SOLVING SCHRÖDINGER EQUATION BY USING MODIFIED VARIATIONAL ITERATION AND HOMOTOPY ANALYSIS METHODS

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Abstract In this paper, a nonlinear Schrödinger equation is solved by using the variational iteration method (VIM), modified variational iteration method (MVIM) and homotopy analysis method (HAM) numerically. For each method, the approximate solution of this equation is calculated based on a recursive relation which its components are computed easily. The existence and uniqueness of the solution and the convergence of the proposed methods are proved. A numerical example is studied to demonstrate the accuracy of the given algorithms.

Keywords Schrödinger equation, Variational iteration method, Modified variational iteration method, Homotopy analysis method.

MSC(2000) 35A15, 34B15, 34C15.

1. Introduction

The Schrödinger equation is a typical partial differential equation that plays a key role in variety of areas in chemistry and mathematical physics. It describes the spatio-temporal evolution of the complex field and many problems in physics. The fields of application varies from optics [27], propagation of the electric field in optical fibers [13], self-focusing and collapse of Langmuir waves in plasma physics [28] to model deep water waves and freak wave(so-called rogue waves) in the ocean [22]. In recent years some works have been done in order to find the numerical solution of this equation [6-10,18,19,23-26]. In this work, we apply the variational iteration method (VIM), modified variational iteration method (MVIM) and homotopy analysis method (HAM) to solve the Schrödinger equation as follows:

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + q \mid u \mid^2 u = 0, \quad t > 0, \tag{1}$$

with the initial condition given by:

$$u(x,0) = f(x), \quad x \in [a,b], \tag{2}$$

where the parameter $q \in R$ corresponds to a focusing $(q > 0)$ or defocusing $(q < 0)$ effect of the nonlinearity.

We can write Eq.(1) as follows:

$$\frac{\partial u}{\partial t} = i\frac{\partial^2 u}{\partial x^2} + iq \mid u \mid^2 u, \quad t > 0. \tag{3}$$

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To obtain the approximate solution of Eq.(3), by integrating one time from Eq.(3) with respect to t and using the initial conditions we obtain,

$$u(x,t) = f(x) + i \int_0^t D^2(u(x,t)) \ dt + i \int_0^t F(u(x,t)) \ dt, \tag{4}$$

where, $F(u(x,t)) = q \mid u(x,t) \mid^2 u(x,t)$, and $D^2(u(x,t)) = \frac{\partial^2 u(x,t)}{\partial x^2}$.

In Eq.(4), we assume $f(x)$ is bounded for all x,t in $J = [a,b]$. Also, we suppose the functions $D^2(u(x,t))$ and $F(u(x,t))$ are Lipschitz continuous as $\mid D^2(u) - D^2(u^*) \mid \leq L_1 \mid u - u^* \mid$, $\mid F(u) - F(u^*) \mid \leq L_2 \mid u - u^* \mid$ where $u = u(x,t)$, $u^* = u(x,t^*)$ and

$$\alpha_1 := b(L_1 + L_2), \ \gamma_1 := b\alpha_1,$$

$$\beta_1 := \begin{cases} (1 - a + b\alpha_1), & 0 < t \leq 1 \\ (b(1 + \alpha_1) - 1), & t > 1. \end{cases}$$

1.1. Description of the VIM and MVIM

We consider the following nonlinear differential equation:

$$L(u(x,t)) + N(u(x,t)) = g(x,t), \tag{5}$$

where L is a linear operator, N is a nonlinear operator and $g(x,t)$ is a known analytical function. In the VIM [12,14-17], a correction functional can be constructed as follows:

$$u_{n+1}(x,t) = u_n(x,t) + \int_0^t \lambda(x,\tau)\{L(u_n(x,\tau)) + N(u_n(x,\tau)) - g(x,\tau)\}d\tau, \quad n \geq 0, \tag{6}$$

