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Gang PANG[1], Yibo YANG[2], Xavier ANTOINE[3], Shaoqiang TANG[4]

Abstract. Based on the discrete artificial boundary condition introduced in [16] for the two-dimensional free Schrödinger equation in a computational rectangular domain, we propose to analyze the stability and convergence rate of the resulting full scheme. We prove that the global scheme is L^2-stable and that the accuracy is second-order in time, confirming then the numerical results reported in [16].

Keywords: Schrödinger equation; artificial boundary condition; stability analysis; convergence analysis.

AMS Subject Classification: 35J10, 65L20, 65L10, 65L12

1 Introduction

Time-dependent Schrödinger equations play a key role in many applications related to physics and engineering [6, 14, 21, 22], including quantum physics, acoustics, electromagnetism and optics. In many cases, the equation is set in the whole space $\mathbb{R}^d$ ($d \geq 1$). Therefore, when one wants to simulate the solution to the initial-value problem, we have to bound the computational domain to get a finite number of spatial degrees of freedom. Doing this, one needs to fix a suitable boundary condition at the fictitious interface of the domain that mimics the behavior of the wave field in the exterior domain. If the physical solution is confined within a finite domain [6], trivially a homogeneous Dirichlet or Neumann boundary condition can be considered. Nevertheless, this is insufficient in some situations. A classical example is when the wave is outgoing, expanding then to infinity. More advanced boundary conditions must be designed, considering transparent, artificial or absorbing boundary conditions, according to the properties of the boundary condition. This usually requires a lot of mathematical and numerical analysis to state well-suited boundary conditions that minimize the spurious reflection at the boundary, but also to lead to accurate and stable numerical schemes. For the Schrödinger equation, and over the past two decades, many contributions were done for the one- and two-dimensional cases, for the linear or nonlinear Schrödinger equation, involving possibly some space and time variable

[1]School of Mathematical Sciences, Beihang University of Aeronautics and Astronautics, Beijing 100191, P.R. China. Email: gangpang@buaa.edu.cn

[2]Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, 3401 Walnut St, Philadelphia, PA 19104, United States. Email: ybyang@seas.upenn.edu

[3]Institut Elie Cartan de Lorraine, Université de Lorraine, Sphinx team, Inria Nancy-Grand Est, F-54506 Vandoeuvre-lès-Nancy Cedex, France. Email: xavier.antoine@univ-lorraine.fr

[4]HEDPS, CAPT and LTCS, College of Engineering, Peking University, Beijing 100871, China. Email: maotang@pku.edu.cn

potentials, with simple or complicate smooth convex fictitious boundaries. We refer to [4, 5, 7, 11, 13, 18] for some examples, the list of references being non exhaustive. Available review papers on artificial boundary conditions are e.g. [12, 15, 23] for general PDEs, and [1, 3] more specifically for Schrödinger-type problems. Many approaches can be developed to build these boundary conditions. Some methods are based on directly working with the continuous PDE, building approximations to the Dirichlet-to-Neumann (DtN) operators, others include constructions of boundary conditions for the semi-discretized equation (in time or space), and finally other techniques are directly applied at the full discrete level. For completeness, let us also mention that Perfectly Matched Layer (PML) [8, 9, 10, 19, 24] can be used for truncating the computational domain.

Here, we consider the time-dependent linear free Schrödinger equation truncated in a rectangular two-dimensional domain. The artificial boundary condition under consideration is the one proposed in [16], based on an exact representation of the boundary operator for a rectangular shaped domain, with a second-order spatial discretization of the Schrödinger equation. Therefore, the corresponding boundary condition falls into the framework of semi-discrete artificial boundary conditions. From some numerical simulations, we have shown in [16] that, based on a Crank-Nicolson scheme, the full approximation is second-order in time. The aim of the present paper is to prove the stability of the fully discrete scheme as well as the second-order error estimate in time. Since this paper is already technical as well as [16], the authors strongly advise the reader to first understand the derivation in [16] before entering into the details of the present paper.

The plan of the paper is the following. After the introduction (Section 1), Section 2 focuses on the problem setting, its semi-discretization in space and some basic properties of the scheme. In Section 3, we develop the results related to the exact artificial boundary condition for the discrete spatial rectangular lattice. We also proceed to the full discretization of the initial boundary-value problem. In Section 4, we prove the L^2-stability of the fully discrete scheme. Section 5 is devoted to the convergence analysis. Finally, we end by a conclusion in Section 6 and an Appendix.

2 Problem setting: semi-discretization and basic properties

Let us consider the two-dimensional linear Schrödinger equation with unknown $u := u(x, y, t)$

$$\iota \dot{u} = -\Big(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\Big), \tag{1}$$

where $(x, y) \in \mathbb{R}^2$ and $t > 0$ are the space and time variables, respectively. The time derivative is denoted by $\dot{u} := \partial_t u$. In addition, a compactly supported initial data $u(x, y, t = 0) = u_0(x, y)$ is added to equation (1). Finally, the complex-valued number ι is such that $\iota := \sqrt{-1}$.

Let us now introduce the uniform spatial steps Δx and Δy in the x- and y-directions, respectively. By discretizing (1) with a second-order five points stencil scheme for the laplacian (with $\Delta x = \Delta y$ here) and after rescaling the time variable through $t = (\Delta x^2)^{-1} t$, we obtain the following semi-discrete system for the exact (e) solution $\psi^e := (\psi^e_{m,n})_{(m,n)\in\mathbb{Z}^2}$

$$\iota \dot{\psi}^e_{m,n} = -(\psi^e_{m+1,n} + \psi^e_{m-1,n} + \psi^e_{m,n+1} + \psi^e_{m,n-1} - 4\psi^e_{m,n}) = -\Delta\psi^e_{m,n}, \tag{2}$$

with compactly supported initial data $\psi^e_{m,n}(0) = u_0(m\Delta x, n\Delta x)$ for the uniform lattice $(m, n) \in \mathbb{Z}^2$. In the above equation, we define the discrete laplacian as: $\Delta := \Delta_x + \Delta_y$, with $\Delta_{x,y} := \Delta^+_{x,y}\Delta^-_{x,y}$ and

denoting by Δ_x^+ (Δ_x^-, respectively) the forward (backward, respectively) finite-difference operator in the x-direction. Similarly, the operators Δ_y^+ and Δ_y^- are introduced in the y-direction. Let us assume that the initial data is square integrable, i.e. $\| \psi^e(0) \|_{*,2} < \infty$, where the semi-discrete L^2-norm on the infinite lattice is defined by

$$\| \psi^e \|_{*,2} = \Big(\sum_{(m,n)\in\mathbb{Z}^2} |\psi^e_{m,n}|^2 \Big)^{1/2}.$$

We furthermore consider the following standard behavior of the solution at infinity

$$|\psi^e_{m,n}(t)| \to 0 \quad \text{for } |m| + |n| \to \infty.$$

We define $\psi^{e,(k)}_{m,n}(t)$ as the k-th order time derivative of $\psi^e_{m,n}(t)$. Then, we have $|\psi^{e,(k)}_{m,n}(t)| \to 0$.

By multiplying Eq. (2) by $\overline{\psi^e_{m,n}(t)}$ ($\bar{z}$ being the conjugate of a complex number z), taking the conjugate of Eq. (2) and multiplying it by $-\psi^e_{m,n}(t)$, then summing up the two equations for (m,n) in $\mathbb{Z}^2$ and integrating by parts the resulting equation, one can prove the semi-discrete L^2-norm conservation

$$\forall t > 0, \quad \| \psi^e(t) \|_{*,2} = \| \psi^e(0) \|_{*,2} \, .$$

In addition, taking the k-th derivative of the semi-discrete equation

$$i\dot{\psi}^e_{m,n} = -(\psi^e_{m,n-1} + \psi^e_{m,n+1} + \psi^e_{m+1,n} + \psi^e_{m-1,n} - 4\psi^e_{m,n}),$$

we obtain

$$i\psi^{e,(k+1)}_{m,n} = -(\psi^{e,(k)}_{m,n-1} + \psi^{e,(k)}_{m,n+1} + \psi^{e,(k)}_{m+1,n} + \psi^{e,(k)}_{m-1,n} - 4\psi^{e,(k)}_{m,n}),$$

which means that

$$|\psi^{e,(k+1)}_{m,n}| \le |\psi^{e,(k)}_{m,n-1}| + |\psi^{e,(k)}_{m,n+1}| + |\psi^{e,(k)}_{m+1,n}| + |\psi^{e,(k)}_{m-1,n}| + 4|\psi^{e,(k)}_{m,n}|.$$

This leads to

$$|\psi^{e,(k+1)}_{m,n}|^2 \le 5|\psi^{e,(k)}_{m,n-1}|^2 + 5|\psi^{e,(k)}_{m,n+1}|^2 + 5|\psi^{e,(k)}_{m+1,n}|^2 + 5|\psi^{e,(k)}_{m-1,n}|^2 + 80|\psi^{e,(k)}_{m,n}|^2.$$

Summing up over all the indices m and n, we have

$$\sum_{m,n} |\psi^{e,(k+1)}_{m,n}|^2 \le 100 \sum_{m,n} |\psi^{e,(k)}_{m,n}|^2.$$

Finally, we conclude that

$$\| \psi^{e,(k+1)}(0) \|_{*,2} \le 10 \, \| \psi^{e,(k)}(0) \|_{*,2} \tag{3}$$

and

$$\| \psi^{e,(k)}(t) \|_{*,2} = \| \psi^{e,(k)}(0) \|_{*,2} \le 10^k \, \| \psi^e(0) \|_{*,2} \, . \tag{4}$$

One also gets the inequality: $|\psi^{e,(k)}_{m,n}(0)| \le 10^k \, \| \psi^e(0) \|_{*,2}$, meaning that each function $\psi^e_{m,n}(t)$ is analytic.

Remark 1. *The discussion above extends to the case of the Schrödinger equation with a compactly supported potential term given by V, i.e.*

$$\iota \dot{u} = -\Big(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \Big) + V(x,y,t)u, \tag{5}$$

where each function $V(m\Delta x, n\Delta x, t)$ is analytic with respect to t.

