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

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Abstract

This article is concerned with the numerical solution to the time-dependent 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 a finite computational domain. The artificial boundary conditions involve the 1/2 order fractional derivative in t. Then, a fully discrete explicit three-level difference scheme is derived. The truncation errors are analyzed in detail. The stability and convergence with the convergence order of $O(h^{3/2} + \tau h^{-1/2})$ are proved under the condition $\tau/h^2 < 1/2$ by the energy method. A numerical example is given to demonstrate the accuracy and efficiency of the proposed method. Two open problems are brought forward at the end of the article.

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Keywords: Schrödinger equation; Finite difference; Convergence; Solvability; Stability; Infinite domain; Artificial boundary condition; Fractional derivative boundary condition

1. Introduction

The time-dependent Schrödinger equation is the basic of quantum mechanics [8,16]. This model equation also arises in many other practical domains of physical and technological interest, e.g. optics, seismology and plasma physics. There are a lot of studies on the numerical solution of initial and initial-boundary problems for solving the linear or nonlinear Schrödinger equation, see e.g. [9–14,22,23,28,31,32,40,43].

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

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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 [15,18,19,35,36,41,42].

In this article, 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:

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

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

$$\lim_{|x|\to\infty}\psi(x,t) = 0, \quad t>0, \tag{1.3}$$

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. The solution to (1.1)–(1.3) is defined on the whole domain $\Omega=\{(x,t)|x\in R, t>0\}$. 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)–(1.3). To this end, let us split the initial domain Ω into three regions. We designate by $\Omega_i=\{(x,t)|x_l\leqslant x\leqslant x_r, t>0\}$ the interior domain where one wishes to compute an approximate solution, and the two other complementary regions can be defined by $\Omega_l=\{(x,t)|x<x_l, t>0\}$ and $\Omega_r=\{(x,t)|x>x_r, t>0\}$. To simplify the problem, we suppose that $\mathrm{supp}(\phi)\subset[x_l,x_r]$ and

$$V(x,t)=V_-\equiv\text{const}, \quad \text{for } x\leqslant x_l, \quad V(x,t)=V_+\equiv\text{const}, \quad \text{for } x\geqslant x_r,$$

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 [2,7,21,29]; Inhomogeneous extensions are analyzed in [1,4]. They are non-local in t and read

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

for the left boundary at $x=x_l$, and

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

for the right boundary at $x=x_r$. Using the notations of the Riemann–Liouville fractional derivative, the boundary conditions (1.4) and (1.5) can be written as

$$\frac{\partial\psi(x_l,t)}{\partial x} = \sqrt{2}\mathrm{e}^{-(\frac{\pi}{4}+V_-t)\mathrm{i}}\frac{\mathrm{d}^{1/2}[\psi(x_l,t)\mathrm{e}^{\mathrm{i}V_-t}]}{\mathrm{d}t^{1/2}},$$
$$\frac{\partial\psi(x_r,t)}{\partial x} = -\sqrt{2}\mathrm{e}^{-(\frac{\pi}{4}+V_+t)\mathrm{i}}\frac{\mathrm{d}^{1/2}[\psi(x_r,t)\mathrm{e}^{\mathrm{i}V_+t}]}{\mathrm{d}t^{1/2}}.$$

There are also an equivalent form to (1.4) and (1.5) as follows

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

for the left boundary at $x=x_l$, and

$$\psi(x_r,t) = -\sqrt{\frac{2}{\pi}}\mathrm{e}^{-(\frac{\pi}{4}+V_+t)i}\int_0^t\frac{\frac{\partial}{\partial x}[\psi(x_r,s)\mathrm{e}^{\mathrm{i}V_+s}]}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.7}$$

for the right boundary at $x = x_r$. Usually, (1.4) and (1.5) are called the Dirichlet–Neumann boundary conditions and (1.6) and (1.7) are called the Neumann–Dirichlet boundary conditions [2]. In [29], (1.6) and (1.7) are also called the impedance formulation.

As a consequence, the Cauchy problem (1.1)–(1.3) on the infinite domain can be reduced to the initial boundary value problem

$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi, \quad x_l \leqslant x \leqslant x_r, \quad t > 0, \tag{1.8}$$

$$\psi(x,0) = \phi(x), \quad x_l \leqslant x \leqslant x_r, \tag{1.9}$$

with the boundary conditions (1.4) and (1.5), or, with the boundary conditions (1.6) and (1.7).

Classically, the density $\|\psi\|_{L_2(R)}$ is decreasing for the problem (1.1)–(1.3) 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 $L_2([x_l,x_r])$-norm of the approximate solution. Arnold [3,5] proved the following result.

Theorem 1. *Let us assume that potential $V \in \Phi(R_t^+, L^\infty(C))$ satisfies: $Im(V(x,t)) \leqslant 0$, for $x \in [x_l, x_r]$ and $t > 0$. Let $\psi(x,t)$ be a solution to the initial boundary value problem (1.8) and (1.9) with (1.4) and 1.5), then, $\psi \in \Phi(R_t^+, H^1([x_l,x_r]))$ and fulfils the following energy inequality*

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

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 $t_n = n\tau, t_{n+\frac{1}{2}} = \left(n+\frac{1}{2}\right)\tau, n = 0,1,2,\ldots$

Eq. (1.8) is often discretized by the Crank–Nicolson scheme

$$\mathrm{i}\cdot\frac{\psi_j^n - \psi_j^{n-1}}{\tau} = -\frac{1}{2}\cdot\frac{1}{h^2}\left(\psi_{j+1}^{n-\frac{1}{2}} - 2\psi_j^{n-\frac{1}{2}} + \psi_{j-1}^{n-\frac{1}{2}}\right) + V\left(x_j, t_{n-\frac{1}{2}}\right)\psi_j^{n-\frac{1}{2}}, \quad 1 \leqslant j \leqslant M-1, \quad n \geqslant 1, \tag{1.10}$$

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. It is well-known that ad-hoc discretizations of analytic TBCs leads to numerical reflections and might render the unconditional stable Crank–Nicolson scheme only conditional stable. This destruction of the unconditional stability was proven in the thesis of Mayfield [27] in the context of underwater acoustics with a homogeneous Dirichlet BC at $x = 0$ and a discretized TBC only at $x = x_r$. Following Mayfield's discretization idea, if $V_- = 0$ and $V_+ = 0$, the TBCs (1.6) and (1.7) can be discretized by

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

and

$$\int_0^{t_N} \frac{\frac{\partial\psi(x_r,s)}{\partial x}}{\sqrt{t_N - s}}\,ds \approx \sum_{n=1}^{N} \frac{\psi(x_r, t_n) - \psi(x_r - h, t_n)}{h} \int_{t_{n-1}}^{t_n} \frac{\mathrm{d}s}{\sqrt{t_N - s}}. \tag{1.12}$$

Arnold and Ehrhardt [6] presented the following result.

Theorem 2. *The difference scheme (1.10)–(1.12) is stable, if and only if*

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

This shows that the chosen boundary discretization destroys the unconditional stability of the underlying Crank–Nicolson scheme. If $V(x,t) \equiv 0$, Baskakov and Popov [7] approximated boundary conditions (1.4) and (1.5) by the piece-wise linear approximations of the functions $\psi(x_l,s)$, $\psi(x_r,s)$ in the integrals:

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\psi(x_1,s)}{\sqrt{t-s}}\,\mathrm{d}s\right]\Bigg|_{t=t_N} = \left[\int_0^t \frac{\frac{\partial\psi(x_1,s)}{\partial s}}{\sqrt{t-s}}\,\mathrm{d}s\right]\Bigg|_{t=t_N} = \sum_{n=1}^{N}\int_{t_{n-1}}^{t_n}\frac{\frac{\partial\psi(x_1,s)}{\partial s}}{\sqrt{t_N-s}}\,\mathrm{d}s$$
$$\approx \sum_{n=1}^{N}\frac{\psi(x_1,t_n)-\psi(x_1,t_{n-1})}{\tau}\int_{t_{n-1}}^{t_n}\frac{\mathrm{d}s}{\sqrt{t_N-s}} \tag{1.13}$$

and

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\psi(x_r,s)}{\sqrt{t-s}}\,\mathrm{d}s\right]\Bigg|_{t=t_N} \approx \sum_{n=1}^{N}\frac{\psi(x_r,t_n)-\psi(x_r,t_{n-1})}{\tau}\int_{t_{n-1}}^{t_n}\frac{\mathrm{d}s}{\sqrt{t_N-s}}. \tag{1.14}$$

For the one-dimensional Schrödinger equation, also see the paper by Schmidt and Yevick [34]. Yevick, Friese and Schmidt [45] presented a comparison of transparent boundary conditions for the Fresnel equation. Schädle [33] 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 by using the finite element method and coupling the boundary conditions by collocation. A numerical example is given. Lubich and Schädle [25] 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 [39], for (1.8) and (1.9) with (1.4) and (1.5), we presented an implicit difference scheme. At each time level, only a tridiagonal system of linear algebraic equations needs to be solved and the Thomas method can be used. The unique solvability, unconditional stability and convergence are proved. The convergence order is of $O(h^{3/2}+\tau^{3/2}h^{-1/2})$. The numerical experiment shew the theoretical results. As a special case, the stability and convergence of the difference scheme (1.10), (1.13) and (1.14) are obtained. The authors of article [20] also derive an implicit difference scheme for (1.8), (1.9) with (1.4), (1.5) by the method of reduction of order [37,38] and analyze the stability and convergence.