where λ is a general Lagrange multiplier which can be identified optimally via variational theory. Here the function $u_n(x,\tau)$ is a restricted variations which means $\delta u_n = 0$. Therefore, we first determine the Lagrange multiplier λ that will be identified optimally via integration by parts. The successive approximation $u_n(x,t)$, $n \geq 0$ of the solution $u(x,t)$ will be readily obtained upon using the obtained Lagrange multiplier and by using any selective function u_0. The zeroth approximation u_0 may be selected any function that just satisfies at least the initial and boundary conditions. With λ determined, then several approximation $u_n(x,t)$, $n \geq 0$ follow immediately. Consequently, the exact solution may be obtained by using

$$u(x,t) = \lim_{n \to \infty} u_n(x,t). \tag{7}$$

The VIM has been shown to solve effectively, easily and accurately a large class of nonlinear problems with approximations converge rapidly to accurate solutions.

To obtain the approximation solution of Eq.(1), according to the VIM, we can write iteration formula (6) as follows:

$$u_{n+1}(x,t) = u_n(x,t) + L_t^{-1}(\lambda[u_n(x,t) - f(x) - i \int_0^t D^2(u_n(x,t)) \ dt \\ -i \int_0^t F(u_n(x,t)) \ dt]), \ n \geq 0, \tag{8}$$

where,

$$L_t^{-1}(.) = \int_0^t (.) \ d\tau.$$

To find the optimal λ, we proceed as

$$\delta u_{n+1}(x,t) = \delta u_n(x,t) + \delta L_t^{-1}(\lambda[u_n(x,t) - f(x) - i \int_0^t D^2(u_n(x,t)) \ dt \\ -i \int_0^t F(u_n(x,t)) \ dt]). \tag{9}$$

From Eq.(9), the stationary conditions can be obtained as follows:
$\lambda' = 0$ and $1 + \lambda = 0$.

Therefore, the Lagrange multipliers can be identified as $\lambda = -1$ and by substituting in (8), the following iteration formula is obtained.

$$u_0(x,t) = f(x), \\ u_{n+1}(x,t) = u_n(x,t) - L_t^{-1}(u_n(x,t) - f(x) - i \int_0^t D^2(u_n(x,t)) \ dt \\ -i \int_0^t F(u_n(x,t)) \ dt, \quad n \geq 0. \tag{10}$$

To obtain the approximation solution of Eq.(1), based on the MVIM [4,5], we can write the following iteration formula:

$$u_{-1}(x,t) = 0, \\ u_0(x,t) = f(x), \\ u_{n+1}(x,t) = u_n(x,t) - L_t^{-1}(-i \int_0^t D^2(u_n(x,t) - u_{n-1}(x,t)) \ dt \\ -i \int_0^t F(u_n(x,t) - u_{n-1}(x,t)) \ dt, \quad n \geq 0. \tag{11}$$

Relations (10) and (11) will enable us to determine the components $u_n(x,t)$ recursively for $n \geq 0$.

1.2. Description of the HAM

Consider

$$N[u] = 0,$$

where N is a nonlinear operator, $u(x,t)$ is unknown function and x is an independent variable. let $u_0(x,t)$ denote an initial guess of the exact solution $u(x,t)$, $h \neq 0$ an auxiliary parameter, $H(x,t) \neq 0$ an auxiliary function, and L an auxiliary linear operator with the property $L[s(x,t)] = 0$ when $s(x,t) = 0$. Then using $q \in [0,1]$ as an embedding parameter, we construct a homotopy as follows:

$$(1-q)L[\phi(x,t;q) - u_0(x,t)] - qhH(x,t)N[\phi(x,t;q)] \\ = \hat{H}[\phi(x,t;q); u_0(x,t), H(x,t), h, q]. \tag{12}$$

It should be emphasized that we have great freedom to choose the initial guess $u_0(x,t)$, the auxiliary linear operator L, the non-zero auxiliary parameter h, and the auxiliary function $H(x,t)$.