3 Exact boundary conditions for the semi-discrete Schrödinger equation on a rectangular domain - full discretization

Let us introduce the Laplace transform

$$\tilde{\psi}^e_{m,n}(s) := \int_0^\infty \psi^e_{m,n}(t) e^{-st} dt. \tag{6}$$

Before presenting the construction of boundary conditions for general compact initial data, we start with a special case, i.e., the so-called point-source problem. We assume that the wave function ψ^e satisfies Eq. (2) and that $\psi^e_{m,n}(0) = 0$, for $(m,n) \neq (0,0)$. For a given function $\psi^e_{0,0}(t)$, we have, for $(m,n) \neq (0,0)$,

$$\psi^e_{m,n}(t) = f^e_{m,n}(t) * \psi^e_{0,0}(t) = \int_0^t f^e_{m,n}(\tilde{t}) \psi^e_{0,0}(t - \tilde{t}) d\tilde{t}, \tag{7}$$

where the function $f^e_{m,n}(t)$ can be numerically computed with high accuracy by a fourth-order Runge-Kutta scheme from the expression

$$g^e_{m,n}(t) = f^e_{m,n}(t) * g^e_{0,0}(t), \tag{8}$$

with

$$\begin{aligned} g^e_{m,n}(t) = (\iota t)^{m+n} e^{-4\iota t} \frac{(m+n)!}{m!n!} \frac{\sqrt{\pi}}{2^{m+n+1}\Gamma(\frac{m+n+1}{2})\Gamma(\frac{m+n}{2}+1)} \times \\ {}_2F_3 \left(\begin{array}{c} \frac{1}{2}(m+n+1), \frac{1}{2}(m+n)+1; -4t^2 \\ m+1, n+1, m+n+1 \end{array} \right). \end{aligned} \tag{9}$$

In the above definition, Γ is the Gamma special function and the generalized hypergeometric function ${}_2F_3$ [17] is given by

$${}_2F_3 \left(\begin{array}{c} a_1, a_2; z \\ b_1, b_2, b_3 \end{array} \right) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k}{k! (b_1)_k (b_2)_k (b_3)_k} z^k, \tag{10}$$

with $(a)_k = a(a+1)...(a+k-1)$, for $k \geq 1$ and $(a)_0 = 1$. This is the inverse Laplace transform of $W((m,n), \frac{4 - \iota s}{2})$, where

$$\begin{aligned} W((m,n), z) = \frac{1}{2^{m+n} z^{m+n+1}} \frac{(m+n)!}{m!n!} \times \\ {}_4F_3 \left(\begin{array}{c} \frac{1}{2}(m+n+1), \frac{1}{2}(m+n+1), \frac{1}{2}(m+n)+1, \frac{1}{2}(m+n)+1; \frac{4}{z^2} \\ m+1, n+1, m+n+1 \end{array} \right), \end{aligned} \tag{11}$$

and $z = (4 - \iota s)/2$. The function ${}_4F_3$ is the generalized hypergeometric function ${}_pF_q$ [17], with $p = 4$ and $q = 3$.

Let us consider now a finite rectangular computational domain and let us assume that the initial data is zero outside the selected rectangular box, including its boundary. To simplify the presentation, we suppose that the domain is the square $L \times L$ (see Fig. 1). The nodes at the boundary are labelled

counterclockwise, with the interior layer set as I_k, for $1 \leq k \leq 4L-4$, and the outer layer as J_k, with $1 \leq k \leq 4L$. Deriving a numerical artificial boundary condition consists in writing $\psi^e_{J_k}(t)$ as a function of the values of the wave field in the interior layer, completing hence the semi-discrete system (2) to get a problem set in a finite computational region.

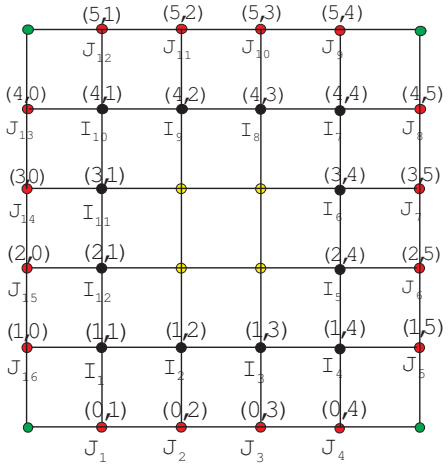

Figure 1: Discrete computational lattice (for $L = 4$): the red bullets represent the outer layer points, the black ones correspond to the interior layer points, the yellow ones are the interior points and the green ones stands for the corner points.

Let us consider that $\psi^e_{I_k}(t)$, for $k = 1, \cdots, 4L-4$, are given values. Following [16], we first decompose them as $4L-4$ unknown independent sources $\chi^e_{I_k}(t)$

$$\psi^e_{I_k}(t) = \sum_{\ell=1}^{4L-4} f^e_{I_k - I_\ell}(t) * \chi^e_{I_\ell}(t). \tag{12}$$

For $1 \leq k \leq 4L-4$ and $z = \dfrac{4-\iota s}{2}$, we have

$$\tilde{\psi}^e_{I_k}(s) = \sum_{\ell=1}^{4L-4} \frac{W\left(I_k - I_\ell, z\right)}{W\left((0,0), z\right)} \tilde{\chi}^e_{I_\ell}(s), \tag{13}$$

where $\tilde{\chi}^e_{I_\ell}(s)$ is the Laplace transform of the function $\chi^e_{I_\ell}(t)$. From the asymptotic estimates

$$\frac{W\left((m,n), z\right)}{W\left((0,0), z\right)} \sim \left(\frac{2}{z}\right)^{m+n}, \qquad |z| \to +\infty,$$

the matrix $\left(\dfrac{W\left(I_k - I_\ell, z\right)}{W\left((0,0), z\right)}\right)_{k,\ell}$ is diagonally dominant for large values s. Consequently, the matrix is invertible, the functions $\tilde{\chi}_{I_\ell}(s)$ exist and can be determined uniquely. One can also prove that $\chi^e_{I_\ell}(0) = 0$. For a point (m,n) outside the inner boundary, we have

$$\tilde{\psi}^e_{m,n}(s) = \sum_{\ell=1}^{4L-4} \frac{W\left((m,n) - I_\ell, z\right)}{W\left((0,0), z\right)} \tilde{\chi}^e_{I_\ell}(s). \tag{14}$$

For any inner boundary point I_ℓ, a direct computation shows that

$$\begin{aligned}(4-\iota s)W\left((m,n)-I_\ell,z\right) = W\left((m+1,n)-I_\ell,z\right)+W\left((m-1,n)-I_\ell,z\right)\\ +W\left((m,n+1)-I_\ell,z\right)+W\left((m,n-1)-I_\ell,z\right).\end{aligned} \tag{15}$$

Injecting the above relation into (14) gives

$$(4-\iota s)\tilde{\psi}^e_{m,n}(s) = \tilde{\psi}^e_{m+1,n}(s)+\tilde{\psi}^e_{m-1,n}(s)+\tilde{\psi}^e_{m,n+1}(s)+\tilde{\psi}^e_{m,n-1}(s), \tag{16}$$

meaning that for any point (m,n) outside the inner boundary, $\psi^e_{m,n}(t)$ satisfies Eq. (2). It can also be checked that $\psi^e_{m,n}(0)=0$. Once the sources $\chi^e_{I_\ell}(t)$ have been obtained, an exact boundary condition reads as follows, for $1\le \ell \le 4L$,

$$\psi^e_{I_\ell}(t) = \sum_{l=1}^{4L-4} f^e_{I_\ell - I_l}(t) * \chi^e_{I_l}(t), \qquad \psi^e_{J_\ell}(t) = \sum_{l=1}^{4L-4} f^e_{J_\ell - I_l}(t) * \chi^e_{I_l}(t). \tag{17}$$

For two sequences $u=\{u^k\}$ and $v=\{v^k\}$, let us now define the discrete convolution

$$(u\star v)^k = \sum_{l=0}^{k} u^l v^{k-l}\Delta t_l := \sum_{l=0}^{k} u^l v^{k-l}\Delta t - u^0 v^k \frac{\Delta t}{2} - u^k v^0 \frac{\Delta t}{2}$$

through the trapezoidal quadrature rule, with $\Delta t_l = \Delta t/2$ for $l=0,k$ and $\Delta t_l = \Delta t$ otherwise. For a fixed time step Δt, $(f^e_{m,n})^k$, $(\psi^e_{m,n})^k$ and $(\chi^e_{m,n})^k$ stand for the quantities $f^e_{m,n}(k\Delta t)$, $\psi^e_{m,n}(k\Delta t)$ and $\chi^e_{m,n}(k\Delta t)$, respectively. In addition, the numerical approximation of $f^e_{m,n}(k\Delta t)$, $\psi^e_{m,n}(k\Delta t)$, $\chi^e_{m,n}(k\Delta t)$ is designated by $f^k_{m,n}$, $\psi^k_{m,n}$, $\chi^k_{m,n}$, respectively. In the present paper, the unknowns $\psi^k_{m,n}$ $(1\le m,n\le L)$ are computed by applying the Crank-Nicolson scheme [2] to Eq. (2)

$$\begin{aligned}-\iota\frac{\psi^k_{m,n}-\psi^{k-1}_{m,n}}{\Delta t} = \frac{1}{2}\Delta(\psi^k_{m,n}+\psi^{k-1}_{m,n}) = \frac{1}{2}(\psi^k_{m-1,n}+\psi^k_{m+1,n}+\psi^k_{m,n-1}+\psi^k_{m,n+1}-4\psi^k_{m,n})\\ +\frac{1}{2}(\psi^{k-1}_{m-1,n}+\psi^{k-1}_{m+1,n}+\psi^{k-1}_{m,n-1}+\psi^{k-1}_{m,n+1}-4\psi^{k-1}_{m,n}),\end{aligned} \tag{18}$$

for $1\le m,n\le L$. Concerning the boundary condition, $\psi^k_{I_\ell}$ and $\psi^k_{J_\ell}$ $(1\le \ell\le 4L)$ can be written from relations (17) as

$$\psi^k_{I_\ell} = \sum_{l=1}^{4L-4} (f_{I_\ell - I_l}\star\chi_{I_l})^k, \qquad \psi^k_{J_\ell} = \sum_{l=1}^{4L-4} (f_{J_\ell - I_l}\star\chi_{I_l})^k. \tag{19}$$

Finally, we can use the values $\psi^k_{I_\ell}$ to complete the fully discretized system given by Eq. (18), for $1\le m,n\le L$, and then prove the stability of the whole system.

4 L^2-stability analysis of the scheme

In this section, we prove the stability of the scheme (18)-(19). Le us first introduce the norm

$$\|\ \psi\ \|_2 = \Big(\sum_{m,n=1}^{L} |\psi_{m,n}|^2\Big)^{1/2} \tag{20}$$

and the $\mathcal{Z}$-transform $\hat{u}$ of a sequence $u := \{u^k\}$ as

$$\hat{u}(z) = \sum_{k=0}^{\infty} \frac{u^k}{z^k}. \tag{21}$$

If $w^k = (u \star v)^k$, one directly gets

$$\hat{w}(z) = \sum_{k=0}^{\infty} \frac{w^k}{z^k} = \sum_{k=0}^{\infty} \frac{1}{z^k} \sum_{l=0}^{k} u^l v^{k-l} \Delta t_l = \hat{u}(z)\hat{v}(z)\Delta t - u^0 \frac{\Delta t}{2} \hat{v}(z) - v^0 \frac{\Delta t}{2} \hat{u}(z). \tag{22}$$

From the relation $(g^e_{m,n})^k = (f_{m,n} \star g^e_{0,0})^k$ and (22), one has

$$\hat{g}^e_{m,n}(z) = \hat{f}_{m,n}(z)\hat{g}^e_{0,0}(z)\Delta t - \hat{g}^e_{0,0}(z) f^e_{m,n}(0) \frac{\Delta t}{2} - \hat{f}^e_{m,n}(z) g^e_{0,0}(0) \frac{\Delta t}{2},$$

leading to

$$\hat{f}_{m,n}(z) = \frac{\hat{g}^e_{m,n}(z) + \hat{g}^e_{0,0}(z) f^e_{m,n}(0) \frac{\Delta t}{2}}{(\hat{g}^e_{0,0}(z) - \frac{g^e_{0,0}(0)}{2})\Delta t}. \tag{23}$$

If $v^k = (u \star f_{m,n})^k$, with $u^0 = 0$, we have

$$\hat{v}(z) = \hat{f}_{m,n}(z)\hat{u}(z)\Delta t - f^e_{m,n}(0)\hat{u}(z)\frac{\Delta t}{2} = \frac{\hat{g}^e_{m,n}(z) + \frac{f^e_{m,n}(0)\Delta t}{4}}{(\hat{g}^e_{0,0}(z) - \frac{g^e_{0,0}(0)}{2})} \hat{u}(z) = h_{m,n}(z)\hat{u}(z). \tag{24}$$

From the definition of the terms $g^e_{m,n}(t)$, the quantities $h_{m,n}(z)$ can be uniformly written as

$$h_{m,n}(z) = \frac{\hat{g}^e_{m,n}(z) - \frac{1}{2}\delta_{0,0} + \frac{i}{4} \triangle t \delta_{0,1}}{\hat{g}^e_{0,0}(z) - \frac{1}{2}}. \tag{25}$$

Here, $\delta_{0,0} = 1$ for $(m,n) = (0,0)$, $\delta_{0,0} = 0$ for other cases. In the same way, $\delta_{0,1} = 1$ for $(m,n) = (0,1)$, $\delta_{0,1} = 0$ otherwise.

