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Stability and convergence analysis of artificial boundary conditions for the Schrödinger equation on a rectangular domain

Gang PANG¹, Yibo YANG², Xavier ANTOINE³, Shaoqiang TANG⁴

Abstract. Based on the semi-discrete artificial boundary condition introduced in [24] for the two-dimensional free Schrödinger equation in a computational rectangular domain, we propose to analyze the stability and convergence rate with respect to time 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 "Ji S., Yang Y., Pang G., Antoine X., *Computer Physics Communications*, 2018" [24].

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 [8, 21, 32, 33], 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 [8], 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 (ABC), 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

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space and time variable potentials, with simple or complicate smooth convex fictitious boundaries. We refer to [5, 6, 9, 17, 20, 27] for some examples, the list of references being non exhaustive. Available review papers on artificial boundary conditions are e.g. [18, 22, 34] for general PDEs, and [1, 4] 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) [3, 14, 15, 16, 30, 35] 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. When the fictitious boundary has some corners, like this is the case for the rectangular domain, then the construction of artificial boundary conditions is known to be more complicate since the existence of corners directly impacts the design of the boundary conditions. For example, specific nontrivial compatibility boundary conditions at the corners need to be added to the artificial boundary conditions to get an increased accuracy for time-domain wave equations [7, 13, 19, 29] and time-harmonic wave scattering [28]. In addition, the numerical analysis of such problems remains difficult to conduct. For the PML problem, corners may lead to instabilities in the time-domain [10] and require a careful choice of the discretization to stabilize the method. In addition, tuning correctly the PML parameters is not so easy and strongly depends on the configuration, i.e. the PDE under study and its discretization [3, 11, 12, 14, 15, 16, 30, 35].

In the present paper, we focus on the artificial boundary condition method proposed in [24] which solves exactly the corner problem for the rectangular shaped domain, and is based on a second-order spatial semi-discretization of the Schrödinger equation. Therefore, the corresponding boundary condition falls into the framework of semi-discrete artificial boundary conditions. From some numerical simulations, it was shown in [24] that, using 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, for fixed spatial discretization steps Δx and Δy . However, the paper does not address the important and difficult question of designing an accelerated numerical method for evaluating the integral operators arising in the definition of these ABCs. This needs further numerical and computational studies which are out of the scope of the present paper. Since this paper is already technical as well as [24], the authors strongly advise the reader to first understand the derivation in [24] before entering into the details of the present paper, even if the material to understand the paper is self-contained. Let us also remark that the method for constructing ABCs [24] has recently been applied with success in [23] to design new artificial boundary conditions for the 1D nonlocal Schrödinger equation. This later work, combined with the design of ABCs on rectangular domains developed in [24], should offer the possibility to extend the ABCs to the 2D nonlocal Schrödinger equation (as well as heat equation) and to some peridynamics models. Therefore, the numerical analysis developed in the present paper for the 2D local Schrödinger equation is valuable for understanding how to obtain the convergence and stability results for the more complicate nonlocal case.

The plan of the paper is the following. After the introduction (Section 1), we develop in Section 2 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 3, we prove the L^2 -stability of the fully discrete scheme. Section 4 is devoted to the convergence analysis. Finally,

we end by a conclusion in Section 5 and two Appendices.

2 Exact boundary conditions for the semi-discrete Schrödinger equation on a rectangular domain

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

$$\iota \dot{\psi} = -\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right), \quad (1)$$

where $(x, y) \in \mathbb{R}^2$ and $t > 0$ are the space and time variables, respectively. The time derivative is denoted by $\dot{\psi} := \partial_t \psi$. In addition, a compactly supported initial data $\psi(x, y, t = 0) = \psi_0(x, y)$ 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 (assuming here that $\Delta x = \Delta y$) 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 $\psi^e := (\psi_{m,n}^e)_{(m,n) \in \mathbb{Z}^2}$ to

$$\iota \dot{\psi}_{m,n}^e = -(\psi_{m+1,n}^e + \psi_{m-1,n}^e + \psi_{m,n+1}^e + \psi_{m,n-1}^e - 4\psi_{m,n}^e) = -\Delta \psi_{m,n}^e, \quad (2)$$

with compactly supported initial data $\psi_{m,n}^e(0) = \psi_0(m\Delta x, n\Delta x)$ 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 we denote by Δ_x^+ (Δ_x^- , respectively) the forward (backward, respectively) finite-difference operator in the x -direction, i.e.

$$\Delta_x^+ \psi_{m,n}^e := \psi_{m+1,n}^e - \psi_{m,n}^e, \quad \Delta_x^- \psi_{m,n}^e := \psi_{m,n}^e - \psi_{m-1,n}^e.$$

Similarly, the operators Δ_y^+ and Δ_y^- are given in the y -direction by

$$\Delta_y^+ \psi_{m,n}^e := \psi_{m,n+1}^e - \psi_{m,n}^e, \quad \Delta_y^- \psi_{m,n}^e := \psi_{m,n}^e - \psi_{m,n-1}^e.$$

Let us define the Laplace transform \tilde{h} of h as

$$\tilde{h}(s) := \int_0^\infty h(t) e^{-st} dt \quad (3)$$

and the convolution $(f * g)$ of f and g as

$$(f * g)(t) := \int_0^t f(\tau) g(t - \tau) d\tau. \quad (4)$$

Therefore, the Laplace transform $\tilde{\psi}_{m,n}^e(s)$ of $\psi_{m,n}^e$ is given by

$$\tilde{\psi}_{m,n}^e(s) := \int_0^\infty \psi_{m,n}^e(t) e^{-st} dt. \quad (5)$$

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 to compute the discrete Green's functions which is needed for the general case. We assume that the wave function ψ^e satisfies Eq. (2) and that $\psi_{m,n}^e(0) = 0$, for $(m, n) \neq (0, 0)$. For a given function $\psi_{0,0}^e(t)$, from [24] we have, for $(m, n) \neq (0, 0)$,

$$\psi_{m,n}^e(t) = f_{m,n}^e(t) * \psi_{0,0}^e(t) = \int_0^t f_{m,n}^e(\tilde{t}) \psi_{0,0}^e(t - \tilde{t}) d\tilde{t}, \quad (6)$$

where the Green's function $f_{m,n}^e(t)$ comes from the expression

$$g_{m,n}^e(t) = f_{m,n}^e(t) * g_{0,0}^e(t), \quad (7)$$

with

$$g_{m,n}^e(t) = (t)^{m+n} e^{-4t} \frac{(m+n)!}{m!n!} \frac{\sqrt{\pi}}{2^{m+n+1} \Gamma(\frac{m+n+1}{2}) \Gamma(\frac{m+n}{2} + 1)} \times {}_2F_3 \left(\begin{matrix} \frac{1}{2}(m+n+1), \frac{1}{2}(m+n)+1; -4t^2 \\ m+1, n+1, m+n+1 \end{matrix} \right). \quad (8)$$

In the above definition, Γ is the Gamma function and the generalized hypergeometric function ${}_2F_3$ [25] is given by

$${}_2F_3 \left(\begin{matrix} a_1, a_2; z \\ b_1, b_2, b_3 \end{matrix} \right) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k}{k! (b_1)_k (b_2)_k (b_3)_k} z^k, \quad (9)$$

with $(a)_k = a(a+1)\dots(a+k-1)$, for $k \geq 1$ and $(a)_0 = 1$. The function ${}_2F_3$ is the inverse Laplace transform of the function $W((m, n), \frac{4-\iota s}{2})$, where

$$W((m, n), z) = \frac{1}{2^{m+n} z^{m+n+1}} \frac{(m+n)!}{m!n!} \times {}_4F_3 \left(\begin{matrix} \frac{1}{2}(m+n+1), \frac{1}{2}(m+n+1), \frac{1}{2}(m+n)+1, \frac{1}{2}(m+n)+1; \frac{4}{z^2} \\ m+1, n+1, m+n+1 \end{matrix} \right), \quad (10)$$

and $z = (4 - \iota s)/2$. The function ${}_4F_3$ is the generalized hypergeometric function ${}_pF_q$ [25], with $p = 4$ and $q = 3$. In particular, we have $f_{0,0}^e(t) = \delta(t)$, where δ is the Dirac distribution.