Enforcing the homotopy (12) to be zero, i.e.,

$$\hat{H}[\phi(x,t;q); u_0(x,t), H(x,t), h, q] = 0, \tag{13}$$

we have the so-called zero-order deformation equation

$$(1-q)L[\phi(x,t;q) - u_0(x,t)] = qhH(x,t)N[\phi(x,t;q)]. \tag{14}$$

When $q = 0$, the zero-order deformation Eq.(14) becomes

$$\phi(x;0) = u_0(x,t), \tag{15}$$

and when $q = 1$, since $h \neq 0$ and $H(x,t) \neq 0$, the zero-order deformation Eq.(14) is equivalent to

$$\phi(x,t;1) = u(x,t). \tag{16}$$

Thus, according to (15) and (16), as the embedding parameter q increases from 0 to 1, $\phi(x,t;q)$ varies continuously from the initial approximation $u_0(x,t)$ to the exact solution $u(x,t)$. Such a kind of continuous variation is called deformation in homotopy [11,20,21].

Due to Taylor's theorem, $\phi(x,t;q)$ can be expanded in a power series of q as follows

$$\phi(x,t;q) = u_0(x,t) + \sum_{m=1}^{\infty} u_m(x,t)q^m, \tag{17}$$

where

$$u_m(x,t) = \frac{1}{m!} \frac{\partial^m \phi(x,t;q)}{\partial q^m} \big|_{q=0} \ .$$

Let the initial guess $u_0(x,t)$, the auxiliary linear operator L, the nonzero auxiliary parameter h and the auxiliary function $H(x,t)$ be properly chosen so that the power series (17) of $\phi(x,t;q)$ converges at $q = 1$, then, we have under these assumptions the solution series

$$u(x,t) = \phi(x,t;1) = u_0(x,t) + \sum_{m=1}^{\infty} u_m(x,t). \tag{18}$$

From Eq.(17), we can write Eq.(14) as follows

$$
\begin{aligned}
&(1-q)L[\phi(x,t,q) - u_0(x,t)] \\
= \ & (1-q)L[\sum_{m=1}^{\infty} u_m(x,t) \ q^m] \\
= \ & q \ h \ H(x,t)N[\phi(x,t,q)] \\
\Rightarrow \ & L[\sum_{m=1}^{\infty} u_m(x,t) \ q^m] - q \ L[\sum_{m=1}^{\infty} u_m(x,t)q^m] \\
= \ & q \ h \ H(x,t)N[\phi(x,t,q)].
\end{aligned} \tag{19}
$$

By differentiating (19) m times with respect to q, we obtain

$$
\begin{aligned}
& \{L[\sum_{m=1}^{\infty} u_m(x,t) \ q^m] - q \ L[\sum_{m=1}^{\infty} u_m(x,t)q^m]\}^{(m)} \\
= \ & \{q \ h \ H(x,t)N[\phi(x,t,q)]\}^{(m)} \\
= \ & m! \ L[u_m(x,t) - u_{m-1}(x,t)] \\
= \ & h \ H(x,t) \ m \ \frac{\partial^{m-1}N[\phi(x,t;q)]}{\partial q^{m-1}} \big|_{q=0} \ .
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
& L[u_m(x,t) - \chi_m u_{m-1}(x,t)] = hH(x,t)\Re_m(u_{m-1}(x,t)), \ m \geq 1 \\
& u_m(0) = 0,
\end{aligned} \tag{20}
$$

where,

$$\Re_m(u_{m-1}(x,t)) = \frac{1}{(m-1)!} \frac{\partial^{m-1} N[\phi(x,t;q)]}{\partial q^{m-1}} \Big|_{q=0}, \tag{21}$$

and

$$\chi_m = \begin{cases} 0, & m \leq 1 \\ 1, & m > 1 \end{cases}$$

Note that the high-order deformation Eq. (20) is governing the linear operator L, and the term $\Re_m(u_{m-1}(x,t))$ can be expressed simply by (21) for any nonlinear operator N.