As is well known, the explicit difference scheme has its own advantages. It is very simple for the numerical implementation. In this article we give an explicit difference scheme for (1.8) and (1.9) with (1.4) and (1.5). The explicit difference scheme considered is as follows:

$$\mathrm{i}\cdot\frac{\psi_0^{n+1}-\psi_0^{n-1}}{2\tau} = -\frac{1}{2}\cdot\frac{2}{h}\left\{\frac{\psi_1^n-\psi_0^n}{h}-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0\frac{\psi_0^{n+1}+\psi_0^{n-1}}{2}-\sum_{l=1}^{n-1}(a_{l-1}-a_l)\frac{\psi_0^{n-l+1}+\psi_0^{n-l-1}}{2}\mathrm{e}^{-\mathrm{i}V_{-}t_l}\right]\right\}$$
$$+V(x_0,t_n)\frac{\psi_0^{n+1}+\psi_0^{n-1}}{2},\quad n\geqslant 1, \tag{1.15}$$
$$\mathrm{i}\cdot\frac{\psi_j^{n+1}-\psi_j^{n-1}}{2\tau} = -\frac{1}{2}\cdot\frac{1}{h^2}(\psi_{j+1}^n-2\psi_j^n+\psi_{j-1}^n)+V(x_j,t_n)\frac{\psi_j^{n+1}+\psi_j^{n-1}}{2},\quad 1\leqslant j\leqslant M-1,\quad n\geqslant 1, \tag{1.16}$$
$$\mathrm{i}\cdot\frac{\psi_M^{n+1}-\psi_M^{n-1}}{2\tau} = -\frac{1}{2}\cdot\frac{2}{h}\left\{-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0\frac{\psi_M^{n+1}+\psi_M^{n-1}}{2}-\sum_{l=1}^{n-1}(a_{l-1}-a_l)\frac{\psi_M^{n-l+1}+\psi_M^{n-l-1}}{2}\mathrm{e}^{-\mathrm{i}V_{+}t_l}\right]\right.$$
$$\left.-\frac{\psi_M^n-\psi_{M-1}^n}{h}\right\}+V(x_M,t_n)\frac{\psi_M^{n+1}+\psi_M^{n-1}}{2},\quad n\geqslant 1, \tag{1.17}$$
$$\psi_j^0=\phi(x_j),\quad \psi_j^1=\phi(x_j)+\tau\phi_1(x_j),\quad 0\leqslant j\leqslant M, \tag{1.18}$$

where

$$\phi_1(x)=\mathrm{i}\left[\frac{1}{2}\phi''(x)-V(x,0)\phi(x)\right], \tag{1.19}$$
$$a_l=\frac{2}{\sqrt{l}+\sqrt{l+1}},\quad l=0,1,2,\ldots \tag{1.20}$$

It is obvious that

$$a_{l-1}-a_l=\frac{2}{\sqrt{l-1}+\sqrt{l}}-\frac{2}{\sqrt{l}+\sqrt{l+1}}=\frac{4}{(\sqrt{l-1}+\sqrt{l})(\sqrt{l}+\sqrt{l+1})(\sqrt{l+1}+\sqrt{l-1})},\quad l=1,2,3,\ldots$$

which is a positive and decreasing sequence.

The interior scheme (1.16) is the leap-frog scheme [24], whose truncation error is $O(\tau^2+h^2)$. For the Dirichlet problem, the leap-frog scheme is conditional stable with the restrictive condition $\tau/h^2 \leqslant 1/2$ [24]. Another common used explicit scheme is the Dufort–Frankel scheme

$$\mathrm{i}\cdot\frac{\psi_j^{n+1}-\psi_j^{n-1}}{2\tau}=-\frac{1}{2}\cdot\frac{1}{h^2}\left[\psi_{j+1}^n-(\psi_j^{n+1}+\psi_j^{n-1})+\psi_{j-1}^n\right]+V(x_j,t_n)\frac{\psi_j^{n+1}+\psi_j^{n-1}}{2}.$$

It can be simply obtained by replacing the term ψ_j^n with $(\psi_j^{n+1}+\psi_j^{n-1})/2$ in the leap-frog scheme (1.16). The truncation error of the Dufort–Frankel scheme is of order $(\tau^2+h^2+(\tau/h)^2)$. For the Dirichlet problem, the Dufort–Frankel scheme is unconditional stable [24]. In order to ensure the consistency, the meshes should satisfy $\tau/h\to 0$ as the meshes τ and h go to zero. Therefore, the key to the convergence is the consistency.

By introducing a dissipative term to the leap-frog scheme, Dai [12] establishes a three level explicit difference scheme for the variable coefficient Schrödinger equation with initial and Dirichlet boundary conditions. The scheme is proved to be unconditional stable by the discrete energy method. The scheme is the same as the Dufort–Frankel scheme in [43] except a constant in the dissipative term.

The organization of this article is the following. In Section 2, we present some preliminary lemmas. Lemma 2 is prepared for the derivation of the difference scheme and Lemma 3 is for the analysis of the difference scheme. In Section 3, we derive the fully discretized explicit difference scheme (1.15)–(1.18) for the problem (1.8) and (1.9) with (1.4) and (1.5). The truncation errors are given in detail, which will be used in the proof of the convergence of the difference scheme. The stability and convergence are proved under the condition $\lambda\equiv\tau/h^2<1/2$ in Section 4. The convergence order is of $O(h^{3/2}+\tau h^{-1/2})$. Finally, Section 5 presents a numerical experiment showing the theoretical results. A brief conclusion is given at the end of the article. Theorems 3 and 4 are our main results. In the following, we suppose that the problem (1.1)–(1.3) has an appropriate smooth solution.

2. Preliminary lemmas

The following two lemmas will be used to derive the difference scheme (1.15)–(1.18).

Lemma 1 [44]. *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. *Suppose $f(t)\in C^2[0,t_{n+1}]$ 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

$$\frac{1}{2}[F(t_{n+1})+F(t_{n-1})]=\frac{1}{\sqrt{\tau}}\left[a_0\frac{f(t_{n+1})+f(t_{n-1})}{2}-\sum_{l=1}^{n-1}(a_{l-1}-a_l)\frac{f(t_{n-l+1})+f(t_{n-l-1})}{2}\mathrm{e}^{-\mathrm{i}vt_l}\right]$$
$$+r_1(a_{n-1}-a_n)\tau^{1/2}+r_2\tau^{3/2},$$

where $\{a_k\}$ is defined in (1.20) and there exists a constant C dependent on f such that

$$|r_1|\leqslant C,\quad |r_2|\leqslant C. \tag{2.1}$$

Proof. Similarly to the proof of Lemma 2.2 in [39], we can obtain

$$\begin{aligned}\frac{1}{2}[F(t_{n+1})+F(t_{n-1})] &= \frac{1}{2}\frac{1}{\sqrt{\tau}}\left\{\left[a_0 f(t_{n+1}) - \sum_{l=1}^{n}(a_{l-1}-a_l)f(t_{n-l+1})\mathrm{e}^{-\mathrm{i}vt_l}\right]\right.\\ &\quad \left. + \left[a_0 f(t_{n-1}) - \sum_{l=1}^{n-2}(a_{l-1}-a_l)f(t_{n-l-1})\mathrm{e}^{-\mathrm{i}vt_l}\right]\right\} + \mathrm{O}(\tau^{3/2})\\ &= \frac{1}{\sqrt{\tau}}\left[a_0\frac{f(t_{n+1})+f(t_{n-1})}{2} - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\frac{f(t_{n-l+1})+f(t_{n-l-1})}{2}\mathrm{e}^{-\mathrm{i}vt_l}\right.\\ &\quad \left. -(a_{n-1}-a_n)\frac{f(t_1)}{2}\mathrm{e}^{-\mathrm{i}vt_n}\right] + \mathrm{O}(\tau^{3/2})\\ &= \frac{1}{\sqrt{\tau}}\left[a_0\frac{f(t_{n+1})+f(t_{n-1})}{2} - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\frac{f(t_{n-l+1})+f(t_{n-l-1})}{2}\mathrm{e}^{-\mathrm{i}vt_l}\right]\\ &\quad -(a_{n-1}-a_n)\frac{f(t_1)}{2\sqrt{\tau}}\mathrm{e}^{-\mathrm{i}vt_n} + \mathrm{O}(\tau^{3/2}).\end{aligned}$$

Noticing that

$$\frac{f(t_1)}{2\sqrt{\tau}} = \frac{f(\tau)-f(0)}{2\sqrt{\tau}} = \frac{1}{2}f'(\eta)\sqrt{\tau}, \quad \eta\in(0,\tau),$$

this completes the proof. □

The following Lemma will be used for the analysis of the difference scheme. It is a discrete counterpart of Lemma 2.1 in [3], which states that the kernel of the Dirichlet-to-Neumann operator $\mathrm{e}^{\mathrm{i}\pi/4}\sqrt{\mathrm{d}/\mathrm{d}t}$ is of positive type in the sense of memory equations (see, e.g. [17]).

Lemma 3 [39]. *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 (1.20).

