Open boundary conditions and computational schemes for Schrödinger equations with general potentials and nonlinearities

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Abstract

This paper addresses the construction of absorbing boundary conditions for the one-dimensional Schrödinger equation with a general variable repulsive potential or with a cubic nonlinearity. Semi-discrete time schemes, based on Crank-Nicolson approximations, are built for the associated initial boundary value problems. Finally, some numerical simulations give a comparison of the various absorbing boundary conditions to analyse their accuracy and efficiency.

1 Introduction

We consider in this paper two kinds of initial value problems. The first one consists in a time-dependent Schrödinger equation with potential V set in an unbounded domain

$$\begin{cases} i\partial_t u + \partial_x^2 u + V\, u = 0, & (x,t) \in \mathbb{R} \times [0;T], \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{1.1}$$

where u_0 in the initial data. The maximal time of computation is denoted by T. We assume in this article that V is a real-valued potential such that $V \in \mathcal{C}^\infty(\mathbb{R}\times\mathbb{R}^+, \mathbb{R})$. This kind of potential then creates acceleration of the field compared to the free-potential equation [10, 17].

Our second interest concerns the one-dimensional cubic nonlinear Schrödinger equation

$$\begin{cases} i\partial_t u + \partial_x^2 u + q\,|u|^2\, u = 0, & (x,t) \in \mathbb{R}\times[0;T], \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{1.2}$$

where the real parameter q corresponds to a focusing ($q > 0$) or defocusing ($q < 0$) effect of the cubic nonlinearity. This equation has the property to possess special solutions which propagate without dispersion, the so-called solitons.

For obvious reasons linked to the numerical solution of such problems, it is usual to truncate the spatial computational domain with a fictitious boundary $\Sigma := \partial\Omega = \{x_l, x_r\}$, where x_l and x_r respectively designate the left and right endpoints introduced to have a bounded domain of computation $\Omega =]x_l; x_r[$. Let us define the time domains $\Omega_T = \Omega\times[0;T]$ and $\Sigma_T = \Sigma\times[0;T]$. Considering the fictitious boundary Σ, we are now led to solve the problem

$$\begin{cases} i\partial_t u + \partial_x^2 u + \mathscr{V}\, u = 0, & (x,t) \in \Omega_T, \\ u(x,0) = u_0(x), & x \in \Omega, \end{cases} \tag{1.3}$$

where $\mathscr{V}$ can denote either the real potential $V(x,t)$ or the cubic nonlinearity $q\,|u|^2\,(x,t)$. In the sequel of the paper, we assume that the initial datum u_0 is compactly supported in the computational domain Ω.

Of course, a boundary condition set on Σ_T must be added to systems (1.3). An ideal exact boundary condition answering the problem is the so-called Transparent Boundary Condition (TBC) which leads to a solution of (1.3) equal to the restriction of the solution of (1.1) or (1.2) on Ω_T. A first well-known case considers $\mathscr{V} = 0$. This situation has been treated by many authors [2]. In this case, which is precisely described in Section 2.2, we are able to build the following TBC in term of the Dirichlet-to-Neumann (DtN) operator

$$\partial_{\mathbf{n}} u + e^{-i\pi/4}\partial_t^{1/2} u = 0, \quad \text{on } \Sigma_T, \tag{1.4}$$

where $\mathbf{n}$ is the outwardly directed unit normal vector to Σ. The operator $\partial_t^{1/2}$ is known as the half-order derivative operator (see Equation (2.7) for its definition). Its nonlocal character related to its convolutional structure has led to many developments concerning its accurate and efficient evaluation in the background of TBCs [2].

A second situation which is related to the above case is when the potential is only time varying: $\mathscr{V} = V(x,t) = V(t)$. In this case, the change of unknown

$$v(x,t) = e^{-i\mathcal{V}(t)} u(x,t), \tag{1.5}$$

with

$$\mathcal{V}(t) = \int_0^t V(s)\, ds \tag{1.6}$$

reduces the initial Schrödinger equation with potential to the free-potential Schrödinger equation [4]. Then, the TBC (1.4) can be used for v and the resulting DtN TBC for u is

$$\partial_{\mathbf{n}} u(x,t) + e^{-i\pi/4} e^{i\mathcal{V}(t)}\, \partial_t^{1/2} \left(e^{-i\mathcal{V}(t)} u(x,t) \right) = 0, \qquad \text{on } \Sigma_T. \tag{1.7}$$

This change of variables is fundamental and, coupled to a factorization theorem, allows to derive accurate approximations of the TBC, which are usually called artificial or Absorbing Boundary Conditions (ABCs), in situations where $\mathscr{V} = V(x,t)$ [5] and $\mathscr{V} = q\,|u|^2$ [4]. Families of ABCs can be computed and are classified following their degree of accuracy. Typically, for a general function $\mathscr{V}$, the first ABC would be exactly (1.7), where $\mathcal{V}(t)$ has to be replaced by $\mathcal{V}(x,t) = \int_0^t \mathscr{V}(x,s) ds$. The ABC gives quite satisfactory accurate results but its evaluation remains costly since it involves the nonlocal time operator $\partial_t^{1/2}$. In [5], an other kind of ABCs was introduced, their numerical treatments being based on Padé approximants. It therefore gives rise to a local approximation scheme which is very competitive.

The aim of the present paper is to present precisely the link between the two different types of ABCs set up in [5] and [4] and to extend the local ABC derived for $\mathscr{V} = V(x,t)$ to the cubic nonlinear Schrödinger equation. Moreover, associated unconditionally stable schemes are given and numerical results are reported.

For completeness, we must mention that recent attempts have been directed towards the derivation of TBCs for special potentials. In [15], the case of a linear potential is considered in the background of parabolic equations in electromagnetism. Using the Airy functions, the TBC can still be written and its accuracy is tested. In [27], Zheng derives the TBC in the special case of a sinusoidal potential using Floquet's theory. All these solutions take care of the very special form of the potential. Let us remark that other solutions based on PML techniques have also been applied e.g. in [26]. Concerning the nonlinear case, using paradifferential operators techniques, Szeftel [24] presented other kinds of ABCs. Moreover, a recent paper [6] gives a comprehensive review of current developments related to the derivation of artificial boundary conditions for nonlinear partial differential equations following various approaches.

The present paper is organized as follows. In Section 2, we recall the derivation of open boundary conditions for linear Schrödinger equations. Subsection 2.1 concerns the derivation of the TBC, and Subsection 2.2 gives some possible extensions and their interpretations in the context of pseudodifferential calculus. This tool is the essential ingredient used in Section 3 where two possible approaches for building ABCs for the one-dimensional Schrödinger equation with a variable repulsive potential are given. Section 4 is devoted to their numerical discretization and the underlying properties of the proposed schemes. Section 5 is concerned with the nonlinear case for which we explain the links between the different approaches and propose a new family of ABCs for the cubic nonlinear Schrödinger equation. Numerical schemes are also analysed. Section 6 presents some numerical computations. These simulations show the high accuracy and efficiency of the proposed ABCs. Moreover, comparisons are provided between the different approaches. Finally, a conclusion is given in Section 7.

2 Open boundary conditions for linear Schrödinger equations

2.1 The constant coefficients case: derivation of the TBC

We recall in this Section the standard derivation of the Transparent Boundary Condition (TBC) in the context of the following 1D Schrödinger equation

$$\begin{aligned} & i\partial_t u + \partial_x^2 u + V(x,t)u = 0, \quad (x,t) \in \Omega_T, \\ & \lim_{|x|\to\infty} u(x,t) = 0, \\ & u(x,0) = u_0(x), \quad x \in \Omega, \end{aligned} \tag{2.1}$$

where the initial datum u_0 is compactly supported in Ω and the given real potential V is zero outside Ω. It is well-known that the previous equation (2.1) is well-posed in $L^2(\mathbb{R})$ (see e.g. [22, 23]) and that the "density" is time preserved, i.e., $\|u(t)\|_{L^2(\mathbb{R})} = \|u_0\|_{L^2(\mathbb{R})}$, $\forall t \geq 0$. The TBC for the Schrödinger equation (2.1) were independently derived by several authors from various application fields [20, 21, 8, 11, 13]. Such a TBC is nonlocal according to the time variable t and connects the Neumann datum $\partial_x v(x_{l,r},t)$ to the Dirichlet one $v(x_{l,r},t)$. As a Dirichlet-to-Neumann (DtN) map it reads

$$\partial_{\mathbf{n}} v(x,t) = -\frac{e^{-i\pi/4}}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{v(x,\tau)}{\sqrt{t-\tau}}\, d\tau \quad \text{on } \Sigma_T, \tag{2.2}$$

where $\partial_{\mathbf{n}}$ is the outwardly directed unit normal derivative to Ω.

