_e-\varphi_{7(25)}]\rvert$
0.1	0.5	6.44218×10^{-1}	6.44218×10^{-1}	6.44218×10^{-1}	0	0
0.2	1.0	7.83327×10^{-1}	7.83326×10^{-1}	7.83327×10^{-1}	4.11900×10^{-7}	0
0.3	1.5	8.91207×10^{-1}	8.91197×10^{-1}	8.91207×10^{-1}	1.00621×10^{-5}	0
0.4	2.0	9.63558×10^{-1}	9.63484×10^{-1}	9.63558×10^{-1}	7.40560×10^{-5}	0
0.5	2.5	9.97495×10^{-1}	9.97305×10^{-1}	9.97495×10^{-1}	1.90261×10^{-4}	0
0.6	3.0	9.91655×10^{-1}	9.92093×10^{-1}	9.91667×10^{-1}	4.27931×10^{-4}	1.83090×10^{-6}
0.7	3.5	9.46300×10^{-1}	9.51688×10^{-1}	9.46324×10^{-1}	5.38785×10^{-3}	2.34274×10^{-5}
0.8	4.0	8.63209×10^{-1}	8.86803×10^{-1}	8.63409×10^{-1}	2.35941×10^{-2}	1.99421×10^{-4}
0.9	4.5	7.45705×10^{-1}	8.13307×10^{-1}	7.46928×10^{-1}	6.76015×10^{-2}	1.22261×10^{-3}
1.0	5.0	5.98472×10^{-1}	7.38013×10^{-1}	6.04102×10^{-1}	1.39540×10^{-1}	5.63020×10^{-3}



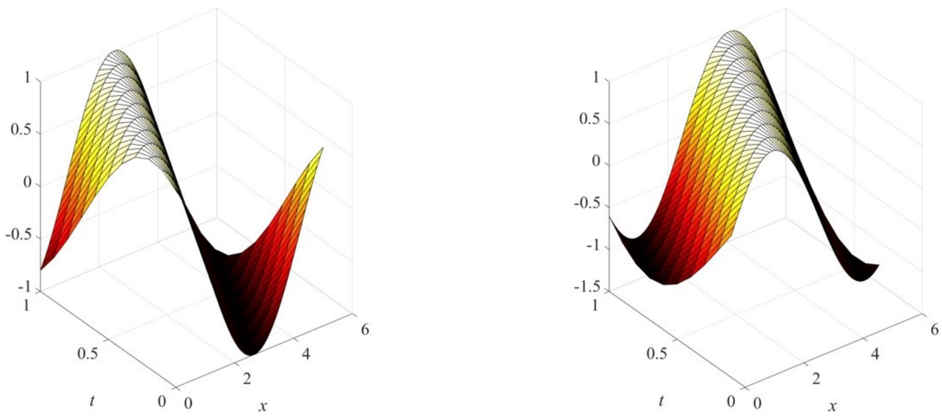
(a) $\mathrm{Re}[\varphi_e]$ (b) $\mathrm{Im}[\varphi_e]$

Figure 1. The real, imaginary parts of solution φ_e in Ex. 5.1.



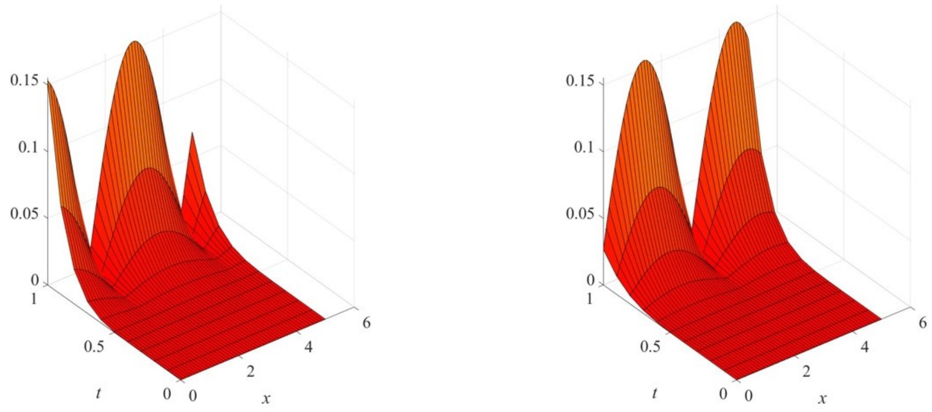
(a) $\mathrm{Re}\left[\varphi_{7(23)}\right]$ (b) $\mathrm{Im}\left[\varphi_{7(23)}\right]$

