

**STABILITY AND ERROR ANALYSIS FOR A SECOND-ORDER
FAST APPROXIMATION OF THE 1D SCHRÖDINGER EQUATION
UNDER ABSORBING BOUNDARY CONDITIONS ***

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Abstract. A second-order Crank-Nicolson finite difference method, integrating a fast approximation of an exact discrete absorbing boundary condition, is proposed for solving the one-dimensional Schrödinger equation in the whole space. The fast approximation is based on Gaussian quadrature approximation of the convolution coefficients in the discrete absorbing boundary conditions. It approximates the time convolution in the discrete absorbing boundary conditions by a system of $\mathcal{O}(\log^2 N)$ ordinary differential equations at each time step, where N denotes the total number of time steps. Stability and error estimate are presented for the numerical solutions given by the proposed fast algorithm. Numerical experiments are provided, which agree with the theoretical results and show the performance of the proposed numerical method.

Key words. Schrödinger equation, absorbing boundary condition, fast algorithm, Gaussian quadrature, stability, error estimate

AMS subject classifications. 65M12, 65R20, 65D30, 65Z05

1. Introduction. This article is concerned with the development and analysis of a fast algorithm for solving Cauchy problem of the one-dimensional Schrödinger equation:

$$i \partial_t u(x, t) = \mathcal{L}(t)u(x, t), \quad \forall x \in \mathbb{R}, \forall t > 0, \quad (1.1a)$$

$$\lim_{|x| \rightarrow +\infty} u(x, t) = 0, \quad \forall t > 0, \quad (1.1b)$$

$$u(x, 0) = u_0(x), \quad \forall x \in \mathbb{R}, \quad (1.1c)$$

where $i = \sqrt{-1}$ denotes the imaginary unit, $u(x, t)$ the complex-valued wave function to be solved, and

$$\mathcal{L}(t) = -[\partial_x + iA(x, t)]^2 + V(x, t) \quad (1.2)$$

the time-dependent Schrödinger operator. The initial wave function $u_0(x)$, the real-valued magnetic potential $A(x, t)$ and the real-valued electric potential $V(x, t)$ are assumed to be smooth functions with compact supports in a bounded interval (x_-, x_+) . The standard Schrödinger equation

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

whose external electric potential $V_{ex}(x, t)$ has constant tails in $(-\infty, x_-] \cup [x_+, \infty)$, can always be converted to (1.1)-(1.2) with $A(x, t) = -\partial_x \int_0^t V_{ex}(x, s) ds$ through a

*The work of Buyang Li is partially supported by a grant from the Research Grants Council of the Hong Kong Special Administrative Region (Project No. 15300817). The work of Jiwei Zhang is partially supported by NSFC under grant NOs. 11771035, 91430216, and NSAF U1530401. Jiwei Zhang also thanks for the hospitality and supports of Beijing Computational Science Research Center during his working period here. The work of Chunxiong Zheng is partially supported by NSFC under grant NOs. 91630205 and 11771248.

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transformation $u(x, t) = e^{i \int_0^t V_{ex}(x, s) ds} \psi(x, t)$; see [21, Section 2].

Under the assumptions above, it is known that the solution of the Cauchy problem (1.1) in the bounded domain (x_-, x_+) coincides with the solution of the following initial-boundary value problem (cf. [3, 4, 18, 21, 31]):

$$i\partial_t u(x, t) = \mathcal{L}(t)u(x, t), \quad \forall x \in (x_-, x_+), \quad \forall t > 0, \quad (1.3a)$$

$$\sqrt{-i\partial_t} u(x_{\pm}, t) + \partial_\nu u(x_{\pm}, t) = 0, \quad \forall t > 0, \quad (1.3b)$$

$$u(x, 0) = u_0(x), \quad \forall x \in [x_-, x_+], \quad (1.3c)$$

where ∂_ν denotes the outward normal derivative at the boundary points x_{\pm} , and (1.3b) is often referred to as an absorbing boundary condition (ABC), with

$$\begin{aligned} \sqrt{-i\partial_t} u(x_{\pm}, \cdot) &:= \mathcal{L}_s^{-1} \left[\sqrt{-is} (\mathcal{L}u)(x_{\pm}, s) \right] \\ &= \frac{\sqrt{-i}}{\sqrt{\pi}} \int_0^t (t-s)^{-\frac{1}{2}} \partial_s u(x_{\pm}, s) ds. \end{aligned} \quad (1.4)$$

Here $\mathcal{L}u$ denotes the Laplace transform of u in time and \mathcal{L}_s^{-1} denotes the inverse Laplace transform with respect to the frequency s . Such ABCs were constructed for various evolution equations in the literature to reduce the computation to a bounded domain of physical interest [2, 7, 9–14, 32]; also see [17, 28, 33–35] on high-dimensional and nonlinear problems. In the more general computational domains, (e.g., nonconvex domains where waves may leave and re-enter the domain), boundary integral equations can be constructed and taken as implicit boundary conditions on an artificial boundary [5, 19, 20, 27, 29].

The ABC (1.3b) contains a convolution operator $\sqrt{-i\partial_t}$ in time, which depends on all the historical values of the solution on the boundary. As a consequence, the direct evaluation of a discrete ABC at the n th time step requires $\mathcal{O}(n)$ operations to evaluate the numerical solutions from all the past n steps. Hence, fast algorithms for the ABC are important when the number of time steps is large. A fast algorithm based on Fourier transform was developed in [16], which can be used to evaluate the convolution integrals in the ABC exactly with $\mathcal{O}(\log^2 N)$ operations and $\mathcal{O}(N)$ storage for the computations up to the N th time step. By using quadrature approximation of the inverse Laplace transform representation of the convolution kernel with error ϵ , the convolution integrals in the ABC can be approximated within $\mathcal{O}(N(\log N) \log \frac{1}{\epsilon})$ operations and $\mathcal{O}((\log N) \log \frac{1}{\epsilon})$ storage [23, 26]. Alternatively, the convolution kernel can be approximated by a sum of exponentials based on a nonlinear least squares algorithm with the same order of complexity and storage [1, 18]. Instead of approximating the convolution integrals directly, one can also approximate the discretized convolution integrals based on quadrature approximation of the weights [30] with complexity $\mathcal{O}(N(\log N) \log \frac{1}{\epsilon})$ and storage $\mathcal{O}((\log N) \log \frac{1}{\epsilon})$.

For the initial-boundary value problem (1.3), an error estimate of $\mathcal{O}(h^{-\frac{1}{2}}(h^2 + \tau^{\frac{3}{2}}))$ was presented in [31] for a Crank-Nicolson finite difference method (with finite difference methods for spatial discretization and ABC), where τ and h denote the time-step size and spatial mesh size. The error estimate is optimal up to a factor $h^{-\frac{1}{2}}$, which was caused by using an L^2 -norm error estimate and controlling the boundary terms from the ABC through utilizing the inverse (trace) inequality. By using a stronger H^1 -norm error estimate, an optimal-order error estimate of $\mathcal{O}(\tau^2 + h^2)$ was proved in [21] for a perturbed Crank-Nicolson method, integrating a fast approximation of the ABC based on Padé's approximation of the generating function of the discrete convolution operator, with complexity $\mathcal{O}(N^{\frac{3}{2}} \log N)$ and storage $\mathcal{O}(N^{\frac{1}{2}} \log N)$ to maintain the

overall second-order accuracy.

In this paper we develop a new fast method to approximate the discrete ABC (described in section 2) without using contour integrals or Padé approximation. Instead, the fast algorithm is based on a simple Gaussian quadrature approximation of the discrete convolution coefficients on the real interval $(0, 1)$. We prove an overall second-order convergence $\mathcal{O}(\tau^2 + h^2)$ for a Crank–Nicolson finite difference method for (1.3a) in the interior domain, with the proposed fast approximation to the convolution quadrature discretization of the ABC (1.3b). The overall complexity and storage up to N th time step are $\mathcal{O}(MN + N \log^2 N)$ and $\mathcal{O}(M + \log^2 N)$, respectively, with M denoting the nodes of spatial finite difference discretization.

2. Discretization of (1.3) with direct evaluation of the ABC. In this section, we first describe a Crank-Nicolson scheme for (1.3) with a discrete ABC, which is derived by first discretizing the original problem (1.1) with the Crank-Nicolson method and then reducing the discrete problem in the whole space to a bounded domain of computational interest. This semi-discretization scheme was introduced in [3]. We then present the stability analysis of time discretization and the finite difference method for spatial discretization. Fast approximation of this discrete ABC will be proposed in the next section.

2.1. \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:

$$\ell^2(\mathcal{H}) = \left\{ g = \{g^n\}_{n=0}^{+\infty} : g^n \in \mathcal{H}, \|g\|_{\ell^2(\mathcal{H})} \equiv \left(\sum_{n=0}^{+\infty} \|g^n\|_{\mathcal{H}}^2 \right)^{\frac{1}{2}} < \infty \right\},$$

$$\ell_0^2(\mathcal{H}) = \left\{ g = \{g^n\}_{n=0}^{+\infty} \in \ell^2(\mathcal{H}) : g^0 = 0 \right\}.$$

Examples of Hilbert spaces to be used in this paper include \mathbb{C}^M and $L^2(I)$, where $M \geq 1$ is an integer and $I \subset \mathbb{R}$ is a finite or infinite interval. The inner product of $L^2(I)$ is defined as

$$(f, g)_{L^2(I)} = \int_I \overline{f(x)} g(x) dx, \quad \forall f, g \in L^2(I),$$

with $\overline{f(x)}$ denoting the complex conjugate of $f(x)$.

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

$$\tilde{g}(z) = \sum_{n=0}^{+\infty} g^n z^n,$$

which is an \mathcal{H} -valued function holomorphic in the unit disk \mathbb{D} . The limit $\tilde{g}(z) = \lim_{r \nearrow 1} \tilde{g}(rz)$ exists in $L^2(\partial\mathbb{D}; \mathcal{H})$, and the following Parseval's identity holds:

$$(f, g)_{\ell^2(\mathcal{H})} = \int_{\partial\mathbb{D}} (\tilde{f}(z), \tilde{g}(z))_{\mathcal{H}} \mu(dz), \quad \forall f, g \in \ell^2(\mathcal{H}), \quad (2.1)$$

where $\mu(dz) = \frac{1}{2\pi} d\theta$ (the Haar measure) through the change of variable $z = e^{i\theta}$, with $\theta \in [-\pi, \pi)$.

