AN EFFICIENT SECOND-ORDER FINITE DIFFERENCE METHOD FOR THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION WITH ABSORBING BOUNDARY CONDITIONS *

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Abstract. A stable and convergent second-order fully discrete finite difference scheme with efficient approximation of the exact absorbing boundary conditions is proposed to solve the Cauchy problem of one-dimensional Schrödinger equation. Our approximation is based on the Padé expansion of the square root function in the complex plane. By introducing a constant damping term to the governing equation and modifying the standard Crank-Nicolson implicit scheme, we show that the fully discrete numerical scheme is unconditionally stable if the order of Padé expansion is chosen from our criterion. In this case, an optimal-order asymptotic error estimate is proved for the numerical solutions. Numerical examples are provided to support the theoretical analysis and illustrate the performance of the proposed numerical scheme.

Key words. Schrödinger equation, absorbing boundary condition, convolution quadrature, Padé approximation, fast algorithm, error estimate

AMS subject classifications. 65M12, 65R20, 65Z05

1. Introduction. The Schrödinger equation describes the time evolution of a physical system in which the quantum effects are significant. It also appears in some other applications, such as underwater acoustics and optics [23, 29, 30]. This work is concerned with an effficient numerical method for the Cauchy problem of one-dimensional Schrödinger equation:

$$i\,\partial_t\psi(x,t) = -\partial_x^2\psi(x,t) + V(x)\psi(x,t) + V_{ex}(x,t)\psi(x,t),\ x\in\mathbb{R}, \tag{1.1}$$

$$\lim_{|x|\to+\infty}\psi(x,t) = 0,\ \psi(x,0) = \psi_0(x),\quad x\in\mathbb{R}, \tag{1.2}$$

where $i=\sqrt{-1}$ denotes the imaginary unit, $\psi(x,t)$ the complex-valued wave function to be determined, $V(x)$ a real-valued nuclear potential, and $V_{ex}(x,t)$ a real-valued external electric potential.

Over the past few decades, great efforts have been made to overcome the numerical difficulties arising from solving PDEs in unbounded domains. Among these efforts, the artificial boundary method turns out to be very successful, see the monograph [19] and the review papers [4, 11, 12, 14, 33]. The key step of the artificial boundary method is the construction of suitable boundary conditions on some artificial boundaries. By this approach, the original problems in the whole space are reduced to problems on bounded domains, which can be solved by grid-based numerical methods. For wave-like problems, these boundary conditions are usually referred to as absorbing boundary conditions (ABCs) in the literature. ABCs are called exact if they render the solutions of truncated domain problems exactly the same as those of unbounded domain problems.

For the Schrödinger equation, the exact ABCs are nonlocal in time, containing some temporal convolutions in the formulations [7, 18]. The nonlocal convolutions in the ex-

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act ABC cause many difficulties in developing and analyzing numerical methods for the truncated problem in bounded domains [5, 31]. On the one hand, only sub-optimal error estimate has been proved for the Schrödinger equation under exact ABCs [31, Theorem 4.3]. On the other hand, fast evaluation of temporal convolutions is important when the number of time steps is large (this occurs in long-time evolution or small time-step simulations, and at the n-th time step $\mathcal{O}(n)$ operations are needed to compute the convolution integral, which results in a total computational cost of $\mathcal{O}(N^2)$ in operations and $\mathcal{O}(N)$ in memory, with N denoting the number of time steps). Fast convolution algorithms with essentially linear complexity $\mathcal{O}(N\ln^2 N)$ and memory $\mathcal{O}(N)$ have been developed in [9, 16]. Fast algorithms with less memory requirements are also extensively studied. This kind of algorithms usually utilizes the summation of exponentials to approximate the convolution kernel (see [21] for an exception), and transform a temporal convolution to a sequence of first order ODE problems. The derivation of exponentials can be done through quadrature approximation in the time domain [8, 22, 36], direct rational approximation of kernel symbols [2, 25], or quadrature approximation of contour integrals in the Laplace domain [28]. While maintaining the almost optimal complexity in terms of operations count, i.e. $\mathcal{O}(N\ln N)$ or $\mathcal{O}(N)$, these algorithms can reduce the memory requirement to at most $\mathcal{O}(\ln N)$.

There are some works on high-order local ABCs for the Schrödinger equation which have considered accelerating long time simulations by using the Padé approximation [6, 32, 34, 35]. However, no analysis has been given for choosing the explicit order of Padé approximation for the fast numerical solutions to achieve optimal-order convergence. In [36], Zheng investigated the convergence of a fast algorithm for the one-dimensional heat equation. However, the analysis technique cannot be directly extended to the Schrödinger equation.

The objective of this paper is to construct a stable and convergent numerical method, integrating an efficient evaluation of the exact ABC as well, for solving the Cauchy problem of one-dimensional Schrödinger equation. To this end, we first reformulate the Schrödinger equation into an equivalent form with a constant damping term σ, and then construct a perturbed Crank-Nicolson scheme to discretize the reformulated problem in time. Specifically, we apply the $\mathcal{Z}$-transform to the reformulated Schrödinger equation to derive a discrete ABC for the temporally discretized problem, and then propose a second-order finite difference scheme for further spatial discretization. By using the (m, m)-Padé rational expansion of the square root function [25], we introduce an efficient algorithm to approximate the discrete convolution involved in the discrete ABC, which is reformulated as a system of differential equations by applying Lindman's idea [24]. The construction of the damping term and the perturbation of the Crank-Nicolson discretization are the key ingredients to maintain the stability of the resulting fully discrete numerical scheme. Finally, we present numerical analysis for the proposed numerical method to guarantee the optimal-order convergence by explicitly prescribing the order of Padé expansion $m = \frac{\ln 1/8(\sigma\tau)^{9/2}}{2\ln\left(1-(\sigma\tau)^{1/2}\right)}$, where τ denotes the step size of time discretization. If T is the length of the time interval, we can choose the the parameter $\sigma = 1/T$ and step size $\tau = T/N$ in the numerical simulations. The number of auxiliary variables, m, behaves asymptotically like $\frac{9}{4}\sqrt{N}\ln N$. Therefore, the proposed algorithm requires $\mathcal{O}(\sqrt{N}\ln N)$ storage and the additional computational cost $\mathcal{O}(N^{\frac{3}{2}}\ln N)$ to evaluate the exact ABCs.

The rest of this paper is organized as follows. In section 2, we introduce the setting of the problem, reformulating the problem by constructing a damping factor in time, and deriving the exact ABC for the reformulated equation. In section 3, we propose temporal and spatial discretizations for the reformulated equation on a truncated computational domain. In sections 4, we introduce the Padé approximation of the fully discrete numerical method, as well as the resulting algorithm for practical computation. In section 5, we determine the order of Padé expansion and prove the optimal-order convergence of the numerical solutions. Numerical examples are provided in section 6 to illustrate the effectiveness of the proposed numerical method.

2. Construction of exact ABCs. We assume that the initial wave function $\psi_0(x)$ and the nuclear potential $V(x)$ in (1.1)-(1.2) are smooth functions with compact supports. Besides, the external electric potential function $V_{ex}(x,t)$ is smooth and has constant tail parts when the location point is suitably far away from the origin. If we set

$$\tilde{V}(x,t) = \int_0^t V_{ex}(x,s)ds, \quad A(x,t) = -\partial_x \tilde{V}(x,t),$$

then the above assumptions imply the existence of two real numbers $x_\pm$ such that

$$\psi_0(x) = 0,\ A(x,t) = 0,\ V(x) = 0, \quad \forall\, x \in (-\infty, x_-] \cup [x_+, \infty). \tag{2.1}$$

Let us introduce a new wave function

$$u(x,t) = e^{i\tilde{V}(x,t)-\sigma t}\psi(x,t),$$

where $\sigma \in [0,1]$ is an auxiliary parameter for controlling the stability of the algorithm to be introduced in this paper. Generally, we set $\sigma = T^{-1}$ with T being the evolutionary time. It is straightforward to verifty that the function $u(x,t)$ solves the following initial value problem:

$$\begin{aligned} &i(\partial_t + \sigma)u(x,t) = \mathcal{L}(t)u(x,t), && \forall x \in \mathbb{R},\ \forall\, t > 0, \\ &u(x,0) = \psi_0(x), && \forall\, x \in \mathbb{R}, \\ &\lim_{|x|\to+\infty} u(x,t) = 0, && \forall\, t > 0, \end{aligned} \tag{2.2}$$

where the time-dependent linear operator $\mathcal{L}(t)$ is defined by

$$\mathcal{L}(t) = -[\partial_x + iA(x,t)]^2 + V(x). \tag{2.3}$$

To obtain exact ABCs for the problem (2.2), we first consider the following exterior problem on the semi-infinite interval $[x_+, +\infty)$:

$$i(\partial_t + \sigma)u(x,t) = -\partial_x^2 u(x,t), \qquad \forall\, x \in [x_+, +\infty),\ \forall\, t > 0, \tag{2.4a}$$

$$u(x,0) = 0, \qquad \forall\, x \in [x_+, +\infty), \tag{2.4b}$$

$$\lim_{x\to+\infty} u(x,t) = 0, \qquad \forall\, t > 0. \tag{2.4c}$$

The Laplace transform of (2.4) in time yields

$$i(z+\sigma)\widehat{u}(x,z) = -\partial_x^2 \widehat{u}(x,z), \qquad \forall\, x \in [x_+, \infty),\ \forall\, z \in \mathbb{C}_+, \tag{2.5}$$

$$\lim_{x\to\infty} \widehat{u}(x,z) = 0, \qquad \forall\, z \in \mathbb{C}_+, \tag{2.6}$$

where $\mathbb{C}_+$ stands for the right half part of the complex plane. The general solution of the equation (2.5) is

$$\widehat{u}(x,z) = c_1(z)\exp\left(-x\sqrt{-i(z+\sigma)}\right) + c_2(z)\exp\left(x\sqrt{-i(z+\sigma)}\right),$$

where $\sqrt{\cdot}$ denotes the square root with nonnegative real part. Clearly, the infinity boundary condition (2.6) implies $c_2(z) = 0$. Consequently, by differentiating the last equation we obtain

$$\partial_x \widehat{u}(x,z) = -\sqrt{-i(z+\sigma)}\,\widehat{u}(x,z), \qquad \forall\, x \in [x_+, +\infty),\ \forall\, z \in \mathbb{C}_+, \tag{2.7}$$

whose inverse Laplace transform yields an absorbing boundary condition at x_+:

$$\sqrt{-i(\partial_t + \sigma)}\,u(x_+,t) + \partial_x u(x_+,t) = 0, \qquad \forall\, t > 0. \tag{2.8}$$

In the above, $\sqrt{-i(\partial_t+\sigma)}$ stands for the multiplier operator (in time) associated with the symbol $\sqrt{-i(z+\sigma)}$, namely,

$$\sqrt{-i(\partial_t+\sigma)}\,u(x_+,t) := \mathscr{L}_z^{-1}[\sqrt{-i(z+\sigma)}\,\widehat{u}(x_+,z)](t), \qquad \forall\, t>0,$$

with $\mathscr{L}_z^{-1}$ denoting the inverse Laplace transform with respect to z-variable.

A similar boundary condition can be derived at x_-:

$$\sqrt{-i(\partial_t+\sigma)}\,u(x_-,t) - \partial_x u(x_-,t) = 0, \qquad \forall\, t>0. \tag{2.9}$$

In view of (2.8) and (2.9), the solution of (2.2) is the same as the solution of the following problem in a bounded domain:

$$\begin{aligned}
&i(\partial_t+\sigma)u(x,t) = \mathcal{L}(t)u(x,t), && \forall x\in(x_-,x_+),\ \forall\, t>0,\\
&\sqrt{-i(\partial_t+\sigma)}\,u(x_\pm,t) + \partial_\nu u(x_\pm,t) = 0, && \forall\, t>0,\\
&u(x,0) = \psi_0(x), && \forall\, x\in[x_-,x_+],
\end{aligned} \tag{2.10}$$

where ∂_ν denotes the outward normal derivative at the boundary points $x_\pm$.

3. Discretization of (2.10). In this section, we discretize (2.10) in time by the Crank-Nicolson scheme with an $\mathcal{O}(\tau^2)$ perturbation, with convolution quadrature for discretizing the fractional time derivative at the boundary points. The $\mathcal{O}(\tau^2)$ perturbation is proposed to guarantee the stability and convergence of an efficient algorithm to be introduced in section 4.

We first introduce the notations of $\mathcal{Z}$-transform in the following subsection.