Let us now come to the construction of the exact boundary conditions for general initial data. We consider a finite rectangular computational domain and we 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 $1 \leq k \leq 4L - 4$. More explicitly, we have $I_\ell = (1, \ell)$ for $1 \leq \ell \leq L - 1$, $I_{\ell+L-1} = (\ell, L)$ for $1 \leq \ell \leq L - 1$, $I_{\ell+2L-2} = (L, L + 1 - \ell)$ for $1 \leq \ell \leq L - 1$ and $I_{\ell+3L-3} = (L + 1 - \ell, 1)$ for $1 \leq \ell \leq L - 1$. The outer layer points are denoted by J_k for $k = 1, \dots, 4L$, with the same orientation. Deriving a numerical artificial boundary condition consists in writing $\psi_{J_k}^e(t)$ 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 the finite computational region.

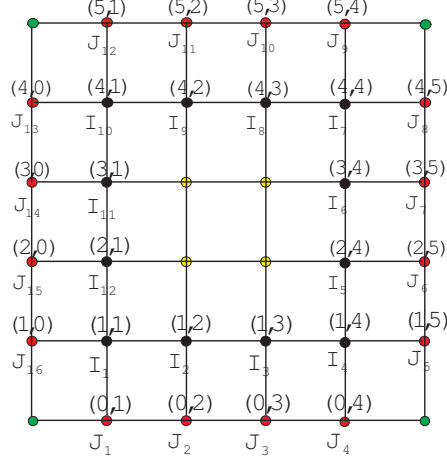


Figure 1: Discrete computational lattice (for $L = 4$): the red bullets represent the outer layer points, the black ones correspond to the interior layer points, the yellow ones are the interior points and the green ones stands for the corner points.

From [24] and for any integers (m, n) , the functions $\psi_{m,n}^e(t)$ are proved to be analytic with respect to t , and $\tilde{\psi}_{m,n}^e(s)$ is analytic around ∞ . Let us consider that $\psi_{I_k}^e(t)$, for $k = 1, \dots, 4L - 4$, are given values. Following [24], we first decompose them as $4L - 4$ unknown independent sources $\chi_{I_k}^e(t)$ thanks to the previous Green's functions $f_{m,n}^e$ following

$$\psi_{I_k}^e(t) = \sum_{\ell=1}^{4L-4} f_{I_k - I_\ell}^e(t) * \chi_{I_\ell}^e(t). \quad (11)$$

For $1 \leq k \leq 4L - 4$ and $z = \frac{4 - \iota s}{2}$, it can be proved [24] that the following relation holds in the Laplace domain

$$\tilde{\psi}_{I_k}^e(s) = \sum_{\ell=1}^{4L-4} \frac{W(I_k - I_\ell, z)}{W((0, 0), z)} \tilde{\chi}_{I_\ell}^e(s), \quad (12)$$

where $\tilde{\chi}_{I_\ell}^e(s)$ denotes the Laplace transform of the function $\chi_{I_\ell}^e(t)$. From (10) and $W((m, n), z) = W(|m|, |n|, z)$ [31], one has the asymptotic estimates [25]

$$\frac{W((m, n), z)}{W((0, 0), z)} \sim C_{|m|+|n|}^{|m|} \left(\frac{1}{2z}\right)^{|m|+|n|}, \quad |z| \rightarrow +\infty,$$

where $C_{|m|+|n|}^{|m|}$ is the binomial coefficient. Therefore, the matrix $\left(\frac{W(I_k - I_\ell, z)}{W((0, 0), z)}\right)_{k,\ell}$ is diagonally dominant for large values of the parameter s . Consequently, the matrix is invertible and the functions $\tilde{\chi}_{I_\ell}^e(s)$ exist and can be determined uniquely. Since $\tilde{\psi}_{I_k}^e(s)$ are analytic near the infinity, then the functions $\tilde{\chi}_{I_\ell}^e(s)$ also share this property and $\chi_{I_\ell}^e(t)$ are analytical functions. It can also be proved that

$\chi_{I_\ell}^e(0) = 0$. For a point (m, n) outside the inner boundary, we have the representation formula

$$\tilde{\psi}_{m,n}^e(s) = \sum_{\ell=1}^{4L-4} \frac{W((m, n) - I_\ell, z)}{W((0, 0), z)} \tilde{\chi}_{I_\ell}^e(s). \quad (13)$$

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

$$(4 - \iota s)W((m, n) - I_\ell, z) = W((m + 1, n) - I_\ell, z) + W((m - 1, n) - I_\ell, z) \\ + W((m, n + 1) - I_\ell, z) + W((m, n - 1) - I_\ell, z). \quad (14)$$

Injecting the above relation into (13) gives

$$(4 - \iota s)\tilde{\psi}_{m,n}^e(s) = \tilde{\psi}_{m+1,n}^e(s) + \tilde{\psi}_{m-1,n}^e(s) + \tilde{\psi}_{m,n+1}^e(s) + \tilde{\psi}_{m,n-1}^e(s), \quad (15)$$

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

$$\psi_{I_\ell}^e(t) = \sum_{l=1}^{4L-4} f_{I_\ell - I_l}^e(t) * \chi_{I_l}^e(t), \quad \psi_{J_\ell}^e(t) = \sum_{l=1}^{4L-4} f_{J_\ell - I_l}^e(t) * \chi_{I_l}^e(t). \quad (16)$$

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 , $(f_{m,n}^e)^k$, $(\psi_{m,n}^e)^k$ and $(\chi_{m,n}^e)^k$ stand for the quantities $f_{m,n}^e(k\Delta t)$, $\psi_{m,n}^e(k\Delta t)$ and $\chi_{m,n}^e(k\Delta t)$, respectively. In addition, the numerical approximation of $f_{m,n}^e(k\Delta t)$, $\psi_{m,n}^e(k\Delta t)$, $\chi_{m,n}^e(k\Delta t)$ is designated by $f_{m,n}^k$, $\psi_{m,n}^k$, $\chi_{m,n}^k$, respectively. In the present paper, the unknowns $\psi_{m,n}^k$ ($1 \leq m, n \leq L$) are computed by applying the Crank-Nicolson scheme [2] to (2)

$$-\iota \frac{\psi_{m,n}^k - \psi_{m,n}^{k-1}}{\Delta t} = \frac{1}{2} \Delta (\psi_{m,n}^k + \psi_{m,n}^{k-1}) = \frac{1}{2} (\psi_{m-1,n}^k + \psi_{m+1,n}^k + \psi_{m,n-1}^k + \psi_{m,n+1}^k - 4\psi_{m,n}^k) \\ + \frac{1}{2} (\psi_{m-1,n}^{k-1} + \psi_{m+1,n}^{k-1} + \psi_{m,n-1}^{k-1} + \psi_{m,n+1}^{k-1} - 4\psi_{m,n}^{k-1}), \quad (17)$$

for $1 \leq m, n \leq L$. Concerning the boundary condition, $\psi_{I_\ell}^k$ and $\psi_{J_\ell}^k$ ($1 \leq \ell \leq 4L$) are discretized from relations (16) as

$$\psi_{I_\ell}^k = \sum_{l=1}^{4L-4} (f_{I_\ell - I_l}^k \star \chi_{I_l}^k), \quad \psi_{J_\ell}^k = \sum_{l=1}^{4L-4} (f_{J_\ell - I_l}^k \star \chi_{I_l}^k). \quad (18)$$

Based on (7), the terms $f_{m,n}^k$ in relation (18) can be numerically computed from

$$(g_{m,n}^e)^k = (f_{m,n}^e \star g_{0,0}^e)^k, \quad (19)$$

where $g_{m,n}^e(t)$ can be approximated accurately e.g. by a fourth-order Runge-Kutta scheme. Finally, we can use the values $\psi_{I_\ell}^k$ to complete the fully discretized system given by (17), for $1 \leq m, n \leq L$, and then prove the stability of the whole system.

Remark 1. If the external potential outside the computational domain is a constant V but not zero, then only the kernel function $\tilde{g}_{m,n}^e(s)$ needs to be changed to $W((m,n), \frac{4+V-\iota s}{2})$, and the resulting boundary condition (16) still holds.

3 L^2 -stability analysis of the scheme

In this section, we prove the stability of the scheme (17)-(18). Let us first introduce the norm

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

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

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

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

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

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

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

leading to

$$\hat{f}_{m,n}(z) = \frac{\hat{g}_{m,n}^e(z) + \hat{g}_{0,0}^e(z) f_{m,n}^e(0) \frac{\Delta t}{2}}{(\hat{g}_{0,0}^e(z) - \frac{g_{0,0}^e(0)}{2}) \Delta t}, \quad (23)$$

where $\hat{g}_{m,n}^e(z) = \sum_{k=0}^{\infty} \frac{g_{m,n}^e(k\Delta t)}{z^k}$. If $v^k = (u \star f_{m,n})^k$, with $u^0 = 0$, we have

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

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

$$h_{m,n}(z) = \frac{\hat{g}_{m,n}^e(z) - \frac{1}{2} \delta_{0,0} + \frac{i}{4} \Delta t \delta_{0,1}}{\hat{g}_{0,0}^e(z) - \frac{1}{2}}. \quad (25)$$

Here, $\delta_{0,0} = 1$ for $(m, n) = (0, 0)$, $\delta_{0,0} = 0$ for the other cases. Similarly, we set $\delta_{0,1} = 1$ for $(m, n) = (0, 1)$, and $\delta_{0,1} = 0$ otherwise.

