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Gang PANG[a,*], Songsong JI[b], Xavier ANTOINE[c]

[a] *School of Mathematical Science, Beijing University of Areonautics and Astronautics, Beijing 100083, China*
[b] *HEDPS,CAPT,and LTCS, College of Engineering, Peking University, Beijing 100871, China*
[c] *Université de Lorraine, CNRS, Inria, IECL, F-54506 Vandoeuvre-lès-Nancy Cedex, France*

Abstract

The construction of exact absorbing boundary conditions (ABCs) for the one-dimensional nonlocal fully-discrete Schrödinger equation is proposed. The computation of the Green's functions for the discrete nonlocal Schrödinger equation is stated and used to build the ABCs. Numerical error estimates are then proved for the case of a singular interaction kernel. The theory and numerical analysis is supported by numerical examples.

Keywords: Nonlocal Schrödinger equation, exact absorbing boundary condition, stability and error analysis

1. Introduction

Two decades ago, Laskin [1, 2, 3, 4] proposed a time-dependent space Fractional Schrödinger Equation (FSE) which can be used e.g. to describe the fractional oscillator of Bohr atom [1] or long-range dispersive interactions properties [5]. The specificity of the FSE is that it involves a fractional Laplacian term $(-\partial_x^2)^{s/2}$, usually for $1 \leq s \leq 2$, instead of the standard local Laplacian ($s = 2$). The FSE led to many developments, from both the applications, theoretical and numerical sides (see e.g. [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]), and has shown to produce specific behaviors compared with the local Schrödinger equation. More generally, fractional PDE models can be embedded into the framework of nonlocal PDEs [17] to include more advanced long range interactions that are not met in the fractional situation. From this view point, the fractional PDE model can be interpreted as a nonlocal model for a specific kernel. In the present paper, we consider the one-dimensional system with nonlocal Schrödinger equation: find the function ψ solution to

$$\left\{ \begin{array}{l} \mathrm{i}\psi_t(x,t) = \mathcal{L}_\delta \psi(x,t), \quad x \in \mathbb{R}, \quad t \in (0,T], \\ \psi(x,0) = \psi^0(x), \quad x \in \mathbb{R}, \\ \lim_{|x|\to+\infty} \psi(x,t) = 0, \quad t \in (0,T], \end{array} \right. \tag{1}$$

where $\mathrm{i} = \sqrt{-1}$ and ψ^0 is a given initial data. The maximal time of computation is T. The nonlocal operator $\mathcal{L}_\delta$ appearing in (1) extends the fractional Laplacian [17] and is given by

$$\mathcal{L}_\delta \psi(x) = \int_{\mathbb{R}} \gamma_\delta(y-x, \frac{y+x}{2})(\psi(x) - \psi(y))dy. \tag{2}$$

We assume that the interaction kernel function γ_δ has the following properties

*Author for correspondence, gangpang@buaa.edu.cn

- positiveness: $\gamma_\delta(a,b) \geq 0$;
- symmetry according to the first argument a: $\gamma_\delta(-a,b) = \gamma_\delta(a,b)$;
- finite horizon: $\exists \delta > 0$ such that $\gamma_\delta(a,b) = 0$ if $|a| > \delta > 0$.

In the above notations, $a = x - y$ measures the distance between the two points x and y, and $(x+y)/2$ controls the local horizon. We also need to precise some additional assumptions that are used later [18, 19] to solve the nonlocal model set in a finite computational domain $]x_-, x_+[$

- A1: we assume that the initial data ψ^0 is compactly supported in $]x_-, x_+[$;
- A2: γ_δ is compactly supported in $[-\delta, \delta] \times \mathbb{R}$ for $\delta \leq (x_+ - x_-)/2$;
- A3: γ_δ is homogeneous in the exterior domain, i.e.

$$\begin{array}{ll} \gamma_\delta(a,b) = \gamma_{\delta,-}(a), & \text{for } b \in (-\infty, x_- + \delta], \\ \gamma_\delta(a,b) = \gamma_{\delta,+}(a), & \text{for } b \in [x_+ - \delta, +\infty). \end{array} \tag{3}$$

Here, we consider that $\gamma_{\delta,\pm} =: \gamma_\infty$ to simplify the presentation. Finally, similar problems to (1) could also arise for nonlocal diffusion [17, 20].

The aim of the paper is to develop truncation techniques for computing the solution to (1) in the finite computational domain $]x_-, x_+[$. Many contributions were proposed to solve this problem for integer order partial differential equations, usually by considering transparent/artificial/absorbing boundary conditions (ABC) at a fictitious boundary, or alternatively absorbing layers or Perfectly Matched Layer (PML). We refer e.g. to [21, 22] for details about this topic in the case of quantum mechanics equations. Developing ABC or absorbing layers/PML truncation techniques for spatially nonlocal and fractional models remains much less studied than for local PDEs. For ABCs, techniques based on DtN operators have been introduced in [23, 24] in the case of nonlocal heat equations. Furthermore, a full numerical analysis of ABCs is available in [25]. For the two-dimensional nonlocal wave equation, ABCs were constructed in [26, 27] while for nonlocal Schrödinger equations, ABCs were proposed and numerically approximated in [19, 28]. In the framework of the absorbing layers/PML approach, efficient and precised methods were designed in [29, 30, 31, 32] for time-dependent heat and Schrödinger equations involving fractional operators, most particularly the fractional Laplacian. It is nevertheless unclear if these approaches can be extended to more general nonlocal models as the one considered here.

The goal of the present paper is to propose the construction of ABCs for a fully discretized version of (1) and to develop the error analysis of the scheme. To this end, in section 2.1, we discretize (1) by using a Crank-Nicolson scheme in time and an asymptotically compatible scheme in space. This allows us to derive the exact ABC for the fully discrete scheme in subsection 2.2. In addition, we propose a numerical algorithm for computing the kernel functions involved in the definition of the ABCs in subsection 2.3. After stating some properties of these kernel functions in section 3, we prove the stability of the boundary condition. We next develop in section 4 the error analysis between the exact solution of (1) and the solution of the semi-discretized system associated with (1) in the nontrivial case of a singular interaction kernel γ_δ. This shows that the error is second-order both in space and time. In section 5, we study the error analysis for the numerical solution of (1) with given boundary condition, showing the second-order convergence of the scheme. We end the paper by some numerical examples in section 6, a conclusion in section 7 and the technical Appendix A.

2. Exact absorbing boundary conditions for the fully discrete nonlocal Schrödinger equation

To design some exact absorbing boundary conditions for the nonlocal Schrödinger equation appearing in system (1), we first fully discretize the equation in subsection 2.1 and next extract the corresponding boundary conditions in subsections 2.2 and 2.3.

2.1. Full discretization of the 1D nonlocal Schrödinger equation

For the spatial discretization, we use the Asymptotic Compatibility (AC) discretization scheme derived in [26] to approximate the nonlocal operator $\mathcal{L}_\delta$ given by (2) (see [33, 34] for other AC schemes). Let us set discretize $[x_-, x_+]$ by using $J+1$ equally spaced grid points $x_j = x_- + jh$, $0 \le j \le J$, for the uniform spatial step $h := (x_+ - x_-)/J > 0$, with $x_0 = x_-$ and $x_J = x_+$. We introduce ϕ_j as the standard hat function of width h centered at point x_j. Then, we have the following spatial approximation, for $j \in \mathbb{Z}$,

$$\mathcal{L}_\delta \psi(x_j) \approx L_{\delta,h}\psi_j = \sum_{k\in\mathbb{Z}} b_{j,k}(\psi_j - \psi_k), \tag{4}$$

where $\psi_j \approx \psi(x_j, \cdot)$ and the real-valued coefficients $b_{j,k}$ are given by

$$b_{j,k} = -c_{j-k} := \begin{cases} \dfrac{1}{(j-k)h}\displaystyle\int_{\mathbb{R}} y\phi_{j-k}(y)\gamma_\delta(y, \frac{x_j+x_k}{2})dy, & j \ne k, \\ 0, & j = k, \end{cases}$$

and $b_{k,j} = b_{j,k}$. Since the kernel function γ_δ is compactly supported, then one gets: $b_{j,k} = 0$ for $|j-k| > K := [\delta/h] + 1$, where $[\cdot]$ is the floor function. Therefore, the sum in (4) is finite with index $k = -K, ..., K$.

Let us now consider a Hilbert space $\mathcal{H}$ equipped with an inner product $(\cdot,\cdot)_{\mathcal{H}}$ and induced norm $\|\cdot\|_{\mathcal{H}}$. We introduce the semi-infinite sequence space

$$\ell^2(\mathcal{H}) = \Big\{ u = \{u^n\}_{n=0}^\infty : u^n \in \mathcal{H},\ \|u\|_{\ell^2(\mathcal{H})} = (\sum_{n=0}^\infty \|u^n\|_{\mathcal{H}}^2)^{\frac{1}{2}} < \infty \Big\},$$

with the inner product: $(u,v)_{\ell^2(\mathcal{H})} \equiv \sum_{n=0}^\infty (u^n, v^n)_{\mathcal{H}}$, $\forall u, v \in \ell^2(\mathcal{H})$. For a sequence $u = \{u^n\}_{n=0}^\infty \in \ell^2(\mathcal{H})$, we define the operator S by: $Su = \{u^{n+1}\}_{n=0}^\infty$. The average operator E and the forward difference quotient operator D_τ with uniform time step τ are given by $E = (S+I)/2$ and $D_\tau = (S-I)/\tau$, respectively. We also need the following notations: $Su^n = (Su)^n$, $Eu^n = (Eu)^n$ and $D_\tau u^n = (D_\tau u)^n$. Let us define the coefficients:

$$a_0 = -2\sum_{k=1}^K c_k, \quad \text{and} \quad a_k = c_k, \quad k = 1, ..., K. \tag{5}$$

After some calculations, we obtain the discretized nonlocal Schrödinger equation approximating (1) and based on the Crank-Nicolson time scheme at time $t_n = n\tau$, $n \in \mathbb{N}$, and AC discretization

$$\mathrm{i}D_\tau \psi_j^n = EL_{\delta,h}\psi_j^n := a_0 E\psi_j^n + \sum_{k=1}^K a_k(E\psi_{j+k}^n + E\psi_{j-k}^n), \quad \text{for } j \in \mathbb{Z}, \tag{6}$$

where we denote by ψ_j^n the numerical approximation of $\psi(x_j, t_n)$.

2.2. Exact absorbing boundary condition for the fully discrete nonlocal Schrödinger equation

For ψ_j^0, $j = 0, ..., J$, compactly supported in $[x_0, x_J]$, we need to introduce some artificial boundary conditions to complete (6) written for $j = 0, ..., J$. To this end, we derive in Theorem 1 a relation between the left exterior unknowns ψ_j^n (red dots in Figure 1), $j \leq -1$, and the interior left values ψ_j^n (blue dots) ($0 \leq j \leq K-1$) in the computational domain, which will play the role of left absorbing boundary condition. A similar relation is given for the right ABC as shown on Figure 1 for the nodes $J+1 \leq j \leq J+K$.

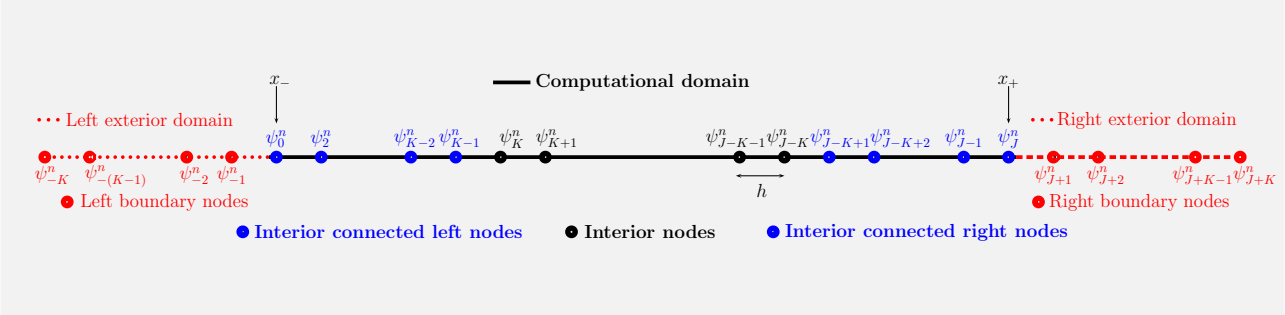

Figure 1: Discretization of the domain and unknowns.

Before giving Theorem 1, we introduce the convolution of two sequences $(g^n)_n$ and $(f^n)_n$ as: $(f \star g)^n := \sum_{r=0}^n g^{n-r} f^n$. For two sequences of matrices $(\mathbb{A}^n)_n$ and $(\mathbb{B}^n)_n$ of size $K \times K$, and for a K components vector sequence $(\mathbf{v}^n)_n$, we define the $K \times K$ matrix $(\mathbb{A} \star \mathbb{B})^n := \sum_{r=0}^n \mathbb{A}^{n-r}\mathbb{B}^r$, and the vector (of size K) $(\mathbb{A} \star \mathbf{v})^n := \sum_{r=0}^n \mathbb{A}^{n-r}\mathbf{v}^r$. For the tools related to the $\mathcal{Z}$-transform, we introduce: $\widehat{f}(z) := \sum_{k=0}^\infty f^n z^{-n}$, $\widehat{\mathbb{A}}(z) := \sum_{n=0}^\infty \mathbb{A}^n z^{-n}$ and $\widehat{\mathbf{v}}(z) := \sum_{n=0}^\infty \mathbf{v}^n z^{-n}$. Finally, we set: $\rho_K(z,x) := \mathrm{i}\frac{z-1}{\tau} - \frac{z+1}{2} A_K(x)$, with $A_K(x) := a_0 + 2\sum_{k=1}^K a_k \cos(kx)$.