3.1. $\mathcal{Z}$-transform of a sequence of functions. Given a Hilbert space $\mathcal{H}$ with the inner product $(\cdot,\cdot)_{\mathcal{H}}$ and the induced norm $\|\cdot\|_{\mathcal{H}}$, let us introduce the semi-infinite sequence spaces:

$$\begin{aligned}
\ell^2(\mathcal{H}) &= \Big\{ g=\{g^n\}_{n=0}^\infty : g^n\in\mathcal{H},\ \|g\|_{\ell^2(\mathcal{H})} \equiv \Big(\sum_{n=0}^\infty \|g^n\|_{\mathcal{H}}^2\Big)^{\frac12} < \infty \Big\},\\
\ell_0^2(\mathcal{H}) &= \Big\{ g=\{g^n\}_{n=0}^\infty \in \ell^2(\mathcal{H}) : g^0 = 0 \Big\}.
\end{aligned}$$

The linear space $\ell^2(\mathcal{H})$ is a Hilbert space with the inner product

$$(f,g)_{\ell^2(\mathcal{H})} \equiv \sum_{n=0}^\infty (f^n,g^n)_{\mathcal{H}}, \quad \forall f,g\in\ell^2(\mathcal{H}).$$

For any element in $g=\{g^n\}_{n=0}^\infty\in\ell^2(\mathcal{H})$, we define its $\mathcal{Z}$-transform as $\widetilde{g}(z)=\sum_{n=0}^\infty g^n z^n$, which is an $\mathcal{H}$-valued function holomorphic in the unit disk $\mathbb{D}$. The limit $\widetilde{g}(z)=\lim_{r\nearrow 1}\widetilde{g}(rz)$ exists in $L^2(\partial\mathbb{D};\mathcal{H})$, and the following Parseval's identity holds:

$$(f,g)_{\ell^2(\mathcal{H})} = \int_{\partial\mathbb{D}} (\widetilde{f}(z),\widetilde{g}(z))_{\mathcal{H}}\ \mu(dz), \qquad \forall f,g\in\ell^2(\mathcal{H}). \tag{3.1}$$

For a sequence $f=\{f^n\}_{n=0}^\infty\in\ell^2(\mathcal{H})$, we define the shift operator S by $Sf=\{f^{n+1}\}_{n=0}^\infty$. The average operator E and the forward difference quotient operator D_τ are defined by

$$E=\frac{S+I}{2} \quad\text{and}\quad D_\tau=\frac{S-I}{\tau},$$

respectively. Besides, we make the following notations our convention:

$$Sf^n=(Sf)^n, \quad Ef^n=(Ef)^n, \quad D_\tau f^n=(D_\tau f)^n.$$

It is straightforward to verify that

$$\widetilde{Sf}(z) = z^{-1}\widetilde{f}(z), \quad \widetilde{Ef}(z) = \frac{z^{-1}+1}{2}\widetilde{f}(z), \quad \widetilde{D_\tau f}(z) = \frac{z^{-1}-1}{\tau}\widetilde{f}(z), \quad \forall f \in \ell_0^2(\mathcal{H}). \tag{3.2}$$

Besides, for all $f, g \in \ell^2(\mathcal{H})$ the following identities hold:

$$D_\tau(f^n g^n) = f^n D_\tau g^n + g^n D_\tau f^n + \tau D_\tau f^n D_\tau g^n, \qquad \forall\, n \geq 0, \tag{3.3}$$

$$\mathrm{Re}(D_\tau f^n, E f^n)_{\mathcal{H}} = \frac{1}{2} D_\tau \|f^n\|_{\mathcal{H}}^2, \qquad \forall\, n \geq 0. \tag{3.4}$$

The identities (3.1) and (3.2)-(3.4) will be used frequently in this paper.

3.2. A perturbed Crank-Nicolson scheme. We shall derive a time-stepping scheme for (2.10) from the time discretization of the original problem (1.1). Let $\tau > 0$ be the time step and let us set $t_n = n\tau$. We discretize (2.2) in the following way:

$$\begin{aligned} & i(D_\tau + \sigma E)u^n(x) = \mathcal{L}^{n+\frac{1}{2}}(E + \sigma\tau^2 D_\tau)u^n(x), && \forall x \in \mathbb{R},\ \forall\, n \geq 0, \\ & u^0(x) = \psi_0(x), && \forall\, x \in \mathbb{R}, \\ & \lim_{|x|\to+\infty} u^n(x) = 0, && \forall\, n \geq 1, \end{aligned} \tag{3.5}$$

where $u^n(x) \approx u(x, t_n)$ and $\mathcal{L}^{n+\frac{1}{2}} = \mathcal{L}(t_{n+\frac{1}{2}})$; see (2.3). The scheme (3.5) differs from the standard Crank-Nicolson scheme by the small term $\mathcal{L}^{n+\frac{1}{2}}\sigma\tau^2 D_\tau u^n(x)$.

In view of assumption (2.1), on the interval $[x_+, +\infty)$ the semi-discrete problem (3.5) reduces to

$$\begin{aligned} & i(D_\tau + \sigma E)u^n(x) = -\partial_x^2(E + \sigma\tau^2 D_\tau)u^n(x), && \forall x \in [x_+, +\infty),\ \forall n \geq 0, \\ & u^0(x) = 0, && \forall x \in [x_+, +\infty), \\ & \lim_{x\to+\infty} u^n(x) = 0, && \forall n \geq 1. \end{aligned} \tag{3.6}$$

Let $\widetilde{u}(x,z)$ denote the $\mathcal{Z}$-transform of the sequence $\{u^n(x)\}_{n=0}^{\infty}$. Applying the $\mathcal{Z}$-transform to (3.6) and using (3.2), we obtain

$$\begin{aligned} & \frac{1}{i\tau}\delta(z,\sigma)\widetilde{u}(x,z) - \partial_x^2\widetilde{u}(x,z) = 0, \quad \forall x \in [x_+, +\infty), \\ & \lim_{x\to+\infty} \widetilde{u}(x,z) = 0, \end{aligned}$$

where

$$\delta(z,\sigma) = \frac{2 - 2z + \sigma\tau(1+z)}{1 + z + 2\sigma\tau(1-z)}$$

may be viewed as the generating function for time discretization [27].

The solution $\widetilde{u}$ of the equation above can be generally expressed as

$$\widetilde{u}(x,z) = c_1^+ \exp\left(x\sqrt{-i\frac{\delta(z,\sigma)}{\tau}}\right) + c_2^+ \exp\left(-x\sqrt{-i\frac{\delta(z,\sigma)}{\tau}}\right).$$

The condition $\lim_{x\to+\infty} \widetilde{u}(x,z) = 0$ implies $c_1^+ = 0$. This leads to the following identity (by differentiating $\widetilde{u}(x,z)$ with respect to x):

$$\partial_x\widetilde{u}(x_+, z) = -\sqrt{-i\frac{\delta(z,\sigma)}{\tau}}\,\widetilde{u}(x_+, z), \quad \forall z \in \mathbb{D}, \tag{3.7}$$

which is in analogy to the continuous case (2.7).

Note that the function

$$\widetilde{K}(z) = \sqrt{-i\delta(z,\sigma)} \tag{3.8}$$

is analytic in the unit disk $\mathbb{D}$. Thus it has a power series expansion

$$\widetilde{K}(z) = \sum_{j=0}^{\infty} K_j z^j, \quad \forall\, z \in \mathbb{D}. \tag{3.9}$$

Substituting (3.9) and $\widetilde{u}(x,z) = \sum_{n=0}^{\infty} u^n(x) z^n$ into (3.7) yields an exact absorbing boundary condition for (3.5) at the right artificial boundary point $x = x_+$:

$$\tau^{-\frac{1}{2}}(\mathcal{K}*u)^n(x_+) + \partial_x u^n(x_+) = 0, \quad \forall\, n \geq 0,$$

where $\mathcal{K}*$ is the convolution quadrature operator corresponding to the symbol $\widetilde{K}(z)$, namely,

$$(\mathcal{K}*u)^n = \sum_{j=0}^{n} K_j u^{n-j}. \tag{3.10}$$

For the simplicity of notations, for a function $u(x,t)$ we denote $\mathcal{K}*u(x,t_n) = \sum_{j=0}^{n} K_j\, u(x, t_{n-j})$.

Analogously, by analyzing the problem (3.5) on $(-\infty, x_-]$, we derive an exact absorbing boundary condition at the left artificial boundary point $x = x_-$:

$$\tau^{-\frac{1}{2}}(\mathcal{K}*u)^n(x_-) - \partial_x u^n(x_-) = 0, \quad \forall\, n \geq 1.$$

Consequently, the semi-discrete problem (3.5), originally defined on the the whole space, can be reduced to the following semi-discrete problem on a bounded domain:

$$\begin{aligned} & i(D_\tau + \sigma E)u^n(x) = \mathcal{L}^{n+\frac{1}{2}}(E + \sigma\tau^2 D_\tau)u^n(x), && \forall x \in (x_-, x_+),\ \forall\, n \geq 0, \\ & \tau^{-\frac{1}{2}}(\mathcal{K}*u)^n(x_\pm) + \partial_\nu u^n(x_\pm) = 0, && \forall\, n \geq 0, \\ & u^0(x) = \psi_0(x), && \forall\, x \in [x_-, x_+]. \end{aligned} \tag{3.11}$$

Comparing (3.11) with (2.10), we see that the equation is discretized by a Crank-Nicolson scheme subject to an $\mathcal{O}(\tau^2)$ perturbation, with a convolution quadrature approximation to the fractional-order time derivative at the boundary points $x_\pm$. Since the time discretization (3.5) in the whole space is of second order, it follows that the induced convolution quadrature at the boundary points $x_\pm$ in (3.11) is also second order:

$$|\tau^{-\frac{1}{2}}(\mathcal{K} * u_\pm)^n - \sqrt{-i(\partial_t + \sigma)}u(x_\pm, t_n)| \leq C\tau^2, \tag{3.12}$$

where $u_\pm^n := u(x_\pm, t_n)$. A proof of (3.12) is presented in Appendix A based on the ideas of [26, 27].

3.3. Spatial discretization. Let M be a positive integer, $h = (x_+ - x_-)/M$ be the mesh size, and $\tau > 0$ be the time step. We define the mesh points

$$\begin{aligned} & x_k = x_- + \left(k - \frac{1}{2}\right) h, && k = 0, 1, \cdots, M+1, \\ & t_n = n\tau, && n = 0, 1, \cdots, N, \end{aligned}$$

with x_0 and x_{M+1} being two ghost points.

Given a vector $v = (v_0, \cdots, v_{M+1}) \in \mathbb{C}^{M+2}$, we introduce the discrete gradient $\nabla_h v$ as the $(M+1)$-dimensional vector $(\nabla_h v_0, \cdots, \nabla_h v_M)$ defined by

$$\nabla_h v_k = \frac{v_{k+1} - v_k}{h}, \quad k = 0, 1, \cdots, M.$$

The linear operator which maps the $(M+2)$-dimensional vector $v=(v_0,\cdots,v_{M+1})$ to the M-dimensional vector $(v_1,\cdots,v_M)$ will be denoted by $\mathcal{P}$. The linear operator which maps v to the $(M+1)$-dimensional vector $(v_0,\cdots,v_M)$ will be denoted by $\mathcal{Q}$. Besides, we define the Neumann and Dirichlet data associated with the $(M+2)$-dimensional vector v as

$$\partial_\nu^- v=\frac{v_0-v_1}{h},\ \partial_\nu^+ v=\frac{v_{M+1}-v_M}{h},\ \gamma^- v=\frac{v_0+v_1}{2},\ \gamma^+ v=\frac{v_{M+1}+v_M}{2}.$$

We introduce an inner product in the M-dimensional vector space as

$$(\phi,\varphi)_h=h\sum_{k=1}^{M}\bar{\phi}_k\varphi_k,$$

and an inner product in the $(M+1)$-dimensional vector space as

$$\langle\chi,\omega\rangle_h=\frac{h}{2}\bar{\chi}_0\omega_0+h\sum_{k=1}^{M-1}\bar{\chi}_k\omega_k+\frac{h}{2}\bar{\chi}_M\omega_M.$$

Correspondingly, the induced norms will be denoted by

$$\|\phi\|_h=\sqrt{(\phi,\phi)_h},\qquad |\chi|_h=\sqrt{\langle\chi,\chi\rangle_h}.$$

We introduce a second-order spatial discretization $\mathcal{L}_h^n$ for the continuous differential operator $\mathcal{L}(t_n)$, which maps the $(M+2)$-dimensional vector space to the M-dimensional vector space:

$$\mathcal{L}_h^n v=((\mathcal{L}_h^n v)_1,\cdots,(\mathcal{L}_h^n v)_M),\quad \forall\, v=(v_0,\cdots,v_{M+1}),$$

with

$$\begin{aligned}(\mathcal{L}_h^n v)_k\ &=\frac{2v_k-v_{k+1}-v_{k-1}}{h^2}+\frac{A(x_{k+\frac{1}{2}},t_n)v_{k+1}-A(x_{k-\frac{1}{2}},t_n)v_{k-1}}{ih}\\ &\quad+[V(x_k)+A^2(x_k,t_n)]v_k.\end{aligned}$$