Let us now introduce the index I^1_m, $1 \leq m \leq 4L$, such that: $I^1_m = (1,m)$, $I^1_{L+m} = (m,L)$, $I^1_{m+2L} = (L, L+1-m)$ and $I^1_{m+3L} = (L+1-m, 1)$, for $1 \leq m \leq L$. Therefore, I^1 and J have both $4L$ elements. Let us set $\beta = e^{\rho \Delta t} > 1$, with $\rho > 0$. We use this term below to act like a phase change in the spectral space of $\mathcal{Z}$-transformation. Doing this, we have some integrals later (e.g. like for (34) or (41)) which are not singular, simplifying the analysis. Taking $\varphi^k_{m,n} = \frac{1}{\beta^k}\psi^k_{m,n}$ in Eq. (18), one obtains

$$-\iota \frac{2}{\Delta t}(\varphi^k_{m,n} - \varphi^{k-1}_{m,n}) = \Delta(\varphi^k_{m,n} + \varphi^{k-1}_{m,n}) + (\beta - 1)(\Delta + \iota \frac{2}{\Delta t})\varphi^k_{m,n} \tag{26}$$

and

$$-\iota \frac{2}{\Delta t}\beta(\varphi^k_{m,n} - \varphi^{k-1}_{m,n}) = \beta\Delta(\varphi^k_{m,n} + \varphi^{k-1}_{m,n}) + (1 - \beta)(\Delta - \iota \frac{2}{\Delta t})\varphi^{k-1}_{m,n}. \tag{27}$$

Let us now multiply the conjugate of Eq. (26) by $\varphi^k_{m,n}$ and Eq. (27) by $-\beta^{-1}\overline{\varphi^{k-1}_{m,n}}$, and sum over $1 \leq m, n \leq L$. Then one gets

$$\begin{aligned}
&\sum_{n=1}^{L}\sum_{m=1}^{L}(|\varphi^k_{m,n}|^2 - |\varphi^{k-1}_{m,n}|^2) \leq -(1-\frac{1}{\beta})\sum_{m=1}^{L}\sum_{n=1}^{L}|\varphi^{k-1}_{m,n}|^2 - (\beta-1)\sum_{m=1}^{L}\sum_{n=1}^{L}|\varphi^k_n|^2 \\
&+ \frac{\Delta t}{2\beta}\mathrm{Im}\sum_{n=1}^{L}\left[\overline{(\varphi^{k-1}_{0,n}+\beta\varphi^k_{0,n})}\triangle^+_x(\varphi^{k-1}_{0,n}+\beta\varphi^k_{0,n}) - \overline{(\varphi^{k-1}_{L+1,n}+\beta\varphi^k_{L+1,n})}\triangle^-_x(\varphi^{k-1}_{L+1,n}+\beta\varphi^k_{L+1,n})\right] \\
&+ \frac{\Delta t}{2\beta}\mathrm{Im}\sum_{m=1}^{L}\left[\overline{(\varphi^{k-1}_{m,0}+\beta\varphi^k_{m,0})}\triangle^+_y(\varphi^{k-1}_{m,0}+\beta\varphi^k_{m,0}) - \overline{(\varphi^{k-1}_{m,L+1}+\beta\varphi^k_{m,L+1})}\triangle^-_y(\varphi^{k-1}_{m,L+1}+\beta\varphi^k_{m,L+1})\right].
\end{aligned} \tag{28}$$

Summing up all these inequalities from $k=1$ to K and integrating by parts yield

$$\| \varphi^K \|_2^2 \leq \| \varphi^0 \|_2^2 + \frac{\Delta t}{2\beta}\mathrm{Im}\sum_{m=1}^{4L}\sum_{k=1}^{K}\left[\overline{(\varphi^{k-1}_{J_m}+\beta\varphi^k_{J_m})}(\varphi^{k-1}_{I^1_m}+\beta\varphi^k_{I^1_m}-\varphi^{k-1}_{J_m}-\beta\varphi^k_{J_m})\right], \tag{29}$$

where $k=K$ is the index corresponding to the time of computation $t_K = K\Delta t$.

Let us now determine the sign of the second term appearing in the right-hand side of the above inequality.

Lemma 1. *Let us consider the scheme (18)-(19). Let ρ be a (relatively large) given positive constant and let us set $\beta = e^{\rho\Delta t} > 1$. Then, there exists a time step Δt_0 such that, for $\Delta t \leq \Delta t_0$, one gets*

$$\sum_{m=1}^{4L}\sum_{k=1}^{K}\left[\overline{(\varphi^{k-1}_{J_m}+\beta\varphi^k_{J_m})}(\varphi^{k-1}_{I^1_m}+\beta\varphi^k_{I^1_m}-\varphi^{k-1}_{J_m}-\beta\varphi^k_{J_m})\right] \leq 0. \tag{30}$$

Proof. For $h_{m,n}$ defined by Eq. (25), we can introduce the three following matrices $\mathbf{A}$, $\mathbf{A}^1$ and $\mathbf{B}$ with elements

$$\mathbf{A}_{\ell,l}(z) = h_{I^1_\ell - I_l}(z), \quad \mathbf{A}^1_{\ell,l}(z) = h_{I_\ell - I_l}(z) \quad \text{and} \quad \mathbf{B}_{\ell,l}(z) = h_{J_\ell - I_l}(z). \tag{31}$$

The matrices $\mathbf{A}$ and $\mathbf{B}$ are of size $4L \times (4L-4)$ while $\mathbf{A}^1$ is a $(4L-4)\times(4L-4)$ matrix. Let us now define the vectors

$$\hat{\psi}_{I^1}(z) = [\hat{\psi}_{I^1_1}, \hat{\psi}_{I^1_2}, ...\hat{\psi}_{I^1_{4L}}]^T, \quad \hat{\psi}_J(z) = [\hat{\psi}_{J_1}, \hat{\psi}_{J_2}, ...\hat{\psi}_{J_{4L}}]^T, \quad \hat{\chi}_I(z) = [\hat{\chi}_{I_1}, \hat{\chi}_{I_2}, ...\hat{\chi}_{I_{4L-4}}]^T, \tag{32}$$

where ^{T} denotes the transposition operation. Therefore, the $\mathcal{Z}$-transform of the boundary conditions can be written in the compact form

$$\hat{\psi}_{I^1}(z) = \mathbf{A}(z)\hat{\chi}_I(z), \quad \hat{\psi}_I(z) = \mathbf{A}^1(z)\hat{\chi}_I(z), \quad \hat{\psi}_J(z) = \mathbf{B}(z)\hat{\chi}_I(z). \tag{33}$$

Following these notations, we obtain

$$\begin{aligned}
&\sum_{l=1}^{4L}\sum_{k=1}^{K}\mathrm{Im}\left[\overline{(\varphi^{k-1}_{J_l}+\beta\varphi^k_{J_l})}(\varphi^{k-1}_{I^1_l}+\beta\varphi^k_{I^1_l}-\varphi^{k-1}_{J_l}-\beta\varphi^k_{J_l})\right] \\
&\qquad = \frac{1}{2\pi}\mathrm{Im}\left[\int_0^{2\pi}|1+\beta e^{\iota\phi}|^2\bar{\hat{\psi}}^T_J(\beta e^{\iota\phi})(\hat{\psi}_{I^1}(\beta e^{\iota\phi}) - \hat{\psi}_J(\beta e^{\iota\phi}))d\phi\right] \\
&\qquad = \frac{1}{2\pi}\mathrm{Im}\left[\int_0^{2\pi}|1+\beta e^{\iota\phi}|^2\bar{\hat{\chi}}^T_I(\beta e^{\iota\phi})\bar{\mathbf{B}}^T(\beta e^{\iota\phi})\mathbf{A}(\beta e^{\iota\phi})\hat{\chi}_I(\beta e^{\iota\phi})d\phi\right].
\end{aligned} \tag{34}$$

To conclude, we only need to prove that

$$\mathrm{Im}\left[\bar{\mathbf{V}}^T\bar{\mathbf{B}}^T(\beta e^{\iota\phi})\mathbf{A}(\beta e^{\iota\phi})\mathbf{V}\right] \leq 0, \tag{35}$$

for any $\phi \in [0, 2\pi]$ and $\mathbf{V} \in \mathbb{C}^{4L-4}$. The analysis is stated by considering three cases for ϕ.

By definition [16]

$$g_{m,n}(t) = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(mx)\cos(ny)e^{-i(4-2\cos(x)-2\cos(y))t}dxdy \tag{36}$$

and by using the definition of $\mathcal{Z}$- transform, we obtain

$$\begin{aligned}\hat{g}_{m,n}(\beta e^{\iota\phi}) &= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(mx)\cos(ny)\sum_{j=0}^{\infty}e^{-K_0(x,y)j\triangle t}/(e^{(\rho\triangle t+\iota\phi)})^j dxdy \\ &= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(mx)\cos(ny)\frac{e^{(K_0(x,y)+\rho)\triangle t+\iota\phi}}{e^{(K_0(x,y)+\rho)\triangle t+\iota\phi}-1}dxdy,\end{aligned} \tag{37}$$

with $K_0(x,y) := 2\iota(2-\cos(x)-\cos(y))$. We set $\alpha = \rho^3$ and $z = \beta e^{\iota\phi}$.