3. The consistency analysis of the overall scheme

We denote by $\Psi_j(t)$ the value of the solution $\psi(x,t)$ at the point (x_j,t).

Considering the differential equation (1.8) at the point (x_j,t), we have

$$\mathrm{i}\frac{\partial\psi(x_j,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi(x_j,t)}{\partial x^2} + V(x_j,t)\psi(x_j,t), \quad 0\leqslant j\leqslant M, \quad t>0. \tag{3.1}$$

Using the Taylor expansion, it follows from (3.1), (1.9) and (1.4), (1.5) that

$$\mathrm{i}\frac{\mathrm{d}\Psi_0(t)}{\mathrm{d}t} = -\frac{1}{2}\cdot\frac{2}{h}\left[\frac{\Psi_1(t)-\Psi_0(t)}{h} - \sqrt{\frac{2}{\pi}}\mathrm{e}^{-\left(\frac{\pi}{4}+V_-t\right)\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t\frac{\Psi_0(s)\mathrm{e}^{\mathrm{i}V_-s}}{\sqrt{t-s}}\,\mathrm{d}s\right] + V(x_0,t)\Psi_0(t) + R_0(t), \quad t>0, \tag{3.2}$$

$$\mathrm{i}\frac{\mathrm{d}\Psi_j(t)}{\mathrm{d}t} = -\frac{1}{2}\cdot\frac{1}{h^2}\left[\Psi_{j+1}(t)-2\Psi_j(t)+\Psi_{j-1}(t)\right] + V(x_j,t)\Psi_j(t) + R_j(t), \quad 1\leqslant j\leqslant M-1, \quad t>0, \tag{3.3}$$

$$\begin{aligned}\mathrm{i}\frac{\mathrm{d}\Psi_M(t)}{\mathrm{d}t} &= -\frac{1}{2}\cdot\frac{2}{h}\left[-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\left(\frac{\pi}{4}+V_+t\right)\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t\frac{\Psi_M(s)\mathrm{e}^{\mathrm{i}V_+s}}{\sqrt{t-s}}\,\mathrm{d}s - \frac{\Psi_M(t)-\Psi_{M-1}(t)}{h}\right]\\ &\quad + V(x_M,t)\Psi_M(t) + R_M(t), \quad t>0,\end{aligned} \tag{3.4}$$

$$\Psi_j(0) = \phi(x_j), \quad 0\leqslant j\leqslant M, \tag{3.5}$$

where there exists a constant c_1 such that

$$|R_0(t)| \leqslant c_1 h, \quad |R_M(t)| \leqslant c_1 h; \quad |R_j(t)| \leqslant c_1 h^2, \quad 1 \leqslant j \leqslant M-1. \tag{3.6}$$

For (3.2) and (3.4), we have used

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

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 (3.2)–(3.5) that

$$\begin{aligned}
&\mathrm{i}\frac{\mathrm{d}\Psi_0(t_n)}{\mathrm{d}t} = -\frac{1}{2}\cdot\frac{2}{h}\left[\frac{\Psi_1(t_n)-\Psi_0(t_n)}{h} - \sqrt{\frac{2}{\pi}}\cdot \mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\cdot\frac{1}{2}[F(t_{n+1})+F(t_{n-1})]\right] + V(x_0,t_n)\cdot\frac{1}{2}[\Psi_0(t_{n+1})+\Psi_0(t_{n-1})]\\
&\qquad + \mathrm{O}\left(h+\frac{\tau^2}{h}\right), \quad n\geqslant 1,\\
&\mathrm{i}\cdot\frac{\mathrm{d}\Psi_j(t_n)}{\mathrm{d}t} = -\frac{1}{2}\cdot\frac{1}{h^2}[\Psi_{j+1}(t_n)-2\Psi_j(t_n)+\Psi_{j-1}(t_n)] + V(x_j,t_n)\cdot\frac{1}{2}[\Psi_j(t_{n+1})+\Psi_j(t_{n-1})] + \mathrm{O}(\tau^2+h^2),\\
&\quad 1\leqslant j\leqslant M-1, \quad n\geqslant 1,\\
&\mathrm{i}\frac{\mathrm{d}\Psi_M(t_n)}{\mathrm{d}t} = -\frac{1}{2}\cdot\frac{2}{h}\left[-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{2}[G(t_{n+1})+G(t_{n-1})] - \frac{\Psi_M(t_n)-\Psi_{M-1}(t_n)}{h}\right] + V(x_M,t_n)\cdot\frac{1}{2}[\Psi_M(t_{n+1})\\
&\qquad + \Psi_M(t_{n-1})] + \mathrm{O}\left(h+\frac{\tau^2}{h}\right), \quad n\geqslant 1,\\
&\Psi_j(t_0) = \phi(x_j), \quad \Psi_j(t_1) = \phi(x_j)+\tau\phi_1(x_j)+\mathrm{O}(\tau^2), \quad 0\leqslant j\leqslant M.
\end{aligned}$$

Denote

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

Using the Taylor expansion and applying Lemma 2, we have

$$\begin{aligned}
\mathrm{i}\cdot\frac{\Psi_0^{n+1}-\Psi_0^{n-1}}{2\tau} &= -\frac{1}{2}\cdot\frac{2}{h}\left\{\frac{\Psi_1^n-\Psi_0^n}{h} - \sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0\frac{\Psi_0^{n+1}+\Psi_0^{n-1}}{2} - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\frac{\Psi_0^{n-l+1}+\Psi_0^{n-l-1}}{2}\mathrm{e}^{-\mathrm{i}V_- t_l}\right]\right.\\
&\quad\left. + (a_{n-1}-a_n)\mathrm{O}(\tau^{1/2}) + \mathrm{O}(\tau^{3/2})\right\} + V(x_0,t_n)\frac{\Psi_0^{n+1}+\Psi_0^{n-1}}{2} + \mathrm{O}\left(h+\frac{\tau^2}{h}\right), \quad n\geqslant 1,
\end{aligned} \tag{3.7}$$

$$\begin{aligned}
&\mathrm{i}\cdot\frac{\Psi_j^{n+1}-\Psi_j^{n-1}}{2\tau} = -\frac{1}{2}\cdot\frac{1}{h^2}(\Psi_{j+1}^n-2\Psi_j^n+\Psi_{j-1}^n) + V(x_j,t_n)\frac{\Psi_j^{n+1}+\Psi_j^{n-1}}{2} + \mathrm{O}(\tau^2+h^2),\\
&\quad 1\leqslant j\leqslant M-1, \quad n\geqslant 1,
\end{aligned} \tag{3.8}$$

$$\begin{aligned}
\mathrm{i}\cdot\frac{\Psi_M^{n+1}-\Psi_M^{n-1}}{\tau} &= -\frac{1}{2}\cdot\frac{2}{h}\left\{-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0\frac{\Psi_M^{n+1}+\Psi_M^{n-1}}{2} - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\frac{\Psi_M^{n-l+1}+\Psi_M^{n-l-1}}{2}\mathrm{e}^{-\mathrm{i}V_+ t_l}\right]\right.\\
&\quad\left. + (a_{n-1}-a_n)\mathrm{O}(\tau^{1/2}) + \mathrm{O}(\tau^{3/2}) - \frac{\Psi_M^n-\Psi_{M-1}^n}{h}\right\} + V(x_M,t_n)\frac{\Psi_M^{n+1}+\Psi_M^{n-1}}{2} + \mathrm{O}\left(h+\frac{\tau^2}{h}\right), \quad n\geqslant 1,
\end{aligned} \tag{3.9}$$

$$\Psi_j^0 = \phi(x_j), \quad \Psi_j^1 = \phi(x_j)+\tau\phi_1(x_j)+\mathrm{O}(\tau^2), \quad 0\leqslant j\leqslant M. \tag{3.10}$$

Omitting the small terms in (3.7)–(3.10), we construct the difference scheme (1.15)–(1.18) for (1.8) and (1.9) with (1.4) and (1.5).

