Analysis of finite element method for one-dimensional time-dependent Schrödinger equation on unbounded domain

Jicheng Jin\textsuperscript{a,*}, Xiaonan Wu\textsuperscript{b,2}

\textsuperscript{a}Department of Mathematics, Xiangtan University, Xiangtan, Hunan Province, China
\textsuperscript{b}Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong

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Abstract

This paper addresses the theoretical analysis of a fully discrete scheme for the one-dimensional time-dependent Schrödinger equation on unbounded domain. We first reduce the original problem into an initial-boundary value problem in a bounded domain by introducing a transparent boundary condition, then fully discretize this reduced problem by applying Crank–Nicolson scheme in time and linear or quadratic finite element approximation in space. By a rigorous analysis, this scheme has been proved to be unconditionally stable and convergent, its convergence order has also been obtained. Finally, two numerical examples are performed to show the accuracy of the scheme.

Keywords: Schrödinger equation; Finite element method; Artificial boundary

1. Introduction

We consider the following initial value problem of Schrödinger equation on $\mathbb{R}^1 \times [0, T]$:

\begin{align}
    i\psi_t(x, t) &= -\frac{1}{2}\psi_{xx}(x, t) + V(x, t)\psi(x, t), \quad \forall (x, t) \in \mathbb{R}^1 \times (0, T],
    
    \psi(x, 0) &= \psi^0(x), \quad \forall x \in \mathbb{R}^1,
\end{align}

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

This model equation arises in many practical domains of physical and technological interest, e.g., quantum mechanics, optics, seismology and plasma physics. To simplify the problem, we suppose that $\psi^0(x)$ is compact with

\begin{equation}
    \text{Supp}\{\psi^0\} \subset (0, 1),
\end{equation}

* Corresponding author.
E-mail addresses: jjc@xtu.edu.cn (J. Jin), xwu@hkbu.edu.hk (X. Wu).

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

\[
V(x, t) = \begin{cases} 
V_1, & 1 < x < +\infty, \quad 0 \leq t \leq T, \\
V_0, & -\infty < x \leq 0, \quad 0 \leq t \leq T.
\end{cases}
\]  

(1.4)

\( V_{tt}(x, t) \) is bounded in \([0, 1] \times [0, T]\), and \( \|V(\cdot, t)\|_{H^1(0,1)} \) is bounded in \([0, T]\). Without loss of generality, we assume that there exists a constant \( \widehat{V} \) such that

\[
V(x, t) \geq \widehat{V} > 0, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq T.
\]  

(1.5)

In fact, if \( V(x, t) \) does not satisfy (1.5), we can let \( \tilde{\psi}(x, t) = e^{i\xi t}\psi(x, t) \) and choose constant \( \lambda \) large enough such that \( \widehat{V}(x, t) = \lambda + V(x, t) \geq \widehat{V} \) in \([0, 1] \times [0, T]\), then \( \tilde{\psi}(x, t) \) satisfies

\[
\imath\tilde{\psi}_t(x, t) = -\frac{1}{2}\tilde{\psi}_{xx}(x, t) + \tilde{V}(x, t)\tilde{\psi}(x, t), \quad \forall (x, t) \in \mathbb{R}^1 \times (0, T),
\]

\[
\tilde{\psi}(x, 0) = \psi^0(x), \quad \forall x \in \mathbb{R}^1.
\]

Solving the time-dependent Schrödinger equation has become one of the main tools of modelling and simulating molecular encounters. In order to solve numerically such whole-space problem, we have to consider a finite subdomain and impose an artificial boundary condition. When the solution of this new problem is equal to the restriction to the subdomain of the original solution, we say that the artificial boundary condition is transparent.

Let \( \Omega = (0, 1) \), introduce two artificial boundaries \( \Gamma_0 = \{x = 0, 0 < t \leq T\} \) and \( \Gamma_1 = \{x = 1, 0 < t \leq T\} \), then \( \mathbb{R}^1 \times (0, T) \) is divided into three parts:

\[
Q_T^- = \{(x, t)| -\infty < x \leq 0, 0 < t \leq T\},
\]

\[
Q_T^+ = \{(x, t)| 1 \leq x < +\infty, 0 < t \leq T\},
\]

\[
Q_T = \{(x, t)| x \in \Omega, 0 < t \leq T\}.
\]

Subdomain \( Q_T \) is our computational domain.

For this problem, several authors in \([8,16,21]\) independently introduced the transparent boundary conditions as the following:

\[
\psi_\lambda(0, t) = \sqrt{\frac{\pi}{2}} \frac{e^{-i\pi/4}e^{-iV_0 t}}{\sqrt{t - \lambda}} \int_0^t \psi(0, \lambda)e^{iV_0 \lambda} d\lambda \quad \text{on } \Gamma_0,
\]  

(1.6)

\[
\psi_\lambda(1, t) = -\sqrt{\frac{\pi}{2}} \frac{e^{-i\pi/4}e^{-iV_1 t}}{\sqrt{t - \lambda}} \int_0^t \psi(1, \lambda)e^{iV_1 \lambda} d\lambda \quad \text{on } \Gamma_1.
\]  

(1.7)

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

\[
i\psi_t(x, t) = -\frac{1}{2}\psi_{xx}(x, t) + V(x, t)\psi(x, t), \quad \forall (x, t) \in Q_T,
\]  

(1.8)

\[
\psi_\lambda(0, t) = \sqrt{\frac{\pi}{2}} \frac{e^{-i\pi/4}e^{-iV_0 t}}{\sqrt{t - \lambda}} \int_0^t \psi(0, \lambda)e^{iV_0 \lambda} d\lambda, \quad 0 < t \leq T,
\]  

(1.9)

\[
\psi_\lambda(1, t) = -\sqrt{\frac{\pi}{2}} \frac{e^{-i\pi/4}e^{-iV_1 t}}{\sqrt{t - \lambda}} \int_0^t \psi(1, \lambda)e^{iV_1 \lambda} d\lambda, \quad 0 < t \leq T,
\]  

(1.10)

\[
\psi(x, 0) = \psi^0(x), \quad x \in \overline{\Omega}.
\]  

(1.11)

This initial-boundary value problem is well-posed and its solution coincides with the solution of the original problem (1.1)–(1.2) restricted to \( Q_T \) [2].