Figure 2. The real, imaginary parts of solution $\varphi_{7(23)}$ in Ex. 5.1.



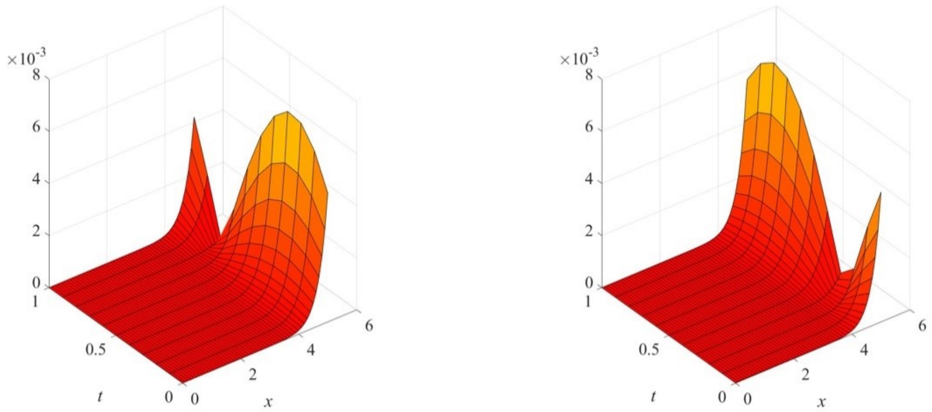
(a) $\mathrm{Re}\left[\varphi_{7(25)}\right]$ (b) $\mathrm{Im}\left[\varphi_{7(25)}\right]$

Figure 3. The real, imaginary parts of solution $\varphi_{7(25)}$ in Ex. 5.1.



(a) $\left|\mathrm{Re}\left[\varphi_e\text{-}\varphi_{7(23)}\right]\right|$ (b) $\left|\mathrm{Im}\left[\varphi_e\text{-}\varphi_{7(23)}\right]\right|$

Figure 4. The real, imaginary parts of absolute error of $\varphi_{7(23)}$ in Ex. 5.1.



(a) $\left|\mathrm{Re}\left[\varphi_e\text{-}\varphi_{7(25)}\right]\right|$ (b) $\left|\mathrm{Im}\left[\varphi_e\text{-}\varphi_{7(25)}\right]\right|$

Figure 5. The real, imaginary parts of absolute error of $\varphi_{7(25)}$ in Ex. 5.1.

Example 5.2.
Consider the following problem for NLTSE

$$\left(i\frac{\partial}{\partial t}+\nabla^2+1-\sin^2 x\sin^2 y\sin^2 z+|\varphi(\mathbf{r},t)|^2\right)\varphi(\mathbf{r},t)=0,\ t>0,\ \mathbf{r}\in\mathbb{R}^3,$$

with the initial condition

$$\varphi(\mathbf{r},0)=\sin x\sin y\sin z,$$

and boundary conditions

$$\varphi(0,y,z,t)=0,\ \frac{\partial\varphi(\mathbf{r},t)}{\partial x}\bigg|_{x=0}=\sin y\sin z\, e^{-2it},$$
$$\varphi(x,0,z,t)=0,\ \frac{\partial\varphi(\mathbf{r},t)}{\partial y}\bigg|_{y=0}=\sin x\sin z\, e^{-2it},$$
$$\varphi(x,y,0,t)=0,\ \frac{\partial\varphi(\mathbf{r},t)}{\partial z}\bigg|_{z=0}=\sin x\sin y\, e^{-2it}.$$

