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ORIGINAL ARTICLE

Numerical solution of the Klein–Gordon equation via He's variational iteration method

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Abstract In this paper, we present the solution of the Klein–Gordon equation. Klein–Gordon equation is the relativistic version of the Schrödinger equation, which is used to describe spinless particles. The He's variational iteration method (VIM) is implemented to give approximate and analytical solutions for this equation. The variational iteration method is based on the incorporation of a general Lagrange multiplier in the construction of correction functional for the equation. Application of variational iteration technique to this problem shows rapid convergence of the sequence constructed by this method to the exact solution. Moreover, this technique reduces the volume of calculations by avoiding discretization of the variables, linearization or small perturbations.

Keywords Klein–Gordon equation · Variational iteration method · Small perturbations · Mesh points schemes · Quantum mechanics

1 Introduction

The Klein–Gordon equation (Klein–Gordon–Fock equation) is the relativistic version of the Schrödinger equation, which is used to describe spinless particles. It was named after Oskar Klein and Walter Gordon [1].

The Schrödinger equation for a free particle is

$$\frac{P^2}{2m}\psi = ih\frac{\partial}{\partial t}\psi,$$

where $P = -ih\nabla$ is the momentum operator (∇ is the del operator). The Schrödinger equation suffers from not being relativistically covariant, meaning it does not take into account Einstein's special relativity.

It is natural to try to use the identity from special relativity

$$E = \sqrt{P^2c^2 + m^2c^4},$$

for the energy; then, just inserting the quantum mechanical momentum operator, yields the free particle wave equation

$$\sqrt{(-ih\nabla)^2c^2 + m^2c^4}\psi = ih\frac{\partial}{\partial t}\psi.$$

This, however, is a cumbersome expression to work with because of the square root. The square root term introduces ambiguity. In addition, this equation, as it stands, is nonlocal and furthermore, it does not satisfy some of the conditions required by special relativity.

Klein and Gordon instead worked with the more general square of this equation (the Klein–Gordon equation

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for a free particle), which in covariant notation reads

$$(\Box^2 + \mu^2)\psi = 0,$$

where

$$\mu = \frac{mc}{h},$$

and

$$\Box^2 = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2.$$

This operator is called the d'Alembert operator. Today this form is interpreted as the relativistic field equation for a scalar (i.e., spin-0) particle.

The Klein–Gordon equation was allegedly first found by Schrödinger, before he made the discovery of the equation that now bears his name. He rejected it because he could not make it include the spin of the electron. The way Schrödinger found his equation was by making simplifications in the Klein–Gordon equation.

In 1926, soon after the Schrödinger equation was introduced, Fock wrote an article about its generalization for the case of magnetic fields, where forces were dependent on velocity, and independently derived this equation. Both Klein and Fock used Kaluza and Klein's method. Fock also determined the gauge theory for the wave equation. The Klein–Gordon equation for a free particle has a simple plane wave solution [1].

Authors of [2] used the properties of four explicit finite difference schemes to integrate the nonlinear Klein–Gordon equation. It turned out that the energy conserving scheme is the most suitable to study the long time behavior of the solutions. They observed undesirable characteristics in some of the numerical schemes, in particular, a loss of spatial symmetry and the onset of instability for large values of a parameter in the initial condition of the equation. In [3], an analysis of the schemes described in [2] as applied to a linear problem is carried out, and these indicate that the instability arises from the use of explicit finite difference schemes rather than any failure of energy conservation. This conjecture is further supported by an analysis of two further schemes.

Lee in [4] investigated the numerical solution of the following two dimensional Klein–Gordon equation by collocation method

$$\frac{\partial^2 u}{\partial t^2} - \Delta u + |u|^\alpha u = f,$$

where f in various areas of mathematical physics is a source term independent of the solution u, and $\alpha > 0$. He showed the stability and convergence for using spectral method.

In [5], a fully implicit and discrete energy conserving finite difference scheme for the solution of an initial-boundary value problem of the nonlinear Klein–Gordon equation is presented. A theoretical analysis is performed, and it has been demonstrated that the numerical scheme is particularly attractive when long-time solutions are sought. In [6]; a C^∞ global existence for the following Klein–Gordon equation is investigated

$$(\Box + m^2)u = f(u, u', u''), \quad (t, x, y) \in R^+ \times R \times \mathbf{M},$$
$$u(0, x, y) = \epsilon u_0(x, y), \quad \partial_t u(0, x, y) = \epsilon u_1(x, y),$$

where $\mathbf{M} = (\mathbf{M}, g)$ is a compact Riemannian manifold without boundary, $m \in]0, \infty[$, $\Box = \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{x^2} - \Delta_g$, is the d'Alembertian on the waveguide, f is a polynomial in (u, u', u''), u_0 and u_1 are real valued and belong to $C_0^\infty(R \times \mathbf{M})$, and $\epsilon > 0$ is a small parameter.

