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The stability and convergence of a difference scheme for the Schrödinger equation on an infinite domain by using artificial boundary conditions

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Abstract

This paper is concerned with the numerical solution to the Schrödinger equation on an infinite domain. Two exact artificial boundary conditions are introduced to reduce the original problem into an initial boundary value problem with computational domain. Then, a fully discrete difference scheme is derived. The truncation errors are analyzed in detail. The unique solvability, stability and convergence with the convergence order of $O(h^{3/2} + \tau^{3/2}h^{-1/2})$ are proved by the energy method. A numerical example is given to demonstrate the accuracy and efficiency of the proposed method. As a special case, the stability and convergence of the difference scheme proposed by Baskakov and Popov in 1991 is obtained.

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1. Introduction

When we wish to solve numerically a differential equation defined on an infinite domain, it is necessary to consider a finite sub-domain and to use artificial boundary conditions in such a way that the solutions in the finite sub-domain approximate the original solution. If the approximation is exact, the transfer is called exact and the corresponding artificial boundary condition is called exact or transparent. For instance, different transparent boundary conditions (TBCs) for the wave equation are derived in [7,8,10,19–22].

In this paper, we study the problem of the numerical approximation of a dispersive wave $\psi(x, t)$, solution to the Schrödinger equation in an unbounded domain. More concretely, we consider the following linear equation:

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$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi, \quad x\in R,\ t>0, \tag{1.1}$$

$$\psi(x,0) = \phi(x), \quad x\in R, \tag{1.2}$$

where the electrostatic potential function $V(x,t)$ is assumed to be given with $\mathrm{Im}(V(x,t))\leqslant 0$, and for the sake of conciseness, we assume that ϕ is a compactly supported datum. This model equation arises in many practical domains of physical and technological interest, e.g., quantum mechanics, optics, seismology and plasma physics.

The solution to (1.1), (1.2) is defined on the whole domain $\Omega = \{(x,t)|x\in R, t>0\}$ and must vanish for $x\to\pm\infty$. However, from a practical point of view, the infinite domain of propagation has to next use a well-adapted discretization scheme for Eqs. (1.1) and (1.2). To this end, let us split the initial domain Ω into three regions. We designate by $\Omega_i = \{(x,t)|x_\mathrm{l}\leqslant x\leqslant x_\mathrm{r}, t>0\}$ the interior domain where one wishes to compute an approximate solution, and two other complementary regions can be defined by $\Omega_\mathrm{l} = \{(x,t)|x\leqslant x_\mathrm{l}, t>0\}$ and $\Omega_\mathrm{r} = \{(x,t)|x\geqslant x_\mathrm{r}, t>0\}$. To simplify the problem, we suppose that $\mathrm{supp}(\phi)\subset[x_\mathrm{l},x_\mathrm{r}]$ and

$$V(x,t) = V_- \equiv \text{const.} \quad \text{for } x\leqslant x_\mathrm{l}, \qquad V(x,t) = V_+ \equiv \text{const.} \quad \text{for } x\geqslant x_\mathrm{r},$$

with $\mathrm{Im}(V_-) = \mathrm{Im}(V_+) = 0$.

The transparent boundary conditions (TBCs) for Schrödinger equation were independently derived by several authors from various application fields [2,6,11,15]; Inhomogeneous extensions are analyzed in [1,5]. They are non-local in t and read

$$\frac{\partial\psi(x_\mathrm{l},t)}{\partial x} = \sqrt{\frac{2}{\pi}}\mathrm{e}^{-\left(\frac{\pi}{4}+V_-t\right)\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\psi(x_\mathrm{l},s)\mathrm{e}^{\mathrm{i}V_-s}}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.3}$$

for the left boundary at $x = x_\mathrm{l}$, and

$$\frac{\partial\psi(x_\mathrm{r},t)}{\partial x} = -\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\left(\frac{\pi}{4}+V_+t\right)\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\psi(x_\mathrm{r},s)\mathrm{e}^{\mathrm{i}V_+s}}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.4}$$

for the right boundary at $x = x_\mathrm{r}$. There are also an equivalent form to (1.3) and (1.4) as follows

$$\psi(x_\mathrm{l},t) = \sqrt{\frac{2}{\pi}}\mathrm{e}^{-\left(\frac{\pi}{4}+V_-t\right)\mathrm{i}}\int_0^t \frac{\frac{\partial}{\partial x}[\psi(x_\mathrm{l},s)\,\mathrm{e}^{\mathrm{i}V_-s}]}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.5}$$

for the left boundary at $x = x_\mathrm{l}$, and

$$\psi(x_\mathrm{r},t) = -\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\left(\frac{\pi}{4}+V_+t\right)\mathrm{i}}\int_0^t \frac{\frac{\partial}{\partial x}[\psi(x_\mathrm{r},s)\,\mathrm{e}^{\mathrm{i}V_+s}]}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.6}$$

for the right boundary at $x = x_\mathrm{r}$. Usually, (1.3) and (1.4) are called the Dirichlet–Neumann boundary conditions and (1.5) and (1.6) are called the Neumann–Dirichlet boundary conditions [2].

As a consequence, the Cauchy problem (1.1), (1.2) on the infinite domain can be reduced to the initial boundary value problem

$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi, \quad x_\mathrm{l}<x<x_\mathrm{r},\ t>0, \tag{1.7}$$

$$\psi(x,0) = \phi(x), \quad x_\mathrm{l}\leqslant x\leqslant x_\mathrm{r} \tag{1.8}$$

with the boundary conditions (1.3), (1.4), or, with the boundary conditions (1.5), (1.6).

Classically, the density $\|\psi\|_{L_2(R)}$ is decreasing for the problem (1.1), (1.2) in the whole space and moreover it is conserved if the potential $V(x,t)$ is real. In the case of a bounded domain, this should also be the case for the $L_2([x_\mathrm{l},x_\mathrm{r}])$-norm of the approximate solution. Arnold [3,4] proved the following result.

Theorem 1.1. *Let us assume that potential* $V\in\Phi(R_t^+,L^\infty(C))$ *satisfies*: $\mathrm{Im}(V(x,t))\leqslant 0$ *for* $x\in[x_\mathrm{l},x_\mathrm{r}]$ *and* $t>0$. *Let* $\psi(x,t)$ *be a solution to the initial boundary value problem (1.7), (1.8) with (1.3), (1.4), then,* $\psi\in\Phi(R_t^+,H^1([x_\mathrm{l},x_\mathrm{r}]))$ *and fulfills the following energy inequality*:

$$\|\psi(\cdot,t)\|_{L_2([x_l,x_r])} \leqslant \|\phi\|_{L_2([x_l,x_r])} \quad \forall t>0 \text{ and } \phi \in H^1([x_l,x_r]).$$

The proof of this theorem is based on the next lemma.

Lemma 1.2. *For any $T>0$, let $u(t) \in H^{\frac{1}{4}}(0,T)$ with the extension $u(t)=0$ for $t>T$. Then*

$$\mathrm{Re}\left\{ e^{\frac{i\pi}{4}} \int_0^\infty \bar{u}(t) \frac{d}{dt}\left[\int_0^t \frac{u(s)}{\sqrt{t-s}}\, ds\right] dt \right\} \geqslant 0,$$

where (and below) $\bar{u}$ denotes the complex conjugate of u.

Let $\omega_h \equiv \{x_j | 0 \leqslant j \leqslant M\}$ be a uniform mesh of the interval $[x_l, x_r]$, where $x_j = x_l + jh$, $0 \leqslant j \leqslant M$ with $h = (x_r - x_l)/M$. Denote $t_n = n\tau, t_{n-\frac{1}{2}} = (n-\frac{1}{2})\tau,\ n = 0,1,2,\ldots$.