Let us now introduce the index I_m^1 , $1 \leq m \leq 4L$, such that: $I_m^1 = (1, m)$, $I_{L+m}^1 = (m, L)$, $I_{m+2L}^1 = (L, L+1-m)$ and $I_{m+3L}^1 = (L+1-m, 1)$, 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 $\varphi_{m,n}^k = \frac{1}{\beta^k} \psi_{m,n}^k$ in (17), we obtain

$$-\iota \frac{2}{\Delta t} (\varphi_{m,n}^k - \varphi_{m,n}^{k-1}) = \Delta (\varphi_{m,n}^k + \varphi_{m,n}^{k-1}) + (\beta - 1) (\Delta + \iota \frac{2}{\Delta t}) \varphi_{m,n}^k \quad (26)$$

and

$$-\iota \frac{2}{\Delta t} \beta (\varphi_{m,n}^k - \varphi_{m,n}^{k-1}) = \beta \Delta (\varphi_{m,n}^k + \varphi_{m,n}^{k-1}) + (1 - \beta) (\Delta - \iota \frac{2}{\Delta t}) \varphi_{m,n}^{k-1}. \quad (27)$$

Let us now multiply the conjugate of (26) by $\varphi_{m,n}^k$ and (27) by $-\beta^{-1} \overline{\varphi_{m,n}^{k-1}}$ (\bar{z} being the conjugate of a complex number z), and sum over $1 \leq m, n \leq L$. Then one gets

$$\begin{aligned} \sum_{n=1}^L \sum_{m=1}^L (|\varphi_{m,n}^k|^2 - |\varphi_{m,n}^{k-1}|^2) &\leq -(1 - \frac{1}{\beta}) \sum_{m=1}^L \sum_{n=1}^L |\varphi_{m,n}^{k-1}|^2 - (\beta - 1) \sum_{m=1}^L \sum_{n=1}^L |\varphi_n^k|^2 \\ &+ \frac{\Delta t}{2\beta} \text{Im} \sum_{n=1}^L \left[\overline{(\varphi_{0,n}^{k-1} + \beta \varphi_{0,n}^k)} \Delta_x^+ (\varphi_{0,n}^{k-1} + \beta \varphi_{0,n}^k) - \overline{(\varphi_{L+1,n}^{k-1} + \beta \varphi_{L+1,n}^k)} \Delta_x^- (\varphi_{L+1,n}^{k-1} + \beta \varphi_{L+1,n}^k) \right] \\ &+ \frac{\Delta t}{2\beta} \text{Im} \sum_{m=1}^L \left[\overline{(\varphi_{m,0}^{k-1} + \beta \varphi_{m,0}^k)} \Delta_y^+ (\varphi_{m,0}^{k-1} + \beta \varphi_{m,0}^k) - \overline{(\varphi_{m,L+1}^{k-1} + \beta \varphi_{m,L+1}^k)} \Delta_y^- (\varphi_{m,L+1}^{k-1} + \beta \varphi_{m,L+1}^k) \right]. \end{aligned} \quad (28)$$

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

$$\|\varphi^K\|_2^2 \leq \|\varphi^0\|_2^2 + \frac{\Delta t}{2\beta} \text{Im} \sum_{m=1}^{4L} \sum_{k=1}^K \left[\overline{(\varphi_{J_m}^{k-1} + \beta \varphi_{J_m}^k)} (\varphi_{I_m^1}^{k-1} + \beta \varphi_{I_m^1}^k - \varphi_{J_m}^{k-1} - \beta \varphi_{J_m}^k) \right], \quad (29)$$

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 (17)-(18). 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 $\Delta t \leq \Delta t_0$, the following inequality holds*

$$\sum_{m=1}^{4L} \sum_{k=1}^K \left[\overline{(\varphi_{J_m}^{k-1} + \beta \varphi_{J_m}^k)} (\varphi_{I_m^1}^{k-1} + \beta \varphi_{I_m^1}^k - \varphi_{J_m}^{k-1} - \beta \varphi_{J_m}^k) \right] \leq 0. \quad (30)$$

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

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

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

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

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

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

Following these notations, we obtain

$$\begin{aligned} & \sum_{l=1}^{4L} \sum_{k=1}^K \operatorname{Im} \left[\overline{(\varphi_{J_l}^{k-1} + \beta \varphi_{J_l}^k)} (\varphi_{I_l}^{k-1} + \beta \varphi_{I_l}^k - \varphi_{J_l}^{k-1} - \beta \varphi_{J_l}^k) \right] \\ &= \frac{1}{2\pi} \operatorname{Im} \left[\int_0^{2\pi} |1 + \beta e^{i\phi}|^2 \bar{\psi}_J^T(\beta e^{i\phi}) (\hat{\psi}_{I^1}(\beta e^{i\phi}) - \hat{\psi}_J(\beta e^{i\phi})) d\phi \right] \\ &= \frac{1}{2\pi} \operatorname{Im} \left[\int_0^{2\pi} |1 + \beta e^{i\phi}|^2 \bar{\chi}_I^T(\beta e^{i\phi}) \bar{\mathbf{B}}^T(\beta e^{i\phi}) \mathbf{A}(\beta e^{i\phi}) \hat{\chi}_I(\beta e^{i\phi}) d\phi \right]. \end{aligned} \quad (34)$$

To conclude, we only need to prove that

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

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 [24], we have

$$g_{m,n}^e(t) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \cos(mx) \cos(ny) e^{-i(4-2\cos(x)-2\cos(y))t} dx dy \quad (36)$$

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

$$\begin{aligned} \hat{g}_{m,n}^e(\beta e^{i\phi}) &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \cos(mx) \cos(ny) \sum_{j=0}^{\infty} e^{-K_0(x,y)j\Delta t} / (e^{(\rho\Delta t+i\phi)})^j dx dy \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \cos(mx) \cos(ny) \frac{e^{(K_0(x,y)+\rho)\Delta t+i\phi}}{e^{(K_0(x,y)+\rho)\Delta t+i\phi} - 1} dx dy, \end{aligned} \quad (37)$$

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

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

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

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

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

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

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

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

$$\frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \cos(mx) \cos(ny) (K_0(x, y) + \rho) dx dy = (\rho + 4\iota) \delta_{0,0} - \iota \delta_{1,0} - \iota \delta_{0,1} \quad (41)$$

and

$$\begin{aligned} \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \cos(mx) \cos(ny) (K_0(x, y) + \rho)^2 dx dy &= (\rho^2 + 8\iota\rho - 20) \delta_{0,0} \\ &- \delta_{2,0} - \delta_{0,2} + (8 - 2\iota\rho) \delta_{0,1} + (8 - 2\iota\rho) \delta_{1,0} - 2\delta_{1,1}. \end{aligned} \quad (42)$$

The matrices \mathbf{A}_0 , \mathbf{A}_1 , \mathbf{B}_1 , \mathbf{B}_2 are given from expressions (105) to (109) in Appendix B. Let us analyze the expansion (39) and its effect on stating the inequality (35) for Case 1.

