Available online at www.sciencedirect.com
SCIENCE DIRECT
An International Journal
computers & mathematics with applications
ELSEVIER Computers and Mathematics with Applications 50 (2005) 1345–1362
www.elsevier.com/locate/camwa

A Finite-Difference Method for the One-Dimensional Time-Dependent Schrödinger Equation on Unbounded Domain

HOUDE HAN*
Department of Mathematical Science, Tsinghua University
Beijing 100084, P.R. China
hhan@math.tsinghua.edu.cn

JICHENG JIN†
Department of Mathematics, Xiangtan University
Hunan Province, P.R. China
and
Department of Mathematics, Hong Kong Baptist University
Kowloon Tong, Hong Kong
jjc@xtu.edu.cn

XIAONAN WU‡
Department of Mathematics, Hong Kong Baptist University
Kowloon Tong, Hong Kong
xwu@math.hkbu.edu.hk

(Received and accepted May 2005)

Abstract—A finite-difference scheme is proposed for the one-dimensional time-dependent Schrödinger equation. We introduce an artificial boundary condition to reduce the original problem into an initial-boundary value problem in a finite-computational domain, and then construct a finite-difference scheme by the method of reduction of order to solve this reduced problem. This scheme has been proved to be uniquely solvable, unconditionally stable, and convergent. Some numerical examples are given to show the effectiveness of the scheme.

Keywords—The Schrödinger equation, Finite-difference method, Artificial boundary conditions.

1. INTRODUCTION

The Schrödinger equation has been widely used in various application areas, e.g., quantum mechanics, optics, seismology, and plasma physics. Here, we consider the following initial value problem of the Schrödinger equation on $R^1 \times [0, T]$,

*The research is partly supported by the Special Funds for Major State Basic Research Projects of China.
† Author to whom all correspondence should be addressed.
‡The research is supported by RGC of Hong Kong and FRG of Hong Kong Baptist University.
The authors wish to thank the referees for many valuable suggestions.

0898-1221/05/$ - see front matter Typeset by $\mathcal{AMS}$-TEX
doi:10.1016/j.camwa.2005.05.006

$$i\psi_t(x,t) = -\frac{1}{2}\psi_{xx}(x,t) + V(x,t)\psi(x,t), \qquad \forall (x,t) \in R^1 \times (0,T], \tag{1.1}$$

$$\psi(x,0) = \psi^0(x), \qquad \forall x \in R^1, \tag{1.2}$$

where $V(x,t)$ is the potential (real valued) function given on $R^1 \times (0,T]$, $\psi^0(x)$ is the complex initial data given on R^1, and the unknown function $\psi(x,t)$ is a complex valued function on $R^1 \times [0,T]$.

In order to solve such whole-space problems by numerical methods, one has to consider a finite subdomain and impose an artificial boundary condition. When the solution of this new problem is equal to the restriction to the subdomain of the original solution, we say that the artificial boundary condition is transparent.

Suppose that $V(x,t)$ is constant outside bounded domain $(0,1) \times (0,T]$ with

$$V(x,t) = \begin{cases} V_+, & 1 \le x < +\infty, \quad 0 < t \le T, \\ V_-, & -\infty < x \le 0, \quad 0 < t \le T, \end{cases} \tag{1.3}$$

and $\psi^0(x)$ is compact with

$$\operatorname{Supp}\{\psi^0\} \subset [0,1]. \tag{1.4}$$

Then, we can introduce two artificial boundaries $\Gamma_0 = \{x = 0, 0 < t \le T\}$ and $\Gamma_1 = \{x = 1, 0 < t \le T\}$, which divide $R^1 \times (0,T]$ into three parts,

$$\Omega_- = \{(x,t) \mid -\infty < x \le 0,\ 0 < t \le T\},$$
$$\Omega_+ = \{(x,t) \mid 1 \le x < +\infty,\ 0 < t \le T\},$$
$$\Omega_e = \{(x,t) \mid 0 < x < 1,\ 0 < t \le T\}.$$

The finite subdomain Ω_e is our computational domain.

Transparent boundary conditions for this problem were independently derived by several authors from various application fields [1–3]. They are nonlocal in t and read,

$$\psi_x(0,t) = \sqrt{\frac{2}{\pi}} e^{-i(\pi/4)} e^{-iV_- t} \frac{d}{dt} \int_0^t \frac{\psi(0,\lambda) e^{iV_-\lambda}}{\sqrt{t-\lambda}} \, d\lambda, \qquad \text{on } \Gamma_0, \tag{1.5}$$

$$\psi_x(1,t) = -\sqrt{\frac{2}{\pi}} e^{-i(\pi/4)} e^{-iV_+ t} \frac{d}{dt} \int_0^t \frac{\psi(1,\lambda) e^{iV_+\lambda}}{\sqrt{t-\lambda}} \, d\lambda, \qquad \text{on } \Gamma_1. \tag{1.6}$$

A simple calculation shows that (1.5),(1.6) are equivalent to the impedance boundary conditions [3],

$$\psi(0,t) = \frac{1}{\sqrt{2\pi}} e^{i(\pi/4)} \int_0^t \frac{\psi_x(0,\lambda) e^{-iV_-\lambda}}{\sqrt{t-\lambda}} \, d\lambda, \qquad \text{on } \Gamma_0, \tag{1.7}$$

$$\psi(1,t) = -\frac{1}{\sqrt{2\pi}} e^{i(\pi/4)} \int_0^t \frac{\psi_x(1,t-\lambda) e^{-iV_+\lambda}}{\sqrt{\lambda}} \, d\lambda, \qquad \text{on } \Gamma_1. \tag{1.8}$$

Therefore, the initial-boundary value problem to approximate is now given by

$$i\psi_t(x,t) = -\frac{1}{2}\psi_{xx}(x,t) + V(x,t)\psi(x,t), \qquad \forall (x,t) \in \Omega_e, \tag{1.9}$$

$$\psi_x(0,t) = \sqrt{\frac{2}{\pi}} e^{-i(\pi/4)} e^{-iV_- t} \frac{d}{dt} \int_0^t \frac{\psi(0,\lambda) e^{iV_-\lambda}}{\sqrt{t-\lambda}} \, d\lambda, \qquad 0 < t \le T, \tag{1.10}$$

$$\psi_x(1,t) = -\sqrt{\frac{2}{\pi}} e^{-i(\pi/4)} e^{-iV_+ t} \frac{d}{dt} \int_0^t \frac{\psi(1,\lambda) e^{iV_+\lambda}}{\sqrt{t-\lambda}} \, d\lambda, \qquad 0 < t \le T, \tag{1.11}$$

$$\psi(x,0) = \psi^0(x), \qquad 0 \le x \le 1. \tag{1.12}$$

This initial-boundary value problem is well-posed and its solution coincides with the solution of the original problem (1.1),(1.2) restricted to $\bar{\Omega}_e$ [4].

The main difficulty of the numerical approximation is linked to the boundary conditions (1.10),(1.11) with the mildly singular convolution kernels, their numerical discretization is far from trivial. In fact, the discretization scheme for the analytic transparent boundary conditions often destroys the unconditional stability of the underlying Crank-Nicolson scheme used for the Schrödinger equation and makes the overall numerical scheme only conditional stable [1,5]. Moreover, the numerical reflections at the artificial boundaries may appear.

So far, several approaches have been proposed. Instead of using a discretization of the analytic transparent boundary conditions like (1.10),(1.11), Arnold and Ehrhard [6–9], first discretized the Schrödinger equation on the whole space by using a Crank-Nicolson scheme and then derived an exact discrete transparent boundary condition directly from the fully discretized Schrödinger equation. The resulting scheme is unconditionally stable and no numerical reflection appears at the boundaries. However, it seems quite difficult to extend this approach to the finite-element method, which has advantages for the problems on two-dimensional domains with curved boundaries. Similarly, Schmidt *et al.* [10–12], first discretized the Schrödinger equation in t direction and then derived the associated nonlocal transparent boundary condition from the semidiscretized Schrödinger equation. This approach has been proved to be efficient and the fully discrete scheme is unconditionally stable when finite-element methods are employed for the spatial discretization. However, this approach can induce small numerical reflections at the boundaries. Mayfield [5] and Baskakov and Popov [1] proposed the most straightforward approaches. They used the Crank-Nicolson scheme for the Schrödinger equation (1.9) and the left-point rectangular quadrature rule or a higher-order quadrature rule to discretize the equivalent boundary conditions (1.7),(1.8) or the conditions (1.10),(1.11). Unfortunately, the resulting schemes have been proved to be conditionally stable and the strong numerical reflections can be induced. Recently, Antoine *et al.* [4] and Friese *et al.* [13] also proposed some unconditionally stable discretization schemes for the transparent boundary condition. In this paper, we also propose a straightforward approach. First, we apply the so-called method of reduction of order to construct a finite-difference scheme for the Schrödinger equation (1.9) and then directly discretize the analytic transparent boundary conditions (1.10),(1.11). Our discretized boundary conditions are exact in spatial direction, the overall scheme has been proved to be unconditionally stable and convergent, and our numerical examples show that almost no numerical reflections are observed at the boundaries. Moreover, this discretization method for the transparent boundary condition can be easily extended to finite-element approximation [14].

The organization of this paper is the following. In Section 2, we derive our fully discrete finite-difference schemes, the stability and convergence are analyzed in Section 3. Section 4 is devoted to presentation of numerical examples to show the effectiveness of our approach.

2. THE CONSTRUCTION OF THE DIFFERENCE SCHEME

Let $\Omega = (0,1)$. For a nonnegative integer k and real number p, $1 \le p \le \infty$, we use $W^{k,p}(\Omega)$ to denote the Sobolev space and $L^p(0,T;\mathbf{X})$ to denote the space of all L^p integrable functions $w(\cdot,t)$ from $[0,T]$ into the Banach space $\mathbf{X}$, and define [15]

$$W^{k,p}(0,T;\mathbf{X}) = \left\{ w \in L^p(0,T;\mathbf{X});\ \frac{\partial^s w}{\partial t^s} \in L^p(0,T;\mathbf{X}),\ \forall\, 0 \le s \le k \right\},$$

with norm,

$$\|w\|_{W^{k,p}(0,T;\mathbf{X})} = \left(\sum_{s=0}^{k} \int_0^T \left\| \frac{\partial^s w}{\partial t^s} \right\|_{\mathbf{X}}^p \right)^{1/p}, \qquad 1 \le p < \infty,$$

$$\|w\|_{W^{k,\infty}(0,T;\mathbf{X})} = \max_{0 \le s \le k} \left\{ \left\| \left\| \frac{\partial^s w}{\partial t^s} \right\|_{\mathbf{X}} \right\|_{L^\infty(0,T)} \right\}.$$

To simplify the notations, we denote $W^{0,p}$ and $W^{k,2}$ by L^p and H^k, respectively.

