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NEW LAPLACE VARIATIONAL ITERATIVE METHOD FOR SOLVING 3D SCHRÖDINGER EQUATIONS

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Abstract: In this research, new semi analytical technique based on Laplace transform and modified variational iterative method is presented for solving 3D Schrodinger equation arising in quantum physics and other branches of sciences. Numerical examples illustrate the accuracy of the proposed method.

Keywords: Laplace transform; modified variational iterative method; 3D Schrodinger equation; numerical examples.

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1. INTRODUCTION

An equation which describes the wave function or state function in quantum mechanical system is called Schrodinger equation. This paper is devoted to the numerical computation of three-dimensional time dependent Schrodinger equation

$$-i\frac{\partial u(x,y,z,t)}{\partial t} = \nabla^2 u(x,y,z,t) + v(x,y,z)u(x,y,z,t),$$

where i is the imaginary unit, u is the time dependent wave function and v is the potential function. This equation has many applications in several branches of science and engineering. Schrodinger equations arises in quantum mechanics for modelling of quantum devices [5], in various quantum calculators [6, 8], in design of certain opto-electronic devices [7], in electromagnetic wave propagation [9] and in underwater acoustics [10].

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In mathematics, Laplace transform based numerical methods plays a major role in the field of computational and applied mathematics. To make it iterative, variational methods have attracts the attention of various researchers and scientists. Combination of these two methods gives numerical results with significant convergence. Variational iteration method has been developed for solving delay differential equations in [1]. Variational iteration technique for nonlinear equations has been presented in [2]. In [3], Variational iteration method has presented for solving autonomous ordinary differential equations. Approximate solution of time fractional telegraph equation has obtained with the help of variational iteration method in [4]. Laplace-variational iteration method has been developed for solving the homogeneous Smoluchowski coagulation equation in [11]. Eighth order boundary value problems have solved with the aid of new modified variational iteration transform method in [12]. A strategy on Laplace transform and variational iteration has been presented in [13] for solving differential equations. Reconstruction of variational iteration algorithms using the Laplace transform has presented in [14]. Time-fractional diffusion equation in porous medium, has solved with variational iteration method and obtained numerical results have presented in [15]. Some drawbacks in the application of the variation iteration method and how Laplace transform method overcome these, have been discussed in [16]. A semi- analytical method has been presented for solving a family of Kuramoto-Shivshinsky equations in [17]. Laplace variational method has presented for modified fractional derivatives with non-singular kernel in [18]. New Laplace variational iteration method has been developed for solving nonlinear partial differential equations in [19]. Efficient numerical technique based on wavelets has been developed for solving three-dimensional partial differential equations in [20]. Haar wavelets based numerical scheme has been presented for solving two-dimensional telegraph equations in [21].

2. PRELIMINARIES

In this section, we discuss some definitions and properties of Laplace transforms:

2.1 LAPLACE TRANSFORM:

Let $g(t)$ be a function of t defined for all positive values of t. Then the Laplace transforms of $g(t)$, represented as $L\{g(t)\}$ and is defined as:

$$L\{g(t)\} = \int_0^\infty e^{-st} g(t) dt = \bar{g}(s),$$

provided the integral exists and $'s'$ is a parameter which may be a real or complex number. Therefore

$$L\{g(t)\} = \bar{g}(s),$$

that is

$$g(t) = L^{-1}\{\bar{g}(s)\}.$$

The term $L^{-1}\{\bar{g}(s)\}$, is called the inverse Laplace transform of $\bar{g}(s)$.

2.2 LINEARITY PROPERTY OF LAPLACE TRANSFORM:

Let $f(t)$, $g(t)$ be two functions of t defined for all positive values of t. Then

$$L\{a.f(t) + b.g(t)\} = a.L\{f(t)\} + b.L\{g(t)\}$$

where a and b are arbitrary constants.

2.3 LAPLACE TRANSFORM FOR DIFFERENTIATION:

Let $f(t)$ be a function of t defined for all positive values of t. Then, the Laplace transform of n^{th} derivative of function $f(t)$ is

$$L\left[\frac{d^n(f(t))}{dt^n}\right] = s^n \bar{f}(s) - s^{n-1} f(0) - s^{n-2} f'(0) - s^{n-3} f''^{(0)} - \cdots - s f^{(n-2)}(0) - f^{(n-1)}(0)$$

where $\bar{f}(s) = L\{f(t)\}$.

2.4 LINEARITY PROPERTY OF INVERSE LAPLACE TRANSFORM:

Let $f(t)$, $g(t)$ be two functions of t defined for all positive values of t. Let $\bar{f}(s)$ and $\bar{g}(s)$ be the functions of s such that $\bar{f}(s) = L\{f(t)\}$ and $\bar{g}(s) = L\{g(t)\}$.