4. The stability and convergence of the difference scheme

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

Let $u \equiv \{u_j | 0 \leqslant j \leqslant M\}$ and $v \equiv \{v_j | 0 \leqslant j \leqslant M\}$ are two grid (complex) functions on ω_h. Introduce the following inner product and the norms:

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

$$\|u\| = \sqrt{(u, u)}, \quad |u|_1^2 = h\sum_{j=1}^{M}\left|\frac{u_j - u_{j-1}}{h}\right|^2.$$

In addition, we denote

$$\delta_x u_{j-\frac{1}{2}} = \frac{1}{h}(u_j - u_{j-1}), \quad \delta_x^2 u_j = \frac{1}{h}\left(\delta_x u_{j+\frac{1}{2}} - \delta_x u_{j-\frac{1}{2}}\right).$$

Theorem 3. *Let $\{\psi_j^n\}$ be the solution of the difference scheme (1.15)–(1.18). Then we have*

$$\|\psi^{n+1}\|^2 + \|\psi^n\|^2 + \tau\cdot\mathrm{Im}\left\{h\sum_{j=1}^{M}\left(\delta_x\psi_{j-\frac{1}{2}}^{n+1}\right)\left(\delta_x\overline{\psi_{j-\frac{1}{2}}^{n}}\right)\right\} \leqslant \|\psi^1\|^2 + \|\psi^0\|^2 + \tau\cdot\mathrm{Im}\left\{h\sum_{j=1}^{M}\left(\delta_x\psi_{j-\frac{1}{2}}^{1}\right)\left(\delta_x\overline{\psi_{j-\frac{1}{2}}^{0}}\right)\right\},$$
$$n = 1, 2, \ldots. \tag{4.1}$$

In addition, if

$$\lambda \equiv \frac{\tau}{h^2} < \frac{1}{2}, \tag{4.2}$$

we have

$$\|\psi^{n+1}\|^2 + \|\psi^n\|^2 \leqslant \frac{1+2\lambda}{1-2\lambda}(\|\psi^1\|^2 + \|\psi^0\|^2), \quad n = 1, 2, \ldots. \tag{4.3}$$

Proof. Let

$$\phi_j^n = \frac{\psi_j^{n+1} + \psi_j^{n-1}}{2}$$

and denote

$$(\phi^n, V(\cdot, t_n)\phi^n) = h\left[\frac{1}{2}V(x_0, t_n)|\phi_0^n|^2 + \sum_{j=1}^{M-1}V(x_j, t_n)|\phi_j^n|^2 + \frac{1}{2}V(x_M, t_n)|\phi_M^n|^2\right].$$

Multiplying (1.15) by $-\mathrm{i}h\overline{\phi_0^n}$, (1.16) by $-2\mathrm{i}h\overline{\phi_j^n}$ and (1.17) by $-\mathrm{i}h\overline{\phi_M^n}$ respectively, then summing up the results, we obtain

$$h\left[\frac{1}{2}(\overline{\psi_0^{n+1}} + \overline{\psi_0^{n-1}})(\psi_0^{n+1} - \psi_0^{n-1}) + \sum_{j=1}^{M-1}(\overline{\psi_j^{n+1}} + \overline{\psi_j^{n-1}})(\psi_j^{n+1} - \psi_j^{n-1}) + \frac{1}{2}(\overline{\psi_M^{n+1}} + \overline{\psi_M^{n-1}})(\psi_M^{n+1} - \psi_M^{n-1})\right]\Big/(2\tau)$$
$$= \mathrm{i}\left[\overline{\phi_0^n}\delta_x\psi_{\frac{1}{2}}^n + h\sum_{j=1}^{M-1}\overline{\phi_j^n}\delta_x^2\psi_j^n - \overline{\phi_M^n}\delta_x\psi_{M-\frac{1}{2}}^n\right] - \mathrm{i}\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{\phi_0^n}\left[a_0\phi_0^n - \sum_{l=1}^{n-1}(a_{l-1} - a_l)\phi_0^{n-l}\mathrm{e}^{-\mathrm{i}V_{-}t_l}\right]$$
$$- \mathrm{i}\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{\phi_M^n}\left[a_0\phi_M^n - \sum_{l=1}^{n-1}(a_{l-1} - a_l)\phi_M^{n-l}\mathrm{e}^{-\mathrm{i}V_{+}t_l}\right] - 2\mathrm{i}(\phi^n, V(\cdot, t_n)\phi^n)$$

$$
\begin{aligned}
&= -\mathrm{i}h\sum_{j=0}^{M-1}\left(\delta_x\overline{\phi^n_{j+\frac12}}\right)\left(\delta_x\psi^n_{j+\frac12}\right) - \sqrt{\frac{2}{\pi}}\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{\phi^n_0}\left[a_0\phi^n_0 - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\phi_0^{n-l}\mathrm{e}^{-\mathrm{i}V_-t_l}\right]\\
&\quad - \sqrt{\frac{2}{\pi}}\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{\phi^n_M}\left[a_0\phi^n_M - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\phi_M^{n-l}\mathrm{e}^{-\mathrm{i}V_+t_l}\right] - 2\mathrm{i}(\phi^n, V(\cdot,t_n)\phi^n).
\end{aligned}
$$

Taking the real part, we have

$$
\begin{aligned}
\frac{1}{2\tau}(\|\psi^{n+1}\|^2 - \|\psi^{n-1}\|^2) &= \mathrm{Im}\left\{h\sum_{j=0}^{M-1}\left(\delta_x\overline{\phi^n_{j+\frac12}}\right)\left(\delta_x\psi^n_{j+\frac12}\right)\right\}\\
&\quad - \sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{\phi^n_0}\left[a_0\phi^n_0 - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\phi_0^{n-l}\mathrm{e}^{-\mathrm{i}V_-t_l}\right]\right\}\\
&\quad - \sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{\phi^n_M}\left[a_0\phi^n_M - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\phi_M^{n-l}\mathrm{e}^{-\mathrm{i}V_+t_l}\right]\right\}\\
&\quad + 2\mathrm{Im}\{(\phi^n, V(\cdot,t_n)\phi^n)\}.
\end{aligned}\tag{4.4}
$$

Substituting

$$
\begin{aligned}
\mathrm{Im}\left\{\left(\delta_x\overline{\phi^n_{j-\frac12}}\right)\left(\delta_x\psi^n_{j-\frac12}\right)\right\} &= \frac12\left[\mathrm{Im}\left\{\left(\delta_x\overline{\psi^{n+1}_{j-\frac12}}\right)\left(\delta_x\psi^n_{j-\frac12}\right)\right\} + \mathrm{Im}\left\{\left(\delta_x\overline{\psi^{n-1}_{j-\frac12}}\right)\left(\delta_x\psi^n_{j-\frac12}\right)\right\}\right]\\
&= \frac12\left[-\mathrm{Im}\left\{\left(\delta_x\psi^{n+1}_{j-\frac12}\right)\left(\delta_x\overline{\psi^n_{j-\frac12}}\right)\right\} + \mathrm{Im}\left\{\left(\delta_x\psi^n_{j-\frac12}\right)\left(\delta_x\overline{\psi^{n-1}_{j-\frac12}}\right)\right\}\right]
\end{aligned}
$$

and (because of $\mathrm{Im}\{V(x,t)\} \leqslant 0$)

$$
\mathrm{Im}\{(\phi^n, V(\cdot,t_n)\phi^n)\} = (\phi^n, \mathrm{Im}\{V(\cdot,t_n)\}\phi^n) \leqslant 0
$$

into (4.4), we get

$$
\begin{aligned}
\frac{1}{\tau}(F^n - F^{n-1}) &\leqslant -\frac12\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{\phi^n_0\mathrm{e}^{\mathrm{i}V_-t_n}}\left[a_0\phi^n_0\mathrm{e}^{\mathrm{i}V_-t_n} - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\phi_0^{n-l}\mathrm{e}^{\mathrm{i}V_-t_{n-l}}\right]\right\}\\
&\quad -\frac12\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{\phi^n_M\mathrm{e}^{\mathrm{i}V_+t_n}}\left[a_0\phi^n_M\mathrm{e}^{\mathrm{i}V_+t_n} - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\phi_M^{n-l}\mathrm{e}^{\mathrm{i}V_+t_{n-l}}\right]\right\}
\end{aligned}\tag{4.5}
$$

where

$$
F^n = \|\psi^{n+1}\|^2 + \|\psi^n\|^2 + \tau\mathrm{Im}\left\{h\sum_{j=1}^{M}\left(\delta_x\psi^{n+1}_{j-\frac12}\right)\left(\delta_x\overline{\psi^n_{j-\frac12}}\right)\right\}.
$$

Since

$$
|\psi^n|_1^2 = h\sum_{j=1}^{M}\left|\frac{\psi^n_j - \psi^n_{j-1}}{h}\right|^2 \leqslant h\sum_{j=1}^{M}\frac{2}{h^2}(|\psi^n_j|^2 + |\psi^n_{j-1}|^2) \leqslant \frac{4}{h^2}\|\psi^n\|^2,
$$

we have

$$
\left|h\sum_{j=1}^{M}\left(\delta_x\psi^{n+1}_{j-\frac12}\right)\left(\delta_x\overline{\psi^n_{j-\frac12}}\right)\right| \leqslant |\psi^{n+1}|_1\cdot|\psi^n|_1 \leqslant \left(\frac{2}{h}\|\psi^{n+1}\|\right)\left(\frac{2}{h}\|\psi^n\|\right) \leqslant \frac{2}{h^2}(\|\psi^{n+1}\|^2 + \|\psi^n\|^2).
$$

Consequently, we have

$$
(1-2\lambda)(\|\psi^{n+1}\|^2 + \|\psi^n\|^2) \leqslant F^n \leqslant (1+2\lambda)(\|\psi^{n+1}\|^2 + \|\psi^n\|^2). \tag{4.6}
$$

It is seen that F^n is equivalent to $\|\psi^{n+1}\|^2 + \|\psi^n\|^2$ if $\lambda < 1/2$.

Letting $u^n = \phi_0^n e^{iV_- t_n}$ and $u^n = \phi_M^n e^{iV_+ t_n}$ in Lemma 3 respectively, we have

$$\mathrm{Re}\left\{e^{\frac{\pi}{4}i}\sum_{n=1}^{N}\overline{\phi_0^n e^{iV_- t_n}}\left[a_0\phi_0^n e^{iV_- t_n} - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\phi_0^{n-l}e^{iV_- t_{n-l}}\right]\right\} \geqslant 0 \tag{4.7}$$

and

$$\mathrm{Re}\left\{e^{\frac{\pi}{4}i}\sum_{n=1}^{N}\overline{\phi_M^n e^{iV_+ t_n}}\left[a_0\phi_M^n e^{iV_+ t_n} - \sum_{l=1}^{n-1}(a_{l-1}-a_l)\phi_M^{n-l}e^{iV_+ t_{n-l}}\right]\right\} \geqslant 0. \tag{4.8}$$

Summing up (4.5) for n from 1 to N, then using (4.7) and (4.8), we get

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

It follows that

$$F^n \leqslant F^0, \quad n = 1,2,\ldots,$$

which is (4.1).