The main difficulty of the numerical approximation is linked to the boundary conditions (1.9) and (1.10) with the mildly singular convolution kernels since the numerical discretization for this kind of boundary conditions often makes the overall numerical scheme only conditionally stable when the Crank–Nicolson scheme or finite element method is used for the interior equation [8,20]. Moreover, the numerical reflections at the artificial boundaries may appear.
So far, several approaches have been proposed. Not discretizing the boundary conditions like (1.9) and (1.10), Arnold and Ehrhard [5–7,11] derived an exact discrete transparent boundary condition directly from the fully discretized Schrödinger equation on the whole space by using a Crank–Nicolson scheme. The resulting scheme is unconditionally stable and does not induce numerical reflection at the boundaries. However, it seems quite difficult to extend this approach to the finite element method. Similarly, Schmidt et al. [23–25], Friese et al. [12], Schädl et al. [22,18], Antoine et al. [2] and Alonso-Mallo et al. [1] first chosen a semi-discrete scheme of the Schrödinger equation and then derived the associated non-local transparent boundary condition or local absorbing boundary condition from the semi-discretized Schrödinger equation. These approaches are efficient, the resulting schemes are unconditionally stable, and no or only small numerical reflections appear at the boundaries. Mayfield [20], Baskakov and Popov (BP) [8] proposed the most straightforward approaches. They used the Crank–Nicolson scheme for the Schrödinger equation and the left-point rectangular quadrature rule or a higher-order quadrature rule to discretize the boundary conditions. Unfortunately, the resulting schemes have been proved to be conditionally stable and the strong numerical reflections can be induced. Recently, Wu et al. developed a new, modified BP approach for the boundary conditions of the heat equation [26] and the Schrödinger equation [13], the discretized boundary conditions are exact in spatial direction, the resulting finite difference scheme is unconditionally stable, and almost no numerical reflections appear at the boundaries.

For this problem, to our knowledge, there has been a lot of work on the finite difference approximation but only a little of work on the finite element approximation. In [1–3,22], the authors introduce some proper non-reflecting boundary conditions or absorbing boundary conditions for the one- or two-dimensional Schrödinger equations, construct the fully discrete schemes for the resulting initial-boundary value problems, where the finite element methods are employed for the spatial discretization. The approaches proposed in these papers are efficient, and the numerical examples also show that the numerical schemes have good accuracy, but no rigorous global error estimates are given for the fully discrete solutions. In this paper, we apply the approach proposed in [13] to discretize the boundary conditions (1.9) and (1.10), the Crank–Nicolson scheme in time and linear or quadratic finite element approximation in space to discretize Eq. (1.8). It is shown, by a rigorous analysis, that this fully discrete scheme is unconditionally stable and convergent, its global error order is also obtained. For time-spatial meshsize \( (\tau, h) \), the \( m \)-degree finite element approximation yields \( O(h^{-(s+1)/2}[h^{m+1}(1 + h^{m-1}|\ln \tau|^{1/2} + \tau^{3/2}]) \) accuracy in \( H^s \) norm, \( m = 1, 2, s = 0, 1 \). We emphasize here that the convergence rate \( \frac{3}{7} \) in time strongly depends on our approach of the boundary conditions which is of order \( \frac{3}{7} \) in time, hence, if a second-order discrete scheme of the boundary conditions is employed, then a global second-order convergence in time can be expected. Of course, this might make the theoretical analysis more lengthy and involved. We hope this paper can provide some insights on how to estimate the convergence order for this kind of problem.

The organization of this paper is the following. In Section 2, we will derive our fully discrete finite element scheme, its stability and convergence will be analyzed in Section 3. Section 4 is devoted to present two numerical examples to show the accuracy of the scheme.

2. Construction of fully discrete finite element scheme

For any complex valued functions \( u(x) \) and \( v(x) \), let \( (u, v) \) denote the inner product

\[
(u, v) = \int_{\Omega} u(x) \bar{v}(x) \, dx,
\]

where \( \bar{v} \) denotes the complex conjugate of \( v \). We introduce the function space

\[
H^{1,1}(Q_T) = \{ w(x, t) | w(x, t), w_x(x, t), w_t(x, t) \text{ are in } L^2(Q_T) \},
\]

and for a non-negative integer \( k \) and real number \( p, 1 \leq p \leq \infty \), we use \( W^{k,p}(\Omega) \) to denote the Sobolev space and \( L^p(0, T; X) \) to denote the space of all \( L^p \) integrable functions \( w(\cdot, t) \) from \( [0, T] \) into the Banach space \( X \), and define [10]

\[
W^{k,p}(0, T; X) = \left\{ w \in L^p(0, T; X), \frac{\partial^s w}{\partial t^s} \in L^p(0, T; X), \forall 0 \leq s \leq k \right\}
\]
where
\[
\|w\|_{W^{k,p}(0,T;X)} = \left( \sum_{s=0}^{k} \int_0^T \left\| \frac{\partial^s w}{\partial t^s} \right\|_X^p \right)^{1/p}, \quad 1 \leq p < \infty,
\]
\[
\|w\|_{W^{k,\infty}(0,T;X)} = \max_{0 \leq s \leq k} \left\{ \left\| \frac{\partial^s w}{\partial t^s} \right\|_{L^\infty(0,T)} \right\}.
\]

To simplify the notations, we denote \(W^0,p\) and \(W^k,2\) by \(L^p\) and \(H^k\), respectively. Then \(\psi(x,t)\), the weak solution of problem (1.8)-(1.11), is defined as the following:

\[
\psi(x,t) \in H^{1,1}(Q_T) \text{ such that for nearly all } t \in (0,T),
\]
\[
i(\psi, v) = A(\psi, v) + \sum_{j=0}^1 \tilde{v}(j,t) b_j(\psi(t)), \quad \forall v(x,t) \in H^{1,1}(Q_T),
\]
(2.1)
\[
\psi(x,0) = \psi^0(x), \quad x \in \overline{\Omega},
\]
(2.2)

where
\[
A(\psi, v) = \int_\Omega \left[ \frac{1}{2} \psi_\lambda(x,t) \tilde{v}_\lambda(x,t) + V(x,t)\psi(x,t)\tilde{v}(x,t) \right] \, dx,
\]
and
\[
b_j(\psi(t)) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{1 + \tau^2}} \int_0^1 \psi(j,\lambda) e^{iV_j\lambda} \, d\lambda, \quad j = 0, 1.
\]
(2.3)

For \(m = 1\) or 2, let \(h = 1/mJ\) and \(\tau = T/N\) be the mesh sizes in space and time with positive integer \(J\) and \(N\), \(x_j = jh, j = 0, 1, \ldots, mJ\), be the nodes in \(\overline{\Omega}\), \(t_n = n\tau, n = 0, 1, \ldots, N\), be the nodes in \([0,T]\) and \(e_j = [x_{m(j-1)}, x_{mj}], j = 1, \ldots, J\), be the elements of \(\overline{\Omega}\). We construct the linear \((m = 1)\) or quadratic \((m = 2)\) Lagrange finite element space:

\[
S^m_0 = \{ v_h(x) \mid v_h(x) \in C(\overline{\Omega}), v_h(x)|_{e_j} \text{ is a polynomial of degree } m, \quad j = 1, \ldots, J \}.
\]

We introduce the following notations. Let \(t^{n-1/2} = \frac{1}{2}(t_n + t_{n-1})\), and

\[
A^{n-1/2}(u,v) = \int_\Omega \left[ \frac{1}{2} u_x \tilde{v}_x + V(x,t_{n-1/2})u \tilde{v} \right] \, dx, \quad A^n(u,v) = \int_\Omega \left[ \frac{1}{2} u_x \tilde{v}_x + V(x,t_n)u \tilde{v} \right] \, dx.
\]