The derivation of the TBC (2.2) is performed from Eq. (2.1) and is based on the decomposition of the Hilbert space $L^2(\mathbb{R})$ as $L^2(\Omega) \oplus L^2(\Omega_r \cup \Omega_l)$ where $\Omega =]x_l, x_r[$, $\Omega_l =]-\infty, x_l]$, and $\Omega_r = [x_r, \infty[$. Eq. (2.1) is equivalent to the coupled system of equations

$$\begin{cases} (i\partial_t + \partial_x^2)v = -V(x,t)v, \ (x,t) \in \Omega_T, \\ \partial_x v(x,t) = \partial_x w(x,t), \ (x,t) \in \Sigma_T \\ v(x,0) = u_0(x), \ x \in \Omega, \end{cases} \tag{2.3}$$

$$\begin{cases} (i\partial_t + \partial_x^2)w = 0, \ x \in \Omega_l \cup \Omega_r, \ t > 0, \\ w(x,t) = v(x,t), \ (x,t) \in \Sigma_T, \\ \lim_{|x| \to \infty} w(x,t) = 0, \ t > 0, \\ w(x,0) = 0, \ x \in \Omega_l \cup \Omega_r. \end{cases} \tag{2.4}$$

This splitting of the spatial domain $\mathbb{R}$ into interior and exterior problems is explained on Fig. 2.1. It shows the basic idea for constructing the TBC. The Transparent Boundary Condition is obtained by applying

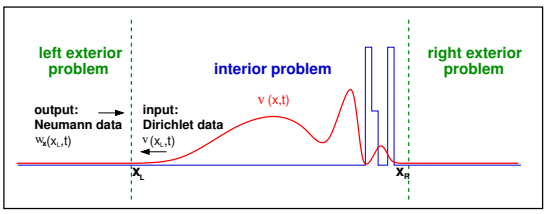

Figure 2.1: Domain decomposition for the construction of the TBC.

the Laplace transformation $\mathcal{L}$ with respect to the time t to the exterior problems (2.4). The Laplace transform is defined through the relation $\hat{w}(s) := \mathcal{L}(w)(s) := \int_{\mathbb{R}^+} w(t)e^{-st}dt$, where $s = \sigma + i\tau$ is the time covariable with $\sigma > 0$.

In the following, we focus on the derivation of the TBC at the right endpoint x_r. The Laplace transformation of (2.4) (on Ω_r) reads $is\widehat{w} + \partial_x^2 \widehat{w} = 0$, $x \in \Omega_r$. The solution to this second-order ode with constant coefficients can be computed as $\hat{w}(x,s) = A^+(s)e^{\sqrt[+]{-is}\,x} + A^-(s)e^{-\sqrt[+]{-is}\,x}$, $x > x_r$, where the branch-cut of the square root $\sqrt[+]{\ }$ is taken such that the real part is positive. However, since the solution is an element of $L^2(\Omega_r)$, the coefficient A^+ must vanish. Using the Dirichlet data at the artificial boundary yields $\hat{w}(x,s) = e^{-\sqrt[+]{-is}\,(x-x_r)}\,\hat{w}(x,s)|_{x=x_r}$. Deriving $\hat{w}(x,s)$ with respect to x gives

$$\partial_x \hat{w}(x,s)|_{x=x_r} = -\sqrt[+]{-is}\,\hat{w}(x,s)|_{x=x_r}. \tag{2.5}$$

The analogous condition at the left boundary is $-\partial_x \hat{w}(x,s)|_{x=x_l} = -\sqrt[+]{-is}\,\hat{w}(x,s)|_{x=x_l}$. Applying an inverse Laplace transformation $\mathcal{L}^{-1}$ allows to obtain an expression of the Neumann datum $\partial_x w(x_{l,r},t)$ as a function of the Dirichlet one. Since we have continuity of the traces on

Σ_T, the boundary condition of equation (2.3) is into

$$\partial_{\mathbf{n}} v(x,t) = \mathcal{L}^{-1}(-\sqrt[+]{-i\cdot}\,\hat{v}(x,\cdot))(t) = \int_0^t f(t-\tau)v(x,\tau)\,d\tau, \quad on \quad \Sigma_T, \tag{2.6}$$

where $\mathcal{L}(f)(s) = -\sqrt[+]{-is}$. By construction we have that u coincides with v on Ω, meaning that we have an exact or a Transparent Boundary Condition (TBC) given by the second equation of (2.6).

All this analysis could also be performed using the time Fourier transform $\mathscr{F}_t$

$$\mathscr{F}_t(u)(x,\tau) = \frac{1}{2\pi}\int_{\mathbb{R}} u(x,t)e^{-it\tau}\mathrm{d}t,$$

which roughly speaking corresponds to let $\sigma \to 0$ in the expression of the Laplace transform and induces the following definition of the square root $\sqrt{\tau} = \sqrt{\tau}$ if $\tau \geq 0$ and $\sqrt{\tau} = -i\sqrt{-\tau}$ if $\tau < 0$. The condition (2.5) is thus replaced by

$$\partial_x \mathscr{F}_t w(x,\tau)|_{x=x_r} = i\sqrt{-\tau}\,\mathscr{F}_t w(x,\tau)|_{x=x_r}.$$

We recover the TBC on Σ_T with $\partial_{\mathbf{n}} v(x,t) = \mathscr{F}_t{}^{-1}(i\sqrt{-\cdot}\,\mathscr{F}_t v(x,\cdot))(t)$. This expression or its Laplace version $\partial_{\mathbf{n}} v(x,t) = \mathcal{L}^{-1}(-\sqrt[+]{-i\cdot}\,\hat{v}(x,\cdot))(t)$ can be simply written at points $x = x_{l,r}$ as follows

$$\partial_{\mathbf{n}} v(x,t) = -e^{-i\pi/4}\partial_t^{1/2} v(x,t).$$

The term $\partial_t^{1/2} = \sqrt{\partial_t}$ has to be interpreted as a fractional half-order time derivative. We recall that the derivative $\partial_t^{k-\alpha} f(t)$ of order $k-\alpha > 0$ of a function f, with $k \in \mathbb{N}$ and $0 < \alpha \leq 1$, is defined by

$$\partial_t^{k-\alpha} f(t) = \frac{1}{\Gamma(\alpha)}\frac{d^k}{dt^k}\int_0^t (t-\tau)^{\alpha-1} f(\tau)d\tau, \tag{2.7}$$

where $\Gamma(z) = \int_0^{+\infty} e^{-t}t^{z-1}dz$ denotes the Gamma function. In the same spirit, one can also define the integration of real order $p > 0$ of a function f, denoted by $I_t^p f(t)$, by

$$I_t^p f(t) = \frac{1}{\Gamma(p)}\int_0^t (t-\tau)^{p-1} f(\tau)d\tau. \tag{2.8}$$

At this point, an interesting remark is that the Schrödinger equation can formally be factorized into left and right traveling waves (cf. [8]):

$$\Big(\partial_x - e^{-i\frac{\pi}{4}}\partial_t^{1/2}\Big)\Big(\partial_x + e^{-i\frac{\pi}{4}}\partial_t^{1/2}\Big)u = 0, \quad x > x_r. \tag{2.9}$$

This remark is crucial since it gives the idea to use a Nirenberg-like theorem in Section 3.2 for general variable coefficients equations (including potentials for instance).