Using (4.6) in (4.1), we get

$$(1-2\lambda)(\|\psi^{n+1}\|^2 + \|\psi^n\|^2) \leqslant (1+2\lambda)(\|\psi^1\|^2 + \|\psi^0\|^2).$$

When $\lambda < \frac{1}{2}$, we obtain

$$\|\psi^{n+1}\|^2 + \|\psi^n\|^2 \leqslant \frac{1+2\lambda}{1-2\lambda}(\|\psi^1\|^2 + \|\psi^0\|^2), \quad n = 1,2,3,\ldots.$$

This completes the proof. $\square$

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

Theorem 4. *Assume (1.8) and (1.9) with (1.4) and (1.5) have solution $\psi(x,t) \in C_{x,t}^{4,3}([x_l,x_r]\times[0,T])$ and $\{\psi_j^n\}$ be the solution of (1.15)–(1.18). Let*

$$U_j^n = \Psi_j^n - \psi_j^n, \quad \Psi_j^n = \psi(x_j,t_n), \quad 0 \leqslant j \leqslant M, \quad n \geqslant 0.$$

Then, if $\lambda < 1/2$ and $\tau \leqslant (1-2\lambda)/2$, we have

$$\|U^n\| \leqslant \frac{\sqrt{2}c}{\sqrt{1-2\lambda}}e^{\frac{T}{1-2\lambda}}\left\{\sqrt{(1+2\lambda)(x_r-x_l)}\tau^2 + \sqrt{T}\left[2\left(h^{3/2}+\frac{\tau^{3/2}}{h^{1/2}}\right)+\sqrt{2(x_r-x_l)}(\tau^2+h^2)\right]+\frac{2\sqrt{2}\tau}{h^{1/2}}\right\},$$
$$\text{when } n\tau \leqslant T,$$

or,

$$\|U^n\| = O(h^{3/2} + \tau h^{-1/2}), \quad \text{when } n\tau \leqslant T, \tag{4.9}$$

where the constant c is defined in (4.14) and (4.15).

Proof. Denote

$$W_j^n = \frac{1}{2}(U_j^{n+1} + U_j^{n-1}).$$

Subtracting (1.15)–(1.18) from (3.7)–(3.10), we can obtain the error equations:

$$\begin{aligned} i\cdot\frac{U_0^{n+1}-U_0^{n-1}}{2\tau} = {} & -\frac{1}{2}\cdot\frac{2}{h}\left\{\frac{U_1^n-U_0^n}{h} - \sqrt{\frac{2}{\pi}}e^{-\frac{\pi}{4}i}\frac{1}{\sqrt{\tau}}\left[a_0W_0^n - \sum_{l=1}^{n-1}(a_{l-1}-a_l)W_0^{n-l}e^{-iV_- t_l}\right]\right\} \\ & + V(x_0,t_n)W_0^n + P_0^n, \quad n \geqslant 1, \end{aligned} \tag{4.10}$$

$$\mathrm{i}\cdot\frac{U_j^{n+1}-U_j^{n-1}}{2\tau}=-\frac{1}{2}\cdot\frac{1}{h^2}(U_{j+1}^n-2U_j^n+U_{j-1}^n)+V(x_j,t_n)W_j^n+P_j^n,$$
$$1\leqslant j\leqslant M-1,\quad n\geqslant 1, \tag{4.11}$$
$$\mathrm{i}\cdot\frac{U_M^{n+1}-U_M^{n-1}}{2\tau}=-\frac{1}{2}\cdot\frac{2}{h}\left\{-\sqrt{\frac{2}{\pi}}\mathrm{e}^{-\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\left[a_0W_M^n-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_M^{n-l}\mathrm{e}^{-\mathrm{i}V_+t_l}\right]-\frac{U_M^n-U_{M-1}^n}{h}\right\}$$
$$+V(x_M,t_n)W_M^n+P_M^n,\quad n\geqslant 1, \tag{4.12}$$
$$U_j^0=0,\quad U_j^1=r_j,\quad 0\leqslant j\leqslant M, \tag{4.13}$$

where there exists a constant c such that

$$|P_0^n|\leqslant c\left[h+\frac{\tau^{3/2}}{h}+(a_{n-1}-a_n)\frac{\tau^{1/2}}{h}\right],\quad |P_M^n|\leqslant c\left[h+\frac{\tau^{3/2}}{h}+(a_{n-1}-a_n)\frac{\tau^{1/2}}{h}\right], \tag{4.14}$$
$$|P_j^{n-\frac{1}{2}}|\leqslant c(h^2+\tau^2),\quad 1\leqslant j\leqslant M-1;\quad |r_j|\leqslant c\tau^2,\quad 0\leqslant j\leqslant M. \tag{4.15}$$

Multiplying (4.10) by $-\mathrm{i}h\overline{W_0^n}$, (4.11) by $-2\mathrm{i}h\overline{W_j^n}$ and (4.12) by $-\mathrm{i}h\overline{W_M^n}$ respectively, then summing up the results, we obtain

$$h\left(\overline{W_0^n}\cdot\frac{U_0^{n+1}-U_0^{n-1}}{2\tau}+2\sum_{j=1}^{M-1}\overline{W_j^n}\cdot\frac{U_j^{n+1}-U_j^{n-1}}{2\tau}+\overline{W_M^n}\cdot\frac{U_M^{n+1}-U_M^{n-1}}{2\tau}\right)$$
$$=-\mathrm{i}h\sum_{j=0}^{M-1}\left(\delta_x\overline{W_{j+\frac{1}{2}}^n}\right)\left(\delta_xU_{j+\frac{1}{2}}^n\right)-\sqrt{\frac{2}{\pi}}\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{W_0^n}\left[a_0W_0^n-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_0^{n-l}\mathrm{e}^{-\mathrm{i}V_-t_l}\right]$$
$$-\sqrt{\frac{2}{\pi}}\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\frac{1}{\sqrt{\tau}}\overline{W_M^n}\left[a_0W_M^n-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_M^{n-l}\mathrm{e}^{-\mathrm{i}V_+t_l}\right]-2\mathrm{i}(W^n,V(\cdot,t_n)W^n)-2\mathrm{i}(W^n,P^n).$$

Similarly to the proof of Theorem 3, taking the real part and noticing $\mathrm{Im}(V(x,t))\leqslant 0$, we get

$$\frac{1}{2\tau}(G^n-G^{n-1})=-\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{W_0^n}\left[a_0W_0^n-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_0^{n-l}\mathrm{e}^{-\mathrm{i}V_-t_l}\right]\right\}$$
$$-\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{W_M^n}\left[a_0W_M^n-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_M^{n-l}\mathrm{e}^{-\mathrm{i}V_+t_l}\right]\right\}$$
$$+2\mathrm{Im}\{(W^n,V(\cdot,t_n)W^n)\}+2\mathrm{Im}\{(W^n,P^n)\}$$
$$\leqslant-\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{W_0^n\mathrm{e}^{\mathrm{i}V_-t_n}}\left[a_0W_0^n\mathrm{e}^{\mathrm{i}V_-t_n}-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_0^{n-l}\mathrm{e}^{\mathrm{i}V_-t_{n-l}}\right]\right\}$$
$$-\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\tau}}\mathrm{Re}\left\{\mathrm{e}^{\frac{\pi}{4}\mathrm{i}}\overline{W_M^n\mathrm{e}^{\mathrm{i}V_+t_n}}\left[a_0W_M^n\mathrm{e}^{\mathrm{i}V_+t_n}-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_M^{n-l}\mathrm{e}^{\mathrm{i}V_+t_{n-l}}\right]\right\}$$
$$+\|W^n\|^2+\|P^n\|^2. \tag{4.16}$$

where

$$G^n=\|U^{n+1}\|^2+\|U^n\|^2+\mathrm{Im}\left\{h\sum_{j=0}^{M-1}\left(\delta_xU_{j+\frac{1}{2}}^{n+1}\right)\left(\delta_x\overline{U_{j+\frac{1}{2}}^n}\right)\right\}.$$

Similarly to (4.6), we have

$$(1-2\lambda)(\|U^{n+1}\|^2+\|U^n\|^2)\leqslant G^n\leqslant(1+2\lambda)(\|U^{n+1}\|^2+\|U^n\|^2). \tag{4.17}$$

Applying Lemma 3 and similarly to the proof of (4.7), (4.8), we have

$$\mathrm{Re}\left\{e^{\frac{\pi}{4}i}\sum_{n=1}^{N}\overline{W_0^n e^{iV_-t_n}}\left[a_0 W_0^n e^{iV_-t_n}-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_0^{n-l}e^{iV_-t_{n-l}}\right]\right\}\geqslant 0 \tag{4.18}$$

and

$$\mathrm{Re}\left\{e^{\frac{\pi}{4}i}\sum_{n=1}^{N}\overline{W_M^n e^{iV_+t_n}}\left[a_0 W_M^n e^{iV_+t_n}-\sum_{l=1}^{n-1}(a_{l-1}-a_l)W_M^{n-l}e^{iV_+t_{n-l}}\right]\right\}\geqslant 0. \tag{4.19}$$