The exact solution is

$$\varphi_e(\mathbf{r},t) = \sin x \sin y \sin z\, e^{-2it}. \tag{26}$$

Case 5.2.1. [iteration formula (17)]
The formula (17) becomes

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + i\int_0^t \Big(i\frac{\partial}{\partial\eta} + \nabla^2 + 1 - \sin^2 x \sin^2 y \sin^2 z + \left|\varphi_j(\mathbf{r},\eta)\right|^2\Big)\varphi_j(\mathbf{r},\eta)d\eta, \tag{27}$$

$j = 0, 1, 2, \ldots$. Starting with $\varphi_0(\mathbf{r},t) = \varphi(\mathbf{r},0)$ and using (27), we have

$$\varphi_1(\mathbf{r},t) = \varphi_0(\mathbf{r},t) + i\int_0^t \Big(i\frac{\partial}{\partial\eta} + \nabla^2 + 1 - \sin^2 x \sin^2 y \sin^2 z + |\varphi_0(\mathbf{r},\eta)|^2\Big)\varphi_0(\mathbf{r},\eta)d\eta$$

$$= (1 - 2it)\varphi_0(\mathbf{r},t),$$

$$\varphi_2(\mathbf{r},t) = (1 - 2it - 2t^2)\varphi_0(\mathbf{r},t),$$

$$\vdots$$

$$\varphi_j(\mathbf{r},t) = \Big(1 - 2it - 2t^2 + \cdots + \frac{(-2it)^j}{j!}\Big)\varphi_0(\mathbf{r},t). \tag{28}$$

The solution is

$$\varphi(\mathbf{r},t) = \lim_{j\to\infty}\varphi_j(\mathbf{r},t) = \varphi_e(\mathbf{r},t).$$

Case 5.2.2. [iteration formula (18)]
From the iteration formula (18), we get

$$\varphi_{j+1}(\mathbf{r},t) = \varphi_j(\mathbf{r},t) + \int_0^x (\gamma - x)\Big(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial\gamma^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + 1 - \sin^2\gamma \sin^2 y \sin^2 z + \left|\varphi_j(\gamma,y,z,t)\right|^2\Big)\varphi_j(\gamma,y,z,t)d\gamma, \tag{29}$$

$j = 0, 1, 2, \ldots$. Starting with $\varphi_0(\mathbf{r},t) = x \sin y \sin z\, e^{-2it}$ and using (29), approximate solutions are

$$\varphi_1(\mathbf{r},t) = \varphi_0(\mathbf{r},t) + \int_0^x (\gamma - x)\Big(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial\gamma^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + 1 - \sin^2\gamma \sin^2 y \sin^2 z + |\varphi_0(\gamma,y,z,t)|^2\Big)\varphi_0(\gamma,y,z,t)d\gamma$$

$$= \Big(x - \frac{x^3}{3!}\Big)\sin y \sin z\, e^{-2it},$$

$$\varphi_2(\mathbf{r},t) = \Big(x - \frac{x^3}{3!} + \frac{x^5}{5!}\Big)\sin y \sin z\, e^{-2it},$$

$$\vdots$$

$$\varphi_j(\mathbf{r},t) = \Big(x - \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots + (-1)^j\frac{x^{2j+1}}{(2j+1)!}\Big)\sin y \sin z\, e^{-2it}. \tag{30}$$

We obtain the solution $\varphi(\mathbf{r},t) = \sin x \sin y \sin z\, e^{-2it}$.

In Figures 6-10, Tables 3-4, the solution φ_e is the exact solution given in (26) when $y = z = 0.25$. Approximations $\varphi_{7(28)}, \varphi_{7(30)}$ are the solutions obtained from approximations φ_j given in equations (28) and (30) for $j = 7$, respectively.