Eq. (1.7) is often discretized by the Crank–Nicolson scheme

$$i \cdot \frac{\psi_j^n - \psi_j^{n-1}}{\tau} = -\frac{1}{2}\cdot\frac{1}{h^2}\left(\psi_{j+1}^{n-\frac{1}{2}} - 2\psi_j^{n-\frac{1}{2}} + \psi_{j-1}^{n-\frac{1}{2}}\right) + V\left(x_j, t_{n-\frac{1}{2}}\right)\psi_j^{n-\frac{1}{2}}, \quad 1 \leqslant j \leqslant M-1,\ n \geqslant 1, \tag{1.9}$$

where $\psi_j^{n-\frac{1}{2}} = \frac{1}{2}(\psi_j^n + \psi_j^{n-1})$. The main difficulty of the numerical approximation is now linked to the presence of a convolution operator in the boundary conditions. If $V_- = 0$ and $V_+ = 0$, Mayfield in [14] used the approximation

$$\int_0^{t_N} \frac{\frac{\partial\psi(x_l,s)}{\partial x}}{\sqrt{t_N - s}}\, ds = \sum_{n=1}^N \frac{\psi(x_l+h,t_n) - \psi(x_l,t_n)}{h} \int_{t_{n-1}}^{t_n} \frac{1}{\sqrt{t_N-s}}\, ds \tag{1.10}$$

and

$$\int_0^{t_N} \frac{\frac{\partial\psi(x_r,s)}{\partial x}}{\sqrt{t_N - s}}\, ds = \sum_{n=1}^N \frac{\psi(x_r,t_n) - \psi(x_r-h,t_n)}{h} \int_{t_{n-1}}^{t_n} \frac{1}{\sqrt{t_N-s}}\, ds \tag{1.11}$$

to approximate (1.5) and (1.6), respectively. For the resulting scheme she obtained the following result.

Theorem 1.3 (cf. [14]). *The difference scheme (1.9)–(1.11) is stable, if and only if*

$$4\pi\frac{\tau}{h^2} \in \bigcup_{j=1}^{\infty}\left[(2j+1)^{-2}, (2j)^{-2}\right].$$

This shows that the chosen boundary discretization destroys the unconditional stability of the underlying Crank–Nicolson scheme. Baskakov and Popov [6] approximated boundary conditions (1.3) and (1.4) by the piecewise linear approximations of the functions $\psi(x_l,s)$, $\psi(x_r,s)$ in the integrals:

$$\left[\frac{d}{dt}\int_0^t \frac{\psi(x_l,s)}{\sqrt{t-s}}\, ds\right]\bigg|_{t=t_N} = \left[\int_0^t \frac{\frac{\partial\psi(x_l,s)}{\partial s}}{\sqrt{t-s}}\, ds\right]\bigg|_{t=t_N} = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \frac{\frac{\partial\psi(x_l,s)}{\partial s}}{\sqrt{t_N-s}}\, ds$$
$$= \sum_{n=1}^N \frac{\psi(x_l,t_n) - \psi(x_l,t_{n-1})}{\tau}\int_{t_{n-1}}^{t_n}\frac{ds}{\sqrt{t_N-s}}$$

and

$$\left[\frac{d}{dt}\int_0^t \frac{\psi(x_r,s)}{\sqrt{t-s}}\, ds\right]\bigg|_{t=t_N} = \sum_{n=1}^N \frac{\psi(x_r,t_n) - \psi(x_r,t_{n-1})}{\tau}\int_{t_{n-1}}^{t_n}\frac{ds}{\sqrt{t_N-s}}.$$

For the one-dimensional Schrödinger equation, also see the paper by Schmidt and Yevick [18]. Yevick et al. [9] presented a comparison of transparent boundary conditions for the Fresnel equation. Schädle [17] considered the numerical solution to the two-dimensional Schrödinger equation. Time discretization is done by the trapezoidal rule in the interior and by convolution quadrature on the boundary. A convergence estimate is declared for the semidiscretization in t. Space discretization is done using the finite element method and coupling the boundary conditions by collocation. A numerical example is given. Lubich and Schädle [12] have shown how the convolution kernel can be effectively compressed so that the required work and storage depends only logarithmically on the number of time steps. To our knowledge, there have been only a very few results on the convergence of the numerical results for the Schrödinger equation in unbounded domain. In the following, we suppose that the problem (1.1), (1.2) has an appropriate smooth solution.

The difference scheme we will consider for (1.7), (1.8) with (1.3), (1.4) is as follows:

$$\mathrm{i}\cdot\frac{\psi_0^n-\psi_0^{n-1}}{\tau}=-\frac{1}{2}\cdot\frac{2}{h}\left\{\frac{\psi_1^{n-\frac{1}{2}}-\psi_0^{n-\frac{1}{2}}}{h}-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0\psi_0^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\psi_0^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_-(t_n-t_k)}\right]\right\}$$
$$+V\left(x_0,t_{n-\frac{1}{2}}\right)\psi_0^{n-\frac{1}{2}},\quad n\geqslant 1,\tag{1.12}$$

$$\mathrm{i}\cdot\frac{\psi_j^n-\psi_j^{n-1}}{\tau}=-\frac{1}{2}\cdot\frac{1}{h^2}\left(\psi_{j+1}^{n-\frac{1}{2}}-2\psi_j^{n-\frac{1}{2}}+\psi_{j-1}^{n-\frac{1}{2}}\right)+V\left(x_j,t_{n-\frac{1}{2}}\right)\psi_j^{n-\frac{1}{2}},\quad 1\leqslant j\leqslant M-1,\ n\geqslant 1,\tag{1.13}$$

$$\mathrm{i}\cdot\frac{\psi_M^n-\psi_M^{n-1}}{\tau}=-\frac{1}{2}\cdot\frac{2}{h}\left\{-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0\psi_M^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\psi_M^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_+(t_n-t_k)}\right]-\frac{\psi_M^{n-\frac{1}{2}}-\psi_{M-1}^{n-\frac{1}{2}}}{h}\right\}$$
$$+V\left(x_M,t_{n-\frac{1}{2}}\right)\psi_M^{n-\frac{1}{2}},\quad n\geqslant 1,\tag{1.14}$$

$$\psi_j^0=\phi(x_j),\quad 0\leqslant j\leqslant M,\tag{1.15}$$

where

$$a_k=\frac{2}{\sqrt{k}+\sqrt{k+1}},\quad k=0,1,2,\ldots.\tag{1.16}$$

At each time level, only a tridiagonal system of linear equations needs to be solved and the Thomas method can be used. It should be pointed out that, when $V_-=0$ and $V_+=0$, the difference scheme (1.12)–(1.15) is equivalent to the difference scheme presented by Baskakov and Popov in [6].

The organization of this paper is the following. In Section 2, we present some preliminary lemmas. Lemma 2.2 is prepared for the derivation of the difference scheme and Lemma 2.5 is for the analysis of the difference scheme. In Section 3, we derive the fully discretized difference scheme (1.12)–(1.15) for the problem (1.7), (1.8) with (1.3), (1.4). The standard Crank–Nicolson finite difference scheme is for the interior domain, together with several implementations at the boundaries. The truncation errors are given in detail, which will be used in the proof of the convergence of the difference scheme. The unique solvability, stability and convergence are proved in Section 4. The convergence order is of $\mathrm{O}(h^{3/2}+\tau^{3/2}h^{-1/2})$. As a special case, the stability and convergence of the difference scheme proposed by Baskakov and Popov in [6] is obtained. Finally, Section 5 presents a numerical experiment showing the theoretical results. A brief conclusion is given at the end of the paper. Theorems 4.1 and 4.3 are our main results.

2. Preliminary lemmas

The following lemmas will be used to derive the difference scheme (1.12)–(1.15).