Summing up (4.16) for n from 1 to N and using (4.18) and (4.19), we get

$$\begin{aligned}\frac{1}{2\tau}\left(G^N-G^0\right)&\leqslant\sum_{n=1}^{N}(\|W^n\|^2+\|P^n\|^2)\leqslant\sum_{n=1}^{N}\left(\frac{\|U^{n+1}\|^2+\|U^{n-1}\|^2}{2}+\|P^n\|^2\right)\\&\leqslant\frac{1}{2}\sum_{n=1}^{N}(\|U^{n+1}\|^2+\|U^n\|^2)+\frac{1}{2}\|U^0\|^2+\sum_{n=1}^{N}\|P^n\|^2,\quad N\geqslant 1.\end{aligned}$$

Using (4.17), we have

$$G^n\leqslant G^0+\tau\|U^0\|^2+2\tau\sum_{k=1}^{n}\|P^k\|^2+\frac{\tau}{1-2\lambda}\sum_{k=1}^{n}G^k,\quad n\geqslant 1.$$

When $\tau\leqslant(1-2\lambda)/2$, it follows that

$$G^n\leqslant 2\left[G^0+\tau\|U^0\|^2+2\tau\sum_{k=1}^{n}\|P^k\|^2+\frac{\tau}{1-2\lambda}\sum_{k=1}^{n-1}G^k\right],\quad n\geqslant 1.$$

The discrete Gronwall inequality [30] gives,

$$G^n\leqslant 2e^{\frac{2n\tau}{1-2\lambda}}\left(G^0+\tau\|U^0\|^2+2\tau\sum_{k=1}^{n}\|P^k\|^2\right),\quad n\geqslant 1,$$

or,

$$\|U^{n+1}\|^2+\|U^n\|^2\leqslant\frac{2}{1-2\lambda}e^{\frac{2n\tau}{1-2\lambda}}\left((1+2\lambda)(\|U^1\|^2+\|U^0\|^2)+\tau\|U^0\|^2+2\tau\sum_{k=1}^{n}\|P^k\|^2\right),\quad n\geqslant 1. \tag{4.20}$$

It follows from (4.13)–(4.15) that

$$\|U^0\|=0,\quad \|U^1\|\leqslant\sqrt{x_r-x_l}\,c\tau^2 \tag{4.21}$$

and

$$\begin{aligned}\|P^n\|^2&\leqslant h\left[c\left(h+\frac{\tau^{3/2}}{h}+(a_{n-1}-a_n)\frac{\tau^{1/2}}{h}\right)\right]^2+(M-1)h\left[c(\tau^2+h^2)\right]^2\\&\leqslant 2c^2\left(h^{3/2}+\frac{\tau^{3/2}}{h^{1/2}}\right)^2+2c^2(a_{n-1}-a_n)^2\frac{\tau}{h}+(x_r-x_l)c^2(\tau^2+h^2)^2.\end{aligned} \tag{4.22}$$

Substituting (4.21) and (4.22) into (4.20) and using

$$\sum_{k=1}^{n}(a_{k-1}-a_k)^2\leqslant\sum_{k=1}^{n}(a_{k-1}-a_k)=a_0-a_n<a_0=2,$$

we obtain

$$\|U^{n+1}\|^2+\|U^n\|^2 \leqslant \frac{2}{1-2\lambda}e^{\frac{2n\tau}{1-2\lambda}}\left\{(1+2\lambda)(x_r-x_l)c^2\tau^4+2\tau\sum_{k=1}^{n}\left[2c^2\left(h^{3/2}+\frac{\tau^{3/2}}{h^{1/2}}\right)^2\right.\right.$$
$$\left.\left.+2c^2(a_{n-1}-a_n)^2\frac{\tau}{h}+(x_r-x_l)c^2(\tau^2+h^2)^2\right]\right\}$$
$$\leqslant \frac{2}{1-2\lambda}e^{\frac{2T}{1-2\lambda}}\left[(1+2\lambda)(x_r-x_l)c^2\tau^4+4c^2T\left(h^{3/2}+\frac{\tau^{3/2}}{h^{1/2}}\right)^2\right.$$
$$\left.+8c^2\frac{\tau^2}{h}+2(x_r-x_l)c^2T(\tau^2+h^2)^2\right],\quad \text{when}\quad (n+1)\tau\leqslant T,$$

which yields

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

when $n\tau\leqslant T$.

This completes the proof. □

5. Numerical results

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

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

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

The exact solution of the problem above is [26]

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

Take a positive integer M. Let $N=4M^2$, $h=1/M$, $\tau=1/N$. Then $\lambda=1/4$, $\tau=h^2/4$. Table 1 gives some numerical solutions obtained by the difference scheme (1.15)–(1.18) and the exact solutions at three points. Table 2 presents the errors of the difference solutions in L_2 norm with different mesh sizes on the line $t=1$. Fig. 1 plots the errors of the difference solutions with $M=8$, 16, 32, 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 different grid number M and step size h, respectively. It is clear that $\|\Psi^N-\psi^N\|$ decreases much quickly as the grid number M increases or as the mesh size h decreases. The values $\max_{1\leqslant n\leqslant N-1}\{\|\psi^n\|^2+\|\psi^{n+1}\|^2\}/(\|\psi^0\|^2+\|\psi^1\|^2)$ are listed at Table 3. The difference scheme (1.15)–(1.18) is stable when $\lambda=1/4$.

Table 1
Some numerical results with $\lambda=1/4$

$M\backslash(x,t)$	(0.0, 1.0)	(0.5, 1.0)	(1.0, 1.0)
8	0.051909 − 0.039143i	0.046943 − 0.047015i	0.051909 − 0.039143i
16	0.052847 − 0.039191i	0.047725 − 0.046029i	0.052847 − 0.039191i
32	0.053081 − 0.039207i	0.048020 − 0.045835i	0.053081 − 0.039207i
64	0.053136 − 0.03921i	0.048117 − 0.045814i	0.053136 − 0.039210i
128	0.053150 − 0.039211i	0.048148 − 0.04581i	0.053150 − 0.039211i
256	0.053153 − 0.039212i	0.048156 − 0.04581i	0.053153 − 0.039212i
Exact solution	0.053154 − 0.039212i	0.048159 − 0.04581i	0.053154 − 0.039212i

Table 2
The errors of the difference solutions at $t = 1$ with $\lambda = 1/4$

M $(N = 4M^2)$	$\|\Psi^N - \psi^N\|$	$\|\Psi^{N/4} - \psi^{N/4}\|/\|\Psi^N - \psi^N\|$
8	1.951271e − 3	*
16	4.987582e − 4	3.912
32	1.243734e − 4	4.010
64	3.113997e − 5	3.994
128	7.882658e − 6	3.950
256	1.991164e − 6	3.950

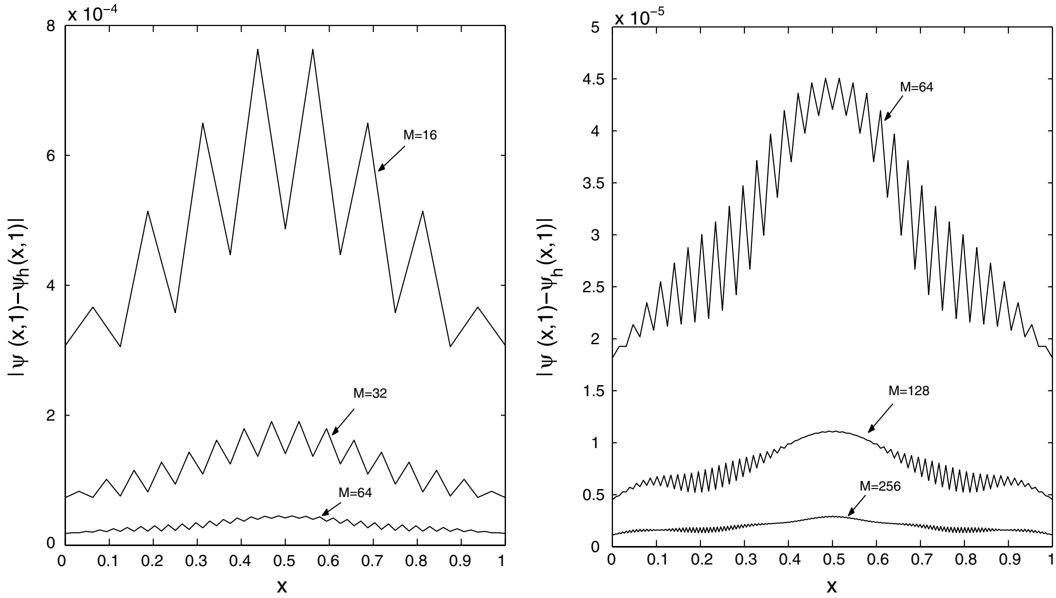

Fig. 1. The errors of the difference solutions at $t = 1$ when $\lambda = 1/4$.