The real (imaginary) parts of the solution φ_e, approximations $\varphi_{7(28)}$, $\varphi_{7(30)}$ and the absolute errors of approximations $\varphi_{7(28)}, \varphi_{7(30)}$ with respect to φ_e are listed in Table 3 (Table 4) by taking different values of t and x. Comparison of absolute errors shows that $\varphi_{7(30)}$ converges φ_e faster than $\varphi_{7(28)}$. The absolute error can be made smaller by using approximate solutions consisting of more terms obtained for larger number j.

The graphs of the solution φ_e and approximations $\varphi_{7(28)}$, $\varphi_{7(30)}$ are given in Figure 6 and Figures 7-8, respectively. The real parts of the solutions are in (a), the imaginary parts are in (b). It is observed that the approximation $\varphi_{7(30)}$ is a closer solution to the φ_e solution than the approximation $\varphi_{7(28)}$.

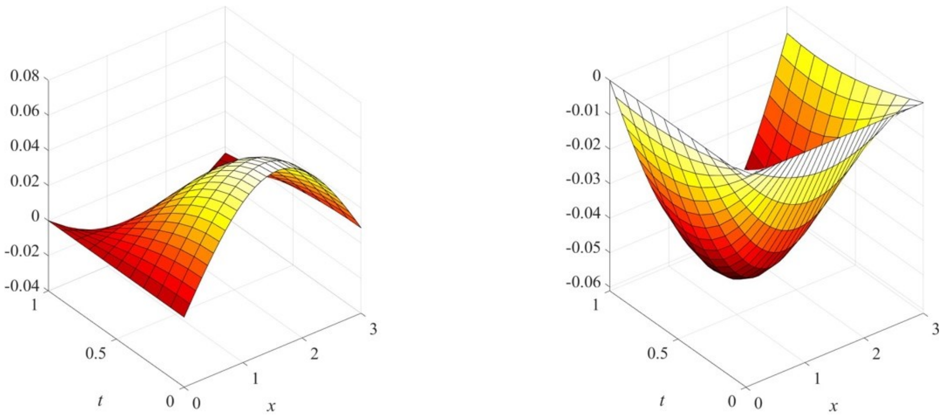
In Figures 9-10, the real parts of the absolute errors of the approximations $\varphi_{7(28)}, \varphi_{7(30)}$ with respect to φ_e are given in (a), and the imaginary parts are plotted in (b), respectively. The graphs depict the error in the approximation $\varphi_{7(30)}$ is much smaller than the error in the approximation $\varphi_{7(28)}$.

Table 3. The real parts of solution φ_e, approximations $\varphi_{7(28)}$, $\varphi_{7(30)}$ and absolute errors of approximations in Ex. 5.2.

t	***x***	**Exact solution**	**VIM solution**		**Absolute error**	
		$\mathbf{Re}[\varphi_e]$	$\mathbf{Re}[\varphi_{7(28)}]$	$\mathbf{Re}[\varphi_{7(30)}]$	$\lvert\mathbf{Re}[\varphi_e - \varphi_{7(28)}]\rvert$	$\lvert\mathbf{Re}[\varphi_e - \varphi_{7(30)}]\rvert$
0.1	0.3	1.77278×10^{-2}	1.77278×10^{-2}	1.77278×10^{-2}	0	0
0.2	0.6	3.18328×10^{-1}	3.18328×10^{-1}	3.18328×10^{-1}	0	0
0.3	0.9	3.95719×10^{-2}	3.95719×10^{-2}	3.95719×10^{-2}	0	0
0.4	1.2	3.97464×10^{-2}	3.97461×10^{-2}	3.97464×10^{-2}	2.35700×10^{-7}	0
0.5	1.5	3.29884×10^{-2}	3.29869×10^{-2}	3.29884×10^{-2}	1.49757×10^{-6}	0
0.6	1.8	2.15994×10^{-2}	2.15932×10^{-2}	2.15994×10^{-2}	6.25612×10^{-6}	0
0.7	2.1	8.98037×10^{-3}	8.96145×10^{-3}	8.98037×10^{-3}	1.89240×10^{-5}	0
0.8	2.4	-1.20723×10^{-3}	-1.25004×10^{-3}	-1.20723×10^{-3}	1.21594×10^{-5}	0
0.9	2.7	-5.94346×10^{-3}	-6.01245×10^{-3}	-5.94346×10^{-3}	5.30100×10^{-5}	0
1.0	3.0	-3.59458×10^{-3}	-3.64706×10^{-3}	-3.59457×10^{-3}	5.24778×10^{-5}	9.01000×10^{-9}