Under these notations, the following result holds.

Theorem 1. *Let $n \in \mathbb{N}$. The left and right absorbing boundary conditions associated with (6) can be respectively written as*

$$\psi_j^n = \sum_{k=1}^K (\mathbb{C}_{-j,k} \star \psi_{k-1})^n, \quad \text{for } -K \leq j \leq -1, \tag{7}$$

$$\psi_{J+j}^n = \sum_{k=1}^K (\mathbb{C}_{j,k} \star \psi_{J+1-k})^n, \quad \text{for } 1 \leq j \leq K, \tag{8}$$

where the sequence of $K \times K$ matrices $(\mathbb{C}^n)_n$ is given by: $\widehat{\mathbb{C}}(z) = \widehat{\mathbb{B}}(z)\widehat{\mathbb{A}}^{-1}(z)$, $z \in \mathbb{C}$. In the above relations, we have: $\mathbb{B}_{j,k}^n = f_{j+k-1}^n$ and $\mathbb{A}_{j,k}^n = f_{|j-k|}^n$, for $1 \leq j,k \leq K$, with

$$\hat{f}_j(z) = \frac{\hat{g}_j(z)}{\hat{g}_0(z)}, \quad \hat{g}_j(z) = \frac{1}{2\pi}\int_0^{2\pi} \rho_K^{-1}(z,x) e^{-\mathrm{i}jx} dx. \tag{9}$$

Let us introduce δ_j^0 as the Krönecker symbol such that $\delta_0^0 = 1$ and $\delta_j^0 = 0$ for $j \neq 0$. To prove Theorem 1, we first state the following Lemma.

Lemma 1. *The functions $\widehat{f}_j(z)$, for $j \in \mathbb{Z}$, satisfy*

$$\mathrm{i}\frac{z-1}{\tau}\widehat{f}_j(z) = \frac{z+1}{2}\Big[a_0\widehat{f}_j(z) + \sum_{k=1}^K a_k(\widehat{f}_{j+k}(z) + \widehat{f}_{j-k}(z))\Big] + \frac{\delta_j^0}{\widehat{g}_0(z)}. \tag{10}$$

Proof of Lemma 1. Let $j \in \mathbb{Z}$. A simple calculation based on (9) leads to

$$a_0\widehat{f}_j + \sum_{k=1}^{K} a_k(\widehat{f}_{j+k} + \widehat{f}_{j-k}) = \frac{1}{2\pi\widehat{g}_0(z)} \int_0^{2\pi} \rho_K^{-1}(z,x) A_K(x) e^{-\mathrm{i}jx} dx$$
$$= \frac{2}{(z+1)\widehat{g}_0(z)} \Big(-\frac{1}{2\pi} \int_0^{2\pi} e^{-\mathrm{i}jx} dx + \mathrm{i}\frac{z-1}{\tau}\widehat{g}_j \Big) = \frac{2}{(z+1)\widehat{g}_0(z)} \left[\mathrm{i}\frac{z-1}{\tau}\widehat{g}_j(z) - \delta_j^0 \right],$$

which provides (10). ■

Let us now prove the following result.

Lemma 2. *Let us assume that the kernel functions $\{f_j^n\}_{n\in\mathbb{N}}$ satisfy (9), for $j \in \mathbb{Z}$, $j \neq 0$. We consider K given sequences $\{u_k^n\}_{n\in\mathbb{N}}$, such that $u_k^0 = 0$, for $0 \leq k \leq K-1$. If we define*

$$\psi_j^n = \sum_{k=0}^{K-1} (f_{j-k} \star u_k)^n, \quad \textit{for } j \leq K-1, \tag{11}$$

then, for any integer $j \leq -1$, we have

$$\mathrm{i}D_\tau \psi_j^n = EL_{\delta,h}\psi_j^n, \tag{12}$$

with $\psi_j^0 = 0$.

Proof of Lemma 2. From (11), we obtain

$$\widehat{\psi}_j(z) = \sum_{k=0}^{K-1} \widehat{f}_{j-k}(z)\widehat{u}_k(z), \quad \text{for } j \leq K-1. \tag{13}$$

For $j \leq -1$, we have $j-k < 0$, with $0 \leq k \leq K-1$, and $\delta_j^0 = 0$. Hence, from (10), the functions $\widehat{\psi}_j(z)$ satisfy

$$i\frac{z-1}{\tau}\hat{\psi}_j(z) = \frac{z+1}{2}\Big[\sum_{k=0}^{K-1} a_0\hat{f}_{j-k}(z)\hat{u}_k(z) + \sum_{k=0}^{K-1}\sum_{p=1}^{K} a_p(\hat{f}_{j-k-p}(z) + \hat{f}_{j-k+p}(z))\hat{u}_k(z)\Big]$$
$$= \frac{z+1}{2}a_0\hat{\psi}_j(z) + \frac{z+1}{2}\sum_{p=1}^{K} a_p(\hat{\psi}_{j-p}(z) + \hat{\psi}_{j+p}(z)),$$

which leads to (12) after $\mathcal{Z}$-inversion. Finally, we have $\psi_j^0 = \sum_{k=0}^{K-1} f_{j-k}^0 u_k^0 = 0$ from (13). ■

Lemma 2 implies that the functions ψ_j^n, $j \leq -1$, satisfy the governing fully discrete nonlocal Schrödinger equation on the left exterior domain. Consequently, if we can compute $\{u_k^n\}_n$, for $0 \leq k \leq K-1$, we obtain the ABC at the left boundary given by (11) and leading to (7).

Let us now admit the following Lemma. Its proof is available at the end of this section since it requires some preliminary analytical results.

Lemma 3. *For K given sequences $\{\psi_j^n\}_n$, with $\psi_j^0 = 0$ and $0 \leq j \leq K-1$, we can find K sequences $\{u_k^n\}_n$, with $0 \leq k \leq K-1$, such that,*

$$\psi_j^n = \sum_{k=0}^{K-1} (f_{j-k} \star u_k)^n, \quad 0 \leq j \leq K-1. \tag{14}$$

Lemma 3 shows that, being given the interior values $\{\psi_j^n\}_n$, $0 \le j \le K-1$, we can compute $\{u_j^n\}_n$ through (14) and then obtain $\{\psi_j^n\}_n$, $j \le K-1$, satisfying (11) and the exterior left problem (12), for $j \le -1$. Based on the two previous Lemmas, we prove Theorem 1.

Proof of Theorem 1. By using Lemma 3, we can find K sequences $\{u_k^n\}_n$, $0 \le k \le K-1$, such that (14) holds for the boundary values $\{\psi_j^n\}_n$, $0 \le j \le K-1$. Now, for the same sequences $\{u_k^n\}_n$, we can define $\{\psi_j^n\}_n$ based on (11), for $j \le -1$. Therefore, $\{\psi_j^n\}_n$ satisfy (12), $-K \le j \le -1$, by Lemma 2. Combining (11) and (14) provides the left boundary condition. More precisely, we have

$$\begin{cases} \psi_j^n = \displaystyle\sum_{k=1}^{K} (f_{-j+k-1} \star u_{k-1})^n, \quad -K \le j \le -1, \\ \psi_{k-1}^n = \displaystyle\sum_{\ell=1}^{K} (f_{k-\ell} \star u_{\ell-1})^n, \quad 1 \le k \le K, \end{cases} \tag{15}$$

since $f_{-j+k-1}^n = f_{1-k+j}^n$. Now, by applying the $\mathcal{Z}$-transform to (15) and eliminating $\widehat{u}(z)$, we directly obtain the equivalent expression $\psi_j^n = \sum_{k=1}^{K} (\mathbb{C}_{-j,k} \star \psi_{k-1})^n$, $-K \le j \le -1$, where $\mathbb{A}$, $\mathbb{B}$ and $\mathbb{C}$ are $K \times K$ matrices such that $\widehat{\mathbb{C}}(z) = \widehat{\mathbb{B}}(z)\widehat{\mathbb{A}}^{-1}(z)$, $(\mathbb{B}^n)_{j,k} = f_{j+k-1}^n$ and $(\mathbb{A}^n)_{j,k} = f_{j-k}^n$, $1 \le j,k \le K$. Similar calculations on the right domain lead to (8). ■

Let us note that, from the definition of $\mathbb{A}$ and $\mathbb{B}$, and since the index of f_{j+k-1}^n is such that $0 \le j+k-1 \le 2K-1$, from $f_{-j}^n = f_j^n$ and $(\mathbb{B}^n)_{j,k} = f_{j+k-1}^n$, we only need to compute f_j^n for $0 \le j \le 2K-1$ to determine $\widehat{\mathbb{C}}(z) = \widehat{\mathbb{B}}(z)\widehat{\mathbb{A}}^{-1}(z)$ in subsection 2.3. In addition, we remark that considering $\widehat{g}_n(z)$ instead of $\widehat{f}_n(z)$ is sufficient to compute $\widehat{\mathbb{C}}$. Indeed, since $\widehat{\mathbb{B}}_{j,k}(z) = \widehat{g}_{j+k-1}(z)/\widehat{g}_0(z)$ and $\widehat{\mathbb{A}}_{j,k}(z) = \widehat{g}_{|j-k|}(z)/\widehat{g}_0(z)$, for $1 \le j,k \le K$, from the relation $\widehat{\mathbb{C}} = \widehat{\mathbb{B}}\widehat{\mathbb{A}}^{-1}$, we can modify the two matrices to be $\widehat{\mathbb{B}}_{j,k}(z) = \widehat{g}_{j+k-1}(z)$ and $\widehat{\mathbb{A}}_{j,k}(z) = \widehat{g}_{|j-k|}(z)$, with $\widehat{g}_j(z)$ given by (9).

2.3. Computation of the functions $\{g_j^n\}_n$, for $0 \le j \le 2K-1$

Let us define $\{g_j^n\}_n$ as the inverse discrete $\mathcal{Z}$-transform of $\widehat{g}_j(z)$. Since $g_j^n = g_{-j}^n$, from (9), we only need to compute g_j^n, for $0 \le j \le 2K-1$, to derive the absorbing boundary conditions (7) and (8). From Lemma 1, the functions $\widehat{g}_j(z)$, for $j \in \mathbb{Z}$, satisfy

$$\mathrm{i}\frac{z-1}{\tau}\widehat{g}_j(z) = \frac{z+1}{2}\Big[a_0\widehat{g}_j(z) + \sum_{k=1}^{K} a_k(\widehat{g}_{j+k}(z) + \widehat{g}_{j-k}(z))\Big] + \delta_j^0, \tag{16}$$

leading to $\mathrm{i}D_\tau g_j^n = EL_{\delta,h}g_j^n + \delta_j^0$, with $g_j^0 = 0$.

Let us now state the following Lemma.

Lemma 4. *The sequences $\{g_j^n\}_n$, for any integer $j \in \mathbb{Z}$ and $n \ge 2$, are such that*

$$\begin{aligned} g_j^n = g_{j-2K}^n + \frac{1}{Ka_K}\sum_{k=1}^{K-1} ka_k(g_{j-K-k}^n - g_{j-K+k}^n) + \frac{(2n-3)}{(n-1)Ka_K}\sum_{k=1}^{K} ka_k(g_{j-K-k}^{n-1} - g_{j-K+k}^{n-1}) \\ + \frac{(n-2)}{(n-1)Ka_K}\sum_{k=1}^{K} ka_k(g_{j-K-k}^{n-2} - g_{j-K+k}^{n-2}) - \frac{4\mathrm{i}(j-K)}{(n-1)Ka_K}\frac{1}{\tau}g_{j-K}^{n-1}. \end{aligned} \tag{17}$$

Proof of Lemma 4. For any integer $j \in \mathbb{Z}$, we define $\hat{h}_j(z) = (z+1)\hat{g}_j(z)$. Then, we have

$$\frac{d}{dz}\sum_{k=1}^{K} ka_k(\hat{h}_{j-k}-\hat{h}_{j+k}) = \frac{1}{2\pi}\frac{d}{dz}\int_0^{2\pi} 2\mathrm{i}(1+z)\rho_K^{-1}(z,x)A_K'(x)e^{-\mathrm{i}jx}dx = -\frac{4\mathrm{i}j}{(z+1)\tau}\hat{g}_j,$$

which leads to

$$\sum_{k=1}^{K} ka_k(\hat{g}_{j-k}(z)-\hat{g}_{j+k}(z)) + (z+1)\sum_{k=1}^{K} ka_k(\frac{d}{dz}\hat{g}_{j-k}(z) - \frac{d}{dz}\hat{g}_{j+k}(z)) = -\frac{4\mathrm{i}j}{(z+1)\tau}\hat{g}_j(z). \quad (18)$$

After multiplying (18) by $(1+z)$, we obtain

$$(z+1)\sum_{k=1}^{K} ka_k\sum_{n=0}^{\infty}(g_{j-k}^n - g_{j+k}^n)z^{-n} + (z+1)^2\sum_{k=1}^{K} ka_k\sum_{n=0}^{\infty}k(g_{j+k}^n - g_{j-k}^n)z^{-(n+1)} = -4\mathrm{i}j\frac{1}{\tau}\sum_{n=0}^{\infty} g_j^n z^{-n}.$$

After some manipulations, we deduce

$$g_{j+K}^{n+1} = g_{j-K}^{n+1} + \frac{1}{Ka_K}\sum_{k=1}^{K-1} ka_k(g_{j-k}^{n+1} - g_{j+k}^{n+1}) + \frac{(2n-1)}{nKa_K}\sum_{k=1}^{K} ka_k(g_{j-k}^n - g_{j+k}^n)$$
$$+\frac{(n-1)}{nKa_K}\sum_{k=1}^{K} ka_k(g_{j-k}^{n-1} - g_{j+k}^{n-1}) - \frac{4\mathrm{i}j}{nKa_K}\frac{1}{\tau}g_j^n.$$