To obtain the approximation solution of Eq. (1), according to HAM, let

$$N[u(x,t)] = u(x,t) - f(x) - i \int_0^t D^2(u(x,t)) \, dt - i \int_0^t F(u(x,t)) \, dt,$$

so,

$$\begin{aligned} &\Re_m(u_{m-1}(x,t)) \\ =\ & u_{m-1}(x,t) - f(x) - i \int_0^t D^2(u_{m-1}(x,t)) \, dt - i \int_0^t F(u_{m-1}(x,t)) \, dt. \end{aligned} \tag{22}$$

Substituting (22) into (20),

$$\begin{aligned} &L[u_m(x,t) - \chi_m u_{m-1}(x,t)] \\ =\ & hH(x,t)[u_{m-1}(x,t) - i \int_0^t D^2(u(x,t)) \, dt - i \int_0^t F(u(x,t)) - (1-\chi_m)f(x)]. \end{aligned} \tag{23}$$

We take an initial guess $u_0(x,t) = f(x)$, an auxiliary linear operator $Lu = u$, a nonzero auxiliary parameter $h = -1$, and auxiliary function $H(x,t) = 1$. This is substituted into (23) to give the recurrence relation

$$\begin{aligned} u_0(x,t) &= f(x), \\ u_{n+1}(x,t) &= i \int_0^t D^2(u_n(x,t)) \, dt + i \int_0^t F(u_n(x,t)) \, dt, \quad n \geq 0. \end{aligned} \tag{24}$$

2. Existence and convergence of the methods

Theorem 2.1. *Let $0 < \alpha_1 < 1$, then Schrödinger equation (1), has a unique solution.*

Proof. Let u and u^* be two different solutions of (4) then

$$\begin{aligned} | u - u^* | &= | \int_0^t D^2(u(x,t)) \, dt + \int_0^t F(u(x,t)) | \\ &\leq \int_0^t | D^2(u(x,t)) - D^2(u^*(x,t)) | \, dt \\ &\quad + \int_0^t | F(u(x,t)) - F(u^*(x,t)) | \, dt \\ &\leq b(L_1 + L_2) \, | u - u^* | \\ &= \alpha_1 \, | u - u^* | \, . \end{aligned}$$

Consequently we get $(1 - \alpha_1) \, | u - u^* | \leq 0$. Since $0 < \alpha_1 < 1$ then $| u - u^* | = 0$ and therefore $u = u^*$. This completes the proof. $\square$

Theorem 2.2. *The solution $u_n(x,t)$ obtained from the relation (10) using VIM converges to the exact solution of the problem (1) when $0 < \alpha_1 < 1$ and $0 < \beta_1 < 1$.*

Proof.   Let $\lim_{n\to\infty} u_n(x,t) = u(x,t)$. According to (10) we have,

$$u(x,t) = u(x,t) - L_t^{-1}([u(x,t) - f(x) - i\int_0^t D^2(u(x,t))\ dt - i\int_0^t F(u(x,t)))\ dt])$$
(25)

By subtracting both sides of relation (25) from (10),

$$
\begin{aligned}
u_{n+1}(x,t) - u(x,t) \ = \ & u_n(x,t) - u(x,t) - L_t^{-1}(u_n(x,t) - u(x,t) \\
& -i\int_0^t [D^2(u_n(x,t)) - D^2(u(x,t))] \\
& -i\int_0^t [F(u_n(x,t))\ dt - F(u(x,t))\ dt]\ dt).
\end{aligned}
$$
(26)