For the simplicity of notations, we use the abbreviation $\mathcal{L}_h^n v_k:=(\mathcal{L}_h^n v)_k$. A direct computation shows that for all $(M+2)$-dimensional vectors v and w, the following discrete Green's formula holds (with element-wise multiplication by U^n and A^n)

$$(\mathcal{P}v,\mathcal{L}_h^n w)_h=\langle\nabla_h^n v,\nabla_h^n w\rangle_h+(\mathcal{P}v,U^n\mathcal{P}w)_h-\overline{\gamma^\pm v}\cdot\partial_\nu^\pm w, \tag{3.13}$$

where $\nabla_h^n=\nabla_h+iA^n\mathcal{Q}$, $A^n=(A_0^n,\cdots,A_M^n)$ and $U^n=(U_1^n,\cdots,U_M^n)$ with the components determined by

$$A_k^n=A(x_{k+\frac{1}{2}},t_n),\quad U_k^n=V(x_k)+A^2(x_k,t_n)-A^2(x_{k+\frac{1}{2}},t_n).$$

In the time-stepping scheme (3.11), replacing the function $u^n(x)$ by the vector $u^n=(u_0^n,\cdots,u_{M+1}^n)$ and replacing the continuous operator $\mathcal{L}^{n+\frac{1}{2}}$ with its discrete analogue $\mathcal{L}_h^{n+\frac{1}{2}}$, we obtain the following fully discrete finite difference scheme:

$$i(D_\tau+\sigma E)\mathcal{P}u^n=\mathcal{L}_h^{n+\frac{1}{2}}(E+\sigma\tau^2 D_\tau)u^n,\qquad \forall\, n\ge 0, \tag{3.14}$$

$$\tau^{-\frac{1}{2}}(\mathcal{K}*\gamma^\pm u)^n+\partial_\nu^\pm u^n=0,\qquad \forall\, n\ge 0, \tag{3.15}$$

$$u^0=(\psi_0(x_0),\cdots,\psi_0(x_{M+1})). \tag{3.16}$$

4. Efficient approximation of (3.14)-(3.16). In this section, we introduce an efficient algorithm for approximating the solution of (3.14)-(3.16). The stability and convergence of the proposed algorithm will be presented in the next section.

4.1. Rational approximation of the convolution quadrature. Prescribed a non-negative integer $m > 0$, the (m, m)-order Padé approximation for the function $\sqrt{1+s}$ can be expressed as (see [25])

$$\sqrt{1+s} \approx 1 + \sum_{j=1}^{m} \frac{a_j s}{1 + b_j s},$$

where

$$a_j = \frac{2}{2m+1} \sin^2 \frac{j\pi}{2m+1}, \quad b_j = \cos^2 \frac{j\pi}{2m+1}, \quad j = 1, \cdots, m.$$

Based on the Padé approximation, we design a rational approximation for the square root function $\sqrt{s}$ on the closed right half complex plane:

$$\sqrt{s} = \sqrt{1+s-1} \approx 1 + \sum_{j=1}^{m} \frac{a_j(s-1)}{1 + b_j(s-1)} \equiv R_m(s), \quad \mathrm{Re}(s) \geq 0.$$

We can rewrite $R_m(s)$ as

$$\begin{aligned} &R_m(s) = \lambda - \sum_{j=1}^{m} \frac{1}{c_j s + d_j}, \\ &\lambda = 1 + \sum_{j=1}^{m} a_j b_j^{-1}, \ c_j = a_j^{-1} b_j^2, \ d_j = a_j^{-1} b_j (1 - b_j), \quad j = 1, \cdots, m. \end{aligned} \tag{4.1}$$

The following result was proved in [25].

Lemma 4.1. *Let*

$$\gamma(s) := \frac{\sqrt{s}-1}{\sqrt{s}+1} \quad \text{and} \quad \mathcal{E}_m(s) := \sqrt{s} - R_m(s), \quad m = 0, 1, 2, \cdots$$

Then the following identity holds:

$$\mathcal{E}_m(s) = 2\sqrt{s} \frac{\gamma^{2m+1}(s)}{1 + \gamma^{2m+1}(s)}, \quad \text{if } \mathrm{Re}(s) \geq 0 \text{ and } s \neq 0. \tag{4.2}$$

For all $\tau > 0$ and $\sigma > 0$, let us introduce the rational approximation $\widetilde{K}^{(m)}(z)$ of the symbol $\widetilde{K}(z)$:

$$\widetilde{K}^{(m)}(z) := i^{-\frac{1}{2}} R_m(\delta(z, \sigma)), \quad \forall\, m \geq 0. \tag{4.3}$$

We denote by $\mathcal{K}^{(m)}*$ the convolution operator analogously defined as (3.10), by replacing the convolution coefficients K_j in (3.10) with the series expansion coefficients of the function $\widetilde{K}^{(m)}(z)$. After replacing the convolution operator $\mathcal{K}*$ in (3.14)-(3.16) with its rational approximation $\mathcal{K}^{(m)}*$, we obtain the following fully discrete scheme:

$$\begin{aligned} &i(D_\tau + \sigma E)\mathcal{P} u^n = \mathcal{L}_h^{n+\frac{1}{2}} (E + \sigma\tau^2 D_\tau) u^n, \quad \forall\, n \geq 0, \\ &\tau^{-\frac{1}{2}} (\mathcal{K}^{(m)} * \gamma^{\pm} u)^n + \partial_\nu^{\pm} u^n = 0, \qquad\qquad \forall\, n \geq 0, \\ &u^0 = (\psi_0(x_0), \cdots, \psi_0(x_{M+1})). \end{aligned} \tag{4.4}$$

In the practical computation, (4.4) can be solved by an efficient algorithm described in the next subsection.

4.2. Implementation algorithm. Let us define $v^n := (E + \sigma\tau^2 D_\tau)u^n$ for $n \geq 0$. Then we have

$$u^{n+1} = \frac{2v^n - (1-2\sigma\tau)u^n}{1+2\sigma\tau}, \qquad \forall\, n \geq 0,$$

$$(D_\tau + \sigma E)\mathcal{P}u^n = \frac{2+\sigma\tau}{\tau(1+2\sigma\tau)}\mathcal{P}v^n - \frac{2-2\sigma^2\tau^2}{\tau(1+2\sigma\tau)}\mathcal{P}u^n, \qquad \forall\, n \geq 0.$$

By applying (4.1) to (4.3), we derive

$$\begin{aligned}
i^{\frac{1}{2}}\widetilde{K}^{(m)}(z) &= \lambda - \sum_{j=1}^{m} \frac{1}{c_j\delta(z,\sigma) + d_j} \\
&= \lambda - \sum_{j=1}^{m} \frac{1}{c_j \frac{2+\sigma\tau+(\sigma\tau-2)z}{1+2\sigma\tau+(1-2\sigma\tau)z} + d_j} \\
&= \lambda - \sum_{j=1}^{m} \frac{e_j + f_j z}{1+g_j z} = \lambda - \sum_{j=1}^{m} e_j - \sum_{j=1}^{m} \frac{(f_j - e_j g_j)z}{1+g_j z},
\end{aligned}$$

where we have set

$$\begin{aligned}
e_j &= \frac{1+2\sigma\tau}{c_j(2+\sigma\tau) + d_j(1+2\sigma\tau)}, \\
f_j &= \frac{1-2\sigma\tau}{c_j(2+\sigma\tau) + d_j(1+2\sigma\tau)}, \\
g_j &= \frac{c_j(\sigma\tau-2) + d_j(1-2\sigma\tau)}{c_j(2+\sigma\tau) + d_j(1+2\sigma\tau)}.
\end{aligned}$$

Therefore, we have

$$\tau^{-\frac{1}{2}}\widetilde{K}^{(m)}(z) = \tilde{\lambda} - \sum_{j=1}^{m} \frac{\tilde{f}_j z}{1+g_j z},$$

where $\tilde{\lambda} = (i\tau)^{-\frac{1}{2}}(\lambda - \sum_{j=1}^m e_j)$ and $\tilde{f}_j = (i\tau)^{-\frac{1}{2}}(f_j - e_j g_j)$. The last identity implies

$$\tau^{-\frac{1}{2}}\widetilde{K}^{(m)}(z)\gamma^{\pm}\tilde{v}(z) = \tilde{\lambda}\gamma^{\pm}\tilde{v}(z) - \sum_{j=1}^{m} \frac{\tilde{f}_j z}{1+g_j z}\gamma^{\pm}\tilde{v}(z).$$

To simplify the notations, we set $\tilde{w}_{j,\pm} = \frac{\tilde{f}_j}{1+g_j z}\gamma^{\pm}\tilde{v}(z)$. Therefore, we derive

$$\begin{aligned}
\tilde{w}_{j,\pm} + g_j z \tilde{w}_{j,\pm} &= \tilde{f}_j \gamma^{\pm}\tilde{v}(z), \\
\tau^{-\frac{1}{2}}\widetilde{K}^{(m)}(z)\gamma^{\pm}\tilde{v}(z) &= \tilde{\lambda}\gamma^{\pm}\tilde{v}(z) - \sum_{j=1}^{m} z\tilde{w}_{j,\pm}.
\end{aligned}$$

The inverse $\mathcal{Z}$-transform of the last two equations yields

$$\begin{aligned}
w_{j,\pm}^n + g_j w_{j,\pm}^{n-1} &= \tilde{f}_j \gamma^{\pm} v^n, \\
\tau^{-\frac{1}{2}}(\mathcal{K}^{(m)} * \gamma^{\pm} v)^n &= \tilde{\lambda}\gamma^{\pm} v^n - \sum_{j=1}^{m} w_{j,\pm}^{n-1}.
\end{aligned}$$

Consequently, the fully discrete scheme (4.4) can be written into an equivalent form:

$$\begin{aligned}
&\frac{i(2+\sigma\tau)}{\tau(1+2\sigma\tau)}\mathcal{P}v^n - \mathcal{L}_h^{n+\frac{1}{2}}v^n = \frac{i(2-2\sigma^2\tau^2)}{\tau(1+2\sigma\tau)}\mathcal{P}u^n, \quad && \forall\, n \ge 0,\\
&\partial_\nu^{\pm} v^n + \tilde{\lambda}\gamma^{\pm} v^n - \sum_{j=1}^{m} w_{j,\pm}^{n-1} = 0, && \forall\, n \ge 0,\\
&w_{j,\pm}^n + g_j w_{j,\pm}^{n-1} = \tilde{f}_j \gamma^{\pm} v^n, && \forall\, n \ge 0,\\
&u^0 = (\psi_0(x_0), \cdots, \psi_0(x_{M+1})) \quad \text{and} \quad w_{j,\pm}^{-1} = 0, && j = 1, \cdots, m.
\end{aligned} \tag{4.5}$$

Given u^n with $n \ge 0$, one can solve v^n and w^n from (4.5), and then update u^{n+1} by using the identity $v^n = (E + \sigma\tau^2 D_\tau)u^n$. The scheme (4.5) is equivalent to (4.4) but does not require evaluating discrete convolutions at the boundary points $x_\pm$.

5. Error estimate. In this section, we prove the following theorem on the convergence of the numerical solutions given by (4.4).

Theorem 5.1. *Assume that the solution u of (2.10) is sufficiently smooth, or equivalently, the solution ψ of (1.1) is sufficiently smooth. Let $\eta^n = (\eta_0^n, \cdots, \eta_{M+1}^n)$, with $\eta_j^n = u(x_j, t_n) - u_j^n$ denoting the error of the numerical solution given by the algorithm (4.4) for solving (2.10). If the time step τ is small enough such that $\sigma\tau \in (0, \frac{1}{2}]$, and the order m of the Padé approximation is sufficiently large such that*

$$2m+1 \ge \frac{\ln\epsilon}{\ln(1-(\sigma\tau)^{\frac{1}{2}})}, \quad \textit{for some } \epsilon \in \left(0, \frac{(\sigma\tau)^{\frac{9}{2}}}{8}\right], \tag{5.1}$$

then we have the following error estimate:

$$\max_{1 \le n \le [T/\tau]} \left(\|\mathcal{P}\eta^n\|_h + |\nabla_h^n \eta^n|_h \right) \le C_T(\tau^2 + h^2), \tag{5.2}$$

where C_T is a constant depending on T.

The proof of Theorem 5.1 is presented in the following two subsections.