2.2 Extensions and interpretations in the context of pseudodifferential operator calculus: introduction to the derivation of ABCs

The first possible extension is to consider a given real potential V which is constant in space outside Ω, *i.e.*, $V(x,t) = V_l(t)$ for $x < x_l$, $V(x,t) = V_r(t)$ for $x > x_r$. An easy computation, which consists in applying the following *gauge change* in (2.1), reduces this case to the zero exterior potential [3] for the new unknown

$$\psi_{l,r} = e^{-i\mathcal{V}_{l,r}(t)} u_{l,r}, \quad \text{with} \quad \mathcal{V}_{l,r}(t) = \int_0^t V_{l,r}(s)ds, \quad \forall t > 0. \tag{2.10}$$

The resulting TBC is then given by

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}_{l,r}(t)} \partial_t^{1/2} (e^{-i\mathcal{V}_{l,r}(t))} u) = 0, \quad \text{on } \Sigma_T. \tag{2.11}$$

The analysis based on Laplace or Fourier transforms and performed in the previous subsection can also be done if the potential is constant outside Ω. This would lead to

$$\partial_{\mathbf{n}} u(x,t) = \int_0^t f(t-\tau) u(x,\tau)\, d\tau, \text{on } \Sigma_T, \tag{2.12}$$

where $\mathcal{L}(f)(s) = -\sqrt[+]{-is - V_{l,r}}$. Therefore, the Schrödinger equation can formally and exactly be factorized into left and right traveling waves (cf. [8]):

$$(\partial_x - e^{-i\frac{\pi}{4}} \sqrt[+]{\partial_t - iV_r})(\partial_x + e^{-i\frac{\pi}{4}} \sqrt[+]{\partial_t - iV_r}) u = 0, \quad x > x_r.$$

To understand and to make clearer the link between expressions (2.11) and (2.12), we have to introduce the notion of pseudodifferential operator. A pseudodifferential operator $P(x,t,\partial_t)$ is given by its symbol $p(x,t,\tau)$ in the Fourier space

$$\begin{aligned} P(x,t,\partial_t)u(x,t) &= \mathscr{F}_t^{-1}\Big(p(x,t,\tau)\hat{u}(x,\tau)\Big) \\ &= \int_{\mathbb{R}} p(x,t,\tau)\, \mathscr{F}_t(u)(x,\tau)\, e^{it\tau}\, \mathrm{d}\tau. \end{aligned} \tag{2.13}$$

The inhomogeneous pseudodifferential operator calculus used in the paper was first introduced in [14]. For self-conciseness reasons, we only present the useful notions required here. Let α be a real number and Ξ an open subset of $\mathbb{R}$. Then (see in [19]), the symbol class $S^\alpha(\Xi \times \Xi)$ denotes the linear space of $\mathcal{C}^\infty$ functions $a(\cdot,\cdot,\cdot)$ in $\Xi \times \Xi \times \mathbb{R}$ such that

for each $K \subseteq \Xi \times \Xi$ and for all indices β, δ, γ, there exists a constant $C_{\beta,\delta,\gamma}(K)$ such that $|\partial_\tau^\beta \partial_t^\delta \partial_x^\gamma a(x,t,\tau)| \leq C_{\beta,\delta,\gamma}(K)(1+|\tau|^2)^{\alpha-\beta}$, for all $(x,t) \in K$ and $\tau \in \mathbb{R}$. A function f is said to be inhomogeneous of degree m if: $f(x,t,\mu^2\tau) = \mu^m f(x,t,\tau)$, for any $\mu > 0$. Then, a pseudodifferential operator $P = P(x,t,\partial_t)$ is inhomogeneous and classical of order M, $M \in \mathbb{Z}/2$, if its total symbol, designated by $p = \sigma(P)$, has an asymptotic expansion in inhomogeneous symbols $\{p_{M-j/2}\}_{j=0}^{+\infty}$ as

$$p(x,t,\tau) \sim \sum_{j=0}^{+\infty} p_{M-j/2}(x,t,\tau),$$

where each function $p_{M-j/2}$ is inhomogeneous of degree $2M-j$, for $j \in \mathbb{N}$. The meaning of $\sim$ is that

$$\forall \widetilde{m} \in \mathbb{N}, \quad p - \sum_{j=0}^{\widetilde{m}} p_{M-j/2} \in S^{M-(\widetilde{m}+1)/2}.$$

A symbol p satisfying the above property is denoted by $p \in S_S^M$ and the associated operator $P = Op(p)$ by inverse Fourier transform (according to (2.13)) by $P \in \mathrm{OPS}_S^M$. Finally, let us remark that smoothness of the potential V is required for applying pseudodifferential operators theory. However, this is crucial into the complementary set of Ω but a much weaker regularity assumption could be expected for the interior problem set in Ω allowing therefore a wide class of potentials.

Let us come back to the comparison of relations (2.11) and (2.12) in the case of a constant potential outside Ω. With the previous definitions, Eqs. (2.11) and (2.12) respectively read

$$\partial_{\mathbf{n}} u(x,t) + i e^{iV_{l,r}t} Op\left(-\sqrt{-\tau}\right)(e^{-iV_{l,r}t}u)(x,t) = 0, \quad \text{on } \Sigma_T, \tag{2.14}$$

and

$$\partial_{\mathbf{n}} u(x,t) + i Op\left(-\sqrt{-\tau + V_{l,r}}\right)(u)(x,t), \quad \text{on } \Sigma_T. \tag{2.15}$$

Actually, these two formulations are equivalent thanks to the following Lemma (see [5] for a proof).

Lemma 2.1. *If a is a t-independent symbol of S^m and $V(x,t) = V(x)$, then the following identity holds*

$$Op\left(a(\tau - V(x))\right) u = e^{itV(x)} Op\left(a(\tau)\right)\left(e^{-itV(x)}u(x,t)\right). \tag{2.16}$$

In our case, since V is also x-independent, one gets

$$iOp\left(-\sqrt{-\tau + V_{l,r}}\right)(u)(x,t) = ie^{iV_{l,r}t} Op\left(-\sqrt{-\tau}\right)(e^{-iV_{l,r}t)}u)(x,t),$$

which explains the close link between (2.11) and (2.12).

Lemma (2.1) has other applications when the potential V depends on the spatial variable x. To emphasize this point, let us develop some approximations of the TBC for the case of a linear potential $V(x,t) = x$. Applying a Fourier transform in time, the Schrödinger equation: $i\partial_t u + \partial_x^2 u + xu = 0$ sets on Ω_T becomes the Airy equation $\partial_x^2 \mathscr{F}_t u + (-\tau + x)\mathscr{F}_t u = 0$. The solution to this equation which is outgoing is given by $\mathscr{F}_t u(x,\tau) = \mathrm{Ai}\left((x-\tau)e^{-i\pi/3}\right)$, where Ai stands for the Airy function [1]. Deriving this expression according to x, we obtain the exact relation expressing the corresponding DtN map in the Fourier space

$$\partial_{\mathbf{n}} \mathscr{F}_t u(x,\tau) = e^{-i\pi/3} \frac{\mathrm{Ai}'\left((x-\tau)e^{-i\pi/3}\right)}{\mathrm{Ai}\left((x-\tau)e^{-i\pi/3}\right)} \mathscr{F}_t u(x,\tau), \tag{2.17}$$

giving therefore the total symbol. The numerical approximation of the corresponding TBC is difficult to handle and approximations are needed. For sufficiently large values of $|\tau|$, one has the following approximation

$$e^{2i\pi/3} \frac{\mathrm{Ai}'\left((x-\tau)e^{-i\pi/3}\right)}{\mathrm{Ai}\left((x-\tau)e^{-i\pi/3}\right)} \approx -e^{-i\pi/6}\sqrt{-\tau + x}.$$

If we replace the total (left) symbol by its approximation, we obtain what is usually called an artificial or Absorbing Boundary Condition (ABC)

$$\partial_{\mathbf{n}} u + iOp\left(-\sqrt{-\tau + x}\right)(u) = 0, \quad \text{on } \Sigma_T. \tag{2.18}$$

Thanks to Lemma (2.1) and since $V(x,t) = x$, this ABC is strictly equivalent to

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} e^{itx_{l,r}} \partial_t^{1/2}(e^{-itx_{l,r}} u) = 0, \quad \text{on } \Sigma_T. \tag{2.19}$$

Let us remark that, in the specific case of a linear potential, a change of unknown allows to transform the Schrödinger equation with linear potential into another Schrödinger equation without potential [10]. Indeed, if v is solution to $i\partial_t v + \partial_x^2 v = 0$, then $u(x,t) = e^{-i(-\alpha t x + \frac{t^3}{3}|\alpha|^2)} v(x - t^2\alpha, t)$ is solution to $i\partial_t u + \partial_x^2 u + \alpha x u = 0$.

At this point, some partial conclusions can be drawn

- Formally, the operator $i\partial_t + \partial_x^2 + V$ can be (exactly or approximately) factorized as

  $$i\partial_t + \partial_x^2 + V = \left(\partial_x + i\sqrt{i\partial_t + V}\right)\left(\partial_x - i\sqrt{i\partial_t + V}\right),$$

  according to the (x,t)-dependence of the potential. In the above right hand side, the second term characterizes the DtN map involved in the TBC or ABC.