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 as our convention (to clarify the meaning of the identities in (2.2)):

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

It is straightforward to verify that for $f \in \ell_0^2(\mathcal{H})$ the following identities hold:

$$\widetilde{S}f(z) = z^{-1}\widetilde{f}(z), \quad \widetilde{E}f(z) = \frac{z^{-1}+1}{2}\widetilde{f}(z), \quad \widetilde{D}_\tau f(z) = \frac{z^{-1}-1}{\tau}\widetilde{f}(z). \quad (2.2)$$

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

$$g^n D_\tau f^n = D_\tau (f^n g^{n-1}) - f^n D_\tau g^{n-1}, \quad \forall n \geq 0, \quad (2.3)$$

$$\operatorname{Re}(D_\tau f^n, E f^n)_\mathcal{H} = \frac{1}{2} D_\tau \|f^n\|_\mathcal{H}^2, \quad \forall n \geq 0, \quad (2.4)$$

where $g^{-1} := g^0$. The identities (2.1)-(2.4) will be used frequently in this paper.

2.2. The Crank-Nicolson scheme with a discrete ABC. We shall derive a time-stepping scheme for (1.3) from the time discretization of the original problem (1.1). To this end, we denote $t_n = n\tau$, $n = 0, 1, 2, \dots$, with $\tau > 0$ the step size for time discretization.

We discretize (1.1) by the standard Crank-Nicolson scheme for the time-dependent Schrödinger equation:

$$\begin{aligned} iD_\tau u^n(x) &= \mathcal{L}^{n+\frac{1}{2}} E u^n(x), \quad \forall x \in \mathbb{R}, \quad \forall n \geq 0, \\ \lim_{|x| \rightarrow +\infty} u^n(x) &= 0, \quad \forall n \geq 1, \\ u^0(x) &= u_0(x), \quad \forall x \in \mathbb{R}, \end{aligned} \quad (2.5)$$

where $u^n(x) \approx u(x, t_n)$ and $\mathcal{L}^{n+\frac{1}{2}} = \mathcal{L}(t_{n+\frac{1}{2}})$; see (1.2).

Since u_0 , A and V have compact supports in $[x_-, x_+]$, on the interval $[x_+, +\infty)$ the semi-discrete problem (2.5) reduces to

$$\begin{aligned} iD_\tau u^n(x) &= -\partial_x^2 E u^n(x), \quad \forall x \in [x_+, +\infty), \quad \forall n \geq 0, \\ u^0(x) &= 0, \quad \forall x \in [x_+, +\infty), \\ \lim_{x \rightarrow +\infty} u^n(x) &= 0, \quad \forall n \geq 1. \end{aligned} \quad (2.6)$$

Let $\tilde{u}(x, z)$ denote the \mathcal{Z} -transform of the sequence $\{u^n(x)\}_{n=0}^{+\infty}$. Applying the \mathcal{Z} -transform to (2.6) and using (2.2), we obtain

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

whose solution can be generally expressed as

$$\tilde{u}(x, z) = c_1^+ \exp\left(\frac{x}{\sqrt{i\tau}} \sqrt{\frac{2-2z}{1+z}}\right) + c_2^+ \exp\left(-\frac{x}{\sqrt{i\tau}} \sqrt{\frac{2-2z}{1+z}}\right),$$

where $\sqrt{\cdot}$ takes nonnegative real parts for numbers in $\mathbb{C} \setminus (-\infty, 0)$. The condition

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

$$\partial_x \tilde{u}(x_+, z) + \frac{1}{\sqrt{i\tau}} \sqrt{\frac{2-2z}{1+z}} \tilde{u}(x_+, z) = 0, \quad \forall z \in \mathbb{D}. \quad (2.7)$$

Note that the function

$$K(z) = \frac{1}{\sqrt{i}} \sqrt{\frac{2-2z}{1+z}} \quad (2.8)$$

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

$$K(z) = \sum_{j=0}^{+\infty} K_j z^j, \quad \forall z \in \mathbb{D}. \quad (2.9)$$

The explicit expression of K_j is given by (cf. [3, 36])

$$K_j = \sqrt{-2i} \alpha_j, \quad \alpha_j = \begin{cases} \beta_k = \frac{(2k)!}{2^{2k}(k!)^2}, & j = 2k, \\ -\beta_k, & j = 2k + 1. \end{cases} \quad (2.10)$$

Substituting (2.9) and $\tilde{u}(x, z) = \sum_{n=0}^{+\infty} u^n(x) z^n$ into (2.7) yields an exact ABC for (2.5) at the right artificial boundary point $x = x_+$:

$$\partial_x u^n(x_+) + \tau^{-\frac{1}{2}} (\mathcal{K} * u)^n(x_+) = 0, \quad \forall n \geq 0, \quad (2.11)$$

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

$$(\mathcal{K} * u)^n = \sum_{j=0}^n K_j u^{n-j}. \quad (2.12)$$

For the simplicity of notation, for a function $u(x, t)$ we denote

$$\mathcal{K} * u(x, t_n) = \sum_{j=0}^n K_j u(x, t_{n-j}). \quad (2.13)$$

Analogously, by analyzing the problem (2.5) on $(-\infty, x_-]$, we derive an exact ABC at the left artificial boundary point $x = x_-$:

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

Consequently, the semi-discrete problem (2.5), originally defined on the the whole space, can be reduced to the following semi-discrete problem on a bounded domain:

$$\begin{aligned} iD_\tau u^n(x) &= \mathcal{L}^{n+\frac{1}{2}} E u^n(x), & \forall x \in (x_-, x_+), \quad \forall n \geq 0, \\ \partial_\nu u^n(x_\pm) + \tau^{-\frac{1}{2}} (\mathcal{K} * u)^n(x_\pm) &= 0, & \forall n \geq 0, \\ u^0(x) &= u_0(x), & \forall x \in [x_-, x_+], \end{aligned} \quad (2.14)$$

where $\nu = \pm 1$ denotes the unit outward normal at the boundary points x_\pm .

Since the time discretization (2.5) in the whole space is of second order, it follows that the induced convolution quadrature at the boundary points x_\pm in (2.14) is also of second order:

$$|\tau^{-\frac{1}{2}} (\mathcal{K} * u_\pm)^n - \sqrt{-i\partial_t} u(x_\pm, t_n)| \leq C\tau^2, \quad (2.15)$$

where $u_\pm^n := u(x_\pm, t_n)$. A proof of (2.15) can be found in [21, Appendix A] (by substituting $\sigma = 0$ therein).

2.3. Stability of time discretization. The discrete operator $\mathcal{K}*$ in (2.14) obtained by convolution quadrature preserves the ‘sign property’ of the continuous convolution operator $\sqrt{-i\partial_t}$, as shown in the following theorem.

Theorem 2.1. *The discrete convolution operator $\mathcal{K}*$ is stable, in the sense that for any sequence $v = (v^0, v^1, \dots)$ with $v^0 = 0$ and any $m \geq 0$, it holds that*

$$\Im \sum_{n=0}^m \overline{Ev^n} \cdot (\mathcal{K} * Ev)^n \leq 0, \quad (2.16)$$

$$\Re \sum_{n=0}^m \overline{D_\tau v^n} \cdot (\mathcal{K} * Ev)^n \geq 0. \quad (2.17)$$

Proof. Let us consider the following exterior problem:

$$iD_\tau \phi^n(x) = -\partial_x^2 E\phi^n(x), \quad \forall x \in [0, +\infty), \quad \forall n \geq 0, \quad (2.18a)$$

$$\phi^0(x) = 0, \quad \forall x \in [0, +\infty), \quad (2.18b)$$

$$\phi^n(0) = v^n, \quad \lim_{x \rightarrow +\infty} \phi^n(x) = 0, \quad \forall n \geq 1. \quad (2.18c)$$

We have seen that (2.6) implies (2.11). Similarly, the problem (2.18) implies

$$\partial_x \phi^n(0) = -\tau^{-\frac{1}{2}} (\mathcal{K} * \phi)^n(0) = -\tau^{-\frac{1}{2}} (\mathcal{K} * v)^n. \quad (2.19)$$

The $L^2(\mathbb{R}_+)$ -inner product between $E\phi^n(x)$ and (2.18a) yields (by taking the imaginary part)

$$\frac{1}{2} D_\tau \|\phi^n\|_{L^2(\mathbb{R}_+)}^2 = \Im \left(\overline{E\phi^n(0)} \partial_x E\phi^n(0) \right) = -\Im \left(\tau^{-\frac{1}{2}} \overline{Ev^n} (\mathcal{K} * Ev)^n \right),$$

where we have used (2.18c)-(2.19) and the following identity in the last equality:

$$E(\mathcal{K} * v)^n = (\mathcal{K} * Ev)^n. \quad (2.20)$$

Summing up the index n from 0 to m yields

$$\Im \sum_{n=0}^m \overline{Ev^n} \cdot (\mathcal{K} * Ev)^n = -\frac{1}{2\tau^{\frac{1}{2}}} \|\phi^{m+1}\|_{L^2(\mathbb{R}_+)}^2 \leq 0.$$

Similarly, the $L^2(\mathbb{R}_+)$ -inner product between $D_\tau \phi^n(x)$ and (2.18a) yields (by taking the real part)

$$\begin{aligned} 0 &= \Re(\overline{D_\tau \phi^n}, -\partial_x^2 E\phi^n)_{L^2(\mathbb{R}_+)} \\ &= \Re(\partial_x D_\tau \phi^n, \partial_x E\phi^n)_{L^2(\mathbb{R}_+)} + \Re\left(\overline{D_\tau \phi^n(0)} \partial_x E\phi^n(0)\right) \\ &= \Re(\partial_x D_\tau \phi^n, \partial_x E\phi^n)_{L^2(\mathbb{R}_+)} - \Re\left(\tau^{-\frac{1}{2}} \overline{D_\tau v^n} (\mathcal{K} * Ev)^n\right), \end{aligned}$$

where we have used (2.18c)-(2.19) and (2.20) in the last equality. Since

$$\Re(\partial_x D_\tau \phi^n, \partial_x E\phi^n)_{L^2(\mathbb{R}_+)} = \frac{1}{2} D_\tau \|\partial_x \phi^n\|_{L^2(\mathbb{R}_+)}^2,$$

it follows that

$$\Re\left(\tau^{-\frac{1}{2}} \overline{D_\tau v^n} (\mathcal{K} * Ev)^n\right) = \frac{1}{2} D_\tau \|\partial_x \phi^n\|_{L^2(\mathbb{R}_+)}^2.$$

Summing up the index n from 0 to m yields

$$\Re \sum_{n=0}^m \overline{D_\tau v^n} \cdot (\mathcal{K} * Ev)^n = \frac{1}{2\tau^{\frac{1}{2}}} \|\partial_x \phi^{m+1}\|_{L^2(\mathbb{R}_+)}^2 \geq 0.$$

This completes the proof of Theorem 2.1. \square

Remark 2.1. In [21, Proposition 5.3] we have proved similar sign properties

$$\operatorname{Im} \sum_{n=0}^m \overline{f^n(\mathcal{K}^{(m)} * f)} \leq 0, \quad \forall m \geq 0, \quad (2.21)$$

$$\operatorname{Re} \sum_{n=0}^m \overline{(D_\tau + \sigma E) f^n(\mathcal{K}^{(m)} * (E + \sigma \tau^2 D_\tau) f)} \geq 0, \quad \forall m \geq 0. \quad (2.22)$$

It is seen that $\sigma = 0$ yields (2.16)-(2.17). However, the proof of [21, Proposition 5.3] does not apply to the case $\sigma = 0$, as the extended sequence $f^n = \frac{1-\sigma}{1+\sigma} f^{n-1}$, $n = m+1, m+2, \dots$, used in the proof of [21, Proposition 5.3] is not in $\ell^2(\mathbb{C})$ in the case $\sigma = 0$.