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

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

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 $(\mathbf{B}_1^T \mathbf{A}_1 + \mathbf{B}_2^T \mathbf{A}_0)$ contribute to the inequality (35). Concerning $(\mathbf{R}_2 \mathbf{A}_0 + \mathbf{B}_1^T \mathbf{R}_1 + \mathbf{B}_2^T \mathbf{A}_1) \Delta t^3$, an analysis shows that its coefficients satisfy

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

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

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

while the order of the elements of $|\mathbf{R}_2^T \mathbf{R}_1 \Delta t^5|$ 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 $\mathbf{V} \in \mathbb{C}^{4L-4}$, the following inequalities

$$\begin{aligned} \left| \hat{g}_{0,0}^e(z) - \frac{1}{2} \right|^2 \text{Im} \left[\bar{\mathbf{V}}^T \bar{\mathbf{B}}^T \mathbf{A} \mathbf{V} \right] &\leq -\frac{\rho}{16} \frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})} \Delta t^2 |\mathbf{V}|^2 \\ &+ \frac{\cot^2(\frac{\phi}{2})}{\sin^2(\frac{\phi}{2})} \Delta t^2 \left(\mathcal{O}\left(\frac{\rho^3}{\alpha}\right) + \mathcal{O}\left(\frac{\rho^4}{\alpha^2}\right) + \mathcal{O}\left(\frac{\rho^5}{\alpha^3}\right) \right) |\mathbf{V}|^2 \leq 0. \end{aligned} \quad (44)$$

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

$$\begin{aligned} &\frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \cos(mx) \cos(ny) \sum_{j=0}^{\infty} e^{-K_0(x,y)j\Delta t} / (e^{(\rho + \iota\phi_{\Delta t})\Delta t})^j \Delta t dx dy - \frac{1}{2} \delta_{0,0} \Delta t + \frac{\iota}{4} \delta_{0,1} \Delta t^2 \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \frac{\cos(mx) \cos(ny)}{\rho + \iota\phi_{\Delta t} + K_0(x,y)} dx dy + \mathcal{O}(\Delta t^2) = \frac{1}{2\iota} W((m,n), \frac{\rho + \iota\phi_{\Delta t}}{2\iota} + 2) + \mathcal{O}(\Delta t^2) \end{aligned} \quad (45)$$

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

Let us recall that ρ is assumed to be relatively large. From (10), we have [25]

$$W((k,l), z) \sim \frac{1}{2^{k+l} z^{k+l+1}} C_{k+l}^k (1 + \mathcal{O}(\frac{1}{z}))$$

when $|z| \rightarrow +\infty$. Therefore, for $I_m^1 - I_n = (k, \ell)$ and ρ large, we obtain

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

From (45) and Δt small enough, we have

$$\begin{aligned} &\hat{g}_{I_m^1 - I_n}^e(z) \Delta t - \frac{1}{2} \delta_{0,0} \Delta t + \frac{\iota}{4} \Delta t^2 \delta_{0,1} \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \frac{\cos(kx) \cos(\ell y)}{\rho + \iota\phi_{\Delta t} + K_0(x,y)} dx dy + \mathcal{O}(\Delta t^2) = \frac{1}{2\iota} W((k,l), \frac{\rho + \iota\phi_{\Delta t}}{2\iota} + 2) + \mathcal{O}(\Delta t^2). \end{aligned} \quad (46)$$

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

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

and

$$\Delta t \left(\hat{g}_{0,0}^e(z) - \frac{1}{2} \right) \mathbf{B} = \frac{\iota}{(\rho + \iota(\phi_{\Delta t} + 4))^2} \mathbf{I}_1 \left(\mathbf{I} + \mathcal{O}\left(\frac{1}{\rho + \iota(\phi_{\Delta t} + 4)}\right) \right) + \mathcal{O}(\Delta t^2). \quad (48)$$

Since $\mathbf{I}_1^T \mathbf{I}_1 = \mathbf{I}_2$, where \mathbf{I}_2 is given by (110) (see Appendix B), then one gets

$$\Delta t^2 \left| \hat{g}_{0,0}^e(z) - \frac{1}{2} \right|^2 \bar{\mathbf{B}}^T \mathbf{A} = \frac{-\iota\rho + (4 + \phi_{\Delta t})}{((\phi_{\Delta t} + 4)^2 + \rho^2)^2} \left(\mathbf{I}_2 + \mathcal{O}\left(\frac{1}{\rho + \iota(\phi_{\Delta t} + 4)}\right) \right) + \mathcal{O}(\Delta t^2), \quad (49)$$

and finally $\text{Im} [\bar{\mathbf{V}}^T \bar{\mathbf{B}}^T \mathbf{A} \mathbf{V}] \leq 0$.

Case 3: $\pi - \alpha\Delta t \leq \phi \leq \pi + \alpha\Delta t$. 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

$$\begin{aligned} \hat{g}_{m,n}^e(e^{\rho\Delta t + \phi\iota}) &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \cos(mx) \cos(ny) \sum_{j=0}^{\infty} e^{-K_0 j \Delta t} / (e^{(\rho + \iota\phi_{\Delta t})\Delta t})^j (-1)^j dx dy \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \cos(mx) \cos(ny) \frac{1}{1 + e^{-K_1 \Delta t}} dx dy = \frac{1}{2} \delta_{0,0} + \left(\frac{K_2}{4}\right) \delta_{0,0} \Delta t - \frac{\iota}{4} \delta_{0,1} \Delta t \\ &\quad - \frac{\iota}{4} \delta_{1,0} \Delta t - (K_2^3 \delta_{0,0} - 3K_2 \delta_{0,2} - 3K_2 \delta_{2,0} + \iota\delta_{3,0} + \iota\delta_{0,3} + \iota(9 - 3K_2^2) \delta_{1,0} \\ &\quad + \iota(9 - 3K_2^2) \delta_{0,1} + 3\iota\delta_{1,2} + 3\iota\delta_{2,1} - 6K_2 \delta_{1,1} - 12K_2) \frac{\Delta t^3}{48} + \mathcal{O}(\Delta t^4), \end{aligned} \quad (50)$$

which means that

$$\left(\hat{g}_{0,0}^e(z) - \frac{1}{2} \right) \mathbf{A} = \Delta t \frac{K_2}{4} \mathbf{I}_1 + \mathcal{O}(\Delta t^2) \quad (51)$$

and

$$\left(\hat{g}_{0,0}^e(z) - \frac{1}{2} \right) \mathbf{B} = \Delta t^3 \left(\frac{\iota K_2^2}{16} \mathbf{I}_1 + \mathcal{O}(1) \right) + \mathcal{O}(\Delta t^4). \quad (52)$$

This leads to

$$\left| \hat{g}_{0,0}^e(z) - \frac{1}{2} \right|^2 \bar{\mathbf{B}}^T \mathbf{A} = -\Delta t^4 (\rho^2 + (4 + \phi_{\Delta t})^2) \frac{\iota K_2}{64} \left(\mathbf{I}_2 + \mathcal{O}\left(\frac{1}{\rho}\right) \right) + \mathcal{O}(\Delta t^5). \quad (53)$$

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

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

$$\text{Im} \sum_{l=1}^{4L} \sum_{k=1}^K \left[\overline{(\varphi_{J_l}^{k-1} + \beta\varphi_{J_l}^k)} (\varphi_{I_l}^{k-1} + \beta_1\varphi_{I_l}^k - \varphi_{J_l}^{k-1} - \beta_1\varphi_{J_l}^k) \right] \leq 0. \quad (54)$$

□

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

Theorem 1. *For the scheme (17)-(18), 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 $T_K = K\Delta t$,*

$$\| \psi^K \|_2 \leq e^{\rho T_K} \| \psi^0 \|_2. \quad (55)$$

Proof. From $\|\varphi^K\|_2^2 \leq \|\varphi^0\|_2^2$, we have: $e^{-\rho K \Delta t} \|\psi^K\|_2 \leq \|\psi^0\|_2$ which gives (55). \square

Remark 2. While the Crank-Nicolson scheme is usually unconditionally stable in $\|\cdot\|_2$ -norm, by the current approach we only proved the discretization (17)-(18) to be conditionally stable in Theorem 1. Further explorations are expected on unconditional stability.

4 Error analysis of the scheme

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

$$\begin{aligned}
(u \star v)^k &= \int_0^{k\Delta t} u(s)v(k\Delta t - s)ds - \frac{1}{2} \int_0^{\Delta t} \sum_{l=0}^{k-1} (u(\cdot)v(k\Delta t - \cdot))''(s + l\Delta t)s(s - \Delta t)ds \\
&= \int_0^{k\Delta t} u(s)v(k\Delta t - s)ds - \frac{1}{4} \int_0^{\Delta t} (u(\cdot)v(k\Delta t - \cdot))''(s)s(s - \Delta t)ds \\
&\quad + \frac{1}{4} \int_0^{\Delta t} (u(\cdot)v(k\Delta t - \cdot))''(k\Delta t + s)s(s - \Delta t)ds \\
&\quad - \frac{1}{2} \int_0^{\Delta t} \int_0^{k\Delta t} (u(\cdot)v(k\Delta t - \cdot))''(s + \tau)d\tau s(s - \Delta t)ds \frac{1}{\Delta t} \\
&\quad + \frac{1}{4} \int_0^{\Delta t} \left(\int_0^{k\Delta t} (u(\cdot)v(k\Delta t - \cdot))''''(s + \tau)\tau(\tau - k\Delta t)d\tau \right) s(s - \Delta t)ds \frac{1}{\Delta t} \\
&= (u * v)(k\Delta t) + r(k\Delta t, \Delta t)\Delta t^2,
\end{aligned} \tag{56}$$

for $k \geq 0$, where

$$\begin{aligned}
r(t, \Delta t) &= -\frac{\Delta t}{4} \int_0^1 (u(\cdot)v(t - \cdot))''(s\Delta t)s(s - 1)ds + \frac{\Delta t}{4} \int_0^1 (u(\cdot)v(t - \cdot))''(t + s\Delta t)s(s - 1)ds \\
&\quad - \frac{1}{2} \int_0^1 \int_0^t (u(\cdot)v(t - \cdot))''(s\Delta t + \tau)d\tau s(s - 1)ds \\
&\quad + \frac{1}{4} \int_0^1 \left(\int_0^t (u(\cdot)v(t - \cdot))''''(s\Delta t + \tau)\tau(\tau - t)d\tau \right) s(s - 1)ds
\end{aligned} \tag{57}$$