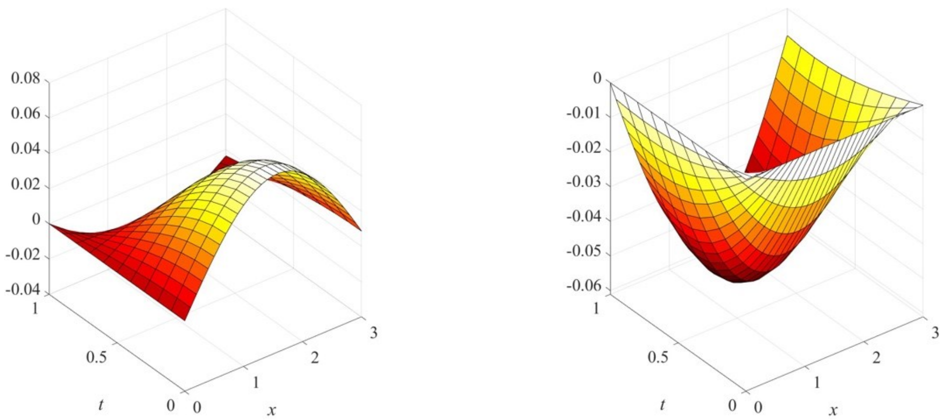
Table 4. The imaginary parts of solution φ_e, approximations $\varphi_{7(28)}$, $\varphi_{7(30)}$ and absolute errors of approximations in Ex. 5.2.

t	***x***	**Exact solution**	**VIM solution**		**Absolute error**	
		$\mathbf{Im}[\varphi_e]$	$\mathbf{Im}[\varphi_{7(28)}]$	$\mathbf{Im}[\varphi_{7(30)}]$	$\lvert\mathbf{Im}[\varphi_e - \varphi_{7(28)}]\rvert$	$\lvert\mathbf{Im}[\varphi_e - \varphi_{7(30)}]\rvert$
0.1	0.3	-3.59361×10^{-3}	-3.59361×10^{-3}	-3.59361×10^{-3}	0	0
0.2	0.6	-1.34587×10^{-2}	-1.34587×10^{-2}	-1.34587×10^{-2}	0	0
0.3	0.9	-2.70726×10^{-2}	-2.70726×10^{-2}	-2.70726×10^{-2}	0	0
0.4	1.2	-4.09244×10^{-2}	-4.09244×10^{-2}	-4.09244×10^{-2}	0	0
0.5	1.5	-5.13763×10^{-2}	-5.13763×10^{-2}	-5.13763×10^{-2}	1.66730×10^{-7}	0
0.6	1.8	-5.55570×10^{-2}	-5.55561×10^{-2}	-5.55570×10^{-2}	8.36570×10^{-7}	0
0.7	2.1	-5.20672×10^{-2}	-5.2062×10^{-2}	-5.20672×10^{-2}	2.95535×10^{-6}	0
0.8	2.4	-4.13266×10^{-2}	-4.13190×10^{-2}	-4.13266×10^{-2}	7.65020×10^{-5}	0
0.9	2.7	-2.54752×10^{-2}	-2.54614×10^{-2}	-2.54752×10^{-2}	1.38868×10^{-5}	0
1.0	3.0	-7.85431×10^{-3}	-7.84255×10^{-3}	-7.85429×10^{-3}	1.17553×10^{-5}	1.96870×10^{-8}