- Transparent Boundary Conditions or Absorbing Boundary Conditions are written through a DtN operator either

$$\partial_{\mathbf{n}} u + iOp\left(-\sqrt{-\tau}\right)(u) = 0, \quad \text{on } \Sigma_T,$$

or

$$\partial_{\mathbf{n}} u + iOp\left(-\sqrt{-\tau + V}\right)(u) = 0, \quad \text{on } \Sigma_T.$$

- If $V(x,t) = V(t)$, the change of unknown $v(x,t) = e^{-i\mathcal{V}(t)}u(x,t)$, with $\mathcal{V}(t) = \int_0^t V(s)ds$, reduces the Schrödinger equation with potential to a free-Schrödinger equation and the TBC is then

$$\partial_{\mathbf{n}} u(x,t) + e^{-i\pi/4} e^{i\mathcal{V}(t)} \partial_t^{1/2}\left(e^{-i\mathcal{V}(t)}\right)(x,t) = 0, \quad \text{on } \Sigma_T.$$

3 ABCs for the linear Schrödinger equation with a general variable potential

3.1 Two possible strategies

It is clear from the above analysis that we cannot expect to get a TBC for real general potentials. We then need to derive some approximations and most specifically to compute ABCs using the previously introduced pseudodifferential operator calculus which extends the Laplace transform based approach to variable coefficients operators. Furthermore, it enables to manipulate symbols of operators at the algebraic level instead of operators at the functional level. The partial conclusions given at the end of the previous section lets to think that two possible strategies to build ABCs can be considered.

The first natural approach would consist in building an approximate boundary condition based on the equation (1.1) with unknown u. However, even if this approach seems direct, it is quite intricate and for this reason it will be designated as strategy 2 in the sequel.

A second possibility, called strategy 1, is the following. Let us consider now that u is the solution to Eq. (1.1) and let us define $\mathcal{V}$ as a primitive in time of the potential V

$$\mathcal{V}(x,t) = \int_0^t V(x,s)\,\mathrm{d}s. \tag{3.1}$$

Following the Gauge change (2.10), let us introduce v as the new unknown defined by

$$v(x,t) = e^{-i\mathcal{V}(x,t)}u(x,t). \tag{3.2}$$

We obviously have $v_0(x) = u_0(x)$. Moreover, plugging u given by (3.1)-(3.2) into the Schrödinger equation with potential shows that v is solution to the variable coefficients Schrödinger equation

$$i\partial_t v + \partial_x^2 v + f\,\partial_x v + g\,v = 0, \quad \text{in } \Omega_T, \tag{3.3}$$

setting $f = 2i\partial_x \mathcal{V}$ and $g = i\partial_x^2 \mathcal{V} - (\partial_x \mathcal{V})^2$. The fundamental reason why considering this change of unknown is crucial is that this first step leads to the TBC (2.11) applied to v and associated to (3.3) for a time-dependent potential (since then $f = g = 0$).

We will see later that these two approaches lead to different absorbing boundary conditions which however coincide in some situations.

3.2 Practical computation of the asymptotic expansion of the DtN operator

We explain here how to compute the asymptotic expansion of the DtN operator for a given model Schrödinger equation with smooth variable coefficients A and B

$$L(x,t,\partial_x,\partial_t)w = i\partial_t w + \partial_x^2 w + A\partial_x w + Bw = 0. \tag{3.4}$$

Since we are trying to build an approximation of the DtN operator at the boundary, we must be able to write the normal derivative trace operator ∂_x (focusing on the right point x_r) as a function of the trace operator through an operator Λ^+ which involves some (fractional) time derivatives/integrals of w as well as the effects of the potential V and its (x,t) variations. This can be done in an approximate way thanks to the factorization of L given by relation (3.4)

$$L(x,t,\partial_x,\partial_t) = (\partial_x + i\Lambda^-)(\partial_x + i\Lambda^+) + R, \tag{3.5}$$

where $R \in \mathrm{OPS}^{-\infty}$ is a smoothing pseudodifferential operator. This relation corresponds to the formal factorization presented at the end of section 2.2. The operators $\Lambda^\pm$ are pseudodifferential operators of order 1/2 (in time) and order zero in x. Computing the operators $\Lambda^\pm$ in an exact way through their respective total symbols $\sigma(\Lambda^\pm)$ cannot be expected in general (which would therefore provide a TBC). A more realistic approach consists in seeking an asymptotic form of the total symbol $\sigma(\Lambda^\pm)$ as

$$\sigma(\Lambda^\pm) = \lambda^\pm \sim \sum_{j=0}^{+\infty} \lambda^\pm_{1/2-j/2}, \tag{3.6}$$

where $\lambda^\pm_{1/2-j/2}$ are symbols corresponding to operators of order $1/2-j/2$.

Now, expanding the factorization (3.5), identifying the terms in L in front of the operators ∂_x with the ones from the expanded factorization and finally using a few symbolic manipulations yield the system of equations

$$\begin{cases} i(\lambda^- + \lambda^+) = a \\ i\partial_x \lambda^+ - \displaystyle\sum_{\alpha=0}^{\infty} \frac{(-i)^\alpha}{\alpha!}\, \partial_\tau^\alpha \lambda^- \, \partial_t^\alpha \lambda^+ = -\tau + b, \end{cases} \tag{3.7}$$

with $a(x,t) = \sigma(A) = A$, $b(x,t) = \sigma(B) = B$, since A and B are two functions of (x,t).

Looking at the first equation of system (3.7), we see that we must have: $\lambda^-_{1/2} = -\lambda^+_{1/2}$. Now, if we identify the highest order symbol in the second equation of system (3.7), then one gets four possibilities

$$\lambda^+_{1/2}(\tau) = \mp\sqrt{-\tau} \tag{3.8}$$

and

$$\lambda^+_{1/2}(x,t,\tau) = \mp\sqrt{-\tau + b(x,t)}. \tag{3.9}$$

The first choice can be viewed as considering a principal classical symbol while the second possibility rather referees to as a semi-classical symbol (see e.g. in [10]).

Let us now consider the strategy 1 based on the gauge change leading to compute v solution to (3.3) for $A = f$ and $B = g$. Following the derivation of the TBCs made in section 2.2, the principal symbol with negative imaginary part characterizes the outgoing part of the solution u. A study of the sign of (3.8) (for a real-valued potential V) shows that the negative sign leads to the correct choice. Since g is a complex-valued potential with no controlled sign, we cannot determine the outgoing wave for (3.9). The only possible choice is then

$$\lambda^+_{1/2} = -\sqrt{-\tau}. \tag{3.10}$$

Let us now consider the second strategy which consists in working on equation (1.1) for u setting $A = 0$ and $B = V$. The study of the sign of (3.8) and (3.9) for a real-valued potential V is possible in both cases and as for the first strategy, the negative sign provides the suitable solution. Therefore, we obtain the two possible symbols $\lambda^+_{1/2} = -\sqrt{-\tau}$ and $\lambda^+_{1/2} = -\sqrt{-\tau + V}$. However, considering $\lambda^+_{1/2} = -\sqrt{-\tau}$ would give some symbols which are approximations of $\lambda^+_{1/2} = -\sqrt{-\tau + V}$ by using a truncated Taylor expansion when $|\tau| \to +\infty$. Since this case leads to less accurate ABCs, we will only consider next the case

$$\lambda^+_{1/2} = -\sqrt{-\tau + V}. \tag{3.11}$$

Choosing the principal symbol is a crucial point since it is directly related to the accuracy of the ABC. Moreover, for a given choice of the principal symbol, the corrective asymptotic terms $\{\lambda^+_{1/2-j/2}\}_{j\geq 1}$ are different since they are computed in cascade developing the infinite sum in the second equation of (3.7) as seen in the following Proposition.

Proposition 3.1. *Let us fix $\lambda^+_{1/2}$ by the expression* (3.10)*. Then, the solution to system* (3.7) *is given by*

$$\lambda^+_0 = \frac{1}{2\lambda^+_{1/2}}\left(-i(\partial_x + a)\lambda^+_{1/2}\right), \tag{3.12}$$

and, for $j \in \mathbb{N}$, $j \geq 1$, by

$$\begin{aligned}\lambda^+_{-j/2} = \frac{1}{2\lambda^+_{1/2}}\Bigg(&b\,\delta_{j,1} - i(\partial_x + a)\lambda^+_{-j/2+1/2} + -\sum_{k=1}^{j}\lambda^+_{-j/2+k/2}\lambda^+_{1/2-k/2}\\ &-\sum_{\alpha=1}^{(j+1)/2}\frac{(-i)^\alpha}{\alpha!}\sum_{k=0}^{j+1-2\alpha}\partial^\alpha_\tau\lambda^+_{-j/2+k/2+\alpha}\partial^\alpha_t\lambda^+_{1/2-k/2}\Bigg)\end{aligned} \tag{3.13}$$

where $\delta_{j,1} = 0$ if $j \neq 1$ and $\delta_{1,1} = 1$.