5.1. Properties of the rational approximation $\widetilde{K}^{(m)}(z)$. By using (3.8) one can prove that the symbol $\widetilde{K}(z)$ satisfies the following inequalities (see Appendix B):

$$\max_{z\in\partial\mathbb{D}} |\widetilde{K}(z)| \le (\sigma\tau)^{-\frac{1}{2}}, \qquad \min_{z\in\partial\mathbb{D}} |\widetilde{K}(z)| \ge (\sigma\tau)^{\frac{1}{2}} \qquad \text{if } \sigma\tau \in \left(0, \frac{1}{2}\right], \tag{5.3}$$

$$\max_{z\in\partial\mathbb{D}} \operatorname{Im} \widetilde{K}(z) \le -\frac{(\sigma\tau)^{\frac{3}{2}}}{2}, \qquad \min_{z\in\partial\mathbb{D}} \operatorname{Re} \widetilde{K}(z) \ge \frac{(\sigma\tau)^{\frac{3}{2}}}{2}, \qquad \text{if } \sigma\tau \in \left(0, \frac{1}{2}\right]. \tag{5.4}$$

Lemma 5.2. *Under the conditions $\sigma\tau \in \left(0, \frac{1}{2}\right]$ and (5.1), we have*

$$\max_{z\in\partial\mathbb{D}} \operatorname{Im} \widetilde{K}^{(m)}(z) \le 0 \quad \textit{and} \quad \max_{z\in\partial\mathbb{D}} \operatorname{Im}\left(\widetilde{K}(z)^2 \overline{\widetilde{K}^{(m)}(z)}\right) \le 0, \tag{5.5}$$

$$\max_{z\in\partial\mathbb{D}} |\widetilde{K}^{(m)}(z) - \widetilde{K}(z)| \le \frac{(\sigma\tau)^4}{2}. \tag{5.6}$$

Proof. Let us set $s(z) = \dfrac{2-2z+\sigma\tau(1+z)}{1+z+2\sigma\tau(1-z)}$, which satisfies the following inequality (see Appendix B):

$$\max_{z\in\partial\mathbb{D}} |\gamma(s(z))| \le 1 - (\sigma\tau)^{\frac{1}{2}}, \quad \forall\, \sigma\tau \in \left(0, \frac{1}{2}\right]. \tag{5.7}$$

If $2m+1 \geq \frac{\ln \epsilon}{\ln(1-(\sigma\tau)^{\frac{1}{2}})}$, then $\left[1-(\sigma\tau)^{\frac{1}{2}}\right]^{2m+1} \leq \epsilon \leq \frac{1}{2}$. As a result, Lemma 4.1 implies

$$\max_{z\in\partial\mathbb{D}} \left|\frac{\widetilde{K}(z)-\widetilde{K}^{(m)}(z)}{\widetilde{K}(z)}\right| = \max_{z\in\partial\mathbb{D}} \left|\frac{2\gamma^{2m+1}(s(z))}{1+\gamma^{2m+1}(s(z))}\right| \leq \max_{z\in\partial\mathbb{D}} \frac{2\left|\gamma(s(z))\right|^{2m+1}}{1-\left|\gamma(s(z))\right|^{2m+1}} \leq 4\epsilon.$$

Consequently, by using (5.3) and (5.1) we have

$$\max_{z\in\partial\mathbb{D}} |\widetilde{K}^{(m)}(z)-\widetilde{K}(z)| \leq 4\epsilon|\widetilde{K}(z)| \leq \frac{(\sigma\tau)^4}{2}.$$

Since $\epsilon \leq \frac{(\sigma\tau)^{\frac{9}{2}}}{8} \leq \frac{(\sigma\tau)^2}{8}$, it follows that

$$\begin{aligned}\max_{z\in\partial\mathbb{D}} \operatorname{Im} \widetilde{K}^{(m)}(z) &= \max_{z\in\partial\mathbb{D}} \left[\operatorname{Im} \widetilde{K}(z) - \operatorname{Im}\big(\widetilde{K}(z)-\widetilde{K}^{(m)}(z)\big)\right] \\ &\leq -\frac{(\sigma\tau)^{\frac{3}{2}}}{2} + 4\epsilon \max_{z\in\partial\mathbb{D}} |\widetilde{K}(z)| \leq -\frac{(\sigma\tau)^{\frac{3}{2}}}{2} + 4\epsilon(\sigma\tau)^{-\frac{1}{2}} \leq 0.\end{aligned}$$

Besides, we have

$$\begin{aligned}\max_{z\in\partial\mathbb{D}} \left(\operatorname{Im} \widetilde{K}(z)^2\overline{\widetilde{K}^{(m)}(z)}\right) &= \max_{z\in\partial\mathbb{D}} \left(\operatorname{Im} \widetilde{K}(z)^2\overline{\widetilde{K}(z)}\right) + \max_{z\in\partial\mathbb{D}} \operatorname{Im} \widetilde{K}(z)^2\overline{(\widetilde{K}^{(m)}(z)-\widetilde{K}(z))} \\ &\leq \max_{z\in\partial\mathbb{D}} \operatorname{Im} \widetilde{K}(z)|\widetilde{K}(z)|^2 + \max_{z\in\partial\mathbb{D}} |\widetilde{K}(z)|^2|\widetilde{K}^{(m)}(z)-\widetilde{K}(z)| \\ &\leq -\frac{(\sigma\tau)^{\frac{5}{2}}}{2} + \max_{z\in\partial\mathbb{D}} |\widetilde{K}(z)|^2\frac{(\sigma\tau)^4}{2} \\ &\leq -\frac{(\sigma\tau)^{\frac{5}{2}}}{2} + \frac{(\sigma\tau)^3}{2} \leq 0.\end{aligned}$$

The proof thus ends. □

The following properties are direct consequences of (5.5).

Proposition 5.3. *For all complex sequences $f=\{f^n\}_{n=0}^{\infty}$ with $f^0=0$, the following inequalities hold:*

$$\operatorname{Im}\sum_{k=0}^{n} \overline{f^k}(\mathcal{K}^{(m)} * f)^k \leq 0, \qquad \forall\, n\geq 0, \tag{5.8}$$

$$\operatorname{Re}\sum_{k=0}^{n} \overline{(D_\tau+\sigma E)f^k}(\mathcal{K}^{(m)} * (E+\sigma\tau^2 D_\tau)f)^k \geq 0, \qquad \forall\, n\geq 0. \tag{5.9}$$

Proof. Without loss of generality, we re-define $f^k=0$ for $k>n$. This does not affect the value of $\operatorname{Im}\sum_{k=0}^{n}\overline{f^k}(\mathcal{K}^{(m)} * f)^k$, and we have

$$\begin{aligned}\operatorname{Im}\sum_{k=0}^{n} \overline{f^k}(\mathcal{K}^{(m)} * f)^k = \operatorname{Im}(f,\mathcal{K}^{(m)} * f)_{\ell^2(\mathbb{C})} &= \operatorname{Im}\int_{\partial\mathbb{D}} (\widetilde{f}(z),\widetilde{K}^{(m)}(z)\widetilde{f}(z))_{\mathbb{C}}\,\nu(dz) \\ &= \operatorname{Im}\int_{\partial\mathbb{D}} |\widetilde{f}(z)|^2\widetilde{K}^{(m)}(z)\,\nu(dz) \leq 0.\end{aligned}$$

Analogously, without loss of generality, we re-define $f^k=\frac{1-\sigma}{1+\sigma}f^{k-1}$ for $k>n$. Then we have $(D_\tau+\sigma E)f^k=0$ for $k>n$ and thus

$$\begin{aligned}&\operatorname{Re}\sum_{k=0}^{n} \overline{(D_\tau+\sigma E)f^k}(\mathcal{K}^{(m)} * (E+\sigma\tau^2 D_\tau)f^k) \\ &= \operatorname{Re}((D_\tau+\sigma E)f,\mathcal{K}^{(m)} * (E+\sigma\tau^2 D_\tau)f)_{\ell^2(\mathbb{C})}\end{aligned}$$

$$
\begin{aligned}
&= \tau^{-1}\mathrm{Re}\int_{\partial\mathbb{D}} |\widetilde{f}(z)|^2\overline{[z^{-1}-1+\sigma\tau(z^{-1}+1)/2]}\widetilde{K}^{(m)}(z)[(z^{-1}+1)/2+\sigma\tau(z^{-1}-1)]\,\nu(dz)\\
&= (4\tau)^{-1}\mathrm{Re}\int_{\partial\mathbb{D}} |z|^{-2}|\widetilde{f}(z)|^2\overline{[2-2z+\sigma\tau(1+z)]}\widetilde{K}^{(m)}(z)[1+z+2\sigma\tau(1-z)]\,\nu(dz)\\
&= (4\tau)^{-1}\mathrm{Re}\int_{\partial\mathbb{D}} |z|^{-2}|\widetilde{f}(z)|^2\overline{i\widetilde{K}(z)^2}\widetilde{K}^{(m)}(z)|1+z+2\sigma\tau(1-z)|^2\,\nu(dz)\\
&= -(4\tau)^{-1}\int_{\partial\mathbb{D}} \mathrm{Im}\Big(\widetilde{K}(z)^2\overline{\widetilde{K}^{(m)}(z)}\Big)|z|^{-2}|\widetilde{f}(z)|^2|1+z+2\sigma\tau(1-z)|^2\,\nu(dz)\geq 0.
\end{aligned}
$$

This ends the proof. □

5.2. Error estimate. Let $u(t_n)=(u(x_0,t_n),u(x_1,t_n),\ldots,u(x_{M+1},t_n))$. It is straightforward to check that the error vector η^n defined in Theorem 5.1 satisfies the following equation:

$$
\begin{aligned}
&i(D_\tau+\sigma E)\mathcal{P}\eta^n=\mathcal{L}^{n+\frac12}(E+\sigma\tau^2D_\tau)\eta^n+f^n, && \forall\, n\geq 0, && (5.10)\\
&\tau^{-\frac12}(\mathcal{K}^{(m)}*\gamma^\pm\eta)^n+\partial_\nu^\pm\eta^n=g_\pm^n, && \forall\, n\geq 0, && (5.11)\\
&\eta^0=0, && && (5.12)
\end{aligned}
$$

where f^n and $g_\pm^n$ are given truncation errors of the time and space discretizations, i.e.

$$
\begin{aligned}
f^n=&[i(D_\tau+\sigma E)\mathcal{P}u(t_n)-i(\partial_t u(t_{n+\frac12})+\sigma u(t_{n+\frac12}))]\\
&-\big[\mathcal{L}^{n+\frac12}Eu(t_n)-\mathcal{L}(t_{n+\frac12})u(t_{n+\frac12})\big]-\sigma\tau^2\mathcal{L}^{n+\frac12}D_\tau u(t_n),
\end{aligned}\tag{5.13}
$$

$$
\begin{aligned}
g_\pm^n=&\tau^{-\frac12}(\mathcal{K}^{(m)}-\mathcal{K})*\gamma^\pm u(t_n)+\big[\tau^{-\frac12}\mathcal{K}*\gamma^\pm u(t_n)-\sqrt{-i(\partial_t+\sigma)}\gamma^\pm u(t_n)\big]\\
&+\big[\sqrt{-i(\partial_t+\sigma)}\gamma^\pm u(t_n)-\sqrt{-i(\partial_t+\sigma)}u(x_\pm,t_n)\big]+\big[\partial_\nu^\pm u(t_n)-\partial_\nu u(x_\pm,t_n)\big].
\end{aligned}\tag{5.14}
$$

By using Taylor expansion, (3.12) and (5.6), it is straightforward to verify the following estimate of the truncation errors (see Appendix C):

$$
\|f^n\|_h+\|D_\tau f^n\|_h+|g_\pm^n|+|D_\tau g_\pm^n|\leq C(\tau^2+h^2). \tag{5.15}
$$

Then Theorem 5.1 is a consequence of the following stability estimate.

Lemma 5.4. *The solution of* (5.10)-(5.12) *satisfies the following stability estimate:*

$$
\begin{aligned}
&\max_{1\leq n\leq[T/\tau]}\big(\|\mathcal{P}\eta^n\|^2+|\nabla_h^n\eta^n|_h^2\big)\\
&\leq C_T\left[\max_{0\leq k\leq n-2}\|D_\tau f^k\|_h^2+\max_{0\leq k\leq n-1}(\|f^k\|_h^2+|D_\tau g_\pm^k|^2)+\max_{0\leq k\leq n}|g_\pm^k|^2\right],
\end{aligned}\tag{5.16}
$$

where C_T is a constant depending on T.