Lemma 2.1 (cf. [23]). *Suppose* $f(t)\in C^2[0,t_n]$. *Then*

$$\left|\int_0^{t_n}\frac{f'(t)}{\sqrt{t_n-t}}\,\mathrm{d}t-\sum_{k=1}^{n}\frac{f(t_k)-f(t_{k-1})}{\tau}\int_{t_{k-1}}^{t_k}\frac{\mathrm{d}t}{\sqrt{t_n-t}}\right|\leqslant\frac{1}{6}(10\sqrt{2}-11)\max_{0\leqslant t\leqslant t_n}|f''(t)|\tau^{3/2}.$$

Lemma 2.2. *Suppose* $f(t)\in C^2[0,t_n]$ *and* $f(0)=0$. *Denote*

$$F(t)=\mathrm{e}^{-\mathrm{i}vt}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t\frac{f(s)\mathrm{e}^{\mathrm{i}vs}}{\sqrt{t-s}}\,\mathrm{d}s.$$

Then, we have

$$\frac{1}{2}[F(t_n)+F(t_{n-1})]=\frac{1}{\sqrt{\tau}}\left[a_0 f^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})f^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}v(t_n-t_k)}\right]+\mathrm{O}(\tau^{3/2}),$$

where $\{a_k\}$ *is defined in* (1.16) *and*

$$f^{k-\frac{1}{2}}=\frac{1}{2}[f(t_k)+f(t_{k-1})],\quad k=1,2,\ldots,n.$$

Proof. It follows from $f(0)=0$ that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t\frac{f(s)\,\mathrm{e}^{\mathrm{i}vs}}{\sqrt{t-s}}\,\mathrm{d}s&=\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t f(s)\,\mathrm{e}^{\mathrm{i}vs}\,\mathrm{d}(-2\sqrt{t-s})=\frac{\mathrm{d}}{\mathrm{d}t}\left[-2\sqrt{t-s}f(s)\,\mathrm{e}^{\mathrm{i}vs}|_{s=0}^{t}+\int_0^t 2\sqrt{t-s}\frac{\mathrm{d}(f(s)\,\mathrm{e}^{\mathrm{i}vs})}{\mathrm{d}s}\,\mathrm{d}s\right]\\&=\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_0^t 2\sqrt{t-s}\frac{\mathrm{d}(f(s)\,\mathrm{e}^{\mathrm{i}vs})}{\mathrm{d}s}\,\mathrm{d}s\right]=\int_0^t\frac{\mathrm{d}(2\sqrt{t-s})}{\mathrm{d}t}\,\frac{\mathrm{d}(f(s)\,\mathrm{e}^{\mathrm{i}vs})}{\mathrm{d}s}\,\mathrm{d}s\\&=\int_0^t\frac{\mathrm{d}(f(s)\,\mathrm{e}^{\mathrm{i}vs})}{\mathrm{d}s}\cdot\frac{\mathrm{d}s}{\sqrt{t-s}}.\end{aligned}$$

Then, according to Lemma 2.1 and noticing

$$\frac{1}{\sqrt{\tau}}\int_{t_{k-1}}^{t_k}\frac{\mathrm{d}s}{\sqrt{t_n-s}}=a_{n-k},\tag{2.1}$$

we have

$$\begin{aligned}F(t_n)&=\mathrm{e}^{-\mathrm{i}vt_n}\int_0^{t_n}\frac{\mathrm{d}(f(s)\,\mathrm{e}^{\mathrm{i}vs})}{\mathrm{d}s}\cdot\frac{\mathrm{d}s}{\sqrt{t_n-s}}=\mathrm{e}^{-\mathrm{i}vt_n}\sum_{k=1}^{n}\frac{f(t_k)\,\mathrm{e}^{\mathrm{i}vt_k}-f(t_{k-1})\,\mathrm{e}^{\mathrm{i}vt_{k-1}}}{\tau}\int_{t_{k-1}}^{t_k}\frac{\mathrm{d}s}{\sqrt{t_n-s}}+\mathrm{O}(\tau^{3/2})\\&=\frac{1}{\sqrt{\tau}}\sum_{k=1}^{n}a_{n-k}\left[f(t_k)\mathrm{e}^{-\mathrm{i}v(t_n-t_k)}-f(t_{k-1})\,\mathrm{e}^{-\mathrm{i}v(t_n-t_{k-1})}\right]+\mathrm{O}(\tau^{3/2})\\&=\frac{1}{\sqrt{\tau}}\left[a_0 f(t_n)-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})f(t_k)\mathrm{e}^{-\mathrm{i}v(t_n-t_k)}\right]+\mathrm{O}(\tau^{3/2}).\end{aligned}$$

Therefore,

$$\begin{aligned}\frac{1}{2}[F(t_n)+F(t_{n-1})]&=\frac{1}{2}\frac{1}{\sqrt{\tau}}\left\{\left[a_0 f(t_n)-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})f(t_k)\,\mathrm{e}^{-\mathrm{i}v(t_n-t_k)}\right]\right.\\&\quad\left.+\left[a_0 f(t_{n-1})-\sum_{k=1}^{n-2}(a_{n-1-k-1}-a_{n-1-k})f(t_k)\,\mathrm{e}^{-\mathrm{i}v(t_{n-1}-t_k)}\right]\right\}+\mathrm{O}(\tau^{3/2})\\&=\frac{1}{\sqrt{\tau}}\left[a_0 f^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})f^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}v(t_n-t_k)}\right]+\mathrm{O}(\tau^{3/2}).\end{aligned}$$

This completes the proof. □

The following lemma with its corollary is for the proof of a discrete counterpart of Lemma 1.2.

Lemma 2.3. *Let*

$$f(x)=\begin{cases}1, & x\in[0,1),\\0, & x\notin[0,1).\end{cases}$$

Then $f\in H^{1/4}(R)$.

Proof. The Fourier transformation of $f(x)$ is

$$\hat{f}(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-\mathrm{i}xy}\,\mathrm{d}x = \frac{1}{\sqrt{2\pi}} \int_{0}^{1} \mathrm{e}^{-\mathrm{i}xy}\,\mathrm{d}x = \frac{1-\mathrm{e}^{-\mathrm{i}y}}{\sqrt{2\pi}\cdot \mathrm{i}y}.$$

Consequently, we have

$$\begin{aligned}\int_{-\infty}^{\infty}(1+y^2)^{1/4}|\hat{f}(y)|^2\,\mathrm{d}y &= \int_{-\infty}^{\infty}(1+y^2)^{1/4}\frac{4\sin^2\left(\frac{y}{2}\right)}{y^2}\,\mathrm{d}y \\ &= \int_{-1}^{1}(1+y^2)^{1/4}\frac{\sin^2\left(\frac{y}{2}\right)}{\left(\frac{y}{2}\right)^2}\,\mathrm{d}y + \int_{|y|\geqslant 1}(1+y^2)^{1/4}\frac{4\sin^2\left(\frac{y}{2}\right)}{y^2}\,\mathrm{d}y \\ &\leqslant \int_{-1}^{1}(1+y^2)^{1/4}\,\mathrm{d}y + \int_{|y|\geqslant 1}(1+y^2)^{1/4}\frac{4}{y^2}\,\mathrm{d}y < \infty.\end{aligned}$$

Therefore $f \in H^{1/4}(R)$. This completes the proof. □

Corollary 2.4. *If*

$$f(x) = \begin{cases} 1, & x \in [a,b), \\ 0, & x \notin [a,b). \end{cases}$$

Then $f \in H^{1/4}(R)$.

The following lemma is a discrete counterpart of Lemma 1.2.

Lemma 2.5. *For* $u = (u^1, u^2, \ldots, u^N)$, *where* u_i *is a complex number*, $1 \leqslant i \leqslant N$, *we have*

$$\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\cdot\tau\sum_{n=1}^{N}\overline{u^n}\frac{1}{\sqrt{\tau}}\left[a_0u^n - \sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})u^k\right]\right\} \geqslant 0,$$

where $\{a_k\}$ *is defined in* (1.16).

Proof. Define the function $u(t)$ as follows:

$$u(t) = \begin{cases} u^n, & t\in[t_{n-1},t_n),\ 1\leqslant n\leqslant N, \\ 0, & t\notin[t_0,t_N). \end{cases}$$

For $n = 1, 2, \ldots, N$, let

$$f_n(t) = \begin{cases} 1, & x\in[t_{n-1},t_n), \\ 0, & t\notin[t_{n-1},t_n). \end{cases}$$

Then

$$u(t) = \sum_{n=1}^{N} u^n f_n(t).$$

It follows from Corollary 2.4 that $u \in H^{1/4}(R)$.

