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Analysis of High-Order Absorbing Boundary Conditions for the Schrödinger Equation

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Abstract. The paper is concerned with the numerical solution of Schrödinger equations on an unbounded spatial domain. High-order absorbing boundary conditions for one-dimensional domain are derived, and the stability of the reduced initial boundary value problem in the computational interval is proved by energy estimate. Then a second order finite difference scheme is proposed, and the convergence of the scheme is established as well. Finally, numerical examples are reported to confirm our error estimates of the numerical methods.

AMS subject classifications: 65M12, 65M06, 65M15

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1 Introduction

Schrödinger equation is one of the basic equations of quantum mechanics, and can be found in many areas of physical and technological interest, e.g., optics, seismology and plasma physics. In this paper, the numerical approximation of Schrödinger equation of the following form is considered:

$$i\partial_t\psi(x,t) = -\partial_x^2\psi(x,t) + V(x,t)\psi, \qquad x\in\mathbb{R}, \quad 0<t\leq T, \tag{1.1a}$$

$$\lim_{|x|\to\infty}\psi(x,t)=0, \qquad t\geq 0, \tag{1.1b}$$

$$\psi(x,0)=\psi_0(x), \qquad x\in\mathbb{R}, \tag{1.1c}$$

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where $V(x,t)$ is the potential function and $V(x,t) \in L^\infty$ with real (or negative complex) part. It is assumed that the initial data is compactly supported on a finite (interior) domain $\Omega_i = \{x | x_l < x < x_r\}$, $V(x,t)$ is constant on the complementary region $\Omega_c = \mathbb{R}/\Omega_i$. If the initial value is not compactly supported, one refers to [13] and references therein to see how to treat it. A great numerical challenge lies on the unboundedness of the definition domain of the model equation (1.1a)-(1.1c), since the traditional methods (finite difference method and finite element method et al.) can not be used directly. In practical numerical simulations, people are concerned about the evolution of the solution in a finite domain of physical interest, rather than the whole space. Thus the equations need to be reduced to a problem on bounded (computational) domain in a neighborhood of the region of physical interest. An often used method is to limit the interest region by an artificial boundary, impose the ideal absorbing boundary conditions (ABCs), and then solve a reduced initial boundary value problem on a bounded domain. This procedure is usually called artificial boundary methods [3, 12, 15, 20–22, 24, 25, 28, 38, 40]. Artificial boundary conditions consist of two categories: nonlocal and local. The nonlocal ABCs in time (and in space for multimensional cases) are well-posed, but are expensive. It is often desirable to design local ABCs which are both computationally efficient and easy to implement. However, the proposed ABCs often result in a degradation of accuracy and stability. Other solutions to address the unboundedness issue are the perfectly matched layer method [8, 45], infinite element or boundary element method [41] and so on.

Many efforts have been continuously devoted to the study of using artificial boundary methods for Schrödinger equations [1,6,9–11,14,23,26,30,36,37,46] and the references therein. For recent development, we shall refer to a review paper [3]. When the simulation is for a long time or high accuracy is needed, high-order ABCs are necessary for efficiently minimizing the unphysical reflection. The high-order method has been widely used in wave equations [7, 16–19], based on which, in this paper we construct a family of high-order ABCs for Schrödinger equation. To differ from ABCs obtained by Di Menza, Szeftel and Antoine etc [2, 10, 11, 36, 37] and use the idea of Kuska [30], a physical parameter k_0 is introduced to adjust the performance of high-order ABCs, which is related to the velocity of wave impinged on the artificial boundary. The boundary condition can efficiently absorb the "fast" or "slow" waves by choosing suitable values k_0. In [2] (with $k_0 = 1$), the authors proposed high-order ABCs for Schrödinger equation with an exterior repulsive potential, which is a more difficult case. The aims of this paper are to establish the theoretical aspects of the reduced problem and design a corresponding finite difference scheme. The focuses of the presentation are on the stability of the initial boundary value problem with high-order ABCs on finite (computational) domain, and then on the difference scheme. We prove the solvability and convergence of the difference scheme and obtain the optimal convergence rate at the order of $\mathcal{O}(h^2 + \tau^2)$ with mesh size h and time step τ (see Theorem 4). One is also recommended to refer to the strategy of proving the well-posedness of the corresponding initial boundary problem in [36]. The theoretical results in this paper have formed a basis to study the stability of ABCs for the nonlinear Schrödinger equation in the future [42, 43].

The remaining part of the paper is organized as follows. Section 2 is devoted to the construction of high-order ABCs. Some auxiliary variables are introduced to avoid high-order derivatives, and the energy estimate of the solution to the approximate initial boundary value problem is proved. Section 3 discusses the Crank-Nicolson type difference scheme for the reduced problem, and gives the stability and convergence analysis. Section 4 presents some numerical examples to demonstrate the effectiveness and efficiency of the proposed methods, and finally, concluding remarks are given in Section 5.

2 Construction of high-order absorbing boundary conditions

In this section the design of high-order local ABCs follows the basic ideas in references [1, 12, 16, 30, 33]. Restricting (1.1a) to the exterior domain Ω_c, we have

$$i\partial_t\psi(x,t)=-\partial_x^2\psi(x,t)+V\psi,\quad x\in\Omega_c,\quad 0<t\le T. \tag{2.1}$$

Since the potential V is a real constant on the region Ω_c, we may assume $V=0$ in Ω_c. Since otherwise a simple change of variable would eliminate the term $V\psi$. Thus, we have

$$i\partial_t\psi(x,t)=-\partial_x^2\psi(x,t),\quad x\in\Omega_c,\quad 0<t\le T. \tag{2.2}$$

The previous works show the transparent boundary conditions in an exact manner:

$$\partial_{\mathbf{n}}\psi+\frac{e^{-\frac{\pi}{4}i}}{\sqrt{\pi}}\partial_t\int_0^t\psi(x,\tau)\frac{d\tau}{\sqrt{t-\tau}}=0, \tag{2.3}$$

where $\mathbf{n}$ denotes the outwardly directed unit normal vector at $x=x_l,x_r$. The equivalent forms are given by the Neumann-Dirichlet map [32]

$$\psi+\frac{e^{\frac{\pi}{4}i}}{\sqrt{\pi}}\int_0^t\partial_{\mathbf{n}}\psi(x,\tau)\frac{d\tau}{\sqrt{t-\tau}}=0. \tag{2.4}$$

For more literature works that focus on the numerical treatment of (2.3) and (2.4), we shall refer to [4,27,29,34,35], etc. To construct local ABCs, the boundary should be almost transparent for a plane wave of the form [30]

$$\psi(x,t)=\exp\left[-i(\omega t-\xi x)\right]. \tag{2.5}$$

The idea underlying this form is, firstly, to get the dispersion relation,

$$\xi^2=\omega, \tag{2.6}$$

then to implement the duality between the $x-t$ space and the $\xi-\omega$ space to obtain a differential equation on the artificial boundary. The expression (2.5) implies that there exist only the scattering waves. We solve (2.6) and arrive at

$$\xi=\pm\sqrt{\omega}, \tag{2.7}$$

where the plus sign in "$\pm$" corresponds to ABCs at boundary x_r, and the minus sign to ABCs at x_l. Without loss of generality, the plus sign and minus sign in "$\pm$" also mean the right boundary condition and left boundary condition in the following discussions, respectively. By Taylor or Padé approximation to $\sqrt{\omega}$, Kuska and Shibata etc [1,30,33] proposed what follows:

$$\text{2nd order:} \qquad i\partial_t\psi \pm i2k_0\partial_x\psi + k_0^2\psi = 0, \tag{2.8a}$$

$$\text{3rd order:} \qquad 3ik_0^2\partial_x\psi - \partial_x\partial_t\psi \pm (k_0^3\psi + 3ik_0\partial_t\psi) = 0. \tag{2.8b}$$

The parameter $k_0 = \sqrt{\omega_0}$ is chosen according to the underlying physical meaning, representing the wavenumber of the wave impinged on the artificial boundary, and ω_0 is a positive constant. To expand $\sqrt{\omega}$ as accurate as possible, we use the expansion:

$$\sqrt{\omega_0}\sqrt{\frac{\omega}{\omega_0}} \approx \sqrt{\omega_0} - \sqrt{\omega_0}\sum_{m=1}^{N}\frac{b_m\left(1-\frac{\omega}{\omega_0}\right)}{1-a_m\left(1-\frac{\omega}{\omega_0}\right)}, \qquad \text{for } \left|1-\frac{\omega}{\omega_0}\right| < 1, \tag{2.9}$$

where

$$a_m = \cos^2\left(\frac{m\pi}{2N+1}\right), \quad b_m = \frac{2}{2N+1}\sin^2\left(\frac{m\pi}{2N+1}\right), \quad m = 1,2,\cdots,N.$$

Substituting (2.9) into (2.7), we have

$$\xi = \pm\left(k_0 - k_0\sum_{m=1}^{N}\frac{b_m(1-\frac{\omega}{k_0^2})}{1-a_m(1-\frac{\omega}{k_0^2})}\right). \tag{2.10}$$

Using the dual relation $\xi \Leftrightarrow -i\partial_x$ and $\omega \Leftrightarrow i\partial_t$, (2.8b) is the simplest case with $N=1$ for (2.10). Obviously (2.10) will put us in trouble when N chosen larger. We perform Lindmann's trick [31] to introduce some auxiliary variables to decrease the order of partial derivatives. The auxiliary variables are defined as

$$\phi_{m,l} = \frac{1}{(1-a_m)k_0^2 + a_m\omega}\psi \quad \text{or} \quad \phi_{m,l} = \frac{(k_0^2-\omega)}{(1-a_m)k_0^2 + a_m\omega}\psi,$$

where $l=1,2$. $l=1$ represents the left-hand-side boundary auxiliary, $l=2$ represents the right-hand-side one. Turning to $\xi \Leftrightarrow -i\partial_x$ and $\omega \Leftrightarrow i\partial_t$, we have two groups of high-order boundary conditions: BC1

$$\begin{cases} i\partial_x\psi \pm \left(k_0\psi - k_0\sum\limits_{m=1}^{N} b_m(k_0^2\phi_{m,l} - i\partial_t\phi_{m,l})\right) = 0, \\ (1-a_m)k_0^2\phi_{m,l} + ia_m\partial_t\phi_{m,l} = \psi, \quad m=1,2,\cdots,N, \end{cases} \tag{2.11}$$

and BC2:

$$\begin{cases} i\partial_x\psi \pm \left(k_0\psi - k_0\sum\limits_{m=1}^{N} b_m\phi_{m,l}\right) = 0, \\ (1-a_m)k_0^2\phi_{m,l} + ia_m\partial_t\phi_{m,l} = k_0^2\psi - i\partial_t\psi, \quad m=1,2,\cdots,N. \end{cases} \tag{2.12}$$

We remark that BC1 and BC2 are similar to Di Menza's [10, 11], Szeftel's ABCs [36, 37] and Antoine etc [2], but different from them by introducing the physical parameter k_0 to adjust ABCs such that they can absorb the "fast" or "slow" waves efficiently. For more recent development in wave equations one refers to [3, 7, 16–20] and references therein.