Proof. Since $\gamma^\pm\eta^0=0$, we have $E\mathcal{K}^{(m)}*\gamma^\pm\eta=\mathcal{K}^{(m)}*E\gamma^\pm\eta$. By applying the discrete Green's formula (3.13) and the boundary conditions (5.11), taking the imaginary part of the inner product between (5.10) and $(E+\sigma\tau^2D_\tau)\mathcal{P}\eta^n$ yields

$$
\begin{aligned}
&\frac12(1+\sigma^2\tau^2)D_\tau\|\mathcal{P}\eta^n\|_h^2\\
&\leq \mathrm{Re}\,((E+\sigma\tau^2D_\tau)\mathcal{P}\eta^n,(D_\tau+\sigma E)\mathcal{P}\eta^n)_h\\
&= -\mathrm{Im}\,\overline{(E+\sigma\tau^2D_\tau)\gamma^\pm\eta^n}\cdot(E+\sigma\tau^2D_\tau)\partial_\nu^\pm\eta^n+\mathrm{Im}\,((E+\sigma\tau^2D_\tau)\mathcal{P}\eta^n,f^n)_h\\
&= \tau^{-\frac12}\mathrm{Im}\overline{(E+\sigma\tau^2D_\tau)\gamma^\pm\eta^n}\cdot(E+\sigma\tau^2D_\tau)(\mathcal{K}^{(m)}*\gamma^\pm\eta)^n\\
&\quad -\mathrm{Im}\,\overline{(E+\sigma\tau^2D_\tau)\gamma^\pm\eta^n}\cdot(E+\sigma\tau^2D_\tau)g_\pm^n+\mathrm{Im}\,((E+\sigma\tau^2D_\tau)\mathcal{P}\eta^n,f^n)_h\\
&\leq \tau^{-\frac12}\mathrm{Im}\overline{(E+\sigma\tau^2D_\tau)\gamma^\pm\eta^n}\cdot\big[\mathcal{K}^{(m)}*(E+\sigma\tau^2D_\tau)\gamma^\pm\eta\big]^n
\end{aligned}
$$

$$+\mathcal{O}(1)\,E\left(|\gamma^{\pm}\eta^n|^2+|g_{\pm}^n|^2+\|\mathcal{P}\eta^n\|_h^2\right)+\mathcal{O}(1)\|f^n\|_h^2.$$

Summing up the index n and using Proposition 5.3, we obtain

$$\|\mathcal{P}\eta^n\|_h^2\le\mathcal{O}(\tau)\sum_{k=1}^{n}\left(|\gamma^{\pm}\eta^k|^2+|g_{\pm}^k|^2+\|\mathcal{P}\eta^k\|_h^2\right)+\mathcal{O}(\tau)\sum_{k=0}^{n-1}\|f^k\|_h^2. \tag{5.17}$$

Next performing the inner product with $(D_\tau+\sigma E)\mathcal{P}\eta^n$ and taking the real part, we derive

$$\mathrm{Re}((D_\tau+\sigma E)\mathcal{P}\eta^n,\mathcal{L}_h^{n+\frac12}(E+\sigma\tau^2D_\tau)\eta^n)_h+\mathrm{Re}((D_\tau+\sigma E)\mathcal{P}\eta^n,f^n)_h=0.$$

Applying the discrete Green's formula (3.13), we derive

$$\begin{aligned}
&\mathrm{Re}((D_\tau+\sigma E)\mathcal{P}\eta^n,\mathcal{L}_h^{n+\frac12}(E+\sigma\tau^2D_\tau)\eta^n)_h\\
=&\,\mathrm{Re}\langle\nabla_h^{n+\frac12}(D_\tau+\sigma E)\eta^n,\nabla_h^{n+\frac12}(E+\sigma\tau^2D_\tau)\eta^n\rangle_h\\
&+\mathrm{Re}\left((D_\tau+\sigma E)\mathcal{P}\eta^n,U^{n+\frac12}(E+\sigma\tau^2D_\tau)\mathcal{P}\eta^n\right)_h\\
&-\mathrm{Re}\,\overline{\gamma^{\pm}(D_\tau+\sigma E)\eta^n}\partial_\nu^{\pm}(E+\sigma\tau^2D_\tau)\eta^n\\
\equiv&\, I_1+I_2+I_3.
\end{aligned}$$

Obviously, we have

$$\begin{aligned}
I_1&\ge(1+\sigma^2\tau^2)\mathrm{Re}\,\langle\nabla_h^{n+\frac12}D_\tau\eta^n,\nabla_h^{n+\frac12}E\eta^n\rangle_h\\
&=\frac12(1+\sigma^2\tau^2)\tau^{-1}\left[\langle\nabla_h^{n+\frac12}\eta^{n+1},\nabla_h^{n+\frac12}\eta^{n+1}\rangle_h-\langle\nabla_h^{n+\frac12}\eta^{n},\nabla_h^{n+\frac12}\eta^{n}\rangle_h\right]\\
&=\frac12(1+\sigma^2\tau^2)\left[D_\tau|\nabla_h^n\eta^n|_h^2+\mathcal{O}(1)\,E\left(|\nabla_h^n\eta^n|_h^2+\|\mathcal{P}\eta^n\|_h^2\right)\right].
\end{aligned}$$

For the term I_2, it holds that

$$\begin{aligned}
I_2&=(1+\sigma^2\tau^2)\mathrm{Re}\,(D_\tau\mathcal{P}\eta^n,U^{n+\frac12}E\mathcal{P}\eta^n)_h+\mathcal{O}(1)\,E\|\mathcal{P}\eta^n\|_h^2\\
&=\frac12(1+\sigma^2\tau^2)D_\tau(\mathcal{P}\eta^n,U^n\mathcal{P}\eta^n)_h+\mathcal{O}(1)\,E\|\mathcal{P}\eta^n\|_h^2.
\end{aligned}$$

For the term I_3, by the discrete Green's formula we have

$$\begin{aligned}
I_3=&\,\tau^{-\frac12}\mathrm{Re}\,\overline{(D_\tau+\sigma E)\gamma^{\pm}\eta^n}(E+\sigma\tau^2D_\tau)(\mathcal{K}^{(m)}*\gamma^{\pm}\eta)^n-\mathrm{Re}\,\overline{(D_\tau+\sigma E)\gamma^{\pm}\eta^n}(E+\sigma\tau^2D_\tau)g_{\pm}^n\\
=&\,\tau^{-\frac12}\mathrm{Re}\,\overline{(D_\tau+\sigma E)\gamma^{\pm}\eta^n}(E+\sigma\tau^2D_\tau)(\mathcal{K}^{(m)}*\gamma^{\pm}\eta)^n\\
&-\mathrm{Re}\,\overline{D_\tau\gamma^{\pm}\eta^n}\,Eg_{\pm}^n+\mathcal{O}(1)\,E\left(|\gamma^{\pm}\eta^n|^2+|g_{\pm}^n|^2\right).
\end{aligned}$$

On the other hand, we have

$$\mathrm{Re}\left((D_\tau+\sigma E)\mathcal{P}\eta^n,f^n\right)_h=\mathrm{Re}\,(D_\tau\mathcal{P}\eta^n,f^n)_h+\mathcal{O}(1)\,E\|\mathcal{P}\eta^n\|_h^2+\mathcal{O}(1)\|f^n\|_h^2.$$

Combining the above together yields

$$\begin{aligned}
&\frac12(1+\sigma^2\tau^2)D_\tau\left[|\nabla_h^n\eta^n|_h^2+(\mathcal{P}u^n,U^n\mathcal{P}\eta^n)_h\right]\\
\le&-\tau^{-\frac12}\mathrm{Re}\,\overline{(D_\tau+\sigma E)\gamma^{\pm}\eta^n}\cdot(E+\sigma\tau^2D_\tau)(\mathcal{K}^{(m)}*\gamma^{\pm}\eta)^n\\
&+\mathrm{Re}\,\overline{D_\tau\gamma^{\pm}\eta^n}\cdot Eg_{\pm}^n-\mathrm{Re}\,(D_\tau\mathcal{P}\eta^n,f^n)_h+\mathcal{O}(1)\|f^n\|_h^2\\
&+\mathcal{O}(1)\,E\left(|\nabla_h^n\eta^n|_h^2+\|\mathcal{P}\eta^n\|_h^2+|\gamma^{\pm}\eta^n|^2+|g_{\pm}^n|^2\right).
\end{aligned}$$

Summing up the index n, using Proposition 5.3, and using summation by parts in time for $\sum_{k=0}^{n-1}\mathrm{Re}\,\overline{D_\tau\gamma^{\pm}\eta^n}\cdot Eg_{\pm}^n$ and $-\sum_{k=0}^{n-1}\mathrm{Re}\,(D_\tau\mathcal{P}\eta^n,f^n)_h$, we derive

$$\frac12(1+\sigma^2\tau^2)\tau^{-1}\left[|\nabla_h^n\eta^n|_h^2+(\mathcal{P}\eta^n,U^n\mathcal{P}\eta^n)_h\right]$$

$$
\begin{aligned}
&\leq \mathcal{O}(1)\tau^{-1}\left(|\gamma^{\pm}\eta^n|^2+|g_{\pm}^{n-1}|^2+|g_{\pm}^{n}|^2+\|\mathcal{P}\eta^n\|_h^2+\|f^{n-1}\|_h^2\right)\\
&\quad+\mathcal{O}(1)\sum_{k=1}^{n}\left(|\nabla_h^k\eta^k|_h^2+\|\mathcal{P}\eta^k\|_h^2+|\gamma^{\pm}\eta^k|^2+|g_{\pm}^k|^2\right)\\
&\quad+\mathcal{O}(1)\sum_{k=0}^{n-1}\left(\|f^k\|_h^2+|D_\tau g_{\pm}^k|^2\right)+\mathcal{O}(1)\sum_{k=0}^{n-2}|D_\tau f^k|_h^2,
\end{aligned}
$$

which leads to

$$
\begin{aligned}
|\nabla_h^n\eta^n|_h^2 \leq\,&\mathcal{O}(1)\left(|\gamma^{\pm}\eta^n|^2+|g_{\pm}^{n-1}|^2+|g_{\pm}^{n}|^2+\|\mathcal{P}\eta^n\|_h^2+\|f^{n-1}\|_h^2\right)\\
&+\mathcal{O}(\tau)\sum_{k=1}^{n}\left(|\nabla_h^k\eta^k|_h^2+\|\mathcal{P}\eta^k\|_h^2+|\gamma^{\pm}\eta^k|^2+|g_{\pm}^k|^2\right)\\
&+\mathcal{O}(\tau)\sum_{k=0}^{n-1}\left(\|f^k\|_h^2+|D_\tau g_{\pm}^k|^2\right)+\mathcal{O}(\tau)\sum_{k=0}^{n-2}|D_\tau f^k|_h^2.
\end{aligned}
\tag{5.18}
$$

By the discrete Sobolev imbedding theorem, we have

$$
|\gamma^{\pm}\eta^n|^2 \leq \mathcal{O}(\epsilon^{-1})\|\mathcal{P}\eta^n\|_h^2+\epsilon|\nabla_h^n\eta^n|_h^2. \tag{5.19}
$$

Combining (5.17), (5.18) and (5.19), choosing ϵ small enough and applying the discrete Gronwall's inequality, we derive (5.16). The proof of Lemma 5.16 is complete. □

Remark 5.1. *A "good" approximation of the exact DtN operator (continuous or discrete) should preserve the "sign property". In other words, upon integration or summation by parts, the boundary contribution due to this approximate DtN should be nonpositive or nonnegative as in the continuous setting. When we perform the error analysis, the boundary conditions are inhomogeneous: there exists a truncation term getting involved. The direct consequence of this quantity is that when we perform the discrete L^2-estimate, the trace of field will get involved. See in (5.17) the first term $\gamma^{\pm}\eta^k$. If such a term does not exist, the discrete Gronwall's inequality will lead to the L^2-stability. In order to handle this term, we have to resort to the H^1-estimate. This is performed below (5.17), until the end of page 13. After the H^1-estimate is established, we can apply a discrete Sobolev embedding to bound the trace term $\gamma^{\pm}\eta^k$ by the H^1-norm of η^k, please see (5.19).*

6. Numerical results. We now provide numerical tests to validate the theoretical results presented in the preceding sections. The convergence order of the proposed numerical scheme will be examined. As applications, we will simulate the spontaneous radiation of a wave packet and the ionization of a ground state due to the action of time-varying electromagnetic field.

In the calculations to guarantee the second order convergence of the proposed scheme above, we always take $\sigma = 1/T$ and determine the number of Padé expansion terms (see Lemma 5.2) by using the following criterion:

$$
m=\frac{\ln\epsilon}{2\ln\left(1-(\sigma\tau)^{\frac{1}{2}}\right)},\quad \epsilon=\frac{(\sigma\tau)^{\frac{9}{2}}}{8}.
$$

Noting that $\sigma\tau = 1/N$, in this situation the m behaves asymptotically like $\frac{9}{4}\sqrt{N}\ln N$. The additional computational cost for evaluating the ABCs obtain u^N is thus $\mathcal{O}(N^{\frac{3}{2}}\ln N)$ flops (see Figs. 6.2 and 6.4 below) and the computational storage requires $\mathcal{O}(\sqrt{N}\ln N)$.