For function \(w(x,t)\) and function series \(u^n(x), n = 0, 1, 2, \ldots\), let

\[
\delta_t w^{n-1/2}(x) = \frac{1}{\tau} [w(x,t_n) - w(x,t_{n-1})], \quad \delta_t u^{n-1/2}(x) = \frac{1}{\tau} [u^n(x) - u^{n-1}(x)],
\]
\[
w^{n-1/2}(x) = \frac{1}{2} [w(x,t_n) + w(x,t_{n-1})], \quad u^{n-1/2}(x) = \frac{1}{2} [u^n(x) + u^{n-1}(x)].
\]

For function or function series \(\varphi, j = 0, 1\), we use the notation:

\[
F_j(\varphi) = e^{-i\pi/4} \left\{ a_0 \varphi^{n-1/2}(j) + \sum_{k=1}^{n-1} (a_{n-k} - a_{n-k-1}) e^{-iV_j(t_{n-k})} \varphi^{k-1/2}(j) \right\},
\]
(2.4)

where
\[
a_k = \sqrt{\frac{2}{\pi \tau}} (\sqrt{k+1} - \sqrt{k}), \quad k = 0, 1, 2, \ldots.
\]
(2.5)

Suppose that \(\psi(x,t)\) is the solution of problem (2.1)-(2.2) and

\[
\psi(x,t) \in W^{2,\infty}(0,T; W^{1,p}(\Omega)), \quad 1 \leq p \leq \infty,
\]
then for nearly all \( t \in [0, T] \),
\[
\frac{\partial^s \psi(x, t)}{\partial t^s} \in W^{1, p}(\Omega),
\]
and by the Sobolev embedding theorem,
\[
\left\| \frac{\partial^s \psi(x, t)}{\partial t^s} \right\|_{C(\Omega)} \leq c \left\| \frac{\partial^s \psi(x, t)}{\partial t^s} \right\|_{W^{1, p}(\Omega)}, \quad s = 0, 1, 2,
\]
where and throughout this paper, \( c \) is a constant independent of \( h \) and \( \tau \), but may have different values at different places.

Using the approach in [13] to discretize the boundary conditions (1.9) and (1.10), we have (see [13])
\[
\frac{1}{2} \left[ b_j \psi(t_n) + b_j \psi(t_{n-1}) \right] = F_j (\psi)^{n-1/2} + \gamma_j^{n-1/2}, \quad 1 \leq n \leq N,
\]
with
\[
|\gamma_j^{n-1/2}| \leq c \tau^{3/2} \| \psi(x, t) \|_{W^{2, \infty}(0, T; W^{1, p}({\Omega}))}.
\]

Then we define the finite element solution \( \Psi^n(x) \) of problem (1.8)–(1.11) as the following:

Find \( \Psi^n(x) \in S^m_h \) such that
\[
i(\delta_t \Psi^{n-1/2}(x), v_h(x)) = A^{n-1/2}(\Psi^{n-1/2}(x), v_h(x))
\]
\[
+ \sum_{j=0}^{1} \tilde{v}_h(j) F_j (\Psi)^{n-1/2}, \quad \forall v_h(x) \in S^m_h, \quad 1 \leq n \leq N,
\]
\[
\Psi^0(x) = \psi^0_I(x), \quad x \in \Omega,
\]
where \( \psi^0_I(x) \in S^m_h \) is the interpolation of \( \psi^0(x) \).

3. Analysis of the fully discrete scheme

We introduce the following lemma [13]:

**Lemma 1.** For any complex vector \( \mathbf{u} = (u^1, u^2, \ldots, u^N) \), the following inequality holds:
\[
\text{Re} \left\{ e^{i\pi/4} \sum_{n=1}^{N} \overline{u^n} \left[ a_0 u^n - \sum_{k=1}^{n-1} (a_{n-k-1} - a_{n-k}) u^k \right] \right\} \geq 0,
\]
where \( a_k \) is defined in (2.5).

By this lemma, we have the following result:

**Theorem 1.** The fully discrete scheme (2.9)–(2.10) is unconditionally stable, and
\[
\| \Psi^n \|_{L^2(\Omega)} \leq \| \Psi^0 \|_{L^2(\Omega)}.
\]

**Proof.** Taking \( v_h(x) = \Psi^{n-1/2}(x) \) in (2.9), we get
\[
\frac{i}{2\tau} \left( \| \Psi^n \|_{L^2(\Omega)}^2 - \| \Psi^{n-1} \|_{L^2(\Omega)}^2 \right) + \frac{i}{2\tau} \left( \langle \Psi^n, \Psi^{n-1} \rangle - \langle \Psi^n, \Psi^{n-1} \rangle \right)
\]
\[
= A^{n-1/2}(\Psi^{n-1/2}, \Psi^{n-1/2}) + \sum_{j=0}^{1} \overline{\Psi^{n-1/2}(j) F_j (\Psi)^{n-1/2}}, \quad 1 \leq n \leq N.
\]
Summing up the above equality for $n$ and comparing the imaginary parts of the results, we get
\[
\frac{1}{2\pi} (\|\Psi^n\|^2_{L^2(\Omega)} - \|\Psi^0\|^2_{L^2(\Omega)}) = \sum_{l=1}^{n} \sum_{j=0}^{l} \text{Im}\{\overline{\psi}^{l-1/2}(j) F_j(\Psi)^{l-1/2}\}. \tag{3.2}
\]
From (2.4),
\[
\overline{\psi}^{l-1/2}(j) F_j(\Psi)^{l-1/2} = -ie^{i\pi/4} \left\{ a_0 |\overline{\psi}^{l-1/2}(j)|^2 + \sum_{k=1}^{l-1} (a_{l-k} - a_{l-k-1}) e^{-iV_j(t_i-t_k)} \overline{\psi}^{k-1/2}(j) \overline{\psi}^{l-1/2}(j) \right\}.
\]
Then according to Lemma 1,
\[
\sum_{l=1}^{n} \text{Im}\{\overline{\psi}^{l-1/2}(j) F_j(\Psi)^{l-1/2}\}
\leq \text{Re}\left\{ e^{i\pi/4} \sum_{l=1}^{n} \overline{\psi}^{l-1/2}(j)e^{iV_jt_i} \left[ a_0 |\overline{\psi}^{l-1/2}(j)|e^{iV_jt_i} - \sum_{k=1}^{l-1} (a_{l-k} - a_{l-k-1}) \overline{\psi}^{k-1/2}(j)e^{iV_jt_i} \right] \right\} \geq 0.
\tag{3.3}
\]
Therefore (3.1) follows from (3.2) and (3.3). \(\square\)

Next we consider the convergence. Notice that $A(u, v)$ is bounded and coercive on $H^1(\Omega) \times H^1(\Omega)$, therefore for any fixed $t \in [0, T]$ and given $w(x, t) \in H^1(\Omega)$, we can define its elliptic projection $R_h w(x, t) \in S_h^m$ such that
\[
A(R_h w(x, t), v_h(x)) = A(w(x, t), v_h(x)), \quad \forall v_h(x) \in S_h^m. \tag{3.4}
\]