Metcalfe and Sogge solved wave and Klein–Gordon equations of the form

$$(\Box + m^2)u = Q(u, u', u''), \quad (t, x, y) \in R^+ \times R^n \times \Omega,$$
$$u(0, x, y) = \epsilon u_0(x, y), \quad \partial_t u(0, x, y) = \epsilon u_1(x, y),$$
$$u|_{\partial\Omega} = 0,$$

where $\Box = \partial_t^2 - \Delta_x - \Delta_\Omega$, $x \in R^n$, $n \geq 3$, $\Delta_x = \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2}$, Δ_Ω denotes the standard Laplacian $\Delta_\Omega = \sum_{j=1}^d \frac{\partial^2}{\partial y_j^2}$, $\Omega \in R^d$ denotes a nonempty, bounded domain with smooth boundary $\partial\Omega$, and Q is a quadratic function in its argument, and affine linear in u'' [7]. The authors of this paper solved this high dimensional problem by the classical argument of wave and Klein–Gordon equations, i.e., uniform estimate and energy estimate in a fashion similar to that used by Klainerman [8].

In [9], by using auxiliary equation method, several types of new exact travelling wave solutions of the nonlinear Klein–Gordon equation with quadratic

nonlinearity

$$u_{tt} - \alpha^2 u_{xx} + \beta u - \gamma u^2 = 0,$$

and with cubic nonlinearity

$$u_{tt} - \alpha^2 u_{xx} + \beta u - \gamma u^3 = 0,$$

are constructed(α, β, and γ are known constants).

Kevrekidis and Konotop studied compactons concentrated on the discrete nonlinear Klein–Gordon model of the form [10]

$$\ddot{u_n} = \Delta_2 u_n + f(u_{n-1}, u_n, u_{n+1}),$$

where $\Delta_2 u_n = u_{n+1} + u_{n-1} - 2u_n$ is the discrete Laplacian (with unit spacing) and the nonlinearity is assumed to be of the type

$$\begin{aligned} &f(su_{n-1}, su_n, su_{n+1}) \\ &\quad = \sum_{k=1}^{m} g_k(su_{n-1}, su_n, su_{n+1}) \\ &\quad = \sum_{k=1}^{m} s^k g_k(su_{n-1}, su_n, su_{n+1}), \end{aligned}$$

where s is any function of time.

In [11] the local and global existence and uniqueness of weak solution of the damped Klein–Gordon equation with Dirichlet boundary condition is established. The Klein–Gordon equation with damping term is described by the following partial differential equation:

$$\frac{\partial^2 y}{\partial t^2} + \alpha \frac{\partial y}{\partial t} - \beta \Delta y + \delta |y|^\gamma = f,$$

where α, β, $\gamma > 0$, $\delta \in R$ are physical parameters, and f is a forcing function. The existence and uniqueness of the strong solutions of the Cauchy problem for the above equation with Dirichlet boundary conditions (with $\beta = \delta = 1$) are studied in [12].

[13] deals with the numerical solution of the damped nonlinear Klein–Gordon equation with Dirichlet boundary condition using variational method and finite element approximation.

In this work, we focus on the following Klein–Gordon equation:

$$(\Box + m^2)u = f(u, u', u''), \tag{1.1}$$

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \partial_t u(\mathbf{x}, 0) = u_1(\mathbf{x}),$$

where $\mathbf{x} = (x_1, \ldots, x_n) \in R^n$, $t \in R^+$ and $\Box = \frac{\partial^2}{\partial t^2} - \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}$.

The solution of this equation is presented by means of variational iteration method, (VIM) and then, several examples are given to show the efficiency of the proposed method for solving this equation.

For simplicity in illustrating the procedure of variational iteration method, we rewrite f as $f = f_1 + f_2$, where f_1 is the linear part of f and f_2 is the nonlinear part of f if it exists.