Finally, we can rewrite the above expression for g_j^n as (17). ■

We still need to compute g_j^1, $j\in\mathbb{Z}$. To this end, we write

$$g_j^1 = \frac{1}{2\pi}\int_0^{2\pi}\frac{e^{\mathrm{i}jx}}{\mathrm{i}/\tau - a_0/2 - \sum_{k=1}^{K} a_k(e^{ikx}+e^{-ikx})/2}\frac{de^{ix}}{ie^{ix}} = \frac{1}{2\pi i}\int_{|z|=1}\frac{z^{K+j-1}}{q(z)}dz,$$

defining: $q(z) = (i/\tau - a_0/2)z^K - \sum_{k=1}^{K} a_k(z^{K+k}+z^{K-k})/2$, which has $2K$ different roots r_k, $1\le k\le 2K$. We suppose that K_1 zeroes are such that: $|r_k|<1$, $1\le k\le K_1\le K$. Then, we have

$$g_j^1 = \frac{1}{2\pi i}\int_{|z|=1}\frac{z^{K+j-1}}{q(z)}dz = \sum_{k=1}^{K_1}\mathrm{Res}\Big(\frac{z^{K+j-1}}{q(z)}\Big)_{z=r_k} = \sum_{k=1}^{K_1}\frac{r_k^{K+j-1}}{q'(r_k)}.$$

Relation (16) can be used to compute the $2K$ sequences $\{g_j^n\}_n$, for $0\le j\le 2K-1$. To this end, the sequences $\{g_j^n\}_n$, for $2K\le j\le 3K-1$ and $-K\le j\le -1$, need to be determined to close (16). Furthermore, $\{g_j^n\}_n$, for $-K\le j\le -1$, can be obtained by the property: $g_{-j}^n = g_j^n$, and the sequences $\{g_j^n\}_n$, for $2K\le j\le 3K-1$, can be computed based on (17). Therefore, we determine the discrete system for $\{g_j^n\}_n$, with $0\le j\le 2K-1$, and obtain $\mathbb{B} = \mathbb{C}\star\mathbb{A}$.

Finally, we prove Lemma 3.

Proof of Lemma 3. To solve (14) with $\psi_j^0 = 0$, $0\le j\le K-1$, we can equivalently consider

$$\widehat{\psi}_j = \sum_{k=0}^{K-1}\widehat{f}_{j-k}(z)\widehat{u}_k(z), \quad 0\le j\le K-1. \quad (19)$$

Since $\widehat{f}_{j-k}(z) = \widehat{g}_{j-k}/\widehat{g}_0$, then one gets the new form of (19)

$$\widehat{g}_0\widehat{\psi}_j = \sum_{k=0}^{K-1}\widehat{g}_{j-k}(z)\widehat{u}_k, \quad 0\le j\le K-1. \quad (20)$$

If we define the two vectors $\widehat{\boldsymbol{\psi}}_K = (\widehat{g}_0\widehat{\psi}_0, \widehat{g}_0\widehat{\psi}_1, ...\widehat{g}_0\widehat{\psi}_{K-1})^T$ and $\widehat{\mathbf{u}}_K = (\widehat{u}_0, \widehat{u}_1, ...\widehat{u}_{K-1})^T$, then (20) can be rewritten under the matrix form: $\widehat{\boldsymbol{\psi}}_K = \widehat{\mathbb{A}}\widehat{\mathbf{u}}_K$, where $\widehat{\mathbb{A}}$ is the $K \times K$ matrix with coefficients: $\widehat{\mathbb{A}}_{j,k}(s) = \widehat{g}_{|j-k|}(z)$, $0 \leq j, k \leq K-1$, since $\widehat{g}_{j-k} = \widehat{g}_{k-j}$. In addition, we obtain

$$\widehat{g}_j(z) = \frac{1}{2\pi}\int_0^{2\pi} \rho_K^{-1}(z,x)e^{-\mathrm{i}jx}dx = \frac{1}{2\pi}\sum_{\ell=0}^{\infty}\frac{1}{(z)^{\ell+1}}\int_0^{2\pi}\frac{(\mathrm{i}/\tau + A_K(x)/2)^\ell}{(\mathrm{i}/\tau - A_K(x)/2)^{\ell+1}}e^{-\mathrm{i}jx}dx$$
$$= \frac{1}{z}\int_0^{2\pi}\frac{1}{2\pi(\mathrm{i}/\tau - A_K(x)/2)}e^{-\mathrm{i}jx}dx + \mathcal{O}(\frac{\tau}{z^2}) = \frac{\gamma_j}{z} + \mathcal{O}(\frac{\tau}{z^2}),$$

for large values of $|z|$. Moreover, we have $\gamma_j = -\mathrm{i}\tau\delta_j^0 + \mathcal{O}(\tau^2)$. Therefore, we deduce that $\widehat{\mathbb{A}} = -\mathrm{i}\tau z^{-1}(\mathbb{I} + \mathcal{O}(\tau) + \mathcal{O}(z^{-1}))$, where $\mathbb{I}$ is the $K \times K$ identity matrix. For z large enough and small τ, we have: $\widehat{\boldsymbol{\psi}}_K \approx \widetilde{\mathbb{A}}\widehat{\mathbf{u}}_K$, where $\widetilde{\mathbb{A}} := -\mathrm{i}\tau z^{-1}\mathbb{I}$, and (20) has a unique sequence solution $\widehat{\mathbf{u}}_K$, ending hence the proof of Lemma 3. ■

3. Properties of the kernel $\{\mathbb{C}^n\}_n$ and stability analysis

3.1. Properties of the kernel $\{\mathbb{C}^n\}_n$

Let us now prove some useful properties of $\{\mathbb{C}^n\}_n$ for the stability and error analysis. From now on, $\bar{z}$ is the complex conjugate of $z \in \mathbb{C}$, and $\mathbb{M}^T$ is the transpose of any complex-valued matrix $\mathbb{M}$.

Proposition 1. *For any sequence $\mathbf{v} = \{\mathbf{v}^n\}_n$ of elements $\mathbf{v}^n \in \mathbb{C}^K$ such that $\mathbf{v}^0 = 0$, the following inequality holds, for $N \geq 1$,*

$$\Im\Big[\sum_{n=0}^{N-1}\overline{(E(\mathbb{C}\star\mathbf{v}))^n}^T \cdot \mathbb{S}(E\mathbf{v})^n\Big] \geq 0, \tag{21}$$

with $\mathbf{v}^n = [v_0^n, v_1^n, ...v_{K-1}^n]^T$ and $\mathbb{S}$ is the $K \times K$ Hankel matrix based on $\{a_k\}_{k=1,...,K}$ defined by (5) (on the first row), with zeroes under the anti-diagonal.

Proof of Proposition 1. Let us first prove (21). By Lemma 3, for any vector sequence $\mathbf{v} = \{\mathbf{v}^n\}_n$ such that $\mathbf{v}^0 = 0$, we can find some sequences $\{u_k^n\}_n$, $1 \leq k \leq K$, such that: $v_j^n = \sum_{k=0}^{K-1}(f_{j-k}\star u_k)^n$, $0 \leq j \leq K-1$. Hence, one can directly define: $v_j^n = \sum_{k=0}^{K-1}(f_{j-k}\star u_k)^n$, for $j \leq -1$. Since $a_0 = -2\sum_{k=1}^K a_k$, then $\{v_j^n\}_n$, $j \leq -1$, satisfy the fully discrete nonlocal Schrödinger equation (12)

$$\mathrm{i}D_\tau v_j^n = a_0 E v_j^n + \sum_{k=1}^K a_k(Ev_{j-k}^n + Ev_{j+k}^n) = \sum_{k=1}^K a_k(Ev_{j-k}^n - Ev_j^n) + \sum_{k=1}^K a_k(Ev_{j+k}^n - Ev_j^n).$$

Multiplying the above equality by $\overline{Ev_j^n}$, and summing from $j = -J$ to $j = -1$ yields

$$\sum_{j=-J}^{-1}\mathrm{i}\frac{v_j^{n+1}-v_j^n}{\tau}\overline{Ev_j^n} = \sum_{j=-J}^{-1}\sum_{k=1}^K a_k(Ev_{j+k}^n - Ev_j^n)(\overline{Ev_j^n} - \overline{Ev_{j+k}^n}) + \sum_{j=-J}^{-1}\sum_{k=1}^K a_k(Ev_{j+k}^n - Ev_j^n)\overline{Ev_{j+k}^n}$$
$$+ \sum_{j=-J}^{-1}\sum_{k=1}^K a_k(Ev_{j-k}^n - Ev_k^n)(\overline{Ev_j^n} - \overline{Ev_{j-k}^n}) + \sum_{j=-J}^{-1}\sum_{k=1}^K a_k(Ev_{j-k}^n - Ev_j^n)\overline{Ev_{j-k}^n}. \tag{22}$$

Computing (22)-$\overline{(22)}$ leads to

$$\sum_{j=-J}^{-1} \mathrm{i}\frac{|v_j^{n+1}|^2-|v_j^n|^2}{\tau} = -\sum_{k=1}^{K}\sum_{j=-k}^{-1} a_k E v_j^n \overline{E v_{j+k}^n} + \sum_{k=1}^{K}\sum_{j=-k}^{-1} a_k \overline{E v_j^n} E v_{j+k}^n$$
$$-\sum_{k=1}^{K}\sum_{j=-J-k}^{-J-1} a_k E v_{j+k}^n \overline{E v_j^n} + \sum_{k=1}^{K}\sum_{j=-J-k}^{-J-1} a_k \overline{E v_{j+k}^n} E v_j^n. \tag{23}$$

Taking $J \to +\infty$ in (23), and since $v_j^n \to 0$ when $|j| \to +\infty$, we obtain

$$\sum_{j=-\infty}^{0} \mathrm{i}\frac{|v_j^{n+1}|^2-|v_j^n|^2}{\tau} = -\sum_{k=1}^{K}\sum_{j=-k}^{-1} a_k E v_j^n \overline{E v_{j+k}^n} + \sum_{k=1}^{K}\sum_{j=-k}^{-1} a_k \overline{E v_j^n} E v_{j+k}^n. \tag{24}$$

Let us define $\mathbf{u}^n = [u_0^n, u_1^n, \cdots, u_{K-1}^n]^T$, $\mathbf{v}^n = [v_0^n, v_1^n, \cdots, v_{K-1}^n]^T$ and $\mathbf{w}^n = [v_{-1}^n, v_{-2}^n, \cdots, v_{-K}^n]^T$. By Lemma 3 we have $\mathbf{v}^n = (\mathbb{A} \star \mathbf{u})^n$ and $\mathbf{w}^n = (\mathbb{B} \star \mathbf{u})^n$, implying that: $\mathbf{w}^n = (\mathbb{C} \star \mathbf{v})^n$. Summing up (24) from $n = 0$ to $N-1$, one finally gets (21) since

$$\mathrm{i}\sum_{j=-\infty}^{-1} \frac{|v_j^N|^2}{\tau} = 2\mathrm{i}\Im\Big(\sum_{n=0}^{N-1} \overline{(E(\mathbb{C}\star\mathbf{v}))^n}^T \cdot \mathbb{S}(E\mathbf{v})^n\Big). \tag{25}$$

■

3.2. Stability analysis

For $\boldsymbol{\psi}^n := (\psi_j^n)_{j=0,\ldots,J}$, $n \in \mathbb{N}$, we introduce the norm $||\boldsymbol{\psi}^n||_{\ell_J^2} := h^{1/2}(\sum_{j=0}^{J} |\psi_j^n|^2)^{1/2}$. We now prove the ℓ_J^2-stability of the fully-discrete scheme with ABC.