By the integration by parts and using (2.1), we have

$$\begin{aligned}\int_0^{\infty}\overline{u(t)}\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_0^t\frac{u(s)}{\sqrt{t-s}}\,\mathrm{d}s\right]\mathrm{d}t &= \int_0^{t_N}\overline{u(t)}\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_0^t\frac{u(s)}{\sqrt{t-s}}\,\mathrm{d}s\right]\mathrm{d}t = \sum_{n=1}^{N}\int_{t_{n-1}}^{t_n}\overline{u(t)}\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_0^t\frac{u(s)}{\sqrt{t-s}}\,\mathrm{d}s\right]\mathrm{d}t \\ &= \sum_{n=1}^{N}\overline{u^n}\int_{t_{n-1}}^{t_n}\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_0^t\frac{u(s)}{\sqrt{t-s}}\,\mathrm{d}s\right]\mathrm{d}t \\ &= \sum_{n=1}^{N}\overline{u^n}\left[\int_0^{t_n}\frac{u(s)}{\sqrt{t_n-s}}\,\mathrm{d}s - \int_0^{t_{n-1}}\frac{u(s)}{\sqrt{t_{n-1}-s}}\,\mathrm{d}s\right]\end{aligned}$$

$$
\begin{aligned}
&= \sum_{n=1}^{N} \overline{u^n}\left[\sum_{k=1}^{n} \int_{t_{k-1}}^{t_k} \frac{u(s)}{\sqrt{t_n - s}}\,\mathrm{d}s - \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{u(s)}{\sqrt{t_{n-1} - s}}\,\mathrm{d}s\right] \\
&= \sum_{n=1}^{N} \overline{u^n}\left[\sum_{k=1}^{n} u^k \int_{t_{k-1}}^{t_k} \frac{\mathrm{d}s}{\sqrt{t_n - s}} - \sum_{k=1}^{n-1} u^k \int_{t_{k-1}}^{t_k} \frac{\mathrm{d}s}{\sqrt{t_{n-1} - s}}\right] \\
&= \sum_{n=1}^{N} \overline{u^n}\left[\sum_{k=1}^{n} \sqrt{\tau} a_{n-k} u^k - \sum_{k=1}^{n-1} \sqrt{\tau} a_{n-k-1} u^k\right] \\
&= \sqrt{\tau} \sum_{n=1}^{N} \overline{u^n}\left[a_0 u^n - \sum_{k=1}^{n-1} (a_{n-k-1} - a_{n-k}) u^k\right].
\end{aligned}
$$

According to Lemma 1.2, we have

$$
\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}} \cdot \tau \sum_{n=1}^{N} \overline{u^n} \frac{1}{\sqrt{\tau}}\left[a_0 u^n - \sum_{k=1}^{n-1}(a_{n-k-1} - a_{n-k}) u^k\right]\right\} = \mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}} \cdot \int_0^{\infty} \overline{u(t)} \frac{\mathrm{d}}{\mathrm{d}t}\left[\int_0^t \frac{u(s)}{\sqrt{t-s}}\,\mathrm{d}s\right]\mathrm{d}t\right\} \geqslant 0.
$$

This completes the proof. □

3. The derivation of the difference scheme

We denote by $\Psi_j(t)$ the value of the solution $\psi(x,t)$ at the point (x_j,t). Using the Taylor expansion, it follows from (1.7), (1.8) with (1.3), (1.4) that

$$
\mathrm{i}\frac{\mathrm{d}\Psi_0(t)}{\mathrm{d}t} = -\frac{1}{2}\cdot\frac{2}{h}\left\{\frac{\Psi_1(t) - \Psi_0(t)}{h} - \sqrt{\frac{2}{\pi}}\mathrm{e}^{-\left(\frac{\pi}{4}+V_{-}t\right)\mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\Psi_0(s)\,\mathrm{e}^{\mathrm{i}V_{-}s}}{\sqrt{t-s}}\,\mathrm{d}s\right\} + V(x_0,t)\Psi_0(t) + R_0(t), \quad t>0, \tag{3.1}
$$

$$
\mathrm{i}\frac{\mathrm{d}\Psi_j(t)}{\mathrm{d}t} = -\frac{1}{2}\cdot\frac{1}{h^2}\left(\Psi_{j+1}(t) - 2\Psi_j(t) + \Psi_{j-1}(t)\right) + V(x_j,t)\Psi_j(t) + R_j(t), \quad 1 \leqslant j \leqslant M-1, t>0, \tag{3.2}
$$

$$
\mathrm{i}\frac{\mathrm{d}\Psi_M(t)}{\mathrm{d}t} = -\frac{1}{2}\cdot\frac{2}{h}\left\{-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\left(\frac{\pi}{4}+V_{+}t\right)\mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\Psi_M(s)\,\mathrm{e}^{\mathrm{i}V_{+}s}}{\sqrt{t-s}}\,\mathrm{d}s - \frac{\Psi_M(t) - \Psi_{M-1}(t)}{h}\right\} + V(x_M,t)\Psi_M(t) + R_M(t), \quad t>0, \tag{3.3}
$$

$$
\Psi_j(0) = \phi(x_j), \quad 0 \leqslant j \leqslant M, \tag{3.4}
$$

where there exists a constant c_1 such that

$$
|R_0(t)| \leqslant c_1 h, \quad |R_M(t)| \leqslant c_1 h, \quad |R_j(t)| \leqslant c_1 h^2, \quad 1 \leqslant j \leqslant M-1. \tag{3.5}
$$

For (3.1) and (3.3), we have used

$$
\frac{\partial^2\psi(x_1,t)}{\partial x^2} = \frac{2}{h}\left\{\frac{\psi(x_1+h,t) - \psi(x_1,t)}{h} - \frac{\partial\psi(x_1,t)}{\partial x}\right\} + \mathrm{O}(h),
$$

$$
\frac{\partial^2\psi(x_r,t)}{\partial x^2} = \frac{2}{h}\left\{\frac{\partial\psi(x_r,t)}{\partial x} - \frac{\psi(x_r,t) - \psi(x_r - h,t)}{h}\right\} + \mathrm{O}(h).
$$

Denote

$$
F(t) = \mathrm{e}^{-\mathrm{i}V_{-}t}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\Psi_0(s)\,\mathrm{e}^{\mathrm{i}V_{-}s}}{\sqrt{t-s}}\,\mathrm{d}s, \quad G(t) = \mathrm{e}^{-\mathrm{i}V_{+}t}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\Psi_M(s)\,\mathrm{e}^{\mathrm{i}V_{+}s}}{\sqrt{t-s}}\,\mathrm{d}s.
$$

It follows from (3.1)–(3.4) that

$$\mathrm{i}\cdot\frac{1}{2}\cdot\left[\frac{\mathrm{d}\Psi_0(t_n)}{\mathrm{d}t}+\frac{\mathrm{d}\Psi_0(t_{n-1})}{\mathrm{d}t}\right]$$
$$=-\frac{1}{2}\cdot\frac{2}{h}\left\{\frac{1}{2}\left[\frac{\Psi_1(t_n)-\Psi_0(t_n)}{h}+\frac{\Psi_1(t_{n-1})-\Psi_0(t_{n-1})}{h}\right]-\sqrt{\frac{2}{\pi}}\cdot\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\cdot\frac{1}{2}[F(t_n)+F(t_{n-1})]\right\}$$
$$+V\left(x_0,t_{n-\frac{1}{2}}\right)\cdot\frac{1}{2}[\Psi_0(t_n)+\Psi_0(t_{n-1})]+\mathrm{O}(\tau^2+h),\quad n\geqslant 1,$$
$$\mathrm{i}\cdot\frac{1}{2}\cdot\left[\frac{\mathrm{d}\Psi_j(t_n)}{\mathrm{d}t}+\frac{\mathrm{d}\Psi_j(t_{n-1})}{\mathrm{d}t}\right]$$
$$=-\frac{1}{4}\cdot\left\{\frac{1}{h^2}\left[\Psi_{j+1}(t_n)-2\Psi_j(t_n)+\Psi_{j-1}(t_n)\right]+\frac{1}{h^2}\left[\Psi_{j+1}(t_{n-1})-2\Psi_j(t_{n-1})+\Psi_{j-1}(t_{n-1})\right]\right\}$$
$$+V\left(x_j,t_{n-\frac{1}{2}}\right)\cdot\frac{1}{2}\left[\Psi_j(t_n)+\Psi_j(t_{n-1})\right]+\mathrm{O}(\tau^2+h^2),\quad 1\leqslant j\leqslant M-1,\ n\geqslant 1,$$
$$\mathrm{i}\cdot\frac{1}{2}\cdot\left[\frac{\mathrm{d}\Psi_M(t_n)}{\mathrm{d}t}+\frac{\mathrm{d}\Psi_M(t_{n-1})}{\mathrm{d}t}\right]$$
$$=-\frac{1}{2}\cdot\frac{2}{h}\left\{-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{2}[G(t_n)+G(t_{n-1})]-\frac{1}{2}\left[\frac{\Psi_M(t_n)-\Psi_{M-1}(t_n)}{h}+\frac{\Psi_M(t_{n-1})-\Psi_{M-1}(t_{n-1})}{h}\right]\right\}$$
$$+V\left(x_M,t_{n-\frac{1}{2}}\right)\cdot\frac{1}{2}[\Psi_M(t_n)+\Psi_M(t_{n-1})]+\mathrm{O}(\tau^2+h),\quad n\geqslant 1,$$
$$\Psi_j(0)=\phi(x_j),\quad 0\leqslant j\leqslant M.$$