Example 1. To demonstrate the performance of our numerical scheme, we first consider the free Schrödinger equation (i.e. $V(x) = 0$) with the following exact beam-like solution

$$\psi(x,t) = \frac{1}{\sqrt{\zeta + it}} \exp\left[ik(x - kt) - \frac{(x - 2kt)^2}{4(\zeta + it)} \right]. \tag{6.1}$$

In the above, k is a real parameter which controls the beam propagation speed, and ζ is a positive parameter which controls the beam width. The parameter ζ should be carefully selected, so that the initial wave function $\psi(x, 0)$ is negligibly small outside of the spatial computation domain $[-3, 3]$. In this numerical simulation, we put $k = 2$ and $\zeta = 0.04$. Besides, we set the evolutionary time as $T = 2$.

The left panel of Fig. 6.1 illustrates the evolution of numerical solutions. No spurious reflection can be detected near the absorbing boundaries. The right panel of Fig. 6.1 plots the numerical errors when we recursively double the parameters $M = N$ from 120 to 3840. A second-order convergence order in the L_∞-norm is clearly observed.

We now take a closer look at the computational cost by comparing with the direct scheme (3.11). The CPU time is investigated in log10 scale by increasing the total number of time steps $N = 70000, \cdots, 250000$ and fixing $M = 100$. Fig. 6.2 shows the CPU times for the efficient evaluation and direct evaluation of the discrete ABC. One can clearly observe the expected slope of 3/2 for the efficient evaluation.

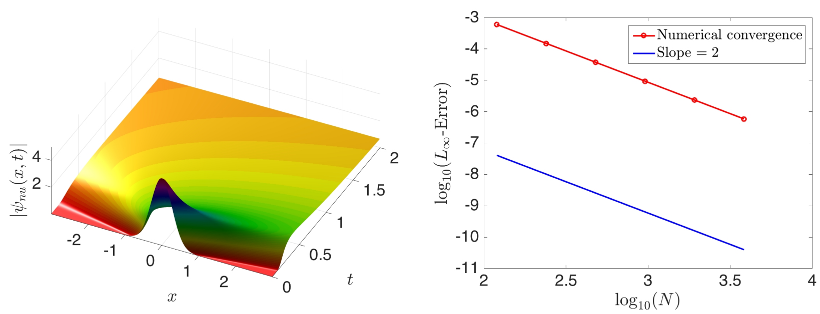

FIG. 6.1. *(Example 1) Left: the evolution of the solution. Right: the convergence order.*

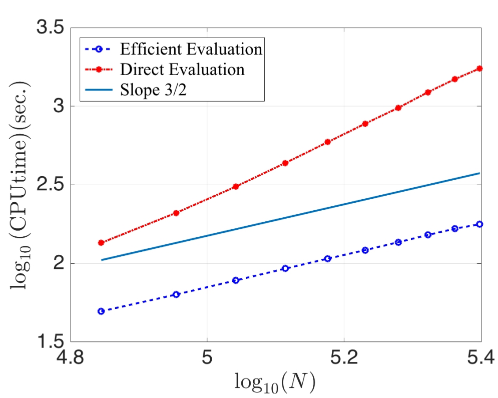

FIG. 6.2. *(Example 1) the* log-log *plot for the CPU time by fixing $M = 100$ with different N.*

Example 2. Bound states are referred to as the L^2-bounded eigenfunctions of the following

Schrödinger eigenvalue problem:

$$[-\partial_x^2 + V(x)]\psi = \lambda\psi. \tag{6.2}$$

Under mild conditions, the spectrums of (6.2) lie in the real axis. The bound state associated with the smallest point spectrum is called ground state. For some well-prepared electric potential function $V(x)$, besides the continuum spectrums, the point spectrums might exist. For example, in the case that

$$V(x) = -3\exp(-x^2),$$

there exists a unique bound state ψ_0 shown as in the left panel of Fig. 6.6 (unnormalized), which is associated with the point spectrum $\lambda_0 = -1.641465$.

If the initial wave packet is not on the state of ψ_0, part of the wave function will radiate spontaneously. To simulate this process, we set the initial wave packet as a Gaussian, i.e.,

$$\psi(x, 0) = 10\exp(-x^2).$$

We take the computational domain of interest as $[-15, 15]$. Note that since the spontaneous radiation is a relatively long time process, introducing absorbing boundaries turns to be a must to reduce the computational cost.

The left panel of Fig. 6.3 illustrates the evolution of numerical solutions until $T = 50$. In this simulation, we have put $M = N = 1280$. The right panel in Fig. 6.3 plots the numerical errors at $T = 10$ by recursively doubling the parameters $M = N$ from 120 to 3840. The reference solution is obtained by the spectral method in a large enough computational domain, see [10]. Again, a second-order convergence order can be clearly observed. The CPU time is investigated in log10 scale by increasing $N = 70000, \cdots, 250000$ and fixing $M = 200$ and $T = 20$. Again, from Fig. 6.4 one can see the advantage of the proposed algorithm over the direct method, and clearly observe the expected slope of 3/2 for the efficient evaluation.

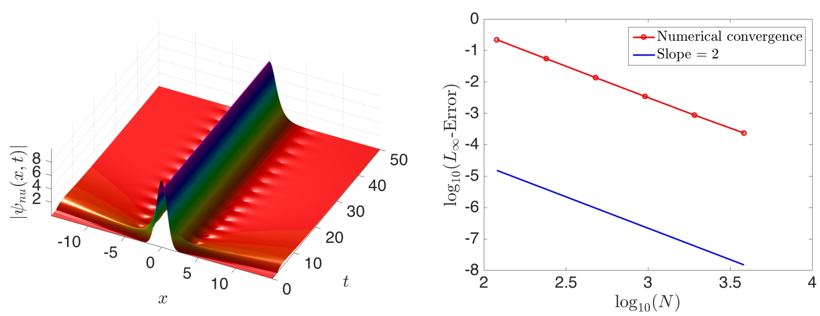

FIG. 6.3. *(Example 2) Left: the evolution of the solution. Right: the convergence order.*

A bound state will remain its profile if there is no interaction between a quantum system and its environment. However, when a time-varying electromagnetic field is imposed, the ionization phenomenon might occur. To simulate this process, we set the magnetic potential as

$$A(x, t) = \frac{2}{\sqrt{\pi}}[1 - \cos(t)]\exp(-x^2).$$

The computational domain is taken as $[-20, 20]$. We present the evolutions of the numerical solution (left) with $M = N = 1280$ and the reference solution (right) in Fig. 6.5. The

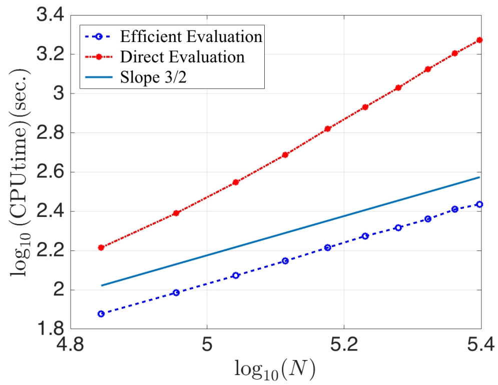

FIG. 6.4. *(Example 2) the* log-log *plot for the CPU time by fixing $M = 200$ and $T = 20$ with different N.*

reference solution is calculated in an enlarged computational domain by employing sufficiently small mesh parameters. We illustrate the field error $|\psi_{nu} - \psi_{ref}|$ in the right panel of Fig. 6.6. Here ψ_{nu} and ψ_{ref} denote the numerical solution and the reference solution, respectively. One can see that the error is always on the scale of 10^{-7} up to the evolutionary time $T = 80$.

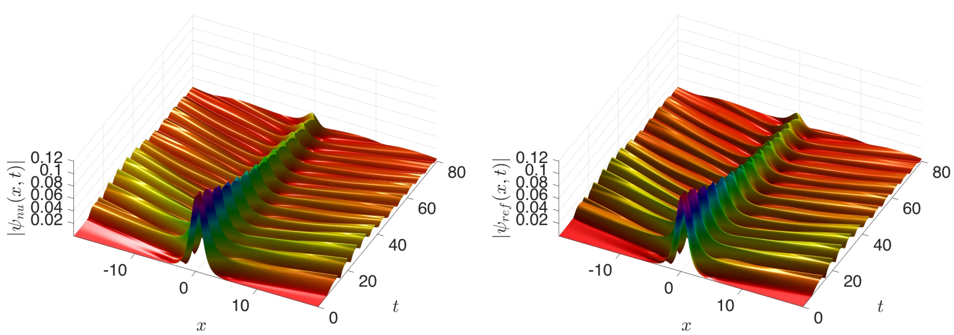

FIG. 6.5. *(Example 2) Left: the evolution of numerical solutions. Right: the evolution of reference solutions.*

7. Conclusion. The one-dimensional Schrödinger equation in an unbounded domain was reformulated into an initial-boundary value problem in a bounded domain of computational interest. A fully discrete perturbed Crank-Nicolson finite difference method was proposed to solve the reformulated initial-boundary value problem. By applying the Padé approximation, the convolution operations in the discrete ABCs were approximated by a system of easily-solved simple finite difference equations. A criterion determining the number of Padé approximation terms was proposed to guarantee the optimal accuracy with respect to the mesh parameters. It was proved that the resulting numerical method preserves the stability and the second-order convergence order of the fully discrete finite difference scheme. Numerical tests validated the theoretical analysis and demonstrated the effectiveness of the proposed numerical method.

We should point out that the complexity of the scheme proposed in this paper requires the computational cost $\mathcal{O}(N^{\frac{3}{2}} \ln N)$ and the storage $\mathcal{O}(\sqrt{N} \ln N)$. While the storage re-

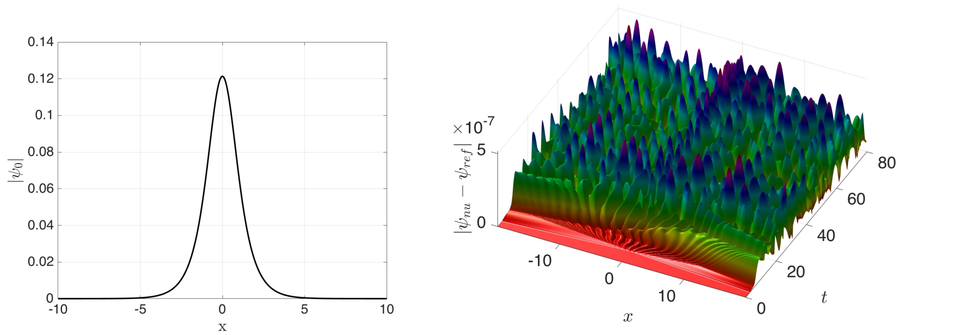

FIG. 6.6. *(Example 2) Left: the initial value (i.e. the eigenfunction of λ_0). Right: the errors between numerical and reference solutions.*

quirement is sub-linear, the computational cost is larger than the fast summation technique developed in [9, 16], where the optimal computational complexity was achieved. Hence, an important issue worthy of further consideration is to accelerate the convolution in the ABCs with almost optimal cost in both complexity and memory.

Acknowledgements. We thank the anonymous referees for the valuable comments and suggestions, which are very helpful for improving the presentation of the paper. In particular, we thank one of the referees for pointing out that the proposed algorithm needs $\mathcal{O}(\sqrt{N}\ln N)$ operations at each time step.

Appendix A. Proof of (3.12).