**Lemma 2.** If for any $t \in [0, T]$, $w(x, t), w_t(x, t) \in H^{m+1}(\Omega)$, then $E(x, t) = w(x, t) - R_h w(x, t)$ has estimates:
\[
\|E\|_{H^s(\Omega)} \leq c h^{m+1-s} \|w\|_{H^{m+1}(\Omega)}, \quad s = 0, 1, \tag{3.5}
\]
\[
\|E_t\|_{H^s(\Omega)} \leq c h^{m+1-s} (\|w_t\|_{H^{m+1}(\Omega)} + \|w\|_{H^{m+1}(\Omega)}), \quad s = 0, 1. \tag{3.6}
\]

**Proof.** Eq. (3.5) is a well-known result. Next we show the validity of (3.6). Let
\[
A_t(u, v) = \int\Omega V_t(x, t) u v \, dx, \quad E_t(x, t) = E_1(x, t) + E_2(x, t),
\]
where
\[
E_1(x, t) = w_t(x, t) - R_h w_t(x, t), \quad E_2(x, t) = R_h w_t(x, t) - \frac{\partial}{\partial t} R_h w(x, t).
\]
For fixed $t \in [0, T]$ and any $v_h(x, t) \in S_h^m$, from (3.4) we have
\[
A(E_2, v_h) = A \left( w_t - \frac{\partial}{\partial t} R_h w, v_h \right) = \frac{d}{dt} A(E, v_h) - A \left( E, \frac{\partial}{\partial t} v_h \right) - A_t(E, v_h) = A_t(E, v_h).
\]
Taking $v_h(x, t) = E_2(x, t)$ and from (1.5), we get
\[
\frac{1}{2} \|E_2\|_{H^1(\Omega)}^2 + \tilde{V} \|E_2\|^2_{L^2(\Omega)} \leq A(E_2, E_2) = A_t(E, E_2) \leq c \|E\|_{L^2(\Omega)} \|E_2\|_{L^2(\Omega)},
\]
which implies that
\[
\|E_2\|_{L^2(\Omega)} \leq c \|E\|_{L^2(\Omega)}, \quad \|E_2\|_{H^1(\Omega)} \leq c \|E\|_{L^2(\Omega)}. \tag{3.7}
\]
Noticing that (3.5) holds when \( w(x, t) \) is replaced by \( w_i(x, t) \), therefore (3.6) follows from (3.7) and the inequality

\[
\|E_i\|_{H^1(\Omega)} \leq \|E_i\|_{H^1(\Omega)} + \|E_2\|_{H^1(\Omega)}. \quad \Box
\]

**Lemma 3.** If for any \( t \in [0, T] \), \( w(x, t), w_i(x, t) \in H^{m+1}(\Omega) \), then at node \( x_j, j = 0, 1, \ldots, mJ \), \( E(x, t) = w(x, t) - R_h w(x, t) \) has estimates:

\[
|E(x, t)| \leq c^2 h^{m+1} \|w\|_{H^{m+1}(\Omega)}, \quad \text{(3.8)}
\]

\[
|E_i(x, t)| \leq c^2 h^{m+1} (\|w_i\|_{H^{m+1}(\Omega)} + \|w\|_{H^{m+1}(\Omega)}). \quad \text{(3.9)}
\]

Moreover, if \( V(x, t) \) is independent of \( t \), then

\[
|E_i(x, t)| \leq c^2 h^m \|w_i\|_{H^{m+1}(\Omega)}. \quad \text{(3.10)}
\]

**Proof.** We follow the idea in [9]. Suppose that \( u(x, t), v(x, t) \) are the solutions of equation

\[
-\frac{1}{2} \phi_x(x, t) + V(x, t) \phi(x, t) = 0, \quad x \in \Omega, \quad t \in [0, T], \quad \text{(3.11)}
\]

with boundary conditions

\[
u(0, t) = 1, \quad u_x(0, t) = 0, \quad v(1, t) = -1, \quad v_x(1, t) = 0,
\]

then \( u(x, t), v(x, t) \in H^{m+1}(\Omega) \).

For any \( t \in [0, T] \), the Wronsky determinant

\[
D(x, t) = \begin{vmatrix} u(x, t) & v(x, t) \\ u_x(x, t) & v_x(x, t) \end{vmatrix} = D(0, t) + \int_0^x [(uv_x)_x - (vu_x)_x] \, dx = D(0, t) = v_x(0, t).
\]

Noticing that the solution of Eq. (3.11) with boundary conditions \( \phi_x(0, t) = \phi_x(1, t) = 0 \) must be identically vanishing, so \( D(0, t) = v_x(0, t) \neq 0 \).

We construct the Green functions as the following:

\[
g(x, t; 0) = -\frac{2v(x, t)}{v_x(0, t)}, \quad g(x, t; 1) = \frac{2u(x, t)}{u_x(1, t)},
\]

\[
g(x, t; z) = \begin{cases} -\frac{2}{D(0, t)} u(x, t)v(z, t), & x \in [0, z) \\ -\frac{2}{D(0, t)} v(x, t)u(z, t), & x \in [z, 1] \end{cases}
\]

for \( z \in (0, 1) \).

It is easy to check that

\[
\varphi(x, t) = A(\varphi, \tilde{g}(; z)), \quad \forall \varphi(x, t) \in H^1(\Omega), \quad t \in [0, T].
\]

Let \( \tilde{g}(x, t; z) \in S_h^m \) is the interpolation of \( g(x, t; z) \). Then for node \( z = x_j, j = 0, 1, \ldots, mJ \), we have

\[
\|\tilde{g}(x, t; x_j) - \tilde{g}(x, t; x_j)\|_{H^1([0, x_j] \cup [x_j, 1])} \leq c h^m \|g(x, t; x_j)\|_{H^{m+1}([0, x_j] \cup [x_j, 1])}. \quad \text{(3.12)}
\]

Therefore (3.8) follows from (3.5), (3.12) and the following inequality:

\[
|E(x, t)| = |A(E, \tilde{g}(x, t; x_j))|
\]

\[
= |A(E, \tilde{g}(x, t; x_j) - \tilde{g}(x, t; x_j))|
\]

\[
\leq c \|E\|_{H^1(\Omega)} \|\tilde{g}(x, t; x_j) - \tilde{g}(x, t; x_j)\|_{H^{m+1}([0, x_j] \cup [x_j, 1])}.
\]

Let \( E_i(x, t) = E_1(x, t) + E_2(x, t) \) with

\[
E_1(x, t) = w_t(x, t) - R_h w(x, t), \quad E_2(x, t) = R_h w(x, t) - \frac{\partial}{\partial t} R_h w(x, t).
\]
Then from (3.7), (3.5), we have
\[
|E_2(x, t)| = |A(E_2, \tilde{g}(\cdot; x_j))| \\
\leq c\|E_2\|_{H^1(\Omega)} \|\tilde{g}(\cdot; x_j)\|_{H^1([0, x_j] \cup(x_j, 1])} \\
\leq c\|E\|_{L^2(\Omega)} \|\tilde{g}(\cdot; x_j)\|_{H^1([0, x_j] \cup(x_j, 1])} \\
\leq \varepsilon^m \|w\|_{H^{m+1}(\Omega)}.
\]
Noticing that (3.8) holds when \(w(x, t)\) is replaced by \(w_t(x, t)\), therefore,
\[
|E_t(x, t)| \leq |E_1(x, t)| + |E_2(x, t)| \leq \varepsilon^m \|w_t\|_{H^{m+1}(\Omega)} + \|w\|_{H^{m+1}(\Omega)},
\]
namely, (3.9) holds.