2.4. Spatial discretization. Let M be a positive integer and $h = (x_+ - x_-)/M$ the mesh size. We define the spatial and temporal mesh points

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

with x_0 and x_{M+1} being two ghost points. Without loss of generality, we assume that the initial data and potentials are zero outside the interval (x_1, x_M) . Otherwise we slightly enlarge the computational domain.

Given a vector $\mathbf{v} = (v_0, \dots, v_{M+1}) \in \mathbb{C}^{M+2}$, we denote

$$\nabla_h \mathbf{v} = (\nabla_h v_0, \dots, \nabla_h v_M), \quad \mathcal{P}\mathbf{v} := (v_1, \dots, v_M) \quad \text{and} \quad \mathcal{Q}\mathbf{v} := (v_0, \dots, v_M),$$

where

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

Besides, we define the Neumann and Dirichlet data

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

The inner product between $\boldsymbol{\phi} = (\phi_1, \dots, \phi_M) \in \mathbb{C}^M$ and $\boldsymbol{\varphi} = (\varphi_1, \dots, \varphi_M) \in \mathbb{C}^M$ is defined as

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

while the inner product between $\boldsymbol{\chi} = (\chi_0, \dots, \chi_M) \in \mathbb{C}^{M+1}$ and $\boldsymbol{\omega} = (\omega_0, \dots, \omega_M) \in \mathbb{C}^{M+1}$ is defined as

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

The induced norms for the inner products on \mathbb{C}^M and \mathbb{C}^{M+1} are denoted by

$$\|\boldsymbol{\phi}\|_h = \sqrt{(\boldsymbol{\phi}, \boldsymbol{\phi})_h} \quad \text{and} \quad |\boldsymbol{\chi}|_h = \sqrt{\langle \boldsymbol{\chi}, \boldsymbol{\chi} \rangle_h},$$

respectively.

A second-order spatial discretization operator \mathcal{L}_h^n for approximating the continuous differential operator $\mathcal{L}(t_n)$ is defined by

$$\mathcal{L}_h^n \mathbf{v} := ((\mathcal{L}_h^n \mathbf{v})_1, \dots, (\mathcal{L}_h^n \mathbf{v})_M), \quad \forall \mathbf{v} = (v_0, \dots, v_{M+1}) \in \mathbb{C}^{M+2},$$

with

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

For the simplicity of notations, we use the abbreviation $\mathcal{L}_h^n \mathbf{v}_k := (\mathcal{L}_h^n \mathbf{v})_k$. A direct computation yields the following discrete Green's formula (with element-wise multiplication by \mathbf{U}^n and \mathbf{A}^n):

$$(\mathcal{P}\mathbf{v}, \mathcal{L}_h^n \mathbf{w})_h = \langle \nabla_h^n \mathbf{v}, \nabla_h^n \mathbf{w} \rangle_h + (\mathcal{P}\mathbf{v}, \mathbf{U}^n \mathcal{P}\mathbf{w})_h - \overline{\gamma^\pm \mathbf{v}} \cdot \partial_\nu^\pm \mathbf{w}, \quad \forall v, w \in \mathbb{C}^{M+2}, \quad (2.23)$$

where

$$\nabla_h^n = \nabla_h + i\mathbf{A}^n \mathcal{Q},$$

with $\mathbf{A}^n = (A_0^n, \dots, A_M^n)$, $\mathbf{U}^n = (U_1^n, \dots, U_M^n)$ and

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

In the time-stepping scheme (2.14), replacing the function $u^n(x)$ by the vector $\mathbf{u}^n = (u_0^n, \dots, u_{M+1}^n)$ 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:

$$iD_\tau \mathcal{P}\mathbf{u}^n = \mathcal{L}_h^{n+\frac{1}{2}} E \mathbf{u}^n, \quad \forall n \geq 0, \quad (2.24a)$$

$$\partial_\nu^\pm \mathbf{u}^n + \tau^{-\frac{1}{2}} (\mathcal{K} * \gamma^\pm \mathbf{u})^n = 0, \quad \forall n \geq 0, \quad (2.24b)$$

$$\mathbf{u}^0 = (u_0(x_0), \dots, u_0(x_{M+1})). \quad (2.24c)$$

3. Fast approximation of (2.24). In this section, we introduce a fast algorithm for approximating the discrete convolution in (2.24b). The stability and convergence of the proposed algorithm will be presented in the next section.

3.1. Approximation by exponential sums. Let us recall the convolution coefficients (2.10). Since

$$\beta_k = \frac{\Gamma(2k+1)}{2^{2k} \Gamma(k+1)^2},$$

applying the Legendre duplication formula (cf. page 29 and 41 in [6]), we derive

$$\begin{aligned} \beta_k &= \frac{1}{\sqrt{\pi}} \frac{\Gamma(k+\frac{1}{2})}{\Gamma(k+1)} = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \sin^{2k} \theta d\theta \\ &= \int_0^1 s^{2k} \mu(ds) \quad \left(\text{with } \mu(ds) = \frac{2ds}{\pi\sqrt{1-s^2}} \right) \\ &= \sum_{l=0}^{L-1} \int_{1-2^{-l}}^{1-2^{-l-1}} s^{2k} \mu(ds) + \int_{1-2^{-L}}^1 s^{2k} \mu(ds) \\ &\approx \sum_{l=0}^{L-1} \sum_{j=1}^L s_{l,j}^{2k} \omega_{l,j} + \sum_{j=1}^L s_{L,j}^{2k} \omega_{L,j} \\ &=: \beta_k^{(L)} = \sum_{m=1}^{L^2} s_m^{2k} \omega_m, \end{aligned} \quad (3.1)$$

where $\sum_{j=1}^L s_{l,j}^{2k} \omega_{l,j}$ is the L -points Gaussian quadrature for the integral

$$\int_{1-2^{-l}}^{1-2^{-l-1}} s^{2k} \mu(ds).$$

Put

$$K_j^{(L)} = \sqrt{-2i} \alpha_j^{(L)}, \quad \alpha_j^{(L)} = \begin{cases} \beta_k^{(L)} & , \quad j = 2k, \\ -\beta_k^{(L)} & , \quad j = 2k + 1, \end{cases} \quad (3.2)$$

and introduce $\mathcal{K}^{(L)*}$ as the discrete convolution associated with the convolution coefficients $K_j^{(L)}$, namely,

$$\mathcal{K}^{(L)*} v^n = \sum_{j=0}^n K_j^{(L)} v^{n-j}. \quad (3.3)$$

Replacing the convolution $\mathcal{K}*$ in (2.24b) by $\mathcal{K}^{(L)*}$ yields the following approximating problem:

$$iD_\tau \mathcal{P} \mathbf{u}^n = \mathcal{L}_h^{n+\frac{1}{2}} E \mathbf{u}^n, \quad \forall n \geq 0, \quad (3.4a)$$

$$\partial_\nu^\pm \mathbf{u}^n + \tau^{-\frac{1}{2}} (\mathcal{K}^{(L)*} \gamma^\pm \mathbf{u})^n = 0, \quad \forall n \geq 0, \quad (3.4b)$$

$$\mathbf{u}^0 = (u_0(x_0), \dots, u_0(x_{M+1})). \quad (3.4c)$$

Problem (3.4) can be solved by a fast algorithm described in the next subsection.

Proposition 3.1. *If $L \geq \log_2(N)$ then*

$$|\beta_k^{(L)} - \beta_k| \leq \frac{e^2 \sqrt{\pi}}{2} L^{\frac{3}{2}} 0.075^L \quad k = 0, 1, \dots, N, \quad (3.5)$$

$$|K_j^{(L)} - K_j| \leq e^2 \sqrt{\frac{\pi}{2}} L^{\frac{3}{2}} 0.075^L, \quad k = 0, 1, \dots, N. \quad (3.6)$$

Proof. Let $f(t) = t^{2k}$. Let $s_{l,j}$, $j = 1, \dots, L$, be the Gaussian quadrature nodes in the interval $[1 - 2^{-l}, 1 - 2^{-l-1}]$, and let $s_{l,j}^*$, $j = 1, \dots, L$, be the uniformly distributed nodes in the interval $[1 - 2^{-l}, 1 - 2^{-l-1}]$. Then a basic property of the Gaussian orthogonal polynomial is the following inequality:

$$\int_{1-2^{-l}}^{1-2^{-l-1}} \prod_{j=1}^L (s - s_{l,j})^2 \mu(ds) \leq \int_{1-2^{-l}}^{1-2^{-l-1}} \prod_{j=1}^L (s - s_{l,j}^*)^2 \mu(ds). \quad (3.7)$$

Moreover, there exists $\xi_l \in [1 - 2^{-l}, 1 - 2^{-l-1}]$ such that

$$\begin{aligned} & \left| \int_{1-2^{-l}}^{1-2^{-l-1}} s^{2k} \mu(ds) - \sum_{j=1}^L s_{l,j}^{2k} \omega_{l,j} \right| \\ & \leq \frac{|f^{(2L)}(\xi_l)|}{(2L)!} \int_{1-2^{-l}}^{1-2^{-l-1}} \prod_{j=1}^L (s - s_{l,j})^2 \mu(ds) \\ & \leq \frac{|f^{(2L)}(\xi)|}{(2L)!} \int_{1-2^{-l}}^{1-2^{-l-1}} \prod_{j=1}^L (s - s_{l,j}^*)^2 \mu(ds) \quad (\text{use (3.7) here}) \\ & \leq \frac{(2k)^{2L} (1 - 2^{-l-1})^{2k-2L}}{(2L)!} \int_{1-2^{-l}}^{1-2^{-l-1}} \prod_{j=1}^L (s - s_{l,j}^*)^2 \mu(ds) \end{aligned}$$

$$\begin{aligned}
&\leq \frac{(2k)^{2L}(1-2^{-l-1})^{2k-2L}}{(2L)!} \int_{1-2^{-l}}^{1-2^{-l-1}} \left(2^{-(l+1)(2L)} \prod_{j=1}^L \frac{j^2}{L^2} \right) \mu(ds) \\
&\leq \frac{(2k)^{2L}(1-2^{-l-1})^{2k-2L}}{(2L)!} 2^{-(l+1)(2L)} \frac{(L!)^2 \pi}{L^{2L} 2} \\
&\leq \frac{(2k)^{2L}(1-2^{-l-1})^{2k-2L}}{(2L)^{2L+\frac{1}{2}} e^{-2L}} 2^{-(l+1)(2L)} \frac{L^{2L+1} e^{-2L}}{L^{2L}} \frac{e^2 \pi}{2\sqrt{2\pi}} \quad (\text{use Stirling's approximation}) \\
&= \frac{(2k)^{2L}(1-2^{-l-1})^{2k-2L} 2^{-(l+1)(2L)}}{2^{2L+\frac{1}{2}} L^{2L-\frac{1}{2}}} \frac{e^2 \pi}{2\sqrt{2\pi}}. \tag{3.8}
\end{aligned}$$