If we set, $e_{n+1}(x,t) = u_{n+1}(x,t) - u_n(x,t)$, $e_n(x,t) = u_n(x,t) - u(x,t)$, $\mid e_n(x,t^*)\mid$ $= max_t\mid e_n(x,t)\mid$ then since e_n is a decreasing function with respect to t from (26) using the mean value theorem we can write,

$$
\begin{aligned}
e_{n+1}(x,t) \ = \ & e_n(x,t) + L_t^{-1}(-e_n(x,t) + i\int_0^t[D^2(u_n(x,t)) - D^2(u(x,t))]\ dt \\
& +i\int_0^t[F(u_n(x,t)) - F(u(x,t))]\ dt) \\
\Rightarrow \quad & \mid e_{n+1}(x,t) - e_n(x,t) + \int_0^t e_n(x,t)\ dt \mid \\
= \quad & \mid L_t^{-1}\int_0^t[D^2(u_n(x,t)) - D^2(u(x,t))]\ dt \\
& +L_t^{-1}\int_0^t[F(u_n(x,t)) - F(u(x,t))]\ dt \mid \\
\Rightarrow \quad & \mid e_{n+1}(x,t) - e_n(x,t) + te_n(x,\eta) \mid \\
\leq \quad & L_t^{-1}\int_0^t \mid D^2(u_n(x,t)) - D^2(u(x,t)) \mid\ dt \\
& +L_t^{-1}\int_0^t \mid F(u_n(x,t)) - F(u(x,t)) \mid\ dt \\
\leq \quad & L_t^{-1}\int_0^t \mid e_n(x,t) \mid (L_1 + L_2)dt \\
\leq \quad & L_t^{-1}\int_0^t \mid e_n(x,t^*) \mid (L_1 + L_2)dt \\
\leq \quad & b^2(L_1 + L_2)\parallel e_n \parallel = b\alpha_1 \parallel e_n \parallel,
\end{aligned}
$$

where $0 \leq \eta \leq t$ and $a \leq t \leq b$. Since $e_n(x,\eta) \geq e_n(x,t)$ hence

$$
\begin{aligned}
& \mid e_{n+1}(x,t) - e_n(x,t) + te_n(x,t) \mid \leq b\alpha_1 \parallel e_n \parallel \Rightarrow \\
& \mid e_{n+1}(x,t) - (1-t)e_n(x,t) \mid \leq b\alpha_1 \parallel e_n \parallel \Rightarrow \\
& \mid e_{n+1}(x,t) - \mid 1-t \mid \mid e_n(x,t) \mid \leq b\alpha_1 \parallel e_n \parallel \Rightarrow \\
& \mid e_{n+1}(x,t) \mid \leq (\mid 1-t \mid + b\alpha_1) \parallel e_n \parallel \leq \begin{cases} (1 - a + b\alpha_1) \parallel e_n \parallel, & 0 < t \leq 1 \\ (b(1+\alpha_1) - 1) \parallel e_n \parallel, & t > 1. \end{cases}
\end{aligned}
$$

Therefore,

$$\|e_{n+1}\| = max_{t\in J}\mid e_{n+1}\mid \leq \beta_1\ max_{t\in J}\mid e_n \mid = \beta_1\|e_n\|.$$

Since $0 < \beta_1 < 1$, then $\|e_n\| \to 0$. So, the series converges and the proof is complete.   □

Theorem 2.3. *The solution $u_n(x,t)$ obtained from the relation (12) using MVIM for the problem (1) converges when $0 < \alpha_1 < 1$, $0 < \gamma_1 < 1$.*

Proof.   The proof is similar to the previous theorem.   □

Theorem 2.4. *If the series solution (24) of problem (1) using HAM is convergent then it converges to the exact solution of the problem (1).*

Proof.   We assume:

$$u(x,t) = \sum_{m=0}^{\infty} u_m(x,t),$$
$$\widehat{F}(u(x,t)) = \sum_{m=0}^{\infty} F(u_m(x,t)),$$
$$\widehat{D^2}(u(x,t)) = \sum_{m=0}^{\infty} D^2(u_m(x,t)).$$

where,

$$\lim_{m \to \infty} u_m(x,t) = 0.$$

We can write,

$$\sum_{m=1}^{n} [u_m(x,t) - \chi_m u_{m-1}(x,t)] = u_1 + (u_2 - u_1) + ... + (u_n - u_{n-1}) = u_n(x,t). \quad (27)$$