If \(V(x, t)\) is independent of \(t\), then from (3.4),
\[
A(E_2, v_h) = A(E_t, v_h) = \frac{d}{dt} A(E, v_h) - A_t(E, v_h) = 0, \quad \forall v_h(x) \in S^m_h,
\]
which implies that \(E_2(x, t) \equiv 0\). Therefore,
\[
|E_t(x, t)| = |E_1(x, t)| \leq \varepsilon^m \|w_t\|_{H^{m+1}(\Omega)}. \quad \square
\]

**Theorem 2.** Assume that \(\Psi^n(x) \in S^m_h, m = 1 \text{ or } 2\), is the finite element solution defined in (2.9)–(2.10), \(\psi(x, t)\) is the solution of problem (2.1)–(2.2), and
\[
\psi^n(x) \in H^{m+1}(\Omega),
\]
\[
\psi(x, t) \in W^{1, \infty}(0, T; H^{m+1}(\Omega)) \cap H^{1, \infty}(0, T; W^{1, 1}(\Omega)) \cap H^{2, 2}(0, T; L^2(\Omega)).
\]
Then
\[
||\psi(\cdot, T_n) - \Psi^n||_{H_s(\Omega)} \leq \varepsilon^{m+1/2}[h^{m+1}(1 + h^m)|\ln \tau|^{1/2} + \tau^{3/2}], \quad s = 0, 1. \tag{3.13}
\]
For \(m = 2\), if \(V(x, t)\) is independent of \(t\), then
\[
||\psi(\cdot, T_n) - \Psi^n||_{H_s(\Omega)} \leq \varepsilon^{m+1/2}[h^{7/2} + h^4|\ln \tau|^{1/2} + \tau^{3/2}], \quad s = 0, 1. \tag{3.14}
\]
**Proof.** Let \(\Psi^n(x) - \psi(x, t_n) = \vartheta^n(x) + \rho^n(x)\) with
\[
\vartheta^n(x) = \Psi^n(x) - R_h \psi(x, t_n), \quad \rho^n(x) = R_h \psi(x, t_n) - \psi(x, t_n).
\]
For any \(v_h(x) \in S^m_h\) and \(1 \leq n \leq N\), from (2.9) we have
\[
i(\delta_t \vartheta^{n-1/2}, v_h) + i(\delta_t (R_h \psi)^{n-1/2}, v_h) = A^{n-1/2}(\vartheta^{n-1/2}, v_h) + \sum_{j=0}^{1} \tilde{v}_h(j) F_j(\vartheta)^{n-1/2} + A^{n-1/2}(\rho^{n-1/2}, v_h) + \sum_{j=0}^{1} \tilde{v}_h(j) F_j(\rho)^{n-1/2} \]
\[
+ A^{n-1/2}(\psi^{n-1/2}, v_h) + \sum_{j=0}^{1} \tilde{v}_h(j) F_j(\psi)^{n-1/2}. \tag{3.15}
\]
Notice that
\[ A^{n-1/2}(\rho^{n-1/2}, \psi_h) = \frac{1}{2} A^{n-1/2}(\rho^n, \psi_h) + \frac{1}{2} A^{n-1/2}(\rho^{n-1}, \psi_h) \]
\[ = \frac{1}{2} \int_{\Omega} [V(x, t_{n-1/2}) - V(x, t_n)]\rho^n \bar{\psi}_h \, dx + \frac{1}{2} \int_{\Omega} [V(x, t_{n-1/2}) - V(x, t_{n-1})]\rho^{n-1} \bar{\psi}_h \, dx, \]
and from (2.1), (2.7),
\[ A^{n-1/2}(\varphi^{n-1/2}, \psi_h) = \frac{1}{2} A^{n-1/2}(\varphi(x, t_n), \psi_h) + \frac{1}{2} A^{n-1/2}(\varphi(x, t_{n-1}), \psi_h) \]
\[ = \frac{1}{2} \int_{\Omega} [V(x, t_{n-1/2}) - V(x, t_n)]\varphi(x, t_n) \bar{\psi}_h \, dx \]
\[ + \frac{1}{2} \int_{\Omega} [V(x, t_{n-1/2}) - V(x, t_{n-1})]\varphi(x, t_{n-1}) \bar{\psi}_h \, dx \]
\[ + i(\psi^{n-1/2}, \psi_h) - \sum_{j=0}^{1} \bar{\psi}_h(j) F_j(\varphi^{n-1/2}) - \sum_{j=0}^{1} \bar{\psi}_h(j) \gamma_j^{n-1/2}, \]
then from (3.15) with \( \psi_h(x) = \varphi^{n-1/2}(x) \), we get
\[ i(\delta_t \varphi^{n-1/2}, \varphi^{n-1/2}) = T_1^n + T_2^n + T_3^n + T_4^n, \quad 1 \leq n \leq N, \tag{3.16} \]
where
\[ T_1^n = A^{n-1/2}(\varphi^{n-1/2}, \varphi^{n-1/2}) + \sum_{j=0}^{1} \bar{\psi}_n^{n-1/2}(j) F_j(\varphi^{n-1/2}) \]
\[ T_2^n = \sum_{j=0}^{1} \bar{\psi}_n^{n-1/2}(j) F_j(\varphi^{n-1/2}), \]
\[ T_3^n = \frac{1}{2} \int_{\Omega} [V(x, t_{n-1/2}) - V(x, t_n)] R_k \varphi(x, t_n) \bar{\psi}_n^{n-1/2} \, dx \]
\[ + \frac{1}{2} \int_{\Omega} [V(x, t_{n-1/2}) - V(x, t_{n-1})] R_k \varphi(x, t_{n-1}) \bar{\psi}_n^{n-1/2} \, dx, \]
\[ T_4^n = i(\psi^{n-1/2} - \delta_t R_k \varphi^{n-1/2}, \varphi^{n-1/2}), \quad T_5^n = - \sum_{j=0}^{1} \bar{\psi}_n^{n-1/2}(j) \gamma_j^{n-1/2}. \]

Noticing that
\[ (\delta_t \varphi^{n-1/2}, \varphi^{n-1/2}) = \frac{1}{2\tau} ([\| \varphi^{n-1/2} \|^2_{L^2(\Omega)} - \| \varphi^{n-1} \|^2_{L^2(\Omega)}) + \frac{1}{2\tau} ([\| \varphi^n \|, \varphi^{n-1} - (\varphi^n, \varphi^{n-1})), \]
then taking the imaginary parts of (3.16) and summing up the result for \( n \), we have
\[ \frac{1}{2\tau} (\| \varphi^n \|^2_{L^2(\Omega)} - \| \varphi^0 \|^2_{L^2(\Omega)}) = \sum_{k=1}^{4} \sum_{l=1}^{n} \text{Im}(T_k^l). \tag{3.17} \]