It is easy to calculate that for any given $l \geq 0$ the function

$$g(y) := (2y)^{2L}(1-2^{-l-1})^{2y-2L}, \quad \forall y \in [0, \infty)$$

achieves maximum value at a point y_{\min} satisfying $g'(y_{\min}) = 0$, i.e.,

$$y_{\min} = \frac{-L}{\ln(1-2^{-l-1})}.$$

By using Taylor's expansion, we have

$$\ln(1-x) = -x - \frac{x^2}{2(1-\theta x)^2}, \quad \text{for some } \theta \in (0, 1) \text{ depending on } x.$$

which implies

$$-2x \leq \ln(1-x) \leq -x, \quad \forall x \in [0, 1/2].$$

As a result, there exists $c_l \in [\frac{1}{2}, 1]$ such that

$$\ln(1-2^{-l-1}) = -2^{-l-1}/c_l \quad \text{and} \quad y_{\min} = L2^{l+1}c_l.$$

Thus

$$\begin{aligned}
(2k)^{2L}(1-2^{-l-1})^{2k-2L} &= g(k) \leq g(y_{\min}) = (L2^{l+1}c_l)^{2L}(1-2^{-l-1})^{2L2^{l+1}c_l-2L} \\
&= (L2^{l+1}c_l)^{2L} e^{(2L2^{l+1}c_l-2L)\ln(1-2^{-l-1})} \\
&= (L2^{l+1}c_l)^{2L} e^{(2L2^{l+1}c_l-2L)(-2^{-l-1}/c_l)} \\
&= L^{2L} 2^{(l+1)2L} c_l^{2L} e^{-(2-c_l^{-1}2^{-l})L}.
\end{aligned}$$

Since $c_0 = 2^{-1}/\ln(2) \approx 0.72$ and $c_l \geq c_0$ for $l \geq 1$, the last equality implies

$$\begin{aligned}
(2k)^{2L}(1-2^{-l-1})^{2k-2L} &\leq \begin{cases} L^{2L} 2^{(l+1)2L} 0.2814^L & \text{if } l = 0, \\ L^{2L} 2^{(l+1)2L} 0.1817^L e^{-(2-0.87^{-1}2^{-1})L} & \text{if } l = 1, \\ L^{2L} 2^{(l+1)2L} e^{-3L/2} & \text{if } l \geq 2. \end{cases} \\
&\leq L^{2L} 2^{(l+1)2L} 0.3^L.
\end{aligned}$$

Substituting the inequality above into (3.8), we obtain

$$\left| \int_{1-2^{-l}}^{1-2^{-l-1}} s^{2k} \mu(ds) - \sum_{j=1}^L s_{L,j}^{2k} \omega_{L,j} \right| \leq \frac{L^{\frac{1}{2}} e^{-L}}{2^{2L+\frac{1}{2}}} \frac{e^2 \pi}{2\sqrt{2\pi}}. \tag{3.9}$$

Similarly, for $L \geq \log_2(k)$

$$\left| \int_{1-2^{-L}}^1 s^{2k} - \sum_{j=1}^L s_{L,j}^{2k} \omega_{L,j} \right| \leq \frac{(2k)^{2L} 2^{-(L+1)(2L)}}{2^{2L+\frac{1}{2}} L^{2L-\frac{1}{2}}} \frac{e^2 \pi}{2\sqrt{2\pi}} \leq \frac{1}{2^{2L+\frac{1}{2}} L^{2L-\frac{1}{2}}} \frac{e^2 \pi}{2\sqrt{2\pi}}. \tag{3.10}$$

Overall, for $L \geq \log_2(N)$ and $0 \leq k \leq N$,

$$|\beta_k^{(L)} - \beta_k| \leq \sum_{l=0}^{L-1} \frac{L^{\frac{1}{2}} 0.3^L}{2^{2L+\frac{1}{2}}} \frac{e^{2\pi}}{2\sqrt{2\pi}} + \frac{1}{2^{2L+\frac{1}{2}} L^{2L-\frac{1}{2}}} \frac{e^{2\pi}}{2\sqrt{2\pi}} \leq \frac{e^2 \sqrt{\pi}}{2} L^{\frac{3}{2}} 0.075^L. \quad (3.11)$$

This proves Proposition 3.1 in view of (3.2). \square

Remark 3.1. The function $\frac{e^2 \sqrt{\pi}}{2} L^{\frac{3}{2}} 0.075^L$ exponentially decays with respect to $L \geq 1$. Thus the approximation $K_j^{(L)}$ of the convolution coefficients K_j is exponentially convergent. For any $0 < \epsilon < \frac{1}{2}$, there exists a unique real number

$$L_\epsilon \geq 1, \quad L_\epsilon = \mathcal{O}(\log_2(1/\epsilon)) \text{ as } \epsilon \rightarrow 0,$$

such that $\frac{e^2 \sqrt{\pi}}{2} L_\epsilon^{\frac{3}{2}} 0.075^{L_\epsilon} = \epsilon$ and thus

$$|K_j^{(L)} - K_j| \leq \epsilon, \quad \text{for } L \geq L_\epsilon.$$

3.2. Implementation algorithm. In this subsection, we describe the fast algorithm for the implementation of the numerical scheme (3.4). By introducing $\mathbf{v}^n = E\mathbf{u}^n$, the problem (3.4) can be rewritten into the following equivalent form:

$$2i\tau^{-1} \mathcal{P}\mathbf{v}^n = \mathcal{L}_h^{n+\frac{1}{2}} \mathbf{v}^n + 2i\tau^{-1} \mathcal{P}\mathbf{u}^n, \quad \forall n \geq 0, \quad (3.12a)$$

$$\partial_\nu^\pm \mathbf{v}^n + \tau^{-\frac{1}{2}} (\mathcal{K}^{(L)} * \gamma^\pm \mathbf{v})^n = 0, \quad \forall n \geq 0, \quad (3.12b)$$

$$\mathbf{u}^{n+1} = 2\mathbf{v}^n - \mathbf{u}^n, \quad \forall n \geq 0, \quad (3.12c)$$

$$\mathbf{u}^0 = (u_0(x_0), \dots, u_0(x_{M+1})). \quad (3.12d)$$

In view of (3.2), the boundary condition (3.12b) is equivalent to

$$\partial_\nu^\pm \mathbf{v}^n + \sqrt{-2i\tau}^{-\frac{1}{2}} \beta_0^{(L)} \gamma^\pm \mathbf{v}^n + \sqrt{-2i\tau}^{-\frac{1}{2}} \sum_{j=1}^n \alpha_j^{(L)} \gamma^\pm \mathbf{v}^{n-j} = 0. \quad (3.13)$$

Since

$$\sum_{j=1}^n \alpha_j^{(L)} \gamma^\pm \mathbf{v}^{n-j} = \begin{cases} \sum_{m=1}^{L^2} \omega_m \left(\sum_{j=1}^k s_m^{2j} \gamma^\pm \mathbf{v}^{2k-2j} - \sum_{j=1}^{k-1} s_m^{2j} \gamma^\pm \mathbf{v}^{2k-1-2j} - \gamma^\pm \mathbf{v}^{2k-1} \right), & n = 2k, \\ \sum_{m=1}^{L^2} \omega_m \left(\sum_{j=1}^k s_m^{2j} \gamma^\pm \mathbf{v}^{2k+1-2j} - \sum_{j=1}^k s_m^{2j} \gamma^\pm \mathbf{v}^{2k-2j} - \gamma^\pm \mathbf{v}^{2k} \right), & n = 2k+1, \end{cases}$$

by setting

$$\mathcal{F}_m^\pm(k) = \sum_{j=1}^k s_m^{2j} \gamma^\pm \mathbf{v}^{2k-2j} \quad \text{and} \quad \mathcal{G}_m^\pm(k) = \sum_{j=1}^k s_m^{2j} \gamma^\pm \mathbf{v}^{2k+1-2j} \quad (3.14)$$

we have (for $n \geq 1$)

$$\sum_{j=1}^n \alpha_j^{(L)} \gamma^\pm \mathbf{v}^{n-j} = \begin{cases} \sum_m \omega_m [\mathcal{F}_m^\pm(k) - \mathcal{G}_m^\pm(k-1) - \gamma^\pm \mathbf{v}^{2k-1}], & n = 2k, \\ \sum_m \omega_m [\mathcal{G}_m^\pm(k) - \mathcal{F}_m^\pm(k) - \gamma^\pm \mathbf{v}^{2k}], & n = 2k+1. \end{cases} \quad (3.15)$$

According to (3.14), it holds that

$$\mathcal{F}_m^\pm(k+1) = s_m^2 [\gamma^\pm \mathbf{v}^{2k} + \mathcal{F}_m^\pm(k)], \quad \mathcal{F}_m^\pm(0) = 0, \quad (3.16)$$

and

$$\mathcal{G}_m^\pm(k+1) = s_m^2 [\gamma^\pm \mathbf{v}^{2k+1} + \mathcal{G}_m^\pm(k)], \quad \mathcal{G}_m^\pm(0) = 0. \quad (3.17)$$

By using (3.15)-(3.17), the summation term involved in (3.13) can be derived within $\mathcal{O}(L^2)$ operations. The total computation cost of the problem (3.4) at a single time step is of order $\mathcal{O}(L^2 + M)$. Thus the computational cost up to N th time step is $\mathcal{O}(N(L^2 + M))$. This significantly reduces the computation when $L^2 \ll N$, compared with the complexity $\mathcal{O}(N(N + M))$ of the direct evaluation method.

4. Stability and accuracy of the numerical solutions. In this section, we present stability analysis and error estimate for the fast algorithm (3.4). In particular, $L = \mathcal{O}(\log N)$ guarantees second-order convergence of the numerical solutions.

4.1. Stability of the discrete problem. To investigate the stability of the fast algorithm (3.4) with perturbed right side, we consider the following problem of $\phi^n \in \mathbb{C}^{M+2}$, $n = 0, 1, \dots, N$:

$$iD_\tau \mathcal{P} \phi^n = \mathcal{L}_h^{n+\frac{1}{2}} E \phi^n + \mathbf{f}^n, \quad \forall n \geq 0, \quad (4.1)$$

$$\tau^{-\frac{1}{2}} (\mathcal{K}^{(L)} * \gamma^\pm \phi)^n + \partial_\nu^\pm \phi^n = g_\pm^n, \quad \forall n \geq 0, \quad (4.2)$$

$$\phi^0 = (0, \dots, 0) \in \mathbb{C}^{M+2}, \quad (4.3)$$

with $g_\pm^0 = 0$, where the discrete convolution operator $\mathcal{K}^{(L)} *$ is defined in (3.3).