Then

$$L^{-1}\{c.\bar{f}(s) + d.\bar{g}(s)\} = c.L^{-1}\{\bar{f}(s)\} + d.L\{\bar{g}(s)\} = c.f(t) + d.g(t)$$

where c and d are arbitrary constants.

3. VARIATIONAL ITERATIVE METHOD (VIM)

Variational iteration method is most powerful technique for solving linear and nonlinear differential equations and is discussed in He [1, 2, 3, 4]. This technique is widely useful to evaluate the exact or approximate solutions of linear or nonlinear problems. The variational iteration method gives the solution in a rapidly infinite convergent series.

The nonlinear terms can be handled with the help of variational iteration method. Consider the differential equations,

$$\boldsymbol{l}u(x,t) + \boldsymbol{n}u(x,t) = \boldsymbol{g}(x,t) \tag{1}$$

with the initial conditions

$$u(x,0) = \boldsymbol{h}(x) \tag{2}$$

where $\boldsymbol{l}$ is a linear operator of the first order, $\boldsymbol{n}$ is nonlinear operator and $\boldsymbol{g}$ is a nonhomogeneous term. From variational iteration method, construct a correction functional as:

$$u_{m+1} = u_m + \int_0^t \lambda[\boldsymbol{l}u_m(x,s) + \boldsymbol{n}\tilde{u}_m(x,s) - \boldsymbol{g}(x,s)]ds \tag{3}$$

where λ is a known as Lagrange's multiplier and $\boldsymbol{m}$ denotes the m^{th} approximations, $\tilde{u}_m$ is restricted function, i.e. $\delta\tilde{u}_m = 0$. The successive approximation u_{m+1} of the solution u will be obtained by using λ and u_0. The solution is

$$u = \lim_{m\to\infty} u_m$$

4. NEW LAPLACE VARIATIONAL ITERATIVE METHOD FOR SOLVING 3D SCHRöDINGER EQUATIONS

In this section, combination of Laplace transform and modified variational iteration method is present to solve three- dimensional Schrodinger equations arising in quantum physics and physical chemistry. Approximate solution of this equation has been obtained in terms of convergent series with very easily computable components.

Assume that $\boldsymbol{l}$ is an operator of the first order $\frac{\partial}{\partial t}$. Equation (1) becomes

$$\frac{\partial}{\partial t}u(x,t) + \boldsymbol{n}u(x,t) = \boldsymbol{g}(x,t) \tag{4}$$

Taking Laplace transform on both sides of (4), we obtain

$$L\left\{\frac{\partial}{\partial t}u(x,t)\right\} + L\{\boldsymbol{n}u(x,t)\} = L\{\boldsymbol{g}(x,t)\} \tag{5}$$

$$sL\{u(x,t)\} - \boldsymbol{h}(x) = L\{\boldsymbol{g}(x,t)\} - L\{\boldsymbol{n}u(x,t)\} \tag{6}$$

Applying inverse Laplace transform on both sides of (6), we obtain

$$u(x,t) = \boldsymbol{G}(x,t) - L^{-1}\left[\frac{1}{s}L\{\boldsymbol{n}u(x,t)\}\right] \tag{7}$$

where $\boldsymbol{G}$ is the term arising from source term and given initial condition. From the correctional functional of the variational iteration method

$$u_{m+1}(x,t) = \boldsymbol{G}(x,t) - L^{-1}\left[\frac{1}{s}L\{\boldsymbol{n}u_m(x,t)\}\right] \tag{8}$$

Equation (8) represents the new modified correction functional of Laplace transform of variational iteration method, the solution is given by

$$u(x,t) = \lim_{m\to\infty} u_m(x,t)$$

5. NUMERICAL RESULTS

In this section, some numerical examples have been presented to illustrate the accuracy and efficiency of the proposed numerical techniques.

Example 1: Consider the following 3D Schrodinger equation

$$-i\frac{\partial u(x,y,z,t)}{\partial t} = \nabla^2 u(x,y,z,t) + v(x,y,z)u(x,y,z,t), \tag{9}$$

with

$$v(x,y,z) = 1 - \frac{2}{x^2} - \frac{2}{y^2} - \frac{2}{z^2}$$

and

$$u(x,y,z,0) = x^2y^2z^2$$

Applying Laplace transform on both sides of (9), we obtain

$$-iL\left\{\frac{\partial u(x,y,z,t)}{\partial t}\right\} = L\{\nabla^2 u(x,y,z,t)\} + L\left\{\left(1 - \frac{2}{x^2} - \frac{2}{y^2} - \frac{2}{z^2}\right)u(x,y,z,t)\right\} \tag{10}$$

This implies

$$sL\{u(x,y,z,t)\} - u(x,y,z,0) = iL\left\{\nabla^2 u(x,y,z,t) + \left(1 - \frac{2}{x^2} - \frac{2}{y^2} - \frac{2}{z^2}\right)u(x,y,z,t)\right\}$$