Let J and N be two positive integers, and let $h = 1/J$ and $\tau = T/N$. We introduce the notations,

$$\Omega_h = \{x_j = jh,\ j = 0,1,\dots,J\}, \qquad \Omega_\tau = \{t_n = n\tau,\ n = 0,1,\dots,N\},$$
$$e_j = [x_{j-1}, x_j], \qquad e_n^* = [t_{n-1}, t_n], \qquad x_{j-1/2} = \frac{1}{2}(x_j + x_{j-1}), \qquad t_{n-1/2} = \frac{1}{2}(t_n + t_{n-1}),$$
$$V_{j-1/2}^{n-1/2} = V\left(x_{j-1/2}, t_{n-1/2}\right), \qquad \Psi_j^n = \psi(x_j, t_n), \qquad U_j^n = u(x_j, t_n),$$

and for a given complex mesh function $\omega = \{\omega_j^n,\ 0 \le j \le J,\ 0 \le n \le N\}$ on $\Omega_h \times \Omega_\tau$, we define

$$\omega_{j-1/2}^n = \frac{1}{2}\left(\omega_j^n + \omega_{j-1}^n\right), \qquad \omega_j^{n-1/2} = \frac{1}{2}\left(\omega_j^n + \omega_j^{n-1}\right),$$
$$\delta_x \omega_{j-1/2}^n = \frac{1}{h}\left(\omega_j^n - \omega_{j-1}^n\right), \qquad \delta_t \omega_j^{n-1/2} = \frac{1}{\tau}\left(\omega_j^n - \omega_j^{n-1}\right),$$
$$\delta_x^2 \omega_j^n = \frac{1}{h^2}\left(\omega_{j+1}^n - 2\omega_j^n + \omega_{j-1}^n\right), \qquad \|\omega^n\|_A = \sqrt{h \sum_{j=1}^{J} \omega_{j-1/2}^n \bar{\omega}_{j-1/2}^n},$$

where $\bar{w}$ denotes the complex conjugate of w.

Let $u(x,t) = \psi_x(x,t)$, then problem (1.9)–(1.12) can be rewritten as the following,

$$i\psi_t(x,t) = -\frac{1}{2}u_x(x,t) + V(x,t)\psi(x,t), \qquad \forall\,(x,t) \in \Omega_e, \tag{2.1}$$
$$u(x,t) = \psi_x(x,t), \qquad \forall\,(x,t) \in \Omega_e, \tag{2.2}$$
$$u(0,t) = \sqrt{\frac{2}{\pi}} e^{-i(\pi/4)} e^{-iV_- t} \frac{d}{dt} \int_0^t \frac{\psi(0,\lambda) e^{iV_-\lambda}}{\sqrt{t-\lambda}} d\lambda, \qquad 0 < t \le T, \tag{2.3}$$
$$u(1,t) = -\sqrt{\frac{2}{\pi}} e^{-i(\pi/4)} e^{-iV_+ t} \frac{d}{dt} \int_0^t \frac{\psi(1,\lambda) e^{iV_+\lambda}}{\sqrt{t-\lambda}} d\lambda, \qquad 0 < t \le T, \tag{2.4}$$
$$\psi(x,0) = \psi^0(x), \qquad u(x,0) = \psi_x^0(x), \qquad 0 \le x \le 1. \tag{2.5}$$

Next, we construct the difference scheme for (2.1)–(2.5).

LEMMA 1. *Suppose $u(t) \in W^{2,\infty}[0,t_n]$. Then,*

$$\left| \int_0^{t_n} u'(t) \frac{dt}{\sqrt{t_n - t}} - \sum_{k=1}^{n} \frac{u(t_k) - u(t_{k-1})}{\tau} \int_{t_{k-1}}^{t_k} \frac{dt}{\sqrt{t_n - t}} \right| \le c\tau^{\frac{3}{2}} \|u\|_{W^{2,\infty}[0,t_n]},$$

where c is a constant independent of h and τ.

PROOF. Similar to the proof of Lemma 1 in [16]. ∎

Suppose that $\psi(x,t)$ is the solution of problem (1.9)–(1.12) and

$$\psi(x,t) \in H^3\left(0,T; H^2(\Omega)\right) \cap W^{2,\infty}\left(0,T; W^{1,1}(\Omega)\right) \cap H^2\left(0,T; H^3(\Omega)\right) \cap H^1\left(0,T; H^4(\Omega)\right).$$

Then, for nearly all $t \in [0,T]$,

$$\frac{\partial^s \psi(x,t)}{\partial t^s} \in W^{1,1}(\Omega), \qquad s = 0,1,2,$$

and by the Sobolev embedding theorem $W^{1,1}(\Omega) \hookrightarrow C(\bar{\Omega})$, we have

$$\left\| \frac{\partial^s \psi(x,t)}{\partial t^s} \right\|_{C(\bar{\Omega})} \le c \left\| \frac{\partial^s \psi(x,t)}{\partial t^s} \right\|_{W^{1,1}(\Omega)}, \qquad s = 0,1,2.$$

Notice that $\psi(0,0)=\psi(1,0)=0$, then

$$\frac{d}{dt}\int_0^t \frac{\psi(0,\lambda)e^{iV_-\lambda}}{\sqrt{t-\lambda}}\,d\lambda=2\frac{d}{dt}\int_0^t \sqrt{t-\lambda}\frac{d}{d\lambda}\left\{\psi(0,\lambda)e^{iV_-\lambda}\right\}d\lambda=\int_0^t \frac{d}{d\lambda}\left\{e^{iV_-\lambda}\psi(0,\lambda)\right\}\frac{d\lambda}{\sqrt{t-\lambda}}.$$

From the boundary condition (2.3) and Lemma 1, we have

$$\begin{aligned}
U_0^n &= \sqrt{\frac{2}{\pi}}e^{-i(\pi/4)}\sum_{k=1}^{n}\int_{t_{k-1}}^{t_k}\frac{d}{d\lambda}\left\{e^{-iV_-(t_n-\lambda)}\psi(0,\lambda)\right\}\frac{d\lambda}{\sqrt{t_n-\lambda}}\\
&= \sqrt{\frac{2}{\pi}}e^{-i(\pi/4)}\sum_{k=1}^{n}\frac{1}{\tau}\left\{e^{-iV_-(t_n-t_k)}\Psi_0^k-e^{-iV_-(t_n-t_{k-1})}\Psi_0^{k-1}\right\}\int_{t_{k-1}}^{t_k}\frac{d\lambda}{\sqrt{t_n-\lambda}}+O\left(\tau^{3/2}\right)\\
&= e^{-i(\pi/4)}\sum_{k=1}^{n}a_{n-k}\left\{e^{-iV_-(t_n-t_k)}\Psi_0^k-e^{-iV_-(t_n-t_{k-1})}\Psi_0^{k-1}\right\}+O\left(\tau^{3/2}\right)\\
&= e^{-i(\pi/4)}\left\{a_0\Psi_0^n+\sum_{k=1}^{n-1}\left(a_{n-k}-a_{n-k-1}\right)e^{-iV_-(t_n-t_k)}\Psi_0^k\right\}+O\left(\tau^{3/2}\right),\qquad 1\le n\le N,
\end{aligned}$$

where

$$a_k=2\sqrt{\frac{2}{\pi\tau}}\left(\sqrt{k+1}-\sqrt{k}\right),\qquad k=0,1,2,\ldots. \tag{2.6}$$

Then,

$$\begin{aligned}
U_0^{n-1} &= e^{-i(\pi/4)}\left\{a_0\Psi_0^{n-1}+\sum_{k=1}^{n-2}\left(a_{n-1-k}-a_{n-k-2}\right)e^{-iV_-(t_{n-1}-t_k)}\Psi_0^k\right\}+O\left(\tau^{3/2}\right)\\
&= e^{-i(\pi/4)}\left\{a_0\Psi_0^{n-1}+\sum_{k=1}^{n-1}\left(a_{n-k}-a_{n-k-1}\right)e^{-iV_-(t_n-t_k)}\Psi_0^{k-1}\right\}+O\left(\tau^{3/2}\right).
\end{aligned}$$

Therefore, for $1\le n\le N$, we have the discretization for (2.3)

$$U_0^{n-1/2}=e^{-i(\pi/4)}\left\{a_0\Psi_0^{n-1/2}+\sum_{k=1}^{n-1}\left(a_{n-k}-a_{n-k-1}\right)e^{-iV_-(t_n-t_k)}\Psi_0^{k-1/2}\right\}+\gamma_0^{n-1/2}, \tag{2.7}$$

and similarly, for (2.4) we have

$$U_J^{n-1/2}=-e^{-i(\pi/4)}\left\{a_0\Psi_J^{n-1/2}+\sum_{k=1}^{n-1}\left(a_{n-k}-a_{n-k-1}\right)e^{-iV_+(t_n-t_k)}\Psi_J^{k-1/2}\right\}+\gamma_J^{n-1/2}, \tag{2.8}$$

with

$$|\gamma_0^{n-1/2}|\le c\tau^{3/2},\qquad |\gamma_J^{n-1/2}|\le c\tau^{3/2}. \tag{2.9}$$

By the Taylor expansion with integral residue, we have

$$\begin{aligned}
f'\left(t_{n-1/2}\right) &= \delta_t f^{n-1/2}+O(\tau)\|f\|_{W^{3,1}(e_n^*)},\\
f\left(t_{n-1/2}\right) &= f^{n-1/2}+O(\tau)\|f\|_{W^{2,1}(e_n^*)},\\
|f(t_n)| &\le \frac{1}{\tau}\|f\|_{L^1(e_n^*)}+\|f\|_{W^{1,1}(e_n^*)}.
\end{aligned}$$