Theorem 2. *Let $N \in \mathbb{N}$. The solution of the fully discrete scheme (6) with ABCs (7)-(8) satisfies the stability inequality*

$$||\boldsymbol{\psi}^N||_{\ell_J^2} \le ||\boldsymbol{\psi}^0||_{\ell_J^2}. \tag{26}$$

Proof of Theorem 2. Repeating the same procedure as in the proof of Proposition 1 by multiplying (6) by $\overline{E\psi_j^n}$ and summing up all the terms from $j = 0$ to $j = J$, we obtain

$$\sum_{j=0}^{J} \mathrm{i}\frac{\psi_j^{n+1}-\psi_j^n}{\tau}\overline{E\psi_j^n} = \sum_{j=0}^{J}\sum_{k=1}^{K} a_k(E\psi_{j+k}^n - E\psi_j^n)(\overline{E\psi_j^n} - \overline{E\psi_{j+k}^n}) + \sum_{j=0}^{J}\sum_{k=1}^{K} a_k(E\psi_{j+k}^n - E\psi_j^n)\overline{E\psi_{j+k}^n}$$
$$+\sum_{j=0}^{J}\sum_{k=1}^{K} a_k(E\psi_{j-k}^n - E\psi_j^n)(\overline{E\psi_j^n} - \overline{E\psi_{j-k}^n}) + \sum_{j=0}^{J}\sum_{k=1}^{K} a_k(E\psi_{j-k}^n - E\psi_j^n)\overline{E\psi_{j-k}^n}. \tag{27}$$

Let us define $(\mathbf{v}_+[\psi])^n = [\psi_J^n, \psi_{J-1}^n, \cdots, \psi_{J-K+1}^n]^T$, $(\mathbf{w}_+[\psi])^n = [\psi_{J+1}^n, \psi_{J+2}^n, \cdots, \psi_{J+K}^n]^T$ and $(\mathbf{v}_-[\psi])^n = [\psi_0^n, \psi_1^n, \cdots, \psi_{K-1}^n]^T$, $(\mathbf{w}_-[\psi])^n = [\psi_{-1}^n, \psi_{-2}^n, \cdots, \psi_{-K}^n]^T$. The boundary conditions read $(\mathbf{w}_+[\psi])^n = (\mathbb{C} \star \mathbf{v}_+[\psi])^n$, $(\mathbf{w}_-[\psi])^n = (\mathbb{C} \star \mathbf{v}_-[\psi])^n$. Computing (27)-$\overline{(27)}$ yields (26)

$$\sum_{j=0}^{J} \mathrm{i}\frac{|\psi_j^N|^2-|\psi_j^0|^2}{\tau} = -2\mathrm{i}\Im\Big(\sum_{n=0}^{N-1} \overline{(E(\mathbb{C}\star\mathbf{v}_-[\psi]))^n}^T \cdot \mathbb{S}E\mathbf{v}_-[\psi]^n + \sum_{n=0}^{N-1} \overline{(E(\mathbb{C}\star\mathbf{v}_+[\psi]))^n}^T \cdot \mathbb{S}E\mathbf{v}_+[\psi]^n\Big).$$

■

4. Truncated and boundary errors analysis

Let us introduce the following norms

$$||f||_{L^\infty} = \max_{x\in\mathbb{R}} |f(x)|, \quad ||f||_{L^2} = (\int_{\mathbb{R}} |f(x)|^2 dx)^{1/2},$$
$$||f||_{L^1_\delta} = \int_{-\delta}^{\delta} |f(x)|dx, \quad ||f||_{L^\infty_{x,\delta}} = \max_{y\in[x-\delta;x+\delta]} |f(y)|,$$

for $\delta > 0$. We recall that γ_δ is assumed to be homogeneous in the exterior domain according to assumption A3 (see (3)). In the computational domain, it may be *a priori* inhomogeneous. However, to simplify the presentation of the proofs, we suppose from now on that γ_δ is also homogeneous inside the computational domain, has a singularity behaviour $\gamma_\delta(a) \sim |a|^{-\alpha}$, $\alpha \leq 1/2$, and that $||\gamma_\delta||_{L^1_\delta} < +\infty$. Nevertheless, if γ_δ is non homogeneous in the domain of computation, the proofs can be adapted for similar singularity types but at the price of more complexity.

4.1. Error estimates: main result

For $\mathbf{u}^n := (u_j^n)_{j\in\mathbb{Z}}$, $n = 0, \cdots, N$, and $\mathbf{U}^N = (\mathbf{u}^n)_{0\leq n\leq N-1}$, with $N \geq 1$, we define the norms

$$||\mathbf{u}^n||_{\ell^\infty} := \max_{j\in\mathbb{Z}} |u_j^n|, \quad ||\mathbf{u}^n||_{\ell^2} := h^{1/2}(\sum_{j\in\mathbb{Z}} |u_j^n|^2)^{1/2}, \quad ||\mathbf{u}^n||_{\ell^2_K} := h^{1/2}(\sum_{k=1}^{K} |u_k^n|^2)^{1/2},$$
$$||\mathbf{U}^N||_{\ell^{\infty,N}} := \max_{0\leq n\leq N-1} ||\mathbf{u}^n||_{\ell^\infty} \quad ||\mathbf{U}^N||_{\ell^{2,N}} := \tau^{1/2}(\sum_{n=0}^{N-1} ||\mathbf{u}^n||^2_{\ell^2})^{1/2}.$$

For ψ solution to (1), we set $\psi_j(t) := \psi(x_j, t)$, for $j \in \mathbb{Z}$. The error e_j^n for (6) is then

$$e_j^n = \mathrm{i}\frac{2}{\tau}(\psi_j(t_{n+1}) - \psi_j(t_n)) - L_{\delta,h}(\psi_j(t_{n+1}) + \psi_j(t_n)),$$

where $0 \leq n \leq N-1$ and $j \in \mathbb{Z}$. We set $\mathbf{e}^n := (e_j^n)_{j\in\mathbb{Z}}$, $n = 0, \cdots, N$, and $\mathbf{E}^N = (\mathbf{e}^n)_{0\leq n\leq N-1}$. We define the backward derivative operator $\nabla_- e_j^n := (e_j^n - e_{j-1}^n)/h$, and $\boldsymbol{\nabla}_-\mathbf{E}^N := (\boldsymbol{\nabla}_-\mathbf{e}^n)_{0\leq n\leq N-1}$, for $\mathbf{e}^n := (e_j^n)_{j\in\mathbb{Z}}$. Let us introduce the time-dependent K components vectors $\mathbf{V}_-\psi = ((\psi_j)_{j=0,\cdots,K-1})^T$, $\mathbf{W}_-\psi = ((\psi_j)_{j=-1,\cdots,-K})^T$, $\mathbf{V}_+\psi = ((\psi_{J-j})_{j=0,\ldots,K-1})^T$ and $\mathbf{W}_+\psi = ((\psi_j)_{j=J+1,\cdots,J+K})^T$. We also need to define the boundary operators $\mathbf{G}_\pm = \mathbb{C}\star\mathbf{V}_\pm - \mathbf{W}_\pm$ such that: $\mathbb{C}\star\mathbf{V}_\pm(t) = \sum_{m=0}^{\infty} \mathbb{C}^m\mathbf{V}_\pm(t - t_m)$, setting $\mathbf{V}_\pm(t) = 0$ for $t < 0$.

The main result of this section concerns the following Theorem which shows that both the truncated and boundary errors of the interior scheme are of order $\mathcal{O}(h^2 + \tau^2)$.

Theorem 3. *For $N \geq 1$, we have the following error bounds*

$$||\mathbf{E}^N||_{\ell^{\infty,N}} \leq C(\tau^2 + h^2), \tag{28}$$
$$||\mathbf{E}^N||_{\ell^{2,N}} \leq C(\tau^2 + h^2), \tag{29}$$
$$||\boldsymbol{\nabla}_-\mathbf{E}^N||_{\ell^{2,N}} \leq C(\tau^2 + h^2), \tag{30}$$
$$||\mathbf{G}_\pm^n||_{\ell^2_K} \leq C(\tau^2 + h^2), \quad 0 \leq n \leq N, \tag{31}$$

where $C > 0$ are some constants that only depend on γ_δ, δ, T and the initial data ψ^0.

4.2. Estimates for the solution ψ of system (1)

We first derive some useful estimates for the solution ψ of the continuous problem (1).

Lemma 5. *Let us assume that $\partial_x^\ell \psi^0$ is in L^2, for a positive integer $\ell \geq 0$. Then, we have: $||\partial_x^\ell \psi||_{L^2} = ||\partial_x^\ell \psi^0||_{L^2}$. In addition, if $\partial_x^{\ell+1}\psi^0$ is in L^∞, then the following bound holds*

$$||\partial_x^\ell \psi||_{L^\infty} \leq C(||\partial_x^{\ell+1}\psi^0||_{L^2} + ||\partial_x^\ell \psi^0||_{L^2}),$$

where $C > 0$ is a constant.

Proof of Lemma 5. Let us consider the governing equation

$$\mathrm{i}\partial_t \psi(x,t) = \int_{-\delta}^{+\delta} \gamma_\delta(y)(\psi(x,t) - \psi(x-y,t))dy. \tag{32}$$

Summing up (32) multiplied by $\overline{\psi}$ and the conjugate of (32) multiplied by $-\psi$, and integrating the equality from $-L$ to $L(>0)$, we obtain

$$\mathrm{i}\partial_t \int_{-L}^{L} |\psi|^2 dx = \int_{-\delta}^{\delta} \gamma_\delta(y)\Big(-\int_{L}^{L+y} + \int_{-L}^{-L+y} \Big)\psi(x,t)\overline{\psi(x-y,t)}dxdy.$$

Since $|\psi(x,t)| \to 0$ as $|x| \to \infty$, taking $L \to +\infty$ in the above expression leads to $\partial_t ||\psi||_{L^2}^2 = 0$, providing $||\psi||_{L^2}^2 = ||\psi^0||_{L^2}^2$. It is easy to see that $||\partial_x^\ell \psi||_{L^2}^2 = ||\partial_x^\ell \psi^0||_{L^2}^2$ also holds. In addition, we have the following inequality which proves the result for $\ell = 0$

$$||\psi||_{L^\infty} \leq \int_{-\infty}^{\infty} (1+|\xi|)^{-1}(1+|\xi|)|\hat{\psi}(\xi)|d\xi \leq C(||\psi||_{L^2} + ||\partial_x \psi||_{L^2}).$$

Similarly, we obtain $||\partial_x^\ell \psi||_{L^2}^2 = ||\partial_x^\ell \psi^0||_{L^2}^2$ by considering $\partial_t \partial_x^\ell \psi$ instead of $\partial_t \psi$ in (32). ■

A consequence of Lemma 5 is given in the next result.

Lemma 6. *Let $k \geq 1$ and $\ell \in \mathbb{N}$. For ψ^0 and ψ sufficiently smooth, and for ψ^0 compactly supported in $]x_-; x_+[$, we have, for $x \in \mathbb{R}$ and $t > 0$,*

$$|\partial_t^k \partial_x^\ell \psi(x,t)| \leq C 2^k ||\gamma_\delta||_{L^1_\delta}^k (||\partial_x^{\ell+1}\psi^0||_{L^2}^2 + ||\partial_x^\ell \psi^0||_{L^2}^2). \tag{33}$$

Proof of Lemma 6. From (32), we have: $|\partial_t \psi(x,t)| \leq ||\gamma_\delta||_{L^1_\delta}\ ||\psi||_{L^\infty}$, and by iteration

$$|\partial_t^k \psi(x,t)| \leq 2||\gamma_\delta||_{L^1_\delta}\ ||\partial_t^{k-1}\psi||_{L^\infty} \leq 2^k ||\gamma_\delta||_{L^1_\delta}^k ||\psi||_{L^\infty} \leq C 2^k ||\gamma_\delta||_{L^1_\delta}^k (||\partial_x \psi^0||_{L^2}^2 + ||\psi^0||_{L^2}^2).$$

Similarly, we prove (33)

$$|\partial_t^k \partial_x^\ell \psi(x,t)| \leq 2||\gamma_\delta||_{L^1_\delta}\ ||\partial_t^{k-1}\partial_x^\ell \psi||_{L^\infty} \leq 2^k ||\gamma_\delta||_{L^1_\delta}^k ||\partial_x^\ell \psi||_{L^\infty} \leq C 2^k ||\gamma_\delta||_{L^1_\delta}^k (||\partial_x^{\ell+1}\psi^0||_{L^2}^2 + ||\partial_x^\ell \psi^0||_{L^2}^2).$$

■

4.3. Boundary error estimates

Let us introduce ϵ_j such that

$$\epsilon_j(t) = a_0\psi_j(t) + \sum_{k=1}^{K} a_k(\psi_{j+k}(t) + \psi_{j-k}(t)) - \mathcal{L}_\delta\psi_j(t), \tag{34}$$

for $j \in \mathbb{Z}$, where ψ designates the solution to (1). We rewrite ϵ_j as,

$$\begin{aligned}\epsilon_j = \sum_{k=1}^{K-1} \frac{\psi_{j-k} - 2\psi_j + \psi_{j+k}}{kh} \int_{(k-1)h}^{(k+1)h} \phi_k(\varsigma)\varsigma\gamma_\delta(\varsigma)d\varsigma \\ + \frac{\psi_{j-K} - 2\psi_j + \psi_{j+K}}{Kh} \int_{(K-1)h}^{Kh} \phi_K(\varsigma)\varsigma\gamma_\delta(\varsigma)d\varsigma \\ - \int_0^\delta (\psi(x_j - \varsigma, t) - 2\psi(x_j, t) + \psi(x_j + \varsigma, t))\gamma_\delta(\varsigma)d\varsigma,\end{aligned} \tag{35}$$

where we recall that ϕ_k is the hat function of width h centered at kh.

Then, the following technical Lemma holds (see Appendix A for the proof).

Lemma 7. *Let us assume that $\psi(x,t) \in \mathcal{C}^5([-\infty,\infty] \times [0,T])$. Then, we have: $\epsilon_j(t) = h^2 Q(x_j,t)$, for $j \in \mathbb{Z}$ and $t > 0$, with*

$$h\sum_{j\in\mathbb{Z}} |Q(x_j,t)|^2 \leq C \int_{\mathbb{R}} \sum_{p=2}^{5} |\partial_x^p \psi(y,0)|^2 dy, \tag{36}$$

setting

$$\begin{aligned}Q(x,t) = h\sum_{k=1}^{K-1} \int_{-1}^{1} \phi_0(\varsigma h)\varsigma^2 d\varsigma \int_0^1 \ddot{q}_k(kh + \varsigma y h, x, t)(1-y)dy \\ + \int_{-1}^{0} \phi_0(\varsigma h)\varsigma d\varsigma \int_0^1 \dot{q}_K(Kh + \varsigma y h, x, t)dy \\ - h\int_0^1 \varsigma^2 \phi_0(\varsigma h)\gamma_\delta(\varsigma h)d\varsigma \int_0^1 \int_0^{\xi_1} (\partial_x^2\psi(x + \varsigma\xi_2 h, t) + \partial_x^2\psi(x - \varsigma\xi_2 h, t))d\xi_2 d\xi_1.\end{aligned} \tag{37}$$

In the above relation, we defined

$$q_k(\varsigma, x, t) = \varsigma\gamma_\delta(\varsigma) \int_0^1 \int_{\varsigma\xi_1}^{kh\xi_1} (\partial_x^2\psi(x + \xi_2, t) + \partial_x^2\psi(x - \xi_2, t))d\xi_2 d\xi_1, \tag{38}$$

and $\ddot{q}(\varsigma, x, t)$ designates the second-order derivative of $q_p(\varsigma, x, t)$ with respect to ς.