Applying initial conditions, we obtain

$$sL\{u(x,y,z,t)\} = x^2y^2z^2 + iL\left\{\nabla^2 u(x,y,z,t) + \left(1 - \frac{2}{x^2} - \frac{2}{y^2} - \frac{2}{z^2}\right)u(x,y,z,t)\right\}$$

Divide by s, we obtain

$$L\{u(x,y,z,t)\} = \frac{x^2y^2z^2}{s} + \frac{i}{s}L\left\{\nabla^2 u(x,y,z,t) + \left(1 - \frac{2}{x^2} - \frac{2}{y^2} - \frac{2}{z^2}\right)u(x,y,z,t)\right\} \tag{11}$$

Applying inverse Laplace transform on both sides of (11), we obtain

$$u = x^2y^2z^2 + L^{-1}\left[\frac{i}{s}L\left\{\nabla^2 u(x,y,z,t) + \left(1 - \frac{2}{x^2} - \frac{2}{y^2} - \frac{2}{z^2}\right)u(x,y,z,t)\right\}\right] \tag{12}$$

Using iteration method, from (12), we obtain

$$u_{m+1} = x^2y^2z^2 + L^{-1}\left[\frac{i}{s}L\left\{\nabla^2 u_m + \left(1 - \frac{2}{x^2} - \frac{2}{y^2} - \frac{2}{z^2}\right)u_m\right\}\right] \tag{13}$$

From (13), we obtain

$$u_0 = x^2y^2z^2$$

$$u_1 = x^2y^2z^2 + ix^2y^2z^2t$$

$$u_2 = x^2y^2z^2 + ix^2y^2z^2t + \frac{x^2y^2z^2(it)^2}{2}$$

$$u_3 = x^2y^2z^2 + x^2y^2z^2it + \frac{x^2y^2z^2(it)^2}{2!} + \frac{x^2y^2z^2(it)^3}{3!}$$

and so on. The solution is

$$u = \lim_{n\to\infty} u_m$$

After simplification, we obtain

$$u = x^2y^2z^2\left(1 + it + \frac{(it)^2}{2!} + \frac{(it)^3}{3!} + \cdots\right) = x^2y^2z^2e^{it} \tag{14}$$

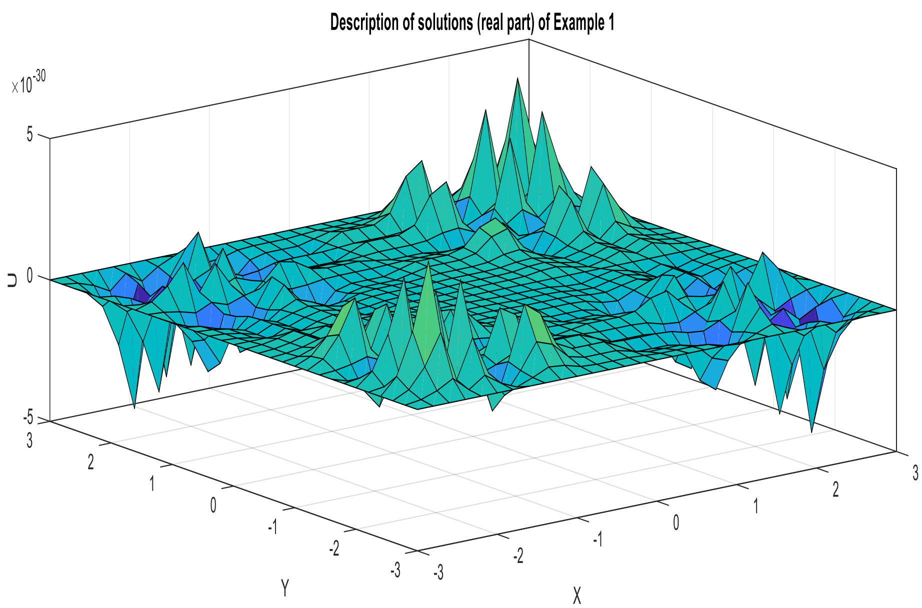

Figure 1: Description of solution (real part) of Example 1 for $t = 0.01$ and $z = 0.5$.

Figure 1 and Figure 2 show the physical behaviour of solutions (real part) of Example 1 and Example 2 respectively.

Example 2: Consider the 3D Schrödinger equation

$$-i\frac{\partial u(x,y,z,t)}{\partial t} = \nabla^2 u(x,y,z,t) + v(x,y,z)u(x,y,z,t), \tag{15}$$

where $v(x,y,z) = 2\pi^2 + 1$ and $u(x,y,z,0) = sin(\pi x)sin(\pi y)sin(\pi z)$.