Case 1: $\alpha\Delta t \leq \phi \leq \pi - \alpha\Delta t$ **or** $\pi + \alpha\Delta t \leq \phi \leq 2\pi - \alpha\Delta t$**.** Let us first write the following expansions

$$\begin{aligned}\left(\hat{g}^e_{0,0}(z) - \frac{1}{2}\right)\boldsymbol{A} &= \boldsymbol{A}_0 + \boldsymbol{A}_1\Delta t + \boldsymbol{R}_1\Delta t^2, \\ \left(\bar{\hat{g}}^e_{0,0}(z) - \frac{1}{2}\right)\bar{\boldsymbol{B}}^T &= \bar{\boldsymbol{B}_1}^T\Delta t + \bar{\boldsymbol{B}_2}^T\Delta t^2 + \boldsymbol{R}_2\Delta t^3.\end{aligned} \tag{38}$$

The four matrices $\boldsymbol{A}_0$, $\boldsymbol{A}_1$, $\bar{\boldsymbol{B}_1}^T$ and $\bar{\boldsymbol{B}_2}^T$ are computed explicitly below. The two residual terms $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ then must be estimated to be controlled. Therefore, one gets

$$\begin{aligned}\left|\hat{g}^e_{0,0}(z) - \frac{1}{2}\right|^2\bar{\boldsymbol{B}}^T\boldsymbol{A} &= \bar{\boldsymbol{B}_1}^T\boldsymbol{A}_0\Delta t + (\boldsymbol{B}_1^T\boldsymbol{A}_1 + \boldsymbol{B}_2^T\boldsymbol{A}_0)\Delta t^2 \\ &+(\boldsymbol{R}_2\boldsymbol{A}_0 + \boldsymbol{B}_1^T\boldsymbol{R}_1 + \boldsymbol{B}_2^T\boldsymbol{A}_1)\Delta t^3 + (\boldsymbol{B}_2^T\boldsymbol{R}_1 + \boldsymbol{R}_2\boldsymbol{A}_1)\Delta t^4 + \boldsymbol{R}_2\boldsymbol{R}_1\Delta t^5.\end{aligned} \tag{39}$$

Now, because the coefficients of $\boldsymbol{A}$ and $\boldsymbol{B}$ are given through $h_{m,n}(z)$ by expressions (31) which are related to $\hat{g}^e_{m,n}(z)$ by Eq. (25), we must derive an expansion of $\hat{g}_{m,n}(\beta e^{\iota\phi})$ thanks to Δt. To this end, let us compute the Taylor's expansion

$$\begin{aligned}\frac{e^{(K_0+\rho)\triangle t+\iota\phi}}{e^{(K_0+\rho)\triangle t+\iota\phi}-1} &= -\frac{\iota}{2}\cot(\frac{\phi}{2}) + \frac{1}{2} + (K_0+\rho)\frac{\Delta t}{4\sin^2(\frac{\phi}{2})} \\ &+(K_0+\rho)^2\iota\frac{\cot(\frac{\phi}{2})}{8\sin^2(\frac{\phi}{2})}\Delta t^2 - (K_0+\rho)^3\frac{\cos(\phi)+2}{48\sin^4(\frac{\phi}{2})}\Delta t^3(1+\mathcal{O}(\frac{\rho}{\alpha})).\end{aligned} \tag{40}$$

Plugging (40) into the expression (37) needs the computation of the following integrals

$$\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(mx)\cos(ny)(K_0(x,y)+\rho)dxdy = (\rho+4\iota)\delta_{0,0} - \iota\delta_{1,0} - \iota\delta_{0,1} \tag{41}$$

and

$$\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(mx)\cos(ny)(K_0(x,y)+\rho)^2dxdy = (\rho^2+8\iota\rho-20)\delta_{0,0} \\ -\delta_{2,0}-\delta_{0,2}+(8-2\iota\rho)\delta_{0,1}+(8-2\iota\rho)\delta_{1,0}-2\delta_{1,1}. \tag{42}$$

The matrices $\boldsymbol{A}_0$, $\boldsymbol{A}_1$, $\boldsymbol{B}_1$, $\boldsymbol{B}_2$ are given from expressions (95) to (99) of the Appendix. Let us analyze the expansion (39) and its effect on stating the inequality (35) for Case 1.

First, since $\bar{\boldsymbol{B}}_1{}^T\boldsymbol{A}_0$ is given by a real-valued diagonal matrix, it does not contribute to (35). Next, the diagonal elements of $(\boldsymbol{B}_1^T\boldsymbol{A}_1+\boldsymbol{B}_2^T\boldsymbol{A}_0)$ are given by

$$-\frac{\rho\cot^2(\frac{\phi}{2})}{8\sin^2(\frac{\phi}{2})}\iota-\frac{3}{2}\frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})} \qquad \text{or} \qquad -\frac{\rho\cot^2(\frac{\phi}{2})}{16\sin^2(\frac{\phi}{2})}\iota-\frac{3}{4}\frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})},$$

the off-diagonal elements consisting in terms $\cot^4(\phi/2)^4$ and $\cot^2(\phi/2)\sin^{-2}(\phi/2)$ multiplied by real-valued constants. Therefore, only the imaginary part of the diagonal elements of $(\boldsymbol{B}_1^T\boldsymbol{A}_1+\boldsymbol{B}_2^T\boldsymbol{A}_0)$ contribute to the inequality (35). Concerning $(\boldsymbol{R}_2\boldsymbol{A}_0+\boldsymbol{B}_1^T\boldsymbol{R}_1+\boldsymbol{B}_2^T\boldsymbol{A}_1)\Delta t^3$, an analysis shows that its coefficients satisfy

$$\left|\frac{\cos(\frac{\phi}{2})}{\sin^5(\frac{\phi}{2})}\mathcal{O}(\rho^3)\Delta t^3\right| = \left|\frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})}\mathcal{O}(\rho^3)\frac{\Delta t^3}{\sin(\phi)}\right| \leq \frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})}\frac{\mathcal{O}(\rho^3)}{\alpha}\Delta t^2. \tag{43}$$

Finally, the order of the coefficients of $\mid(\boldsymbol{B}_2^T\boldsymbol{R}_1+\boldsymbol{R}_2^T\boldsymbol{A}_1)\Delta t^4\mid$ is at most

$$\frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})}\frac{\mathcal{O}(\rho^4)}{\alpha^2}\Delta t^2$$

while the order of the elements of $\mid\boldsymbol{R}_2^T\boldsymbol{R}_1\Delta t^5\mid$ is

$$\frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})}\frac{\mathcal{O}(\rho^5)}{\alpha^3}\Delta t^2.$$

From the above discussion, if ρ is large enough and Δt small enough, we have, for any vector $\mathbf{V}\in\mathbb{C}^{4L-4}$,

$$\left|\hat{g}^e_{0,0}(z)-\frac{1}{2}\right|^2\mathrm{Im}\left[\bar{\mathbf{V}}^T\bar{\boldsymbol{B}}^T\boldsymbol{A}\mathbf{V}\right] \leq -\frac{\rho}{16}\frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})}\Delta t^2\left|\mathbf{V}\right|^2 \\ +\frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})}\Delta t^2\left(\mathcal{O}(\frac{\rho^3}{\alpha})+\mathcal{O}(\frac{\rho^4}{\alpha^2})+\mathcal{O}(\frac{\rho^5}{\alpha^3})\right)\left|\mathbf{V}\right|^2\leq 0. \tag{44}$$

Case 2: $-\alpha\Delta t \le \phi \le \alpha\Delta t$**.** Any angle ϕ can be written as $\phi = \phi_{\Delta t}\Delta t$, where $-\alpha \le \phi_{\Delta t} \le \alpha$. When $\Delta t \to 0$, we can write

$$\begin{aligned}&\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(mx)\cos(ny)\sum_{j=0}^{\infty}e^{-K_0(x,y)j\triangle t}/(e^{(\rho+\iota\phi_{\Delta t})\Delta t})^j\Delta t dxdy - \frac{1}{2}\delta_{0,0}\Delta t + \frac{\iota}{4}\delta_{0,1}\Delta t^2\\ &= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{\cos(mx)\cos(ny)}{\rho+\iota\phi_{\Delta t}+K_0(x,y)}dxdy + \mathcal{O}(\Delta t^2) = \frac{1}{2\iota}W(m,n,\frac{\rho+\iota\phi_{\Delta t}}{2\iota}+2) + \mathcal{O}(\Delta t^2)\end{aligned} \tag{45}$$

uniformly for $-\alpha\Delta t \le \phi \le \alpha\Delta t$, with an error $\mathcal{O}(\Delta t^2)$.

Now for ρ large enough, there exists Δt_0 such that if $\Delta t \le \Delta t_0$ and $I_m^1 - I_n = (k,\ell)$, we have

$$W(m,n,\frac{\rho+\iota\phi_{\Delta t}}{2\iota}+2) \sim \frac{1}{2^{k+\ell}}C_{k+\ell}^k(\frac{2\iota}{\rho+\iota(\phi_{\Delta t}+4)})^{k+\ell+1}\left(1+\mathcal{O}\left(\frac{1}{\rho+\iota(\phi_{\Delta t}+4)}\right)\right).$$

Let us define $\mathbf{I}$ as the $(4L-4)\times(4L-4)$ unitary matrix. Then we have

$$\Delta t\Big(\hat{g}_{0,0}^e(z)-\frac{1}{2}\Big)\mathbf{A} = \frac{1}{\rho+\iota(\phi_{\Delta t}+4)}\mathbf{I}_1(\mathbf{I}+\mathcal{O}(\frac{1}{\rho+\iota(\phi_{\Delta t}+4)})) + \mathcal{O}(\Delta t^2) \tag{46}$$

and

$$\Delta t\Big(\hat{g}_{0,0}^e(z)-\frac{1}{2}\Big)\mathbf{B} = \frac{\iota}{(\rho+\iota(\phi_{\Delta t}+4))^2}\mathbf{I}_1(\mathbf{I}+\mathcal{O}(\frac{1}{\rho+\iota(\phi_{\Delta t}+4)})) + \mathcal{O}(\Delta t^2). \tag{47}$$

Since $\mathbf{I}_1^T\mathbf{I}_1 = \mathbf{I}_2$, where $\mathbf{I}_2$ is given by formula (100) in the Appendix, then one gets

$$\Delta t^2\Big|\hat{g}_{0,0}^e(z)-\frac{1}{2}\Big|^2\bar{\mathbf{B}}^T\mathbf{A} = \frac{-\iota\rho+(4+\phi_{\Delta t})}{((\phi_{\Delta t}+4)^2+\rho^2)^2}(\mathbf{I}_2+\mathcal{O}(\frac{1}{\rho+\iota(\phi_{\Delta t}+4)})) + \mathcal{O}(\Delta t^2), \tag{48}$$

and finally $\mathrm{Im}\left[\bar{\mathbf{V}}^T\bar{\mathbf{B}}^T\mathbf{A}\mathbf{V}\right] \le 0$.