Denote

$$\Psi_j^n=\Psi_j(t_n).$$

Using Taylor expansion and applying Lemma 2.2, we have

$$\mathrm{i}\cdot\frac{\Psi_0^n-\Psi_0^{n-1}}{\tau}=-\frac{1}{2}\cdot\frac{2}{h}\left\{\frac{\Psi_1^{n-\frac{1}{2}}-\Psi_0^{n-\frac{1}{2}}}{h}-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0\Psi_0^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\Psi_0^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_-(t_n-t_k)}\right]+\mathrm{O}(\tau^{3/2})\right\}$$
$$+V\left(x_0,t_{n-\frac{1}{2}}\right)\Psi_0^{n-\frac{1}{2}}+\mathrm{O}(\tau^2+h),\quad n\geqslant 1,\tag{3.6}$$
$$\mathrm{i}\cdot\frac{\Psi_j^n-\Psi_j^{n-1}}{\tau}=-\frac{1}{2}\cdot\frac{1}{h^2}\left(\Psi_{j+1}^{n-\frac{1}{2}}-2\Psi_j^{n-\frac{1}{2}}+\Psi_{j-1}^{n-\frac{1}{2}}\right)+V\left(x_j,t_{n-\frac{1}{2}}\right)\Psi_j^{n-\frac{1}{2}}+\mathrm{O}(\tau^2+h^2),\quad 1\leqslant j\leqslant M-1,\ n\geqslant 1,\tag{3.7}$$
$$\mathrm{i}\cdot\frac{\Psi_M^n-\Psi_M^{n-1}}{\tau}=-\frac{1}{2}\cdot\frac{2}{h}\left\{-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0\Psi_M^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\Psi_M^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_+(t_n-t_k)}\right]+\mathrm{O}(\tau^{3/2})-\frac{\Psi_M^{n-\frac{1}{2}}-\Psi_{M-1}^{n-\frac{1}{2}}}{h}\right\}$$
$$+V\left(x_M,t_{n-\frac{1}{2}}\right)\Psi_M^{n-\frac{1}{2}}+\mathrm{O}(\tau^2+h),\quad n\geqslant 1,\tag{3.8}$$
$$\Psi_j^0=\phi(x_j),\quad 0\leqslant j\leqslant M.\tag{3.9}$$

Omitting the small terms in (3.6)–(3.9), we construct the difference scheme (1.12)–(1.15) for (1.7), (1.8) with (1.3), (1.4).

4. The stability and convergence of the difference scheme

In this section, we will discuss the stability and convergence of the difference scheme.

If $u\equiv\{u_0,u_1,\ldots,u_M\}$ and $v\equiv\{v_0,v_1,\ldots,v_M\}$ are two grid (complex) functions on ω_h, introduce the following inner product and the norm:

$$(u,v)=h\left(\frac{1}{2}\overline{u_0}v_0+\sum_{j=1}^{M-1}\overline{u_j}v_j+\frac{1}{2}\overline{u_M}v_M\right),\quad \|u\|=\sqrt{(u,u)}.$$

Theorem 4.1. *Let* $\{\psi_j^n\}$ *be the solution of the difference scheme* (1.12)–(1.15). *Then, we have*

$$\|\psi^n\| \leqslant \|\phi\|, \quad n = 1, 2, \ldots.$$

Proof. Multiplying (1.12) by $-\frac{1}{2}\mathrm{i}h\overline{\psi_0^{n-\frac{1}{2}}}$, (1.13) by $-\mathrm{i}h\overline{\psi_j^{n-\frac{1}{2}}}$ and (1.14) by $-\frac{1}{2}\mathrm{i}h\overline{\psi_M^{n-\frac{1}{2}}}$, respectively, then summing up the results, we obtain

$$h\left(\frac{1}{2}\overline{\psi_0^{n-\frac{1}{2}}}\frac{\psi_0^n-\psi_0^{n-1}}{\tau}+\sum_{j=1}^{M-1}\overline{\psi_j^{n-\frac{1}{2}}}\frac{\psi_j^n-\psi_j^{n-1}}{\tau}+\frac{1}{2}\overline{\psi_M^{n-\frac{1}{2}}}\frac{\psi_M^n-\psi_M^{n-1}}{\tau}\right)$$
$$=-\frac{1}{2}\mathrm{i}h\sum_{j=0}^{M-1}\left|\frac{\psi_{j+1}^{n-\frac{1}{2}}-\psi_j^{n-\frac{1}{2}}}{h}\right|^2-\frac{1}{2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{\psi_0^{n-\frac{1}{2}}}\left[a_0\psi_0^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\psi_0^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_-(t_n-t_k)}\right]$$
$$-\frac{1}{2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{\psi_M^{n-\frac{1}{2}}}\left[a_0\psi_M^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\psi_M^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_+(t_n-t_k)}\right]-\mathrm{i}\left(\psi^{n-\frac{1}{2}},V\left(\cdot,t_{n-\frac{1}{2}}\right)\psi^{n-\frac{1}{2}}\right).$$

Taking the real part, we have

$$\frac{1}{2\tau}\left(\|\psi^n\|^2-\|\psi^{n-1}\|^2\right)=-\frac{1}{2}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{\psi_0^{n-\frac{1}{2}}}\left[a_0\psi_0^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\psi_0^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_-(t_n-t_k)}\right]\right\}$$
$$-\frac{1}{2}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{\psi_M^{n-\frac{1}{2}}}\left[a_0\psi_M^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\psi_M^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_+(t_n-t_k)}\right]\right\}$$
$$+\mathrm{Re}\left\{-\mathrm{i}\left(\psi^{n-\frac{1}{2}},V(\cdot,t_{n-\frac{1}{2}})\psi^{n-\frac{1}{2}}\right)\right\}. \tag{4.1}$$

Let

$$\omega_j=1,\quad 1\leqslant j\leqslant M-1\quad\text{and}\quad \omega_0=\omega_M=\frac{1}{2}.$$

Since

$$-\mathrm{i}\left(\psi^{n-\frac{1}{2}},V\left(\cdot,t_{n-\frac{1}{2}}\right)\psi^{n-\frac{1}{2}}\right)=-\mathrm{i}h\sum_{j=0}^{M}\omega_jV\left(x_j,t_{n-\frac{1}{2}}\right)\left|\psi_j^{n-\frac{1}{2}}\right|^2$$
$$=-\mathrm{i}h\sum_{j=0}^{M}\omega_j\left[\mathrm{Re}\left(V(x_j,t_{n-\frac{1}{2}})\right)+\mathrm{i}\,\mathrm{Im}\left(V\left(x_j,t_{n-\frac{1}{2}}\right)\right)\right]\left|\psi_j^{n-\frac{1}{2}}\right|^2$$
$$=h\sum_{j=0}^{M}\omega_j\,\mathrm{Im}\left(V\left(x_j,t_{n-\frac{1}{2}}\right)\right)\left|\psi_j^{n-\frac{1}{2}}\right|^2-\mathrm{i}h\sum_{j=0}^{M}\omega_j\,\mathrm{Re}\left(V\left(x_j,t_{n-\frac{1}{2}}\right)\right)\left|\psi_j^{n-\frac{1}{2}}\right|^2,$$

we have

$$\mathrm{Re}\left\{-\mathrm{i}\left(\psi^{n-\frac{1}{2}},V\left(\cdot,t_{n-\frac{1}{2}}\right)\psi^{n-\frac{1}{2}}\right)\right\}=h\sum_{j=0}^{M}\omega_j\,\mathrm{Im}\left(V\left(x_j,t_{n-\frac{1}{2}}\right)\right)\left|\psi_j^{n-\frac{1}{2}}\right|^2.$$