From (15), we obtain

$$-i\frac{\partial u(x,y,z,t)}{\partial t} = \nabla^2 u(x,y,z,t) + (2\pi^2+1)u(x,y,z,t) \tag{16}$$

Applying Laplace transform on both sides of (16), we obtain

$$-iL\left\{\frac{\partial u(x,y,z,t)}{\partial t}\right\} = \mathrm{L}\{\nabla^2 u(x,y,z,t)\} + L\{(2\pi^2+1)u(x,y,z,t)\}$$

This implies

$$sL\{u(x,y,z,t)\} - u(x,y,z,0) = iL\{\nabla^2 u(x,y,z,t) + (2\pi^2+1)u(x,y,z,t)\}$$

Applying initial conditions, we obtain

$$sL\{u(x,y,z,t)\} = sin(\pi x)sin(\pi y)sin(\pi z) + iL\{\nabla^2 u(x,y,z,t) + (2\pi^2+1)u(x,y,z,t)\}$$

Divide by s, we obtain

$$L\{u(x,y,z,t)\} = \frac{sin(\pi x)sin(\pi y)sin(\pi z)}{s} + \frac{i}{s}L\{\nabla^2 u(x,y,z,t) + (2\pi^2+1)u(x,y,z,t)\} \tag{17}$$

Applying inverse Laplace transform on both sides of (17), we obtain

$$u = sin(\pi x)sin(\pi y)sin(\pi z) + L^{-1}\left[\frac{i}{s}L\{\nabla^2 u(x,y,z,t) + (2\pi^2+1)u(x,y,z,t)\}\right] \tag{18}$$

Using iteration method, from (18), we obtain

$$u_{m+1} = sin(\pi x)sin(\pi y)sin(\pi z) + L^{-1}\left[\frac{i}{s}L\{\nabla^2 u_m + (2\pi^2+1)u_m\}\right] \tag{19}$$

From (19), we obtain

$$u_0 = sin(\pi x)sin(\pi y)sin(\pi z)$$

$$u_1 = sin(\pi x)sin(\pi y)sin(\pi z)(1+it)$$

$$u_2 = sin(\pi x)sin(\pi y)sin(\pi z)\left(1+it+\frac{(it)^2}{2!}\right)$$

$$u_3 = sin(\pi x)sin(\pi y)sin(\pi z)\left(1+it+\frac{(it)^2}{2!}+\frac{(it)^3}{3!}\right)$$

and so on. The solution is obtained as

$$u = \lim_{n\to\infty} u_m$$

$$u = sin(\pi x)sin(\pi y)sin(\pi z)\left(1+it+\frac{(it)^2}{2!}+\frac{(it)^3}{3!}+\cdots\right) = sin(\pi x)sin(\pi y)sin(\pi z)e^{it}$$

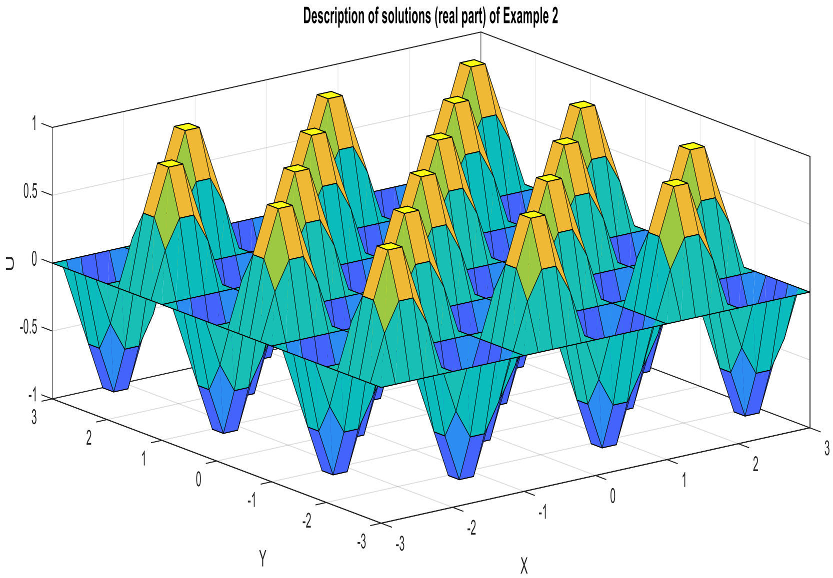

Figure 2: Description of solutions (real part) of Example 2 for $t = 0.01$ and $z = 0.5$.

CONCLUSION

From the above numerical experiments, it is concluded that numerical technique based on the combination of two well-known numerical methods such as Laplace transform method and variational iteration method, is a powerful semi analytical technique for solving three- dimensional partial differential equations. For future scope, these techniques will be applicable for solving three-dimensional nonlinear partial differential equations.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests.

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