Case 3: $\pi - \alpha\Delta t \le \phi \le \pi + \alpha\Delta t$**.** Let us assume that: $\phi = \pi + \Delta t\phi_{\Delta t}$. If we take

$$K_1 = K_0 + \rho + \iota\phi_{\Delta t} \quad \text{and} \quad K_2 = \rho + \iota(4+\phi_{\Delta t}),$$

then we can write

$$\begin{aligned}&\hat{g}_{m,n}(e^{\rho\Delta t+\phi\iota}) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(mx)\cos(ny)\sum_{j=0}^{\infty}e^{-K_0 j\triangle t}/(e^{(\rho+\iota\phi_{\Delta t})\Delta t})^j(-1)^j dxdy\\ &= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(mx)\cos(ny)\frac{1}{1+e^{-K_1\Delta t}}dxdy = \frac{1}{2}\delta_{0,0} + (\frac{K_2}{4})\delta_{0,0}\Delta t - \frac{\iota}{4}\delta_{0,1}\Delta t\\ &-\frac{\iota}{4}\delta_{1,0}\Delta t - (K_2^3\delta_{0,0} - 3K_2\delta_{0,2} - 3K_2\delta_{2,0} + \iota\delta_{3,0} + \iota\delta_{0,3} + \iota(9-3K_2^2)\delta_{1,0}\\ &+\iota(9-3K_2^2)\delta_{0,1} + 3\iota\delta_{1,2} + 3\iota\delta_{2,1} - 6K_2\delta_{1,1} - 12K_2)\frac{\Delta t^3}{48} + \mathcal{O}(\Delta t^4),\end{aligned} \tag{49}$$

which means that

$$\Big(\hat{g}_{0,0}^e(z)-\frac{1}{2}\Big)\mathbf{A} = \Delta t\frac{K_2}{4}\mathbf{I}_1 + \mathcal{O}(\Delta t^2) \tag{50}$$

and

$$\Big(\hat{g}_{0,0}^e(z)-\frac{1}{2}\Big)\mathbf{B} = \Delta t^3\Big(\frac{\iota K_2^2}{16}\mathbf{I}_1 + \mathcal{O}(1)\Big) + \mathcal{O}(\Delta t^4). \tag{51}$$

This leads to

$$\left|\hat{g}^e_{0,0}(z)-\frac{1}{2}\right|^2\bar{\mathbf{B}}^T\mathbf{A}=-\Delta t^4(\rho^2+(4+\phi_{\Delta t})^2)\frac{\iota K_2}{64}\Big(\mathbf{I}_2+\mathcal{O}(\frac{1}{\rho})\Big)+\mathcal{O}(\Delta t^5). \tag{52}$$

In this case, for any small enough Δt, we have : $\mathrm{Im}\left[\bar{\mathbf{V}}^T\bar{\mathbf{B}}^T\mathbf{A}\mathbf{V}\right]\leq 0$.

Collecting the results from the three above cases, we conclude that

$$\mathrm{Im}\sum_{l=1}^{4L}\sum_{k=1}^{K}\left[\overline{(\varphi^{k-1}_{J_l}+\beta\varphi^k_{J_l})}(\varphi^{k-1}_{I^1_l}+\beta_1\varphi^k_{I^1_l}-\varphi^{k-1}_{J_l}-\beta_1\varphi^k_{J_l})\right]\leq 0. \tag{53}$$

□

By using the previous inequality, we can state the following L^2-stability result.

Theorem 1. *For the scheme (18)-(19), if ρ is a given and large enough positive constant, then there exists Δt_0 such that, if $\Delta t\leq\Delta t_0$ and $T_K=K\Delta t$,*

$$\parallel\psi^K\parallel_2\leq e^{\rho T_K}\parallel\psi^0\parallel_2. \tag{54}$$

Proof. From $\parallel\varphi^K\parallel_2^2\leq\parallel\varphi^0\parallel_2^2$, we have: $e^{-\rho K\Delta t}\parallel\psi^K\parallel_2\leq\parallel\psi^0\parallel_2$ which gives (54). □

5 Error analysis of the scheme

For two analytic functions $u(t)$ and $v(t)$, we have the following equalities, by using iterated integration by parts,

$$\begin{aligned}
(u\star v)^k&=\int_0^{k\Delta t}u(s)v(k\Delta t-s)ds-\frac{1}{2}\int_0^{\Delta t}\sum_{l=0}^{k-1}(u(\cdot)v(k\Delta t-\cdot))''(s+l\Delta t)s(s-\Delta t)ds\\
&=\int_0^{k\Delta t}u(s)v(k\Delta t-s)ds-\frac{1}{4}\int_0^{\Delta t}(u(\cdot)v(k\Delta t-\cdot))''(s)s(s-\Delta t)ds\\
&\quad+\frac{1}{4}\int_0^{\Delta t}(u(\cdot)v(k\Delta t-\cdot))''(k\Delta t+s)s(s-\Delta t)ds\\
&\quad-\frac{1}{2}\int_0^{\Delta t}\int_0^{k\Delta t}(u(\cdot)v(k\Delta t-\cdot))''(s+\tau)d\tau s(s-\Delta t)ds\frac{1}{\Delta t}\\
&\quad+\frac{1}{4}\int_0^{\Delta t}(\int_0^{k\Delta t}(u(\cdot)v(k\Delta t-\cdot))''''(s+\tau)\tau(\tau-k\Delta t)d\tau)s(s-\Delta t)ds\frac{1}{\Delta t}\\
&=(u*v)(k\Delta t)+r(k\Delta t,\Delta t)\Delta t^2,
\end{aligned} \tag{55}$$

for $k\geq 0$, where

$$\begin{aligned}
r(t,\Delta t)&=-\frac{\Delta t}{4}\int_0^1(u(\cdot)v(t-\cdot))''(s\Delta t)s(s-1)ds+\frac{\Delta t}{4}\int_0^1(u(\cdot)v(t-\cdot))''(t+s\Delta t)s(s-1)ds\\
&\quad-\frac{1}{2}\int_0^1\int_0^t(u(\cdot)v(t-\cdot))''(s\Delta t+\tau)d\tau s(s-1)ds\\
&\quad+\frac{1}{4}\int_0^1(\int_0^t(u(\cdot)v(t-\cdot))''''(s\Delta t+\tau)\tau(\tau-t)d\tau)s(s-1)ds
\end{aligned} \tag{56}$$

has a series expansion thanks to Δt, with coefficients which are analytic functions with respect to t. For any analytic functions $u_1(t)$,..., $u_n(t)$, by induction, one has

$$(u_n \star ...(u_3 \star (u_2 \star u_1))...)^k = (u_n * ...(u_3 * (u_2 * u_1))...)(k\Delta t) + r_n(k\Delta t, \Delta t)\Delta t^2. \tag{57}$$

Let us now state the following lemma.

Lemma 2. *If ρ is a given and large enough positive real-valued constant, then there exists Δt_0, such that, for any $\Delta t \leq \Delta t_0$, for any angle ϕ and $z = e^{\rho\Delta t + \iota\phi}$, one gets, for $1 \leq m, n \leq L$, the representation*

$$\hat{f}^e_{m,n}(z) = \hat{f}_{m,n}(z) + \frac{\hat{r}_{m,n}(z, \Delta t)}{\hat{g}^e_{0,0}(z) - \frac{1}{2}}\Delta t, \tag{58}$$

where $r_{m,n}(t, \Delta t)$ is an analytic function such that there exists a constant $C_{m,n,\rho}$ with

$$\left| \frac{\hat{r}_{m,n}(z, \Delta t)}{\hat{g}^e_{0,0}(z) - \frac{1}{2}} \right| \leq C_{m,n,\rho}. \tag{59}$$

We also have

$$|h_{m,n}(z)| \leq C_{m,n,\rho}. \tag{60}$$

Proof. By using the representation given by Eq. (55) we have

$$g^e_{m,n}(k\Delta t) = (f^e_{m,n} * g^e_{0,0})(k\Delta t) = (f^e_{m,n} \star g^e_{0,0})^k + r_{m,n}(k\Delta t, \Delta t)\Delta t^2,$$

which leads to

$$\hat{f}^e_{m,n}(z) = \frac{\hat{g}^e_{m,n}(z) + \hat{g}^e_{0,0}(z) f^e_{m,n}(0)\frac{\Delta t}{2}}{(\hat{g}^e_{0,0}(z) - \frac{1}{2})\Delta t} + \frac{\hat{r}_{m,n}(z, \Delta t)}{\hat{g}^e_{0,0}(z) - \frac{1}{2}}\Delta t$$

which is nothing else than Eq. (58) since we have the representation (23) for $\hat{f}_{m,n}(z)$.

Now, let $u(t)$ be a real analytic function such that its Laplace transform $\tilde{u}(s)$ is analytic at $s = \infty$ and can be written as $\tilde{u}(s) = \sum_{k=1}^{\infty} u_k s^{-k}$. Let us remark here that $g_{m,n}(t)$ and $r_{m,n}(t, \Delta t)$ fullfil these properties. Let us consider η and ρ as two large enough real-valued constants, with $\rho > \eta$, and $z = e^{\rho\Delta t + \iota\phi}$. Then we have

$$\begin{aligned} \hat{u}(z) - \frac{u(0)}{2} &= \frac{1}{2\pi\iota}\int_{\eta-\iota\infty}^{\eta+\iota\infty} \sum_{k=0}^{\infty} \tilde{u}(s)\frac{e^{sk\Delta t}}{z^k} ds - \frac{u(0)}{2} = \frac{1}{4\pi\iota}\int_{\eta-\iota\infty}^{\eta+\iota\infty} \sum_{k=0}^{\infty} \frac{u_k}{s^{k+1}} \frac{1 + e^{-(\rho-s)\Delta t - \iota\phi}}{1 - e^{-(\rho-s)\Delta t - \iota\phi}} ds \\ &= \frac{1}{2}\sum_{k=0}^{\infty} \frac{1}{k!}\frac{d^k}{ds^k}\left(\frac{1 + e^{s-\rho\Delta t - \iota\phi}}{1 - e^{s-\rho\Delta t - \iota\phi}}\right)_{s=0} u_k \Delta t^k. \end{aligned} \tag{61}$$

Some computations show that, for any $l \geq 1$, we have

$$\frac{\Delta t^l}{2}\frac{1}{l!}\frac{d^l}{ds^l}\left(\frac{1 + e^{s-\rho\Delta t - \iota\phi}}{1 - e^{s-\rho\Delta t - \iota\phi}}\right)_{s=0} = \frac{\Delta t^l}{2}\sum_{m=1}^{l} \frac{(e^{-\rho\Delta t - \iota\phi})^m}{(1 - e^{-\rho\Delta t - \iota\phi})^{m+1}} \sum_{|\alpha|=l, \alpha_i \geq 1} \frac{1}{\alpha!}, \tag{62}$$

setting $|\alpha| := \sum_{i=1}^m \alpha_i$ and $\alpha! := \alpha_1!...\alpha_m!$, for a multi-index $\alpha := (\alpha_1, ..., \alpha_m)$. In addition, one gets

$$\begin{aligned}\sum_{|\alpha|=l,\alpha_i\geq 1} \frac{1}{\alpha!} \leq \sum_{|\alpha|=l} \frac{1}{\alpha!} &= \frac{1}{2\pi\iota} \oint_{|z|=1} \frac{1}{z^{l+1}}(1 + z + \frac{z^2}{2!} + ...)^m dz \\ &= \frac{1}{2\pi\iota} \oint_{|z|=1} \frac{1}{z^{l+1}} e^{mz} dz = \frac{1}{2\pi} \int_0^{2\pi} e^{me^{\iota\theta} - \iota(l-1)\theta} d\theta \leq e^m.\end{aligned} \tag{63}$$

Case 1. $\pi - \alpha\Delta t \leq \phi \leq \pi + \alpha\Delta t$**.** Let us introduce $\phi = \pi + \phi_{\Delta t}\Delta t$ and take $\alpha = \rho^3$ as in the previous section. For Δt small enough and from the inequalities (62)-(63), we have

$$\frac{\Delta t^l}{2} \frac{1}{l!} \frac{d^l}{ds^l} \left(\frac{1 + e^{s-\rho\Delta t-\iota\phi}}{1 - e^{s-\rho\Delta t-\iota\phi}} \right)_{s=0} \leq \frac{\Delta t^l}{2} \sum_{m=1}^{l} \frac{(e^{-\rho\Delta t})^m}{|1 + e^{-\rho\Delta t-\iota\phi_{\Delta t}\Delta t}|^{m+1}} e^m \leq C_l (e\Delta t)^l. \tag{64}$$