Theorem 4.1. *For $\epsilon = \mathcal{O}(\tau^{\frac{5}{2}})$, there exists a positive constant τ_0 such that for $\tau \leq \tau_0$ the solutions of (4.1)-(4.3) satisfy the following stability estimate for $k = 1, \dots, N$:*

$$\begin{aligned} & \|\mathcal{P} \phi^k\|_h^2 + |\nabla_h^n \phi^k|_h^2 \\ & \leq C \left(\|\mathbf{f}^{k-1}\|_h^2 + |g_\pm^k|^2 + |g_\pm^{k-1}|^2 + \tau \sum_{n=0}^{k-1} (\|\mathbf{f}^n\|_h^2 + \|D_\tau \mathbf{f}^{n-1}\|_h^2 + |g_\pm^n|^2 + |D_\tau g_\pm^{n-1}|^2) \right). \end{aligned} \quad (4.4)$$

Proof. Applying the operator E to (4.2) yields

$$\tau^{-\frac{1}{2}} \mathcal{K}^{(L)} * \gamma^\pm E \phi^n + \partial_\nu^\pm E \phi^n = E g_\pm^n, \quad \forall n \geq 0. \quad (4.5)$$

We further rewrite (4.5) as

$$\tau^{-\frac{1}{2}} \mathcal{K} * \gamma^\pm E \phi^n + \partial_\nu^\pm E \phi^n = E g_\pm^n + \eta^n, \quad \forall n \geq 0, \quad (4.6)$$

with

$$\eta^n = \tau^{-\frac{1}{2}} (\mathcal{K} - \mathcal{K}^{(L)}) * \gamma^\pm E \phi^n,$$

which satisfies

$$|\eta^n| \leq \sum_{j=0}^n \tau^{-\frac{1}{2}} |K_{n-j} - K_{n-j}^{(L)}| |\gamma^\pm E \phi^j|,$$

and thus

$$\begin{aligned} \|(\eta^n)_{n=0}^k\|_{\ell^2(\mathbb{C})} & \leq \tau^{-\frac{1}{2}} \|(K_{n-j} - K_{n-j}^{(L)})_{n=0}^k\|_{\ell^1(\mathbb{C})} \|(\gamma^\pm E \phi^n)_{n=0}^k\|_{\ell^2(\mathbb{C})} \\ & \leq \epsilon T \tau^{-\frac{3}{2}} \|(\gamma^\pm E \phi^n)_{n=0}^k\|_{\ell^2(\mathbb{C})} \\ & \leq \epsilon T \tau^{-\frac{3}{2}} E \|(\gamma^\pm \phi^n)_{n=0}^k\|_{\ell^2(\mathbb{C})}. \end{aligned} \quad (4.7)$$

We define

$$\mathbf{f}^{-1} = \mathbf{f}^0, \quad g_{\pm}^{-1} = g_{\pm}^0, \quad \eta^{-1} = \eta^0 \quad \text{and} \quad \mathbf{U}^{-1} = \mathbf{U}^0.$$

The inner product between $\mathcal{P}E\phi^n$ and (4.1) yields (by taking the imaginary part)

$$\Re(\mathcal{P}E\phi^n, D_{\tau}\mathcal{P}\phi^n)_h = \Im(\mathcal{P}E\phi^n, \mathcal{L}_h^{n+\frac{1}{2}}E\phi^n)_h + \Im(\mathcal{P}E\phi^n, \mathbf{f}^n)_h. \quad (4.8)$$

Applying the discrete Green formula (2.23) and (4.6) yields

$$\begin{aligned} & \frac{1}{2}D_{\tau}\|\mathcal{P}\phi^n\|_h^2 \\ &= \Im(\mathcal{P}E\phi^n, U^n\mathcal{P}E\phi^n)_h - \Im\left(\overline{\gamma^{\pm}E\phi^n} \cdot \partial_{\nu}^{\pm}E\phi^n\right) + \Im(\mathcal{P}E\phi^n, \mathbf{f}^n)_h \\ &= \Im(E\mathcal{P}\phi^n, U^nE\mathcal{P}\phi^n)_h + \tau^{-\frac{1}{2}}\Im\left(\overline{\gamma^{\pm}E\phi^n}\mathcal{K} * \gamma^{\pm}E\phi^n\right) - \Im\left(\overline{\gamma^{\pm}E\phi^n}(Eg_{\pm}^n + \eta^n)\right) \\ & \quad + \Im(E\mathcal{P}\phi^n, \mathbf{f}^n)_h \\ &\leq \Im(E\mathcal{P}\phi^n, U^nE\mathcal{P}\phi^n)_h - \Im\left(\overline{\gamma^{\pm}E\phi^n}(Eg_{\pm}^n + \eta^n)\right) + \Im(E\mathcal{P}\phi^n, \mathbf{f}^n)_h \\ &\leq CE\|\mathcal{P}\phi^n\|_h^2 + |\gamma^{\pm}\phi^n|(|Eg_{\pm}^n| + |\eta^n|) + E\|\mathcal{P}\phi^n\|_h\|\mathbf{f}^n\|_h. \end{aligned} \quad (4.9)$$

Multiplying the inequality above by τ and summing up the results for $n = 0, \dots, k-1$, we obtain

$$\begin{aligned} & \frac{1}{2}\|\mathcal{P}\phi^k\|_h^2 \\ &\leq C\tau\sum_{n=0}^k\|\mathcal{P}\phi^n\|_h^2 + \left(\tau\sum_{n=0}^{k-1}|\gamma^{\pm}\phi^n|^2\right)^{\frac{1}{2}}\left(\tau\sum_{n=0}^{k-1}|Eg_{\pm}^n|^2 + \tau\sum_{n=0}^{k-1}|\eta^n|^2\right)^{\frac{1}{2}} \\ & \quad + \left(\tau\sum_{n=0}^{k-1}\|\mathcal{P}\phi^n\|_h\right)^{\frac{1}{2}}\left(\tau\sum_{n=0}^{k-1}\|\mathbf{f}^n\|_h\right)^{\frac{1}{2}} \\ &\leq C\tau\sum_{n=0}^k\|\mathcal{P}\phi^n\|_h^2 + \left(\tau\sum_{n=0}^{k-1}|\gamma^{\pm}\phi^n|^2\right)^{\frac{1}{2}}\left(\tau\sum_{n=0}^k|g_{\pm}^n|^2 + (\epsilon T\tau^{-\frac{3}{2}})^2\tau\sum_{n=0}^{k-1}|\gamma^{\pm}\phi^n|^2\right)^{\frac{1}{2}} \\ & \quad + \left(\tau\sum_{n=0}^{k-1}\|\mathcal{P}\phi^n\|_h\right)^{\frac{1}{2}}\left(\tau\sum_{n=0}^{k-1}\|\mathbf{f}^n\|_h\right)^{\frac{1}{2}} \\ &\leq C\tau\sum_{n=0}^k\|\mathcal{P}\phi^n\|_h^2 + \left(\delta + \epsilon T\tau^{-\frac{3}{2}}\right)\tau\sum_{n=0}^{k-1}|\gamma^{\pm}\phi^n|^2 + \delta^{-1}\left(\tau\sum_{n=0}^k|g_{\pm}^n|^2 + \tau\sum_{n=0}^{k-1}\|\mathbf{f}^n\|_h^2\right), \end{aligned} \quad (4.10)$$

which holds for arbitrary $\delta > 0$ and $k = 1, \dots, N$.

On the other hand, the inner product between $D_{\tau}\mathcal{P}\phi^n$ and (4.1) yields (by taking the real part)

$$\begin{aligned} \Re(D_{\tau}\mathcal{P}\phi^n, \mathcal{L}_h^{n+\frac{1}{2}}E\phi^n)_h &= -\Re(D_{\tau}\mathcal{P}\phi^n, \mathbf{f}^n)_h \\ &= -D_{\tau}\Re(\mathcal{P}\phi^n, \mathbf{f}^{n-1})_h + \Re(\mathcal{P}\phi^n, D_{\tau}\mathbf{f}^{n-1})_h, \end{aligned} \quad (4.11)$$

where we have used (2.3) in to derive the last equality. By denoting

$$d_{\tau}v^n := \frac{v^{n+\frac{1}{2}} - v^n}{\tau},$$

it is straightforward to verify that

$$\nabla_h^{n+\frac{1}{2}}D_{\tau}\phi^n = D_{\tau}\nabla_h^n\phi^n - id_{\tau}A^{n+\frac{1}{2}}\mathcal{Q}\phi^{n+1} - id_{\tau}A^n\mathcal{Q}\phi^n,$$

$$\nabla_h^{n+\frac{1}{2}} E\phi^n = E\nabla_h^n \phi^n - \frac{\tau}{2} d_\tau A^{n+\frac{1}{2}} \mathcal{Q}\phi^{n+1} - \frac{\tau}{2} d_\tau A^n \mathcal{Q}\phi^n.$$