In view of mathematical theory, BC1 and BC2 are equivalent to each other. Therefore, we only concentrate on the approximate problem coupled with the above BC1 (approximate problem I)

$$i\partial_t\psi(x,t)=-\partial_x^2\psi(x,t)+V(x,t)\psi(x,t),\quad x_l<x<x_r,\quad 0<t\le T, \tag{2.13a}$$

$$i\partial_x\psi(x_l,t)-k_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\psi(x_l,t)-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,1}(t)\Big]=0,\quad 0<t\le T, \tag{2.13b}$$

$$i\partial_x\psi(x_r,t)+k_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\psi(x_r,t)-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,2}(t)\Big]=0,\quad 0<t\le T, \tag{2.13c}$$

$$(1-a_m)k_0^2\phi_{m,1}(t)+ia_m\partial_t\phi_{m,1}(t)=\psi(x_l,t),\quad 1\le m\le N,\quad 0<t\le T, \tag{2.13d}$$

$$(1-a_m)k_0^2\phi_{m,2}(t)+ia_m\partial_t\phi_{m,2}(t)=\psi(x_r,t),\quad 1\le m\le N,\quad 0<t\le T, \tag{2.13e}$$

$$\psi(x,0)=\psi_0(x),\quad x_l\le x\le x_r,\quad \phi_{m,1}(0)=0,\quad \phi_{m,2}(0)=0,\quad 1\le m\le N, \tag{2.13f}$$

where we solved $\partial_t\phi_{m,l}(t)$ from the second equality of (2.11) and then substituted the result to the first equality of (2.11).

Theorem 2.1. *Let* $\{\psi(x,t)\}$ *be the solution of* (2.13a)-(2.13f) *and denote*

$$c=\Big(\sum_{m=1}^{N}\frac{b_m}{a_m^2}\Big)\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)^{-1}. \tag{2.14}$$

Then we have

$$\begin{aligned}&\int_{x_l}^{x_r}|\psi(x,t)|^2dx+k_0^3\sum_{m=1}^{N}b_m\big(|\phi_{m,1}(t)|^2+|\phi_{m,2}(t)|^2\big)\\ \le& e^{ck_0^2t}\int_{x_l}^{x_r}|\psi_0(x)|^2dx,\quad 0<t\le T.\end{aligned} \tag{2.15}$$

Proof. Multiplying (2.13a) by $\overline{\psi}(x,t)$ and integrating the result for x from x_l to x_r, we obtain

$$\begin{aligned}&i\int_{x_l}^{x_r}\overline{\psi}(x,t)\partial_t\psi(x,t)dx\\ =&-\overline{\psi}(x,t)\partial_x\psi(x,t)\big|_{x=x_l}^{x_r}+\int_{x_l}^{x_r}|\partial_x\psi(x,t)|^2dx+\int_{x_l}^{x_r}V(x,t)|\psi(x,t)|^2dx.\end{aligned} \tag{2.16}$$

Taking the imaginary part, we get

$$\frac{1}{2}\frac{d}{dt}\int_{x_l}^{x_r}|\psi(x,t)|^2dx\le\mathrm{Im}\big\{\overline{\psi}(x_l,t)\partial_x\psi(x_l,t)-\overline{\psi}(x_r,t)\partial_x\psi(x_r,t)\big\}. \tag{2.17}$$

It follows from (2.13b) and (2.13c) that

$$\partial_x\psi(x_l,t)=-ik_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\psi(x_l,t)-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,1}(t)\Big],\qquad 0<t\le T, \tag{2.18a}$$

$$\partial_x\psi(x_r,t)=ik_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\psi(x_r,t)-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,2}(t)\Big],\qquad 0<t\le T. \tag{2.18b}$$

Substituting (2.18a) and (2.18b) into (2.17), we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_{x_l}^{x_r}|\psi(x,t)|^2dx\le&-k_0\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\big(|\psi(x_l,t)|^2+|\psi(x_r,t)|^2\big)\\&+k_0^3\mathrm{Re}\Big\{\overline{\psi}(x_l,t)\sum_{m=1}^{N}\frac{b_m}{a_m}\phi_{m,1}(t)+\overline{\psi}(x_r,t)\sum_{m=1}^{N}\frac{b_m}{a_m}\phi_{m,2}(t)\Big\}.\end{aligned} \tag{2.19}$$

Multiplying (2.13d) by $\overline{\phi}_{m,1}(t)$, we have

$$(1-a_m)k_0^2|\phi_{m,1}(t)|^2+ia_m\overline{\phi}_{m,1}(t)\partial_t\phi_{m,1}(t)=\overline{\phi}_{m,1}(t)\psi(x_l,t),\quad 1\le m\le N,\ 0<t\le T. \tag{2.20}$$

Taking the imaginary part, we obtain

$$\frac{1}{2}a_m\frac{d}{dt}|\phi_{m,1}(t)|^2=\mathrm{Im}\{\overline{\phi}_{m,1}(t)\psi(x_l,t)\}. \tag{2.21}$$

Multiplying the equality above by $k_0^3b_m/a_m$ and summing up for m from 1 to N, we have

$$\frac{1}{2}k_0^3\frac{d}{dt}\sum_{m=1}^{N}b_m|\phi_{m,1}(t)|^2=k_0^3\ \mathrm{Im}\Big\{\psi(x_l,t)\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,1}(t)\Big\}. \tag{2.22}$$

Similarly, from (2.13e), we can obtain

$$\frac{1}{2}k_0^3\frac{d}{dt}\sum_{m=1}^{N}b_m|\phi_{m,2}(t)|^2=k_0^3\ \mathrm{Im}\Big\{\psi(x_r,t)\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,2}(t)\Big\}. \tag{2.23}$$

Adding (2.19), (2.22) and (2.23), we get

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}\Big\{\int_{x_l}^{x_r}|\psi(x,t)|^2dx+k_0^3\sum_{m=1}^{N}b_m\big(|\phi_{m,1}(t)|^2+|\phi_{m,2}(t)|^2\big)\Big\}\\ \le&-k_0\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\big(|\psi(x_l,t)|^2+|\psi(x_r,t)|^2\big)\\&+k_0^3\mathrm{Re}\Big\{\psi(x_l,t)\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,1}(t)+\psi(x_r,t)\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,2}(t)\Big\}\\&+k_0^3\mathrm{Im}\Big\{\psi(x_l,t)\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,1}(t)+\psi(x_r,t)\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,2}(t)\Big\}.\end{aligned} \tag{2.24}$$

Using $|\mathrm{Re}(Z)|+|\mathrm{Im}(Z)|\le\sqrt{2}|Z|$ and the ϵ inequality, we have

$$\begin{aligned}
A\equiv& k_0^3\mathrm{Re}\Big\{\psi(x_l,t)\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,1}(t)+\psi(x_r,t)\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,2}(t)\Big\}\\
&+k_0^3\mathrm{Im}\Big\{\psi(x_l,t)\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,1}(t)+\psi(x_r,t)\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,2}(t)\Big\}\\
\le&\sqrt{2}k_0^3\Big(\Big|\psi(x_l,t)\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,1}(t)\Big|+\Big|\psi(x_r,t)\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,2}(t)\Big|\Big)\\
\le&\epsilon\big(|\psi(x_l,t)|^2+|\psi(x_r,t)|^2\big)+\frac{k_0^6}{2\epsilon}\Big(\Big|\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,1}(t)\Big|^2+\Big|\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,2}(t)\Big|^2\Big)\\
\le&\epsilon\big(|\psi(x_l,t)|^2+|\psi(x_r,t)|^2\big)+\frac{k_0^6}{2\epsilon}\Big(\sum_{m=1}^N\frac{b_m}{a_m^2}\Big)\sum_{m=1}^N b_m\Big(|\phi_{m,1}(t)|^2+|\phi_{m,2}(t)|^2\Big).
\end{aligned}\tag{2.25}$$

Taking

$$\epsilon=k_0\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big),$$

we arrive at

$$\begin{aligned}
A\le&k_0\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\big(|\psi(x_l,t)|^2+|\psi(x_r,t)|^2\big)+\frac{\sum_{m=1}^N\frac{b_m}{a_m^2}}{1+\sum_{m=1}^N\frac{b_m}{a_m}}\cdot\frac{1}{2}k_0^5\sum_{m=1}^N b_m\big(|\phi_{m,1}(t)|^2+|\phi_{m,2}(t)|^2\big)\\
=&k_0\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\big(|\psi(x_l,t)|^2+|\psi(x_r,t)|^2\big)+c\cdot\frac{1}{2}k_0^5\sum_{m=1}^N b_m\big(|\phi_{m,1}(t)|^2+|\phi_{m,2}(t)|^2\big).
\end{aligned}\tag{2.26}$$

Inserting the inequality above into (2.24), we obtain

$$\begin{aligned}
&\frac{d}{dt}\Big\{\int_{x_l}^{x_r}|\psi(x,t)|^2dx+k_0^3\sum_{m=1}^N b_m\big(|\phi_{m,1}(t)|^2+|\phi_{m,2}(t)|^2\big)\Big\}\\
\le&c\cdot k_0^5\sum_{m=1}^N b_m\big(|\phi_{m,1}(t)|^2+|\phi_{m,2}(t)|^2\big).
\end{aligned}\tag{2.27}$$

Noticing (2.27), Gronwall inequality yields (2.15). This completes the proof. □

We remark that if the parameter k_0 is a function of time t, the analysis above will be complicate since the inequality (2.27) can not be achieved. For this case, one may also give the stability analysis (see the details in [44]). Above, the first half of the proof is standard (refer to [5]) under the assumption of the existence of the solution of (2.13a)-(2.13f).