Now, taking $\hat{u}(z) := \hat{r}_{m,n}(z, \Delta t)$ in Eq. (61) (with $z = e^{\rho\Delta t+\iota\phi}$), using Eqs. (62)-(63) and noticing that $r_{m,n}(0, \Delta t) = 0$ (by setting $t = 0$ in Eq. (56)) leads to

$$|\hat{r}_{m,n}(z, \Delta t)| \leq \sum_{k=1}^{\infty} C_k (e\Delta t)^k r_{m,n}(k\Delta t, \Delta t) = \mathcal{O}(\Delta t). \tag{65}$$

In addition, a direct computation yields

$$\begin{aligned}\hat{g}^e_{0,0}(e^{\rho\Delta t+\iota\phi}) - \frac{1}{2} &= \frac{1}{2} \frac{1 - e^{-\rho\Delta t-\iota\phi_{\Delta t}\Delta t}}{1 + e^{-\rho\Delta t-\iota\phi_{\Delta t}\Delta t}} - \frac{2e^{-\rho\Delta t-\iota\phi_{\Delta t}\Delta t}}{(1 + e^{-\rho\Delta t-\iota\phi_{\Delta t}\Delta t})^2} \Delta t + \mathcal{O}(\Delta t^2) \\ &= \Big(\frac{\rho + \iota\phi_{\Delta t}}{4} - 1 \Big) \Delta t + \mathcal{O}(\Delta t)^2,\end{aligned} \tag{66}$$

giving then the inequality (59).

Case 2. $-\alpha\Delta t \leq \phi \leq \alpha\Delta t$**.** We again set: $\phi = \Delta t\phi_{\Delta t}$. For small enough Δt and by using (62)-(63), we obtain

$$\begin{aligned}&\left| \frac{\Delta t^l}{2} \frac{1}{l!} \frac{d^l}{ds^l} \left(\frac{1 + e^{s-\rho\Delta t-\iota\phi}}{1 - e^{s-\rho\Delta t-\iota\phi}} \right)_{s=0} \right| \leq \frac{\Delta t^l}{2} \sum_{m=1}^{l} \left| \frac{(e^{-\rho\Delta t})^m}{(1 - e^{-\rho\Delta t-\iota\phi})^{m+1}} \right| \sum_{|\alpha|=l,\alpha_i\geq 1} \frac{1}{\alpha!} \\ &\leq C_l \frac{1}{|1 - e^{-\rho\Delta t-\iota\phi_{\Delta t}\Delta t}|} \sum_{m=1}^{l} (\frac{e}{|\rho + \phi_{\Delta t}|})^m \Delta t^{l-m} \leq C_l \frac{1}{|1 - e^{-\rho\Delta t-\iota\phi_{\Delta t}\Delta t}|} \left(\frac{e}{|\rho + \phi_{\Delta t}|} \right)^l,\end{aligned} \tag{67}$$

which means

$$\hat{r}_{m,n}(e^{\rho\Delta t+\iota\phi}, \Delta t) = \frac{1}{1 - e^{-\rho\Delta t-\iota\phi}} \left(\dot{r}_{m,n}(0, \Delta t)\mathcal{O}(\frac{1}{\rho + |\phi_{\Delta t}|}) + \mathcal{O}(\frac{1}{|\rho + \phi_{\Delta t}|^2}) \right).$$

We use $\dot{r}_{m,n}(z, \Delta t)$ to denote the first-order derivative of $r_{m,n}(z, \Delta t)$ with respective to z.

We also have

$$\hat{g}^e_{0,0}(e^{\rho\Delta t+\iota\phi}) - \frac{1}{2} = \frac{1}{1 - e^{-\rho\Delta t-\iota\phi}} \left(\frac{(1 + e^{-\rho\Delta t-\iota\phi})}{2} + \mathcal{O}(\frac{1}{\rho + |\phi_{\Delta t}|}) \right),$$

leading to (59).

Case 3. $\alpha\Delta t \leq \phi \leq \pi - \alpha\Delta t$ **or** $\pi + \alpha\Delta t \leq \phi \leq 2\pi - \alpha\Delta t$**.** From the inequality (with $\alpha = \rho^3$)

$$\left|\frac{\Delta t}{1-e^{-\rho\Delta t-\iota\phi}}\right| = \left|\frac{\Delta t}{1-e^{-\iota\phi}}\right| \left|\left(1+\frac{e^{-\iota\phi}(1-e^{-\rho\Delta t})}{1-e^{-\iota\phi}}\right)^{-1}\right| \leq C\frac{1}{\alpha}(1+\mathcal{O}(\frac{\rho}{\alpha})) \leq \frac{C}{\alpha}, \tag{68}$$

we deduce that

$$\begin{aligned}\left|\frac{\Delta t^l}{2}\frac{1}{l!}\frac{d^l}{ds^l}\left(\frac{1+e^{s-\rho\Delta t-\iota\phi}}{1-e^{s-\rho\Delta t-\iota\phi}}\right)_{s=0}\right| &= \frac{\Delta t^l}{2}\sum_{m=1}^{l}\left|\frac{(e^{-\rho\Delta t-\iota\phi})^m}{(1-e^{-\rho\Delta t-\iota\phi})^{m+1}}\right| \sum_{|\alpha|=l,\alpha_i\geq 1}\frac{1}{\alpha!} \\ &\leq C\frac{1}{|1-e^{-\rho\Delta t-\iota\phi}|}\sum_{m=1}^{l}\frac{C_m}{\alpha^m}\Delta t^{l-m} \leq \frac{1}{|1-e^{-\rho\Delta t-\iota\phi}|}\frac{CC_l}{\alpha^l},\end{aligned} \tag{69}$$

which means

$$\hat{r}_{m,n}(e^{\rho\Delta t+\iota\phi},\Delta t) = \frac{1}{1-e^{-\rho\Delta t-\iota\phi}}\left(\frac{\dot{r}_{m,n}(0,\Delta t)e^{-\rho\Delta t-\iota\phi}\Delta t}{2(1-e^{-\rho\Delta t-\iota\phi})} + \mathcal{O}(\frac{1}{\alpha^2})\right).$$

Furthermore, we also have

$$\hat{g}^e_{0,0}(e^{\rho\Delta t+\iota\phi}) - \frac{1}{2} = \frac{1}{1-e^{-\rho\Delta t-\iota\phi}}\left(\frac{(1+e^{-\rho\Delta t-\iota\phi})}{2} + \mathcal{O}(\frac{1}{\alpha})\right),$$

finally leading to (59).

Concerning the inequality (60), a similar proof can be adapted, starting from the definition of $h_{m,n}$ given by Eq. (25).

□

Let now us introduce the following indices: $N^1_{m,n} = I_m - I_n$ and $N^2_{m,n} = J_m - I_n$. We also define I^k_1, I^k_2, ...I^k_{4L-5} as the ordered indices I_1, I_2 ... I_{4L-4} excluding the k-th one ($1 \leq k \leq 4L-4$). Finally, let us set $N^{1,k,l}_{m,n} = I^k_m - I^l_n$.

From the boundary condition (17), we have by Laplace transform

$$\begin{aligned}\tilde{\psi}^e_{I_m}(s) &= \sum_{n=1}^{4L-4}\tilde{f}^e_{I_m-I_n}(s)\tilde{\chi}^e_{I_n}(s), \qquad 1 \leq m \leq 4L-4, \\ \tilde{\psi}^e_{J_m}(s) &= \sum_{n=1}^{4L-4}\tilde{f}^e_{J_m-I_n}(s)\tilde{\chi}^e_{I_n}(s), \qquad 1 \leq m \leq 4L.\end{aligned} \tag{70}$$

We define $\mathbf{A}^{1,e}$ as the $(4L-4)\times(4L-4)$ matrix such that the (m,n)-th matrix element of $\mathbf{A}^{1,e}$ is $f^e_{N^1_{m,n}}$. In a similar way, $\mathbf{B}^e$ is a $4L\times(4L-4)$ matrix such that its (m,n)-th element is equal to $f^e_{N^2_{m,n}}$. As a consequence, system (70) leads to

$$\tilde{\psi}^e_J = \tilde{\mathbf{B}}^e(\tilde{\mathbf{A}}^{1,e})^{-1}\tilde{\psi}^e_I = \tilde{\mathbf{F}}^e\tilde{\psi}^e_I. \tag{71}$$

(The inversion of the matrix $\tilde{\mathbf{A}}^{1,e}$ can be obtained from the expression (10).) Let us denote by σ_{4L-5} the set of all permutations of the indices 1 to $4L-5$, an element of the set being written as $\mathrm{i} := (i_1, i_2, ..., i_{4L-5}) \in \sigma_{4L-5}$. Following Cramer's rule, for $1 \leq l \leq 4L$, one can write that

$$\begin{aligned}\tilde{\psi}^e_{J_l} &= \sum_{1\leq m,n\leq 4L-4} (\tilde{\mathbf{B}}^e)_{l,m}((\tilde{\mathbf{A}}^{1,e})^{-1})_{m,n}\tilde{\psi}^e_{I_n} \\ &= \sum_{1\leq m,n\leq 4L-4} \tilde{\psi}^e_{I_n} \frac{1}{\det(\tilde{\mathbf{A}}^{1,e})} \tilde{f}^e_{N^2_{l,m}} (-1)^{m+n} \sum_{\mathrm{i}\in\sigma_{4L-5}} \delta^{\mathrm{i}} \prod_{p=1}^{4L-5} \tilde{f}^e_{N^{1,n,m}_{p,i_p}},\end{aligned} \tag{72}$$

where δ^{i} is the signature of the permutation for a given index $\mathrm{i} \in \sigma_{4L-5}$. Let us now define σ^0_{4L-4} as the set σ_{4L-4} excluding $(1, 2, ..., 4L-4)$. Multiplying by $\det(\tilde{\mathbf{A}}^{1,e})$ on both sides of Eq. (72), then inverting by Laplace transform, one has

$$\begin{aligned}&\psi^e_{J_l} + \sum_{\mathrm{j}\in\sigma^0_{4L-4}} \delta^{\mathrm{j}} f^e_{h^1_{1,j_1}} * (... * (f^e_{N^1_{4L-4,j_{4L-4}}} * \psi^e_{J_l})...) \\ &= \sum_{1\leq m,n\leq 4L-4} f^e_{N^2_{l,m}} (-1)^{m+n} * (\sum_{\mathrm{i}\in\sigma_{4L-5}} \delta^{\mathrm{i}} f^e_{N^{1,n,m}_{1,i_1}} * (...(f^e_{N^{1,n,m}_{4L-5,i_{4L-5}}} * \psi^e_{I_n})...)).\end{aligned} \tag{73}$$