Therefore, we can obtain the following difference scheme of (2.1),(2.2),

$$i\delta_t\Psi_{j-1/2}^{n-1/2}=-\frac{1}{2}\delta_x U_{j-1/2}^{n-1/2}+V_{j-1/2}^{n-1/2}\Psi_{j-1/2}^{n-1/2}+\varepsilon_{j-1/2}^{n-1/2},\quad 1\le j\le J,\quad 1\le n\le N, \tag{2.10}$$

$$U_{j-1/2}^{n-1/2}=\delta_x\Psi_{j-1/2}^{n-1/2}+\delta_{j-1/2}^{n-1/2},\qquad 1\le j\le J,\quad 1\le n\le N, \tag{2.11}$$

where

$$\varepsilon_{j-1/2}^{n-1/2} = O(\tau)\left[\|\psi\|_{W^{3,1}(e_n^*;W^{1,1}(\Omega))} + \|\psi\|_{W^{2,1}(e_n^*;W^{3,1}(\Omega))}\right] + O\left(\frac{h}{\tau}\right)\left[\|\psi\|_{W^{1,1}(e_n^*;W^{2,1}(e_j))} + \|\psi\|_{L^1(e_n^*;W^{4,1}(e_j))}\right] + O(h)\left[\|\psi\|_{W^{2,1}(e_n^*;W^{2,1}(e_j))} + \|\psi\|_{W^{1,1}(e_n^*;W^{4,1}(e_j))}\right],$$

$$\delta_{j-1/2}^{n-1/2} = O(\tau)\|\psi\|_{W^{2,1}(e_n^*;W^{2,1}(\Omega))} + O\left(\frac{h}{\tau}\right)\|\psi\|_{L^1(e_n^*;W^{3,1}(e_j))} + O(h)\|\psi\|_{W^{1,1}(e_n^*;W^{3,1}(e_j))}.$$

It is easy to check that

$$h\sum_{j=1}^{J}\|\psi\|^2_{W^{k,1}(e_n^*;W^{l,1}(\Omega))} = \|\psi\|^2_{W^{k,1}(e_n^*;W^{l,1}(\Omega))} \le c\tau\|\psi\|^2_{H^k(e_n^*;H^l(\Omega))},$$

$$h\sum_{j=1}^{J}\|\psi\|^2_{W^{k,1}(e_n^*;W^{l,1}(e_j))} \le c\tau h^2\|\psi\|^2_{H^k(e_n^*;H^l(\Omega))}.$$

So, we have

$$\left\|\varepsilon^{n-1/2}\right\|_A^2 \le c\tau^3\left[\|\psi\|^2_{H^3(e_n^*;H^1(\Omega))} + \|\psi\|^2_{H^2(e_n^*;H^3(\Omega))}\right] + c\frac{h^4}{\tau}\left[\|\psi\|^2_{H^1(e_n^*;H^2(\Omega))} + \|\psi\|^2_{L^2(e_n^*;H^4(\Omega))}\right] + c\tau h^4,$$

$$\left\|\delta^{n-1/2}\right\|_A^2 \le c\tau^3\|\psi\|^2_{H^2(e_n^*;H^2(\Omega))} + c\frac{h^4}{\tau}\|\psi\|^2_{L^2(e_n^*;H^3(\Omega))} + c\tau h^4,$$

and then

$$\sum_{k=1}^{n}\left\|\varepsilon^{k-1/2}\right\|_A^2 \le c\tau^3\left[\|\psi\|^2_{H^3(0,T;H^1(\Omega))} + \|\psi\|^2_{H^2(0,T;H^3(\Omega))}\right] + c\frac{h^4}{\tau}\left[\|\psi\|^2_{H^1(0,T;H^2(\Omega))} + \|\psi\|^2_{L^2(0,T;H^4(\Omega))}\right] + ch^4, \tag{2.12}$$

$$\sum_{k=1}^{n}\left\|\delta^{k-1/2}\right\|_A^2 \le c\tau^3\|\psi\|^2_{H^2(0,T;H^2(\Omega))} + c\frac{h^4}{\tau}\|\psi\|^2_{L^2(0,T;H^3(\Omega))} + ch^4. \tag{2.13}$$

Therefore, we obtain a finite difference-scheme of problem (2.1)–(2.5) as the following,

$$i\delta_t\psi_{j-1/2}^{n-1/2} + \frac{1}{2}\delta_x u_{j-1/2}^{n-1/2} - V_{j-1/2}^{n-1/2}\psi_{j-1/2}^{n-1/2} = 0, \qquad 1\le j\le J, \quad 1\le n\le N, \tag{2.14}$$

$$u_{j-1/2}^{n-1/2} - \delta_x\psi_{j-1/2}^{n-1/2} = 0, \qquad 1\le j\le J, \quad 1\le n\le N, \tag{2.15}$$

$$u_0^{n-1/2} = e^{-i(\pi/4)}\left\{a_0\psi_0^{n-1/2} + \sum_{k=1}^{n-1}(a_{n-k}-a_{n-k-1})\,e^{-iV_-(t_n-t_k)}\psi_0^{k-1/2}\right\}, \quad 1\le n\le N, \tag{2.16}$$

$$u_J^{n-1/2} = -e^{-i(\pi/4)}\left\{a_0\psi_J^{n-1/2} + \sum_{k=1}^{n-1}(a_{n-k}-a_{n-k-1})\,e^{-iV_+(t_n-t_k)}\psi_J^{k-1/2}\right\}, \quad 1\le n\le N, \tag{2.17}$$

$$\psi_j^0 = \psi^0(x_j), \qquad u_j^0 = \psi_x^0(x_j), \quad 0\le j\le J. \tag{2.18}$$

The finite-difference scheme (2.14)–(2.18) contains two complex mesh functions $\{\psi_j^n,\, u_j^n,\, 0 \le j \le J,\, 0 \le n \le N\}$, by eliminating u_j^n, $0 \le j \le J$, $0 \le n \le N$, we obtain a finite-difference scheme which contains only mesh function ψ_j^n, $0 \le j \le J$, $0 \le n \le N$,

$$\begin{gathered} i\delta_t \left\{ \frac{1}{2}\left(\psi_{j+1/2}^{n-1/2} + \psi_{j-1/2}^{n-1/2} \right) \right\} + \frac{1}{2}\delta_x^2 \psi_j^{n-1/2} \\ -\frac{1}{2}\left\{ V_{j+1/2}^{n-1/2}\psi_{j+1/2}^{n-1/2} + V_{j-1/2}^{n-1/2}\psi_{j-1/2}^{n-1/2} \right\} = 0, \\ 1 \le j \le J-1, \qquad 1 \le n \le N, \end{gathered} \tag{2.19}$$

$$\begin{aligned} &\delta_x \psi_{1/2}^{n-1/2} - h\left\{ -i\delta_t \psi_{1/2}^{n-1/2} + V_{1/2}^{n-1/2}\psi_{1/2}^{n-1/2} \right\} \\ &= e^{-i(\pi/4)} \left\{ a_0 \psi_0^{n-1/2} + \sum_{k=1}^{n-1} \left(a_{n-k} - a_{n-k-1} \right) e^{-iV_-(t_n - t_k)} \psi_0^{k-1/2} \right\}, \qquad 1 \le n \le N, \end{aligned} \tag{2.20}$$

$$\begin{aligned} &\delta_x \psi_{J-1/2}^{n-1/2} + h\left\{ -i\delta_t \psi_{J-1/2}^{n-1/2} + V_{J-1/2}^{n-1/2}\psi_{J-1/2}^{n-1/2} \right\} \\ &= -e^{-i(\pi/4)} \left\{ a_0 \psi_J^{n-1/2} + \sum_{k=1}^{n-1} \left(a_{n-k} - a_{n-k-1} \right) e^{-iV_+(t_n - t_k)} \psi_J^{k-1/2} \right\}, \qquad 1 \le n \le N, \end{aligned} \tag{2.21}$$

$$\psi_j^0 = \psi^0(x_j), \qquad 0 \le j \le J. \tag{2.22}$$

We have the following theorem.

THEOREM 1.

(i) *Suppose that* $\{\psi_j^n,\, u_j^n,\, 0 \le j \le J,\, 0 \le n \le N\}$ *is a solution of problem (2.14)–(2.18), then* $\{\psi_j^n,\, 0 \le j \le J,\, 0 \le n \le N\}$ *is a solution of problem (2.19)–(2.22).*

(ii) *Suppose that* $\{\psi_j^n,\, 0 \le j \le J,\, 0 \le n \le N\}$ *is a solution of problem (2.19)–(2.22), let*

$$u_j^0 = \psi_x^0(x_j), \qquad 0 \le j \le J, \tag{2.23}$$

$$u_0^n = -u_0^{n-1} + 2\left\{ \delta_x \psi_{1/2}^{n-1/2} - h\left(-i\delta_t \psi_{1/2}^{n-1/2} + V_{1/2}^{n-1/2}\psi_{1/2}^{n-1/2} \right) \right\}, \qquad 1 \le n \le N, \tag{2.24}$$

$$u_j^n = -u_{j-1}^n - \left(u_j^{n-1} + u_{j-1}^{n-1} \right) + 4\delta_x \psi_{j-1/2}^{n-1/2}, \qquad 1 \le j \le J, \qquad 1 \le n \le N. \tag{2.25}$$

Then, $\{\psi_j^n,\, u_j^n,\, 0 \le j \le J,\, 0 \le n \le N\}$ *is a solution of problem (2.14)–(2.18).*

In the above sense, we say that problem (2.19)–(2.22) is equivalent to problem (2.14)–(2.18).

PROOF.