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

$$(u_n \star \dots (u_3 \star (u_2 \star u_1)) \dots)^k = (u_n * \dots (u_3 * (u_2 * u_1)) \dots)(k\Delta t) + r_n(k\Delta t, \Delta t)\Delta t^2. \tag{58}$$

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 $z = e^{\rho \Delta t + i\phi}$, one gets, for $1 \leq m, n \leq L$, the representation

$$\hat{f}_{m,n}^e(z) = \hat{f}_{m,n}(z) + \frac{\hat{r}_{m,n}(z, \Delta t)}{\hat{g}_{0,0}^e(z) - \frac{1}{2}} \Delta t, \tag{59}$$

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

$$\left| \frac{\hat{r}_{m,n}(z, \Delta t)}{\hat{g}_{0,0}^e(z) - \frac{1}{2}} \right| \leq C_{m,n,\rho}. \quad (60)$$

We also have

$$|h_{m,n}(z)| \leq C_{m,n,\rho}. \quad (61)$$

Proof. By using the representation given by (56), we have

$$g_{m,n}^e(k\Delta t) = (f_{m,n}^e * g_{0,0}^e)(k\Delta t) = (f_{m,n}^e \star g_{0,0}^e)^k + r_{m,n}(k\Delta t, \Delta t)\Delta t^2,$$

which leads to

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

which is nothing else than (59) 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 $r_{m,n}(t, \Delta t)$ fulfill 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

$$\begin{aligned} \hat{u}(z) - \frac{u(0)}{2} &= \frac{1}{2\pi\iota} \int_{\eta-\iota\infty}^{\eta+\iota\infty} \sum_{k=0}^{\infty} \tilde{u}(s) \frac{e^{sk\Delta t}}{z^k} ds - \frac{u(0)}{2} = \frac{1}{4\pi\iota} \int_{\eta-\iota\infty}^{\eta+\iota\infty} \sum_{k=0}^{\infty} \frac{u_k}{s^{k+1}} \frac{1 + e^{-(\rho-s)\Delta t - \iota\phi}}{1 - e^{-(\rho-s)\Delta t - \iota\phi}} ds \\ &= \frac{1}{2} \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k}{ds^k} \left(\frac{1 + e^{s-\rho\Delta t - \iota\phi}}{1 - e^{s-\rho\Delta t - \iota\phi}} \right)_{s=0} u_k \Delta t^k. \end{aligned} \quad (62)$$

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

$$\frac{\Delta t^l}{2} \frac{1}{l!} \frac{d^l}{ds^l} \left(\frac{1 + e^{s-\rho\Delta t - \iota\phi}}{1 - e^{s-\rho\Delta t - \iota\phi}} \right)_{s=0} = \frac{\Delta t^l}{2} \sum_{m=1}^l \frac{(e^{-\rho\Delta t - \iota\phi})^m}{(1 - e^{-\rho\Delta t - \iota\phi})^{m+1}} \sum_{|\alpha|=l, \alpha_i \geq 1} \frac{1}{\alpha!}, \quad (63)$$

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

$$\begin{aligned} \sum_{|\alpha|=l, \alpha_i \geq 1} \frac{1}{\alpha!} &\leq \sum_{|\alpha|=l} \frac{1}{\alpha!} = \frac{1}{2\pi\iota} \oint_{|z|=1} \frac{1}{z^{l+1}} (1 + z + \frac{z^2}{2!} + \dots)^m dz \\ &= \frac{1}{2\pi\iota} \oint_{|z|=1} \frac{1}{z^{l+1}} e^{mz} dz = \frac{1}{2\pi} \int_0^{2\pi} e^{me^{i\theta} - \iota(l-1)\theta} d\theta \leq e^m. \end{aligned} \quad (64)$$

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 (63)-(64), we have

$$\frac{\Delta t^l}{2} \frac{1}{l!} \frac{d^l}{ds^l} \left(\frac{1 + e^{s-\rho\Delta t - \iota\phi}}{1 - e^{s-\rho\Delta t - \iota\phi}} \right)_{s=0} \leq \frac{\Delta t^l}{2} \sum_{m=1}^l \frac{(e^{-\rho\Delta t})^m}{|1 + e^{-\rho\Delta t - \iota\phi_{\Delta t}\Delta t}|^{m+1}} e^m \leq C_l (e\Delta t)^l. \quad (65)$$

Now, taking $\hat{u}(z) := \hat{r}_{m,n}(z, \Delta t)$ in (62) (with $z = e^{\rho\Delta t + \iota\phi}$), using (63)-(64) and noticing that $r_{m,n}(0, \Delta t) = 0$ (by setting $t = 0$ in (57)) leads to

$$|\hat{r}_{m,n}(z, \Delta t)| \leq \sum_{k=1}^{\infty} C_k (e\Delta t)^k r_{m,n}(k\Delta t, \Delta t) = \mathcal{O}(\Delta t). \quad (66)$$

In addition, a direct computation yields

$$\begin{aligned} \hat{g}_{0,0}^e(e^{\rho\Delta t + \iota\phi}) - \frac{1}{2} &= \frac{1}{2} \frac{1 - e^{-\rho\Delta t - \iota\phi\Delta t}}{1 + e^{-\rho\Delta t - \iota\phi\Delta t}} - \frac{2e^{-\rho\Delta t - \iota\phi\Delta t}}{(1 + e^{-\rho\Delta t - \iota\phi\Delta t})^2} \Delta t + \mathcal{O}(\Delta t^2) \\ &= \left(\frac{\rho + \iota\phi\Delta t}{4} - 1 \right) \Delta t + \mathcal{O}(\Delta t)^2, \end{aligned} \quad (67)$$

giving then the inequality (60).

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 (63)-(64), we obtain

$$\begin{aligned} \left| \frac{\Delta t^l}{2} \frac{1}{l!} \frac{d^l}{ds^l} \left(\frac{1 + e^{s-\rho\Delta t - \iota\phi}}{1 - e^{s-\rho\Delta t - \iota\phi}} \right)_{s=0} \right| &\leq \frac{\Delta t^l}{2} \sum_{m=1}^l \left| \frac{(e^{-\rho\Delta t})^m}{(1 - e^{-\rho\Delta t - \iota\phi})^{m+1}} \right| \sum_{|\alpha|=l, \alpha_i \geq 1} \frac{1}{\alpha!} \\ &\leq C_l \frac{1}{|1 - e^{-\rho\Delta t - \iota\phi\Delta t}|} \sum_{m=1}^l \left(\frac{e}{|\rho + \phi_{\Delta t}|} \right)^m \Delta t^{l-m} \leq C_l \frac{1}{|1 - e^{-\rho\Delta t - \iota\phi\Delta t}|} \left(\frac{e}{|\rho + \phi_{\Delta t}|} \right)^l, \end{aligned} \quad (68)$$

which means

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

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

We also have

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

leading to (60).

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 $\alpha = \rho^3$)

$$\left| \frac{\Delta t}{1 - e^{-\rho\Delta t - \iota\phi}} \right| = \left| \frac{\Delta t}{1 - e^{-\iota\phi}} \right| \left| \left(1 + \frac{e^{-\rho\Delta t}(1 - e^{-\rho\Delta t})}{1 - e^{-\iota\phi}} \right)^{-1} \right| \leq C \frac{1}{\alpha} (1 + \mathcal{O}\left(\frac{\rho}{\alpha}\right)) \leq \frac{C}{\alpha}, \quad (69)$$

we deduce that

$$\begin{aligned} \left| \frac{\Delta t^l}{2} \frac{1}{l!} \frac{d^l}{ds^l} \left(\frac{1 + e^{s-\rho\Delta t - \iota\phi}}{1 - e^{s-\rho\Delta t - \iota\phi}} \right)_{s=0} \right| &= \frac{\Delta t^l}{2} \sum_{m=1}^l \left| \frac{(e^{-\rho\Delta t - \iota\phi})^m}{(1 - e^{-\rho\Delta t - \iota\phi})^{m+1}} \right| \sum_{|\alpha|=l, \alpha_i \geq 1} \frac{1}{\alpha!} \\ &\leq C \frac{1}{|1 - e^{-\rho\Delta t - \iota\phi}|} \sum_{m=1}^l \frac{C_m}{\alpha^m} \Delta t^{l-m} \leq \frac{1}{|1 - e^{-\rho\Delta t - \iota\phi}|} \frac{CC_l}{\alpha^l}, \end{aligned} \quad (70)$$

which means

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

Furthermore, we also have

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

finally leading to (60).