3 The difference method

For the finite difference approximation, let M and K be two positive integers, and let $h=(x_r-x_l)/M$ and $\tau=T/K$. Cover the domain $[x_l,x_r]\times[0,T]$ by $\Omega_h\times\Omega_\tau$, where $\Omega_h=\{x_j|x_j=$

$x_l+jh,\ 0\le j\le M\}$ and $\Omega_\tau=\{t_n|t_n=n\tau,\ 0\le n\le K\}$. Suppose $\psi=\{\psi_j^n|0\le j\le M,\ 0\le n\le K\}$ be a grid function on $\Omega_h\times\Omega_\tau$. Introduce the following notations:

$$\psi_{j-\frac{1}{2}}^n=\frac{1}{2}(\psi_j^n+\psi_{j-1}^n),\qquad \delta_x\psi_{j-\frac{1}{2}}^n=\frac{1}{h}(\psi_j^n-\psi_{j-1}^n),\qquad \psi_j^{n-\frac{1}{2}}=\frac{1}{2}(\psi_j^n+\psi_j^{n-1}),$$
$$\delta_t\psi_j^{n-\frac{1}{2}}=\frac{1}{\tau}(\psi_j^n-\psi_j^{n-1}),\qquad \delta_x^2\psi_j^n=\frac{1}{h^2}(\psi_{j+1}^n-2\psi_j^n+\psi_{j-1}^n),$$
$$\|\psi^n\|=\Big[h\Big(\frac{1}{2}|\psi_0^n|^2+\sum_{j=1}^{M-1}|\psi_j^n|^2+\frac{1}{2}|\psi_M^n|^2\Big)\Big]^{\frac{1}{2}}.$$

In addition, denote

$$x_{j-\frac{1}{2}}=\frac{1}{2}(x_j+x_{j-1}),\quad t_{n-\frac{1}{2}}=\frac{1}{2}(t_n+t_{n-1}),\quad V_j^{n-\frac{1}{2}}=V(x_j,t_{n-\frac{1}{2}}).$$

Now, we introduce the two fictitious points $x_{-1}=x_0-h$ and $x_{M+1}=x_M+h$. The problem (2.13a)-(2.13f) can be approximated by

$$i\delta_t\psi_j^{n-\frac{1}{2}}=-\delta_x^2\psi_j^{n-\frac{1}{2}}+V_j^{n-\frac{1}{2}}\psi_j^{n-\frac{1}{2}},\quad 0\le j\le M,\ 1\le n\le K, \tag{3.1a}$$
$$i\cdot\frac{1}{2}\big(\delta_x\psi_{-\frac{1}{2}}^{n-\frac{1}{2}}+\delta_x\psi_{\frac{1}{2}}^{n-\frac{1}{2}}\big)-k_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_0^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,1}^{n-\frac{1}{2}}\Big]=0,\qquad 1\le n\le K, \tag{3.1b}$$
$$i\cdot\frac{1}{2}\big(\delta_x\psi_{M-\frac{1}{2}}^{n-\frac{1}{2}}+\delta_x\psi_{M+\frac{1}{2}}^{n-\frac{1}{2}}\big)+k_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_M^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,2}^{n-\frac{1}{2}}\Big]=0,\qquad 1\le n\le K, \tag{3.1c}$$
$$(1-a_m)k_0^2\phi_{m,1}^{n-\frac{1}{2}}+ia_m\delta_t\phi_{m,1}^{n-\frac{1}{2}}=\psi_0^{n-\frac{1}{2}},\quad 1\le m\le N,\ 1\le n\le K, \tag{3.1d}$$
$$(1-a_m)k_0^2\phi_{m,2}^{n-\frac{1}{2}}+ia_m\delta_t\phi_{m,2}^{n-\frac{1}{2}}=\psi_M^{n-\frac{1}{2}},\quad 1\le m\le N,\ 1\le n\le K, \tag{3.1e}$$
$$\psi_j^0=\psi_0(x_j),\quad 0\le j\le M,\quad \phi_{m,1}^0=0,\quad \phi_{m,2}^0=0,\quad 1\le m\le N. \tag{3.1f}$$

At the n-th time level, we regard (3.1a)-(3.1f) as a system of linear algebraic equations about the unknowns $\{\psi_j^n|-1\le j\le M+1\}\cup\{\phi_{m,1}^n,\ \phi_{m,2}^n|1\le m\le N\}$.

Using (3.1a) for $j=0$ to remove $\psi_{-1}^{n-\frac{1}{2}}$ in (3.1b), we obtain

$$\begin{aligned}i\delta_t\psi_0^{n-\frac{1}{2}}=&-\frac{2}{h}\Big\{\delta_x\psi_{\frac{1}{2}}^{n-\frac{1}{2}}+ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_0^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,1}^{n-\frac{1}{2}}\Big]\Big\}\\&+V_0^{n-\frac{1}{2}}\psi_0^{n-\frac{1}{2}},\quad 1\le n\le K.\end{aligned} \tag{3.2}$$

Using (3.1a) for $j=M$ to remove $\psi_{M+1}^{n-\frac{1}{2}}$ in (3.1c), we obtain

$$\begin{aligned}i\delta_t\psi_M^{n-\frac{1}{2}}=&-\frac{2}{h}\Big\{ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_M^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,2}^{n-\frac{1}{2}}\Big]-\delta_x\psi_{M-\frac{1}{2}}^{n-\frac{1}{2}}\Big\}\\&+V_M^{n-\frac{1}{2}}\psi_M^{n-\frac{1}{2}},\quad 1\le n\le K.\end{aligned} \tag{3.3}$$

Then the difference scheme (3.1a)-(3.1f) is reduced to

$$i\delta_t\psi_j^{n-\frac{1}{2}}=-\delta_x^2\psi_j^{n-\frac{1}{2}}+V_j^{n-\frac{1}{2}}\psi_j^{n-\frac{1}{2}},\quad 1\le j\le M-1,\ 1\le n\le K, \tag{3.4a}$$

$$\begin{aligned}i\delta_t\psi_0^{n-\frac{1}{2}}=&-\frac{2}{h}\Big\{\delta_x\psi_{\frac{1}{2}}^{n-\frac{1}{2}}+ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_0^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,1}^{n-\frac{1}{2}}\Big]\Big\}\\&+V_0^{n-\frac{1}{2}}\psi_0^{n-\frac{1}{2}},\quad 1\le n\le K,\end{aligned} \tag{3.4b}$$

$$\begin{aligned}i\delta_t\psi_M^{n-\frac{1}{2}}=&-\frac{2}{h}\Big\{ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_M^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,2}^{n-\frac{1}{2}}\Big]-\delta_x\psi_{M-\frac{1}{2}}^{n-\frac{1}{2}}\Big\}\\&+V_M^{n-\frac{1}{2}}\psi_M^{n-\frac{1}{2}},\quad 1\le n\le K,\end{aligned} \tag{3.4c}$$

$$(1-a_m)k_0^2\phi_{m,1}^{n-\frac{1}{2}}+ia_m\delta_t\phi_{m,1}^{n-\frac{1}{2}}=\psi_0^{n-\frac{1}{2}},\quad 1\le m\le N,\quad 1\le n\le K, \tag{3.4d}$$

$$(1-a_m)k_0^2\phi_{m,2}^{n-\frac{1}{2}}+ia_m\delta_t\phi_{m,2}^{n-\frac{1}{2}}=\psi_M^{n-\frac{1}{2}},\quad 1\le m\le N,\quad 1\le n\le K, \tag{3.4e}$$

$$\psi_j^0=\psi_0(x_j),\quad 0\le j\le M,\quad \phi_{m,1}^0=0,\quad \phi_{m,2}^0=0,\quad 1\le m\le N. \tag{3.4f}$$

If $\{\psi_j^{n-1}|0\le j\le M\}\cup\{\phi_{m,1}^{n-1},\phi_{m,2}^{n-1}|1\le m\le N\}$ has been determined, then it follows from (3.4d) and (3.4e) that

$$\phi_{m,1}^{n-\frac{1}{2}}=\frac{ia_m\phi_{m,1}^{n-1}+\frac{\tau}{2}\psi_0^{n-\frac{1}{2}}}{ia_m+\frac{\tau}{2}(1-a_m)k_0^2},\quad \phi_{m,2}^{n-\frac{1}{2}}=\frac{ia_m\phi_{m,2}^{n-1}+\frac{\tau}{2}\psi_M^{n-\frac{1}{2}}}{ia_m+\frac{\tau}{2}(1-a_m)k_0^2},\quad 1\le m\le N, \tag{3.5}$$

and

$$\phi_{m,1}^n=2\phi_{m,1}^{n-\frac{1}{2}}-\phi_{m,1}^{n-1},\quad \phi_{m,2}^n=2\phi_{m,2}^{n-\frac{1}{2}}-\phi_{m,2}^{n-1},\quad 1\le m\le N. \tag{3.6}$$

Substituting (3.5) into (3.4b) and (3.4c) respectively, we find that the system (3.4a), (3.4b) and (3.4c) is a tri-diagonal system of linear algebraic equations about the unknowns $\{\psi_j^n|0\le j\le M\}$. After this system has been solved, we obtain $\{\phi_{m,1}^n,\phi_{m,2}^n|1\le m\le N\}$ from (3.6).

3.1 Stability and solvability

Theorem 3.1. *Let* $\{\psi_j^n|0\le j\le M,0\le n\le K\}$ *be the solution of* (3.1a)-(3.1f)*, or, of* (3.4a)-(3.4f)*. Then we have*

$$\|\psi^n\|^2+k_0^3\sum_{m=1}^N b_m\big(|\phi_{m,1}^n|^2+|\phi_{m,2}^n|^2\big)\le e^{\frac{3}{2}ck_0^2T}\|\psi^0\|^2,\quad 1\le n\le K, \tag{3.7}$$

where c is defined in (2.14)*.*

Proof. Multiplying (3.4a) by $h\overline{\psi}_j^{n-\frac{1}{2}}$, (3.4b) by $h\overline{\psi}_0^{n-\frac{1}{2}}/2$, (3.4c) by $h\overline{\psi}_M^{n-\frac{1}{2}}/2$, then adding the results, we obtain

$$\begin{aligned}
&i\cdot h\Big(\frac{1}{2}\overline{\psi}_0^{n-\frac{1}{2}}\delta_t\psi_0^{n-\frac{1}{2}}+\sum_{j=1}^{M-1}\overline{\psi}_j^{n-\frac{1}{2}}\delta_t\psi_j^{n-\frac{1}{2}}+\frac{1}{2}\overline{\psi}_M^{n-\frac{1}{2}}\delta_t\psi_M^{n-\frac{1}{2}}\Big)\\
=&-\overline{\psi}_0^{n-\frac{1}{2}}\delta_x\psi_{\frac{1}{2}}^{n-\frac{1}{2}}-h\sum_{j=1}^{M-1}\overline{\psi}_j^{n-\frac{1}{2}}\delta_x^2\psi_j^{n-\frac{1}{2}}+\overline{\psi}_M^{n-\frac{1}{2}}\delta_x\psi_{M-\frac{1}{2}}^{n-\frac{1}{2}}\\
&-ik_0\overline{\psi}_0^{n-\frac{1}{2}}\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\psi_0^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,1}^{n-\frac{1}{2}}\Big]\\
&-ik_0\overline{\psi}_M^{n-\frac{1}{2}}\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\psi_M^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,2}^{n-\frac{1}{2}}\Big]\\
&+h\Big(\frac{1}{2}V_0^{n-\frac{1}{2}}|\psi_0^{n-\frac{1}{2}}|^2+\sum_{j=1}^{M-1}V_j^{n-\frac{1}{2}}|\psi_j^{n-\frac{1}{2}}|^2+\frac{1}{2}V_M^{n-\frac{1}{2}}|\psi_M^{n-\frac{1}{2}}|^2\Big).
\end{aligned}\tag{3.8}$$