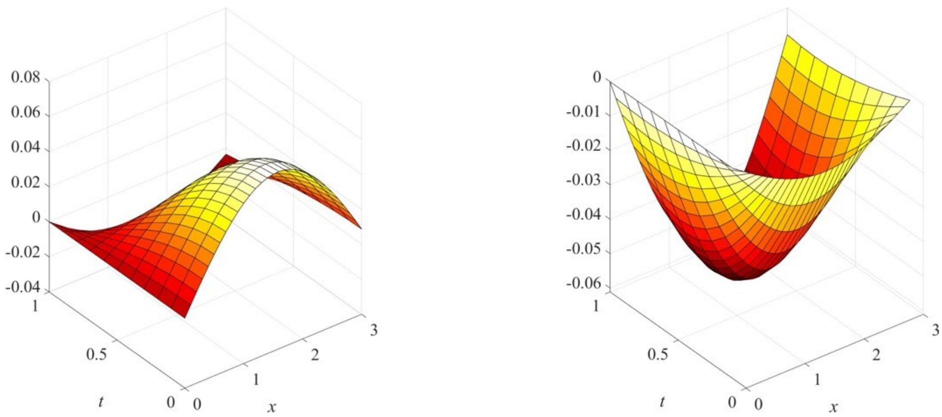
(a) Re$[\varphi_e]$ (b) Im$[\varphi_e]$

Figure 6. The real, imaginary parts of solution φ_e in Ex. 5.2.



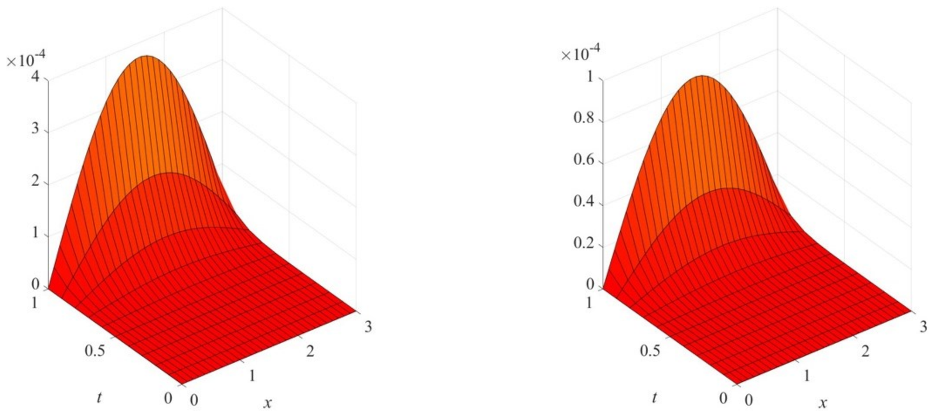
(a) Re$[\varphi_{7(28)}]$ (b) Im$[\varphi_{7(28)}]$

Figure 7. The real, imaginary parts of solution $\varphi_{7(28)}$ in Ex. 5.2.



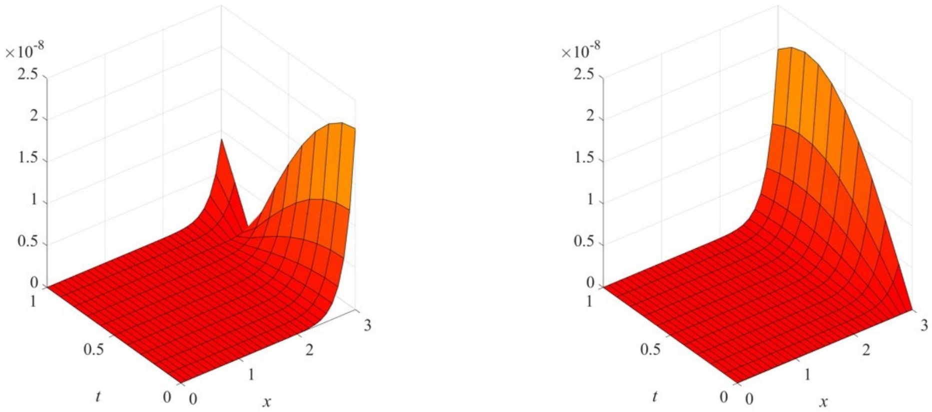
(a) Re$[\varphi_{7(30)}]$ (b) Im$[\varphi_{7(30)}]$

Figure 8. The real, imaginary parts of solution $\varphi_{7(30)}$ in Ex. 5.2.