By the similar derivations to obtain inequality (3.3), we can get
\[ \sum_{l=1}^{n} \text{Im}(T_k^l) = \sum_{j=0}^{n} \sum_{l=1}^{n} \text{Im}(\bar{\psi}^{n-1/2}(j) F_j(\varphi)^{l-1/2}) \leq 0. \tag{3.18} \]
Now we estimate $\sum_{l=1}^{n} \text{Im}\{T_l^j\}$. For $j = 0, 1$, let

$$G_j(\rho)^n = \frac{1}{\sqrt{2\pi}} e^{-in\pi/4} \sum_{k=1}^{n} \frac{1}{\tau} \left( e^{-iV_j(t_{n-k})} \rho^k(j) - e^{-iV_j(t_{n-k-1})} \rho^{k-1}(j) \right) \int_{t_{k-1}}^{t_k} \frac{d\lambda}{\sqrt{t_n - \lambda}},$$

then

$$G_j(\rho)^n = e^{-in\pi/4} \sum_{k=1}^{n} a_{n-k} \left( e^{-iV_j(t_{n-k})} \rho^k(j) - e^{-iV_j(t_{n-k-1})} \rho^{k-1}(j) \right)$$

$$= e^{-in\pi/4} \left\{ a_0 \rho^n(j) + \sum_{k=1}^{n-1} (a_{n-k} - a_{n-k-1}) e^{-iV_j(t_{n-k})} \rho^k(j) - a_{n-1} e^{-iV_j t_n} \rho^0(j) \right\}.$$

Therefore,

$$\frac{1}{2} (G_j(\rho)^n + G_j(\rho)^{n-1}) = F_j(\rho)^{n-1/2} - \frac{a_{n-1}}{2} (e^{-iV_j t_n + \pi/4}) + e^{-iV_j t_n - \pi/4} \rho^0(j).$$

Let $E(x, t) = \psi(x, t) - R_h \psi(x, t)$, then from (3.8) and (3.9), we get

$$|G_j(\rho)^n| \leq \epsilon \sum_{l=1}^{n} \frac{1}{\tau} \int_{t_{k-1}}^{t_k} \left| \frac{\partial}{\partial t} e^{-iV_j(t_{n-t})} E(j, t) \right| dt \int_{t_{k-1}}^{t_k} \frac{d\lambda}{\sqrt{t_n - \lambda}}$$

$$\leq \epsilon \sum_{l=1}^{n} \int_{t_{k-1}}^{t_k} \left( |E(j, t)| + |E_t(j, t)| \right) dt \int_{t_{k-1}}^{t_k} \frac{d\lambda}{\sqrt{t_n - \lambda}}$$

$$\leq c h^{m+1} \|\psi\|_{W^{1,\infty}(0, T; H^{m+1}(\Omega))} \int_{0}^{t_n} \frac{d\lambda}{\sqrt{t_n - \lambda}}$$

$$\leq c h^{m+1} \|\psi\|_{W^{1,\infty}(0, T; H^{m+1}(\Omega))}.$$

From (3.20), by the $\epsilon$-inequality with $\epsilon = 1/8 T$ and inverse inequality

$$\|v_h\|_{C(\Omega)} \leq c h^{-1/2} \|v_h\|_{L^2(\Omega)}, \quad \forall v_h(x) \in S_h,$$

we get

$$|\tilde{T}^{1/2}(j) F_j(\rho)^{n-1/2}| \leq c h^{-1/2} \|\tilde{T}^{1/2}\|_{L^2(\Omega)} \| F_j(\rho)^{n-1/2} |$$

$$\leq c h^{-1} \| F_j(\rho)^{n-1/2} \| + \frac{1}{16 T} \|\tilde{T}^{1/2}\|^2_{L^2(\Omega)}$$

$$\leq c h^{2m+1} \left[ \|\psi\|^2_{W^{1,\infty}(0, T; H^{m+1}(\Omega))} + a_{n-1}^2 \|\psi^0\|^2_{H^{m+1}(\Omega)} \right] + \frac{1}{16 T} \|\tilde{T}^{1/2}\|^2_{L^2(\Omega)}.$$

Because

$$\sum_{l=1}^{n} a_l^2 = \frac{2}{\pi} \sum_{l=0}^{n} \frac{1}{(l^2 + 1 + \sqrt{l})^2} \leq c \tau^{-1} \ln \tau,$$
we have

$$
\sum_{l=1}^{n} |T_{3}^{l}| = \sum_{l=1}^{n} \sum_{j=0}^{1} |\partial^{n-1/2} (j) F_{j}(\rho)^{n-1/2} | \\
\leq c \tau^{-1} T^{2m+1} \left[ \| \psi \|_{W^{1,\infty}(0, T; H^{m+1}(\Omega))} + h^{2(m-1)} \ln \tau \| \psi \|_{H^{H+1}(\Omega)}^{2} \right] + \frac{1}{8 T} \sum_{l=1}^{n} \| \partial^{n-1/2} \|_{L^{2}(\Omega)}^{2} . \quad (3.22)
$$

Next, we estimate \( \sum_{l=1}^{n} |T_{3}^{l}| \). Noticing that

$$
[V(x, t_{n-1/2}) - V(x, t_{n})] R_{h} \psi(x, t_{n}) + [V(x, t_{n-1/2}) - V(x, t_{n-1})] R_{h} \psi(x, t_{n-1}) \\
= [2V(x, t_{n-1/2}) - V(x, t_{n}) - V(x, t_{n-1})] R_{h} \psi(x, t_{n-1}) + [V(x, t_{n-1/2}) - V(x, t_{n})] \int_{t_{n-1}}^{t_{n}} (R_{h} \psi)(x, t) \, dt,
$$

therefore, we get

$$
|T_{3}^{l}| \leq \frac{1}{8 T} \| \partial^{n-1/2} \|_{L^{2}(\Omega)}^{2} c \tau^{3} \left[ \tau \| R_{h} \psi(\cdot, t_{n-1}) \|_{L^{2}(\Omega)}^{2} + \int_{t_{n-1}}^{t_{n}} \| (R_{h} \psi)(t, t) \|_{L^{2}(\Omega)}^{2} \, dt \right]
$$

So we have

$$
\sum_{l=1}^{n} |T_{3}^{l}| \leq \frac{1}{8 T} \sum_{l=1}^{n} \| \partial^{n-1/2} \|_{L^{2}(\Omega)}^{2} c \tau^{3} \| \psi \|_{W^{1,\infty}(0, T; H^{1}(\Omega))}^{2} . \quad (3.23)
$$