Taking the imaginary part, we get

$$\begin{aligned}
\frac{1}{2\tau}\left(\|\psi^n\|^2-\|\psi^{n-1}\|^2\right)\le&-k_0\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\Big(|\psi_0^{n-\frac{1}{2}}|^2+|\psi_M^{n-\frac{1}{2}}|^2\Big)\\
&+k_0^3\mathrm{Re}\Big\{\overline{\psi}_0^{n-\frac{1}{2}}\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,1}^{n-\frac{1}{2}}+\overline{\psi}_M^{n-\frac{1}{2}}\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,2}^{n-\frac{1}{2}}\Big\}.
\end{aligned}\tag{3.9}$$

Multiplying (3.4d) by $\overline{\phi}_{m,1}^{n-\frac{1}{2}}$, we have

$$(1-a_m)k_0^2|\phi_{m,1}^{n-\frac{1}{2}}|^2+ia_m\overline{\phi}_{m,1}^{n-\frac{1}{2}}\,\delta_t\phi_{m,1}^{n-\frac{1}{2}}=\overline{\phi}_{m,1}^{n-\frac{1}{2}}\,\psi_0^{n-\frac{1}{2}},\quad 1\le m\le N,\ 1\le n\le K.\tag{3.10}$$

Taking the imaginary part, we obtain

$$\frac{a_m}{2\tau}\Big(|\phi_{m,1}^{n}|^2-|\phi_{m,1}^{n-1}|^2\Big)=\mathrm{Im}\Big\{\overline{\phi}_{m,1}^{n-\frac{1}{2}}\,\psi_0^{n-\frac{1}{2}}\Big\},\quad 1\le m\le N,\ 1\le n\le K.\tag{3.11}$$

Multiplying the equality above by $k_0^3 b_m/a_m$ and then summing up for m from 1 to N, we get

$$\frac{1}{2\tau}\Big(k_0^3\sum_{m=1}^{N}b_m|\phi_{m,1}^{n}|^2-k_0^3\sum_{m=1}^{N}b_m|\phi_{m,1}^{n-1}|^2\Big)=k_0^3\mathrm{Im}\Big\{\psi_0^{n-\frac{1}{2}}\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,1}^{n-\frac{1}{2}}\Big\},\quad 1\le n\le K.\tag{3.12}$$

Similarly, we can obtain from (3.4e) that

$$\frac{1}{2\tau}\Big(k_0^3\sum_{m=1}^{N}b_m|\phi_{m,2}^{n}|^2-k_0^3\sum_{m=1}^{N}b_m|\phi_{m,2}^{n-1}|^2\Big)=k_0^3\mathrm{Im}\Big\{\psi_M^{n-\frac{1}{2}}\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,2}^{n-\frac{1}{2}}\Big\},\quad 1\le n\le K.\tag{3.13}$$

Adding (3.9), (3.12) and (3.13), we get

$$\begin{aligned}&\frac{1}{2\tau}\Big[\Big(\|\psi^n\|^2+k_0^3\sum_{m=1}^N b_m|\phi_{m,1}^n|^2+k_0^3\sum_{m=1}^N b_m|\phi_{m,2}^n|^2\Big)\\&\quad-\Big(\|\psi^{n-1}\|^2+k_0^3\sum_{m=1}^N b_m|\phi_{m,1}^{n-1}|^2+k_0^3\sum_{m=1}^N b_m|\phi_{m,2}^{n-1}|^2\Big)\Big]\\\leq&-k_0\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\Big(|\psi_0^{n-\frac{1}{2}}|^2+|\psi_M^{n-\frac{1}{2}}|^2\Big)\\&+k_0^3\mathrm{Re}\Big\{\psi_0^{n-\frac{1}{2}}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,1}^{n-\frac{1}{2}}+\psi_M^{n-\frac{1}{2}}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,2}^{n-\frac{1}{2}}\Big\}\\&+k_0^3\mathrm{Im}\Big\{\psi_0^{n-\frac{1}{2}}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,1}^{n-\frac{1}{2}}+\psi_M^{n-\frac{1}{2}}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\phi}_{m,2}^{n-\frac{1}{2}}\Big\}.\end{aligned}\tag{3.14}$$

Similarly to the derivation of (2.27), we may get

$$\begin{aligned}&\frac{1}{\tau}\Big[\Big(\|\psi^n\|^2+k_0^3\sum_{m=1}^N b_m|\phi_{m,1}^n|^2+k_0^3\sum_{m=1}^N b_m|\phi_{m,2}^n|^2\Big)\\&\quad-\Big(\|\psi^{n-1}\|^2+k_0^3\sum_{m=1}^N b_m|\phi_{m,1}^{n-1}|^2+k_0^3\sum_{m=1}^N b_m|\phi_{m,2}^{n-1}|^2\Big)\Big]\\\leq&ck_0^5\sum_{m=1}^N b_m\Big(|\phi_{m,1}^{n-\frac{1}{2}}|^2+|\phi_{m,2}^{n-\frac{1}{2}}|^2\Big).\end{aligned}\tag{3.15}$$

This is a discrete analog of (2.27). Denoting

$$E^n=\big\|\psi^n\big\|^2+k_0^3\sum_{m=1}^N b_m\big|\phi_{m,1}^n\big|^2+k_0^3\sum_{m=1}^N b_m\big|\phi_{m,2}^n\big|^2,$$

we have

$$\frac{1}{\tau}(E^n-E^{n-1})\leq\frac{1}{2}ck_0^2(E^n+E^{n-1}),\quad 1\leq n\leq K.$$

When $\tau\leq 2(3ck_0^2)^{-1}$, this implies

$$E^n\leq\Big(1+\frac{3}{2}ck_0^2\tau\Big)E^{n-1},\quad 1\leq n\leq K.$$

The Gronwall inequality yields

$$E^n\leq e^{\frac{3}{2}ck_0^2n\tau}E^0,\quad 1\leq n\leq K,$$

or,

$$\big\|\psi^n\big\|^2+k_0^3\sum_{m=1}^N b_m\big(\big|\phi_{m,1}^n\big|^2+\big|\phi_{m,2}^n\big|^2\big)\leq e^{\frac{3}{2}ck_0^2T}\big\|\psi^0\big\|^2,\quad 1\leq n\leq K.$$

This completes the proof. $\square$

Now we consider the uniqueness of the difference scheme.

Theorem 3.2. *The difference scheme* (3.1a)-(3.1f)*, or* (3.4a)-(3.4f) *is uniquely solvable.*

Proof. One proves the theorem by induction method.

From (3.4f), $\{\psi_j^0|0\le j\le M\}\cup\{\phi_{m,1}^0,\phi_{m,2}^0|1\le m\le N\}$ is given. Suppose we have determined $\{\psi_j^{n-1}|0\le j\le M\}\cup\{\phi_{m,1}^{n-1},\phi_{m,2}^{n-1}|1\le m\le N\}$. Then (3.4a)-(3.4e) is a system of linear algebraic equations about unknowns $\{\psi_j^n|0\le j\le M\}\cup\{\phi_{m,1}^n,\phi_{m,2}^n|1\le m\le N\}$:

$$i\delta_t\psi_j^{n-\frac12}=-\delta_x^2\psi_j^{n-\frac12}+V_j^{n-\frac12}\psi_j^{n-\frac12},\quad 1\le j\le M-1, \tag{3.16a}$$

$$i\delta_t\psi_0^{n-\frac12}=-\frac{2}{h}\Big\{\delta_x\psi_{\frac12}^{n-\frac12}+ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_0^{n-\frac12}-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,1}^{n-\frac12}\Big]\Big\}+V_0^{n-\frac12}\psi_0^{n-\frac12}, \tag{3.16b}$$

$$i\delta_t\psi_M^{n-\frac12}=-\frac{2}{h}\Big\{ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_M^{n-\frac12}-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,2}^{n-\frac12}\Big]-\delta_x\psi_{M-\frac12}^{n-\frac12}\Big\}+V_M^{n-\frac12}\psi_M^{n-\frac12}, \tag{3.16c}$$

$$(1-a_m)k_0^2\phi_{m,1}^{n-\frac12}+ia_m\delta_t\phi_{m,1}^{n-\frac12}=\psi_0^{n-\frac12},\quad 1\le m\le N, \tag{3.16d}$$

$$(1-a_m)k_0^2\phi_{m,2}^{n-\frac12}+ia_m\delta_t\phi_{m,2}^{n-\frac12}=\psi_M^{n-\frac12},\quad 1\le m\le N. \tag{3.16e}$$

Consider the homogenous system of (3.16a)-(3.16e):

$$\frac{i}{\tau}\psi_j^n=-\frac12\delta_x^2\psi_j^n+\frac12V_j^{n-\frac12}\psi_j^n,\quad 1\le j\le M-1, \tag{3.17a}$$

$$\frac{i}{\tau}\psi_0^n=-\frac1h\Big\{\delta_x\psi_{\frac12}^n+ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_0^n-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,1}^n\Big]\Big\}+\frac12V_0^{n-\frac12}\psi_0^n, \tag{3.17b}$$

$$\frac{i}{\tau}\psi_M^n=-\frac1h\Big\{ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\psi_M^n-k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,2}^n\Big]-\delta_x\psi_{M-\frac12}^n\Big\}+\frac12V_M^{n-\frac12}\psi_M^n, \tag{3.17c}$$

$$\frac12(1-a_m)k_0^2\phi_{m,1}^n+\frac{i}{\tau}a_m\phi_{m,1}^n=\frac12\psi_0^n,\quad 1\le m\le N, \tag{3.17d}$$

$$\frac12(1-a_m)k_0^2\phi_{m,2}^n+\frac{i}{\tau}a_m\phi_{m,2}^n=\frac12\psi_M^n,\quad 1\le m\le N. \tag{3.17e}$$

It suffices to prove that (3.17a)-(3.17e) has only zero solution.