Applying the above proposition to our situation, one obtains the following corollary.

Corollary 3.2. *In strategy 1 ($a = f$ and $b = g$), if we fix the principal symbol $\lambda^+_{1/2} = -\sqrt{-\tau}$ in* (3.7)*, then the next three terms of the asymptotic symbolic expansion are given by using (3.12) as*

$$\lambda^+_0 = \partial_x\mathcal{V}, \quad \lambda^+_{-1/2} = 0 \quad \textit{and} \quad \lambda^+_{-1} = \frac{i\partial_x V}{4\tau}. \tag{3.14}$$

In the case of the second strategy ($a = 0$ and $b = V$) and for $\lambda^+_{1/2} = -\sqrt{-\tau + V}$, we cannot obtain a general formula as for Proposition 3.1. However, the first terms can still be computed to as

$$\lambda^+_0 = 0, \quad \lambda^+_{-1/2} = 0, \quad \text{and} \quad \lambda^+_{-1} = \frac{-i}{4}\frac{\partial_x V}{-\tau + V}. \tag{3.15}$$

In the case of a linear potential $V = x$, we saw that the total symbol is

$$\lambda^+ = e^{2i\pi/3}\,\frac{\mathrm{Ai}'\left((x-\tau)e^{-i\pi/3}\right)}{\mathrm{Ai}\left((x-\tau)e^{-i\pi/3}\right)}. \tag{3.16}$$

The application of Corollary 3.2 in the context of strategy 2 gives the first and second-order approximate symbols $\sigma_1 = i\lambda^+_{1/2} = -i\sqrt{-\tau + x}$

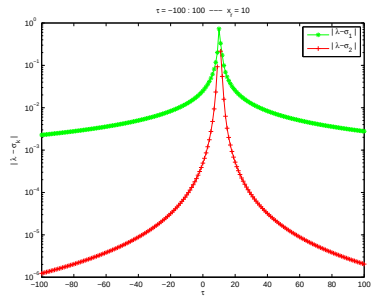

Figure 3.1: Logarithm of the absolute error $|\lambda^+ - \sigma_1|$ and $|\lambda^+ - \sigma_2|$ with respect to τ. A singularity is observed at $|\tau - x_r| = 0$, with $x_r = 10$.

and $\sigma_2 = i\lambda^+_{1/2} + i\lambda^+_0 = \sigma_1 + \frac{1}{4}\frac{1}{-\tau+x}$, setting $V = x$. These two relations give good approximations of $\lambda^+(x,\tau)$ for sufficiently large values of $|x-\tau|$ (see Fig. 3.1 for $x = 10$), corresponding to a high frequency spectrum approximation. This test case shows the validity of our approach in this situation.

3.3 Choosing the ABC in the context of strategy 1

If we assume that V is a real-valued smooth function, then the $L^2(\mathbb{R})$-norm of the solution u to system (1.1) is conserved. If we truncate the domain by introducing a fictitious boundary, then one can expect that the $L^2(\Omega)$-norm of the solution is bounded by $||u_0||_{L^2(\Omega)}$. This is for example proved in [3] in the case of the free-potential. In the case of a general potential, the expression of the artificial boundary condition is essential in the proof of a similar result. In particular, by adapting the proof given in [7] using the Plancherel theorem for Laplace transform, the following Lemma is the keypoint for proving a well-posedness result.

Lemma 3.3. *Let $\varphi \in H^{1/4}(0,T)$ be a function extended by zero for any time $s > T$. Then, we have the properties $\Re\left(e^{i\pi/4}\int_0^\infty \overline{\varphi}\,\partial_t^{1/2}\varphi\,\mathrm{d}t\right) \geq 0$ and $\Re\left(\int_0^{+\infty}\overline{\varphi}\,I_t\,\varphi\,\mathrm{d}t\right) = 0$.*

This Lemma emphasizes the fact that the absorbing boundary condition must have a symmetrical form. Since our approach gives the principal symbol of an operator, an infinite choice of corresponding operators with this principal symbol is possible. For symmetrization reasons, we propose to fix the choice of the artificial boundary condition based on the principal symbol $\lambda^+_{1/2} = -\sqrt{-\tau}$ and (3.14) as follows.

Cancelling the outgoing wave corresponding to $\lambda^+_{1/2}$ for v writes down

$$\partial_{\mathbf{n}} v + i\Lambda^+ v = 0, \qquad \text{on } \Sigma_T. \tag{3.17}$$

Retaining the M first symbols $\{\lambda^+_{1/2-j/2}\}_{M-1\geq j\geq 0}$, we consider the associated ABC

$$\partial_{\mathbf{n}} u_M - i(\partial_x \mathcal{V})\, u_M + ie^{i\mathcal{V}} \sum_{j=0}^{M-1} Op\left(\lambda^+_{1/2-j/2}\right)\left(e^{-i\mathcal{V}} u_M\right) = 0, \quad \text{on } \Sigma_T, \tag{3.18}$$

after replacing v in (3.17) by its expression (3.2). In Equation (3.18), u_M designates an approximation of u since we do not have a TBC. However, u_M will be denoted by u in the sequel for conciseness. We adopt the following compact notation of (3.18)

$$\partial_{\mathbf{n}} u + \Lambda^M_\ell(x,t,\partial_t)\, u = 0, \quad \text{on } \Sigma_T, \tag{3.19}$$

where $M \geq 1$ corresponds to the order of the boundary condition and is equal to the total number of terms $\lambda^+_{j/2}$ retained in the sum. The subscript $\ell = 1$ (respectively $\ell = 2$) refers to as the choice (3.10) (respectively (3.11)) of the principal symbol $\lambda^+_{1/2}$, and therefore to the two different strategies.

Let us begin by considering $\ell = 1$ and $M = 2$. Then one directly obtains

$$\Lambda^2_1(x,t,\partial_t)\, u = e^{-i\pi/4} e^{i\mathcal{V}(x,t)} \partial_t^{1/2}(e^{-i\mathcal{V}(x,t)} u) \tag{3.20}$$

which is a symmetrical operator. The case $M = 4$ is more ambiguous. Indeed, we only have access to the principal symbol $\lambda^+_{-1} = i\partial_x V/(4\tau)$ of an operator. In order to conserve a symmetrical operator for the definition of the ABC, our choice of operator is

$$Op\left(\lambda^+_{-1}\right) v = \mathrm{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, I_t\left(\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, v\right) \quad \mathrm{mod}(\mathrm{OPS}_S^{-3/2}). \tag{3.21}$$

In the above equation, $\mathrm{sg}(\cdot)$ designates the sign function.

We finally obtain the following Proposition.

Proposition 3.4. *For $\ell = 1$, the ABC of order M is given by*

$$\partial_{\mathbf{n}} u + \Lambda^M_1 u = 0, \quad \text{on } \Sigma_T, \tag{3.22}$$

with

$$\Lambda^2_1(x,t,\partial_t)\, u = e^{-i\pi/4} e^{i\mathcal{V}(x,t)} \partial_t^{1/2}\left(e^{-i\mathcal{V}(x,t)} u\right) \tag{3.23}$$

and

$$\Lambda_1^4(x,t,\partial_t)\,u = \Lambda_1^2(x,t,\partial_t)\,u + i\,\mathrm{sg}(\partial_{\mathbf{n}}V)\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}e^{i\mathcal{V}(x,t)}I_t\left(\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}e^{-i\mathcal{V}(x,t)}u\right). \tag{3.24}$$

The boundary condition (3.22) *is referred to as* ABC_1^M *in the sequel.*

Considering the ABCs (3.22) of Proposition 3.4, we get the following well-posedness result (see proof in [5]).