Thus applying the discrete Green formula (2.23) yields

$$\begin{aligned} & \Re(D_\tau \mathcal{P}\phi^n, \mathcal{L}_h^{n+\frac{1}{2}} E\phi^n)_h \\ &= \Re(\nabla_h^{n+\frac{1}{2}} D_\tau \phi^n, \nabla_h^{n+\frac{1}{2}} E\phi^n)_h + \Re(D_\tau \mathcal{P}\phi^n, U^{n+\frac{1}{2}} E\mathcal{P}\phi^n)_h - \Re(\overline{\gamma^\pm D_\tau \phi^n} \partial_\nu^\pm E\phi^n) \\ &= \Re(D_\tau \nabla_h^n \phi^n - id_\tau A^{n+\frac{1}{2}} \mathcal{Q}\phi^{n+1} - id_\tau A^n \mathcal{Q}\phi^n, E\nabla_h^n \phi^n - \frac{\tau}{2} d_\tau A^{n+\frac{1}{2}} \mathcal{Q}\phi^{n+1} - \frac{\tau}{2} d_\tau A^n \mathcal{Q}\phi^n)_h \\ &\quad + \sum_{j=1}^M hU_j^{n+\frac{1}{2}} \frac{1}{2} D_\tau |\mathcal{P}\phi_j^n|^2 - \Re(\overline{\gamma^\pm D_\tau \phi^n} \partial_\nu^\pm E\phi^n) \\ &= \frac{1}{2} D_\tau |\nabla_h^n \phi^n|_h^2 + \Re(D_\tau \nabla_h^n \phi^n, -\frac{\tau}{2} d_\tau A^{n+\frac{1}{2}} \mathcal{Q}\phi^{n+1} - \frac{\tau}{2} d_\tau A^n \mathcal{Q}\phi^n)_h \\ &\quad + \Re(-id_\tau A^{n+\frac{1}{2}} \mathcal{Q}\phi^{n+1} - id_\tau A^n \mathcal{Q}\phi^n, E\nabla_h^n \phi^n)_h \\ &\quad + \sum_{j=1}^M hU_j^{n+\frac{1}{2}} \frac{1}{2} D_\tau |\mathcal{P}\phi_j^n|^2 - \Re(\overline{\gamma^\pm D_\tau \phi^n} \partial_\nu^\pm E\phi^n) \\ &= \frac{1}{2} D_\tau |\nabla_h^n \phi^n|_h^2 + \Re(D_\tau \nabla_h^n \phi^n, -\frac{\tau}{2} d_\tau A^{n+\frac{1}{2}} \mathcal{Q}\phi^{n+1} - \frac{\tau}{2} d_\tau A^n \mathcal{Q}\phi^n)_h \\ &\quad + \Re(-id_\tau A^{n+\frac{1}{2}} \mathcal{Q}\phi^{n+1} - id_\tau A^n \mathcal{Q}\phi^n, E\nabla_h^n \phi^n)_h \\ &\quad + \frac{1}{2} D_\tau \sum_{j=1}^M hU_j^{n-\frac{1}{2}} |\mathcal{P}\phi_j^n|^2 - \frac{1}{2} \sum_{j=1}^M hD_\tau U_j^{n-\frac{1}{2}} |\mathcal{P}\phi_j^n|^2 \\ &\quad - \Re(\overline{\gamma^\pm D_\tau \phi^n} (Eg_\pm^n + \eta^n - \tau^{-\frac{1}{2}} \mathcal{K} * \gamma^\pm E\phi^n)) \\ &\geq \frac{1}{2} D_\tau |\nabla_h^n \phi^n|_h^2 + \frac{1}{2} D_\tau \sum_{j=1}^M hU_j^{n-\frac{1}{2}} |\mathcal{P}\phi_j^n|^2 - \frac{1}{2} \sum_{j=1}^M h|D_\tau U_j^{n-\frac{1}{2}}| |\mathcal{P}\phi_j^n|^2 \\ &\quad - CE|\nabla_h^n \phi^n|_h |E|\mathcal{Q}\phi^n|_h - \Re(\overline{\gamma^\pm D_\tau \phi^n} (Eg_\pm^n + \eta^n)), \end{aligned}$$

where we have used (2.3) in the last equality, and (2.17) in the last inequality. By using (2.3) again we obtain

$$\begin{aligned} & \Re(\overline{\gamma^\pm D_\tau \phi^n} (Eg_\pm^n + \eta^n)) \\ &= \Re D_\tau (\overline{\gamma^\pm \phi^n} (Eg_\pm^{n-1} + \eta^{n-1})) - \Re(\overline{\gamma^\pm \phi^n} D_\tau (Eg_\pm^{n-1} + \eta^{n-1})) \\ &\leq D_\tau \Re(\overline{\gamma^\pm \phi^n} (Eg_\pm^{n-1} + \eta^{n-1})) + C|\gamma^\pm \phi^n| (|D_\tau Eg_\pm^{n-1}| + |D_\tau \eta^{n-1}|). \end{aligned}$$

Substituting the last two estimates into (4.11), we have

$$\begin{aligned} \frac{1}{2} D_\tau |\nabla_h^n \phi^n|_h^2 &\leq -\frac{1}{2} D_\tau \sum_{j=1}^M hU_j^{n-\frac{1}{2}} |\mathcal{P}\phi_j^n|^2 + C\|\mathcal{P}\phi^n\|_h^2 + CE|\nabla_h^n \phi^n|_h |E|\mathcal{Q}\phi^n|_h \\ &\quad + D_\tau \Re(\overline{\gamma^\pm \phi^n} (Eg_\pm^{n-1} + \eta^{n-1})) + C|\gamma^\pm \phi^n| (|D_\tau Eg_\pm^{n-1}| + |D_\tau \eta^{n-1}|) \\ &\quad - D_\tau \Re(\mathcal{P}\phi^n, \mathbf{f}^{n-1})_h + \|\mathcal{P}\phi^n\|_h \|D_\tau \mathbf{f}^{n-1}\|_h \\ &\leq -\frac{1}{2} D_\tau \sum_{j=1}^M hU_j^{n-\frac{1}{2}} |\mathcal{P}\phi_j^n|^2 + C\|\mathcal{P}\phi^n\|_h^2 + CE|\nabla_h^n \phi^n|_h (E|\nabla_h^n \phi^n|_h + E\|\mathcal{P}\phi^n\|_h) \end{aligned}$$

$$\begin{aligned}
& + D_\tau \Re \left(\overline{\gamma^\pm \phi^n} (Eg_\pm^{n-1} + \eta^{n-1}) \right) + C |\gamma^\pm \phi^n| (|D_\tau Eg_\pm^{n-1}| + |D_\tau \eta^{n-1}|) \\
& - D_\tau \Re(\mathcal{P}\phi^n, \mathbf{f}^{n-1})_h + \|\mathcal{P}\phi^n\|_h \|D_\tau \mathbf{f}^{n-1}\|_h, \tag{4.12}
\end{aligned}$$

where we have used the discrete Sobolev embedding $|\mathcal{Q}\phi^n|_h \leq C(|\nabla_h^n \phi^n|_h + \|\mathcal{P}\phi^n\|_h)$ in the last inequality above.

Multiplying the inequality above by τ and summing up the results for $n = 0, \dots, k-1$, we obtain

$$\begin{aligned}
\frac{1}{2} |\nabla_h^n \phi^k|_h^2 & \leq -\frac{1}{2} \sum_{j=1}^M h U_j^{k-\frac{1}{2}} |\mathcal{P}\phi_j^k|^2 + C\tau \sum_{n=0}^{k-1} E \|\mathcal{P}\phi^n\|_h + C\tau \sum_{n=0}^{k-1} E |\nabla_h^n \phi^n|_h \\
& + \Re \left(\overline{\gamma^\pm \phi^k} (Eg_\pm^{k-1} + \eta^{k-1}) \right) \\
& + C \left(\tau \sum_{n=0}^{k-1} |\gamma^\pm \phi^n|^2 \right)^{\frac{1}{2}} \left(\tau \sum_{n=0}^{k-1} |D_\tau Eg_\pm^{n-1}|^2 + \tau \sum_{n=0}^{k-1} |D_\tau \eta^{n-1}|^2 \right)^{\frac{1}{2}} \\
& - \Re(\mathcal{P}\phi^k, \mathbf{f}^{k-1})_h + \left(\tau \sum_{n=0}^{k-1} \|\mathcal{P}\phi^n\|_h \right)^{\frac{1}{2}} \left(\tau \sum_{n=0}^{k-1} \|D_\tau \mathbf{f}^{n-1}\|_h \right)^{\frac{1}{2}} \\
& \leq C\tau \sum_{n=0}^k |\nabla_h^n \phi^n|_h + C\tau \sum_{n=0}^k \|\mathcal{P}\phi^n\|_h^2 + \delta |\gamma^\pm \phi^k|^2 + \delta^{-1} |Eg_\pm^{k-1} + \eta^{k-1}|^2 \\
& + \delta \tau \sum_{n=0}^{k-1} |\gamma^\pm \phi^n|^2 + C\delta^{-1} \left(\tau \sum_{n=0}^k |D_\tau g_\pm^{n-1}|^2 + \tau^{-1} \sum_{n=0}^{k-1} |\eta^n|^2 \right) \\
& + \delta \|\mathcal{P}\phi^k\|_h^2 + \delta^{-1} \|\mathbf{f}^{k-1}\|_h^2 + C\tau \sum_{n=0}^{k-1} \|\mathcal{P}\phi^n\|_h^2 + C\tau \sum_{n=0}^{k-1} \|D_\tau \mathbf{f}^{n-1}\|_h^2 \\
& \leq C\tau \sum_{n=0}^k |\nabla_h^n \phi^n|_h + \delta \|\mathcal{P}\phi^k\|_h^2 + C\tau \sum_{n=0}^k \|\mathcal{P}\phi^n\|_h^2 \\
& + \delta |\gamma^\pm \phi^k|^2 + (\delta + 2\delta^{-1}\epsilon T\tau^{-\frac{5}{2}} + \delta^{-1}\epsilon^2 T^2\tau^{-5}) \tau \sum_{n=0}^{k-1} |\gamma^\pm \phi^n|^2 \\
& + 2\delta^{-1} |Eg_\pm^{k-1}|^2 + \delta^{-1} \tau \sum_{n=0}^k |D_\tau g_\pm^{n-1}|^2 \\
& + \delta^{-1} \|\mathbf{f}^{k-1}\|_h^2 + C\tau \sum_{n=0}^{k-1} \|D_\tau \mathbf{f}^{n-1}\|_h^2, \tag{4.13}
\end{aligned}$$

where we have used (4.7) to derive the last inequality, which holds for arbitrary $\delta > 0$ and $k = 1, \dots, N$.

Summing up (4.10) and (4.13) yields

$$\begin{aligned}
& \frac{1}{2} \|\mathcal{P}\phi^k\|_h^2 + \frac{1}{2} |\nabla_h^n \phi^k|_h^2 \\
& \leq C\tau \sum_{n=0}^k |\nabla_h^n \phi^n|_h + \delta \|\mathcal{P}\phi^k\|_h^2 + C\tau \sum_{n=0}^k \|\mathcal{P}\phi^n\|_h^2 + \delta |\gamma^\pm \phi^k|^2 \\
& + \left(2\delta + 2\delta^{-1}\epsilon T\tau^{-\frac{5}{2}} + \epsilon T\tau^{-\frac{3}{2}} + \delta^{-1}\epsilon^2 T^2\tau^{-5} \right) \tau \sum_{n=0}^{k-1} |\gamma^\pm \phi^n|^2
\end{aligned}$$

$$\begin{aligned}
& + 2\delta^{-1}|Eg_{\pm}^{k-1}|^2 + \delta^{-1}\tau \sum_{n=0}^k (|g_{\pm}^n|^2 + |D_{\tau}g_{\pm}^{n-1}|^2) \\
& + \delta^{-1}\|\mathbf{f}^{k-1}\|_h^2 + C\tau \sum_{n=0}^{k-1} (\|\mathbf{f}^n\|_h^2 + \|D_{\tau}\mathbf{f}^{n-1}\|_h^2) \\
\leq & C\tau \sum_{n=0}^k |\nabla_h^n \phi^n|_h + \delta\|\mathcal{P}\phi^k\|_h^2 + C\tau \sum_{n=0}^k \|\mathcal{P}\phi^n\|_h^2 + C\delta(\|\mathcal{P}\phi^k\|_h^2 + |\nabla_h^k \phi^k|_h^2) \\
& + \left(2\delta + 2\delta^{-1}\epsilon T\tau^{-\frac{5}{2}} + \epsilon T\tau^{-\frac{3}{2}} + \delta^{-1}\epsilon^2 T^2\tau^{-5}\right) \tau \sum_{n=0}^k (\|\mathcal{P}\phi^n\|_h^2 + |\nabla_h^n \phi^n|_h^2) \\
& + 2\delta^{-1}|Eg_{\pm}^{k-1}|^2 + \delta^{-1}\tau \sum_{n=0}^k (|g_{\pm}^n|^2 + |D_{\tau}g_{\pm}^{n-1}|^2) \\
& + \delta^{-1}\|\mathbf{f}^{k-1}\|_h^2 + C\tau \sum_{n=0}^{k-1} (\|\mathbf{f}^n\|_h^2 + \|D_{\tau}\mathbf{f}^{n-1}\|_h^2), \tag{4.14}
\end{aligned}$$

where we have used the discrete H^1 norm to bound the trace at x_{\pm} . By choosing δ sufficiently small and $\epsilon = \mathcal{O}(\tau^{\frac{5}{2}})$, we obtain

$$\begin{aligned}
\|\mathcal{P}\phi^k\|_h^2 + |\nabla_h^n \phi^k|_h^2 & \leq C\tau \sum_{n=0}^k (\|\mathcal{P}\phi^n\|_h^2 + |\nabla_h^n \phi^n|_h^2) \\
& + C(\|\mathbf{f}^{k-1}\|_h^2 + |g_{\pm}^k|^2 + |g_{\pm}^{k-1}|^2) \\
& + C\tau \sum_{n=0}^{k-1} (\|\mathbf{f}^n\|_h^2 + \|D_{\tau}\mathbf{f}^{n-1}\|_h^2 + |g_{\pm}^n|^2 + |D_{\tau}g_{\pm}^{n-1}|^2). \tag{4.15}
\end{aligned}$$