(i) Suppose that $\{\psi_j^n,\, u_j^n,\, 0 \le j \le J,\, 0 \le n \le N\}$ is a solution of problem (2.14)–(2.18). From equality (2.14),(2.15), we have

$$\frac{1}{2}u_j^{n-1/2} = \frac{1}{2}u_{j-1}^{n-1/2} + h\left\{ -i\delta_t \psi_{j-1/2}^{n-1/2} + V_{j-1/2}^{n-1/2}\psi_{j-1/2}^{n-1/2} \right\}, \qquad 1 \le j \le J, \quad 1 \le n \le N, \tag{2.26}$$

$$\frac{1}{2}u_j^{n-1/2} = -\frac{1}{2}u_{j-1}^{n-1/2} + \delta_x \psi_{j-1/2}^{n-1/2}, \qquad 1 \le j \le J, \quad 1 \le n \le N. \tag{2.29}$$

Summing up equation (2.26) and (2.27), we arrive at

$$u_j^{n-1/2} = \delta_x \psi_{j-1/2}^{n-1/2} + h\left\{ -i\delta_t \psi_{j-1/2}^{n-1/2} + V_{j-1/2}^{n-1/2}\psi_{j-1/2}^{n-1/2} \right\}, \qquad 1 \le j \le J, \quad 1 \le n \le N. \tag{2.28}$$

Subtracting equation (2.26) from (2.27), we get

$$u_{j-1}^{n-1/2} = \delta_x \psi_{j-1/2}^{n-1/2} - h\left\{-i\delta_t \psi_{j-1/2}^{n-1/2} + V_{j-1/2}^{n-1/2}\psi_{j-1/2}^{n-1/2}\right\}, \quad 1 \le j \le J, \quad 1 \le n \le N, \tag{2.29}$$

namely,

$$u_{j}^{n-1/2} = \delta_x \psi_{j+1/2}^{n-1/2} - h\left\{-i\delta_t \psi_{j+1/2}^{n-1/2} + V_{j+1/2}^{n-1/2}\psi_{j+1/2}^{n-1/2}\right\}, \quad 0 \le j \le J-1, \quad 1 \le n \le N. \tag{2.30}$$

Therefore, we can get (2.19) by combining (2.28) and (2.30), get (2.20) by substituting (2.29) with $j = 1$ into (2.16), and get (2.21) similarly. Namely, $\{\psi_j^n,\ 0 \le j \le J,\ 0 \le n \le N\}$ is a solution of problem (2.19)–(2.22).

(ii) Suppose that $\{\psi_j^n,\ 0 \le j \le J,\ 0 \le n \le N\}$ is a solution of problem (2.19)–(2.22). By formulations (2.23)–(2.25) we obtain a mesh function $\{u_j^n,\ 0 \le j \le J,\ 0 \le n \le N\}$. Obviously, (2.15) follows from (2.25). Substituting (2.25) with $j = 1$ into (2.24), we can get (2.14) with $j = 1$. Once (2.14) with $j = j_0$, $1 \le j_0 \le J-1$, holds, then we can get (2.14) with $j = j_0 + 1$ by subtracting (2.14) with $j = j_0$ from (2.19) with $j = j_0$, so (2.14) holds for any j, $1 \le j \le J$. (2.16) follows from (2.20) and (2.24). (2.17) can be obtained by subtracting (2.14) with $j = J$ from (2.21) and combining the resulting equality and (2.15). ∎

At n^{th} time level, scheme (2.19)–(2.22) is a tridiagonal system of linear algebraic equations in the complex number space with respect to $\{\psi_j^n,\ 0 \le j \le J\}$. Let v_j^n and w_j^n be the real part and imaginary part of ψ_j^n respectively, then we can obtain the corresponding system of the following form in the real number space,

$$\begin{bmatrix} A_1 & A_2 \\ -A_2 & A_1 \end{bmatrix} \begin{bmatrix} v^n \\ w^n \end{bmatrix} = F^n, \tag{2.31}$$

where

$$v^n = \left[v_0^n, v_1^n, \cdots, v_J^n\right]^t, \qquad w^n = \left[w_0^n, w_1^n, \cdots, w_J^n\right]^t,$$

$(J+1) \times (J+1)$ real-valued matrices A_1 and A_2, are symmetric and tridiagonal. This system can be solved by some iteration methods, for example, the GMRES method.

3. ANALYSIS OF THE DIFFERENCE SCHEME

First, we introduce the following lemma [17].

LEMMA 2. *For any $T > 0$, let $u(t) \in H^{1/4}(0,T)$ with the extension $u(t) = 0$, for $t > T$. Then,*

$$\operatorname{Re}\left\{e^{i\pi/4}\int_0^\infty \bar{u}(t)\frac{d}{dt}\left[\int_0^t \frac{u(\lambda)}{\sqrt{t-\lambda}}\,d\lambda\right]dt\right\} \ge 0.$$

Based on this lemma, we obtain the following lemma (see also [18]).

LEMMA 3. *For any complex vector $\mathbf{u} = (u^1, u^2, \cdots, u^N)$, the following inequality holds,*

$$\operatorname{Re}\left\{e^{i\pi/4}\sum_{n=1}^{N}\bar{u}^n\left[a_0 u^n - \sum_{k=1}^{n-1}\left(a_{n-k-1} - a_{n-k}\right)u^k\right]\right\} \ge 0,$$

where a_k is defined in (2.6).

PROOF. We define function $u(t)$ by

$$u(t) = \begin{cases} u^n, & t_{n-1} \le t < t_n, \qquad 1 \le n < N, \\ 0, & t \ge t_N. \end{cases}$$

We can easily check that $u(t) \in H^{1/4}(0,T)$. Then, we have

$$\begin{aligned}\int_0^\infty \bar{u}(t)\frac{d}{dt}\left[\int_0^t \frac{u(\lambda)}{\sqrt{t-\lambda}}\,d\lambda\right]dt &= \sum_{n=1}^{N}\int_{t_{n-1}}^{t_n} \bar{u}(t)\frac{d}{dt}\left[\int_0^t \frac{u(\lambda)}{\sqrt{t-\lambda}}\,d\lambda\right]dt \\ &= \sum_{n=1}^{N}\bar{u}^n\left[\sum_{k=1}^{n}u^k\int_{t_{k-1}}^{t_k}\frac{d\lambda}{\sqrt{t_n-\lambda}} - \sum_{k=1}^{n-1}u^k\int_{t_{k-1}}^{t_k}\frac{d\lambda}{\sqrt{t_{n-1}-\lambda}}\right] \\ &= \tau\sqrt{\frac{\pi}{2}}\sum_{n=1}^{N}\bar{u}^n\left[\sum_{k=1}^{n}a_{n-k}u^k - \sum_{k=1}^{n-1}a_{n-k-1}u^k\right] \\ &= \tau\sqrt{\frac{\pi}{2}}\sum_{n=1}^{N}\bar{u}^n\left[a_0u^n - \sum_{k=1}^{n-1}\left(a_{n-k-1}-a_{n-k}\right)u^k\right].\end{aligned}$$

According to Lemma 2, we have

$$\begin{aligned}&\operatorname{Re}\left\{e^{i\pi/4}\sum_{n=1}^{N}\bar{u}^n\left[a_0u^n - \sum_{k=1}^{n-1}\left(a_{n-k-1}-a_{n-k}\right)u^k\right]\right\} \\ &= \frac{1}{\tau}\sqrt{\frac{2}{\pi}}\operatorname{Re}\left\{e^{i\pi/4}\int_0^\infty \bar{u}(t)\frac{d}{dt}\left[\int_0^t \frac{u(\lambda)}{\sqrt{t-\lambda}}\,d\lambda\right]dt\right\} \geq 0. \qquad \blacksquare\end{aligned}$$

THEOREM 2. *Difference scheme (2.19)–(2.22) is uniquely solvable.*

PROOF. From Theorem 1, it suffices to prove that difference scheme (2.14)–(2.18) is uniquely solvable. Suppose that we have determined $\{\psi_j^k,\ 0 \leq j \leq J,\ 0 \leq k \leq n-1\}$. We consider the homogenous equations, about $\{\psi_j^n,\ u_j^{n-1/2},\ 0 \leq j \leq J\}$, of (2.14)–(2.18),

$$\frac{i}{\tau}\psi_{j-1/2}^n + \frac{1}{2}\delta_x u_{j-1/2}^{n-1/2} - \frac{1}{2}V_{j-1/2}^{n-1/2}\psi_{j-1/2}^n = 0, \qquad 1 \leq j \leq J, \tag{3.1}$$

$$u_{j-1/2}^{n-1/2} - \frac{1}{2}\delta_x\psi_{j-1/2}^n = 0, \qquad 1 \leq j \leq J, \tag{3.2}$$

$$u_0^{n-1/2} = \frac{1}{2}a_0e^{-i(\pi/4)}\psi_0^n, \tag{3.3}$$

$$u_J^{n-1/2} = -\frac{1}{2}a_0e^{-i(\pi/4)}\psi_J^n. \tag{3.4}$$

Multiplying (3.1) by $\bar{\psi}_{j-1/2}^n$, (3.2) by $\bar{u}_{j-1/2}^{n-1/2}$, and adding the results, we get

$$\begin{aligned}\frac{i}{\tau}\left|\psi_{j-1/2}^n\right|^2 + \left|u_{j-1/2}^{n-1/2}\right|^2 = \frac{1}{2}&\left(\bar{u}_{j-1/2}^{n-1/2}\delta_x\psi_{j-1/2}^n - \bar{\psi}_{j-1/2}^n\delta_x u_{j-1/2}^{n-1/2}\right) \\ &+ \frac{1}{2}V_{j-1/2}^{n-1/2}\left|\psi_{j-1/2}^n\right|^2 = T_1 + T_2,\end{aligned}$$

where the imaginary valued term T_1 and the real valued term T_2 are given by

$$\begin{aligned}T_1 &= \frac{1}{4h}\left(\bar{u}_j^{n-1/2}\psi_j^n - u_j^{n-1/2}\bar{\psi}_j^n - \bar{u}_{j-1}^{n-1/2}\psi_{j-1}^n + u_{j-1}^{n-1/2}\bar{\psi}_{j-1}^n\right), \\ T_2 &= \frac{1}{4h}\left(-\bar{u}_j^{n-1/2}\psi_{j-1}^n - u_j^{n-1/2}\bar{\psi}_{j-1}^n + \bar{u}_{j-1}^{n-1/2}\psi_j^n + u_{j-1}^{n-1/2}\bar{\psi}_j^n\right) \\ &\quad + \frac{1}{2}V_{j-1/2}^{n-1/2}\left|\psi_{j-1/2}^n\right|^2.\end{aligned}$$