Proposition 3.5. *Let* $u_0 \in L^2(\Omega)$ *be a compactly supported initial datum such that* $\mathrm{Supp}(u_0) \subset \Omega$. *Let* $V \in \mathcal{C}^\infty(\mathbb{R}\times\mathbb{R}^+,\mathbb{R})$ *be a real-valued potential. Let us denote by* u *a solution of the initial boundary value problem*

$$\begin{cases} i\partial_t u + \partial_x^2 u + Vu = 0, & \text{in } \Omega_T,\\ \partial_{\mathbf{n}}u + \Lambda_1^M u = 0, & \text{on } \Sigma_T,\\ u(x,0) = u_0(x), & \forall x\in\Omega, \end{cases} \tag{3.25}$$

where the operators Λ_1^M, $M = 2, 4$, *are defined in Proposition 3.4. Then,* u *fulfils the following energy bound*

$$\forall t > 0, \quad ||u(t)||_{L^2(\Omega)} \le ||u_0||_{L^2(\Omega)}, \tag{3.26}$$

for $M = 2$. *Moreover, if* $\mathrm{sg}(\partial_{\mathbf{n}}V)$ *is constant on* Σ_T, *then the inequality* (3.26) *holds for* $M = 4$. *In particular, this implies that we have the uniqueness of the solution* u *of the initial boundary value problem* (3.25).

3.4 Choosing the ABC in the context of strategy 2

Let us now consider the second strategy for building the absorbing boundary conditions ABC_2^M, for $M = 2$ and $M = 4$.

Proposition 3.6. *For* $\ell = 2$, *the ABC of order* M *based on the second strategy for symbols* (3.15) *is given by*

$$\partial_{\mathbf{n}}u + \Lambda_2^M u = 0, \quad \text{on } \Sigma_T, \tag{3.27}$$

with

$$\Lambda_2^2(x,t,\partial_t)\,u = Op\left(-i\sqrt{-\tau+V}\right)u \tag{3.28}$$

and

$$\Lambda_2^4(x,t,\partial_t)\,u = \Lambda_2^2(x,t,\partial_t)\,u + \frac{1}{4}Op\left(\frac{\partial_x V}{-\tau+V}\right)u. \tag{3.29}$$

The boundary condition (3.27) *is referred to as* ABC_2^M *in the sequel of the paper.*

Studying the well-posedness of the initial boundary value problem related to the boundary condition ABC_2^M (3.27)-(3.29) is more difficult than ABC_1^M except for the case $V(x,t) = V(x)$. Indeed, the well-posedness result is trivial since ABC_2^M is strictly equivalent to ABC_1^M. A direct application of Lemma 2.1 gives the following Corollary.

Corollary 3.7. *If the potential V is time independent, then ABC_1^M is equivalent ABC_2^M, for a fixed value of $M = 2, 4$, with $\mathcal{V}(x,t) = tV(x)$. In particular, the well-posedness of the associated bounded initial value problem is immediate from Proposition 3.5.*

4 Semi-discretization schemes and their properties

The aim of this Section is to proceed to the semi-discretization in time of the initial value problem

$$\begin{cases} i\partial_t u + \partial_x^2 u + V\,u = 0, \quad \text{in } \Omega_T, \\ \partial_{\mathbf{n}} u + \Lambda_{1,2}^M u = 0, \quad \text{on } \Sigma_T, \text{ for } M = 2 \text{ or } 4, \\ u(\cdot,0) = u_0, \quad \text{in } \Omega, \end{cases} \tag{4.1}$$

for a maximal time of computation T.

We consider an interior Crank-Nicolson scheme for the time discretization of system (4.1). The interval $[0;T]$ is uniformly discretized using N intervals. Let $\Delta t = T/N$ be the time step and let us set $t_n = n\Delta t$. Furthermore, u^n stands for an approximation of $u(t_n)$ and $V^n = V(x,t_n)$. If $V = V(x)$ is a time-independent potential, then the Crank-Nicolson discretization of the Schrödinger equation is given by $i\,(u^{n+1} - u^n)/\Delta t + \partial_x^2(u^{n+1} + u^n)/2 + V\,(u^{n+1} + u^n)/2 = 0$, for $n = 0, \ldots, N-1$. If $V = V(x,t)$, for matters of symmetry, we choose the following time-discretization of the interior equation

$$i\,\frac{u^{n+1} - u^n}{\Delta t} + \partial_x^2 \frac{u^{n+1} + u^n}{2} + \frac{V^{n+1} + V^n}{2}\,\frac{u^{n+1} + u^n}{2} = 0. \tag{4.2}$$

Let us remark that, for implementation issues, it is often useful to set $v^{n+1} = (u^{n+1} + u^n)/2 = u^{n+1/2}$, with $u^{-1} = 0$ and $u^0 = u_0$. Similarly, we define $W^{n+1} = (V^{n+1} + V^n)/2 = V^{n+1/2}$. Then, the time scheme (4.2) reads

$$2i\,\frac{v^{n+1}}{\Delta t} + \partial_x^2 v^{n+1} + W^{n+1} v^{n+1} = 2i\,\frac{u^n}{\Delta t}. \tag{4.3}$$

We propose here one approximation for each kind of ABC. The approach for strategy 1 is based on semi-discrete convolutions for the fractional operators involved in (4.4)–(4.5), which leads to an unconditionally stable semi-discrete scheme. Considering strategy 2, we propose a

scheme based on the approximation of the fractional operators through the solution of auxiliary differential equations which can be solved explicitly. The evaluation is then extremely efficient but at the same time, no stability proof is at hand.

4.1 Discrete convolutions based discretizations for ABC_1^M

We first consider the boundary conditions ABC_1^M. According to Proposition 3.4, we have

$$\mathrm{ABC}_1^2: \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left(e^{-i\mathcal{V}} u\right) = 0, \tag{4.4}$$

and

$$\begin{aligned} \mathrm{ABC}_1^4: \quad & \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left(e^{-i\mathcal{V}} u\right) \\ & + i\,\mathrm{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{i\mathcal{V}} I_t \left(\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{-i\mathcal{V}} u \right) = 0. \end{aligned} \tag{4.5}$$

We use the symmetrical form of ABC_1^4, which is a keypoint in the case $V = V(x,t)$. The associated initial boundary value problem is then

$$\begin{cases} i\partial_t u + \partial_x^2 u + V\, u = 0, \quad \text{in } \Omega_T, \\ \partial_{\mathbf{n}} u + \Lambda_1^M u = 0, \quad \text{on } \Sigma_T, \text{ for } M = 2 \text{ or } 4, \\ u(\cdot, 0) = u_0, \quad \text{in } \Omega. \end{cases} \tag{4.6}$$

We will use in the sequel the following discrete convolutions approximating the continuous convolution operators.

Proposition 4.1. *If $\{f^n\}_{n\in\mathbb{N}}$ is a sequence of complex numbers approximating $\{f(t_n)\}_{n\in\mathbb{N}}$, then the approximations of $\partial_t^{1/2} f(t_n)$, $I_t^{1/2} f(t_n)$ and $I_t\, f(t_n)$ with respect to the Crank-Nicolson scheme for a time step Δt are given by the numerical quadrature formulas $\partial_t^{1/2} f(t_n) \approx \sqrt{\dfrac{2}{\Delta t}} \displaystyle\sum_{k=0}^{n} \beta_{n-k} f^k$, $I_t^{1/2} f(t_n) \approx \sqrt{\dfrac{\Delta t}{2}} \displaystyle\sum_{k=0}^{n} \alpha_{n-k} f^k$, $I_t\, f(t_n) \approx \dfrac{\Delta t}{2} \displaystyle\sum_{k=0}^{n} \gamma_{n-k} f^k$, where the sequences $(\alpha_n)_{n\in\mathbb{N}}$, $(\beta_n)_{n\in\mathbb{N}}$ and $(\gamma_n)_{n\in\mathbb{N}}$ are such that*

$$\begin{cases} (\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, ...) = (1, 1, \frac{1}{2}, \frac{1}{2}, \frac{3}{8}, \frac{3}{8}, ...), \\ \beta_k = (-1)^k \alpha_k, \quad \forall k \geq 0, \\ (\gamma_0, \gamma_1, \gamma_2, \gamma_3, ...) = (1, 2, 2, ...). \end{cases}$$

The weak formulation of (4.2) writes, for any test-function ψ in $H^1(\Omega)$,

$$\frac{2i}{\Delta t}\int_{x_l}^{x_r}(v^{n+1}-u^n)\psi\mathrm{d}x+\left[\partial_x v^{n+1}\psi\right]_{x_l}^{x_r}-\int_{x_l}^{x_r}\partial_x v^{n+1}\partial_x\psi\mathrm{d}x \\ +\int_{x_l}^{x_r}W^{n+1}v^{n+1}\psi\mathrm{d}x=0. \tag{4.7}$$