It is easy to check that

$$
\psi^{n-1/2}(x) = \delta_{t} \psi^{n-1/2}(x) - \frac{1}{\tau} \int_{t_{n-1}}^{t_{n}} \psi_{s+}(x, \lambda) (t_{n-1/2} - \lambda) \, d\lambda
$$

$$
= \delta_{t} \psi^{n-1/2}(x) - \frac{1}{\tau} \int_{t_{n-1}}^{t_{n}} \left[ \int_{t_{n-1}}^{t} \psi_{s+}(x, s) \, ds \right] (t_{n-1/2} - \lambda) \, d\lambda,
$$

then

$$
|T_{4}^{n}| \leq \left| (\delta_{t} E^{n-1/2}, \partial^{n-1/2} ) \right| + \tau \| \psi \|_{H^{1}(\cdot, t)}^{2} \| \psi \|_{H^{2}(\Omega)} \int_{t_{n-1}}^{t_{n}} \| \psi \|_{H^{2}(\Omega)} \, dt
$$

$$
= \frac{1}{\tau} \left( \int_{t_{n-1}}^{t_{n}} E_{t}(x, \lambda) \, d\lambda, \psi^{n-1/2} \right) + \tau \| \psi \|_{H^{1}(\cdot, t)}^{2} \| \psi \|_{H^{2}(\Omega)} \int_{t_{n-1}}^{t_{n}} \| \psi \|_{H^{2}(\Omega)} \, dt
$$

$$
\leq \frac{1}{\tau} \| \psi \|_{H^{1}(\cdot, t)}^{2} \| \psi \|_{H^{2}(\Omega)} \int_{t_{n-1}}^{t_{n}} \| E_{t}(\cdot, t) \|_{H^{2}(\Omega)} \, dt + \tau \| \psi \|_{H^{1}(\cdot, t)}^{2} \| \psi \|_{H^{2}(\Omega)} \int_{t_{n-1}}^{t_{n}} \| \psi \|_{H^{2}(\Omega)} \, dt
$$

$$
\leq \frac{1}{8 T} \| \psi \|_{H^{1}(\cdot, t)}^{2} \| \psi \|_{H^{2}(\Omega)} \int_{t_{n-1}}^{t_{n}} \| E_{t}(\cdot, t) \|_{H^{2}(\Omega)} \, dt + \tau \| \psi \|_{H^{1}(\cdot, t)}^{2} \| \psi \|_{H^{2}(\Omega)} \int_{t_{n-1}}^{t_{n}} \| \psi \|_{H^{2}(\Omega)} \, dt
$$

Therefore, from (3.6) we have

$$
\sum_{l=1}^{n} |T_{3}^{l}| \leq \frac{1}{8 T} \left[ h^{2(m+1)} \| \psi \|_{W^{1,2}(0, T; H^{m+1}(\Omega))}^{2} + \tau^{4} \| \psi \|_{W^{3,2}(0, T; L^{2}(\Omega))}^{2} \right] + \frac{1}{8 T} \sum_{l=1}^{n} \| \partial^{n-1/2} \|_{L^{2}(\Omega)}^{2} . \quad (3.24)
$$
Finally, from (3.21), (2.8) we have
\[
|T^n_2| \leq ch^{-1/2} \|\varphi\|_{L^2(\Omega)}^{n-1/2} \sum_{j=0}^{1} |\gamma_j^{n-1/2}|
\]
\[
\leq \frac{1}{8T} \|\varphi\|_{L^2(\Omega)}^{n-1/2} + ch^{-1} \tau^3 \|\psi\|_{W^{2,\infty}(0,T;W^{1,1}(\Omega))}^2
\]
then,
\[
\sum_{i=1}^{n} |T^n_2| \leq \frac{1}{8T} \sum_{i=1}^{n} \|\varphi\|_{L^2(\Omega)}^{n-1/2} + ch^{-1} \tau^2 \|\psi\|_{W^{2,\infty}(0,T;W^{1,1}(\Omega))}^2
\]
(3.25)
Therefore, from (3.17), (3.18) and (3.22)–(3.25), we have
\[
\frac{1}{2\tau} (\|\varphi\|_{L^2(\Omega)}^2 - \|\varphi^0\|_{L^2(\Omega)}^2)
\]
\[
\leq \frac{1}{2T} \sum_{i=1}^{n} \|\varphi\|_{L^2(\Omega)}^{n-1/2} + c[\tau^{-1}h^{-2m+1}(1 + h^{2(m-1)}|\ln \tau|) + h^{-1}\tau^3].
\]
(3.26)
Noticing that
\[
\|\varphi\|_{L^2(\Omega)} \leq \|\varphi^0 - \psi_0\|_{L^2(\Omega)} + \|\psi_0 - R_h\psi_0\|_{L^2(\Omega)} \leq ch^{m+1} \|\varphi^0\|_{H^{m+1}(\Omega)}^2
\]
\[
\|\varphi\|_{L^2(\Omega)}^{n-1/2} \leq \frac{1}{2} (\|\varphi\|_{L^2(\Omega)}^2 + \|\varphi\|_{L^2(\Omega)}^{n-1/2})
\]
then from (3.26) we have
\[
\frac{1}{2} \|\varphi\|_{L^2(\Omega)}^2 \leq \left(1 - \frac{\tau}{2T}\right) \|\varphi\|_{L^2(\Omega)}^2
\]
\[
\leq \frac{\tau}{T} \sum_{i=1}^{n-1} \|\varphi\|_{L^2(\Omega)}^2 + c[h^{2m+1}(1 + h^{2(m-1)}|\ln \tau|) + h^{-1}\tau^3].
\]
Using the discrete Gronwall inequality to the above inequality and noticing that \(n\tau \leq T\), we have
\[
\|\varphi\|_{L^2(\Omega)}^2 \leq ch^{-1}[h^{2m+1}(1 + h^{2(m-1)}|\ln \tau|) + h^{-1}\tau^3]e^{2n\tau/T}
\]
\[
\leq ch^{-1}[h^{2m+1}(1 + h^{2(m-1)}|\ln \tau|) + \tau^3].
\]
By the inverse inequality
\[
\|\varphi\|_{H^1(\Omega)} \leq ch^{-1} \|\varphi\|_{L^2(\Omega)},
\]
we have
\[
\|\varphi\|_{H^1(\Omega)} \leq ch^{-(s+1/2)}[h^{m+1}(1 + h^{m-1}|\ln \tau|^{1/2}) + \tau^{3/2}], \quad s = 0, 1.
\]
(3.27)
Therefore, (3.13) follows from (3.5), (3.27) and the following inequality:
\[
\|\psi(\cdot, t_n) - \psi^n\|_{H^1(\Omega)} \leq \|\rho^n\|_{H^1(\Omega)} + \|\varphi^n\|_{H^1(\Omega)}.
\]
(3.28)
For \(m = 2\), if \(V(x, t)\) is independent of \(t\), then we only need to change the estimate of \(|G_0(\rho)|\) by using error estimate (3.10) for \(E_1(0, t)\). In this case, we have
\[
\sum_{i=1}^{n} |T^n_2| \leq c\tau^{-1}h^2 [\|\psi\|_{W^{1,\infty}(0,T;H^1(\Omega))}^2 + |\ln \tau|\|\psi^0\|_{H^1(\Omega)}^2] + \frac{1}{8T} \sum_{i=1}^{n} \|\varphi\|_{L^2(\Omega)}^{n-1/2}^2,
So we can get
\[ \| \partial^p \|_{H^s(\Omega)} \leq c h^{-(s+1)/2} [h^4 \ln \tau]^{1/2} + h^{7/2} + \tau^{3/2}], \quad s = 0, 1. \]

The above inequality and (3.28) have shown the validity of (3.14). □

4. Numerical examples

In this section, we present two examples. The first example is used to check the stability and the convergence order of our numerical approximation. The second example, in which the exact solution is a travelling wave, is used to see whether any numerical reflections appear at the artificial boundaries, and also to compare with other numerical method.