The rest of this paper is organized as follows:

In Section 2, we review the procedure of variational iteration method and apply this technique to Equation (1.1). To show the efficiency of this method, we present some examples and numerical results in Section 3. A conclusion is given in Section 4.

2 Variational iteration method

The He's VIM, which is a modified general Lagrange multiplier method, has been shown to solve effectively, easily, and accurately a large class of linear and nonlinear problems. The main feature of the method is that the solution of a mathematical problem with linearization assumption is used as initial approximation or trial function, then, a more highly precise approximation at some special points can be obtained [14, 15]. This approximation converges rapidly to accurate solution.

In [16], the applications of the present method to coupled *Schrodinger–(KdV)* and shallow water equations are provided. The *Bratu's* problem, which has various important applications in science and engineering is easily solved in [17] with high accuracy by the variational iteration method. The variational iteration technique is employed to solve the nonlinear *dispersive* equation, which is a nonlinear partial differential equation that arise in the process of understanding the role of nonlinear dispersion and in the forming of structures like liquid drops and exhibits compactons [18].

In [19], the generalized *Burgers–Fisher* and *Burgers* equations have been analyzed using the variational iteration method. In [20], the solution for the generalized regularized long wave equation, which is an alternative description of nonlinear dispersive waves to the more usual KdV equation based on variational iteration method is exactly obtained. The variational iteration technique is employed in [21] for solving three types of nonlinear partial differential equations such as coupled Schrodinger–KdV, generalized KdV and shallow water equations. The exact and numerical solutions obtained by variational iteration method for these three important models of mathematical physics are compared to that obtained using Adomian decomposition method. The results reported by these authors [21] show that the variational iteration method is a powerful mathematical tool for finding the exact and numerical solutions of nonlinear partial differential equations. Authors of [22] used the variational iteration procedure to solve several kinds of interesting nonlinear partial differential equations such as coupled nonlinear reaction diffusion equations, Hirota–Satsuma coupled KdV system and Drinefel'd-Sokolov-Wilson equations. The approximate solutions obtained by this method are compared with the exact solutions. The obtained results [22] show that the variational iteration method is of high accuracy, efficient and can overcome the difficulties arising in calculating Adomian polynomials in decomposition technique of Adomian [23]. Author of [24] employed the variational iteration method for determining rational solutions for the *KdV*, the $K(2, 2)$, the Burgers, and the *cubic Boussinesq* equations. This approach is used to solve numerically the harmonic wave generation in a nonlinear, one-dimensional elastic half-space model subjected initially to a prescribed harmonic displacement [25]. Recently, authors of [26] employed this technique for solving several problems in calculus of variations. In [27], He's variational iteration method is used for computing an unknown time-dependent parameter in an inverse quasilinear parabolic partial differential equation. This approach is successfully and effectively applied to *delay* differential equations [28], *autonomous* ordinary differential equations [29], *Blasius* equation [30], etc. The convergence of variational iteration technique of He is proved in [31] for various partial differential models.

It is shown in [32] that the application of VIM to a special kind of nonlinear differential equations leads to calculation of unneeded terms and more time consumed in repeated calculations for series solutions. A modified VIM is introduced to eliminate the shortcomings and in [33] the Padé technique was successfully linked with this modification.

The idea of this method is constructing a correction functional by a general *Lagrange multiplier*. The multiplier in the functional should be chosen such that its correction solution is superior to its initial approximation(trial function) and is the best within the flexibility of trial function, and accordingly, we can identify the multiplier by variational theory. The initial approximation can be freely chosen with possible unknowns, which can be determined by imposing the boundary/initial conditions.

To illustrate the procedure of this approach, we consider the following general differential equation

$$Lu + Nu = g, \tag{2.1}$$

where L is a linear operator, N is a nonlinear operator, and $g(t)$ is an inhomogeneous term.

According to the variational iteration method, the terms of a sequence $\{u_n\}$ are constructed such that this sequence converges to the exact solution. The terms of u_ns are calculated by a correction functional as follows:

$$u_{n+1}(t) = u_n(t) + \int_0^t \lambda\{Lu_n(s) + N\tilde{u}_n(s) - g(s)\}\, ds, \tag{2.2}$$

where λ is the general Lagrange multiplier, which can be identified optimally via the variational theory, the subscript n denotes the nth approximation and $\tilde{u}_n$ is considered as a restricted variation, i.e., $\delta\tilde{u}_n = 0$. For linear problems, the exact solution can be obtained by only one iteration step due to the fact that the Lagrange multiplier can be exactly identified. In nonlinear problems, in order to determine the Lagrange multiplier in a simple manner as possible, the nonlinear terms have to be considered as restricted variations.