Let us now prove Theorem 3.

Proof of Theorem 3. Let us start with (28) and (29). Using Taylor's expansions of $\psi(x, t_n)$ and $\psi(x, t_{n+1})$ and after some computations, we deduce

$$\begin{aligned}e^n(x) := \mathrm{i}\frac{2}{\tau}(\psi(x,t_{n+1}) - \psi(x,t_n)) - L_{\delta,h}(\psi(x,t_{n+1}) + \psi(x,t_n)) \\ = -2h^2 Q(x,t_{n+1/2}) - \frac{\tau^2 h^2}{12}\partial_t^2 Q(x,t_{n+1/2}) - \Big(\mathcal{L}_\delta\partial_t^2\psi(x,t_{n+1/2}) + h^2\partial_t^2 Q(x,t_{n+1/2})\Big)\tau^2/6 \\ + \frac{\mathrm{i}}{12\tau}\int_0^{\tau/2} (\partial_t^5\psi(x,t_{n+1/2}+\varsigma) - \partial_t^5\psi(x,t_{n+1/2}-\varsigma))(\tau/2-\varsigma)^4 d\varsigma \\ - \frac{1}{6}\int_0^{\tau/2} (L_{\delta,h}\partial_t^4\psi(x,t_{n+1/2}+\varsigma) + L_{\delta,h}\partial_t^4\psi(x,t_{n+1/2}-\varsigma)\Big)(\tau/2-\varsigma)^3 d\varsigma.\end{aligned}$$

By using: $L_{\delta,h}\partial_t^k\psi(x_j,t) = \mathcal{L}_\delta\partial_t^k\psi(x_j,t) + h^2\partial_t^k Q(x_j,t)$, and since

$$\Big(\int_0^{\tau/2}(L_{\delta,h}\partial_t^4\psi(x,t_{n+1/2}+\varsigma) + L_{\delta,h}\partial_t^4\psi(x,t_{n+1/2}-\varsigma))(\tau/2-\varsigma)^3 d\varsigma\Big)^2$$
$$\leq C\tau^7\int_{-\tau/2}^{\tau/2}\Big|L_{\delta,h}\partial_t^4\psi(x,t_{n+1/2}+\varsigma)\Big|^2 d\varsigma,$$

one gets

$$|e_j^n|^2 = |e^n(x_j)|^2 \leq Ch^4|Q(x_j,t_{n+1/2})|^2 + \tau^4h^4|\partial_t^2Q(x_j,x_{n+1/2})|^2 + C\tau^4|\mathcal{L}_\delta\partial_t^2\psi(x_j,t_{n+1/2})|^2$$
$$+C\tau^7\int_{-\tau/2}^{\tau/2}\Big(|\mathcal{L}_\delta\partial_t^4\psi(x_j,t_{n+1/2}+\varsigma)|^2 + h^4|\partial_t^4Q(x_j,t_{n+1/2}+\varsigma)|^2 + |\partial_t^5\psi(x_j,t_{n+1/2}+\varsigma)|^2\Big)d\varsigma.$$

From Lemmas 5-7 and the above equality, we deduce (28) since from (A.10) (see page 23) we have

$$|\partial_t^\ell Q(x,t)| \leq C\Big(||\partial_y^2\partial_t^\ell\psi(y,t)||_{L^\infty_{x,\delta}} + ||\partial_y^3\partial_t^\ell\psi(y,t)||_{L^\infty_{x,\delta}}\Big), \quad \ell = 0,2,4,$$

with $\mathcal{L}_\delta\partial_t^2\psi(x,t) = \mathrm{i}\partial_t^3\psi(x,t)$ and $\mathcal{L}_\delta\partial_t^4\psi(x,t) = \mathrm{i}\partial_t^5\psi(x,t)$.

To prove (29), we remark for example that, for $N\tau \leq T$, we have

$$\tau\sum_{n=0}^{N-1}|Q(x,t_{n+1/2})|^2 \leq C\int_0^T|Q(x,t)|^2dt.$$

All the other terms can be treated similarly. This yields

$$\sum_{n=0}^{N-1}\sum_{j=-\infty}^{-1}|e_j^n|^2h\tau \leq C(h^4+\tau^4)\int_0^T\int_{\mathbb{R}}\sum_{0\leq p,\ell\leq 5}|\partial_x^p\partial_t^\ell\psi(x,t)|^2dxdt \leq C(h^4+\tau^4),$$

which provides (29). We obtain (30) similarly.

Let us now prove (31). For the sequence $\{\psi_j^n\}_n = \{\psi_j(t_n)\}_n$ based on the solution of (1), with $\psi_j^0 = 0$, for $0 \leq j \leq K-1$, from Lemma 2 we can find K sequences $\{u_k^n\}_n$, with $0 \leq k \leq K-1$, such that

$$\psi_j^n = \sum_{k=0}^{K-1}(f_{j-k}\star u_k)^n, \quad 0 \leq j \leq K-1. \tag{39}$$

Then, the values ψ_j^n, for $j \leq -1$, can be defined by

$$\psi_j^n = \sum_{k=1}^{K}(f_{j-k}\star u_k)^n, \quad j \leq -1. \tag{40}$$

In this case, the solution satisfies: $\mathrm{i}(\psi_j^{n+1}-\psi_j^n)/\tau = L_{\delta,h}E\psi_j^n$, $j \leq -1$, with $|\psi_j^n| \to 0$ as $j \to -\infty$. Now, let us consider $w_j^n = \psi_j^n - \psi(x_j,t_n)$. For $j \leq -1$, we have

$$\mathrm{i}D_\tau w_j^n = a_0Ew_j^n + \sum_{k=1}^{K}a_k(Ew_{j-k}^n + Ew_{j+k}^n) - \frac{1}{2}e_j^n.$$

Multiplying the above equality by $\overline{Ew_j^n}$, and summing up all the term from $j=-J$ to -1 we get

$$\sum_{j=-J}^{-1} i\frac{w_j^{n+1}-w_j^n}{\tau}\overline{Ew_j^n}$$
$$= \sum_{j=-J}^{-1}\Big[\sum_{k=1}^{K} a_k(Ew_{j+k}^n - Ew_j^n)\overline{Ew_j^n} + \sum_{k=1}^{K} a_k(Ew_{j-k}^n - Ew_j^n)\overline{Ew_j^n}\Big] - \frac{1}{2}\sum_{j=-J}^{-1} e_j^n\overline{Ew_j^n}. \quad (41)$$

Repeating the same procedures, we compute (41)-$\overline{(41)}$. Taking $J\to\infty$, since $\psi_j^n\to 0$ as $|j|\to\infty$ we have

$$\sum_{j=-\infty}^{0} \mathrm{i}\frac{|w_j^{n+1}|^2-|w_j^n|^2}{\tau}$$
$$= 2i\Im\Big(\sum_{n=0}^{N-1}\overline{(E(\mathbf{w}_-[w]))^n}^T\cdot\mathbb{S}(E(\mathbf{v}_-[w]))^n\Big) - \frac{1}{2}\sum_{j=-\infty}^{-1} e_j^n\overline{Ew_j^n} + \frac{1}{2}\sum_{j=-\infty}^{-1}\overline{e_j^n}Ew_j^n. \quad (42)$$

From the choice of $\{\psi_j^n\}_n$ for $0\le j\le K-1$, it is clear that: $w_j^n=\psi_j^n-\psi(x_j,t_n)=0$ for $0\le j\le K-1$, and hence $\mathbf{v}_-[w]=0$. Summing up (42) from $n=0$ to $N-1$, we obtain

$$\sum_{j=-\infty}^{-1}\frac{|w_j^N|^2}{\tau}\le C\sum_{j=-\infty}^{-1}\sum_{n=0}^{N-1}|e_j^n|^2+\sum_{j=-\infty}^{-1}\sum_{n=0}^{N-1}|w_j^n|^2.$$

Then, using (29) and Gronwall's inequality [35] leads to

$$h\sum_{j=-\infty}^{-1}|w_j^N|^2\le C\tau h\sum_{j=-\infty}^{-1}\sum_{n=0}^{N-1}|e_j^n|^2\le(h^4+\tau^4)C(\psi(x,0),\gamma,\delta,T).$$

From (39) and (40), we have $(\mathbf{w}_-[\psi])^n=(\mathbb{C}\star\mathbf{v}_-[\psi])^n=(\mathbb{C}\star\mathbf{V}_-[\psi])^n$. Therefore, we deduce: $[w_{-1}^n,w_{-2}^n,...w_{-K}^n]^T=(\mathbf{w}_-[\psi])^n-\mathbf{W}_-(t)=(\mathbb{C}\star\mathbf{V}_-[\psi])^n-\mathbf{W}_-(t)=\mathbf{G}_-(t)$. ■

5. Error estimates of the scheme

Let us recall that $w_j^n=\psi_j^n-\psi(x_j,t_n)$, where $\psi(x_j,t_n)$ is the solution of the nonlocal Schrödinger equation (1) evaluated at (x_j,t_n), and ψ_j^n solves the fully discrete version (6). In addition, let us define the norm: $||\mathbf{w}^n||_{\ell_J^\infty}:=\max_{0\le j\le J}|w_j^n|$. We set the discrete forward derivatives as: $\nabla_+\psi(x_j,t_n)=(\psi(x_{j+1},t_n)-\psi(x_j,t_n))/h$ and $\nabla_+\psi_j^n=(\psi_{j+1}^n-\psi_j^n)/h$.

Let us give the main result concerning the error estimate.

Theorem 4. *For $\tau>0$ and $N\tau\le T$, we have the error bounds*

$$\|\mathbf{w}^N\|_{\ell_J^2}\le C\tau^2, \quad (43)$$
$$\|\nabla_+\mathbf{w}^N\|_{\ell_{J-1}^2}\le C\tau^2, \quad (44)$$
$$||\mathbf{w}^N||_{\ell_J^\infty}\le C\tau^2, \quad (45)$$

for some constants $C>$ that only depend on γ_δ, δ, T and ψ^0.

It is straightforward to check that the error w_j^n satisfies for $n \geq 0$

$$i\frac{1}{\tau}(w_j^{n+1} - w_j^n) = \frac{1}{2}L_{\delta,h}(w_j^{n+1} + w_j^n) - \frac{1}{2}e_j^n,$$
$$(\mathbb{C} \star \mathbf{v}_\pm[w])^n - (\mathbf{w}_\pm[w])^n = \mathbf{G}_\pm(t_n),$$

with $w_n^0 = 0$, where e_j^n (respectively $\mathbf{G}_\pm(t_n)$) is the interior (respectively boundary truncation) error according to the time and space discretizations defined in Theorem 3.

The proof of Theorem 4 is a consequence of Theorem 3 and the following Lemma.

Lemma 8. *Let us assume that the singular behavior of γ_δ around 0 is $\gamma_\delta(a) \sim |a|^{-\alpha}$, $\alpha \leq 1/2$. Then, the coefficients a_k in $L_{\delta,h}$ given by (5)-(6) satisfy the following inequality: $|a_k| \leq Ch^{1-\alpha}$, for $k = 1, ..., K$.*

Proof of Lemma 8. Since $a_k = a_{-k}$, we only need to estimate a_k for $k \geq 0$. For $k = 1$, one gets

$$|a_k| = \Big| \int_0^{2h} \frac{\phi_k(\varsigma)\varsigma\gamma_\delta(\varsigma)}{kh} d\varsigma \Big| \leq C \Big| \int_0^{2h} \frac{\varsigma^{1-\alpha}}{h} d\varsigma \Big| \leq Ch^{1-\alpha},$$

for a constant $C > 0$. In addition, for $k \geq 2$, we obtain

$$|a_k| = \Big| \int_{(k-1)h}^{(k+1)h} \frac{\phi_k(\varsigma)\varsigma\gamma_\delta(\varsigma)}{kh} d\varsigma \Big| \leq C \Big| \int_{(k-1)h}^{(k+1)h} \frac{\varsigma^{1-\alpha}}{kh} d\varsigma \Big| \leq \frac{C}{h^\alpha} \int_{(k-1)h}^{(k+1)h} \frac{\varsigma}{kh} d\varsigma \leq Ch^{1-\alpha}.$$

■

We can now prove Theorem 4.