By using Taylor's expansion, it is straightforward to verify that

$$\left|\tau^{-\frac{1}{2}}\widetilde{K}(e^{-i\tau\xi}) - \sqrt{-i(i\xi+\sigma)}\right| \le C\tau^2\sqrt{|i\xi+\sigma|}|\xi|^2. \tag{A.1}$$

Assumption (2.1) and equation (1.1) imply that $\psi(x_\pm,t)$ and its time derivatives are zero at $t=0$. Consequently, by extending $\psi(x_\pm,t)$ to be zero on $t\in(-\infty,0]$, we obtain a sufficiently smooth function $\psi(x_\pm,t)$ defined for $t\in\mathbb{R}$. We define

$$\tau^{-\frac{1}{2}}\mathcal{K}*u(x_\pm,t) := \tau^{-\frac{1}{2}}\sum_{j=0}^{\infty}K_j u(x_\pm,t-j\tau), \quad \forall\, t\in\mathbb{R}, \tag{A.2}$$

which is consistent with the definition (3.10) at $t=t_n$. The Fourier transform in time of the last equation is

$$\begin{aligned}
&\mathcal{F}_t[\tau^{-\frac{1}{2}}\mathcal{K}*u(x_\pm,t)](\xi) = \int_{\mathbb{R}}\tau^{-\frac{1}{2}}\mathcal{K}*u(x_\pm,t)e^{-it\xi}dt\\
&= \sum_{j=0}^{\infty}\int_{\mathbb{R}}\tau^{-\frac{1}{2}}K_j u(x_\pm,t-j\tau)e^{-it\xi}dt = \tau^{-\frac{1}{2}}\widetilde{K}(e^{-i\tau\xi})\mathcal{F}_t u(x_\pm,\xi)\\
&= \sqrt{-i(i\xi+\sigma)}\mathcal{F}_t u(x_\pm,\xi) + \big(\tau^{-\frac{1}{2}}\widetilde{K}(e^{-i\tau\xi}) - \sqrt{-i(i\xi+\sigma)}\big)\mathcal{F}_t u(x_\pm,\xi)\\
&= \mathcal{F}_t[\sqrt{-i(\partial_t+\sigma)}u(x_\pm,t)](\xi) + \big(\tau^{-\frac{1}{2}}\widetilde{K}(e^{-i\tau\xi}) - \sqrt{-i(i\xi+\sigma)}\big)\mathcal{F}_t u(x_\pm,\xi),
\end{aligned}$$

which implies that

$$\begin{aligned}
&\big|\tau^{-\frac{1}{2}}\mathcal{K}*u(x_\pm,t) - \sqrt{-i(\partial_t+\sigma)}u(x_\pm,t)\big|\\
&= \big|\mathcal{F}_\xi^{-1}\big[\big(\tau^{-\frac{1}{2}}\widetilde{K}(e^{-i\tau\xi}) - \sqrt{-i(i\xi+\sigma)}\big)\mathcal{F}_t u(x_\pm,\xi)\big](t)\big|
\end{aligned}$$

$$
\begin{aligned}
&\le \int_{\mathbb{R}} \big|\tau^{-\frac{1}{2}}\widetilde{K}(e^{-i\tau\xi}) - \sqrt{-i(i\xi+\sigma)}\big||\mathcal{F}_t u(x_\pm,\xi)|d\xi \\
&\le C\tau^2 \int_{\mathbb{R}} \sqrt{|i\xi+\sigma|}\,\xi^2 \mathcal{F}_t u(x_\pm,\xi)|d\xi \\
&\le C\tau^2 \int_{\mathbb{R}} \frac{1}{1+|\xi|}(1+|\xi|^4)|\mathcal{F}_t u(x_\pm,\xi)|d\xi \\
&\le C\tau^2 \bigg(\int_{\mathbb{R}} \frac{1}{(1+|\xi|)^2}\mathrm{d}\xi\bigg)^{\frac{1}{2}} \bigg(\int_{\mathbb{R}} (1+|\xi|^4)^2|\mathcal{F}_t u(x_\pm,\xi)|^2 d\xi\bigg)^{\frac{1}{2}} \\
&= C\tau^2 \bigg(\int_0^\infty (|u(x_\pm,t)|^2 + |\partial_t^4 u(x_\pm,t)|^2)\mathrm{d}t\bigg)^{\frac{1}{2}}.
\end{aligned}
$$

By choosing $t = t_n$ in the preceding expression, we obtain (3.12).

Appendix B. Proof of (5.3)-(5.4) and (5.7).

Let $\rho = i^{-1}\dfrac{2(1-z)}{1+z}$. Then $\rho \in \mathbb{R}$ for $z \in \partial\mathbb{D}$ and we have

$$
\begin{aligned}
\widetilde{K}(z) &= \frac{1}{\sqrt{i\sigma\tau}}\sqrt{\frac{i\rho+\sigma\tau}{i\rho+(\sigma\tau)^{-1}}} \\
&= (\sigma\tau)^{-\frac{1}{2}}\bigg(\frac{\rho^2+(\sigma\tau)^2}{\rho^2+(\sigma\tau)^{-2}}\bigg)^{\frac{1}{4}}\bigg(\cos\Big(\frac{\pi}{4}-\frac{\theta}{2}\Big) - i\sin\Big(\frac{\pi}{4}-\frac{\theta}{2}\Big)\bigg),
\end{aligned} \tag{B.1}
$$

where

$$
\theta = \arg\bigg(\frac{i\rho+\sigma\tau}{i\rho+(\sigma\tau)^{-1}}\bigg) = \arctan\bigg(\frac{\rho(\sigma\tau)^{-1}-\rho\sigma\tau}{1+\rho^2}\bigg) \in \Big(-\frac{\pi}{2},\frac{\pi}{2}\Big). \tag{B.2}
$$

It is straightforward to verify that

$$
(\sigma\tau)^{\frac{1}{2}} \le (\sigma\tau)^{-\frac{1}{2}}\bigg(\frac{\rho^2+(\sigma\tau)^2}{\rho^2+(\sigma\tau)^{-2}}\bigg)^{\frac{1}{4}} \le (\sigma\tau)^{-\frac{1}{2}}, \qquad \text{if } \sigma\tau \in (0,1]. \tag{B.3}
$$

This proves (5.3).

It is not difficult to verify that, for fixed $\sigma\tau \in (0,1)$ and varying ρ, the angle θ attains maximum $\theta_{\max} = \arctan\Big(\frac{(\sigma\tau)^{-1}-\sigma\tau}{2}\Big)$ when $\rho = 1$. Consequently, we have

$$
\sin\Big(\frac{\pi}{4}-\frac{\theta}{2}\Big) = \sqrt{\frac{1-\sin(\theta)}{2}} \ge \sqrt{\frac{1-\sin(\theta_{\max})}{2}} = \sqrt{\frac{\sigma\tau}{(\sigma\tau)^{-1}+\sigma\tau}} \ge \frac{\sigma\tau}{\sqrt{2}}. \tag{B.4}
$$

Substituting (B.3)-(B.4) into (B.1) yields $\mathrm{Im}\,\widetilde{K}(z) \le -\frac{(\sigma\tau)^{\frac{3}{2}}}{\sqrt{2}}$. The result $\mathrm{Re}\,\widetilde{K}(z) \ge \frac{(\sigma\tau)^{\frac{3}{2}}}{\sqrt{2}}$ can be proved in the same way. This proves (5.4).

Note that

$$
\begin{aligned}
\sqrt{s(z)} = \sqrt{i}\widetilde{K}(z) &= (\sigma\tau)^{-\frac{1}{2}}\bigg(\frac{\rho^2+(\sigma\tau)^2}{\rho^2+(\sigma\tau)^{-2}}\bigg)^{\frac{1}{4}}\bigg(\cos\Big(\frac{\theta}{2}\Big) + i\sin\Big(\frac{\theta}{2}\Big)\bigg) \\
&= |\widetilde{K}(z)|\bigg(\cos\Big(\frac{\theta}{2}\Big) + i\sin\Big(\frac{\theta}{2}\Big)\bigg),
\end{aligned} \tag{B.5}
$$

with $\cos\left(\frac{\theta}{2}\right) \geq \frac{1}{\sqrt{2}}$ for $\theta \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$. Using the last expression of $\sqrt{s(z)}$, we have

$$\begin{aligned}
\left|\frac{\sqrt{s(z)}-1}{\sqrt{s(z)}+1}\right| &= \sqrt{1-\frac{4|\widetilde{K}(z)|\cos\left(\frac{\theta}{2}\right)}{|\widetilde{K}(z)|^2+2|\widetilde{K}(z)|\cos\left(\frac{\theta}{2}\right)+1}} \\
&\leq \sqrt{1-\frac{2\sqrt{2}|\widetilde{K}(z)|}{|\widetilde{K}(z)|^2+\sqrt{2}|\widetilde{K}(z)|+1}} \\
&\leq 1-\frac{\sqrt{2}|\widetilde{K}(z)|}{|\widetilde{K}(z)|^2+\sqrt{2}|\widetilde{K}(z)|+1},
\end{aligned} \tag{B.6}$$

where the last inequality is due to Taylor's expansion $(1-x)^{\frac{1}{2}} = 1-\frac{1}{2}x-\frac{1}{8}x^2+\cdots \leq 1-\frac{1}{2}x$. By considering

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{r}{r^2+\sqrt{2}r+1}\right) = \frac{1-r^2}{(r^2+\sqrt{2}r+1)^2},$$

we see that the minimum value of $\frac{\sqrt{2}|\widetilde{K}(z)|}{|\widetilde{K}(z)|^2+\sqrt{2}|\widetilde{K}(z)|+1}$ is attained at either $|\widetilde{K}(z)| = (\sigma\tau)^{\frac{1}{2}}$ or $|\widetilde{K}(z)| = (\sigma\tau)^{-\frac{1}{2}}$, i.e.

$$\frac{\sqrt{2}|\widetilde{K}(z)|}{|\widetilde{K}(z)|^2+\sqrt{2}|\widetilde{K}(z)|+1} \geq \min\left(\frac{\sqrt{2}(\sigma\tau)^{\frac{1}{2}}}{\sigma\tau+\sqrt{2}(\sigma\tau)^{\frac{1}{2}}+1}\ ,\ \frac{\sqrt{2}(\sigma\tau)^{-\frac{1}{2}}}{(\sigma\tau)^{-1}+\sqrt{2}(\sigma\tau)^{-\frac{1}{2}}+1}\right) \geq (\sigma\tau)^{\frac{1}{2}}.$$

Substituting the last inequality into (B.6) yields (5.7).

Appendix C. Proof of (5.15).

We divide the proof into the following four steps.

Step 1: Note that $f^n = (f_1^n, \ldots, f_M^n)$ with

$$\begin{aligned}
f_j^n =& [i(D_\tau+\sigma E)u(x_j,t_n) - i(\partial_t u(x_j,t_{n+\frac{1}{2}})+\sigma u(x_j,t_{n+\frac{1}{2}}))] \\
&- \left[\mathcal{L}^{n+\frac{1}{2}}Eu(x_j,t_n) - \mathcal{L}(t_{n+\frac{1}{2}})u(x_j,t_{n+\frac{1}{2}})\right] - \sigma\tau^2\mathcal{L}^{n+\frac{1}{2}}D_\tau u(x_j,t_n).
\end{aligned} \tag{C.1}$$

We estimate the three terms in the expression of f_j^n separately. Firstly, we have

$$\begin{aligned}
& i(D_\tau+\sigma E)u(x_j,t_n) - i(\partial_t u(x_j,t_{n+\frac{1}{2}})+\sigma u(x_j,t_{n+\frac{1}{2}})) \\
=& i\left(\frac{u(x_j,t_{n+1})-u(x_j,t_n)}{\tau} - \partial_t u(x_j,t_{n+\frac{1}{2}})\right) \\
&+ i\sigma\left(\frac{u(x_j,t_n)+u(x_j,t_{n+1})}{2} - u(x_j,t_{n+\frac{1}{2}})\right) = \mathcal{O}(\tau^2).
\end{aligned} \tag{C.2}$$

Secondly, it holds that

$$\begin{aligned}
& \mathcal{L}_h^{n+\frac{1}{2}}Eu(x_j,t_n) - \mathcal{L}(t_{n+\frac{1}{2}})u(x_j,t_{n+\frac{1}{2}}) \\
=& (\mathcal{L}_h^{n+\frac{1}{2}}Eu(x_j,t_n) - \mathcal{L}_h^{n+\frac{1}{2}}u(x_j,t_{n+\frac{1}{2}})) + (\mathcal{L}_h^{n+\frac{1}{2}}u(x_j,t_{n+\frac{1}{2}}) - \mathcal{L}(t_{n+\frac{1}{2}})u(x_j,t_{n+\frac{1}{2}})) \\
=& (\mathcal{L}_h^{n+\frac{1}{2}}Eu(x_j,t_n) - \mathcal{L}_h^{n+\frac{1}{2}}u(x_j,t_{n+\frac{1}{2}})) + (\mathcal{L}_h^{n+\frac{1}{2}}u(x_j,t_{n+\frac{1}{2}}) - \mathcal{L}(t_{n+\frac{1}{2}})u(x_j,t_{n+\frac{1}{2}})) \\
=&: I_1 + I_2,
\end{aligned} \tag{C.3}$$