Multiplying (3.17a)-(3.17c) by $h\overline{\psi}_j^n$, $h\overline{\psi}_0^n/2$ and $h\overline{\psi}_M^n/2$, respectively, then adding the results and taking the imaginary part, we get

$$\begin{aligned}\frac1\tau\|\psi^n\|^2\le&-\frac12k_0\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\Big(|\psi_0^n|^2+|\psi_M^n|^2\Big)\\&+\frac12k_0^3\mathrm{Re}\Big\{\overline{\psi}_0^n\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,1}^n+\overline{\psi}_M^n\sum_{m=1}^N\frac{b_m}{a_m}\,\phi_{m,2}^n\Big\}.\end{aligned} \tag{3.18}$$

Multiplying (3.17d) by $b_mk_0^3\overline{\phi}_{m,1}^n{a_m}^{-1}$ and taking the imaginary part, we obtain

$$\frac1\tau k_0^3b_m|\phi_{m,1}^n|^2=\frac12k_0^3\mathrm{Im}\Big\{\frac{b_m}{a_m}\psi_0^n\overline{\phi}_{m,1}^n\Big\},\quad 1\le m\le N.$$

Summing the equality above for m, we have

$$\frac{1}{\tau}k_0^3\sum_{m=1}^{N}b_m|\phi_{m,1}^n|^2=\frac{1}{2}k_0^3\mathrm{Im}\Big\{\psi_0^n\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,1}^n\Big\}. \tag{3.19}$$

Similarly, it is easy to obtain from (3.17e) that

$$\frac{1}{\tau}k_0^3\sum_{m=1}^{N}b_m|\phi_{m,2}^n|^2=\frac{1}{2}k_0^3\mathrm{Im}\Big\{\psi_M^n\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,2}^n\Big\}. \tag{3.20}$$

Adding (3.18), (3.19) and (3.20), we get

$$\begin{aligned}
&\frac{1}{\tau}\Big[\|\psi^n\|^2+k_0^3\sum_{m=1}^{N}b_m\big(|\phi_{m,1}^n|^2+k_0^3|\phi_{m,2}^n|^2\big)\Big]\\
\le&-\frac{1}{2}k_0\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\big(|\psi_0^n|^2+|\psi_M^n|^2\big)+\frac{1}{2}k_0^3\mathrm{Re}\Big\{\overline{\psi}_0^n\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,1}^n+\overline{\psi}_M^n\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,2}^n\Big\}\\
&+\frac{1}{2}k_0^3\mathrm{Im}\Big\{\psi_0^n\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,1}^n+\psi_M^n\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\phi}_{m,2}^n\Big\}\\
\le&\frac{1}{2}ck_0^5\sum_{m=1}^{N}b_m\big(|\phi_{m,1}^n|^2+|\phi_{m,2}^n|^2\big)\le\frac{1}{2}ck_0^2\Big[\|\psi^n\|^2+k_0^3\sum_{m=1}^{N}b_m\big(|\phi_{m,1}^n|^2+k_0^3|\phi_{m,2}^n|^2\big)\Big],
\end{aligned} \tag{3.21}$$

which follows, when $\tau\le 2(ck_0^2)^{-1}$,

$$\|\psi^n\|^2+k_0^3\sum_{m=1}^{N}b_m\big(|\phi_{m,1}^n|^2+k_0^3|\phi_{m,2}^n|^2\big)=0.$$

This completes the proof. $\square$

3.2 Convergence

Define the grid functions

$$\begin{aligned}
&\Psi_j^n=\psi(x_j,t_n), && 0\le j\le M,\quad 0\le n\le K,\\
&\Phi_{m,1}^n=\phi_{m,1}(t_n),\quad \Phi_{m,2}^n=\phi_{m,2}(t_n), && 1\le m\le N,\quad 0\le n\le K.
\end{aligned}$$

Let

$$p_j^{n-\frac{1}{2}}=i\delta_t\Psi_j^{n-\frac{1}{2}}-\Big\{-\delta_x^2\Psi_j^{n-\frac{1}{2}}+V_j^{n-\frac{1}{2}}\Psi_j^{n-\frac{1}{2}}\Big\},\quad 1\le j\le M-1,\ 1\le n\le K, \tag{3.22a}$$

$$\begin{aligned}
p_0^{n-\frac{1}{2}}=&i\delta_t\Psi_0^{n-\frac{1}{2}}+\frac{2}{h}\Big\{\delta_x\Psi_{\frac{1}{2}}^{n-\frac{1}{2}}+ik_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\Psi_0^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\Phi_{m,1}^{n-\frac{1}{2}}\Big]\Big\}\\
&-V_0^{n-\frac{1}{2}}\psi_0^{n-\frac{1}{2}},\quad 1\le n\le K,
\end{aligned} \tag{3.22b}$$

$$
\begin{aligned}
p_M^{n-\frac{1}{2}} = & i\delta_t \Psi_M^{n-\frac{1}{2}} + \frac{2}{h}\Big\{ik_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\Psi_M^{n-\frac{1}{2}} - k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\Phi_{m,2}^{n-\frac{1}{2}}\Big] - \delta_x \Psi_{M-\frac{1}{2}}^{n-\frac{1}{2}}\Big\} \\
& - V_M^{n-\frac{1}{2}}\Psi_M^{n-\frac{1}{2}}, \quad 1\le n\le K, \qquad (3.22c)\\
r_{m,1}^{n-\frac{1}{2}} = & (1-a_m)k_0^2\Phi_{m,1}^{n-\frac{1}{2}} + ia_m\delta_t\Phi_{m,1}^{n-\frac{1}{2}} - \Psi_0^{n-\frac{1}{2}}, \quad 1\le m\le N, \quad 1\le n\le K, \qquad (3.22d)\\
r_{m,2}^{n-\frac{1}{2}} = & (1-a_m)k_0^2\Phi_{m,2}^{n-\frac{1}{2}} + ia_m\delta_t\Phi_{m,2}^{n-\frac{1}{2}} - \Psi_M^{n-\frac{1}{2}}, \quad 1\le m\le N, \quad 1\le n\le K. \qquad (3.22e)
\end{aligned}
$$

Then noticing (2.13a)-(2.13e) and using the Taylor expansion, there exists a constant c_1 such that

$$
\begin{aligned}
&|p_j^{n-\frac{1}{2}}| \le c_1(\tau^2+h^2), \quad 1\le j\le M-1, \quad 1\le n\le K, \qquad (3.23a)\\
&|p_0^{n-\frac{1}{2}}| \le c_1(\tau^2+h), \quad |p_M^{n-\frac{1}{2}}| \le c_1(\tau^2+h), \quad 1\le n\le K, \qquad (3.23b)\\
&|r_{m,1}^{n-\frac{1}{2}}| \le c_1\tau^2, \quad |r_{m,2}^{n-\frac{1}{2}}| \le c_1\tau^2, \quad 1\le n\le K. \qquad (3.23c)
\end{aligned}
$$

In the derivation of (3.23b), we have used

$$
\begin{aligned}
i\partial_t\psi(x_0,t) = & -\partial_x^2\psi(x_0,t) + V(x_0,t)\psi(x_0,t)\\
= & -\frac{2}{h}\Big\{\frac{1}{h}\big[\psi(x_1,t)-\psi(x_0,t)\big] - \partial_x\psi(x_0,t)\Big\} + V(x_0,t)\psi(x_0,t) + \mathcal{O}(h)\\
= & -\frac{2}{h}\Big\{\frac{1}{h}\big[\psi(x_1,t)-\psi(x_0,t)\big] + ik_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\psi(x_0,t) - k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,1}(t)\Big]\Big\}\\
& + V(x_0,t)\psi(x_0,t) + \mathcal{O}(h), \quad 0<t\le T,
\end{aligned}
$$

and

$$
\begin{aligned}
i\partial_t\psi(x_M,t) = & -\partial_x^2\psi(x_M,t) + V(x_M,t)\psi(x_M,t)\\
= & -\frac{2}{h}\Big\{\partial_x\psi(x_M,t) - \frac{1}{h}\big[\psi(x_M,t)-\psi(x_{M-1},t)\big]\Big\} + V(x_M,t)\psi(x_M,t) + \mathcal{O}(h),\\
= & -\frac{2}{h}\Big\{ik_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\psi(x_M,t) - k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\phi_{m,2}(t)\Big] - \frac{1}{h}\big[\psi(x_M,t)-\psi(x_{M-1},t)\big]\Big\}\\
& + V(x_M,t)\psi(x_M,t) + \mathcal{O}(h), \quad 0<t\le T.
\end{aligned}
$$

From (3.22a)-(3.22e) and (2.13f), we have

$$
\begin{aligned}
i\delta_t\Psi_j^{n-\frac{1}{2}} = & -\delta_x^2\Psi_j^{n-\frac{1}{2}} + V_j^{n-\frac{1}{2}}\Psi_j^{n-\frac{1}{2}} + p_j^{n-\frac{1}{2}}, \quad 1\le j\le M-1, \quad 1\le n\le K, \qquad (3.24a)\\
i\delta_t\Psi_0^{n-\frac{1}{2}} = & -\frac{2}{h}\Big\{\delta_x\Psi_{\frac{1}{2}}^{n-\frac{1}{2}} + ik_0\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\Psi_0^{n-\frac{1}{2}} - k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\,\Phi_{m,1}^{n-\frac{1}{2}}\Big]\Big\}\\
& + V_0^{n-\frac{1}{2}}\psi_0^{n-\frac{1}{2}} + p_0^{n-\frac{1}{2}}, \quad 1\le n\le K, \qquad (3.24b)
\end{aligned}
$$

$$i\delta_t\Psi_M^{n-\frac{1}{2}} = -\frac{2}{h}\Big\{ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\Psi_M^{n-\frac{1}{2}} - k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\Phi_{m,2}^{n-\frac{1}{2}}\Big] - \delta_x\Psi_{M-\frac{1}{2}}^{n-\frac{1}{2}}\Big\}$$
$$+V_M^{n-\frac{1}{2}}\Psi_M^{n-\frac{1}{2}} + p_M^{n-\frac{1}{2}}, \quad 1\le n\le K, \tag{3.24c}$$
$$(1-a_m)k_0^2\Phi_{m,1}^{n-\frac{1}{2}} + ia_m\delta_t\Phi_{m,1}^{n-\frac{1}{2}} = \Psi_0^{n-\frac{1}{2}} + r_{m,1}^{n-\frac{1}{2}}, \quad 1\le m\le N, \quad 1\le n\le K, \tag{3.24d}$$
$$(1-a_m)k_0^2\Phi_{m,2}^{n-\frac{1}{2}} + ia_m\delta_t\Phi_{m,2}^{n-\frac{1}{2}} = \Psi_M^{n-\frac{1}{2}} + r_{m,2}^{n-\frac{1}{2}}, \quad 1\le m\le N, \quad 1\le n\le K, \tag{3.24e}$$
$$\Psi_j^0 = \psi_0(x_j), \quad 0\le j\le M, \quad \Phi_{m,1}^0 = 0, \quad \Phi_{m,2}^0 = 0, \quad 1\le m\le N. \tag{3.24f}$$

Denote

$$\tilde{\psi}_j^n = \Psi_j^n - \psi_j^n, \qquad 0\le j\le M, \quad 0\le n\le K,$$
$$\tilde{\phi}_{m,1}^n = \Phi_{m,1}^n - \phi_{m,1}^n, \quad \tilde{\phi}_{m,2}^n = \Phi_{m,2}^n - \phi_{m,2}^n, \qquad 1\le m\le N, \quad 0\le n\le K.$$