Proof of Theorem 4. Let us start with (43). For a time step τ, we have

$$i\frac{1}{\tau}(w_j^{n+1} - w_j^n) = \frac{1}{2}L_{\delta,h}(w_j^{n+1} + w_j^n) - \frac{1}{2}e_j^n.$$

By a procedure similar to the one given in Proposition 1, we obtain

$$\begin{aligned} \frac{i}{\tau}\sum_{j=0}^{J}(|w_j^N|^2 - |w_j^0|^2) &= -2i\Im\Big(\sum_{n=0}^{N-1} \overline{(E(\mathbf{w}_-[w]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_-[w]))^n \\ &+ \sum_{n=0}^{N-1} \overline{(E(\mathbf{w}_+[w]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_+[w]))^n \Big) + \sum_{n=0}^{N-1}\sum_{j=0}^{J} \frac{1}{2}\Big(-\overline{e_j^n} E w_j^n + e_j^n \overline{E e_j^n} \Big), \end{aligned} \tag{46}$$

which leads to

$$\begin{aligned} &\sum_{j=0}^{J} h(|w_j^N|^2 - |w_j^0|^2) \\ &\leq -2\tau h\Im\Big(\sum_{n=0}^{N-1} \overline{(E(\mathbb{C} \star \mathbf{v}_+[w]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_+[w]))^n - \sum_{n=0}^{N-1} \overline{E(\mathbf{G}_+(t_n))}^T \cdot \mathbb{S}(E(\mathbf{v}_+[w]))^n \Big) \\ &-2\tau h\Im\Big(\sum_{n=0}^{N-1} \overline{(E(\mathbb{C} \star \mathbf{v}_-[w]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_-[e]))^n - \sum_{n=0}^{N-1} \overline{E(\mathbf{G}_-(t_n))}^T \cdot \mathbb{S} \cdot (E(\mathbf{v}_-[e]))^n \Big) \\ &+\frac{\tau h}{2} \sum_{n=0}^{N-1}\sum_{j=0}^{J} \Big(|e_j^n||w_j^n| + |e_j^n||w_j^{n+1}| \Big). \end{aligned} \tag{47}$$

In addition, from $a_k = \mathcal{O}(h^{1-\alpha})$, for $1 \leq k \leq K$, and the expression of $\mathbb{S}$, we derive

$$\Big|\Big(\mathbb{S}(E(\mathbf{v}_{\pm}[w]))^n\Big)_k\Big| \leq Ch^{1-\alpha}\Big(\sum_{q=1}^{K}|w^n_{J+1-q}| + \sum_{q=1}^{K}|w^{n+1}_{J+1-q}|\Big). \tag{48}$$

Thus, for $\alpha \leq 1/2$, from (48) and (31), (47) can be written as

$$\begin{aligned}
&-2\tau h\Im\Big(\sum_{n=0}^{N-1}\overline{(E(\mathbb{C}\star\mathbf{v}_{\pm}[w]))^n}^T\cdot\mathbb{S}(E(\mathbf{v}_{\pm}[w]))^n - \sum_{n=0}^{N-1}\overline{E(\mathbf{G}_{\pm}(t_n))}^T\cdot\mathbb{S}(E(\mathbf{v}_{\pm}[w]))^n\Big)\\
&\leq C(h^2+\tau^2)^2 + C\tau\sum_{n=0}^{N}||\mathbf{w}^n||^2_{\ell^2_J}.
\end{aligned} \tag{49}$$

Finally, (29), (46) and (49) lead to

$$||\mathbf{w}^N||^2_{\ell^2_J} - ||\mathbf{w}^0||^2_{\ell^2_J} \leq C(\tau^2+h^2)^2 + C\tau\sum_{n=0}^{N}||\mathbf{w}^n||^2_{\ell^2_J},$$

which proves (43): $\|\mathbf{w}^N\|_{\ell^2_J} \leq Ce^{CN\tau}(\tau^2+h^2) \leq Ce^{CT}(\tau^2+h^2)$.

Let us now focus on (44). For $\{\psi^n_j\}_n$ solution to (6), with $\psi^0_j = 0$ for $0 \leq j \leq K-1$, from Lemma 3 we can find K sequences $\{u^n_k\}_n$, with $0 \leq k \leq K-1$, such that: $\psi^n_j = \sum_{k=0}^{K-1}(f_{j-k}\star u_k)^n$, $0 \leq n \leq K-1$. Then, ψ^n_j, for $j \leq -1$, can be defined by: $\psi^n_j = \sum_{k=1}^{K}(f_{j-k}\star u_k)^n$. In this case, the solution satisfies: $\mathrm{i}\tau^{-1}(\psi^{n+1}_j - \psi^n_j) = L_{\delta,h}E\psi^n_j$, $j \leq 0$, and $|\psi^n_j| \to 0$ as $j \to -\infty$. This leads to

$$\mathrm{i}\frac{\nabla_+\psi^{n+1}_j - \nabla_+\psi^n_j}{\tau} = L_{\delta,h}E\nabla_+\psi^n_j, \quad j \leq -1.$$

Introducing $\varphi^n_j = \nabla_+\psi^n_j$, for $0 \leq j \leq K-1$, from Lemma 2 we can find K sequences $\{v^n_k\}_n$, with $1 \leq k \leq K$, such that: $\varphi^n_j = \sum_{k=0}^{K-1}(f_{j-k}\star v_k)^n$, $0 \leq j \leq K-1$. The terms φ^n_j, for $j \leq -1$, can be defined by: $\varphi^n_j = \sum_{k=1}^{K}(f_{j-k}\star v_k)^n$, $j \leq -1$. In this case, we have

$$\mathrm{i}\frac{\varphi^{n+1}_j - \varphi^n_j}{\tau} = L_{\delta,h}E\varphi^n_j, \quad j \leq -1,$$

and $|\varphi^n_j| \to 0$ as $j \to -\infty$. By defining $\omega^n_j = \nabla_+\psi^n_j - \varphi^n_j$, we obtain

$$\mathrm{i}\frac{\omega^{n+1}_j - \omega^n_j}{\tau} = L_{\delta,h}E\omega^n_j, \quad j \leq -1,$$

and $(\mathbf{v}_-[\omega])^n = [\nabla_+\psi^n_k - \varphi^n_k]^T_{k=0,\dots,K-1} = \mathbf{0}$. Repeating the procedure as for (25), we deduce

$$\sum_{j=-\infty}^{-1}\frac{|\omega^N_j|^2}{\tau} = 2\Im\Big(\sum_{n=0}^{N-1}\overline{(E(\mathbf{w}_-[\omega]))^n}^T\cdot\mathbb{S}(E\mathbf{v}_-[\omega])^n\Big) = 0.$$

Then, we have $\nabla_+\psi^n_j - \varphi^n_j = \omega^n_j = 0$ for $j \leq -1$. By defining $(\mathbf{v}_-[\nabla_+\psi])^n = [\nabla_+\psi^n_k]^T_{k=0,\dots,K-1}$ and $(\mathbf{w}_-[\nabla_+\psi])^n = [\nabla_+\psi^n_{-k}]^T_{k=1,\dots K}$, we obtain: $(\mathbf{w}_-[\omega])^n = (\mathbf{w}_-[\nabla_+\psi])^n - (\mathbf{v}_-[\varphi])^n = 0$. From $(\mathbf{w}_-[\varphi])^n = (\mathbb{C}\star\mathbf{v}_-[\varphi])^n$, one gets

$$(\mathbf{w}_-[\nabla_+\psi])^n = (\mathbf{w}_-[\varphi])^n = (\mathbb{C}\star\mathbf{v}_-[\varphi])^n = (\mathbb{C}\star\mathbf{v}_-[\nabla_+\psi])^n. \tag{50}$$

Similarly, we derive: $(\mathbf{w}_+[\nabla_-\psi])^n = (\mathbb{C} \star \mathbf{v}_+[\nabla_-\psi])^n$, with $(\mathbf{v}_+[\nabla_-\psi])^n = [\nabla_-\psi^n_{L-k}]^T_{k=0,\dots,K-1}$ and $(\mathbf{w}_+[\nabla_-\psi])^n = [\nabla_-\psi^n_{L+k+1}]^T_{k=0,\dots,K-1}$. From (34) and Lemma 7, we have

$$\nabla_+\epsilon_j(t) = a_0\nabla_+\psi_j(t) + \sum_{k=1}^{K} a_k(\nabla_+\psi_{j+k}(t) + \nabla_+\psi_{j-k}(t)) - \mathcal{L}_\delta\nabla_+\psi_j(t) = h^2\nabla_+Q(x_j,t),$$

for $\nabla_+u_j(t) = (u_{j+1}(t) - u_j(t))/h$. From Lemma 7, we deduce

$$h\sum_{j\in\mathbb{Z}} |\nabla_+Q(x_j,t)|^2 \le C\int_{\mathbb{R}} \sum_{p=3}^{6} |\partial_y^p\psi(y,0)|^2 dy.$$

Therefore, we obtain

$$\sum_{n=0}^{N-1}\sum_{j=-\infty}^{-1} |\nabla_+e_j^n|^2 h\tau \le C(h^4+\tau^4)\int_0^T\int_{\mathbb{R}} \sum_{0\le p\le 6, 0\le k\le 5} |\partial_x^p\partial_t^k\psi(x,t)|^2 dxdt \le C(h^4+\tau^4).$$

For the sequence $\{\psi_j(t_n)\}_n$ solution of (1), with $\psi_j^0 = 0$, for $0 \le j \le K-1$, from Lemma 2 we can find K sequences $\{u_k^n\}_n$, with $0 \le k \le K-1$, such that

$$\chi_j^n = \nabla_+\psi_j(t_n) = \sum_{k=0}^{K-1} (f_{j-k} \star u_k)^n, \quad 0 \le j \le K-1. \tag{51}$$

Then, the values χ_j^n, for $j \le -1$, can be defined by

$$\chi_j^n = \sum_{k=1}^{K} (f_{j-k} \star u_k)^n, \quad j \le -1. \tag{52}$$

In this case, the solution satisfies

$$\mathrm{i}\frac{\chi_j^{n+1} - \chi_j^n}{\tau} = L_{\delta,h}E\chi_j^n, \quad j \le -1,$$

with $|\chi_j^n| \to 0$ as $j \to -\infty$. Now, let us consider $d_j^n = \chi_j^n - \nabla_+\psi(x_j,t_n)$. For $j \le -1$, we have

$$\mathrm{i}D_\tau d_j^n = a_0Ed_j^n + \sum_{k=1}^{K} a_k(Ed_{j-k}^n + Ed_{j+k}^n) - \frac{1}{2}\nabla_+e_j^n.$$

Multiplying the above equality by $\overline{Ed_j^n}$, and summing from $j = -J$ to -1 we get

$$\sum_{j=-J}^{-1} i\frac{d_j^{n+1} - d_j^n}{\tau}\overline{Ed_j^n} = \sum_{j=-J}^{-1}\Big[\sum_{k=1}^{K} a_k(Ed_{j+k}^n - Ed_j^n)\overline{Ed_j^n} + \sum_{k=1}^{K} a_k(Ed_{j-k}^n - Ed_j^n)\overline{Ed_j^n}\Big]$$
$$-\frac{1}{2}\sum_{j=-J}^{-1}\nabla_+e_j^n\overline{Ed_j^n}. \tag{53}$$

Computing (53)-$\overline{(53)}$, taking $J \to \infty$ in (53), since $\varphi_j^n \to 0$ when $|j| \to \infty$ we have

$$\sum_{j=-\infty}^{0} \mathrm{i}\frac{|d_j^{n+1}|^2 - |d_j^n|^2}{\tau} = 2i\Im\Big(\sum_{n=0}^{N-1}\overline{(E(\mathbf{w}_-[d]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_-[d]))^n\Big)$$
$$-\frac{1}{2}\sum_{j=-\infty}^{-1}\nabla_+e_j^n\overline{Ed_j^n} + \frac{1}{2}\sum_{j=-\infty}^{-1}\nabla_+\overline{e_j^n}Ed_j^n. \tag{54}$$

From the choice of $\{\chi_j^n\}_n$ for $0 \le j \le K-1$, we have: $d_j^n = \chi_j^n - \nabla_+\psi(x_j,t_n) = 0$ for $0 \le j \le K-1$, and then $\mathbf{v}_-[d] = 0$. Next summing up (54) from $n=0$ to $N-1$ provides

$$\sum_{j=-\infty}^{-1} \frac{|d_j^N|^2}{\tau} = \sum_{n=0}^{N-1}\sum_{j=-\infty}^{0} \frac{|d_j^{n+1}|^2 - |d_j^n|^2}{\tau} = \frac{1}{2\mathrm{i}}\Big(- \sum_{n=0}^{N-1}\sum_{j=-\infty}^{-1} \nabla_+ e_j^n \overline{E d_j^n} + \sum_{n=0}^{N-1}\sum_{j=-\infty}^{-1} \nabla_+ \overline{e_j^n} E d_j^n\Big)$$
$$\le C \sum_{j=-\infty}^{-1}\sum_{n=0}^{N-1} |\nabla_+ e_j^n|^2 + \sum_{j=-\infty}^{-1}\sum_{n=0}^{N-1} |d_j^n|^2.$$

Then, combining (51) and a Gronwall inequality [35] yields

$$h \sum_{j=-\infty}^{-1} |d_j^N|^2 \le C\tau h \sum_{j=-\infty}^{-1}\sum_{n=0}^{N-1} |\nabla_+ e_j^n|^2 \le (h^4+\tau^4) C(\psi^0, \gamma_\delta, \delta, T).$$

From (51) and (52), we have $(\mathbf{w}_-[\chi])^n = (\mathbb{C} \star \mathbf{v}_-[\chi])^n = (\mathbb{C} \star \mathbf{V}_-[\nabla_+\psi_j(t_n)])^n$. We deduce

$$\begin{aligned}[d_{-1}^n, d_{-2}^n, ...d_{-K}^n]^T &= [\chi_{-1}^n - \nabla_+\psi_{-1}(t_n), \chi_{-2}^n - \nabla_+\psi_{-2}(t_n), ...\chi_{-K}^n - \nabla_+\psi_{-K}(t_n)]^T \\ &= (\mathbf{w}_-[\chi])^n - \nabla_+ \mathbf{W}_-(t_n) = (\mathbb{C} \star \mathbf{V}_-[\nabla_+\psi_j(t_n)])^n - \nabla_+ \mathbf{W}_-(t_n) = \nabla_+ \mathbf{G}_-(t_n),\end{aligned}$$

and similarly to the previous calculations, by (51),

$$||\boldsymbol{\nabla}_+ \mathbf{e}^n||_{\ell^2_{J-1}} \le C(\tau^2+h^2), \quad ||\nabla_\mp \mathbf{G}_\pm^n||_{\ell^2_K} \le C(\tau^2+h^2), \quad 0 \le n \le N.$$