Then the discrete Gronwall's inequality implies (4.4). \square

4.2. Error estimate. Let $\mathbf{u}_*^n = (u(x_0, t_n), u(x_1, t_n), \dots, u(x_{M+1}, t_n))$ denote the vector whose entries are the nodal values of the exact solution of (1.3) at the time t_n , and let \mathbf{u}^n denote the numerical solution given by the numerical scheme (3.4). Let $\phi^n = \mathbf{u}_*^n - \mathbf{u}^n$ denote the error of the numerical solution, which satisfies the error equation (4.1)-(4.3) with \mathbf{f}^n and g_{\pm}^n denoting the truncation errors of the numerical scheme, given by

$$\mathbf{f}^n = iD_{\tau}\mathcal{P}u(t_n) - i\partial_t u(t_{n+\frac{1}{2}}) - [\mathcal{L}^{n+\frac{1}{2}}Eu(t_n) - \mathcal{L}(t_{n+\frac{1}{2}})u(t_{n+\frac{1}{2}})], \tag{4.16}$$

$$\begin{aligned}
g_{\pm}^n & = \tau^{-\frac{1}{2}}(\mathcal{K}^{(L)} - \mathcal{K}) * \gamma^{\pm} \mathbf{u}_*^n + [\tau^{-\frac{1}{2}}\mathcal{K} * \gamma^{\pm} \mathbf{u}_*^n - \sqrt{-i(\partial_t + \sigma)}\gamma^{\pm} \mathbf{u}_*^n] \\
& + [\sqrt{-i\partial_t}\gamma^{\pm} \mathbf{u}_*^n - \sqrt{-i\partial_t}u(x_{\pm}, t_n)] + [\partial_{\nu}^{\pm} \mathbf{u}_*^n - \partial_{\nu}u(x_{\pm}, t_n)]. \tag{4.17}
\end{aligned}$$

By using Taylor's expansion, the following truncation error estimate can be verified, provided the solution of the PDE problem (1.1) is sufficiently smooth (cf. [21, Appendix C] with $\sigma = 0$):

$$\|\mathbf{f}^n\|_h + \|D_{\tau}\mathbf{f}^{n-1}\|_h \leq C(\tau^2 + h^2), \quad n = 0, 1, \dots, N-1, \tag{4.18}$$

$$|g_{\pm}^n| + |D_{\tau}g_{\pm}^{n-1}| \leq C(\tau^2 + h^2), \quad n = 0, 1, \dots, N, \tag{4.19}$$

where $\mathbf{f}^{-1} := \mathbf{f}^0$ and $g^{-1} := g^0$.

Substituting the truncation error estimates above into Theorem 4.1, we immediately obtain the following estimate for the error of the numerical solutions.

Theorem 4.2. *If the solution of the PDE problem (1.3) is sufficiently regular, or equivalently, the solution of the original problem (1.1) is sufficiently smooth, then the following error estimate holds:*

$$\max_{1 \leq n \leq N} (\|\mathcal{P}(\mathbf{u}_*^n - \mathbf{u}^n)\|_h + |\nabla_h^n(\mathbf{u}_*^n - \mathbf{u}^n)|_h) \leq C(\tau^2 + h^2). \quad (4.20)$$

5. Numerical examples. As discussed in Proposition 3.1 and Theorem 4.1, we use

$$\frac{e^2 \sqrt{\pi}}{2} L_\epsilon^{\frac{3}{2}} 0.075 L_\epsilon = \epsilon$$

to adaptively determine the number of Gaussian points $L = \lceil L_\epsilon \rceil$ for any given tolerance error ϵ . In all the numerical examples below, we take $\epsilon = \tau^{\frac{5}{2}}$ with the time step $\tau = T/N$. In this case we have $L = \mathcal{O}(\ln N)$. The resulting complexity for evaluating the ABCs up to N th time step is $\mathcal{O}(N \ln^2 N)$, with storage of $\mathcal{O}(\ln^2 N)$.

Two numerical examples are provided below. The first example demonstrates the convergence and complexity of the proposed numerical method. The second example simulates the interaction between an external magnetic potential and the ground state of two nuclei with fixed locations [24]. All the computations are performed by Matlab with double precision.

Example 1. We study the Schrödinger equation with $V(x) = 0$ and $A(x, t) = 0$, whose exact beam-like solution can be given explicitly as

$$u(x, t) = \frac{1}{\sqrt{\zeta + it}} \exp \left[ik(x - kt) - \frac{(x - 2kt)^2}{4(\zeta + it)} \right], \quad (5.1)$$

where k is a parameter to determine the propagation speed of the beam, and ζ is a positive parameter to adjust the beam width such that the initial wave function $u_0(x)$ is negligibly small outside of the spatial computation domain $[-3, 3]$. In the calculations, we set $k = 2$, $\zeta = 0.04$ and the final time $T = 2$.

The errors of numerical solutions in the \log_{10} scale are shown in Fig. 5 by increasing the mesh points with $M = N$ from 120 to 3840. Obviously, second-order convergence is observed by comparing the second order slope.

We now investigate the computational complexity of our numerical method. The CPU time (in seconds) is plotted in the right panel of Fig. 5 by comparing the direct method and the fast method proposed in this paper. To observe the dependence of CPU time on the number of time steps, we fix $M = 100$ and increase the number of time steps with $N = 50000, 70000, 90000, \dots, 300000$. We observe that CPU times of the direct method and the fast algorithm are consistent with the theoretical complexity $\mathcal{O}(N^2)$ and $\mathcal{O}(N \log^2 N)$, respectively.

Example 2. A bound state will keep its profile if there is no interaction between a quantum system and its environment, while the ionization phenomenon may occur when a time-varying electromagnetic field is applied. To simulate this process, we take the electric potential

$$V(x) = -10 \exp(-10(x - 1)^2) - 10 \exp(-10(x + 1)^2)$$

and magnetic potential

$$A(x, t) = \frac{5}{\sqrt{\pi}} (1 - \cos(10t)) \exp(-x^2)$$

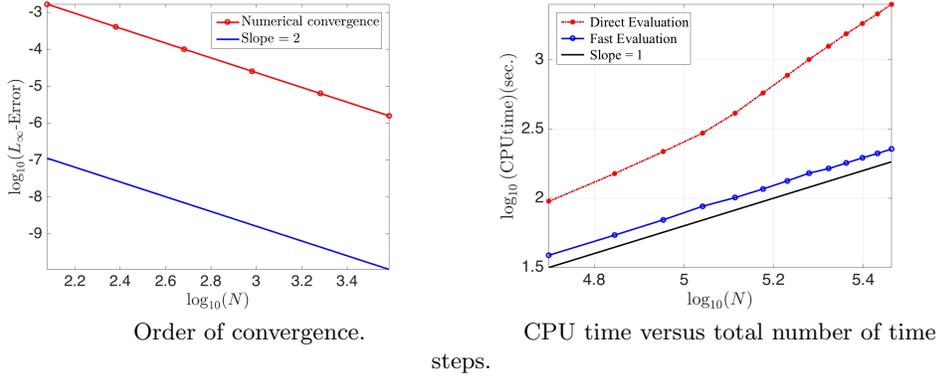


Fig. 5.1. Numerical results for Example 1.

to model the influence on the nuclei.

To obtain the bound states, we solve the L^2 -bounded eigenfunctions of the following Schrödinger eigenvalue problem:

$$[-\partial_x^2 + V(x)]u(x) = \lambda u(x). \quad (5.2)$$

The bound state associated with the smallest point spectrum is referred to as the ground state, whose energy is $\lambda_0 = -3.7332$, see the left panel of Fig. 5, which is chosen as the initial value of problem (1.3) with the above space-dependent nuclear potential.

We take the computational domain $[-20, 20]$ and the final time $T = 100$. The evolutions of numerical solution (left) with $M = 2560$ and $N = 10240$, and the reference solution (right) are plotted in Fig. 5.3. The reference solution is calculated in an enlarged computational domain by employing sufficiently refined mesh parameters. The errors between numerical solutions and reference solutions are plotted in Fig. 5. One can see that the errors are in the scale of 10^{-5} .

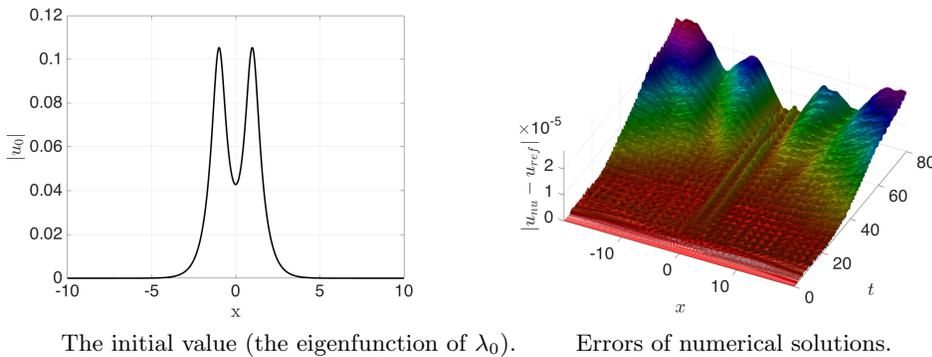
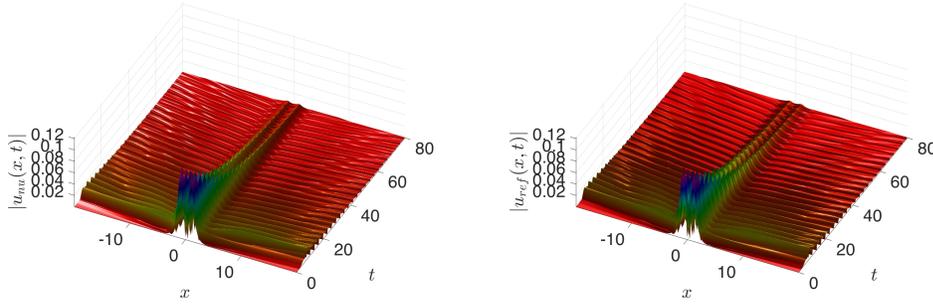


Fig. 5.2. (Example 2): Initial state and error of numerical solutions.