From Eq. (73) and by using (57), one gets

$$\begin{aligned}&(\psi^e_{J_l})^k + \sum_{\mathrm{j}\in\sigma^0_{4L-4}} \delta^{\mathrm{j}} [f^e_{N^1_{1,j_1}} \star (... \star (f^e_{N^1_{4L-4,j_{4L-4}}} \star \psi^e_{J_l})...)]^k \\ &= \sum_{1\leq m,n\leq 4L-4} [f^e_{N^2_{l,m}} (-1)^{m+n} \star (\sum_{\mathrm{i}\in\sigma_{4L-5}} \delta^{\mathrm{i}} f^e_{N^{1,n,m}_{1,i_1}} \star (...(f^e_{N^{1,n,m}_{4L-5,i_{4L-5}}} \star \psi^e_{I_n})...))]^k + H_l(k\Delta t, \Delta t)\Delta t^2,\end{aligned} \tag{74}$$

where $H_l(t, \Delta t)$ is an analytic function of t and Δt which can be expanded thanks to Δt, the coefficients being some analytic functions of t. From the relation

$$\widehat{(u \star v)}(z) = \hat{u}(z)\hat{v}(z)\Delta t - \hat{u}(z)\frac{v^0}{2}\Delta t - \hat{v}(z)\frac{u^0}{2}\Delta t,$$

and applying a $\mathcal{Z}$-transform on both sides of Eq. (74) leads to

$$\begin{aligned}&\hat{\psi}^e_{J_l}(z) + \hat{\psi}^e_{J_l}(z) \sum_{\mathrm{j}\in\sigma^0_{4L-4}} \delta^{\mathrm{j}} \prod_{p=1}^{4L-4} \left(\hat{f}^e_{h^1_{p,j_p}}(z)\Delta t - f^e_{h^1_{p,j_p}}(0)\Delta t/2 \right) \\ &= \sum_{1\leq m,n\leq 4L-4} \hat{\psi}^e_{I_n}(z) \left(\hat{f}^e_{h^2_{l,m}}(z)\Delta t - f^e_{h^2_{l,m}}(0)\Delta t/2 \right) (-1)^{m+n} \\ &\quad \sum_{\mathrm{i}\in\sigma_{4L-5}} \delta^{\mathrm{i}} \prod_{p=1}^{4L-5} \left(\hat{f}^e_{h^{1,n,m}_{p,i_p}}(z)\Delta t - \hat{f}^e_{h^{1,n,m}_{p,i_p}}(0)\Delta t/2 \right) + \hat{H}_l(z, \Delta t)\Delta t^2.\end{aligned} \tag{75}$$

Now, thanks to (58), one has

$$\begin{aligned}
&\hat{\psi}^e_{J_l}(z) + \hat{\psi}^e_{J_l}(z) \sum_{\mathrm{j}\in\sigma^0_{4L-4}} \delta^{\mathrm{j}} \prod_{p=1}^{4L-4} \left(\hat{f}_{h^1_{p,j_p}}(z)\Delta t - f^e_{h^1_{p,j_p}}(0)\Delta t/2 \right) \\
&= \sum_{1\le m,n\le 4L-4} \hat{\psi}^e_{I_n}(z) \left(\hat{f}_{h^2_{l,m}}(z)\Delta t - f^e_{h^2_{l,m}}(0)\Delta t/2 \right) (-1)^{m+n} \\
&\quad \sum_{\mathrm{i}\in\sigma_{4L-5}} \delta^{\mathrm{i}} \prod_{p=1}^{4L-5} \left(\hat{f}_{h^{1,n,m}_{p,i_p}}(z)\Delta t - \hat{f}_{h^{1,n,m}_{p,i_p}}(0)\Delta t/2 \right) \\
&+ (\sum_{1\le m,n\le 4L-4} G_{1,l,m,n}(z,\Delta t)\hat{\psi}^e_{I_n}(z))\Delta t^2 + G_{2,l}(z,\Delta t)\hat{\psi}^e_{J_l}(z)\Delta t^2 + \hat{H}_l(z,\Delta t)\Delta t^2,
\end{aligned} \tag{76}$$

where $G_{1,l,m,n}(z,\Delta t)$ and $G_{2,l}(z,\Delta t)$ are some analytic functions equal to linear combinations of products of the functions $h_{p,q}$ and

$$\frac{\hat{r}_{p,q}(z,\Delta t)}{\hat{g}_{0,0}(z) - g_{0,0}(0)/2}.$$

Next, by using Lemma 2, we can prove the following bounds

$$|G_{1,l,m,n}(z,\Delta t)| \le C_{1,l,m,n,\rho}, \qquad |G_{2,l}(z,\Delta t)| \le C_{2,l,\rho}, \tag{77}$$

for some well-chosen positive real-valued constants $C_{1,l,m,n,\rho}$ and $C_{2,l,\rho}$.

Now, by using (31), Eq. (76) is

$$\begin{aligned}
\hat{\psi}^e_{J_l}(z) &= \sum_{1\le m,n\le 4L-4} (\mathbf{B})_{l,m}((\mathbf{A}^1)^{-1})_{m,n}\hat{\psi}^e_{I_n}(z) + R_l(z,\Delta t)\Delta t^2 \\
&= \sum_{1\le n\le 4L-4} (\mathbf{F})_{l,n}\hat{\psi}^e_{I_n}(z) + R_l(z,\Delta t)\Delta t^2,
\end{aligned} \tag{78}$$

where $\mathbf{F}(z)$ is defined by

$$\hat{\psi}_J(z) = \mathbf{F}(z)\hat{\psi}_I(z) := \mathbf{B}(z)(\mathbf{A}^1(z))^{-1}\hat{\psi}_I(z) \tag{79}$$

and

$$R_l(z,\Delta t) = \frac{1}{\det(\mathbf{A^1})} \left[\sum_{1\le m,n\le 4L-4} G_{1,l,m,n}(z,\Delta t)\hat{\psi}^e_{I_n}(z) + G_{2,l}(z,\Delta t)\hat{\psi}^e_{J_l}(z) + \hat{H}_l(z,\Delta t) \right]. \tag{80}$$

Let us also remark that, if ρ is a given large enough positive constant, then there exists Δt_0, such that, for $\Delta t \le \Delta t_0$, $\mathbf{F}$ being given by (79), for any vector $\mathbf{V}$ of size $4L-4$ and angle ϕ, we have

$$\mathrm{Im}\left[\bar{\mathbf{V}}^T \bar{\mathbf{F}}^T (e^{\rho\Delta t + \iota\phi}) \mathbf{I}_1 \mathbf{V} \right] \le 0. \tag{81}$$

Let us now prove the following error estimate.

Theorem 2. *Let us consider the scheme (18)-(19). Let ρ be a large enough given positive constant, following Theorem 1. Then there exists Δt_0, such that, for any $\Delta t \leq \Delta t_0$ and $t_K = K\Delta t \leq T$, we have the following estimate*

$$\| \psi^K - \psi^e(t_K) \|_2 \leq C(L, T, \psi^e(0))\Delta t^2, \tag{82}$$

where the positive constant C depends on the length L, the maximal time T and the initial data $\psi^e(0)$.

Proof. Let us fix $\rho_1 > \rho$, where ρ is given in Theorem 1. We define the local error: $e^k_{m,n} = (\psi^e_{m,n})^k - \psi^k_{m,n}$. Then one can see that

$$-\frac{2\iota}{\Delta t}(e^k_{m,n} - e^{k-1}_{m,n}) = \Delta(e^{k-1}_{m,n} + e^k_{m,n}) + r_{m,n,k-\frac{1}{2}}, \tag{83}$$

where $r_{m,n,k-\frac{1}{2}}$ is the local residual. From Eq. (78), the $\mathcal{Z}$-transform of the boundary conditions leads to

$$\begin{aligned} \hat{e}_{J_m}(z) &= \sum_{n=1}^{4L-4} \mathbf{F}_{m,n}(z)\hat{\psi}^e_{I_n}(z) + R_m(z, \Delta t)\Delta t^2 - \sum_{n=1}^{4L-4} \mathbf{F}_{m,n}(z)\hat{\psi}_{I_n}(z) \\ &= \sum_{n=1}^{4L-4} \mathbf{F}_{m,n}(z)\hat{e}_{I_n}(z) + R_m(z, \Delta t)\Delta t^2, \end{aligned} \tag{84}$$

where $1 \leq m \leq 4L-4$. If we define $\eta^k_{m,n} = \beta^{-k} e^k_{m,n}$, with $\beta = e^{\rho_1 \Delta t}$, and after some long calculations, one obtains the following expression for the discrete L^2-norm of the error

$$\begin{aligned} \| \eta^K \|_2^2 \leq \frac{1-\beta^2}{\beta^2} \sum_{k=0}^{K-1} \| \eta^k \|_2^2 + \sum_{k=1}^{K} [\frac{\Delta t}{2\beta} \sum_{n=1}^{L} \sum_{m=1}^{L} (\eta^{k-1}_{m,n}\beta^{-k}|r_{m,n,k-\frac{1}{2}}| + \eta^k_{m,n}\beta^{-k+1}|r_{m,n,k-\frac{1}{2}}|)] \\ + \mathrm{Im}\frac{\Delta t}{2\beta^2} \sum_{k=1}^{K} \sum_{m=1}^{4L} [\overline{(\eta^{k-1}_{J_m} + \beta\eta^k_{J_m})}(\eta^{k-1}_{I^1_m} + \beta\eta^k_{I^1_m} - \eta^{k-1}_{J_m} - \beta\eta^k_{J_m})]. \end{aligned} \tag{85}$$

Now, based on Eq. (84), one gets

$$\begin{aligned} &\mathrm{Im} \sum_{k=1}^{K} \sum_{m=1}^{4L} [\overline{(\eta^{k-1}_{J_m} + \beta\eta^k_{J_m})}(\eta^{k-1}_{I^1_m} + \beta\eta^k_{I^1_m} - \eta^{k-1}_{J_m} - \beta\eta^k_{J_m})] \\ &= \mathrm{Im}\frac{1}{2\pi} \int_0^{2\pi} \left[\left|1 + \beta e^{\iota\phi}\right|^2 \sum_{m=1}^{4L} \bar{\hat{e}}_{J_m}(\beta e^{\iota\phi})(\hat{e}_{I^1_m}(\beta e^{\iota\phi}) - \hat{e}_{J_m}(\beta e^{\iota\phi})) \right] d\phi \\ &= \frac{1}{2\pi}\mathrm{Im} \int_0^{2\pi} \left|1 + \beta e^{\iota\phi}\right|^2 \bar{\hat{e}}^T_I(\beta e^{\iota\phi})\bar{\mathbf{F}}^T(\beta e^{\iota\phi})(\mathbf{I}_1 - \mathbf{F}(\beta e^{\iota\phi}))\hat{e}_I(\beta e^{\iota\phi}) d\phi \\ &+ \frac{1}{2\pi}\mathrm{Im} \int_0^{2\pi} \left|1 + \beta e^{\iota\phi}\right|^2 \left[\sum_{m=1}^{4L} \bar{R}_m(\beta e^{\iota\phi}, \Delta t)\hat{e}_{I^1_m}(\beta e^{\iota\phi}) \right] d\phi \Delta t^2. \end{aligned} \tag{86}$$