Since a Taylor's expansion yields

$$Eu(x_j,t_n) - u(x_j,t_{n+\frac{1}{2}}) = \int_{t_n}^{t_{n+1}} \min(t_{n+1}-t, t-t_n)\partial_{tt}u(x_j,t)\mathrm{d}t, \tag{C.4}$$

it follows that

$$
\begin{aligned}
|I_1| &= \left| \int_{t_n}^{t_{n+1}} \min(t_{n+1}-t, t-t_n)\mathcal{L}_h^{n+\frac{1}{2}}\partial_{tt}u(x_j,t)\mathrm{d}t \right| \\
&\le C\tau^2 \max_{t\in[0,T]} \max_{1\le j\le M} |\mathcal{L}_h^{n+\frac{1}{2}}\partial_{tt}u(x_j,t)| \\
&\le C\tau^2 \|u\|_{C^4(\overline{\Omega}\times[0,T])}. \qquad \text{(C.5)}
\end{aligned}
$$

On the other hand, by the definition of $\mathcal{L}_h^{n+\frac{1}{2}}$ and $\mathcal{L}(t_{n+\frac{1}{2}})$, we have

$$
\begin{aligned}
|I_2| = &\frac{-u(x_{j-1},t_{n+\frac{1}{2}}) + 2u(x_j,t_{n+\frac{1}{2}}) - u(x_{j+1},t_{n+\frac{1}{2}})}{h^2} \\
&+ \frac{A(x_{j+\frac{1}{2}},t_{n+\frac{1}{2}})u(x_{j+1},t_{n+\frac{1}{2}}) - A(x_{j-\frac{1}{2}},t_{n+\frac{1}{2}})u(x_{j-1},t_{n+\frac{1}{2}})}{ih} \\
&+ [V(x_j) + A^2(x_j,t_{n+\frac{1}{2}})]u(x_j,t_{n+\frac{1}{2}}) \\
&+ \partial_x^2 u(x_j,t_{n+\frac{1}{2}}) + \partial_x\Big(iA(x,t_{n+\frac{1}{2}})u(x,t_{n+\frac{1}{2}})\Big)\Big|_{x=x_j} + iA(x_j,t_{n+\frac{1}{2}})\partial_x u(x_j,t_{n+\frac{1}{2}}) \\
&- A^2(x_j,t_{n+\frac{1}{2}})u(x_j,t_{n+\frac{1}{2}}) - V(x_j)u(x_j,t_{n+\frac{1}{2}}) \\
=:& \, I_3 + I_4, \qquad \text{(C.6)}
\end{aligned}
$$

where

$$
\begin{aligned}
|I_3| &= \left| \frac{-u(x_{j-1},t_{n+\frac{1}{2}}) + 2u(x_j,t_{n+\frac{1}{2}}) - u(x_{j+1},t_{n+\frac{1}{2}})}{h^2} + \partial_x^2 u(x_j,t_{n+\frac{1}{2}}) \right| \\
&\le Ch^2\|u\|_{C^4(\overline{\Omega}\times[0,T])}, \quad \text{(standard central difference scheme)} \qquad \text{(C.7)}
\end{aligned}
$$

and

$$
\begin{aligned}
I_4 = &\frac{A(x_{j+\frac{1}{2}},t_{n+\frac{1}{2}})u(x_{j+1},t_{n+\frac{1}{2}}) - A(x_{j-\frac{1}{2}},t_{n+\frac{1}{2}})u(x_{j-1},t_{n+\frac{1}{2}})}{ih} \\
&+ \partial_x\Big(iA(x,t_{n+\frac{1}{2}})u(x,t_{n+\frac{1}{2}})\Big)\Big|_{x=x_j} + iA(x_j,t_{n+\frac{1}{2}})\partial_x u(x_j,t_{n+\frac{1}{2}}) \\
= &-i\frac{A(x_{j+\frac{1}{2}},t_{n+\frac{1}{2}})u(x_{j+1},t_{n+\frac{1}{2}}) - A(x_{j-\frac{1}{2}},t_{n+\frac{1}{2}})u(x_{j-1},t_{n+\frac{1}{2}})}{h} \\
&+ i\partial_x A(x_j,t_{n+\frac{1}{2}})u(x_j,t_{n+\frac{1}{2}}) + 2iA(x_j,t_{n+\frac{1}{2}})\partial_x u(x_j,t_{n+\frac{1}{2}}) \\
= &-i\frac{A(x_{j+\frac{1}{2}},t_{n+\frac{1}{2}}) - A(x_{j-\frac{1}{2}},t_{n+\frac{1}{2}})}{h}u(x_j,t_{n+\frac{1}{2}}) \\
&- i\Big(A(x_{j+\frac{1}{2}},t_{n+\frac{1}{2}})\frac{u(x_{j+1},t_{n+\frac{1}{2}}) - u(x_j,t_{n+\frac{1}{2}})}{h} + A(x_{j-\frac{1}{2}},t_{n+\frac{1}{2}})\frac{u(x_j,t_{n+\frac{1}{2}}) - u(x_{j-1},t_{n+\frac{1}{2}})}{h}\Big) \\
&+ i\partial_x A(x_j,t_{n+\frac{1}{2}})u(x_j,t_{n+\frac{1}{2}}) + 2iA(x_j,t_{n+\frac{1}{2}})\partial_x u(x_j,t_{n+\frac{1}{2}}) \\
=:& \, I_5 + I_6, \qquad \text{(C.8)}
\end{aligned}
$$

where

$$
\begin{aligned}
I_5 &= \left| -i\frac{A(x_{j+\frac{1}{2}},t_{n+\frac{1}{2}}) - A(x_{j-\frac{1}{2}},t_{n+\frac{1}{2}})}{h}u(x_j,t_{n+\frac{1}{2}}) + i\partial_x A(x_j,t_{n+\frac{1}{2}})u(x_j,t_{n+\frac{1}{2}}) \right| \\
&\le Ch^2\|A\|_{C^2(\overline{\Omega}\times[0,T])}\|u\|_{C(\overline{\Omega}\times[0,T])}, \qquad \text{(C.9)} \\
I_6 &= -iA(x_{j+\frac{1}{2}},t_{n+\frac{1}{2}})\frac{u(x_{j+1},t_{n+\frac{1}{2}}) - u(x_j,t_{n+\frac{1}{2}})}{h}
\end{aligned}
$$

$$
\begin{aligned}
&- iA(x_{j-\frac{1}{2}}, t_{n+\frac{1}{2}})\frac{u(x_j, t_{n+\frac{1}{2}}) - u(x_{j-1}, t_{n+\frac{1}{2}})}{h} + 2iA(x_j, t_{n+\frac{1}{2}})\partial_x u(x_j, t_{n+\frac{1}{2}})\\
&= \Big(- iA(x_j, t_{n+\frac{1}{2}}) - i\partial_x A(x_j, t_{n+\frac{1}{2}})\frac{h}{2} + \mathcal{O}(h^2)\Big)\Big(\partial_x u(x_j, t_{n+\frac{1}{2}}) + \frac{1}{2}\partial_{xx}u(x_j, t_{n+\frac{1}{2}})h + \mathcal{O}(h^2)\Big)\\
&+ \Big(- iA(x_j, t_{n+\frac{1}{2}}) + i\partial_x A(x_j, t_{n+\frac{1}{2}})\frac{h}{2} + \mathcal{O}(h^2)\Big)\Big(\partial_x u(x_j, t_{n+\frac{1}{2}}) - \frac{1}{2}\partial_{xx}u(x_j, t_{n+\frac{1}{2}})h + \mathcal{O}(h^2)\Big)\\
&= \mathcal{O}(h^2). \qquad \text{(C.10)}
\end{aligned}
$$

The last estimate requires $\partial_{xxx}u$ to be bounded. Substituting (C.7)-(C.10) into (C.6) yields

$$I_2 = \mathcal{O}(h^2). \qquad \text{(C.11)}$$

Then substituting (C.5) and (C.11) into (C.3) yields

$$\mathcal{L}_h^{n+\frac{1}{2}} Eu(x_j, t_n) - \mathcal{L}(t_{n+\frac{1}{2}})u(x_j, t_{n+\frac{1}{2}}) = \mathcal{O}(h^2). \qquad \text{(C.12)}$$

Thirdly,

$$\left|\sigma\tau^2\mathcal{L}^{n+\frac{1}{2}}D_\tau u(t_n)\right| \le C\tau^2\|u\|_{C^3(\overline{\Omega}\times[0,T])}. \qquad \text{(C.13)}$$

Finally, by substituting (C.2) and (C.12)-(C.13) into the expression (C.1), we obtain

$$\|f^n\|_h = \mathcal{O}(\tau^2 + h^2).$$

Step 2: In the similar way (Taylor expansion), one can prove

$$\|D_\tau f^n\|_h \le C\|u\|_{C^5(\overline{\Omega}\times[0,T])}h^2.$$

Step 3: Inequliaty (5.6) of Lemma 5.2 implies $|\widetilde{K}^{(m)}(z) - \widetilde{K}(z)| \le C\tau^4$. Then

$$K_j^{(m)} = \int_{\partial\mathbb{D}} \widetilde{K}^{(m)}(z)z^{-j}\mu(\mathrm{d}z) \quad \text{and} \quad K_j = \int_{\partial\mathbb{D}} \widetilde{K}(z)z^{-j}\mu(\mathrm{d}z)$$

imply that

$$|K_j^{(m)} - K_j| \le \int_{\partial\mathbb{D}} |\widetilde{K}^{(m)}(z) - \widetilde{K}(z)|\mu(\mathrm{d}z) \le C\tau^4.$$

Thus it holds that

$$\left|\sum_{j=0}^{n} K_j^{(m)}u^{n-j} - \sum_{j=0}^{n} K_j u^{n-j}\right| \le \sum_{j=0}^{n} |K_j^{(m)} - K_j|u^{n-j} \le \sum_{j=0}^{n} C\tau^4 \le C\tau^3,$$

which implies

$$\tau^{-\frac{1}{2}}(\mathcal{K}^{(m)} - \mathcal{K}) * \gamma^{\pm}u(t_n) = \mathcal{O}(\tau^{2.5}). \qquad \text{(C.14)}$$

Besides, (3.12) implies that

$$\tau^{-\frac{1}{2}}\mathcal{K} * \gamma^{\pm}u(t_n) - \sqrt{-i(\partial_t + \sigma)}\gamma^{\pm}u(t_n) = \mathcal{O}(\tau^2). \qquad \text{(C.15)}$$

Since $\gamma^+ v = \frac{v_{M+1}+v_M}{2}$ and $x_+ = \frac{x_{M+1}+x_M}{2} = x_{M+\frac{1}{2}}$, it follows that

$$
\begin{aligned}
&\left|(\sqrt{-i(\partial_t + \sigma)}\gamma^{\pm}u(t_n) - \sqrt{-i(\partial_t + \sigma)}u(x_{\pm}, t_n))\right|\\
=&\left|\frac{\sqrt{-i(\partial_t + \sigma)}u(x_{M+1}, t_n) + \sqrt{-i(\partial_t + \sigma)}u(x_M, t_n)}{2} - \sqrt{-i(\partial_t + \sigma)}u(x_{M+\frac{1}{2}}, t_n)\right|\\
=&\mathcal{O}(h^2), \qquad \text{(central difference of } \sqrt{-i(\partial_t + \sigma)}u) \qquad \text{(C.16)}
\end{aligned}
$$

and

$$\partial_\nu^+ u(t_n) - \partial_\nu u(x_+, t_n) = \frac{u(x_{M+1}, t_n) - u(x_M, t_n)}{h} - \partial_x u(x_{M+\frac{1}{2}}, t_n) = \mathcal{O}(h^2),$$
$$\partial_\nu^- u(t_n) - \partial_\nu u(x_-, t_n) = -\frac{u(x_1, t_n) - u(x_0, t_n)}{h} + \partial_x u(x_{\frac{1}{2}}, t_n) = \mathcal{O}(h^2). \tag{C.17}$$

Substituting (C.14)-(C.17) into (5.14) yields

$$g_\pm^n = \mathcal{O}(\tau^2 + h^2). \tag{C.18}$$

Step 4: Since

$$\begin{aligned} D_\tau g_\pm^n =& \tau^{-\frac{1}{2}} (\mathcal{K}^{(m)} - \mathcal{K}) * \gamma^\pm D_\tau u(t_n) \\ &+ \left[\tau^{-\frac{1}{2}} \mathcal{K} * \gamma^\pm D_\tau u(t_n) - \sqrt{-i(\partial_t + \sigma)}\gamma^\pm D_\tau u(t_n)\right] \\ &+ \left[\sqrt{-i(\partial_t + \sigma)}\gamma^\pm D_\tau u(t_n) - \sqrt{-i(\partial_t + \sigma)} D_\tau u(x_\pm, t_n)\right] \\ &+ \left[\partial_\nu^\pm D_\tau u(t_n) - \partial_\nu D_\tau u(x_\pm, t_n)\right], \end{aligned} \tag{C.19}$$

it follows that (C.19) can be estimated similarly as (5.14) (replacing $u(x, t_n)$ by $D_\tau u(x, t_n)$).

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