Therefore, we have

$$\frac{i}{\tau}\left|\psi_{j-1/2}^n\right|^2 = T_1.$$

Multiplying the above equality by h and summing up for j, from (3.3),(3.4), we get

$$\frac{ih}{\tau}\sum_{j=1}^{J}\left|\psi_{j-1/2}^{n}\right|^2 = \frac{1}{4}\left(\bar{u}_J^{n-1/2}\psi_J^n - u_J^{n-1/2}\bar{\psi}_J^n - \bar{u}_0^{n-1/2}\psi_0^n + u_0^{n-1/2}\bar{\psi}_0^n\right)$$
$$= -\frac{i\sqrt{2}a_0}{8}\left(|\psi_J^n|^2 + |\psi_0^n|^2\right),$$

therefore, $\psi_J^n = \psi_0^n = \psi_{j-1/2}^n = 0$, $1 \le j \le J$, which means that $\psi_j^n = 0$, $0 \le j \le J$. From (3.2)–(3.4), we have

$$u_{j-1/2}^{n-1/2} = u_J^{n-1/2} = u_0^{n-1/2} = 0, \qquad 1 \le j \le J,$$

so $u_j^{n-1/2} = 0$, $0 \le j \le J$. ∎

THEOREM 3. *Difference scheme (2.19)–(2.22) is unconditionally stable, and*

$$\|\psi^n\|_A \le \|\psi^0\|_A. \tag{3.5}$$

PROOF. From Theorem 1, it suffices to prove that (3.5) holds for difference scheme (2.14)–(2.18). Multiplying (2.14) by $2\bar{\psi}_{j-1/2}^{n-1/2}$, we get

$$\begin{aligned}\frac{i}{\tau}\left(\left|\psi_{j-1/2}^{n}\right|^2 - \left|\psi_{j-1/2}^{n-1}\right|^2\right) + \frac{i}{\tau}\left(\psi_{j-1/2}^{n}\bar{\psi}_{j-1/2}^{n-1} - \bar{\psi}_{j-1/2}^{n}\psi_{j-1/2}^{n-1}\right)\\ +\frac{1}{2h}\left(u_j^{n-1/2}\bar{\psi}_j^{n-1/2} - u_{j-1}^{n-1/2}\bar{\psi}_{j-1}^{n-1/2}\right)\\ +\frac{1}{2h}\left(u_j^{n-1/2}\bar{\psi}_{j-1}^{n-1/2} - u_{j-1}^{n-1/2}\bar{\psi}_j^{n-1/2}\right) - 2V_{j-1/2}^{n-1/2}\left|\psi_{j-1/2}^{n-1/2}\right|^2 = 0.\end{aligned} \tag{3.6}$$

Multiplying (2.15) by $\bar{u}_{j-1/2}^{n-1/2}$, we get

$$\begin{aligned}\left|u_{j-1/2}^{n-1/2}\right|^2 = \frac{1}{2h}\left(\bar{u}_j^{n-1/2}\psi_j^{n-1/2} - \bar{u}_{j-1}^{n-1/2}\psi_{j-1}^{n-1/2}\right)\\ +\frac{1}{2h}\left(\bar{u}_{j-1}^{n-1/2}\psi_j^{n-1/2} - \bar{u}_j^{n-1/2}\psi_{j-1}^{n-1/2}\right).\end{aligned} \tag{3.7}$$

Summing up (3.6),(3.7), comparing the imaginary parts of the results, we get

$$\frac{1}{\tau}\left(\left|\psi_{j-1/2}^{n}\right|^2 - \left|\psi_{j-1/2}^{n-1}\right|^2\right) = \frac{1}{h}\operatorname{Im}\left\{u_{j-1}^{n-1/2}\bar{\psi}_{j-1}^{n-1/2} - u_j^{n-1/2}\bar{\psi}_j^{n-1/2}\right\}. \tag{3.8}$$

Multiplying the above equality by h and summing up for j, we have

$$\frac{1}{\tau}\left(\|\psi^n\|_A^2 - \|\psi^{n-1}\|_A^2\right) = \operatorname{Im}\left\{u_0^{n-1/2}\bar{\psi}_0^{n-1/2} - u_J^{n-1/2}\bar{\psi}_J^{n-1/2}\right\}. \tag{3.9}$$

Summing up the above equality for n, we get

$$\frac{1}{\tau}\left(\|\psi^n\|_A^2 - \|\psi^0\|_A^2\right) = \sum_{l=1}^{n}\operatorname{Im}\left\{u_0^{l-1/2}\bar{\psi}_0^{l-1/2} - u_J^{l-1/2}\bar{\psi}_J^{l-1/2}\right\}. \tag{3.10}$$

From (2.16),(2.17),

$$\begin{aligned}&u_0^{l-1/2}\bar{\psi}_0^{l-1/2}\\ &= -ie^{i(\pi/4)}\left\{a_0\left|\psi_0^{l-1/2}\right|^2 + \sum_{k=1}^{l-1}\left(a_{l-k} - a_{l-k-1}\right)e^{-iV_-(t_l-t_k)}\psi_0^{k-1/2}\bar{\psi}_0^{l-1/2}\right\},\end{aligned} \tag{3.11}$$

$$u_J^{l-1/2}\bar{\psi}_J^{l-1/2}$$
$$= ie^{i(\pi/4)}\left\{a_0\left|\psi_J^{l-1/2}\right|^2+\sum_{k=1}^{l-1}(a_{l-k}-a_{l-k-1})\,e^{-iV_+(t_l-t_k)}\psi_J^{k-1/2}\bar{\psi}_J^{l-1/2}\right\}. \tag{3.12}$$

Then, according to Lemma 3,

$$\begin{aligned}
&\sum_{l=1}^{n}\mathrm{Im}\left\{u_0^{l-1/2}\bar{\psi}_0^{l-1/2}-u_J^{l-1/2}\bar{\psi}_J^{l-1/2}\right\}\\
&\quad=-\mathrm{Re}\left\{e^{i(\pi/4)}\sum_{l=1}^{n}\overline{\psi_0^{l-1/2}e^{iV_-t_l}}\left[a_0\psi_0^{l-1/2}e^{iV_-t_l}\right.\right.\\
&\qquad\left.\left.-\sum_{k=1}^{l-1}(a_{l-k-1}-a_{l-k})\,\psi_0^{k-1/2}e^{iV_-t_k}\right]\right\}\\
&\qquad-\mathrm{Re}\left\{e^{i(\pi/4)}\sum_{l=1}^{n}\overline{\psi_J^{l-1/2}e^{iV_+t_l}}\left[a_0\psi_J^{l-1/2}e^{iV_+t_l}\right.\right.\\
&\qquad\left.\left.-\sum_{k=1}^{l-1}(a_{l-k-1}-a_{l-k})\,\psi_J^{k-1/2}e^{iV_+t_k}\right]\right\}\\
&\quad\le 0.
\end{aligned} \tag{3.13}$$

Therefore, (3.5) follows from (3.10) and the above inequality. ∎

Next, we give the convergence result.

THEOREM 4. *Assume that $\psi(x,t)$ is the solution of problem (1.9)–(1.12), and*

$$\psi(x,t)\in H^3\left(0,T;H^2(\Omega)\right)\cap W^{2,\infty}\left(0,T;W^{1,1}(\Omega)\right)\cap H^2\left(0,T;H^3(\Omega)\right)\cap H^1\left(0,T;H^4(\Omega)\right).$$

Let $\{\psi_j^n\}$ be the solution of problem (2.19)–(2.22), and let $\varphi_j^n=\psi(x_j,t_n)-\psi_j^n$. Then, we have

$$\|\varphi^n\|_A\le ch_\tau^{-1/2}\left(h^2+\tau^{3/2}\right), \tag{3.14}$$

where $h_\tau=\min\{h,\tau\}$.

PROOF. Denote $\omega_j^n=u(x_j,t_n)-u_j^n$. Subtracting (2.14)–(2.17) from (2.10),(2.11) and (2.7),(2.8), respectively, we obtain the following error equations,

$$i\delta_t\varphi_{j-1/2}^{n-1/2}=-\frac{1}{2}\delta_x\omega_{j-1/2}^{n-1/2}+V_{j-1/2}^{n-1/2}\varphi_{j-1/2}^{n-1/2}+\varepsilon_{j-1/2}^{n-1/2},\qquad 1\le j\le J,\quad 1\le n\le N, \tag{3.15}$$

$$\omega_{j-1/2}^{n-1/2}=\delta_x\varphi_{j-1/2}^{n-1/2}+\delta_{j-1/2}^{n-1/2},\qquad 1\le j\le J,\quad 1\le n\le N, \tag{3.16}$$

$$\omega_0^{n-1/2}=e^{-i(\pi/4)}\left\{a_0\varphi_0^{n-1/2}+\sum_{k=1}^{n-1}(a_{n-k}-a_{n-k-1})\,e^{-iV_-(t_n-t_k)}\varphi_0^{k-1/2}\right\}+\gamma_0^{n-1/2},\quad 1\le n\le N, \tag{3.17}$$

$$\omega_J^{n-1/2}=-e^{-i(\pi/4)}\left\{a_0\varphi_J^{n-1/2}+\sum_{k=1}^{n-1}(a_{n-k}-a_{n-k-1})\,e^{-iV_+(t_n-t_k)}\varphi_J^{k-1/2}\right\}+\gamma_J^{n-1/2},\qquad 1\le n\le N, \tag{3.18}$$

$$\varphi_j^0=0,\qquad \omega_j^0=0,\quad 0\le j\le J. \tag{3.19}$$

From (3.16), we have

$$\begin{aligned}\delta_x\omega_{j-1/2}^{n-1/2}\bar{\varphi}_{j-1/2}^{n-1/2}+\left|\delta_x\varphi_{j-1/2}^{n-1/2}\right|^2&=\delta_x\omega_{j-1/2}^{n-1/2}\bar{\varphi}_{j-1/2}^{n-1/2}\\&\quad+\left(\omega_{j-1/2}^{n-1/2}-\delta_{j-1/2}^{n-1/2}\right)\delta_x\bar{\varphi}_{j-1/2}^{n-1/2}\\&=\frac{1}{h}\left(\omega_j^{n-1/2}\bar{\varphi}_j^{n-1/2}-\omega_{j-1}^{n-1/2}\bar{\varphi}_{j-1}^{n-1/2}\right)\\&\quad-\delta_{j-1/2}^{n-1/2}\delta_x\bar{\varphi}_{j-1/2}^{n-1/2}.\end{aligned}\tag{3.20}$$