The first integral of the above last equality does not contribute to the computation since it is less than

zero. This then leads to

$$\begin{aligned}\Delta t \mathrm{Im}\sum_{k=1}^{K}\sum_{m=1}^{4L}[\overline{(\eta_{J_m}^{k-1}+\beta\eta_{J_m}^{k})}(\eta_{I_m^1}^{k-1}+\beta\eta_{I_m^1}^{k}-\eta_{J_m}^{k-1}-\beta\eta_{J_m}^{k})] \\ \leq \Delta t^3\frac{1}{2\pi}\left|\int_0^{2\pi}\left|1+\beta e^{\iota\phi}\right|^2\sum_{m=1}^{4L}\bar{R}_m(\beta e^{\iota\phi},\Delta t)\hat{e}_{I_m^1}(\beta e^{\iota\phi})d\phi\right|.\end{aligned} \tag{87}$$

From relations (77), (80) and (4), we conclude that

$$\begin{aligned}&\Delta t^3\left|\frac{1}{2\pi}\int_0^{2\pi}\left|1+\beta e^{\iota\phi}\right|^2\bar{R}_l(\beta e^{\iota\phi},\Delta t)\hat{e}_{I_l^1}(\beta e^{\iota\phi})d\phi\right| \leq \frac{\beta^2-1}{4\beta^2}\sum_{k=0}^{K}\left|\eta_{I_l^1}^{k}\right|^2 \\ &+\frac{C\Delta t^5\beta^2}{(\beta^2-1)}(\max_{1\leq m,n\leq 4L-4}\parallel(\det\hat{\mathbf{F}}_{\mathbf{1}}(\beta e^{\iota\phi}))^{-1}G_{1,l,m,n}(\beta e^{\iota\phi},\Delta t)\parallel_{L^\infty[0,2\pi]} \\ &+\parallel(\det\hat{\mathbf{F}}_{\mathbf{1}}(\beta e^{\iota\phi}))^{-1}G_{2,l}(\beta e^{\iota\phi},\Delta t)\parallel_{L^\infty[0,2\pi]}+\parallel(\hat{\mathbf{F}}_{\mathbf{1}}(\beta e^{\iota\phi}))^{-1}\parallel_{L^\infty[0,2\pi]})^2 \\ &\times(\max_{1\leq m\leq 4L}\Delta t\sum_{k=0}^{K}\left|\psi_{J_m}^{e,k}\right|^2+\max_{1\leq n\leq 4L}\Delta t\sum_{k=0}^{K}\left|\psi_{I_n}^{e,k}\right|^2+\Delta t\sum_{k=0}^{K}\left|H_l^k\right|^2) \\ &\leq \frac{\beta^2-1}{4\beta^2}\sum_{k=0}^{K}\left|\eta_{I_l^1}^{k}\right|^2+\Delta t^4 C(L,T,\psi^e(0)),\end{aligned} \tag{88}$$

which provides

$$\begin{aligned}\Delta t \mathrm{Im}\sum_{k=1}^{K}\sum_{m=1}^{4L}[\overline{(\eta_{J_m}^{k-1}+\beta\eta_{J_m}^{k})}(\eta_{I_m^1}^{k-1}+\beta\eta_{I_m^1}^{k}-\eta_{J_m}^{k-1}-\beta\eta_{J_m}^{k})] \\ \leq \frac{\beta^2-1}{2\beta^2}\sum_{k=0}^{K}\parallel\eta^k\parallel_2^2+\Delta t^4 C(L,T,\psi^e(0)).\end{aligned} \tag{89}$$

To get (89) from (88), we use the following estimate for three sequences $\{a_n\}$, $\{b_n\}$ and $\{c_n\}$, where their $\mathcal{Z}$- transforms are $\hat{a}(z)$, $\hat{b}(z)$ and $\hat{c}(z)$, respectively,

$$\begin{aligned}\frac{1}{2\pi}\int_0^{2\pi}|\hat{a}(e^{i\varphi})\hat{b}(e^{i\varphi})\hat{c}(e^{i\varphi})|d\varphi &\leq \frac{1}{2\pi}\parallel\hat{a}(e^{i\varphi})\parallel_{L^\infty[0,2\pi]}\parallel\hat{b}(e^{i\varphi})\parallel_{L^2[0,2\pi]}\parallel\hat{c}(e^{i\varphi})\parallel_{L^2[0,2\pi]} \\ &= \frac{1}{2\pi}\parallel\hat{a}(e^{i\varphi})\parallel_{L^\infty[0,2\pi]}\parallel b\parallel_{l^2}\parallel c\parallel_{l^2}\leq\varepsilon\parallel c\parallel_{l^2}^2+C(\varepsilon)(\parallel\hat{a}(e^{i\varphi})\parallel_{L^\infty[0,2\pi]}\parallel b\parallel_{l^2})^2,\end{aligned} \tag{90}$$

setting $\parallel a\parallel_{l^2}^2=\sum_{k=0}^{K}|a_k|^2$. The terms with indices I_l^1 belong to the computational domain, $1\leq m,n\leq L$, and so they can be controlled by $\parallel\eta^k\parallel_2$ The indices η_{J_l} are not in the computational domain. However, the terms which contain an index η_{J_l} are negative in (86), so they do not need to be estimated in L^2-norm [20]. By using Eq. (4), we obtain: $|r_{m,n,k+\frac{1}{2}}|\leq C(\psi^e(0))\Delta t^2$. Then, by combining with (85), one gets

$$\begin{aligned}\parallel\eta^K\parallel_2^2\leq\frac{1-\beta^2}{\beta^2}\sum_{k=0}^{K-1}\parallel\eta^k\parallel_2^2+\frac{\beta^2-1}{2\beta^2}\sum_{k=0}^{K}\parallel\eta^k\parallel_2^2+C(L,\psi^e(0))\Delta t^4 \\ +\frac{\beta^2-1}{2\beta^2}\sum_{k=0}^{K}\parallel\eta^k\parallel_2^2+\frac{C\Delta t^2}{(\beta^2-1)}\sum_{k=1}^{K}\sum_{1\leq m,n\leq L}\left|r_{m,n,k-\frac{1}{2}}\right|^2.\end{aligned} \tag{91}$$

Finally, we have

$$\| \eta^K \|_2^2 \leq C(L,T,\psi^e(0))\Delta t^4, \tag{92}$$

yielding

$$\| \psi^K - \psi^e(K\Delta t) \|_2 \leq C(L,T,\psi^e(0))\Delta t^2. \tag{93}$$

□

6 Conclusion

In this paper, we proved the L^2-stability of the Crank-Nicolson discretization of the Schrödinger equation with the artificial boundary condition derived in [16]. In addition, the full scheme is proved to be second-order in time. These results confirm the numerical simulations presented in [16].

A Appendices

The matrix $\mathbf{I}_1$ can be written as

$$\mathbf{I}_1 = \begin{bmatrix} 1 & & & & & & & & \\ & \mathbf{I}_{L-2} & & & & & & & \\ & & 1_2 & & & & & & \\ & & & \mathbf{I}_{L-2} & & & & & \\ & & & & 1_2 & & & & \\ & & & & & \mathbf{I}_{L-2} & & & \\ & & & & & & 1_2 & & \\ & & & & & & & \mathbf{I}_{L-2} & \\ 1 & & & & & & & & \end{bmatrix}, \tag{94}$$

where $\mathbf{I}_{L-2}$ is the identity matrix of order $(L-2)$, $1_2 = [1 \quad 1]^T$, and all other entries are zero. In addition, some computations show that

$$\boldsymbol{A}_0 = -\frac{i\cot(\frac{\phi}{2})}{2}\boldsymbol{I}_1, \qquad \boldsymbol{B}_1 = -\frac{i\cot^2(\frac{\phi}{2})}{4}\boldsymbol{I}_1 \tag{95}$$

and

$$\mathbf{A}_1 = \begin{bmatrix} a_1 & b_1 & & & & & & b_1 \\ & \mathbf{C}_1 & & & & & & \\ & b_1 & a_1 & b_1 & & & & \\ & b_1 & a_1 & b_1 & & & & \\ & & & \mathbf{C}_1 & & & & \\ & & & b_1 & a_1 & b_1 & & \\ & & & b_1 & a_1 & b_1 & & \\ & & & & & \mathbf{C}_1 & & \\ & & & & & b_1 & a_1 & b_1 \\ & & & & & b_1 & a_1 & b_1 \\ & & & & & & & \mathbf{C}_1 \\ a_1 & b_1 & & & & & & b_1 \end{bmatrix}, \tag{96}$$

with

$$a_1 = -\frac{\rho + 4i}{4\sin^2(\frac{\phi}{2})}, \qquad\qquad b_1 = -\frac{i\cot^2(\frac{\phi}{2})}{4},$$

and the $(L-2)\times L$ matrix $\mathbf{C}_1$ is given by

$$\mathbf{C}_1 = \begin{bmatrix} b_1 & a_1 & b_1 & & & & & \\ & b_1 & a_1 & b_1 & & & & \\ & & b_1 & a_1 & b_1 & & & \\ & & & . & & & & \\ & & & . & & & & \\ & & & . & & & & \\ & & & & & b_1 & a_1 & b_1 \end{bmatrix}. \tag{97}$$

We also can prove that the matrix $\mathbf{B}_2$ is such that

$$\mathbf{B}_2 = \begin{bmatrix} a_2 & 2b_2 & & & & & & b_2 \\ & \mathbf{C}_2 & & & & & & \\ & 2b_2 & a_2 & b_2 & & & & \\ & b_2 & a_2 & 2b_2 & & & & \\ & & & \mathbf{C}_2 & & & & \\ & & & 2b_2 & a_2 & b_2 & & \\ & & & b_2 & a_2 & 2b_2 & & \\ & & & & & \mathbf{C}_2 & & \\ & & & & & 2b_2 & a_2 & b_2 \\ & & & & & b_2 & a_2 & 2b_2 \\ & & & & & & & \mathbf{C}_2 \\ a_2 & b_2 & & & & & & 2b_2 \end{bmatrix}, \tag{98}$$

with

$$a_2 = -\frac{(2\rho + 8i)\cot(\frac{\phi}{2})}{8\sin^2(\frac{\phi}{2})}, \qquad\qquad b_2 = -\frac{i\cot(\frac{\phi}{2})}{8\sin^2(\frac{\phi}{2})}.$$

The $(L-2)\times L$ matrix $\mathbf{C}_2$ has the following form

$$\mathbf{C}_2 = \begin{bmatrix} 2b_2 & a_2 & 2b_2 & & & & & \\ & 2b_2 & a_2 & 2b_2 & & & & \\ & & 2b_2 & a_2 & 2b_2 & & & \\ & & & . & & & & \\ & & & . & & & & \\ & & & . & & & & \\ & & & & & 2b_2 & a_2 & 2b_2 \end{bmatrix}. \tag{99}$$

It is finally easy to get $\mathbf{I}_1^T\mathbf{I}_1 = \mathbf{I}_2$. The matrix $\mathbf{I}_2$ can be written as

$$\mathbf{I}_2 = \begin{bmatrix} 2 & & & & & & & & \\ & \mathbf{I}_{L-2} & & & & & & & \\ & & 2 & & & & & & \\ & & & \mathbf{I}_{L-2} & & & & & \\ & & & & 2 & & & & \\ & & & & & \mathbf{I}_{L-2} & & & \\ & & & & & & 2 & & \\ & & & & & & & \mathbf{I}_{L-2} \end{bmatrix}. \tag{100}$$

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