If we apply this procedure to Equations (1.1), (2.2) reduces to:

$$u_{n+1}(\mathbf{x}, t) = u_n(\mathbf{x}, t) + \psi_n(\mathbf{x}, t), \tag{2.3}$$

where ψ_n is in the following form:

$$\psi_n(\mathbf{x},t)=\int_0^t \lambda\left\{\frac{\partial^2 u_n}{\partial s^2}(\mathbf{x},s)+m^2u_n(\mathbf{x},s)-f_1 - \sum_{j=1}^{n}\frac{\partial^2\tilde{u}_n}{\partial x_j^2}(\mathbf{x},s)-\tilde{f}_2\right\}ds. \tag{2.4}$$

By taking variation of (2.3) with respect to the independent variable u_n and making the correction functional stationary, λ, the Lagrange multiplier, will be specified. Then, starting with an initial approximation, we can identify the next approximations successively.

3 Test examples

In this section, we present some examples with analytical solution to show efficiency of the method described in previous section for solving Equation (1.1).

3.1 Example 1

As the first example, consider Equation (1.1) with $m=2$, $n=3(\mathbf{x}=(x_1,x_2,x_3))$, $f=5u$, and the following initial conditions

$$u(\mathbf{x},0)=x_1x_2x_3, \tag{3.1}$$

$$\frac{\partial u}{\partial t}(\mathbf{x},0)=-x_1x_2x_3. \tag{3.2}$$

$u(\mathbf{x},t)=x_1x_2x_3e^{-t}$ is the exact solution of this equation. We apply variational iteration method to this equation. To construct the correction functional, it is sufficient to use (2.3) and (2.4):

$$u_{n+1}(\mathbf{x},t)=u_n(\mathbf{x},t)+\psi_n(\mathbf{x},t),$$

where

$$\psi_n(\mathbf{x},t)=\int_0^t \lambda\left\{\frac{\partial^2 u_n}{\partial s^2}(\mathbf{x},s)+4u_n(\mathbf{x},s)-5u_n(\mathbf{x},s) - \sum_{j=1}^{3}\frac{\partial^2\tilde{u}_n}{\partial x_j^2}(\mathbf{x},s)\right\}ds.$$

Taking variation with respect to the independent variable u_n and making the correction functional stationary, we obtain

$$\delta u_{n+1}(\mathbf{x},t)=0,$$

and therefore, we have:

$$\begin{aligned}\delta u_n(\mathbf{x},t)&+\delta\int_0^t\lambda\left\{\frac{\partial^2u_n}{\partial s^2}(\mathbf{x},s)-u_n(\mathbf{x},s) - \sum_{j=1}^{3}\frac{\partial^2\tilde{u}_n}{\partial x_j^2}(\mathbf{x},s)\right\}ds\\ &=\delta u_n(\mathbf{x},t)+\lambda\delta\frac{\partial u_n}{\partial s}(\mathbf{x},s)|_{s=t}-\lambda'\delta u_n(\mathbf{x},s)|_{s=t}\\ &\quad+\int_0^t(\lambda''-\lambda)\delta u_n(\mathbf{x},s)ds=0.\end{aligned}$$

These conditions imply the following stationary conditions:

$$\begin{aligned}\delta u_n &: 1-\lambda'(t)=0,\\ \delta\frac{\partial u_n}{\partial t} &: \lambda(t)=0,\\ \delta u_n &: \lambda-\lambda''=0,\end{aligned}$$

and therefore, we get

$$\lambda(s)=-\frac{1}{2}(e^{t-s}-e^{s-t}).$$

As a result, we have the following variational iteration formula

$$u_{n+1}(\mathbf{x},t)=u_n(\mathbf{x},t)+\psi_n(\mathbf{x},t),$$

where

$$\psi_n(\mathbf{x},t)=-\int_0^t\frac{1}{2}(e^{t-s}-e^{s-t})\left\{\frac{\partial^2u_n}{\partial s^2}(\mathbf{x},s) - u_n(\mathbf{x},s)-\sum_{j=1}^{3}\frac{\partial^2u_n}{\partial x_j^2}(\mathbf{x},s)\right\}ds.$$