According to the interior scheme (4.2), the semi-discretization of ABC_1^2 for v at time t_{n+1} is given by

$$\partial_{\mathbf{n}}v^{n+1}(x_{l,r})=-e^{-i\pi/4}e^{i\mathscr{W}^{n+1}}\sqrt{\frac{2}{\Delta t}}\sum_{k=0}^{n+1}\beta_{n+1-k}e^{-i\mathscr{W}^k}v^k(x_{l,r}),$$

and, for ABC_1^4, by

$$\partial_{\mathbf{n}}v^{n+1}(x_{l,r})=-e^{-i\pi/4}e^{i\mathscr{W}^{n+1}}\sqrt{\frac{2}{\Delta t}}\sum_{k=0}^{n+1}\beta_{n+1-k}e^{-i\mathscr{W}^k}v^k(x_{l,r}) \\ -i\,\mathrm{sg}(\partial_{\mathbf{n}}W^{n+1})\frac{\sqrt{|\partial_{\mathbf{n}}W^{n+1}|}}{2}e^{i\mathscr{W}^{n+1}}\frac{\Delta t}{2}\sum_{k=0}^{n+1}\gamma_{n+1-k}\frac{\sqrt{|\partial_{\mathbf{n}}W^k|}}{2}e^{-i\mathscr{W}^k}v^k(x_{l,r}), \tag{4.8}$$

with the notation $\mathscr{W}^{n+1}=(\mathcal{V}^{n+1}+\mathcal{V}^n)/2$. Then, the following Proposition can be proved (see [5]).

Proposition 4.2. *The semi-discrete Crank-Nicolson scheme for the initial boundary value problem* (4.6) *is given by*

$$\begin{cases} 2i\,\dfrac{v^{n+1}-u^n}{\Delta t}+\partial_x^2 v^{n+1}+W^{n+1}\,v^{n+1}=0, \quad \text{in } \Omega,\\ \partial_{\mathbf{n}}v^{n+1}+\Lambda_1^{M,n+1}v^{n+1}=0, \quad \text{on } \Sigma, \quad \text{for } M=2 \text{ or } 4,\\ u^0=u_0, \quad \text{in } \Omega, \end{cases} \tag{4.9}$$

for $n=0,...,N-1$, setting $v^{n+1}=(u^{n+1}+u^n)/2$, $W^{n+1}=(V^{n+1}+V^n)/2$, and where the semi-discrete operators $\Lambda_1^{2,n+1}$ and $\Lambda_1^{4,n+1}$ are defined by

$$\Lambda_1^{2,n+1}v^{n+1}=e^{-i\pi/4}e^{i\mathscr{W}^{n+1}}\sqrt{\frac{2}{\Delta t}}\sum_{k=0}^{n+1}\beta_{n+1-k}e^{-i\mathscr{W}^k}v^k, \tag{4.10}$$

$$\Lambda_1^{4,n+1}v^{n+1}=\Lambda_1^{2,n+1}v^{n+1} \tag{4.11}$$

$$+\,i\,\mathrm{sg}(\partial_{\mathbf{n}}W^{n+1})\frac{\sqrt{|\partial_{\mathbf{n}}W^{n+1}|}}{2}e^{i\mathscr{W}^{n+1}}\frac{\Delta t}{2}\sum_{k=0}^{n+1}\gamma_{n+1-k}\frac{\sqrt{|\partial_{\mathbf{n}}W^k|}}{2}e^{-i\mathscr{W}^k}v^k. \tag{4.12}$$

Here, $\mathscr{W}^{n+1}$ is defined by $\mathscr{W}^{n+1} = (\mathcal{V}^{n+1} + \mathcal{V}^n)/2$, $\mathcal{V}^n(x)$ being the approximation of $\mathcal{V}(x, t_n)$ using the trapezoidal rule ($\mathcal{V}$ is given by (3.1)*). Moreover, for $M = 2$, one has the following energy inequality*

$$\forall n \in \{0, \ldots, N\}, \quad \|u^n\|_{L^2(\Omega)} \leq \left\|u^0\right\|_{L^2(\Omega)}, \tag{4.13}$$

and if $\mathrm{sg}(\partial_{\mathbf{n}} W^k)$ *is constant, then* (4.13) *also holds for $M = 4$. This proves the $L^2(\Omega)$ stability of the scheme. Inequality* (4.13) *is the semi-discrete version of* (3.26) *under the corresponding assumptions.*

4.2 Auxiliary functions based discretizations for ABC_2^M

While the previous strategy based on discrete convolution operators is accurate and provides a stability result, it may lead to significantly long computational times. For ABC_2^M, the discretizations of the resulting pseudodifferential operators involved is not easy to obtain. In particular, the operators with square-root symbols cannot be expressed in terms of fractional time operators since Lemma 2.1 cannot be applied. Let us consider the following additional approximations which will provide a more suitable way to discretize the ABCs.

Lemma 4.3. *We have the approximations $Op\left(\sqrt{-\tau + V}\right) = \sqrt{i\partial_t + V}$, mod($OPS_S^{-3/2}$) and $Op\left(\frac{\partial_x V}{4} \frac{1}{-\tau + V}\right) = \mathrm{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} (i\partial_t + V)^{-1} \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}$, mod($OPS_S^{-3}$).*

Thanks to Lemma 4.3, we now define the new approximations of ABC_2^M (see Proposition 3.6)

$$\widetilde{\mathrm{ABC}_2^2}: \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V}\, u = 0, \tag{4.14}$$

and

$$\begin{aligned} \widetilde{\mathrm{ABC}_2^4}: \quad & \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V}\, u + \\ & \mathrm{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} (i\partial_t + V)^{-1} \left(\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, u \right) = 0. \end{aligned} \tag{4.15}$$

Let us begin by the second-order condition (4.14). An alternative approach to discrete convolutions (which cannot be applied here) consists in approximating the square-root operator $\sqrt{i\partial_t + V}$ by using rational functions. More specifically here, we consider the m-th order Padé approximants [18]

$$\sqrt{z} \approx R_m(z) = a_0^m + \sum_{k=1}^{m} \frac{a_k^m\, z}{z + d_k^m} = \sum_{k=0}^{m} a_k^m - \sum_{k=1}^{m} \frac{a_k^m\, d_k^m}{z + d_k^m}, \tag{4.16}$$

where the coefficients $(a_k^m)_{0\le k\le m}$ and $(d_k^m)_{1\le k\le m}$ are given by

$$a_0^m = 0 \quad , \quad a_k^m = \frac{1}{m\cos^2\left(\frac{(2k+1)\pi}{4m}\right)} \quad , \quad d_k^m = \tan^2\left(\frac{(2k+1)\pi}{4m}\right).$$

Formally, $\sqrt{i\partial_t + V}$ is approximated by

$$R_m(i\partial_t + V) = \sum_{k=0}^{m} a_k^m - \sum_{k=1}^{m} a_k^m\, d_k^m (i\partial_t + V + d_k^m)^{-1}. \tag{4.17}$$

Applying this process to the equation (4.14), we have the new relation

$$\partial_{\mathbf{n}} u - i\sum_{k=0}^{m} a_k^m\, u + i\sum_{k=1}^{m} a_k^m\, d_k^m (i\partial_t + V + d_k^m)^{-1}\, u = 0, \tag{4.18}$$

defining then a second-order artificial boundary condition referred to as $\mathrm{ABC}_{2,m}^2$ in the sequel. To write a suitable form of the equation in view of an efficient numerical treatment, we classically introduce m auxiliary functions φ_k, for $1 \le k \le m$, (see Lindmann [16]) as follows

$$\varphi_k = (i\partial_t + V + d_k^m)^{-1}\, u, \tag{4.19}$$

leading to the following equation

$$i\partial_t \varphi_k + (V + d_k^m)\,\varphi_k = u, \qquad \text{for } 1 \le k \le m, \text{ at } x = x_{l,r}, \tag{4.20}$$

with the initial condition $\varphi_k(x,0) = 0$. The corresponding complete local artificial boundary condition is written as a system

$$\begin{cases} \partial_{\mathbf{n}} u - i\sum_{k=0}^{m} a_k^m u + i\sum_{k=1}^{m} a_k^m\, d_k^m\, \varphi_k = 0, \\ i\partial_t \varphi_k + (V + d_k^m)\,\varphi_k = u, \qquad \text{for } 1 \le k \le m,\ x = x_{l,r}, \\ \varphi_k(x,0) = 0. \end{cases} \tag{4.21}$$

The semi-discretization of the interior scheme remains the same as before (4.2), and consequently, (4.21) becomes in terms of v_k^n functions

$$\begin{cases} \partial_{\mathbf{n}} v^{n+1} - i\sum_{k=0}^{m} a_k^m v^{n+1} + i\sum_{k=1}^{m} a_k^m d_k^m \varphi_k^{n+1/2} = 0, \\ i\,\dfrac{\varphi_k^{n+1} - \varphi_k^n}{\Delta t} + (W^{n+1} + d_k^m)\,\varphi_k^{n+1/2} = v^{n+1}, \\ \varphi_k^0 = 0. \end{cases} \tag{4.22}$$

for $1 \le k \le m$ and $x = x_{l,r}$.