Again, the CPU times by using the direct method and fast algorithm are shown in Fig. 5.4 in the \log_{10} scale with $N = 50000, 70000, \dots, 300000$. We can see a significant reduction of the CPU time by the fast algorithm, which behaves linearly with respect to the total number of time steps.



Evolution of the numerical solutions.

Evolution of the reference solutions.

Fig. 5.3. (Example 2): Evolution of the solutions.

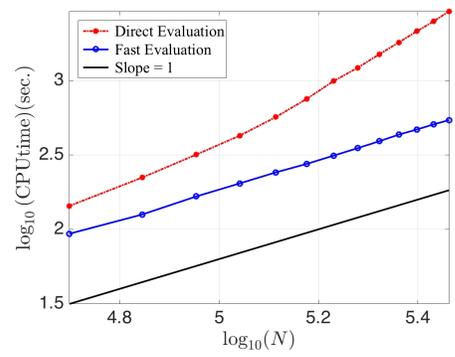


Fig. 5.4. (Example 2): log-log plot of the CPU time versus N (total number of time steps).

6. Conclusion. The one-dimensional Schrödinger equation in the whole space was reformulated into an initial-boundary value problem in a bounded domain of computational interest with an artificial boundary. The Crank-Nicolson finite difference method, together with a new fast algorithm for approximating the ABC, was proposed to solve the initial-boundary value problem. The new fast algorithm approximates the discrete convolution coefficients by a sum of exponentials derived through applying the Gauss quadrature on dyadically decomposed subintervals. A criterion determining the number of quadrature points was proposed to guarantee an overall second-order accuracy of the fully discrete numerical method. Numerical examples were provided to support the theoretical analysis and to demonstrate the effectiveness of the proposed numerical method.

Compared with the existing fast algorithms for convolution quadrature (e.g. [23, 30]), the fast algorithm presented in this paper does not require $\log(N)$ contours for quadrature points, though the total number of quadrature points are of the same order. The spatial discretization in this paper is based on the finite difference method. We have tested (4.1) by $D_\tau \mathcal{P}\phi^n$ (discrete time derivative of the solution) to derive a stability estimate for the finite difference method, which together with the estimate (4.18) for the defect yields an optimal-order error estimate for the numerical solutions. The stability analysis can be extended to finite element spatial discretization of any order (see [3]), but the defect estimate would be one-order lower than the finite

difference method (due to the Ritz projection error of the finite element method). Therefore, for the piecewise linear finite element method, convergence of $O(\tau^2 + h)$ in the H^1 norm can be proved similarly.

We have assumed that the initial value u_0 has a compact support. Strategies to overcome this restriction are given in, e.g., [8] and [22].

We have defined the \mathcal{Z} -transform as a power series of z (instead of a Lorent series of z) so that the \mathcal{Z} -transform of a sequence in $\ell^2(\mathcal{H})$ is always holomorphic in the unit disk \mathbb{D} and has traces in $L^2(\partial\mathbb{D}; \mathcal{H})$. This is the same notation as the generating functions that have been widely used in the community of ordinary differential equations; see [15, 25].

REFERENCES

- [1] B. Alpert, L. Greengard, and T. Hagstrom, Rapid evaluation of nonreflecting boundary kernels for time-domain wave propagation, *SIAM J. Numer. Anal.*, 37 (2000), pp. 1138–1164.
- [2] X. Antoine, A. Arnold, C. Besse, M. Ehrhardt, and A. Schädle, A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations, *Commun. Comput. Phys.*, 4 (2008), pp. 729–796.
- [3] X. Antoine and C. Besse, Unconditionally stable discretization schemes of non-reflecting boundary conditions for the one-dimensional Schrödinger equation, *J. Comput. Phys.* 188 (2003), pp. 157–175.
- [4] A. Arnold, M. Ehrhardt, and I. Sofronov, Discrete transparent boundary conditions for the Schrödinger equation: fast calculation, approximation, and stability, *Commun. Math. Sci.*, 1 (2003), pp. 501–556.
- [5] L. Banjai, C. Lubich, F.-J. Sayas, Stable numerical coupling of exterior and interior problems for the wave equation, *Numer. Math.*, 129 (2015), pp. 611–646.
- [6] W. Bell, Special functions for scientists and engineers, D. Van Nostrand Company, Ltd, 1968.
- [7] B. Engquist and A. Majda, Absorbing boundary conditions for the numerical simulation of waves. *Math. Comput.*, 31 (1977), pp. 629–651.
- [8] M. Ehrhardt, Discrete transparent boundary conditions for Schrödinger-type equations for non-compactly supported initial data, *Appl. Numer. Math.*, 58 (2008), pp. 660–673.
- [9] S. Eriksson and J. Nordström, Exact Non-reflecting Boundary Conditions Revisited: Well-Posedness and Stability, *Found. Comput. Math.*, 17 (2017), pp. 957–986.
- [10] D. Givoli, Non-reflecting boundary conditions: A review, *J. Comput. Phys.*, 94 (1991) pp. 1–29.
- [11] D. Givoli, High-order local non-reflecting boundary conditions: A review, *Wave Motion*, 39 (2004), pp. 319–326.
- [12] B. Gustafsson, Far-field boundary conditions for time-dependent hyperbolic systems. *SIAM J. Sci. Statist. Comput.*, 9 (1988), pp. 812–828.
- [13] T. Hagstrom. Radiation boundary conditions for the numerical simulation of waves. *Acta Numer.*, 8 (1999), pp. 47–106.
- [14] T. Hagstrom, New results on absorbing layers and radiation boundary conditions, in *Topics in Computational Wave Propagation*, M. Ainsworth et al., eds., Springer-Verlag, New York, 2003, pp. 1–42.
- [15] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II.: Stiff and differential-algebraic problems*, Springer, Second edition, 1996.
- [16] E. Hairer, Ch. Lubich, and M. Schlichte, Fast numerical solution of nonlinear Volterra convolution equations, *SIAM J. Sci. and Stat. Comput.*, 6(3) (1985), 532–541.
- [17] H. Han and C. Zheng, Exact nonreflecting boundary conditions for an acoustic problem in three dimensions, *J. Comput. Math.*, 21 (2003), pp. 15–24.
- [18] S. D. Jiang and L. Greengard, Fast evaluation of nonreflecting boundary conditions for the Schrödinger equation in one dimension, *Comput. Math. Appl.*, 47(2004), pp. 955–966.
- [19] B. Kovács and C. Lubich, Stable and convergent fully discrete interior–exterior coupling of Maxwell’s equations, *Numer. Math.*, 137 (2017), pp. 91–117.
- [20] A. R. Laliena, F.-J. Sayas, Theoretical aspects of the application of convolution quadrature to scattering of acoustic waves, *Numer. Math.*, 112 (2009), pp. 637–678.
- [21] B. Li, J. Zhang, and C. Zheng: An efficient second-order finite difference method for the one-dimensional Schrödinger equation with absorbing boundary conditions. *SIAM J. Numer. Anal.*, 56 (2018), pp. 766–791.
- [22] M. F. Levy, Non-local boundary conditions for radiowave propagation, in: *Third International*

- Conference on Mathematical and Numerical Aspects of Wave Propagation Phenomena*, Juan-les-Pins, France, 24-28 April 1995, ed. G. Cohen, SIAM 1995, pp. 499–505.
- [23] M. López-Fernández, C. Lubich, and A. Schädle, Adaptive, fast, and oblivious convolution in evolution equations with memory, *SIAM J. SCI. COMPUT.* 30 (2008), pp. 1015–1037.
 - [24] E. Lorin and X. Yang, Frozen Gaussian approximation-based two-level methods for multi-frequency time dependent Schrödinger equation, *Comput. Phys. Commun.*, 207 (2016), pp. 145–159.
 - [25] C. Lubich, Convolution quadrature revisited, *BIT Numer. Math.*, 44 (2004), pp. 503–514.
 - [26] C. Lubich and A. Schädle, Fast convolution for nonreflecting boundary conditions, *SIAM J. Sci. Comput.*, 24 (2002), pp. 161–182.
 - [27] J. M. Melenk and A. Rieder, Runge-Kutta convolution quadrature and FEM-BEM coupling for the time-dependent linear Schrödinger equation, *J. Integr. Equat. Appl.*, 29 (2017), pp. 189–250.
 - [28] G. Pang, Y. Yang, and S. Tang, Exact boundary condition for semidiscretized Schrödinger equation and heat equation in a rectangular domain, *J. Sci. Comp.*, 72 (2017), pp. 1–13.
 - [29] T. Sánchez-Vizuet and F.-J. Sayas, Symmetric Boundary-Finite Element Discretization of Time Dependent Acoustic Scattering by Elastic Obstacles with Piezoelectric Behavior, *J. Sci. Comput.*, 70 (2017), pp. 1290–1315.
 - [30] A. Schädle, M. López-Fernández, and C. Lubich, Fast and oblivious convolution quadrature, *SIAM J. Sci. Comput.*, 28 (2006), pp. 421–438.
 - [31] Z. Z. Sun, X. Wu, The stability and convergence of a difference scheme for the Schrödinger equation on an infinite domain by using artificial boundary conditions, *J. Comput. Phys.*, 214 (2006), pp. 209–223.
 - [32] S. V. Tsynkov, Numerical solution of problems on unbounded domains: A review, *Appl. Numer. Math.*, 27 (1998), pp. 465–532.
 - [33] X. Wang and S. Tang, Matching boundary conditions for lattice dynamics, *Int. J. Numer. Meth. Engin.*, 93 (2013), pp. 1255–1285.
 - [34] X. Yang and J. Zhang, Computation of the Schrödinger equation in the semiclassical regime on an unbounded domain, *SIAM J. Numer. Anal.*, 52 (2014), pp. 808–831.
 - [35] C. Zheng, A perfectly matched layer approach to the nonlinear Schrödinger wave equations, *J. Comput. Phys.*, 227 (2007), pp. 537–556.
 - [36] C. Zheng, Approximation, stability and fast evaluation of exact artificial boundary condition for one-dimensional heat equation, *J. Comput. Math.*, 25 (2007), pp. 730–745.