Theorem 3.3. *Let* $\{\psi_j^n \,|\, 0\le j\le M,\ 0\le n\le K\}$ *be the solution of the difference scheme* (3.1a)-(3.1f), *or* (3.4a)-(3.4f). *Then we have*

$$\|\tilde{\psi}^n\|^2 + k_0^3\sum_{m=1}^N b_m\Big(\big|\tilde{\phi}_{m,1}^n\big|^2 + \big|\tilde{\phi}_{m,2}^n\big|^2\Big) \le c_2(\tau^2+h^2)^2, \quad 1\le n\le K,$$

where

$$c_2 = \exp\big\{3(1+ck_0^2)T\big\}\cdot\frac{1}{4(1+ck_0^2)}\Big[\frac{1}{k_0} + (x_r-x_l) + 2k_0^3\sum_{m=1}^N\frac{b_m}{a_m^2}\Big]c_1^2.$$

Proof. Subtracting (3.4a)-(3.4f) from (3.24a)-(3.24f), we obtain the error equations

$$i\delta_t\tilde{\psi}_j^{n-\frac{1}{2}} = -\delta_x^2\tilde{\psi}_j^{n-\frac{1}{2}} + V_j^{n-\frac{1}{2}}\tilde{\psi}_j^{n-\frac{1}{2}} + p_j^{n-\frac{1}{2}}, \quad 1\le j\le M-1, \quad 1\le n\le K, \tag{3.25a}$$
$$i\delta_t\tilde{\psi}_0^{n-\frac{1}{2}} = -\frac{2}{h}\Big\{\delta_x\tilde{\psi}_{\frac{1}{2}}^{n-\frac{1}{2}} + ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\tilde{\psi}_0^{n-\frac{1}{2}} - k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\tilde{\phi}_{m,1}^{n-\frac{1}{2}}\Big]\Big\}$$
$$+V_0^{n-\frac{1}{2}}\tilde{\psi}_0^{n-\frac{1}{2}} + p_0^{n-\frac{1}{2}}, \quad 1\le n\le K, \tag{3.25b}$$
$$i\delta_t\tilde{\psi}_M^{n-\frac{1}{2}} = -\frac{2}{h}\Big\{ik_0\Big[\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\tilde{\psi}_M^{n-\frac{1}{2}} - k_0^2\sum_{m=1}^N\frac{b_m}{a_m}\,\tilde{\phi}_{m,2}^{n-\frac{1}{2}}\Big] - \delta_x\tilde{\psi}_{M-\frac{1}{2}}^{n-\frac{1}{2}}\Big\}$$
$$+V_M^{n-\frac{1}{2}}\tilde{\psi}_M^{n-\frac{1}{2}} + p_M^{n-\frac{1}{2}}, \quad 1\le n\le K, \tag{3.25c}$$
$$(1-a_m)k_0^2\tilde{\phi}_{m,1}^{n-\frac{1}{2}} + ia_m\delta_t\tilde{\phi}_{m,1}^{n-\frac{1}{2}} = \tilde{\psi}_0^{n-\frac{1}{2}} + r_{m,1}^{n-\frac{1}{2}}, \quad 1\le m\le N, \quad 1\le n\le K, \tag{3.25d}$$
$$(1-a_m)k_0^2\tilde{\phi}_{m,2}^{n-\frac{1}{2}} + ia_m\delta_t\tilde{\phi}_{m,2}^{n-\frac{1}{2}} = \tilde{\psi}_M^{n-\frac{1}{2}} + r_{m,2}^{n-\frac{1}{2}}, \quad 1\le m\le N, \quad 1\le n\le K, \tag{3.25e}$$
$$\tilde{\psi}_j^0 = 0, \quad 0\le j\le M, \quad \tilde{\phi}_{m,1}^0 = 0, \quad \tilde{\phi}_{m,2}^0 = 0, \quad 1\le m\le N. \tag{3.25f}$$

Multiplying (3.25a) by $h\overline{\tilde{\psi}}_j^{n-\frac{1}{2}}$, (3.25b) by $h\overline{\tilde{\psi}}_0^{n-\frac{1}{2}}/2$, (3.25c) by $h\overline{\tilde{\psi}}_M^{n-\frac{1}{2}}/2$, respectively, then adding the results, we obtain

$$
\begin{aligned}
&i\cdot h\Big(\frac{1}{2}\overline{\tilde{\psi}}_0^{n-\frac{1}{2}}\delta_t\tilde{\psi}_0^{n-\frac{1}{2}}+\sum_{j=1}^{M-1}\overline{\tilde{\psi}}_j^{n-\frac{1}{2}}\delta_t\tilde{\psi}_j^{n-\frac{1}{2}}+\frac{1}{2}\overline{\tilde{\psi}}_M^{n-\frac{1}{2}}\delta_t\tilde{\psi}_M^{n-\frac{1}{2}}\Big)\\
=&-\overline{\tilde{\psi}}_0^{n-\frac{1}{2}}\delta_x\tilde{\psi}_{\frac{1}{2}}^{n-\frac{1}{2}}-h\sum_{j=1}^{M-1}\overline{\tilde{\psi}}_j^{n-\frac{1}{2}}\delta_x^2\tilde{\psi}_j^{n-\frac{1}{2}}+\overline{\tilde{\psi}}_M^{n-\frac{1}{2}}\delta_x\tilde{\psi}_{M-\frac{1}{2}}^{n-\frac{1}{2}}-ik_0\overline{\tilde{\psi}}_0^{n-\frac{1}{2}}\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\tilde{\psi}_0^{n-\frac{1}{2}}\\
&-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\tilde{\phi}_{m,1}^{n-\frac{1}{2}}\Big]-ik_0\overline{\tilde{\psi}}_M^{n-\frac{1}{2}}\Big[\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\tilde{\psi}_M^{n-\frac{1}{2}}-k_0^2\sum_{m=1}^{N}\frac{b_m}{a_m}\tilde{\phi}_{m,2}^{n-\frac{1}{2}}\Big]+h\Big(\frac{1}{2}V_0^{n-\frac{1}{2}}|\psi_0^{n-\frac{1}{2}}|^2\\
&+\sum_{j=1}^{M-1}V_j^{n-\frac{1}{2}}|\psi_j^{n-\frac{1}{2}}|^2+\frac{1}{2}V_M^{n-\frac{1}{2}}|\psi_M^{n-\frac{1}{2}}|^2\Big)+h\Big(\frac{1}{2}\overline{\tilde{\psi}}_0^{n-\frac{1}{2}}p_0^{n-\frac{1}{2}}+\sum_{j=1}^{M-1}\overline{\tilde{\psi}}_j^{n-\frac{1}{2}}p_j^{n-\frac{1}{2}}+\frac{1}{2}\overline{\tilde{\psi}}_M^{n-\frac{1}{2}}p_M^{n-\frac{1}{2}}\Big).
\end{aligned}
$$

Taking the imaginary part, we get

$$
\begin{aligned}
\frac{1}{2\tau}\Big(\|\tilde{\psi}^n\|^2-\|\tilde{\psi}^{n-1}\|^2\Big)\le&-k_0\Big(1+\sum_{m=1}^{N}\frac{b_m}{a_m}\Big)\Big(|\tilde{\psi}_0^{n-\frac{1}{2}}|^2+|\tilde{\psi}_M^{n-\frac{1}{2}}|^2\Big)\\
&+k_0^3\mathrm{Re}\Big\{\overline{\tilde{\psi}}_0^{n-\frac{1}{2}}\sum_{m=1}^{N}\frac{b_m}{a_m}\tilde{\phi}_{m,1}^{n-\frac{1}{2}}+\overline{\tilde{\psi}}_M^{n-\frac{1}{2}}\sum_{m=1}^{N}\frac{b_m}{a_m}\tilde{\phi}_{m,2}^{n-\frac{1}{2}}\Big\}\\
&+\mathrm{Im}\Big\{h\Big[\frac{1}{2}\overline{\tilde{\psi}}_0^{n-\frac{1}{2}}p_0^{n-\frac{1}{2}}+\sum_{j=1}^{M-1}\overline{\tilde{\psi}}_j^{n-\frac{1}{2}}p_j^{n-\frac{1}{2}}+\frac{1}{2}\overline{\tilde{\psi}}_M^{n-\frac{1}{2}}p_M^{n-\frac{1}{2}}\Big]\Big\}. \qquad (3.26)
\end{aligned}
$$

Multiplying (3.25d) by $\overline{\tilde{\phi}}_{m,1}^{n-\frac{1}{2}}$, we have

$$
(1-a_m)k_0^2|\tilde{\phi}_{m,1}^{n-\frac{1}{2}}|^2+ia_m\overline{\tilde{\phi}}_{m,1}^{n-\frac{1}{2}}\delta_t\tilde{\phi}_{m,1}^{n-\frac{1}{2}}=\overline{\tilde{\phi}}_{m,1}^{n-\frac{1}{2}}\tilde{\psi}_0^{n-\frac{1}{2}}+\overline{\tilde{\phi}}_{m,1}^{n-\frac{1}{2}}r_{m,1}^{n-\frac{1}{2}},\quad 1\le m\le N,\ 1\le n\le K.
$$

Taking the imaginary part, we obtain

$$
\frac{1}{2\tau}a_m\big(|\tilde{\phi}_{m,1}^{n}|^2-|\tilde{\phi}_{m,1}^{n-1}|^2\big)=\mathrm{Im}\big\{\overline{\tilde{\phi}}_{m,1}^{n-\frac{1}{2}}\tilde{\psi}_0^{n-\frac{1}{2}}+\overline{\tilde{\phi}}_{m,1}^{n-\frac{1}{2}}r_{m,1}^{n-\frac{1}{2}}\big\},\quad 1\le m\le N,\ 1\le n\le K.
$$

Multiplying the equality above by $k_0^3b_m/a_m$ and then summing up for m from 1 to N, we get

$$
\begin{aligned}
&\frac{1}{2\tau}\Big(k_0^3\sum_{m=1}^{N}b_m|\tilde{\phi}_{m,1}^{n}|^2-k_0^3\sum_{m=1}^{N}b_m|\tilde{\phi}_{m,1}^{n-1}|^2\Big)\\
=&k_0^3\mathrm{Im}\Big\{\tilde{\psi}_0^{n-\frac{1}{2}}\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\tilde{\phi}}_{m,1}^{n-\frac{1}{2}}+\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\tilde{\phi}}_{m,1}^{n-\frac{1}{2}}r_{m,1}^{n-\frac{1}{2}}\Big\},\quad 1\le n\le K. \qquad (3.27)
\end{aligned}
$$