Multiplying (3.15) by $2\bar{\varphi}_{j-1/2}^{n-1/2}$, from (3.20), we get

$$\begin{aligned}&\frac{i}{\tau}\left(\left|\varphi_{j-1/2}^{n}\right|^2-\left|\varphi_{j-1/2}^{n-1}\right|^2\right)+\frac{i}{\tau}\left(\varphi_{j-1/2}^{n}\bar{\varphi}_{j-1/2}^{n-1}-\bar{\varphi}_{j-1/2}^{n}\varphi_{j-1/2}^{n-1}\right)\\&=\left|\delta_x\varphi_{j-1/2}^{n-1/2}\right|^2+\frac{1}{h}(\omega_{j-1}^{n-1/2}\bar{\varphi}_{j-1}^{n-1/2}-\omega_j^{n-1/2}\bar{\varphi}_j^{n-1/2})+2V_{j-1/2}^{n-1/2}\left|\varphi_{j-1/2}^{n-1/2}\right|^2\\&\quad+2\varepsilon_{j-1/2}^{n-1/2}\bar{\varphi}_{j-1/2}^{n-1/2}+\delta_{j-1/2}^{n-1/2}\delta_x\bar{\varphi}_{j-1/2}^{n-1/2},\qquad 1\le j\le J,\quad 1\le n\le N.\end{aligned}$$

Multiplying the above equality by h and summing up for j, comparing the real part and imaginary part of the result, respectively, we obtain

$$\begin{aligned}\left\|\delta_x\varphi^{n-1/2}\right\|_A^2&=\mathrm{Re}\left\{\omega_J^{n-1/2}\bar{\varphi}_J^{n-1/2}-\omega_0^{n-1/2}\bar{\varphi}_0^{n-1/2}\right\}\\&\quad-2\sum_{j=1}^{J}hV_{j-1/2}^{n-1/2}\left|\varphi_{j-1/2}^{n-1/2}\right|^2\\&\quad-\frac{2}{\tau}\mathrm{Im}\left\{\sum_{j=1}^{J}h\varphi_{j-1/2}^{n}\bar{\varphi}_{j-1/2}^{n-1}\right\}\\&\quad-\mathrm{Re}\left\{\sum_{j=1}^{J}h\left(2\varepsilon_{j-1/2}^{n-1/2}\bar{\varphi}_{j-1/2}^{n-1/2}+\delta_{j-1/2}^{n-1/2}\delta_x\bar{\varphi}_{j-1/2}^{n-1/2}\right)\right\},\end{aligned}\tag{3.21}$$

$$\begin{aligned}\frac{1}{\tau}\left(|\varphi^n|_A^2-|\varphi^{n-1}|_A^2\right)&=-\mathrm{Im}\left\{\omega_J^{n-1/2}\bar{\varphi}_J^{n-1/2}-\omega_0^{n-1/2}\bar{\varphi}_0^{n-1/2}\right\}\\&\quad+\mathrm{Im}\left\{\sum_{j=1}^{J}h\left(2\varepsilon_{j-1/2}^{n-1/2}\bar{\varphi}_{j-1/2}^{n-1/2}+\delta_{j-1/2}^{n-1/2}\delta_x\bar{\varphi}_{j-1/2}^{n-1/2}\right)\right\}.\end{aligned}\tag{3.22}$$

Using ε-inequality with $\varepsilon=1$, we have

$$\begin{aligned}\pm\mathrm{Re}\left\{2\varepsilon_{j-1/2}^{n-1/2}\bar{\varphi}_{j-1/2}^{n-1/2}+\delta_{j-1/2}^{n-1/2}\delta_x\bar{\varphi}_{j-1/2}^{n-1/2}\right\}&\le\left|\varepsilon_{j-1/2}^{n-1/2}\right|^2+\left|\varphi_{j-1/2}^{n-1/2}\right|^2\\&\quad+\frac{1}{2}\left|\delta_{j-1/2}^{n-1/2}\right|^2+\frac{1}{2}\left|\delta_x\varphi_{j-1/2}^{n-1/2}\right|^2.\end{aligned}$$

Let $V_m=\|V(x,t)\|_{\infty,\Omega}$ and notice that $Jh=1$, then from (3.21) we have

$$\begin{aligned}\frac{1}{2}\left\|\delta_x\varphi^{n-1/2}\right\|_A^2&\le\mathrm{Re}\left\{\omega_J^{n-1/2}\bar{\varphi}_J^{n-1/2}-\omega_0^{n-1/2}\bar{\varphi}_0^{n-1/2}\right\}\\&\quad+(2V_m+1)\left\|\varphi^{n-1/2}\right\|_A^2\\&\quad+\frac{1}{\tau}\left(\|\varphi^n\|_A^2+\|\varphi^{n-1}\|_A^2\right)+\left\|\varepsilon^{n-1/2}\right\|_A^2+\frac{1}{2}\left\|\delta^{n-1/2}\right\|_A^2\\&\le\mathrm{Re}\left\{\omega_J^{n-1/2}\bar{\varphi}_J^{n-1/2}-\omega_0^{n-1/2}\bar{\varphi}_0^{n-1/2}\right\}\\&\quad+\left\|\varepsilon^{n-1/2}\right\|_A^2+\frac{1}{2}\left\|\delta^{n-1/2}\right\|_A^2\\&\quad+\left(V_m+\frac{1}{2}+\frac{1}{\tau}\right)\left(\|\varphi^n\|_A^2+\|\varphi^{n-1}\|_A^2\right).\end{aligned}\tag{3.23}$$

Similarly, for any $\varepsilon > 0$, from (3.22) we have

$$\begin{aligned}\frac{1}{\tau}\left(\|\varphi^n\|_A^2 - \|\varphi^{n-1}\|_A^2\right) \le \operatorname{Im}\left\{\omega_0^{n-1/2}\bar{\varphi}_0^{n-1/2} - \omega_J^{n-1/2}\bar{\varphi}_J^{n-1/2}\right\} \\ +\frac{\varepsilon}{2}\left(\|\varphi^n\|_A^2 + \|\varphi^{n-1}\|_A^2\right) \\ +\frac{\varepsilon}{2}\left\|\delta_x\varphi^{n-1/2}\right\|_A^2 + \frac{1}{\varepsilon}\left[\left\|\varepsilon^{n-1/2}\right\|_A^2 + \frac{1}{2}\left\|\delta^{n-1/2}\right\|_A^2\right].\end{aligned} \tag{3.24}$$

From (3.17),(3.18),

$$\omega_0^{n-1/2}\bar{\varphi}_0^{n-1/2} - \omega_J^{n-1/2}\bar{\varphi}_J^{n-1/2} = S_{n,0} - S_{n,J} + S_{n,r} \tag{3.25}$$

with

$$S_{n,0} = \left(\omega_0^{n-1/2} - \gamma_0^{n-1/2}\right)\bar{\varphi}_0^{n-1/2}, \qquad S_{n,J} = \left(\omega_J^{n-1/2} - \gamma_J^{n-1/2}\right)\bar{\varphi}_J^{n-1/2},$$

and

$$\begin{aligned}S_{n,r} &= \gamma_0^{n-1/2}\bar{\varphi}_0^{n-1/2} - \gamma_J^{n-1/2}\bar{\varphi}_J^{n-1/2} \\ &= \gamma_0^{n-1/2}\left(\bar{\varphi}_{1/2}^{n-1/2} - \frac{h}{2}\delta_x\bar{\varphi}_{1/2}^{n-1/2}\right) - \gamma_J^{n-1/2}\left(\bar{\varphi}_{J-1/2}^{n-1/2} + \frac{h}{2}\delta_x\bar{\varphi}_{J-1/2}^{n-1/2}\right).\end{aligned}$$

Therefore, for any $\varepsilon_1 > 0$,

$$\begin{aligned}|S_{n,r}| &\le \varepsilon_1\left(\left|\varphi_{J-1/2}^{n-1/2}\right|^2 + \left|\varphi_{1/2}^{n-1/2}\right|^2\right) + \frac{\varepsilon_1 h^2}{4}\left(\left|\delta_x\varphi_{J-1/2}^{n-1/2}\right|^2 + \left|\delta_x\varphi_{1/2}^{n-1/2}\right|^2\right) \\ &\quad + \frac{1}{2\varepsilon_1}\left(\left|\gamma_J^{n-1/2}\right|^2 + \left|\gamma_0^{n-1/2}\right|^2\right) \\ &\le \frac{\varepsilon_1 h^{-1}}{2}\left(\|\varphi^n\|_A^2 + \|\varphi^{n-1}\|_A^2\right) + \frac{\varepsilon_1 h}{4}\left\|\delta_x\varphi^{n-1/2}\right\|_A^2 + \frac{1}{\varepsilon_1}O\left(\tau^3\right).\end{aligned} \tag{3.26}$$

From (3.23), (3.25), and (3.26) with $\varepsilon_1 = 1$, we have

$$\begin{aligned}\left\|\delta_x\varphi^{n-1/2}\right\|_A^2 \le 4\operatorname{Re}\{S_{n,J} - S_{n,0}\} + 4\left\|\varepsilon^{n-1/2}\right\|_A^2 + 2\left\|\delta^{n-1/2}\right\|_A^2 + O\left(\tau^3\right) \\ +4\left(V_m + \frac{1}{2} + \frac{1}{h} + \frac{1}{\tau}\right)\left(\|\varphi^n\|_A^2 + \|\varphi^{n-1}\|_A^2\right).\end{aligned} \tag{3.27}$$