Concerning the inequality (61), a similar proof can be adapted, starting from the definition of $h_{m,n}$ given by (25). □

Let now us introduce the following indices: $N_{m,n}^1 = I_m - I_n$ and $N_{m,n}^2 = J_m - I_n$. We also define $I_1^k, I_2^k, \dots, I_{4L-5}^k$ as the ordered indices $I_1, I_2, \dots, I_{4L-4}$ excluding the k -th one ($1 \leq k \leq 4L-4$). Finally, let us set $N_{m,n}^{1,k,l} = I_m^k - I_n^l$. From the boundary condition (16), we have by Laplace transform

$$\begin{aligned} \tilde{\psi}_{I_m}^e(s) &= \sum_{n=1}^{4L-4} \tilde{f}_{I_m-I_n}^e(s) \tilde{\chi}_{I_n}^e(s), & 1 \leq m \leq 4L-4, \\ \tilde{\psi}_{J_m}^e(s) &= \sum_{n=1}^{4L-4} \tilde{f}_{J_m-I_n}^e(s) \tilde{\chi}_{I_n}^e(s), & 1 \leq m \leq 4L. \end{aligned} \tag{71}$$

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 $f_{N_{m,n}^1}^e$. In a similar way, \mathbf{B}^e is a $4L \times (4L-4)$ matrix such that its (m,n) -th element is equal to $f_{N_{m,n}^2}^e$. As a consequence, system (71) leads to

$$\tilde{\psi}_J^e = \tilde{\mathbf{B}}^e (\tilde{\mathbf{A}}^{1,e})^{-1} \tilde{\psi}_I^e = \tilde{\mathbf{F}}^e \tilde{\psi}_I^e. \tag{72}$$

(The inversion of the matrix $\tilde{\mathbf{A}}^{1,e}$ can be obtained from the expression (9).) Let us denote by σ_{4L-5} the set of all permutations of the indices from 1 to $4L-5$, an element of the set being written as $i := (i_1, i_2, \dots, i_{4L-5}) \in \sigma_{4L-5}$. Following Cramer's rule, for $1 \leq l \leq 4L$, one can write that

$$\begin{aligned} \tilde{\psi}_{J_l}^e &= \sum_{1 \leq m, n \leq 4L-4} (\tilde{\mathbf{B}}^e)_{l,m} ((\tilde{\mathbf{A}}^{1,e})^{-1})_{m,n} \tilde{\psi}_{I_n}^e \\ &= \sum_{1 \leq m, n \leq 4L-4} \tilde{\psi}_{I_n}^e \frac{1}{\det(\tilde{\mathbf{A}}^{1,e})} \tilde{f}_{N_{l,m}^2}^e (-1)^{m+n} \sum_{i \in \sigma_{4L-5}} \delta^i \prod_{p=1}^{4L-5} \tilde{f}_{N_{p,i_p}^1}^e, \end{aligned} \tag{73}$$

where δ^i is the signature of the permutation for a given index $i \in \sigma_{4L-5}$. Let us now define σ_{4L-4}^0 as the set σ_{4L-4} excluding $(1, 2, \dots, 4L-4)$. Multiplying by $\det(\tilde{\mathbf{A}}^{1,e})$ on both sides of (73), then inverting by Laplace transform, one has

$$\begin{aligned} \psi_{J_l}^e + \sum_{j \in \sigma_{4L-4}^0} \delta^j f_{h_{1,j_1}^1}^e * (\dots * (f_{N_{4L-4,j_{4L-4}}^1}^e * \psi_{J_l}^e) \dots) \\ = \sum_{1 \leq m, n \leq 4L-4} f_{N_{l,m}^2}^e (-1)^{m+n} * \left(\sum_{i \in \sigma_{4L-5}} \delta^i f_{N_{1,i_1}^1}^e * (\dots * (f_{N_{4L-5,i_{4L-5}}^1}^e * \psi_{I_n}^e) \dots) \right). \end{aligned} \tag{74}$$

From (74) and by using (58), one gets

$$\begin{aligned}
& (\psi_{J_l}^e)^k + \sum_{j \in \sigma_{4L-4}^0} \delta^j [f_{N_{1,j_1}^e}^e \star (\dots \star (f_{N_{4L-4,j_{4L-4}}^e}^e \star \psi_{J_l}^e) \dots)]^k \\
&= \sum_{1 \leq m, n \leq 4L-4} [f_{N_{l,m}^e}^e (-1)^{m+n} \star (\sum_{i \in \sigma_{4L-5}} \delta^i f_{N_{1,i_1}^{1,n,m}}^e \star (\dots (f_{N_{4L-5,i_{4L-5}}^{1,n,m}}^e \star \psi_{I_n}^e) \dots))]^k + H_l(k\Delta t, \Delta t) \Delta t^2,
\end{aligned} \tag{75}$$

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 (75) leads to

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

Now, thanks to (59), one has

$$\begin{aligned}
& \hat{\psi}_{J_l}^e(z) + \hat{\psi}_{J_l}^e(z) \sum_{j \in \sigma_{4L-4}^0} \delta^j \prod_{p=1}^{4L-4} \left(\hat{f}_{h_{p,j_p}^1}^e(z) \Delta t - f_{h_{p,j_p}^1}^e(0) \Delta t / 2 \right) \\
&= \sum_{1 \leq m, n \leq 4L-4} \hat{\psi}_{I_n}^e(z) \left(\hat{f}_{h_{l,m}^2}^e(z) \Delta t - f_{h_{l,m}^2}^e(0) \Delta t / 2 \right) (-1)^{m+n} \\
&\quad \sum_{i \in \sigma_{4L-5}} \delta^i \prod_{p=1}^{4L-5} \left(\hat{f}_{h_{p,i_p}^{1,n,m}}^e(z) \Delta t - \hat{f}_{h_{p,i_p}^{1,n,m}}^e(0) \Delta t / 2 \right) \\
&+ \left(\sum_{1 \leq m, n \leq 4L-4} G_{1,l,m,n}(z, \Delta t) \hat{\psi}_{I_n}^e(z) \Delta t^2 + G_{2,l}(z, \Delta t) \hat{\psi}_{J_l}^e(z) \Delta t^2 + \hat{H}_l(z, \Delta t) \Delta t^2 \right),
\end{aligned} \tag{77}$$

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 $h_{p,q}$

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

Next, by using Lemma 2, (58) and (99) (Lemma 4, Appendix A), we can prove the following bounds

$$|G_{1,l,m,n}(z, \Delta t)| \leq C_{1,l,m,n,\rho}, \quad |G_{2,l}(z, \Delta t)| \leq C_{2,l,\rho}, \tag{78}$$

for some well-chosen positive real-valued constants $C_{1,l,m,n,\rho}$ and $C_{2,l,\rho}$ which depend on the bounds of $\psi_{m,n}^e(t)$ and of its derivatives.

Now, by using (31), (77) is

$$\begin{aligned}\hat{\psi}_{J_l}^e(z) &= \sum_{1 \leq m, n \leq 4L-4} (\mathbf{B})_{l,m} ((\mathbf{A}^1)^{-1})_{m,n} \hat{\psi}_{I_n}^e(z) + R_l(z, \Delta t) \Delta t^2 \\ &= \sum_{1 \leq n \leq 4L-4} (\mathbf{F})_{l,n} \hat{\psi}_{I_n}^e(z) + R_l(z, \Delta t) \Delta t^2,\end{aligned}\tag{79}$$

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

$$\hat{\psi}_J(z) = \mathbf{F}(z) \hat{\psi}_I(z) := \mathbf{B}(z) (\mathbf{A}^1(z))^{-1} \hat{\psi}_I(z)\tag{80}$$

and

$$R_l(z, \Delta t) = \frac{1}{\det(\mathbf{A}^1)} \left[\sum_{1 \leq m, n \leq 4L-4} G_{1,l,m,n}(z, \Delta t) \hat{\psi}_{I_n}^e(z) + G_{2,l}(z, \Delta t) \hat{\psi}_{J_l}^e(z) + \hat{H}_l(z, \Delta t) \right].\tag{81}$$

Let us also remark that, if ρ is a given large enough positive constant, then there exists Δt_0 , such that, for $\Delta t \leq \Delta t_0$, \mathbf{F} being given by (80), for any vector \mathbf{V} of size $4L - 4$ and angle ϕ , we have

$$\text{Im} \left[\bar{\mathbf{V}}^T \bar{\mathbf{F}}^T (e^{\rho \Delta t + i\phi}) \mathbf{I}_1 \mathbf{V} \right] \leq 0.\tag{82}$$

Let us now prove the following error estimate.