We start with initial approximation $u_0(\mathbf{x},t)=a+bt$, where a and b are constant in t. Regarding initial conditions (3.1) and (3.2), a and b can be considered as $a=x_1x_2x_3$ and $b=-x_1x_2x_3$. By the above iteration

formula, we have:

$$u_1(\mathbf{x}, t) = u_0(\mathbf{x}, t) + \psi_0(\mathbf{x}, t),$$

where

$$\begin{aligned}\psi_0(\mathbf{x}, t) = -\int_0^t \frac{1}{2}(e^{t-s} - e^{s-t})\Bigg\{ &\frac{\partial^2 u_0}{\partial s^2}(\mathbf{x}, s) \\ &- u_0(\mathbf{x}, s) - \sum_{j=1}^{3} \frac{\partial^2 u_0}{\partial x_j^2}(\mathbf{x}, s)\Bigg\} ds \\ = -x_1x_2x_3 + x_1x_2x_3t + x_1x_2x_3e^{-t},\end{aligned}$$

and therefore,

$$u_1(\mathbf{x}, t) = x_1x_2x_3e^{-t},$$

which is the exact solution.

3.2 Example 2

Consider Equation (1.1) with $m = 1$, $n = 2(\mathbf{x} = (x_1, x_2))$, $f = -2 + u$, and the following initial conditions

$$u(x, 0) = x_1^2 + x_2^2, \tag{3.3}$$

$$\frac{\partial u}{\partial t}(x, 0) = x_2^2. \tag{3.4}$$

The exact solution of this equation is

$$u(\mathbf{x}, t) = x_1^2 + x_2^2 + x_2^2t + \frac{1}{3}t^3 + t^2.$$

To apply the variational iteration method to this equation, according to (2.3) and (2.4), we have:

$$u_{n+1}(\mathbf{x}, t) = u_n(\mathbf{x}, t) + \mu_n(\mathbf{x}, t), \tag{3.5}$$

where

$$\psi_n(\mathbf{x}, t) = \int_0^t \lambda \left\{ \frac{\partial^2 u_n}{\partial s^2}(\mathbf{x}, s) - \sum_{j=1}^{2} \frac{\partial^2 \tilde{u}_n}{\partial x_j^2}(\mathbf{x}, s) + 2 \right\} ds.$$

By the same manipulation as previous example, we can obtain the following stationary conditions:

$$\delta u_n : 1 - \lambda'(t) = 0,$$

$$\delta \frac{\partial u_n}{\partial t} : \lambda(t) = 0,$$

$$\delta u_n : \lambda'' = 0,$$

which yield

$$\lambda(s) = s - t.$$

Consider $u_0(\mathbf{x}, t) = a + bt$, where a and b are constant in t and with respect to the initial conditions (3.3) and (3.4), can be considered as $a = x_1^2 + x_2^2$ and $b = x_2^2$. By the above formula, u_1 is obtained in the following form

$$u_1(\mathbf{x}, t) = u_0(\mathbf{x}, t) + \psi_0(\mathbf{x}, t),$$

where

$$\begin{aligned}\psi_0(\mathbf{x}, t) = \int_0^t (s - t)\Bigg\{ &\frac{\partial^2 u_0}{\partial s^2}(\mathbf{x}, s) \\ &- \sum_{j=1}^{2} \frac{\partial^2 u_0}{\partial x_j^2}(\mathbf{x}, s) + 2\Bigg\} ds \\ = \frac{1}{3}t^3 + t^2,\end{aligned}$$

and therefore,

$$u_1(\mathbf{x}, t) = x_1^2 + x_2^2(1 + t) + \frac{1}{3}t^3 + t^2,$$

which is the exact solution.

3.3 Example 3

In this example we solve Equation (1.1) with $m = \frac{\sqrt{3}}{8}$, $n = 1(\mathbf{x} = (x))$, $f = 0$, and initial conditions

$$u(x, 0) = \sin\left(\frac{1}{8}x\right), \tag{3.6}$$

$$\frac{\partial u}{\partial t}(x, 0) = -\frac{1}{4}\sin\left(\frac{1}{8}x\right). \tag{3.7}$$

The exact solution of this equation is:

$$u(x, t) = \sin\left(\frac{1}{8}x\right)\left(\cos\left(\frac{1}{4}t\right) + \sin\left(\frac{-1}{4}t\right)\right).$$