In addition, thanks to the assumption $\mathrm{Im}\,V(x,t)\leqslant 0$, we arrive at

$$\mathrm{Re}\left\{-\mathrm{i}\left(\psi^{n-\frac{1}{2}},V\left(\cdot,t_{n-\frac{1}{2}}\right)\psi^{n-\frac{1}{2}}\right)\right\}\leqslant 0. \tag{4.2}$$

Combining (4.1) and (4.2), we get

$$\frac{1}{2\tau}t(\|\psi^n\|^2-\|\psi^{n-1}\|^2)\leqslant-\frac{1}{2}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{\psi_0^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{n-\frac{1}{2}}}}\left[a_0\psi_0^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{n-\frac{1}{2}}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\psi_0^{k-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{k-\frac{1}{2}}}\right]\right\}$$
$$-\frac{1}{2}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{\psi_M^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{n-\frac{1}{2}}}}\left[a_0\psi_M^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{n-\frac{1}{2}}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})\psi_M^{k-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{k-\frac{1}{2}}}\right]\right\}. \tag{4.3}$$

Letting $u^n = \psi_0^{n-\frac{1}{2}} \mathrm{e}^{\mathrm{i}V_- t_{n-\frac{1}{2}}}$ and $u^n = \psi_M^{n-\frac{1}{2}} \mathrm{e}^{\mathrm{i}V_+ t_{n-\frac{1}{2}}}$ in Lemma 2.5, respectively, we have

$$\mathrm{Re}\left\{ \mathrm{e}^{\frac{\pi}{4}\mathrm{i}} \sum_{n=1}^{N} \overline{\psi_0^{n-\frac{1}{2}} \mathrm{e}^{\mathrm{i}V_- t_{n-\frac{1}{2}}}} \left[a_0 \psi_0^{n-\frac{1}{2}} \mathrm{e}^{\mathrm{i}V_- t_{n-\frac{1}{2}}} - \sum_{k=1}^{n-1} (a_{n-k-1} - a_{n-k}) \psi_0^{k-\frac{1}{2}} \mathrm{e}^{\mathrm{i}V_- t_{k-\frac{1}{2}}} \right] \right\} \geqslant 0 \tag{4.4}$$

and

$$\mathrm{Re}\left\{ \mathrm{e}^{\frac{\pi}{4}\mathrm{i}} \sum_{n=1}^{N} \overline{\psi_M^{n-\frac{1}{2}} \mathrm{e}^{\mathrm{i}V_+ t_{n-\frac{1}{2}}}} \left[a_0 \psi_M^{n-\frac{1}{2}} \mathrm{e}^{\mathrm{i}V_+ t_{n-\frac{1}{2}}} - \sum_{k=1}^{n-1} (a_{n-k-1} - a_{n-k}) \psi_M^{k-\frac{1}{2}} \mathrm{e}^{\mathrm{i}V_+ t_{k-\frac{1}{2}}} \right] \right\} \geqslant 0. \tag{4.5}$$

Summing up (4.3) for n from 1 to N, then using (4.4) and (4.5), we get

$$\frac{1}{2\tau}(\|\psi^N\|^2 - \|\psi^0\|^2) \leqslant 0, \quad N = 1, 2, \ldots,$$

or

$$\|\psi^n\| \leqslant \|\psi^0\|, \quad n = 1, 2, \ldots.$$

This completes the proof. □

Since the difference scheme (1.12)–(1.15) is a system of linear algebraic equations at each time level, it is easy to obtain

Corollary 4.2. *The difference scheme (1.12)–(1.15) has a unique solution.*

Next we turn to the question of the convergence of the difference scheme.

Theorem 4.3. *Assume (1.7), (1.8) with (1.3), (1.4) have solution $\psi(x,t) \in C_{x,t}^{4,3}([x_\mathrm{l}, x_\mathrm{r}] \times [0,T])$ and $\{\psi_j^n\}$ be the solution of (1.12)–(1.15). Then, we have*

$$\|\Psi^n - \psi^n\| \leqslant \mathrm{e}^{\frac{3T}{5}} \sqrt{\frac{6T}{5}} c \left(h^{3/2} + \frac{\tau^{3/2}}{h^{1/2}} + \sqrt{x_\mathrm{r} - x_\mathrm{l}} (\tau^2 + h^2) \right), \quad n\tau \leqslant T,$$

where the constant c is defined in (4.10).

Proof. Let

$$U_j^n = \Psi_j^n - \psi_j^n.$$

Subtracting (1.12)–(1.15) from (3.6)–(3.9), we can obtain the error equations:

$$\mathrm{i} \cdot \frac{U_0^n - U_0^{n-1}}{\tau} = -\frac{1}{2} \cdot \frac{2}{h} \left\{ \frac{U_1^{n-\frac{1}{2}} - U_0^{n-\frac{1}{2}}}{h} - \sqrt{\frac{2}{\pi}} \mathrm{e}^{-\frac{\pi}{4}\mathrm{i}} \frac{1}{\sqrt{\tau}} \left[a_0 U_0^{n-\frac{1}{2}} - \sum_{k=1}^{n-1} (a_{n-k-1} - a_{n-k}) U_0^{k-\frac{1}{2}} \mathrm{e}^{-\mathrm{i}V_-(t_n - t_k)} \right] \right\}$$
$$+ V(x_0, t_{n-\frac{1}{2}}) U_0^{n-\frac{1}{2}} + P_0^{n-\frac{1}{2}}, \quad n \geqslant 1, \tag{4.6}$$

$$\mathrm{i} \cdot \frac{U_j^n - U_j^{n-1}}{\tau} = -\frac{1}{2} \cdot \frac{1}{h^2} \left[U_{j+1}^{n-\frac{1}{2}} - 2U_j^{n-\frac{1}{2}} + U_{j-1}^{n-\frac{1}{2}} \right] + V\left(x_j, t_{n-\frac{1}{2}}\right) U_j^{n-\frac{1}{2}} + P_j^{n-\frac{1}{2}}, \quad 1 \leqslant j \leqslant M-1, \ n \geqslant 1, \tag{4.7}$$

$$\mathrm{i} \cdot \frac{U_M^n - U_M^{n-1}}{\tau} = -\frac{1}{2} \cdot \frac{2}{h} \left\{ -\sqrt{\frac{2}{\pi}} \mathrm{e}^{-\frac{\pi}{4}\mathrm{i}} \frac{1}{\sqrt{\tau}} \left[a_0 U_M^{n-\frac{1}{2}} - \sum_{k=1}^{n-1} (a_{n-k-1} - a_{n-k}) U_M^{k-\frac{1}{2}} \mathrm{e}^{-\mathrm{i}V_+(t_n - t_k)} \right] - \frac{U_M^{n-\frac{1}{2}} - U_{M-1}^{n-\frac{1}{2}}}{h} \right\}$$
$$+ V\left(x_M, t_{n-\frac{1}{2}}\right) U_M^{n-\frac{1}{2}} + P_M^{n-\frac{1}{2}}, \quad n \geqslant 1, \tag{4.8}$$

$$U_j^0 = 0, \quad 0 \leqslant j \leqslant M, \tag{4.9}$$

where there exists a constant c such that

$$|P_0^{n-\frac{1}{2}}| \leqslant c\left(h + \frac{\tau^{3/2}}{h}\right), \quad |P_M^{n-\frac{1}{2}}| \leqslant c\left(h + \frac{\tau^{3/2}}{h}\right), \quad |P_j^{n-\frac{1}{2}}| \leqslant c(h^2 + \tau^2), \quad 1 \leqslant j \leqslant M-1. \tag{4.10}$$