From $w_j^n = \psi_j^n - \psi(x_j,t_n)$, we have

$$i\frac{1}{\tau}(\nabla_+ w_j^{n+1} - \nabla_+ w_j^n) = L_{\delta,h}(\nabla_+ w_j^{n+1} + \nabla_+ w_j^n) - \frac{1}{2}\nabla_+ e_j^n.$$

By $(\mathbf{w}_\mp[\nabla_\pm\psi])^n = (\mathbb{C}\star\mathbf{v}_\mp[\nabla_\pm\psi])^n$ in (50), we have $(\mathbf{w}_-[\nabla_+ w])^n = (\mathbf{w}_-[\nabla_+\psi])^n - (\mathbf{w}_-[\nabla_+\psi(t_n)]) = (\mathbb{C}\star\mathbf{v}_-[\nabla_+\psi])^n - (\mathbf{w}_-[\nabla_+\psi(t_n)])$ which leads to: $(\mathbf{w}_-[\nabla_+ w])^n - (\mathbb{C}\star\mathbf{v}_-[\nabla_+ w])^n = (\mathbb{C}\star\mathbf{v}_-[\nabla_+\psi(t_n)]) - (\mathbf{w}_-[\nabla_+\psi(t_n)]) = \nabla_+\mathbf{G}_-(t_n)$. Thus repeating a procedure similar as in Proposition 1, we obtain

$$\frac{\mathrm{i}}{\tau}\sum_{j=0}^{J-1}(|\nabla_+ w_j^N|^2 - |\nabla_+ w_j^0|^2) = -2i\Im\Big(\sum_{n=0}^{N-1} \overline{(E(\mathbf{w}_-[\nabla_+ w]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_-[\nabla_+ w]))^n$$
$$+ \sum_{n=0}^{N-1} \overline{(E(\mathbf{w}_+[\nabla_- w]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_+[\nabla_- w]))^n\Big) + \sum_{n=0}^{N-1}\sum_{j=0}^{J-1} \frac{1}{2}\Big(- \overline{\nabla_+ e_j^n} E \nabla_+ w_j^n + \nabla_+ e_j^n \overline{E\nabla_+ w_j^n}\Big),$$

which leads to

$$\sum_{j=0}^{J-1} h(|\nabla_+ w_j^N|^2 - |\nabla_+ w_j^0|^2)$$
$$= -2\tau h\Im\Big(\sum_{n=0}^{N-1} \overline{(E(\mathbb{C}\star\mathbf{v}_+[\nabla_- w]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_+[\nabla_- w]))^n - \sum_{n=0}^{N-1} \overline{E(\mathbf{G}_+(t_n))}^T \cdot \mathbb{S}(E(\mathbf{v}_+[\nabla_- w]))^n\Big)$$
$$-2\tau h\Im\Big(\sum_{n=0}^{N-1} \overline{(E(\mathbb{C}\star\mathbf{v}_-[\nabla_+ w]))^n}^T \cdot \mathbb{S}(E(\mathbf{v}_-[\nabla_+ w]))^n - \sum_{n=0}^{N-1} \overline{E(\mathbf{G}_-(t_n))}^T \cdot \mathbb{S}\cdot(E(\mathbf{v}_-[\nabla_+ w]))^n\Big)$$
$$+\frac{\tau h}{2}\sum_{n=0}^{N-1}\sum_{j=0}^{J-1}\Big(|\nabla_+ e_j^n||\nabla_+ w_j^n| + |\nabla_+ e_j^n||\nabla_+ w_j^{n+1}|\Big).$$

We have

$$
\begin{aligned}
&||\nabla_+\mathbf{w}^N||^2_{\ell^2_{J-1}} - ||\nabla_+\mathbf{w}^0||^2_{\ell^2_{J-1}} \\
&\leq C(\tau^2+h^2)^2 + C\tau\sum_{n=0}^{N}||\nabla_+\mathbf{w}^n||^2_{\ell^2_{J-1}} + \frac{\tau h}{2}\sum_{n=0}^{N-1}\sum_{j=0}^{J-1}\Big(|\nabla_+e_j^n||\nabla_+w_j^n| + |\nabla_+e_j^n||\nabla_+w_j^{n+1}|\Big) \\
&\leq C(\tau^2+h^2)^2 + C\tau\sum_{n=0}^{N}||\nabla_+\mathbf{w}^n||^2_{\ell^2_{J-1}},
\end{aligned}
$$

which implies: $||\nabla_+\mathbf{w}^N||_{\ell^2_{J-1}} \leq Ce^{CT}(\tau^2+h^2)$, and proves (44). Finally, by the discrete Sobolev imbedding theorem, we obtain (45). ■

6. Numerical examples

6.1. Example 1

Let us start by considering the nonlocal Schrödinger equation (1) with the constant kernel function $\gamma_\delta(a,b) = 2\delta^{-3}$, for $a \in [-\delta,\delta]$. The computational domain is $[x_-,x_+] := [-3,3]$, and the final time is set to $T=2$, for the initial gaussian data $\psi(x,0) = 5e^{2ix-25x^2/4}$.

Let us fix the spatial discretization step to $h = 5\times10^{-2}$ and analyze the ℓ^∞_J-norm error defined by: $e^{h,\tau}_{\infty,T} := ||\psi^N_j - \psi^{N,\text{ref}}||_{\ell^\infty_J}$ thanks to τ, with $N\tau = T$. Here, we introduced $||u_j||_{\ell^\infty_J} := \max_{0\leq j\leq J}|u_j|$. The reference solution $\psi^{n,\text{ref}}$ is computed for the discretization parameters $h = 5\times10^{-2}$ and $\tau = 1\times10^{-4}$. For different values of δ, we report the error $e^{h,\tau}_{\infty,T}$ at time $T=2$ in Table 1. This example shows that the scheme is second-order in time as expected. Let us now fix the time step to $\tau = 1\times10^{-3}$. The reference solution $\psi^{n,\text{ref}}$ is obtained for $h = 2.5\times10^{-3}$ and $\tau = 1\times10^{-3}$. We give in Table 2 the error $e^{h,\tau}_{\infty,T}$ at $T=2$ with respect to the mesh refinement h where we observe that the convergence rate is equal to 2.

$e^{h,\tau}_{\infty,T}$	$\tau = 1\times10^{-2}$	$\tau = 5\times10^{-3}$	$\tau = 4\times10^{-3}$	$\tau = 2.5\times10^{-3}$	rate
$\delta = 0.4$	4.00×10^{-2}	1.01×10^{-2}	6.44×10^{-3}	2.52×10^{-3}	2.00
$\delta = 0.5$	3.16×10^{-2}	5.06×10^{-3}	7.79×10^{-3}	1.98×10^{-3}	1.99
$\delta = 0.8$	5.71×10^{-3}	1.43×10^{-3}	9.13×10^{-4}	3.56×10^{-4}	2.00
$\delta = 1$	2.20×10^{-3}	5.50×10^{-4}	3.52×10^{-4}	1.37×10^{-4}	1.99

Table 1: **Example 1:** ℓ^∞_J-norm error $e^{h,\tau}_{\infty,T}$ ($h = 5\times10^{-2}$) and convergence rate vs. τ for various values δ.

$e^{h,\tau}_{\infty,T}$	$h = 5\times10^{-2}$	$h = 2.5\times10^{-2}$	$h = 2\times10^{-2}$	$h = 1.25\times10^{-2}$	rate
$\delta = 0.4$	3.76×10^{-2}	9.30×10^{-3}	5.92×10^{-3}	2.25×10^{-3}	2.02
$\delta = 0.5$	4.74×10^{-2}	1.17×10^{-2}	7.46×10^{-3}	2.84×10^{-3}	2.02
$\delta = 0.8$	2.41×10^{-2}	5.98×10^{-3}	3.80×10^{-3}	1.45×10^{-3}	2.02
$\delta = 1$	1.39×10^{-2}	3.45×10^{-3}	2.19×10^{-3}	8.36×10^{-4}	2.03

Table 2: **Example 1:** ℓ^∞_J-norm error $e^{h,\tau}_{\infty,T}$ ($\tau = 1\times10^{-3}$) and convergence rate vs. h for various values δ.

Figure 2 (left) gives the evolution of the numerical solution with discrete ABC in the bounded domain by setting $\tau = 1\times10^{-3}$ and $h = 1.25\times10^{-2}$, for $\delta = 0.4$. For completeness, we also provide

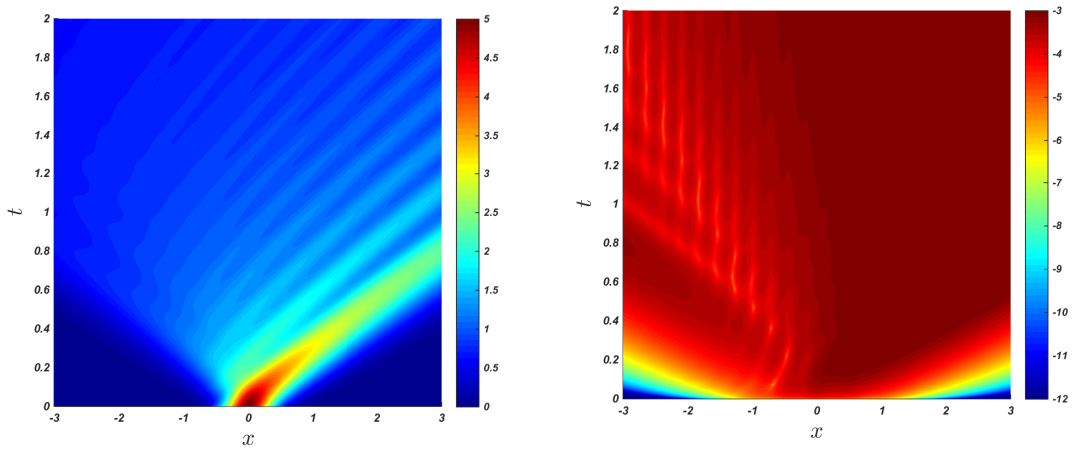

Figure 2: **Example 1 for $\delta = 0.4$:** left: numerical solution; right: error between the reference and numerical solutions (in $\log_{10}$ scale).

on Figure 2 (right) the pointwise error $|\psi_j^n - \psi_j^{n,\mathrm{ref}}|$ (in $\log_{10}$ scale) between the computed solution $\boldsymbol{\psi}^n$ (in $[-3;3] \times [0;2]$) and a reference solution $\boldsymbol{\psi}^{n,\mathrm{ref}}$ computed on a very large spatial domain for $h = 2.5 \times 10^{-3}$ and $\tau = 1 \times 10^{-3}$ and then restricted to the smaller computational domain $[-3;3] \times [0;2]$. We observe that the reflection at the boundary related to the ABC is small and has an amplitude similar to the numerical error of the interior scheme.

6.2. Example 2

We consider now the singular kernel $\gamma(a,b) = \frac{21}{8\delta^{21/8}a^{3/8}}$, with $a \in [-\delta, \delta]$ and the singular kernel exponent $\alpha = 3/8$. We still have $[x_-, x_+] = [-3, 3]$ and $T = 2$, with the same initial data as in Example 1. We choose a fixed spatial discretization step $h = 5 \times 10^{-2}$ and analyze the error $e_{\infty,T}^{h,\tau}$ at $T = 2$ vs τ in Table 3 for various values of δ. The reference solution $\psi^{n,\mathrm{ref}}$ is evaluated for the parameters $h = 5 \times 10^{-2}$ and $\tau = 1 \times 10^{-4}$. We again observe that the scheme is second-order accurate in time. Let us now fix the time step to $\tau = 1 \times 10^{-3}$. The reference solution $\psi^{n,\mathrm{ref}}$ is obtained for $h = 2.5 \times 10^{-3}$ and $\tau = 1 \times 10^{-3}$. We report in Table 4 the error $e_{\infty,T}^{h,\tau}$ at $T = 2$ with respect to the mesh refinement h. For the various values of δ, we observe that the convergence rate is equal to 2 according to h in Table 4. For the same parameters values, we finally plot in Figure 3 (left) the evolution of the solution and the error (right) between the numerical and the reference solutions which again attest of the accuracy of both the scheme and discrete ABC.

$e_{\infty,T}^{h,\tau}$	$\tau = 1 \times 10^{-2}$	$\tau = 5 \times 10^{-3}$	$\tau = 4 \times 10^{-3}$	$\tau = 2.5 \times 10^{-3}$	rate
$\delta = 0.4$	6.88×10^{-2}	1.96×10^{-2}	1.26×10^{-2}	4.94×10^{-3}	1.90
$\delta = 0.5$	8.14×10^{-2}	2.06×10^{-2}	1.32×10^{-2}	5.15×10^{-3}	1.99
$\delta = 0.8$	2.06×10^{-2}	5.17×10^{-3}	3.30×10^{-3}	1.29×10^{-3}	2.00
$\delta = 1$	8.58×10^{-3}	2.15×10^{-3}	1.37×10^{-3}	5.36×10^{-4}	2.00

Table 3: **Example 2:** ℓ_J^∞-norm error $e_{\infty,T}^{h,\tau}$ ($h = 5 \times 10^{-2}$) and convergence rate vs. τ for various values δ.