Example 1. We use (2.9) and (2.10) to solve the following initial value problem of Schrödinger equation on \( R^1 \times [0, 5] \):

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

\[ \psi(x, 0) = \begin{cases} x(1-x)(1+2i), & \forall x \in [0, 1], \\ 0 & \text{otherwise}, \end{cases} \tag{4.2} \]

its exact solution is the following [19]:

\[ \psi(x, t) = \frac{1}{\sqrt{2\pi i}} \int_0^1 \tilde{\psi}(1 - \tilde{x})(1 + 2i) e^{i(x-\tilde{x})^2/2t-\pi/4} d\tilde{x}. \tag{4.3} \]

We denote the time step length by \( \tau \), the distance between adjacent space nodes by \( h \), and the relative error of the \( m \)-degree finite element solution by

\[ e_{h, \tau, s}(t_n) = \frac{\| \psi(\cdot, t_n) - \psi_n \|_{H^s(\Omega)}}{\| \psi(\cdot, t_n) \|_{H^s(\Omega)}}, \quad s = 0, 1. \]

We take \( \tau = h^2 \) and \( h = h_0 = 0.5, h_0/2, h_0/4, h_0/8 \), the corresponding errors \( e_{h, \tau, s}(t_n) \) at time level \( t_n = 5.0 \) are listed in Table 1. We can see that \( e_{h, \tau, 0}(t_n) \approx O(h^{2m}) \), \( e_{h, \tau, 1}(t_n) \approx O(h^{m+2}) \), \( x > 0 \), the numerical results are much better than the theoretical results \( e_{h, \tau, s}(t_n) \approx O(h^{m+1/2-s}) \), which are given in Theorem 2. In the case \( \tau = h \) and \( h = h_0 = 1/20 \), \( h_0/2 \), \( h_0/4 \), \( h_0/8 \), \( h_0/16 \), \( h_0/32 \), the numerical results are listed in Table 2. We can see that the numerical solution converges with the first-order rate under \( L^2 \)-norm, which is coincident with the theoretical result \( e_{h, \tau, s}(t_n) \approx O(h^{1-s}) \), \( s = 0 \).

### Table 1

<table>
<thead>
<tr>
<th>Mesh</th>
<th>( h = h_0 = 0.5 )</th>
<th>( h = h_0/2 )</th>
<th>( h = h_0/4 )</th>
<th>( h = h_0/8 )</th>
</tr>
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<tr>
<td>( e_{h, \tau, 0}^{(1)}(5.0) )</td>
<td>2.45D – 01</td>
<td>1.61D – 02</td>
<td>1.56D – 02</td>
<td>3.92D – 03</td>
</tr>
<tr>
<td>( e_{h, \tau, 0}^{(2)}(5.0) )</td>
<td>9.64D – 02</td>
<td>1.41D – 03</td>
<td>8.35D – 05</td>
<td>4.84D – 06</td>
</tr>
<tr>
<td>( e_{h, \tau, 1}^{(1)}(5.0) )</td>
<td>4.24D – 01</td>
<td>6.32D – 02</td>
<td>1.73D – 02</td>
<td>5.35D – 03</td>
</tr>
<tr>
<td>( e_{h, \tau, 1}^{(2)}(5.0) )</td>
<td>7.12D – 01</td>
<td>1.45D – 03</td>
<td>1.15D – 04</td>
<td>2.06D – 05</td>
</tr>
</tbody>
</table>

### Table 2

<table>
<thead>
<tr>
<th>Mesh</th>
<th>( h = h_0 = 1/20 )</th>
<th>( h = h_0/2 )</th>
<th>( h = h_0/4 )</th>
<th>( h = h_0/8 )</th>
<th>( h = h_0/16 )</th>
<th>( h = h_0/32 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( e_{h, \tau, 0}^{(1)}(5.0) )</td>
<td>1.13D – 01</td>
<td>6.30D – 02</td>
<td>3.14D – 02</td>
<td>1.70D – 02</td>
<td>8.81D – 03</td>
<td>4.62D – 03</td>
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<tr>
<td>( e_{h, \tau, 0}^{(2)}(5.0) )</td>
<td>1.21D – 01</td>
<td>6.23D – 02</td>
<td>3.13D – 02</td>
<td>1.70D – 02</td>
<td>8.80D – 03</td>
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<tr>
<td>( e_{h, \tau, 1}^{(1)}(5.0) )</td>
<td>5.23D00</td>
<td>4.52D00</td>
<td>3.75D00</td>
<td>3.15D00</td>
<td>2.58D00</td>
<td>2.11D00</td>
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<tr>
<td>( e_{h, \tau, 1}^{(2)}(5.0) )</td>
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<td>4.69D00</td>
<td>3.87D00</td>
<td>3.21D00</td>
<td>2.61D00</td>
<td>2.13D00</td>
</tr>
</tbody>
</table>
Under $H^1$-norm, although the error is large, we can still see the convergence of the numerical solution, which has the order about 0.28, and is slightly better than the theoretical result.

**Example 2.** We consider the right travelling Gaussian beam [2] with a wave number $k_0 = 8$:

$$\psi(x, t) = \sqrt{-\frac{i}{200t + i}} \exp \left( \frac{i[200t^2 - (10x - 5)^2] - k_0(10x - 5) + (50k_0^2 + 1)t}{-200t + i} \right).$$
It is the exact solution of the Schrödinger equation (1.1) with \( V(x, t) = 1 \), its evolution at different times are shown graphically in Fig. 1.

In the computation interval \([0, 1]\), we take \( \tau = 2 \times 10^{-5}, h = \frac{1}{160} \), and solve the finite element solution by the (2.9) and (2.10). As comparison, another finite element solution is also solved by applying the DN discrete boundary conditions given in [2]. The evolutions of the exact solution and the numerical solutions at different times are shown graphically in Figs. 2–6. We can see in these figures that our method only induces a very small numerical reflection, and only very small differences between these two numerical solutions can be observed.
5. Conclusions

In this paper, a finite element approximation for the one-dimensional time-dependent Schrödinger equation on unbounded domain is considered. By introducing the artificial boundaries, the original problem on unbounded domain is reduced into an initial-boundary value problem on bounded domain. By applying the approach given in [13] to discretize the transparent boundary conditions, a fully discrete scheme based on finite element method is constructed. By a rigorous analysis, this scheme has been proved to be unconditionally stable and convergent, its convergence order has also be obtained.
References