Hence, from (27),

$$\lim_{n \to \infty} u_n(x,t) = 0. \quad (28)$$

So, using (28) and the definition of the linear operator L, we have

$$\sum_{m=1}^{\infty} L[u_m(x,t) - \chi_m u_{m-1}(x,t)] = L[\sum_{m=1}^{\infty} [u_m(x,t) - \chi_m u_{m-1}(x,t)]] = 0.$$

Therefore from (20), we can obtain that,

$$\sum_{m=1}^{\infty} L[u_m(x,t) - \chi_m u_{m-1}(x,t)] = hH(x,t) \sum_{m=1}^{\infty} \Re_{m-1}(u_{m-1}(x,t)) = 0.$$

Since $h \neq 0$ and $H(x,t) \neq 0$, we have

$$\sum_{m=1}^{\infty} \Re_{m-1}(u_{m-1}(x,t)) = 0. \quad (29)$$

By substituting $\Re_{m-1}(u_{m-1}(x,t))$ into the relation (29) and simplifying it , we have

$$
\begin{aligned}
&\sum_{m=1}^{\infty} \Re_{m-1}(u_{m-1}(x,t)) \\
=\ &\sum_{m=1}^{\infty} [u_{m-1}(x,t) - i \int_0^t D^2(u_{m-1}(x,t))\ dt \\
&-i \int_0^t F(u_{m-1}(x,t))\ dt - (1 - \chi_m)f(x)] \\
=\ &u(x,t) - f(x) - i \int_0^t \widehat{D^2}(u(x,t))\ dt - i \int_0^t \widehat{F}(u(x,t))\ dt.
\end{aligned}
\quad (30)
$$

From (29) and (30), we have

$$u(x,t) = f(x) + i \int_0^t \widehat{D^2}(u(x,t))\ dt + i \int_0^t \widehat{F}(u(x,t))\ dt,$$

therefore, $u(x,t)$ must be the exact solution of the equation. $\square$

3. Numerical example

In this section, we compute a numerical example which is solved by the VIM, MVIM and HAM. The programs have been provided with Mathematica 6 according to the following algorithm where ε is a given positive value.

Algorithm 1: (VIM and MVIM)

Step 1. Set $n \leftarrow 0$,

Step 2. Calculate the recursive relations (10) (for VIM) and (11) (for MVIM).

Step 3. If $\mid u_{n+1} - u_n \mid < \varepsilon$ then go to step 4, else $n \leftarrow n + 1$ and go to step 2,

Step 4. Print $u_n(x, t)$ as the approximate of the exact solution.

Algorithm 2: (HAM)

Step 1. Set $n \leftarrow 0$,

Step 2. Calculate the recursive relation (24)

Step 3. If $\mid u_{n+1} - u_n \mid < \varepsilon$ then go to step 4, else $n \leftarrow n + 1$ and go to step 2,

Step 4. Print $u(x, t) = \sum_{i=0}^{n} u_i(x, t)$ as the approximate of the exact solution.

Example 3.1. Consider the Schrödinger equation as follows:

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + \mid u \mid^2 u = 0,$$

subject to the initial condition $u(x, 0) = \cos(x)$, with the exact solution is $u(x, t) = \cos(x + \frac{t}{4})$.

$$\alpha_1 := 0.1533, \ \beta_1 := 0.65401(t > 1), \ \beta_1 := 0.69599(0 \leq t < 1), \ \gamma_1 := 0.04599.$$

Figure 1 shows the errors obtained from the mentioned algorithms by comparing the results of the HAM, VIM and MVIM.