Similarly, we can obtain from (3.25e) that

$$
\begin{aligned}
&\frac{1}{2\tau}\Big(k_0^3\sum_{m=1}^{N}b_m|\tilde{\phi}_{m,2}^{n}|^2-k_0^3\sum_{m=1}^{N}b_m|\tilde{\phi}_{m,2}^{n-1}|^2\Big)\\
=&k_0^3\mathrm{Im}\Big\{\tilde{\psi}_M^{n-\frac{1}{2}}\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\tilde{\phi}}_{m,2}^{n-\frac{1}{2}}+\sum_{m=1}^{N}\frac{b_m}{a_m}\overline{\tilde{\phi}}_{m,2}^{n-\frac{1}{2}}r_{m,2}^{n-\frac{1}{2}}\Big\},\quad 1\le n\le K. \qquad (3.28)
\end{aligned}
$$

Denote

$$F^n=\big\|\tilde{\psi}^n\big\|^2+k_0^3\sum_{m=1}^N b_m\big|\tilde{\phi}^n_{m,1}\big|^2+k_0^3\sum_{m=1}^N b_m\big|\tilde{\phi}^n_{m,2}\big|^2.$$

Adding (3.26), (3.27) and (3.28), we get

$$\begin{aligned}\frac{1}{2\tau}(F^n-F^{n-1})\le&-k_0\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\Big(|\tilde{\psi}_0^{n-\frac12}|^2+|\tilde{\psi}_M^{n-\frac12}|^2\Big)\\&+k_0^3\mathrm{Re}\Big\{\tilde{\psi}_0^{n-\frac12}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,1}^{n-\frac12}+\tilde{\psi}_M^{n-\frac12}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,2}^{n-\frac12}\Big\}\\&+k_0^3\mathrm{Im}\Big\{\tilde{\psi}_0^{n-\frac12}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,1}^{n-\frac12}+\tilde{\psi}_M^{n-\frac12}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,2}^{n-\frac12}\Big\}\\&+k_0^3\mathrm{Im}\Big\{\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,1}^{n-\frac12}r_{m,1}^{n-\frac12}+\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,2}^{n-\frac12}r_{m,2}^{n-\frac12}\Big\}\\&+\mathrm{Im}\Big\{h\Big(\frac12\overline{\tilde{\psi}}{}_0^{n-\frac12}p_0^{n-\frac12}+\sum_{j=1}^{M-1}\overline{\tilde{\psi}}{}_j^{n-\frac12}p_j^{n-\frac12}+\frac12\overline{\tilde{\psi}}{}_M^{n-\frac12}p_M^{n-\frac12}\Big)\Big\}.\end{aligned}\tag{3.29}$$

Similarly to (2.25), we have

$$\begin{aligned}B\equiv&k_0^3\mathrm{Re}\Big\{\tilde{\psi}_0^{n-\frac12}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,1}^{n-\frac12}+\tilde{\psi}_M^{n-\frac12}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,2}^{n-\frac12}\Big\}\\&+k_0^3\mathrm{Im}\Big\{\tilde{\psi}_0^{n-\frac12}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,1}^{n-\frac12}+\tilde{\psi}_M^{n-\frac12}\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,2}^{n-\frac12}\Big\}\\\le&\epsilon\Big(|\tilde{\psi}_0^{n-\frac12}|^2+|\tilde{\psi}_M^{n-\frac12}|^2\Big)+\frac{k_0^6}{2\epsilon}\Big(\sum_{m=1}^N\frac{b_m}{a_m^2}\Big)\cdot\sum_{m=1}^N b_m\Big(|\tilde{\phi}_{m,1}^{n-\frac12}|^2+|\tilde{\phi}_{m,2}^{n-\frac12}|^2\Big).\end{aligned}$$

Taking

$$\epsilon=\frac12 k_0\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big),$$

we obtain

$$B\le\frac{k_0}{2}\Big(1+\sum_{m=1}^N\frac{b_m}{a_m}\Big)\Big(|\tilde{\psi}_0^{n-\frac12}|^2+|\tilde{\psi}_M^{n-\frac12}|^2\Big)+c\cdot k_0^5\sum_{m=1}^N b_m\Big(|\tilde{\phi}_{m,1}^{n-\frac12}|^2+|\tilde{\phi}_{m,2}^{n-\frac12}|^2\Big).\tag{3.30}$$

In addition, we have

$$\begin{aligned}&k_0^3\Big|\mathrm{Im}\Big\{\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,1}^{n-\frac12}r_{m,1}^{n-\frac12}+\sum_{m=1}^N\frac{b_m}{a_m}\overline{\tilde{\phi}}{}_{m,2}^{n-\frac12}r_{m,2}^{n-\frac12}\Big\}\Big|\\\le&k_0^3\Big[\sum_{m=1}^N b_m\Big(|\tilde{\phi}_{m,1}^{n-\frac12}|^2+|\tilde{\phi}_{m,2}^{n-\frac12}|^2\Big)+\frac14\sum_{m=1}^N\frac{b_m}{a_m^2}\Big(|r_{m,1}^{n-\frac12}|^2+|r_{m,2}^{n-\frac12}|^2\Big)\Big],\end{aligned}\tag{3.31}$$

and

$$
\begin{aligned}
&\Big|h\Big[\frac{1}{2}\overline{\tilde{\psi}}_0^{n-\frac{1}{2}}p_0^{n-\frac{1}{2}}+\sum_{j=1}^{M-1}\overline{\tilde{\psi}}_j^{n-\frac{1}{2}}p_j^{n-\frac{1}{2}}+\frac{1}{2}\overline{\tilde{\psi}}_M^{n-\frac{1}{2}}p_M^{n-\frac{1}{2}}\Big]\Big|\\
\le&\frac{1}{2}h|\tilde{\psi}_0^{n-\frac{1}{2}}|\cdot|p_0^{n-\frac{1}{2}}|+h\sum_{j=1}^{M-1}|\tilde{\psi}_j^{n-\frac{1}{2}}|\cdot|p_j^{n-\frac{1}{2}}|+\frac{1}{2}h|\tilde{\psi}_M^{n-\frac{1}{2}}|\cdot|p_M^{n-\frac{1}{2}}|\\
\le&\frac{k_0}{2}|\tilde{\psi}_0^{n-\frac{1}{2}}|^2+\frac{h^2}{8k_0}|p_0^{n-\frac{1}{2}}|^2+h\sum_{j=1}^{M-1}\Big(|\tilde{\psi}_j^{n-\frac{1}{2}}|^2+\frac{1}{4}|p_j^{n-\frac{1}{2}}|^2\Big)+\frac{k_0}{2}|\tilde{\psi}_M^{n-\frac{1}{2}}|^2+\frac{h^2}{8k_0}|p_M^{n-\frac{1}{2}}|^2\\
\le&\frac{k_0}{2}\Big(|\tilde{\psi}_0^{n-\frac{1}{2}}|^2+|\tilde{\psi}_M^{n-\frac{1}{2}}|^2\Big)+\|\tilde{\psi}^{n-\frac{1}{2}}\|^2+\frac{h^2}{8k_0}\Big(|p_0^{n-\frac{1}{2}}|^2+|p_M^{n-\frac{1}{2}}|^2\Big)+\frac{1}{4}h\sum_{j=1}^{M-1}|p_j^{n-\frac{1}{2}}|^2.
\end{aligned}
\tag{3.32}
$$

Inserting (3.30)-(3.32) into (3.29) and noticing (3.23a)-(3.23c), we get

$$
\begin{aligned}
\frac{1}{2\tau}(F^n-F^{n-1})\le&\|\tilde{\psi}^{n-\frac{1}{2}}\|^2+(1+ck_0^2)k_0^3\sum_{m=1}^{N}b_m\Big(|\tilde{\phi}_{m,1}^{n-\frac{1}{2}}|^2+|\tilde{\phi}_{m,2}^{n-\frac{1}{2}}|^2\Big)\\
&+\frac{h^2}{8k_0}\Big(|p_0^{n-\frac{1}{2}}|^2+|p_M^{n-\frac{1}{2}}|^2\Big)+\frac{1}{4}h\sum_{j=1}^{M-1}|p_j^{n-\frac{1}{2}}|^2+\frac{1}{4}k_0^3\sum_{m=1}^{N}\frac{b_m}{a_m^2}\Big(|r_{m,1}^{n-\frac{1}{2}}|^2+|r_{m,2}^{n-\frac{1}{2}}|^2\Big)\\
\le&\frac{1}{2}(1+ck_0^2)(F^n+F^{n-1})+\frac{1}{4}\Big[\frac{1}{k_0}+(x_r-x_l)+2k_0^3\sum_{m=1}^{N}\frac{b_m}{a_m^2}\Big]c_1^2(\tau^2+h^2)^2,\quad 1\le n\le K.
\end{aligned}
$$

When $\tau\le[3(1+ck_0^2)]^{-1}$, it holds that

$$
F^n\le\big[1+3(1+ck_0^2)\tau\big]F^{n-1}+\frac{3}{4}\Big[\frac{1}{k_0}+(x_r-x_l)+2k_0^3\sum_{m=1}^{N}\frac{b_m}{a_m^2}\Big]c_1^2\tau(\tau^2+h^2)^2,\quad 1\le n\le K.
$$

The Gronwall inequality yields

$$
\begin{aligned}
F^n\le&\exp\big\{3(1+ck_0^2)n\tau\big\}\cdot\Big\{F^0+\frac{1}{4(1+ck_0^2)}\Big[\frac{1}{k_0}+(x_r-x_l)+2k_0^3\sum_{m=1}^{N}\frac{b_m}{a_m^2}\Big]c_1^2(\tau^2+h^2)^2\Big\}\\
\le&\exp\{3(1+ck_0^2)T\}\cdot\frac{1}{4(1+ck_0^2)}\Big[\frac{1}{k_0}+(x_r-x_l)+2k_0^3\sum_{m=1}^{N}\frac{b_m}{a_m^2}\Big]c_1^2(\tau^2+h^2)^2,\quad 1\le n\le K.
\end{aligned}
$$

This ends the proof. □

4 Numerical examples

In this section, three numerical tests are given to verify the theoretical results. We first verify the second order accuracy of the difference scheme both in space and in time for given k_0 and N. Then we investigate the influence of the parameters k_0 and N on the efficiency of the high-order local ABCs. At last, the superposition of a Gaussian field with different wave numbers is considered. Let $\psi_{\text{exact}}(x,t)$ be the solution of (1.1a)-(1.1c) and $\{\psi_j^n | 0 \le j \le M,\ 0 \le n \le K\}$ be the solution of (3.1a)-(3.1f), or (3.4a)-(3.4f). Define the error grid function

$$\hat{e}_j^n = \psi_{\text{exact}}(x_j,t_n) - \psi_j^n, \quad 0 \le j \le M, \quad 0 \le n \le K,$$

and the global error

$$E(h,\tau) = \max_{0 \le n \le K} \|\hat{e}^n\|.$$

If

$$E(h,\tau) \approx \alpha h^p + \beta \tau^q,$$

then, we have

1. when τ is sufficiently small, $E(h,\tau) \approx \alpha h^p$ and $p \approx \log_2\left(\frac{E(2h,\tau)}{E(h,\tau)}\right)$.
2. when h is sufficiently small, $E(h,\tau) \approx \beta \tau^q$ and $q \approx \log_2\left(\frac{E(h,2\tau)}{E(h,\tau)}\right)$.