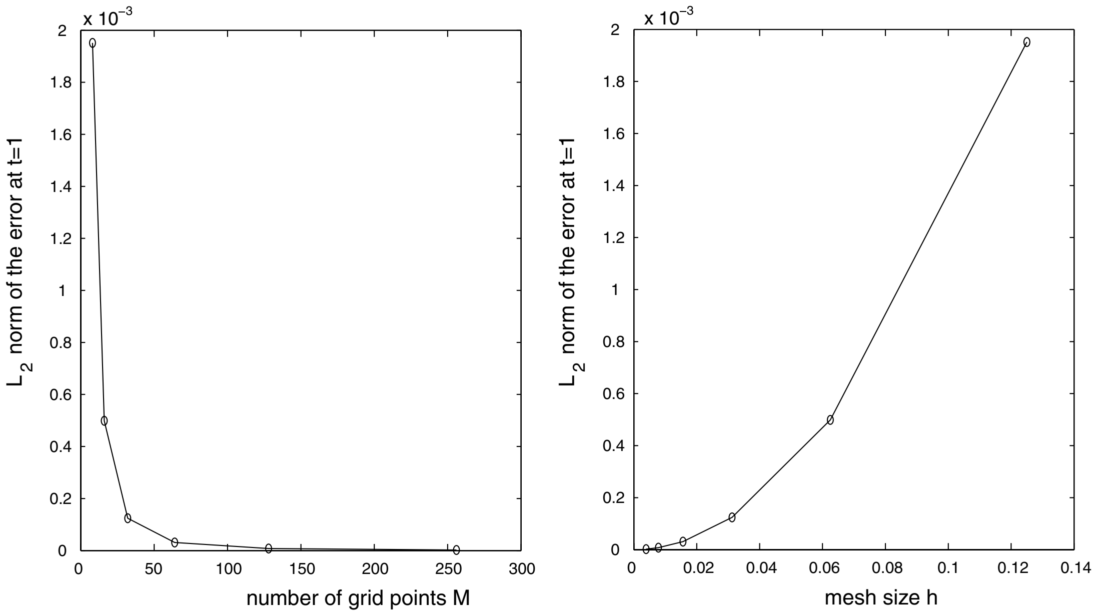

Fig. 2. The errors of the difference solutions at $t = 1$ with respect to h when $\lambda = 1/4$.

Table 3
The numerical stability of the difference solutions with $\lambda = 1/4$

M ($N = 4M^2$)	$\max_{1 \leqslant n \leqslant N-1}\{\|\psi^n\|^2 + \| \psi^{n+1}\|^2\}/(\|\psi^0\|^2 + \|\psi^1\|^2)$
8	1.002829
16	1.000345
32	1.000042
64	1.000005
128	1.000001

Table 4
Some numerical results with $\lambda = 1/3$

$M\backslash(x, t)$	(0.0, 1.0)	(0.5, 1.0)	(1.0, 1.0)
8	0.052013 − 0.039292i	0.046645 − 0.046626i	0.052013 − 0.039292i
16	0.052871 − 0.039217i	0.047476 − 0.045738i	0.052871 − 0.039217i
32	0.053077 − 0.039208i	0.047925 − 0.045837i	0.053077 − 0.039208i
64	0.053135 − 0.039211i	0.048107 − 0.045803i	0.053135 − 0.039211i
128	0.053149 − 0.039212i	0.048147 − 0.045812i	0.053149 − 0.039212i
256	0.053153 − 0.039212i	0.048155 − 0.045809i	0.053153 − 0.039212i
Exact solution	0.053154 − 0.039212i	0.048159 − 0.045810i	0.053154 − 0.039212i

Table 5
The errors of the difference solutions at $t = 1$ with $\lambda = 1/3$

M ($N = 3M^2$)	$\|\Psi^N - \psi^N\|$	$\|\Psi^{N/4} - \psi^{N/4}\|/\|\Psi^N - \psi^N\|$
8	2.012736e − 3	*
16	5.463110e − 4	3.684
32	1.414815e − 4	3.861
64	3.630773e − 5	3.897
128	9.268045e − 6	3.918
256	2.339402e − 6	3.962

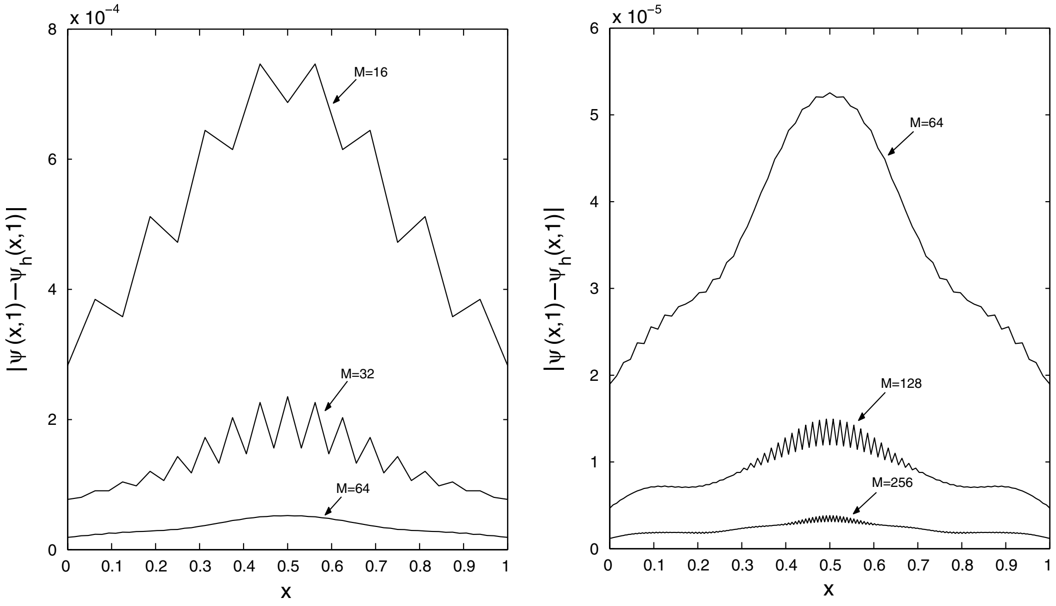

Fig. 3. The errors of the difference solutions at $t = 1$ when $\lambda = 1/3$.

Take a positive integer M. Let $N = 3\ M^2$, $h = 1/M$, $\tau = 1/N$. Then $\lambda = 1/3$, $\tau = h^2/3$. Table 4 gives some numerical solutions obtained by the difference scheme (1.15)–(1.18) and the exact solutions at three points. Table 5 presents the errors of difference solutions in L_2 norm with different mesh sizes on the line $t = 1$. Fig. 3 plots the errors of the difference solutions with $M = 8$, 16, 32, 64, 128, 256 on the line $t = 1$. Fig. 4 plots the errors of the difference solutions in L_2 norm on the line $t = 1$ with respect to the different grid number M and step size h, respectively. The values $\max_{1 \leqslant n \leqslant N-1}\{\|\psi^n\|^2 + \|\psi^{n+1}\|^2\}/(\|\psi^0\|^2 + \|\psi^1\|^2)$ are listed at Table 6. The difference scheme (1.15)–(1.18) is stable if $\lambda = 1/3$.

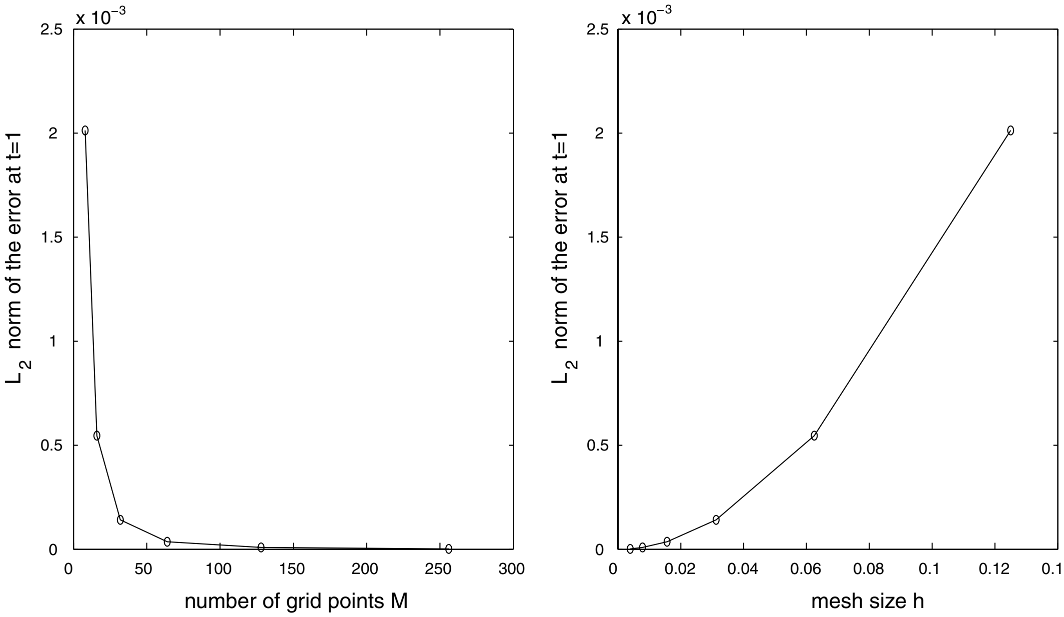

Fig. 4. The errors of the difference solutions at $t = 1$ with respect to h when $\lambda = 1/3$.