Theorem 2. *Let us consider the scheme (17)-(18). 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*

$$\| \psi^K - \psi^e(t_K) \|_2 \leq C(L, T, \psi^e(0)) \Delta t^2,\tag{83}$$

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: $e_{m,n}^k = (\psi_{m,n}^e)^k - \psi_{m,n}^k$. Then one can see that

$$-\frac{2l}{\Delta t} (e_{m,n}^k - e_{m,n}^{k-1}) = \Delta (e_{m,n}^{k-1} + e_{m,n}^k) + r_{m,n,k-\frac{1}{2}},\tag{84}$$

where $r_{m,n,k-\frac{1}{2}}$ is the local residual. From (79), the \mathcal{Z} -transform of the boundary conditions leads to

$$\begin{aligned}\hat{e}_{J_m}(z) &= \sum_{\substack{n=1 \\ 4L-4}}^{4L-4} \mathbf{F}_{m,n}(z) \hat{\psi}_{I_n}^e(z) + R_m(z, \Delta t) \Delta t^2 - \sum_{n=1}^{4L-4} \mathbf{F}_{m,n}(z) \hat{\psi}_{I_n}(z) \\ &= \sum_{n=1}^{4L-4} \mathbf{F}_{m,n}(z) \hat{e}_{I_n}(z) + R_m(z, \Delta t) \Delta t^2,\end{aligned}\tag{85}$$

where $1 \leq m \leq 4L - 4$. If we define $\eta_{m,n}^k = \beta^{-k} e_{m,n}^k$, 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

$$\begin{aligned} \|\eta^K\|_2^2 &\leq \frac{1 - \beta^2}{\beta^2} \sum_{k=0}^{K-1} \|\eta^k\|_2^2 + \sum_{k=1}^K \left[\frac{\Delta t}{2\beta} \sum_{n=1}^L \sum_{m=1}^L (\eta_{m,n}^{k-1} \beta^{-k} |r_{m,n,k-\frac{1}{2}}| + \eta_{m,n}^k \beta^{-k+1} |r_{m,n,k-\frac{1}{2}}|) \right] \\ &+ \text{Im} \frac{\Delta t}{2\beta^2} \sum_{k=1}^K \sum_{m=1}^{4L} \overline{[(\eta_{J_m}^{k-1} + \beta \eta_{J_m}^k)(\eta_{I_m}^{k-1} + \beta \eta_{I_m}^k - \eta_{J_m}^{k-1} - \beta \eta_{J_m}^k)]}. \end{aligned} \quad (86)$$

Now, based on (85), one gets

$$\begin{aligned} &\text{Im} \sum_{k=1}^K \sum_{m=1}^{4L} \overline{[(\eta_{J_m}^{k-1} + \beta \eta_{J_m}^k)(\eta_{I_m}^{k-1} + \beta \eta_{I_m}^k - \eta_{J_m}^{k-1} - \beta \eta_{J_m}^k)]} \\ &= \text{Im} \frac{1}{2\pi} \int_0^{2\pi} \left[|1 + \beta e^{\iota\phi}|^2 \sum_{m=1}^{4L} \bar{\hat{e}}_{J_m}(\beta e^{\iota\phi}) (\hat{e}_{I_m}(\beta e^{\iota\phi}) - \hat{e}_{J_m}(\beta e^{\iota\phi})) \right] d\phi \\ &= \frac{1}{2\pi} \text{Im} \int_0^{2\pi} |1 + \beta e^{\iota\phi}|^2 \bar{\hat{e}}_I^T(\beta e^{\iota\phi}) \bar{\mathbf{F}}^T(\beta e^{\iota\phi}) (\mathbf{I}_1 - \mathbf{F}(\beta e^{\iota\phi})) \hat{e}_I(\beta e^{\iota\phi}) d\phi \\ &+ \frac{1}{2\pi} \text{Im} \int_0^{2\pi} |1 + \beta e^{\iota\phi}|^2 \left[\sum_{m=1}^{4L} \bar{R}_m(\beta e^{\iota\phi}, \Delta t) \hat{e}_{I_m}(\beta e^{\iota\phi}) \right] d\phi \Delta t^2. \end{aligned} \quad (87)$$

The first integral of the above last equality does not contribute to the computation since it is less than zero. This then leads to

$$\begin{aligned} &\Delta t \text{Im} \sum_{k=1}^K \sum_{m=1}^{4L} \overline{[(\eta_{J_m}^{k-1} + \beta \eta_{J_m}^k)(\eta_{I_m}^{k-1} + \beta \eta_{I_m}^k - \eta_{J_m}^{k-1} - \beta \eta_{J_m}^k)]} \\ &\leq \Delta t^3 \frac{1}{2\pi} \left| \int_0^{2\pi} |1 + \beta e^{\iota\phi}|^2 \sum_{m=1}^{4L} \bar{R}_m(\beta e^{\iota\phi}, \Delta t) \hat{e}_{I_m}(\beta e^{\iota\phi}) d\phi \right|. \end{aligned} \quad (88)$$

From relations (78), (81) and (99) (Lemma 4, Appendix A), we conclude that

$$\begin{aligned} &\Delta t^3 \left| \frac{1}{2\pi} \int_0^{2\pi} |1 + \beta e^{\iota\phi}|^2 \bar{R}_l(\beta e^{\iota\phi}, \Delta t) \hat{e}_{I_l}(\beta e^{\iota\phi}) d\phi \right| \leq \frac{\beta^2 - 1}{4\beta^2} \sum_{k=0}^K \left| \eta_{I_l}^k \right|^2 \\ &+ \frac{C \Delta t^5 \beta^2}{(\beta^2 - 1)} \left(\max_{1 \leq m, n \leq 4L-4} \|(\det \hat{\mathbf{F}}_1(\beta e^{\iota\phi}))^{-1} G_{1,l,m,n}(\beta e^{\iota\phi}, \Delta t)\|_{L^\infty[0,2\pi]} \right. \\ &+ \left. \|(\det \hat{\mathbf{F}}_1(\beta e^{\iota\phi}))^{-1} G_{2,l}(\beta e^{\iota\phi}, \Delta t)\|_{L^\infty[0,2\pi]} + \|(\hat{\mathbf{F}}_1(\beta e^{\iota\phi}))^{-1}\|_{L^\infty[0,2\pi]} \right)^2 \\ &\times \left(\max_{1 \leq m \leq 4L} \Delta t \sum_{k=0}^K \left| \psi_{J_m}^{e,k} \right|^2 + \max_{1 \leq n \leq 4L} \Delta t \sum_{k=0}^K \left| \psi_{I_n}^{e,k} \right|^2 + \Delta t \sum_{k=0}^K \left| H_l^k \right|^2 \right) \\ &\leq \frac{\beta^2 - 1}{4\beta^2} \sum_{k=0}^K \left| \eta_{I_l}^k \right|^2 + \Delta t^4 C(L, T, \psi^e(0)), \end{aligned} \quad (89)$$

which provides

$$\begin{aligned} \Delta t \operatorname{Im} \sum_{k=1}^K \sum_{m=1}^{4L} \overline{[(\eta_{J_m}^{k-1} + \beta \eta_{J_m}^k)(\eta_{I_m^1}^{k-1} + \beta \eta_{I_m^1}^k - \eta_{J_m}^{k-1} - \beta \eta_{J_m}^k)]} \\ \leq \frac{\beta^2 - 1}{2\beta^2} \sum_{k=0}^K \|\eta^k\|_2^2 + \Delta t^4 C(L, T, \psi^e(0)). \end{aligned} \quad (90)$$