From (3.24)–(3.27), we have

$$\begin{aligned}\frac{1}{\tau}\left(\|\varphi^n\|_A^2 - \|\varphi^{n-1}\|_A^2\right) &\le \operatorname{Im}\{S_{n,0} - S_{n,J}\} + \frac{2\varepsilon + \varepsilon_1 h}{4}\left\|\delta_x\varphi^{n-1/2}\right\|_A^2 \\ &\quad + \frac{\varepsilon_1 h^{-1} + \varepsilon}{2}\left(\|\varphi^n\|_A^2 + \|\varphi^{n-1}\|_A^2\right) \\ &\quad + \frac{1}{\varepsilon}\left(\left\|\varepsilon^{n-1/2}\right\|_A^2 + \frac{1}{2}\left\|\delta^{n-1/2}\right\|_A^2\right) + \frac{1}{\varepsilon_1}O\left(\tau^3\right) \\ &\le \operatorname{Im}\{S_{n,0} - S_{n,J}\} + (2\varepsilon + \varepsilon_1 h)\operatorname{Re}\{S_{n,J} - S_{n,0}\} \\ &\quad + \left[(2\varepsilon + \varepsilon_1 h)\left(V_m + \frac{1}{2} + \frac{1}{h} + \frac{1}{\tau}\right) + \frac{\varepsilon_1 h^{-1} + \varepsilon}{2}\right] \\ &\quad \cdot\left(\|\varphi^n\|_A^2 + \|\varphi^{n-1}\|_A^2\right) \\ &\quad + \left[2\varepsilon + \varepsilon_1 h + \frac{1}{\varepsilon} + \frac{1}{\varepsilon_1}\right]\left[\left\|\varepsilon^{n-1/2}\right\|_A^2 + \frac{1}{2}\left\|\delta^{n-1/2}\right\|_A^2 + O\left(\tau^3\right)\right].\end{aligned}$$

Let $h_\tau = \min\{h, \tau\}$, take $\varepsilon_1 = \varepsilon = h_\tau \cdot \min\{1/3, 1/[6(V_m+3)T]\}$, then

$$\begin{aligned}\frac{1}{\tau}\left(\|\varphi^n\|_A^2 - \|\varphi^{n-1}\|_A^2\right) &\le \operatorname{Im}\{S_{n,0} - S_{n,J}\} + (2+h)\,\varepsilon \operatorname{Re}\{S_{n,J} - S_{n,0}\} \\ &\quad + \frac{1}{2T}\left(\|\varphi^n\|_A^2 + \|\varphi^{n-1}\|_A^2\right) + O\left(h_\tau^{-1}\right) \\ &\quad \cdot \left[\left\|\varepsilon^{n-1/2}\right\|_A^2 + \frac{1}{2}\left\|\delta^{n-1/2}\right\|_A^2\right] + h_\tau^{-1} O\left(\tau^3\right) \\ &= [1 - (2+h)\,\varepsilon] \operatorname{Im}\{S_{n,0} - S_{n,J}\} + (2+h)\,\varepsilon\,[\operatorname{Re}\{S_{n,J} - S_{n,0}\} \\ &\quad - \operatorname{Im}\{S_{n,J} - S_{n,0}\}] + \frac{1}{2T}\left(\|\varphi^n\|_A^2 + \|\varphi^{n-1}\|_A^2\right) + O\left(h_\tau^{-1}\right) \\ &\quad \cdot \left[\left\|\varepsilon^{n-1/2}\right\|_A^2 + \frac{1}{2}\left\|\delta^{n-1/2}\right\|_A^2\right] + h_\tau^{-1} O\left(\tau^3\right).\end{aligned} \tag{3.28}$$

Similarly to the derivation of (3.11)–(3.13) and from (3.17),(3.18), and Lemma 3, we have

$$\sum_{k=1}^{n} \operatorname{Im}\{S_{k,0} - S_{k,J}\} \le 0. \tag{3.29}$$

We define a real symmetric matrix,

$$B_{2n} = \begin{bmatrix} 1 & 0 & \beta_1 & 0 & \dots & \beta_{n-1} & 0 \\ 0 & 1 & 0 & \beta_1 & \dots & 0 & \beta_{n-1} \\ \beta_1 & 0 & 1 & 0 & \dots & \beta_{n-2} & 0 \\ 0 & \beta_1 & 0 & 1 & \dots & 0 & \beta_{n-2} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \beta_{n-1} & 0 & \beta_{n-2} & 0 & \dots & 1 & 0 \\ 0 & \beta_{n-1} & 0 & \beta_{n-2} & \dots & 0 & 1 \end{bmatrix},$$

with

$$\beta_k = \frac{1}{2}\sqrt{\frac{\pi\tau}{2}}\,\frac{a_k - a_{k-1}}{2} = \frac{1}{2}\left(\sqrt{k+1} - 2\sqrt{k} + \sqrt{k-1}\right), \qquad k = 1, 2, \dots, n-1.$$

Then, B_{2n} is diagonally dominant and is then positive definite. Therefore, if we let $e^{iV_- t_k}$ $\varphi_0^{k-1/2} = R_k + iI_k$ and $\mathbf{X} = (R_1, I_1, R_2, I_2, \dots, R_n, I_n)^t$, R_k, and I_k are real numbers, then the following quadratic form,

$$\begin{aligned}\sum_{k=1}^{n} [\operatorname{Re}\{S_{k,0}\} - \operatorname{Im}\{S_{k,0}\}] &= \sqrt{2}\sum_{k=1}^{n}\left\{a_0\left(R_k^2 + I_k^2\right) + \sum_{s=1}^{k-1}(a_{k-s} - a_{k-s-1})(R_k R_s + I_k I_s)\right\} \\ &= \frac{4}{\sqrt{\pi\tau}}\mathbf{X}^t B_{2n}\mathbf{X} \ge 0.\end{aligned} \tag{3.30}$$

Similarly, we have

$$\sum_{k=1}^{n} [\operatorname{Re}\{S_{k,J}\} - \operatorname{Im}\{S_{k,J}\}] \le 0. \tag{3.31}$$

Summing up (3.28) for n, from (3.29)–(3.31) and (2.12),(2.13), we get

$$\frac{1}{\tau}\|\varphi^n\|_A^2 \le \frac{1}{2T}\sum_{k=1}^{n}\left(\|\varphi^k\|_A^2 + \|\varphi^{k-1}\|_A^2\right) + h_\tau^{-1} O\left(\frac{h^4}{\tau} + \tau^2\right)$$

or

$$\frac{1}{2}\|\varphi^n\|_A^2 \le \left(1 - \frac{\tau}{2T}\right)\|\varphi^n\|_A^2 \le \frac{\tau}{T}\sum_{k=1}^{n-1}\|\varphi^k\|_A^2 + h_\tau^{-1} O\left(h^4 + \tau^3\right).$$

Using the discrete Gronwall inequality to the above inequality and noticing that $n\tau \le T$, we have

$$\|\varphi^n\|_A^2 \le h_\tau^{-1} O\left(h^4 + \tau^3\right) e^{2n\tau/T} = h_\tau^{-1} O\left(h^4 + \tau^3\right).$$

This completes the proof. ∎

4. NUMERICAL EXAMPLE

In this section, we present two examples to show the effectiveness of our scheme. In the first example, we check the stability and convergence of our numerical method, and compare the numerical solution with the known exact solution. In the second example, the exact solution is also known, which is a travelling wave. The purpose here is to see whether there are any numerical reflections on the boundaries, and also to compare with other numerical methods.

EXAMPLE 1. We use scheme (2.19)–(2.22) to solve the following initial value problem of the Schrödinger equation on $R^1 \times [0,5]$,

$$i\psi_t(x,t) = -\frac{1}{2}\psi_{xx}(x,t) + \psi(x,t), \qquad \forall\,(x,t) \in R^1 \times (0,5], \tag{4.1}$$

$$\psi(x,0) = \begin{cases} x(1-x)(1+2i), & \forall x \in [0,1], \\ 0, & \text{otherwise.} \end{cases}$$

Its exact solution is the following [19],

$$\psi(x,t) = \frac{1}{\sqrt{2\pi t}} \int_0^1 \xi(1-\xi)(1+2i)\, e^{i\left[(x-\xi)^2/2t - t - \pi/4\right]}\, d\xi.$$

For mesh size (h,τ), we denote the relative error of the solution by

$$e_{h,\tau}(t_n) = \frac{\left\|\psi(x_j,t_n) - \psi_j^n\right\|_A}{\left\|\psi(x_j,t_n)\right\|_A}.$$

We take $\tau = h$ and $h = h_0 = 0.1$, $h_0/2$, $h_0/4$, $h_0/8$, the corresponding errors $e_{h,\tau}(t_n)$ at time levels $t_n = 1,2,3,4,5$ are listed in Table 1. We can see that $e_{h,\tau}(t_n) \approx O(h)$, which is coincident with the theoretical result given in Theorem 4. In the case that $\tau = h^2$, the errors $e_{h,\tau}(t_n)$ are listed in Table 2. We can see that $e_{h,\tau}(t_n) \approx O(h^2)$, which is better than the theoretical result. This suggests that the error bound obtained in (3.14) may not be optimal, further improvement might be possible.

Table 1. Relative error $e_{h,\tau}(t_n), \tau = h$.

Mesh	$h = h_0 = 0.1$	$h = \frac{h_0}{2}$	$h = \frac{h_0}{4}$	$h = \frac{h_0}{8}$
$e_{h,\tau}(1)$	1.503D − 01	8.609D − 02	4.928D − 02	2.512D − 02
$e_{h,\tau}(2)$	1.796D − 01	9.300D − 02	5.043D − 02	2.770D − 02
$e_{h,\tau}(3)$	1.592D − 01	9.908D − 02	5.527D − 02	2.854D − 02
$e_{h,\tau}(4)$	1.587D − 01	9.423D − 02	5.332D − 02	2.932D − 02
$e_{h,\tau}(5)$	1.706D − 01	9.521D − 02	5.701D − 02	2.940D − 02

Table 2. Relative error $e_{h,\tau}(t_n), \tau = h^2$.