Table 6
The numerical stability of the difference solutions with $\lambda = 1/3$

M ($N = 3M^2$)	$\max_{1 \leqslant n \leqslant N-1}\{\|\psi^n\|^2 + \|\psi^{n+1}\|^2\}/(\|\psi^0\|^2 + \|\psi^1\|^2)$
8	1.004586
16	1.000549
32	1.000067
64	1.000008
128	1.000001

Table 7
Some numerical results at $t = 1$ with $\lambda = 1/2$

$M \backslash (x,t)$	$(0.0, 1.0)$	$(0.5, 1.0)$	$(1.0, 1.0)$
8	0.068505 − 0.068088i	0.062318 − 0.075926i	0.068505 − 0.068088i
16	0.060698 − 0.053681i	0.055177 − 0.060539i	0.060698 − 0.053681i
32	0.056888 − 0.04644i	0.051722 − 0.053083i	0.056888 − 0.046440i
64	0.055011 − 0.042823i	0.049968 − 0.049427i	0.055011 − 0.042823i
128	0.054080 − 0.041017i	0.049072 − 0.047615i	0.054080 − 0.041017i
256	0.053616 − 0.040114i	0.048618 − 0.046712i	0.053616 − 0.040114i
Exact solution	0.053154 − 0.039212i	0.048159 − 0.04581i	0.053154 − 0.039212i

Table 8
The errors of the difference solutions at $t = 1$ with $\lambda = 1/2$

M ($N = 2M^2$)	$\|\Psi^N - \psi^N\|$	$\|\Psi^{N/4} - \psi^{N/4}\|/\|\Psi^N - \psi^N\|$
8	3.343530e − 2	*
16	1.645601e − 2	2.032
32	8.165368e − 3	2.015
64	4.067780e − 3	2.007
128	2.030282e − 3	2.004
256	1.014255e − 3	2.002

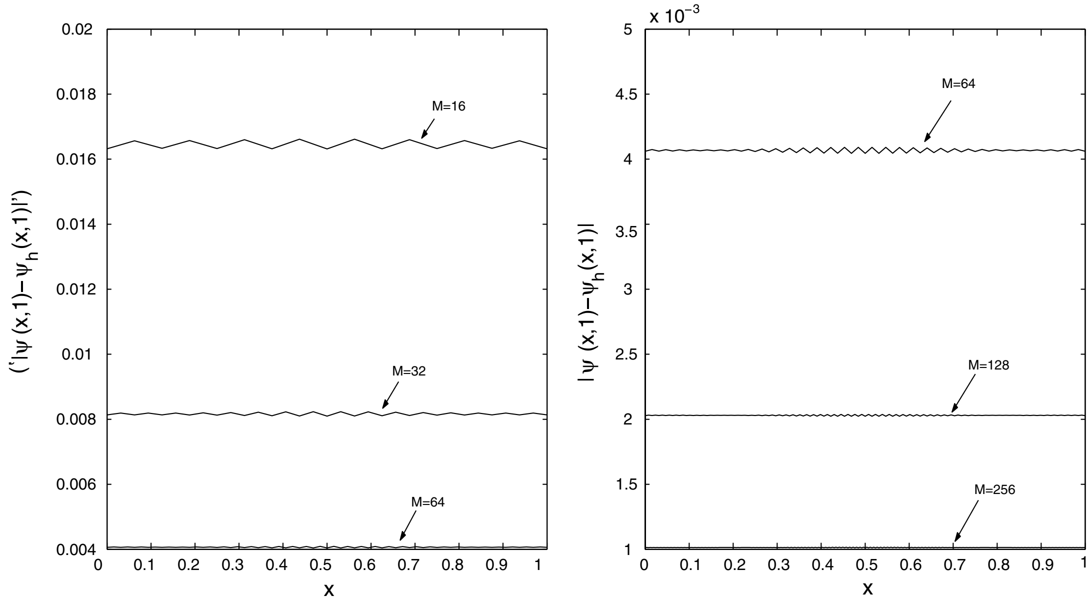

Fig. 5. The errors of the difference solutions at $t = 1$ when $\lambda = 1/2$.

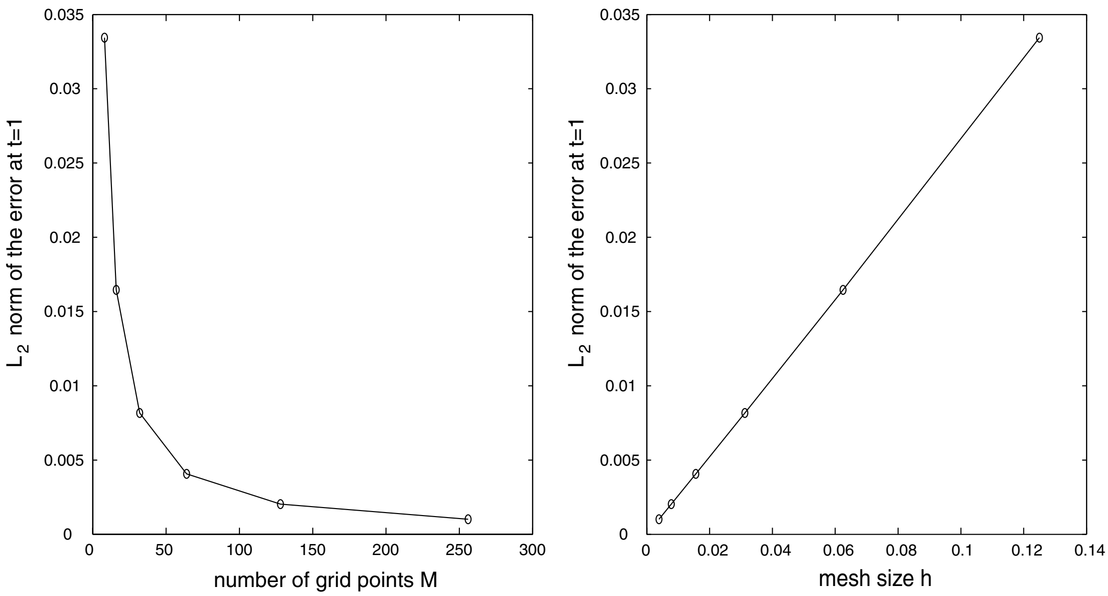

Fig. 6. The errors of the difference solutions at $t = 1$ with respect to h when $\lambda = 1/2$.

Table 9
The numerical stability of the difference solutions with $\lambda = 1/2$

M ($N = 2M^2$)	$\max_{1\leqslant n\leqslant N-1}\{\|\psi^n\|^2 + \|\psi^{n+1}\|^2\}/(\|\psi^0\|^2 + \|\psi^1\|^2)$
8	1.008996
16	1.001046
32	1.000125
64	1.000015
128	1.000002

Table 10
The numerical un-stability of the difference solutions with $M = 8$ and $N = 2M^2 - 1$

n	$\|\psi^n\|^2$	n	$\|\psi^n\|^2$
0	0.0333	37	0.0418
1	0.0334	47	0.0804
2	0.0339	57	0.1836
3	0.0327	67	0.4468
4	0.0333	77	1.1164
5	0.0328	87	2.8036
6	0.0330	97	7.0735
7	0.0324	107	17.4383
17	0.0316	117	45.0414
27	0.0298	127	113.6755

We find that the scheme is also convergent at the critical value $\lambda = 1/2$, but the convergence order is only 1 in space. Take $N = 2M^2$. Some numerical results obtained by the difference scheme (1.15)–(1.18) and the errors of the difference solutions on the line $t = 1$ in L_2 norm are presented in Tables 7 and 8. Fig. 5 plots the errors of the difference solutions with $M = 8$, 16, 32, 64, 128, 256 on the line $t = 1$. Fig. 6 plots the errors of the difference solutions in L_2 norm on the line $t = 1$ with respect to the different grid number M and step size h, respectively. The values $\max_{1\leqslant n\leqslant N-1}\{\|\psi^n\|^2 + \|\psi^{n+1}\|^2\}/\ (\|\psi^0\|^2 + \|\psi^1\|^2)$ are listed at Table 9. The difference scheme (1.15)–(1.18) is stable when $\lambda = 1/2$.

If we take $N = 2M^2 - 1$, numerical computation shows that the difference scheme is unstable. Some values $\|\psi^n\|^2$ are listed at Table 10. The difference scheme (1.15)–(1.18) is unstable.

6. Conclusion and two open problems

In this paper, a numerical solution to the time-dependent 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 a finite computational domain. A fully discrete three-level explicit difference scheme is presented. The stability and convergence are analyzed by the energy method, where Lemma 3 plays an important role. If $\tau/h^2 = O(1)$, then the convergence rate is order of $O(h^{3/2})$.

A numerical example is shown to demonstrate the effectiveness of the difference scheme. Seeing Tables 2 and 5, a second order reduction can be observed for the L_2 norm. There remains an open problem whether the estimate (4.9) is optimal or not. Moreover, at the critical value $\tau/h^2 = 1/2$, the numerical results show that the proposed scheme is still convergent, but with a less order 1. Could this be proved? This is an another open problem.

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