Multiplying (4.6) by $-\frac{1}{2}\mathrm{i}h\overline{U_0^{n-\frac{1}{2}}}$, (4.7) by $-\mathrm{i}h\overline{U_j^{n-\frac{1}{2}}}$ and (4.8) by $-\frac{1}{2}\mathrm{i}h\overline{U_M^{n-\frac{1}{2}}}$, respectively, then summing up the results, we obtain

$$h\left(\frac{1}{2}\overline{U_0^{n-\frac{1}{2}}}\cdot\frac{U_0^n-U_0^{n-1}}{\tau}+\sum_{j=1}^{M-1}\overline{U_j^{n-\frac{1}{2}}}\cdot\frac{U_j^n-U_j^{n-1}}{\tau}+\frac{1}{2}\overline{U_M^{n-\frac{1}{2}}}\cdot\frac{U_M^n-U_M^{n-1}}{\tau}\right)$$
$$=-\frac{1}{2}\mathrm{i}h\sum_{j=0}^{M-1}\left|\frac{U_{j+1}^{n-\frac{1}{2}}-2U_j^{n-\frac{1}{2}}}{h}\right|^2-\frac{1}{2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{U_0^{n-\frac{1}{2}}}\left[a_0U_0^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})U_0^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_-(t_n-t_k)}\right]$$
$$-\frac{1}{2}\sqrt{\frac{2}{\pi}}\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{U_M^{n-\frac{1}{2}}}\left[a_0U_M^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})U_M^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_+(t_n-t_k)}\right]-\mathrm{i}\left(U^{n-\frac{1}{2}},V(\cdot,t_{n-\frac{1}{2}})U^{n-\frac{1}{2}}\right)-\mathrm{i}\left(U^{n-\frac{1}{2}},P^{n-\frac{1}{2}}\right).$$

Taking the real part and noticing $\mathrm{Im}(V(x,t))\leqslant 0$, we get

$$\frac{1}{2\tau}(\|U^n\|^2-\|U^{n-1}\|^2)=-\frac{1}{2}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\ \mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{U_0^{n-\frac{1}{2}}}\left[a_0U_0^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})U_0^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_-(t_n-t_k)}\right]\right\}$$
$$-\frac{1}{2}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{U_M^{n-\frac{1}{2}}}\left[a_0U_M^{n-\frac{1}{2}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})U_M^{k-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}V_+(t_n-t_k)}\right]\right\}$$
$$+\left(U^{n-\frac{1}{2}},\left(\mathrm{Im}V\left(\cdot,t_{n-\frac{1}{2}}\right)\right)U^{n-\frac{1}{2}}\right)+\mathrm{Im}\left(\left(U^{n-\frac{1}{2}},P^{n-\frac{1}{2}}\right)\right)$$
$$\leqslant-\frac{1}{2}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{U_0^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{n-\frac{1}{2}}}}\left[a_0U_0^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{n-\frac{1}{2}}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})U_0^{k-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{k-\frac{1}{2}}}\right]\right\}$$
$$-\frac{1}{2}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{U_M^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{n-\frac{1}{2}}}}\left[a_0U_M^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{n-\frac{1}{2}}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})U_M^{k-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{k-\frac{1}{2}}}\right]\right\}$$
$$+\frac{1}{2}\left(\|U^{n-\frac{1}{2}}\|^2+\|P^{n-\frac{1}{2}}\|^2\right). \tag{4.11}$$

Applying Lemma 2.5 and similarly to the proof of (4.4), (4.5), we have

$$\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\sum_{n=1}^{N}\overline{U_0^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{n-\frac{1}{2}}}}\left[a_0U_0^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{n-\frac{1}{2}}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})U_0^{k-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_-t_{k-\frac{1}{2}}}\right]\right\}\geqslant 0 \tag{4.12}$$

and

$$\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\sum_{n=1}^{N}\overline{U_M^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{n-\frac{1}{2}}}}\left[a_0U_M^{n-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{n-\frac{1}{2}}}-\sum_{k=1}^{n-1}(a_{n-k-1}-a_{n-k})U_M^{k-\frac{1}{2}}\mathrm{e}^{\mathrm{i}V_+t_{k-\frac{1}{2}}}\right]\right\}\geqslant 0. \tag{4.13}$$

Summing up (4.11) for n from 1 to N and using (4.12) and (4.13), we get

$$\frac{1}{2\tau}\left(\|U^N\|^2-\|U^0\|^2\right)\leqslant\frac{1}{2}\sum_{n=1}^{N}\left(\|U^{n-\frac{1}{2}}\|^2+\|P^{n-\frac{1}{2}}\|^2\right),\quad N=1,2,\ldots,$$

or,

$$\|U^n\|^2\leqslant\|U^0\|^2+\frac{1}{2}\tau\sum_{k=1}^{n}\left(\|U^k\|^2+\|U^{k-1}\|^2\right)+\tau\sum_{k=1}^{n}\|P^{k-\frac{1}{2}}\|^2,\quad n=1,2,\ldots. \tag{4.14}$$

Since $1/(1-\frac{\tau}{2})\leqslant 6/5$ when $\tau\leqslant 1/3$, it follows from (4.14) that

$$\|U^n\|^2\leqslant\frac{6}{5}\left(\|U^0\|^2+\tau\sum_{k=0}^{n-1}\|U^k\|^2+\tau\sum_{k=1}^{n}\|P^{k-\frac{1}{2}}\|^2\right),\quad n=1,2,\ldots.$$

The discrete Gronwall inequality [16] gives

$$\|U^n\|^2 \leqslant \frac{6}{5}\,e^{\frac{6}{5}n\tau}\left(\|U^0\|^2 + \tau\sum_{k=1}^{n}\|P^{k-\frac{1}{2}}\|^2\right), \quad n = 1, 2, \ldots. \tag{4.15}$$

It follows from (4.9) and (4.10) that

$$\|U^0\| = 0 \tag{4.16}$$

and

$$\|P^{k-\frac{1}{2}}\|^2 \leqslant h\left[c\left(h + \frac{\tau^{3/2}}{h}\right)\right]^2 + (M-1)h\left[c(\tau^2 + h^2)\right]^2. \tag{4.17}$$

Substituting (4.16) and (4.17) into (4.15), we obtain

$$\|U^n\| \leqslant e^{\frac{3}{5}T}\sqrt{\frac{6T}{5}}c\left(h^{3/2} + \frac{\tau^{3/2}}{h^{1/2}} + \sqrt{x_r - x_l}(\tau^2 + h^2)\right), \quad n\tau \leqslant T.$$

This completes the proof. □

5. Numerical results

In order to demonstrate the effectiveness of our difference scheme, we compute the following problem:

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}, \quad x \in R,\ t > 0, \tag{5.1}$$

$$\psi(x,0) = \begin{cases} x(1-x), & x \in [0,1], \\ 0, & x \notin [0,1]. \end{cases} \tag{5.2}$$

The exact solution of the problem above is [13]

Table 1
Some numerical results

$M\backslash(x,t)$	(0.0, 1.0)	(0.5, 1.0)	(1.0, 1.0)
8	(0.07287, −0.05322)	(0.04519, −0.02713)	(0.07287, −0.05322)
16	(0.05258, −0.04603)	(0.05350, −0.03796)	(0.05258, −0.04603)
32	(0.05687, −0.04681)	(0.04065, −0.04507)	(0.05687, −0.04681)
64	(0.05526, −0.03981)	(0.04944, −0.04797)	(0.05526, −0.03981)
128	(0.05521, −0.04096)	(0.04680, −0.04449)	(0.05521, −0.04096)
256	(0.05439, −0.04009)	(0.04886, −0.04568)	(0.05438, −0.04008)
Exact solution	(0.05315, −0.03921)	(0.04816, −0.04581)	(0.05315, −0.03921)

Table 2
The errors of the difference solutions at $t = 1$

M	$\|\Psi^M - \psi^M\|$
8	0.152846E − 01
16	0.881551E − 02
32	0.436230E − 02
64	0.223932E − 02
128	0.118164E − 02
256	0.607033E − 03