Example 4.1. Let the computational domain be $[-5,5]$, $V(x,t) \equiv 0$, and let the initial value be given by

$$\psi_0(x) = \exp(-x^2).$$

Then the exact solution of (1.1a)-(1.1c) corresponding to the above initial value on $\mathbb{R}$ is

$$\psi_{\text{exact}}(x,t) = \frac{1}{\sqrt{1+4it}} \exp\left(\frac{-x^2}{1+4it}\right).$$

Using fixed parameters $k_0 = 1.0$, $N = 40$, and $T = 5$, we list the three cases as follows:

1. Fix τ =1.0e-4. Taking $h = 1/8, 1/16, 1/32, 1/64$, respectively, Table 1 shows the second order convergence of $E(h,\tau)$ in h.
2. Fix $h =$ 2.0e-4. Taking $\tau = 1/16, 1/32, 64, 1/128$, respectively, Table 2 shows the second order convergence of $E(h,\tau)$ in τ.
3. Taking $h = \tau = 1/16, 1/32, 1/64, 1/128$, respectively. We observe that the difference scheme are second order convergent both in space and in time in Table 3.

For different parameters k_0 and N, Table 4 shows the global error $E(h,\tau)$ with $h = \tau = 1/1280$.

Table 1: The global error and convergence order in h when $\tau = 1.0\text{e}-4$ for Example 4.1.

h	1/8	order	1/16	order	1/32	order	1/64	order
$E(h,\tau)$	9.367e-3	*	2.320e-3	2.014	5.784e-4	2.004	1.445e-4	2.001

Table 2: The global error and convergence order in τ when $h=2.0\text{e}-4$ for Example 4.1.

τ	1/16	order	1/32	order	1/64	order	1/128	order
$E(h,\tau)$	1.957e-2	*	4.883e-3	2.003	1.212e-3	2.010	3.025e-4	2.003

Table 3: The global error and convergence order when $h=\tau$ for Example 4.1.

$h=\tau$	1/16	order	1/32	order	1/64	order	1/128	order
$E(h,\tau)$	1.388e-2	*	3.425e-3	2.018	8.534e-4	2.005	2.132e-4	2.001

Table 4: The global error $E(h,\tau)$ with different N and k_0 with $h=\tau=1/1280$ for Example 4.1.

$k_0\backslash N$	1	3	5	7	10	20	40
0.5	9.2158e-2	1.4475e-2	3.1787e-3	8.5344e-4	4.2008e-4	8.6432e-5	1.3417e-5
0.8	3.4254e-2	3.1599e-3	1.1213e-3	5.2838e-4	2.6362e-4	3.4596e-5	4.0263e-6
1.0	2.2618e-2	3.3776e-3	1.0711e-3	4.6489e-4	1.7987e-4	2.3413e-5	3.3431e-6
2.0	8.0027e-2	1.0680e-2	2.4561e-3	7.8611e-4	2.0884e-4	1.2367e-5	3.3428e-6
4.0	2.2432e-1	6.0722e-2	1.9620e-2	7.0785e-3	1.8032e-3	5.3560e-5	3.3427e-6
10	4.5262e-1	2.4390e-1	1.3942e-1	8.3093e-2	4.0265e-2	4.6131e-3	1.1415e-4

Example 4.2. In this example, we compare the numerical solution of (2.13a)-(2.13f) with the exact solution, of (1.1a)-(1.1c):

$$\psi_{\text{exact}}(x,t)=\frac{\exp(-i\pi/4)}{\sqrt{4t-i}}\exp\Big(\frac{ix^2-6x-36t}{4t-i}\Big).$$

Let the computational interval be $[-5,5]$. The bound of the initial function remains under 1.0e-10 beyond the computational interval. The wave will pass through the left boundary ($x=-5$) between $t=0$ and $t=1$.

For fixed parameters $k_0=6.0$, $N=40$, and $T=1$, we also list the three cases as follows:

1. Let τ=1.0e-4. Table 5 shows the second order convergence of global error $E(h,\tau)$ in τ by taking $h=1/16,1/32,1/64$ and $1/128$.
2. Let $h=$ 2.0e-4. Table 6 shows the second order convergence of global error $E(h,\tau)$ in h by taking $\tau=1/160,1/320,1/640$ and $1/1280$.
3. Table 7 presents global error $E(h,\tau)$ when $h=\tau=1/160,1/320,1/640,1/1280$.

Take $h=\tau=1/5120$. We study the global error $E(h,\tau)$ for different parameters k_0 and N. Some results are shown in Table 8.

We remark that from Tables 1-3 and Tables 5-7, one can observe that the difference scheme has the accuracy of second order in time and in space when the parameter N is chosen larger (here $N=40$). From Table 4 and Table 8, one can see that the global error $E(h,\tau)$ is sensitive to the choice of k_0. The global error $E(h,\tau)$ tends to be smaller and smaller when N is chosen larger and larger. Hence we conclude that when N is taken

Table 5: The global error and convergence order in h when $\tau=1.0\text{e}-4$ for Example 4.2.

h	1/16	order	1/32	order	1/64	order	1/128	order
$E(h,\tau)$	1.812e-1	*	4.498e-2	2.010	1.123e-2	2.001	2.823e-3	1.992

Table 6: The global error and convergence order in τ when $h=2.0\text{e}-4$ for Example 4.2.

τ	1/160	order	1/320	order	1/640	order	1/1280	order
$E(h,\tau)$	9.070e-2	*	2.267e-2	2.000	5.665e-3	2.001	1.417e-3	1.999

Table 7: The global error and convergence order when $h=\tau$ for Example 4.2.

$h=\tau$	1/160	order	1/320	order	1/640	order	1/1280	order
$E(h,\tau)$	1.820e-1	*	4.517e-2	2.011	1.127e-2	2.004	2.815e-3	2.001

Table 8: The global error $E(h,\tau)$ with different N and k_0 with $h=\tau=1/5120$ for Example 4.2.

$k_0\backslash N$	1	2	4	6	10	20	40
1.0	4.0807e-1	2.1471e-1	6.2692e-2	1.9354e-2	2.0892e-3	9.0887e-5	9.0160e-5
3.0	5.1861e-2	8.4734e-3	3.0384e-4	9.1021e-5	9.0161e-5	9.0194e-5	9.0160e-5
6.0	3.4199e-3	3.2694e-4	9.0159e-5	9.0160e-5	9.0156e-5	9.0156e-5	9.0156e-5
9.0	2.2323e-2	3.3231e-3	1.6136e-4	9.0160e-5	9.0160e-5	9.0160e-5	9.0160e-5
12	5.9666e-2	1.2206e-2	9.1779e-4	1.0948e-4	9.0160e-5	9.0160e-5	9.0160e-5
20	1.9273e-1	6.6941e-2	1.0344e-2	2.0970e-3	1.4682e-4	9.0160e-5	9.0160e-5

larger enough, the obtained high-order ABCs will work well, and the influence of the parameter k_0 can be ignored. For $N=40$. Tables 1-8 verified the efficiency of the high-order LABCs to absorb the "fast" or "slow" waves.

Example 4.3. We consider an example (see, e.g., Section 6.2 in [3]) about the superposition of a few Gaussian fields with different wave numbers. Let the potential $V\equiv 0$ and the Gaussian initial condition

$$\psi_0=\sum_{\iota=1}^{4}\exp\big\{-(x-x_\iota)^2+ik_\iota(x-x_\iota)\big\}, \tag{4.1}$$

with $x_1=-9, x_2=-6, x_3=-2, x_4=0$ and $k_1=5, k_2=-7, k_3=-12, k_4=2$. The computational domain is chosen to be $]x_l,x_r[=]-12,3[$ and the error E_T is defined by $E_T=\max_{n=K}\|\hat{e}^n\|$.

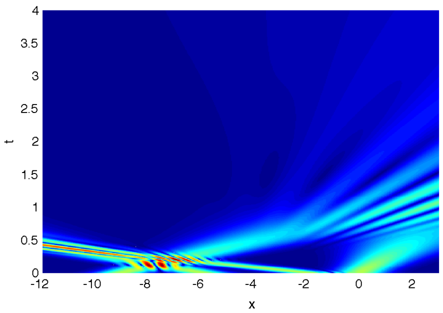
For fixed parameters $k_0=6.0$, $N=40$, and $T=4$, we also list the two cases as follows:

1. Fig. 1 shows the evolution of reference solution (left) and the evolution of numerical solution (right). In the calculation, the mesh sizes are chosen to be $h=1.0\text{e-}2$ and $\tau=1.0\text{e-}3$.
2. Let $\tau=1.0e-4$. Table 9 shows the error $E_T(h,\tau)$ and the corresponding convergence order in h by taking $h=1/20, 1/40.1/80$ and $1/160$.

Table 9: The error E_T and convergence order in h when $\tau = 1.0\text{e}-4$ for Example 4.3.

h	1/160	order	1/320	order	1/640	order	1/1280	order
$E(h,\tau)$	3.346e-3	*	1.577e-3	1.085	7.554e-4	1.062	3.678e-4	1.038

From Fig. 1, no reflection wave is obviously observed. Table 9 shows that the convergence is of first-order, since k_0 is fixed. Generally speaking, the parameter k_0 should be taken approximately as the wave-number of the wave impinged on the boundary. In practical computations, we can turn to a suitable wave-number picked adaptively by applying the Gabor transform [39, 43]. Thus the parameter k_0 will be a function of time t, and the analysis for this case would be more complicated.



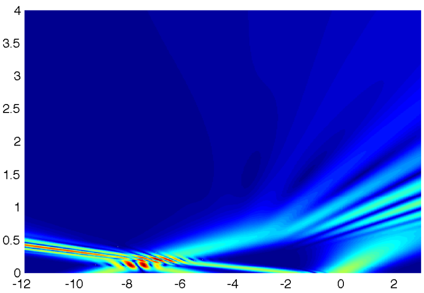


Figure 1: The reference solution (left) and the numerical solution (right).

5 Concluding remarks

We have successfully constructed the high order ABCs for the Schrödinger equations, and illustrated that the reduced initial boundary value problems are stable. The second part of the article is on the difference approximation (a Crank-Nicolson type difference scheme). The unique solvability, unconditional stability and convergence are proved. The convergence order is two both in time and in space. Numerical examples have verified the theoretical results for single wave numbers. For the superposition of a few Gaussian fields with different wave-numbers, we need to apply better ABCs (to refer to [3]).

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