Table 1 Comparison of the exact and approximate values by VIM in Example 3

(x, t)	Exact value	Approximate value by VIM	Absolute error
$(-5, 5)$	0.37075405851278	0.37075405355941	$4.953372212401774 \times 10^{-9}$
$(-4, 4)$	0.14438795611141	0.14438795565649	$4.549206011894569 \times 10^{-10}$
$(-3, 3)$	−0.01833197994970	−0.01833197997004	$2.033529594713812 \times 10^{-11}$
$(-2, 2)$	−0.09850562396599	−0.09850562396624	$2.463723669521301 \times 10^{-13}$
$(-1, 1)$	−0.08995387519190	−0.08995387519190	$1.387778780781446 \times 10^{-16}$
$(0, 0)$	0	0	0
$(1, 1)$	0.08995387519190	0.08995387519190	$1.387778780781446 \times 10^{-16}$
$(2, 2)$	0.09850562396599	0.09850562396624	$2.463723669521301 \times 10^{-13}$
$(3, 3)$	0.01833197994970	0.01833197997004	$2.033529594713812 \times 10^{-11}$
$(4, 4)$	−0.14438795611141	−0.14438795565649	$4.549206011894569 \times 10^{-10}$
$(5, 5)$	−0.37075405851278	−0.37075405355941	$4.953372212401774 \times 10^{-9}$

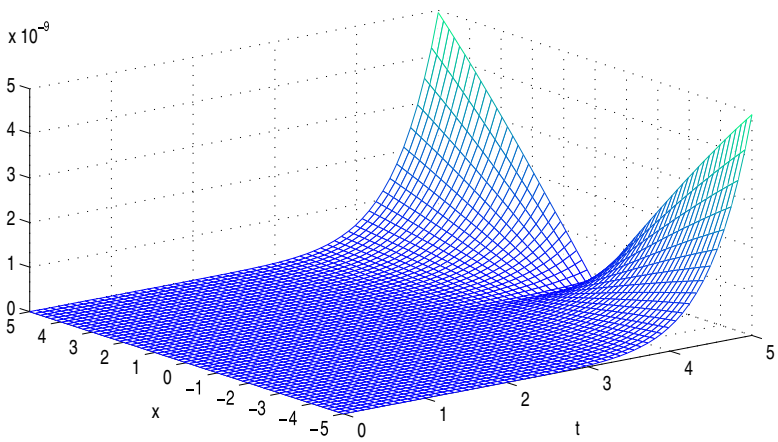

Fig. 1 Plot of absolute error in Example 3

To solve this equation by variational iteration method, we use (2.3) and (2.4):

$$u_{n+1}(x, t) = u_n(x, t) + \psi_n(x, t),$$

where

$$\psi_n(x, t) = \int_0^t \lambda \left\{ \frac{\partial^2 u_n}{\partial s^2} + \frac{3}{64} u_n(x, s) - \frac{\partial^2 \tilde{u}_n}{\partial x^2}(x, s) \right\} ds.$$

Such as previous examples, we obtain the following stationary conditions:

$$\delta u_n : 1 - \lambda'(t) = 0,$$
$$\delta \frac{\partial u_n}{\partial t} : \lambda(t) = 0,$$
$$\delta u_n : \lambda'' + \frac{3}{64}\lambda = 0,$$

and therefore, we get

$$\lambda(s) = \frac{8\sqrt{3}}{3} \sin\left(\frac{\sqrt{3}}{8}(s - t)\right).$$

We consider initial approximation u_0 as $u_0(\mathbf{x}, t) = a + bt$, where a and b are constant in t. Regarding initial conditions (3.6) and (3.7), a and b can be considered as $a = \sin(\frac{1}{8}x)$ and $b = -\frac{1}{4}\sin(\frac{1}{8}x)$.

By the above recurrent formula, we get u_1, u_2, u_3, u_4 and consider u_4 as an approximation of the exact solution. Numerical results by this approximation are summarized in Table 1 and the absolute error function $|u_4(x, t) - u(x, t)|$ is plotted in Fig. 1. These results show the high accuracy of the approximate solution obtained by the variational iteration method.

4 Conclusion

In this work, the *variational iteration method* has been successfully implemented to the *Klein–Gordon*

equation. Application of this procedure shows that the proposed method is very simple and straightforward. Furthermore, this approach unlike the mesh points schemes [35] does not provide any linear or nonlinear system of equations. It does not require any discretization, linearization, or small perturbations [36], and therefore, is capable of greatly reducing the size of calculations while still maintaining high accuracy of the numerical solution.

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