To get (90) from (89), 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,

$$\begin{aligned} \frac{1}{2\pi} \int_0^{2\pi} |\hat{a}(e^{i\varphi}) \hat{b}(e^{i\varphi}) \hat{c}(e^{i\varphi})| d\varphi &\leq \frac{1}{2\pi} \|\hat{a}(e^{i\varphi})\|_{L^\infty[0,2\pi]} \|\hat{b}(e^{i\varphi})\|_{L^2[0,2\pi]} \|\hat{c}(e^{i\varphi})\|_{L^2[0,2\pi]} \\ &= \frac{1}{2\pi} \|\hat{a}(e^{i\varphi})\|_{L^\infty[0,2\pi]} \|b\|_{l^2} \|c\|_{l^2} \leq \varepsilon \|c\|_{l^2}^2 + C(\varepsilon) (\|\hat{a}(e^{i\varphi})\|_{L^\infty[0,2\pi]} \|b\|_{l^2})^2, \end{aligned} \quad (91)$$

setting $\|a\|_{l^2}^2 = \sum_{k=0}^K |a_k|^2$. 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 $\|\eta^k\|_2$. The indices η_{J_l} are not in the computational domain. However, the terms which contain an index η_{J_l} are negative in (87), so they do not need to be estimated in L^2 -norm [31]. By using (99), we obtain: $|r_{m,n,k+\frac{1}{2}}| \leq C(\psi^e(0)) \Delta t^2$. Then, by combining with (86), one gets

$$\begin{aligned} \|\eta^K\|_2^2 &\leq \frac{1 - \beta^2}{\beta^2} \sum_{k=0}^{K-1} \|\eta^k\|_2^2 + \frac{\beta^2 - 1}{2\beta^2} \sum_{k=0}^K \|\eta^k\|_2^2 + C(L, \psi^e(0)) \Delta t^4 \\ &\quad + \frac{\beta^2 - 1}{2\beta^2} \sum_{k=0}^K \|\eta^k\|_2^2 + \frac{C \Delta t^2}{(\beta^2 - 1)} \sum_{k=1}^K \sum_{1 \leq m, n \leq L} |r_{m,n,k-\frac{1}{2}}|^2. \end{aligned} \quad (92)$$

Finally, we have

$$\|\eta^K\|_2^2 \leq C(L, T, \psi^e(0)) \Delta t^4, \quad (93)$$

yielding

$$\|\psi^K - \psi^e(K \Delta t)\|_2 \leq C(L, T, \psi^e(0)) \Delta t^2, \quad (94)$$

ending hence the proof. \square

5 Discussion and Conclusion

In this paper, we proved the L^2 -stability of the Crank-Nicolson discretization of the semi-discrete Schrödinger equation with the artificial boundary condition derived in [24]. In addition, the full scheme is proved to be second-order in time. These results confirm the numerical simulations presented in [24].

Nevertheless, to fully analyze the scheme, some points remain to prospect. For example, the presented convergence analysis of the scheme does not include yet the spatial convergence analysis which will be studied in a forthcoming paper. Furthermore, fast evaluation schemes for integral operators should be used in conjunction with the ABC method to have an efficient scheme. This needs to be further prospected from the point of view of the design of the algorithm but also concerning

the effect of these additional approximations on the numerical analysis of the full scheme. Finally, the extension to the nonlinear case can be obtained thanks to time-splitting schemes [3, 26] and the methodology should also yield the construction of ABCs for 2D nonlocal Schrödinger equations in rectangular domains, combined with the recent results in [23].

A Proof of Lemma 4

Since the initial condition is compactly supported, then it is square integrable, i.e. $\|\psi^e(0)\|_{*,2} < \infty$, where the L^2 -norm on the infinite lattice is defined by

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

Lemma 3. *The behavior of the exact solution $\psi_{m,n}^e$ of (2) at infinity is such that*

$$|\psi_{m,n}^e(t)| \sim \mathcal{O}\left(\frac{1}{|m| + |n|}\right) \quad \text{for } |m| + |n| \rightarrow \infty.$$

Proof. Setting $\tilde{\lambda}_{I_k}^e(s) = \frac{\tilde{\chi}_{I_k}^e(s)}{\tilde{g}_{0,0}^e(s)}$, for $1 \leq k \leq 4L - 4$, and from (16), the boundary conditions can be written as

$$\psi_{I_k}^e(t) = \sum_{\ell=1}^{4L-4} g_{I_k - I_\ell}^e(t) * \lambda_{I_\ell}^e(t), \quad 1 \leq k \leq 4L - 4. \quad (95)$$

Then, for any term $\psi_{m,n}^e(t)$ outside the computational domain, one has from (13)

$$\psi_{m,n}^e(t) = \sum_{\ell=1}^{4L-4} g_{(m,n) - I_\ell}^e * \lambda_{I_\ell}^e(t). \quad (96)$$

By integration by parts for (36) and for fixed t , we have

$$|g_{m,n}^e(t)| \sim \mathcal{O}\left(\frac{1}{\max(|m|, |n|)}\right) \sim \mathcal{O}\left(\frac{1}{|m| + |n|}\right) \quad (97)$$

and

$$|\psi_{m,n}^e(t)| = \left| \sum_{\ell=1}^{4L-4} g_{(m,n) - I_\ell}^e * \lambda_{I_\ell}^e(t) \right| \sim \mathcal{O}\left(\frac{1}{|m| + |n|}\right) \quad \text{for } |m| + |n| \rightarrow \infty,$$

leading to

$$|\psi_{m,n}^e(t)| \rightarrow 0 \quad \text{for } |m| + |n| \rightarrow \infty. \quad (98)$$

□

If we define $\psi_{m,n}^{e,(k)}(t)$ as the k -th order time derivative of $\psi_{m,n}^e(t)$, then, we can also prove that $|\psi_{m,n}^{e,(k)}(t)| \sim \mathcal{O}\left(\frac{1}{|m| + |n|}\right)$ when $|m| + |n| \rightarrow \infty$.

Let us now prove the following Lemma.

Lemma 4. *We have the following L^2 -norm (mass) conservation property*

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

Furthermore, the following inequality holds

$$\|\psi^{e,(k)}(t)\|_{*,2} = \|\psi^{e,(k)}(0)\|_{*,2} \leq 10^k \|\psi^e(0)\|_{*,2}, \quad (99)$$

and $\psi^e : \mathbb{R}_0^+ \rightarrow \ell^2(\mathbb{Z}^2)$ is an analytic function.

Proof. By multiplying (2) by $\overline{\psi_{m,n}^e(t)}$, taking the complex conjugate of (2) and multiplying it by $-\psi_{m,n}^e(t)$, then summing up the two equations for (m,n) such that $-N \leq m, n \leq N$, and summing by parts the resulting equation, one gets

$$\begin{aligned} & \sum_{n=-N}^N \sum_{m=-N}^N (|\psi_{m,n}^e(t)|^2 - |\psi_{m,n}^e(0)|^2) = \\ & + \operatorname{Im} \sum_{n=-N}^N \left[\overline{(\psi_{-N,n}^e(0) + \psi_{-N,n}^e(t))} \Delta_x^+ (\psi_{-N,n}^e(0) + \psi_{-N,n}^e(t)) \right. \\ & \left. - \overline{(\psi_{N,n}^e(0) + \psi_{N,n}^e(t))} \Delta_x^- (\psi_{N,n}^e(0) + \psi_{N,n}^e(t)) \right] \\ & + \operatorname{Im} \sum_{m=-N}^N \left[\overline{(\psi_{m,-N}^e(0) + \psi_{m,-N}^e(t))} \Delta_y^+ (\psi_{m,-N}^e(0) + \psi_{m,-N}^e(t)) \right. \\ & \left. - \overline{(\psi_{m,N}^e(0) + \psi_{m,N}^e(t))} \Delta_y^- (\psi_{m,N}^e(0) + \psi_{m,N}^e(t)) \right]. \end{aligned} \quad (100)$$

When $N \rightarrow \infty$, from Lemma 3, the left side of (100) behaves like $8N \times \mathcal{O}(1/N^2) = \mathcal{O}(8/N)$, and thus we obtain

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

In addition, taking the k -th derivative of the semi-discrete equation (2), we have

$$\iota \psi_{m,n}^{e,(k+1)} = -(\psi_{m,n-1}^{e,(k)} + \psi_{m,n+1}^{e,(k)} + \psi_{m+1,n}^{e,(k)} + \psi_{m-1,n}^{e,(k)} - 4\psi_{m,n}^{e,(k)}),$$

which means that

$$|\psi_{m,n}^{e,(k+1)}| \leq |\psi_{m,n-1}^{e,(k)}| + |\psi_{m,n+1}^{e,(k)}| + |\psi_{m+1,n}^{e,(k)}| + |\psi_{m-1,n}^{e,(k)}| + 4|\psi_{m,n}^{e,(k)}|.$$

This leads to

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

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

$$\sum_{m,n} |\psi_{m,n}^{e,(k+1)}|^2 \leq 100 \sum_{m,n} |\psi_{m,n}^{e,(k)}|^2.$$

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