In this example, the approximate solution of the Schrödinger equation is convergent with two iterations by using the HAM. By comparing the results of Figure 1, we observe that the HAM is more rapid convergence than the VIM and MVIM.

Example 3.2. Consider the Schrödinger equation as follows:

$$i\frac{\partial u}{\partial t} = -\frac{1}{2}\frac{\partial^2 u}{\partial x^2} - \mid u \mid^3 u, \quad t \geq 0.$$

Subject to the initial condition: $u(x, 0) = e^{ix}$.

With the exact solution is $u(x, t) = e^{i(x + \frac{1}{2}t)}$. $\alpha_1 = 0.3678, \ \beta_1 = 0.5463(t > 1), \beta_1 = 0.5688(0 < t < 1), \gamma_1 = 0.22068, \epsilon = 10^{-2}$.

Table 1. Numerical results for Example 2

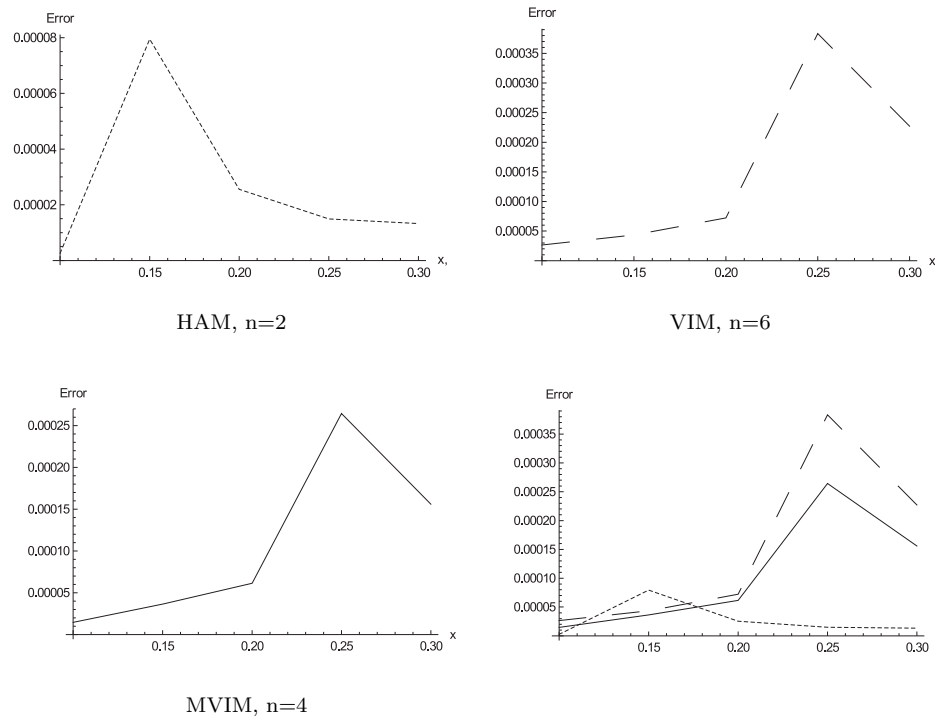| (x,t)	Errors		
	VIM(n=10)	MVIM(n=8)	HAM(n=4)
(0.3,0.2)	0.0725267	0.0654478	0.0348465
(0.4,0.25)	0.0741196	0.0654478	0.0437432
(0.5,0.3)	0.0745569	0.0676829	0.0424038
(0.6,0.35)	0.0762653	0.0701516	0.0556712

Fig. 1. The Comparison between the errors of the methods in the example for $t = 0.35$.

4.   Conclusion

The HAM has been shown to solve effectively, easily and accurately a large class of nonlinear problems with the approximations which convergent are rapidly to exact solutions. In this work, the HAM has been successfully employed to obtain the approximate solution of the Schrodinger equation. In this case, the numerical results are more accurate and the number of iterations is less than the VIM and MVIM.

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