(a) $\left|\mathrm{Re}\left[\varphi_e\text{-}\varphi_{7(28)}\right]\right|$ (b) $\left|\mathrm{Im}\left[\varphi_e\text{-}\varphi_{7(28)}\right]\right|$

Figure 9. The real, imaginary parts of absolute error of $\varphi_{7(28)}$ in Ex. 5.2.



(c) $\left|\mathrm{Re}\left[\varphi_e\text{-}\varphi_{7(30)}\right]\right|$ (d) $\left|\mathrm{Im}\left[\varphi_e\text{-}\varphi_{7(30)}\right]\right|$

Figure 10. The real, imaginary parts of absolute error of $\varphi_{7(30)}$ in Ex. 5.2.

6. Results and discussion

The solution function of the Schrödinger equation allows to analyze the behavior of a quantum mechanical system. We searched for the solution functions of the time dependent Schrödinger equations using VIM, because it preserves the physical properties of the equation and provides analytical and faster approximate solutions. We extended VIM to three-dimensional LTSE and NLTSE. Different Lagrange multipliers were determined. We formed different iteration formulas with Lagrange multipliers. Examples are given to demonstrate the accuracy and applicability of the proposed iteration formulas. In each example, two cases were considered depending on the choice of iteration formulas for the time dependent Schrödinger equation. Figures and tables are given to compare the approximations obtained using different iteration formulas with each other and with the exact solution. In Tables 1-2, the exact solution, the approximations obtained from the iteration formulas in the two cases and the absolute errors of the approximations with respect to the exact solution were calculated for different t and x values. Comparing the real (imaginary) parts of the numerical results of Table 1 (Table 2) for the same t and x values, it is shown that in the second case, the approximation obtained from the iteration formula converges to the exact solution faster than in the first case. Comparison of Tables 3-4 gives similar results. When Figures 1-3

(Figures 6-8) are compared, it is observed that the real and imaginary parts of the approximate solutions are compatible with the real and imaginary parts of the exact solution, and in the second case, the approximation obtained from the iteration formula is closer to the exact solution than in the first case. Comparing Figures 4-5, it is seen that in the second case, the real (imaginary) part of the absolute error of the approximation obtained from the iteration formula with respect to the exact solution is smaller than in the first case. When Figures 9-10 are examined, similar results are found. In the examples, it is observed that the approximations obtained from different iteration formulas converge to the exact solution, but the convergence speeds are different. The results show that VIM is an effective method for solving three dimensional time dependent Schrödinger equations and the choice of the iteration formula has a significant effect on the accuracy of the approximate solution. In the future, VIM can be applied to different differential equations by developing new iteration formulas.

7. Conclusion

In this paper, we apply VIM to three dimensional LTSE and NLTSE. We have been formed different iteration formulas of VIM for three dimensional LTSE and NLTSE. Two cases are considered in which different iteration formulas are used in the sample problems. In both cases, approximate solutions converging to the exact solution are obtained. When the approximations obtained in the examples are compared, it is seen that the approximations obtained in the second case converge to the exact solution faster than the first case. This rapid convergence highlights the importance of choosing the appropriate iteration formula. Obtaining approximate solutions that converge more rapidly to the exact solution depends on choice of the iteration formula. Using different iteration formulas of VIM for linear and nonlinear Schrödinger equations increases the convergence speed and accuracy of the solutions. With different iteration formulas, VIM has the potential to produce efficient and highly accurate solutions.

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