Mesh	$h = h_0 = 0.1$	$h = \frac{h_0}{2}$	$h = \frac{h_0}{4}$	$h = \frac{h_0}{8}$
$e_{h,\tau}(1)$	1.100D − 02	2.823D − 03	7.061D − 04	1.736D − 04
$e_{h,\tau}(2)$	1.020D − 02	2.561D − 03	6.518D − 04	1.640D − 04
$e_{h,\tau}(3)$	1.007D − 02	2.520D − 03	6.345D − 04	1.607D − 04
$e_{h,\tau}(4)$	1.002D − 02	2.510D − 03	6.289D − 04	1.589D − 04
$e_{h,\tau}(5)$	1.000D − 02	2.505D − 03	6.270D − 04	1.577D − 04

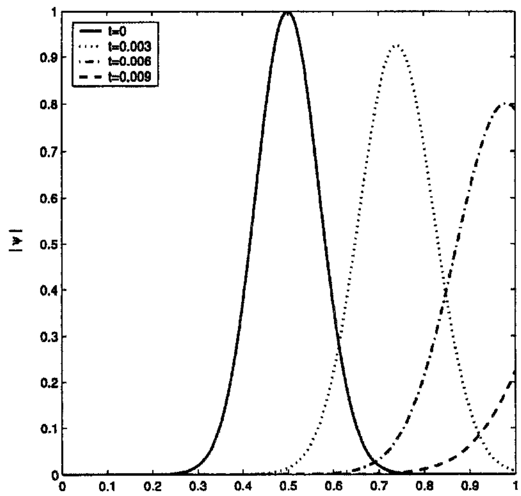

Figure 1. The exact solution $|\psi(x,t)|$ at different times.

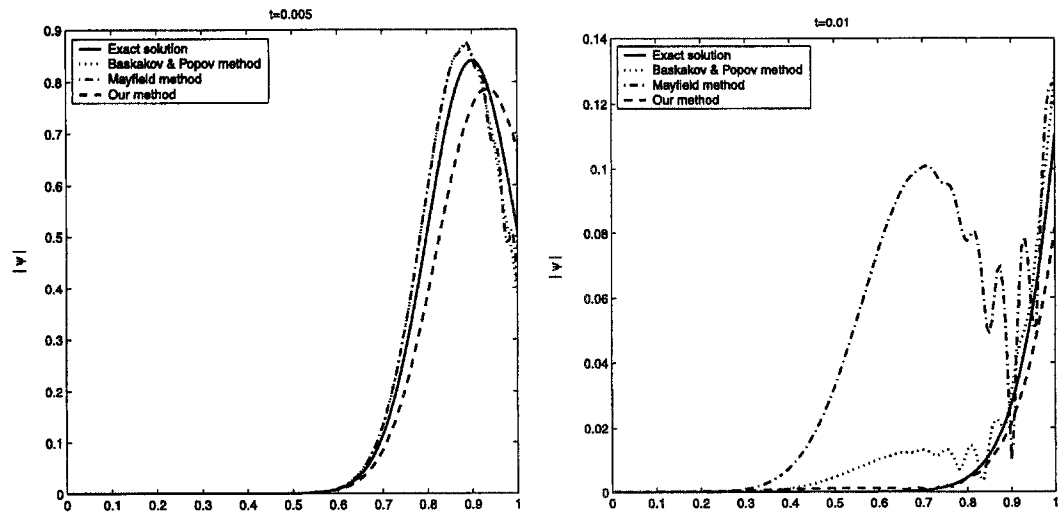

Figure 2. The solutions $|\psi(x,t)|$ at $t = 0.005$ and $t = 0.01$.

EXAMPLE 2. We consider the right travelling Gaussian beam [4], with a wave number $k_0 = 8$,

$$\psi(x,t) = \sqrt{\frac{i}{-200t+i}} \exp\left(\frac{-i(10x-5)^2 - k_0(10x-5) + 50k_0^2 t}{-200t+i}\right).$$

It is the exact solution of the Schrödinger equation (1.1) with $V(x,t) = 0$, its evolution at different times are shown graphically in Figure 1.

In order to compare the numerical results using our method to the solutions using other discretization methods of the analytic transparent boundary conditions, we consider the computational interval $[0,1]$, take the space step $h = 1/160$ and the time step $\tau = 2 \times 10^{-5}$ and solve the numerical solutions by our method, the Mayfield method [5] and the Baskakov and Popov method [1], respectively. The evolutions of the exact solution and the numerical solutions at different times are shown graphically in Figures 2 and 3. We can see in these figures that our method almost does not induce the numerical reflection, but the other two methods induce strong reflections travelling to the left. At time $t = 0.015$, the numerical solution using our method has almost completely left the domain $[0,1]$ but the numerical solutions using the other two methods

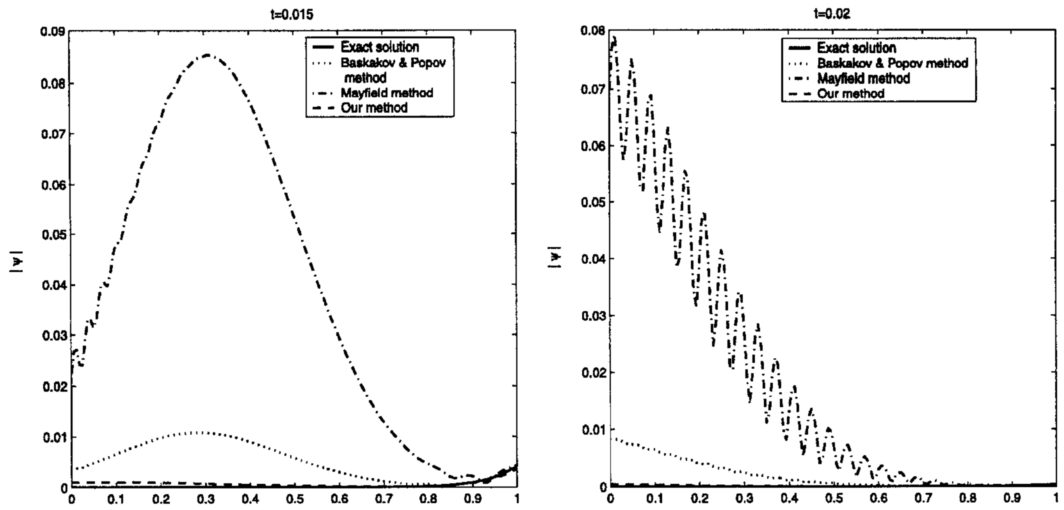

Figure 3. The solutions $|\psi(x,t)|$ at $t = 0.015$ and $t = 0.02$.

contain a reflected wave packet with the maximum modulus (which corresponds to the maximum error) of about 0.086 for the Mayfield method and around 0.011 for the Baskakov and Popov method.

5. CONCLUSIONS

In this paper, we consider a finite-difference approximation for the one-dimensional time-dependent Schrödinger equation on unbounded domain. Artificial boundary conditions are introduced to reduce the original problem to an initial-boundary value problem in a finite-computational domain. Using the method of reduction of order, a finite-difference scheme is constructed to solve the reduced problem. This scheme has been proved to be uniquely solvable, unconditionally stable and convergent. Numerical examples showed the effectiveness of our scheme.

REFERENCES

1. V.A. Baskakov and A.V. Popov, Implementation of transparent boundaries for numerical solution of the Schrödinger equation, *Wave Motion* **14**, 123–128, (1991).
2. J.R. Hellums and W.R. Frensley, Non-Markovian open-system boundary conditions for the time-dependent Schrödinger equation, *Phys. Rev. B* **49**, 2904–2906, (1994).
3. J.S. Papadakis, NORDA Parabolic Equation Workshop, NORDA Tech. Note, Volume 143, (1982).
4. X. Antoine and C. Besse, Unconditionally stable discretization schemes of nonreflecting boundary conditions for the one-dimensional Schrödinger equation, *J. Comput. Phys.* **188**, 157–175, (2003).
5. B. Mayfield, Nonlocal boundary conditions for the Schrödinger equation, Ph.D. Thesis, University of Rhode Island, Providence, RI, (1989).
6. A. Arnold, Mathematical concept of open quantum boundary conditions, *Theory Stat. Phys.* **30** (4-6), 561–584, (2001).
7. A. Arnold and M. Ehrhardt, Discrete transparent boundary conditions for wide angle parabolic equations in underwater acoustics, *J. Comput. Phys.* **145**, 611-638, (1998).
8. A. Arnold and M. Ehrhardt, Discrete transparent boundary conditions for the Schrödinger equation, *Revista di Mathematic della Universita di Parma* **6** (4), 57–108, (2001).
9. M. Ehrhardt, Disctete transparent boundary conditions for general Schrödinger-type equations, *VLSI Design* **9** (4), 325–338, (1999).
10. F. Schmidt, Construction of discrete transparent boundary conditions for Schrödinger-type equations, *Surv. Math. Ind.* **9** (2), 87–100, (1999).
11. F. Schmidt and P. Deuflhard, Discrete transparent boundary conditions for the numerical solution of Fresnel's equation, *Computers Math. Applic.* **29** (9), 53–76, (1995).
12. F. Schmidt and D. Yevick, Discrete transparent boundary conditions for Schrödinger-type equations, *J. Comput. Phys.* **134**, 96–107, (1997).

13. T. Friese, F. Schmidt and D. Yevick, A comparison of transparent boundary conditions for the Fresnel equation, *J. Comput. Phys.* **168**, 433–444, (2001).
14. J. Jin, Finite element methods for some elliptic problems with singularity and problems on unboundary domains, Ph. D. Thesis, Hong Kong Baptist University, (2004).
15. E.T. Chung, Q. Du and J. Zou, Convergence analysis of a finite volume method for Maxwell's equations in nonhomogeneous media, *SIAM J. Numer. Anal.* **41**, 37–63, (2003).
16. X. Wu and Z.Z. Sun, Convergence of difference scheme for heat equation in unbounded domains using artificial boundary conditions, *Appl. Numer. Math.* **50**, 261–277, (2004).
17. A. Arnold, Numerical absorbing boundary conditions for quantum evolution equations, *VLSI Design* **6**, 313–319, (1998).
18. Z.Z. Sun and X. Wu, Numerical computation for the Schrödinger equations on an infinite domain (to appear).
19. L. Mandel and E. Wolf, *Optical Coherence and Quantum Optics*, pp. 266–267, Cambridge University Press, Cambridge, (1995).