$e^{h,\tau}_{\infty,T}$	$h = 5 \times 10^{-2}$	$h = 2.5 \times 10^{-2}$	$h = 2 \times 10^{-2}$	$h = 1.25 \times 10^{-2}$	rate
$\delta = 0.4$	3.07×10^{-2}	7.70×10^{-3}	4.90×10^{-3}	1.87×10^{-3}	2.02
$\delta = 0.5$	5.06×10^{-2}	1.25×10^{-2}	7.97×10^{-3}	3.04×10^{-3}	2.03
$\delta = 0.8$	3.07×10^{-2}	7.60×10^{-3}	4.84×10^{-3}	1.84×10^{-3}	2.03
$\delta = 1$	2.19×10^{-2}	5.42×10^{-3}	3.45×10^{-3}	1.31×10^{-3}	2.03

Table 4: **Example 2:** ℓ^∞_J-norm error $e^{h,\tau}_{\infty,T}$ ($\tau = 1 \times 10^{-3}$) and convergence rate vs. h for various values δ.

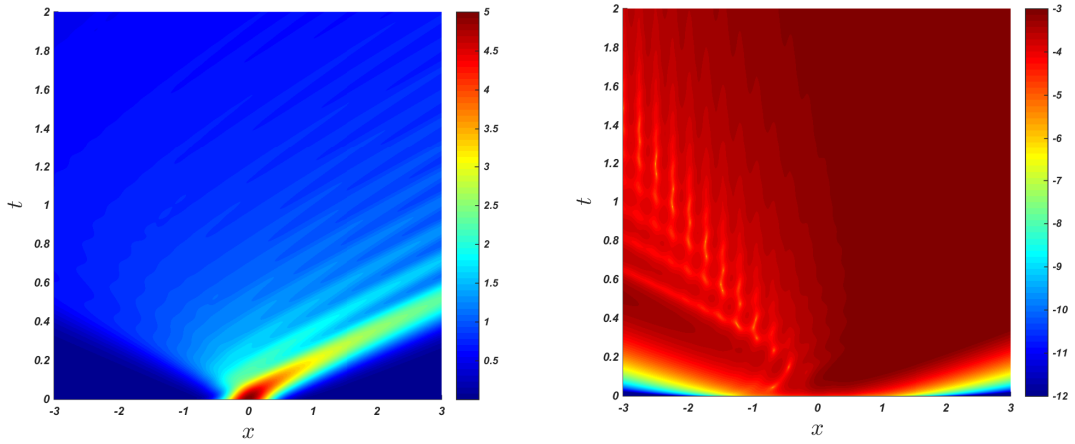

Figure 3: **Example 2 ($\delta = 0.4$):** left: numerical solution; right: error between the reference and numerical solutions (in $\log_{10}$ scale).

7. Conclusion

We provided the construction of fully discrete ABCs for the one-dimensional nonlocal Schrödinger equation discretized by the Crank-Nicolson scheme in time and an asymptotically compatible scheme in space. An algorithm is given for evaluating these ABCs. In addition, the stability and error analysis of the scheme are developed for a singular kernel. Numerical examples confirm the accuracy of the ABCs. Further works include the extension to the singular cases for $\alpha \geq 1/2$, higher dimensional problems as well as considering nonlinearities into the equation.

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Appendix A. Proof of Lemma 7

From the identity $u(x-\varsigma)-2u(x)+u(x+\varsigma)=\varsigma^2\int_0^1\int_0^{\xi_1}(u''(x+\varsigma\xi_2)+u''(x-\varsigma\xi_2))d\xi_2 d\xi_1$, the third term on the right hand side of (35) can be written as

$$\begin{aligned}
&\int_0^\delta(\psi(x_j-\varsigma,t)-2\psi(x_j,t)+\psi(x_j+\varsigma,t))\gamma_\delta(\varsigma)d\varsigma\\
&=h^3\int_0^1\varsigma^2\phi_0(\varsigma h)\gamma_\delta(\varsigma h)d\varsigma\int_0^1\int_0^{\xi_1}(\partial_x^2\psi(x_j+\varsigma\xi_2 h,t)+\partial_x^2\psi(x_j-\varsigma\xi_2 h,t))d\xi_2 d\xi_1\\
&+\sum_{k=1}^K\int_0^\delta\phi_k(\varsigma)\Big[\varsigma^2\gamma_\delta(\varsigma)d\varsigma\int_0^1\int_0^{\xi_1}(\partial_x^2\psi(x_j+\varsigma\xi_2,t)+\partial_x^2\psi(x_j-\varsigma\xi_2,t))d\xi_2 d\xi_1\Big].
\end{aligned}\tag{A.1}$$

In the same way, the two first terms on the right hand side can be recast as

$$\begin{aligned}
&\sum_{k=1}^{K-1}\frac{\psi_{j-k}-2\psi_j+\psi_{j+k}}{kh}\int_{x_{k-1}}^{x_{k+1}}\phi_k(\varsigma)\varsigma\gamma_\delta(\varsigma)d\varsigma+\frac{\psi_{j-K}-2\psi_j+\psi_{j+K}}{Kh}\int_{x_{K-1}}^{x_K}\phi_K(\varsigma)\varsigma\gamma_\delta(\varsigma)d\varsigma\\
&\quad=\sum_{k=1}^K\int_0^\delta\phi_k(\varsigma)\Big[kh\varsigma\gamma_\delta(\varsigma)d\varsigma\int_0^1\int_0^{\xi_1}(\partial_x^2\psi(x_j+\xi_2 kh,t)+\partial_x^2\psi(x_j-\xi_2 kh,t))d\xi_2 d\xi_1\Big].
\end{aligned}\tag{A.2}$$

Thus, from (A.1) and (A.2), (35) can be rewritten as

$$\begin{aligned}
&\epsilon_j(t)=\sum_{k=1}^K\int_0^\delta\phi_k(\varsigma)q_k(\varsigma,x_j,t)d\varsigma\\
&-h^3\int_0^1\varsigma^2\phi_0(\varsigma h)\gamma_\delta(\varsigma h)d\tau\int_0^1\int_0^{\xi_1}(\partial_x^2\psi(x_j+\varsigma\xi_2 h,t)+\partial_x^2\psi(x_j-\varsigma\xi_2 h,t))d\xi_2 d\xi_1,
\end{aligned}\tag{A.3}$$

where $q_k(\varsigma,x,t)$ is defined by (38). It is easy to see that

$$\begin{aligned}
q_k(\varsigma,x,t)&=q_k(kh,x,t)+\dot q_k(kh,x,t)(\varsigma-kh)+\int_{kh}^\varsigma\ddot q_k(y,x,t)(\varsigma-y)dy,\\
q_k(\varsigma,x,t)&=q_k(kh,x,t)+\int_{kh}^\varsigma\dot q_k(y,x,t)dy,
\end{aligned}\tag{A.4}$$

where we use the dots to represent the derivative of $q_k(\varsigma,x,t)$ with respect to the first variable ς. By using (A.4) and $q_k(kh,x,t)=0$, we deduce after some calculations

$$\begin{aligned}
&\sum_{k=1}^K\int_0^\delta\phi_k(\varsigma)q_k(\varsigma,x_j,t)d\varsigma=\sum_{k=1}^{K-1}h^3\int_{-1}^1\phi_0(\varsigma h)\varsigma^2 d\varsigma\int_0^1\ddot q_k(kh+\varsigma yh,x_j,t)(1-y)dy\\
&+h^2\int_{-1}^0\phi_0(\varsigma h)\varsigma d\varsigma\int_0^1\dot q_K(Kh+\varsigma yh,x_j,t)dy.
\end{aligned}\tag{A.5}$$

Therefore from (A.3) and (A.5), we obtain: $\epsilon_j(t)=h^2Q(x_j,t)$, with $Q(x,t)$ defined by (37).

Now, the last term of (37) satisfies

$$\begin{aligned}
&|h\int_0^1\varsigma^2\phi_0(\varsigma h)\gamma_\delta(\varsigma h)d\varsigma\int_0^1\int_0^{\xi_1}(\partial_x^2\psi(x+\varsigma\xi_2 h,t)+\partial_x^2\psi(x-\varsigma\xi_2 h,t))d\xi_2 d\xi_1|\\
&\le\frac{C}{h^\alpha}\int_{-h}^h|\partial_x^2\psi(x+y,t)|dy.
\end{aligned}$$

Consequently, we deduce

$$|Q(x,t)|^2 \leq C\sum_{k=1}^{K-1}\int_0^1 d\varsigma\int_{-\varsigma h}^{\varsigma h}(\varsigma h-|y|)^2|\ddot{q}_k(kh+y,x,t)|^2dy/h^2$$
$$+C\int_0^1 d\varsigma\int_{-\varsigma h}^{0}|\dot{q}_K(Kh+y,x,t)|^2dy/h+C\int_{-h}^{h}|\partial_x^2\psi(x+y,t)|^2dy/h^{2\alpha-1}. \quad (A.6)$$

From (38), the terms $\dot{q}_k(\varsigma,x,t)$ and $\ddot{q}_k(\varsigma,x,t)$ satisfy

$$\ddot{q}_k(\varsigma,x,t)=\frac{d^2}{d\varsigma^2}(\varsigma\gamma_\delta(\varsigma))\int_0^1\int_{\varsigma\xi_1}^{kh\xi_1}(\partial_x^2\psi(x+\xi_2,t)+\partial_x^2\psi(x-\xi_2,t))d\xi_2d\xi_1 \quad (A.7)$$
$$-2\frac{d}{d\varsigma}(\varsigma\gamma_\delta(\varsigma))\int_0^1(\xi_1\partial_x^2\psi(x+\xi_1\varsigma,t)+\xi_1\partial_x^2\psi(x-\xi_1\varsigma,t))d\xi_1$$
$$-\varsigma\gamma_\delta(\varsigma)\int_0^1(\xi_1^2\partial_x^3\psi(x+\xi_1\varsigma,t)-\xi_1^2\partial_x^3\psi(x-\xi_1\varsigma,t))d\xi_1$$

and

$$\dot{q}_K(\varsigma,x,t)=\frac{d}{d\varsigma}(\varsigma\gamma_\delta(\varsigma))\int_0^1\int_{\varsigma\xi_1}^{Kh\xi_1}(\partial_x^2\psi(x+\xi_2,t)+\partial_x^2\psi(x-\xi_2,t))d\xi_2d\xi_1$$
$$-(\varsigma\gamma_\delta(\varsigma))\int_0^1(\xi_1\partial_x^2\psi(x+\xi_1\varsigma,t)+\xi_1\partial_x^2\psi(x-\xi_1\varsigma,t))d\xi_1.$$

Now, γ_δ takes its values on $[-\delta,\delta]$ and has a singularity at 0 of the form $|\varsigma|^{-\alpha}$. Thus, we can find a constant $C>0$ such that: $|\frac{d^m}{d\varsigma^m}\gamma_\delta(\varsigma)|\leq C|\varsigma^{-(\alpha+m)}|$, for $\varsigma\in[-\delta,\delta]$ and $m=0,1,2$. In addition, in (A.5), $\ddot{q}_k(\varsigma,x,t)$ only takes its values ς on $[(k-1)h,(k+1)h]$. Recalling that $kh\leq Kh=\delta$, for example the function $\partial_x^2\psi(x+\xi_2,t)$ in (A.7) has values for $\xi_2\in[-\delta,\delta]$. Thus, for $(k-1)h\leq\varsigma\leq(k+1)h$, from the above expression and (38), we have

$$|\ddot{q}_k(\varsigma,x,t)|^2\leq C(h^2\varsigma^{-2(1+\alpha)}+\varsigma^{-2\alpha}+\varsigma^{2-2\alpha})||(|\partial_x^2\psi(y,t)|+|\partial_x^3\psi(y,t)|)^2||_{L^\infty_{x,\delta}},$$
$$|\dot{q}_K(\varsigma,x,t)|^2\leq C(h^2\varsigma^{-2\alpha}+\varsigma^{2-2\alpha})\||\partial_x^2\psi(y,t)|^2||_{L^\infty_{x,\delta}}.$$

The above inequality gives after some computations

$$\int_0^1 d\varsigma\int_{-\varsigma h}^{\varsigma h}(\varsigma h-y)^2|\ddot{q}_k(kh+y,x,t)|^2dy/h^2 \quad (A.8)$$
$$\leq C\|(|\partial_x^2\psi(y,t)|+|\partial_x^3\psi(y,t)|)^2||_{L^\infty_{x,\delta}}\int_{(k-1)h}^{(k+1)h}\frac{1}{|y|^{2\alpha}}dy+Ch\|(|\partial_x^2\psi(y,t)|+|\partial_x^3\psi(y,t)|)^2||_{L^\infty_{x,\delta}},$$

and

$$\int_0^1 d\varsigma\int_{-\varsigma h}^{0}|\dot{q}_k(Kh+y,x,t)|^2dy/h\leq C\||\partial_x^2\psi(y,t)|^2||_{L^\infty_{x,\delta}}. \quad (A.9)$$

Taking (A.8), (A.9) into (A.6), for $\alpha<1/2$ we have

$$|Q(x,t)|^2\leq C\|(|\partial_x^2\psi(y,t)|+|\partial_x^3\psi(y,t)|)^2||_{L^\infty_{x,\delta}}. \quad (A.10)$$

On the other hand, there exists $x_\delta \in [x-\delta, x+\delta]$ such that

$$\||\partial_x^2\psi(y,t)|^2\|_{L^\infty_{x,\delta}} = |\partial_x^2\psi(x_\delta,t)|^2 \le C|\partial_x^2\psi(x,t)|^2 + C\int_{-\delta}^{\delta}|\partial_x^3\psi(x+y,t)|^2dy. \tag{A.11}$$

Combining (A.10) and (A.11), we have

$$h\sum_{j=-\infty}^{\infty}|Q(x_j,t)|^2 \le C\int_{\mathbb{R}}\sum_{p=2}^{4}|\partial_x^p\psi(y,0)|^2dy$$

from Lemma 5. Thus, this ends the proof of (36). ■

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