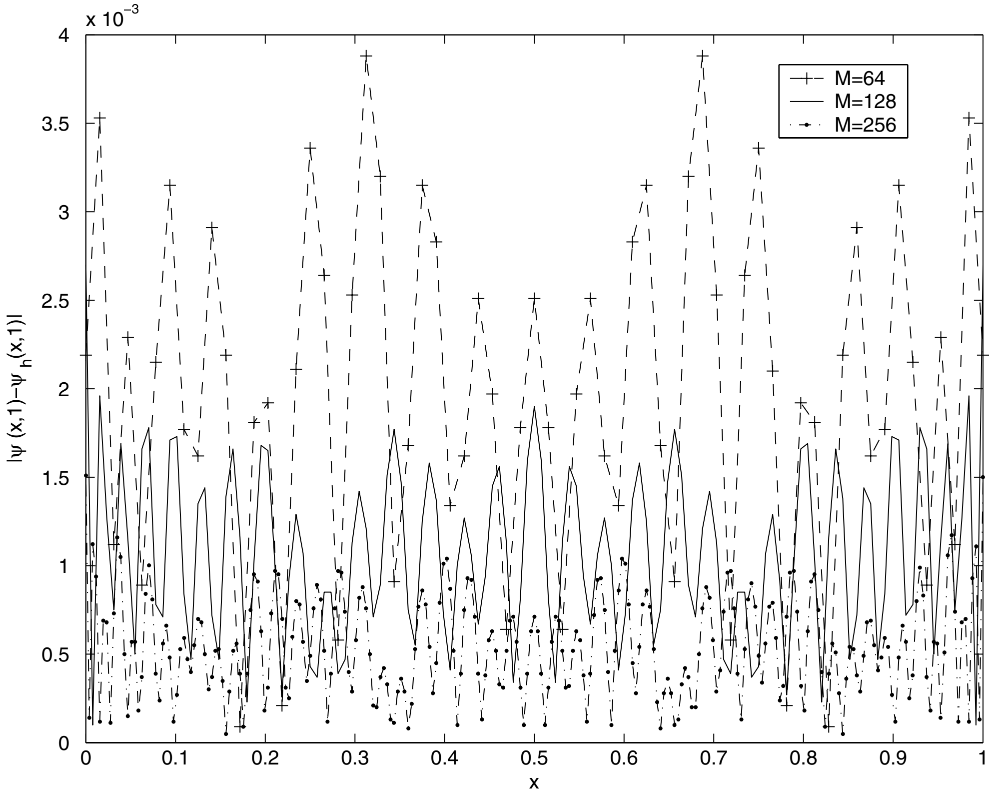

Fig. 1. The errors of the difference solutions at $t = 1$ with $M = 64, 128, 256$.

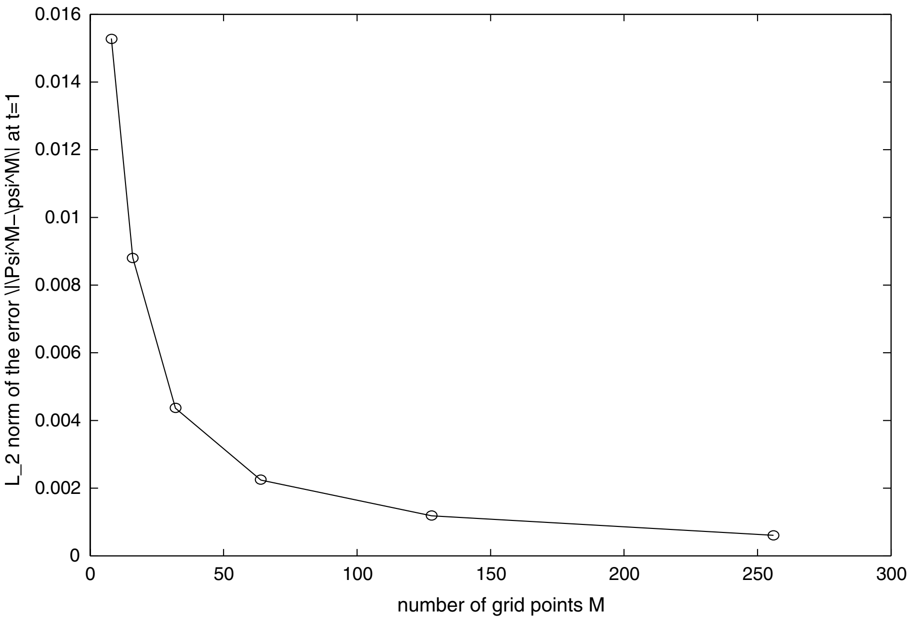

Fig. 2. The errors of the difference solutions at $t = 1$ with respect to M.

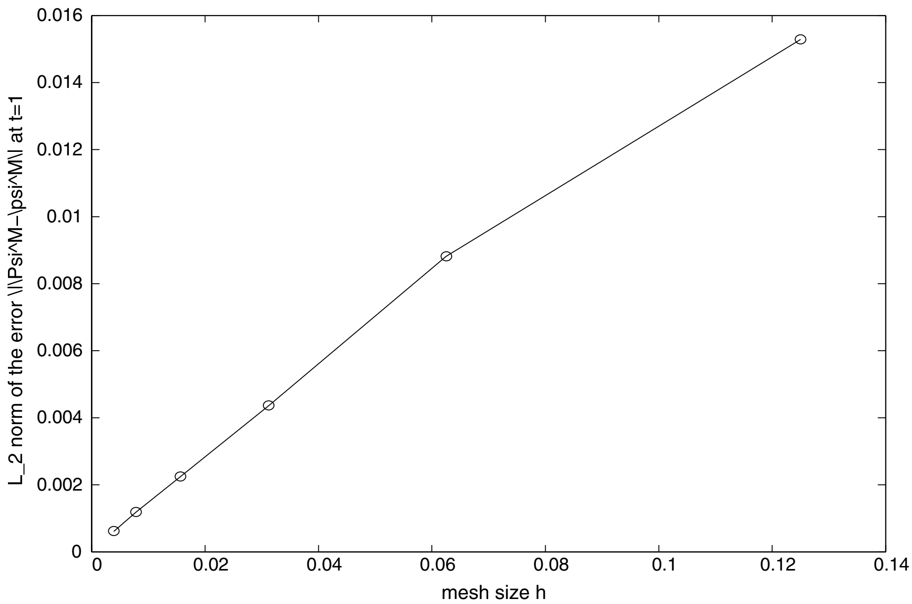

Fig. 3. The errors of the difference solutions at $t = 1$ with respect to h.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi t}} \int_0^1 \xi(1-\xi)\,\mathrm{e}^{\mathrm{i}\left[\frac{(x-\xi)^2}{2t}-\frac{\pi}{4}\right]}\,\mathrm{d}\xi. \tag{5.3}$$

Take $h = \tau = 1/M$. Table 1 gives some numerical solutions obtained by difference scheme (1.12)–(1.15) and exact solutions at three points. Table 2 presents the errors of difference solutions in L_2 norms with different mesh sizes on the line $t = 1$. Fig. 1 plots the errors of the difference solutions with $M = 64,128,256$ on the line $t = 1$. Fig. 2 plots the errors of the difference solutions in L_2 norm on the line $t = 1$ with respect to the grid number M. It is clear that $\|\Psi^M - \psi^M\|$ decreases much quickly as the grid number M increases. Fig. 3 plots the errors of the difference solutions in L_2 norm on the line $t = 1$ with respect to the mesh size h. It may be seen that the error $\|\Psi^M - \psi^M\|$ is approximately linearly dependent on h, i.e., there is a constant C such that

$$\|\Psi^M - \psi^M\| \approx Ch.$$

Using the least squares method and the data in Table 2, we obtain

$$\|\Psi^M - \psi^M\| \approx 0.127h.$$

This is in concordance with as our theoretical results.

6. Conclusion

In this paper, a numerical solution to the Schrödinger equation on an infinite domain is considered. Two exact artificial boundary conditions are introduced to reduce the original problem into an initial boundary value problem with computational domain. A fully discrete difference scheme are presented. The solvability, stability and convergence are analyzed by the energy method, where Lemma 2.5 plays an important role. A numerical example is shown to demonstrate the effectiveness of the difference scheme.

We have tried to construct some high order difference scheme, but we met a difficulty that no result similar to Lemma 2.5 can be obtained when we want to prove the stability and convergence.

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