Now, let us consider the fourth-order condition $\widetilde{\mathrm{ABC}_2^4}$ given by (4.15)

$$\begin{aligned}\partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V}\, u \\ + \mathrm{sg}(\partial_{\mathbf{n}} V)\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}(i\partial_t + V)^{-1}\left(\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, u\right) = 0, \quad \text{on } \Sigma \times \mathbb{R}.\end{aligned} \tag{4.23}$$

Then, one has to introduce one more additional auxiliary function ψ such that $(i\partial_t + V)\,\psi = \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, u$.

We call $\mathrm{ABC}_{2,m}^4$ the resulting approximation of $\widetilde{\mathrm{ABC}_2^4}$. Using again a Crank-Nicolson discretization of ψ, one gets the following approximate representation of $\mathrm{ABC}_{1,m}^4$

$$\begin{cases} \partial_{\mathbf{n}} v^{n+1} - i\displaystyle\sum_{k=0}^{m} a_k^m v^{n+1} + i\sum_{k=1}^{m} a_k^m d_k^m \varphi_k^{n+1/2} \\ \qquad\qquad + \mathrm{sg}(\partial_{\mathbf{n}} W^{n+1})\dfrac{\sqrt{|\partial_{\mathbf{n}} W^{n+1}|}}{2}\psi^{n+1/2} = 0, \\ i\,\dfrac{\varphi_k^{n+1} - \varphi_k^n}{\Delta t} + (W^{n+1} + d_k^m)\,\varphi_k^{n+1/2} = v^{n+1}, \\ i\,\dfrac{\psi^{n+1} - \psi^n}{\Delta t} + W^{n+1}\,\psi^{n+1/2} = \dfrac{\sqrt{|\partial_{\mathbf{n}} W^{n+1}|}}{2} v^{n+1}, \\ \varphi_k^0 = \psi^0 = 0. \end{cases} \tag{4.24}$$

for $1 \le k \le m$ and $x = x_{l,r}$.

5 Extensions to nonlinear problems

Following the developments in [4] for the cubic nonlinear Schrödinger (NLS), one can extend the derivation performed in section 3.2 to cases in which the potential is formally replaced by a nonlinearity. To be more precise, we consider the following cubic (NLS) equation

$$\begin{cases} i\partial_t u + \partial_x^2 u + q|u|^2 u = 0, \ (x,t) \in \Omega_T, \\ u(x,0) = u_0(x), \qquad\qquad x \in \Omega. \end{cases} \tag{5.1}$$

The role of the potential $V(x,t)$ is now replaced by the cubic nonlinear term $q|u|^2(x,t)$. If $q > 0$ (resp. $q < 0$), the (NLS) equation is said to be focusing (resp. defocusing). This equation is well posed and has special solutions when dispersion and nonlinearity compensate, namely the soliton solution, which exhibits the specific behavior to propagate without modification of its amplitude. The cubic NLS equation is extremely interesting since it is the prototype of more general nonlinear dispersive equations and therefore it has received many attentions among the years.

In the context of TBCs and ABCs, contributions can be found in the papers [4, 24, 26, 6].

If we formally replace the potential by the nonlinearity $q|u|^2$, the two strategies developped in the previous sections lead respectively to two different ABCs of order M that will be denoted by NLABC_1^M for the first strategy and $\widetilde{\mathrm{NLABC}}_2^M$-$\mathrm{NLABC}_{2,m}^M$ for strategy 2. For strategy 1, the ABCs of order M are given by

$$\partial_{\mathbf{n}} u + \Upsilon_1^M u = 0, \quad \text{on } \Sigma_T, \tag{5.2}$$

with (NLABC_1^2)

$$\Upsilon_1^2\, u = e^{-i\pi/4} e^{i\mathbb{V}(x,t)} \partial_t^{1/2} \left(e^{-i\mathbb{V}(x,t)} u \right)$$

and (NLABC_1^4)

$$\Upsilon_1^4\, u = \Upsilon_1^2\, u + i\,\mathrm{sg}(\partial_{\mathbf{n}} q|u|^2) \frac{\sqrt{|\partial_{\mathbf{n}} q|u|^2|}}{2} e^{i\mathbb{V}(x,t)} I_t \left(\frac{\sqrt{|\partial_{\mathbf{n}} q|u|^2|}}{2} e^{-i\mathbb{V}(x,t)} u \right),$$

setting $\mathbb{V}(x,t) = \int_0^t q|u|^2(x,s)\, ds$.

For the second strategy, one gets $\widetilde{\mathrm{NLABC}}_2^2$: $\partial_{\mathbf{n}} u - i\sqrt{i\partial_t + q|u|^2} u = 0$ and $\widetilde{\mathrm{NLABC}}_2^4$:

$$\begin{aligned} &\partial_{\mathbf{n}} u - i\sqrt{i\partial_t + q|u|^2} u \\ &\quad + \mathrm{sg}(\partial_{\mathbf{n}} q|u|^2) \frac{\sqrt{|\partial_{\mathbf{n}} q|u|^2|}}{2} (i\partial_t + q|u|^2)^{-1} \left(\frac{\sqrt{|\partial_{\mathbf{n}} q|u|^2|}}{2} u \right) = 0. \end{aligned}$$

The numerical treatment is slightly different from the linear Schrödinger equation with potential. Indeed, the semi-discrete approximation of the nonlinear term $q|u|^2 u$ is done following the Durán and Sanz-Serna scheme [12]. More precisely, we use the midpoint approximation $q|(u^{n+1} + u^n)/2|^2 (u^{n+1} + u^n)/2$. This differs from $q(|u^{n+1}|^2 + |u^n|^2)(u^{n+1} + u^n)/4$ which is the classical Crank-Nicolson approximation and corresponds to Eq. (4.2). Therefore, the semi-discrete time scheme reads

$$i\frac{u^{n+1} - u^n}{\Delta t} + \partial_x^2 \frac{u^{n+1} + u^n}{2} + q \left| \frac{u^{n+1} + u^n}{2} \right|^2 \frac{u^{n+1} + u^n}{2} = 0$$

which can be recast as follows

$$2i\frac{v^{n+1}}{\Delta t} + \partial_x^2 v^{n+1} + q|v^{n+1}|^2 v^{n+1} = 2i\frac{u^n}{\Delta t}, \tag{5.3}$$

where v^{n+1} denotes the midpoint term $(u^{n+1} + u^n)/2$. Since this scheme is now nonlinear, we solve it by a fixed-point procedure with error tolerance ε. The algorithm is described below:

```
let ζ^0 = v^n , s = 0
repeat
        solve the linear elliptic problem
        2i ζ^{s+1}/Δt + ∂_x^2 ζ^{s+1} = 2i u^n/Δt − q|ζ^s|^2 ζ^s
        s = s + 1
until ‖ζ^{s+1} − ζ^s‖_{L^2(Ω)} ≤ ε
v^{n+1} = ζ^{s+1} , u^{n+1} = 2v^{n+1} − u^n
```

The rule is to replace v^{n+1} by ζ^{s+1} if the corresponding term is linear and by ζ^s if one deals with a nonlinear one. We do not detail this step further and this principle is also applied to the numerical treatment of other nonlinear ABCs.

The numerical approximation of NLABC_1^4 is

$$\partial_{\mathbf{n}}\zeta^{s+1} + e^{-i\frac{\pi}{4}}\sqrt{\frac{2}{\Delta t}}\zeta^{s+1} = g^s \text{ on } \Sigma_T, \tag{5.4}$$

with

$$\begin{aligned} g^s = &-e^{-i\frac{\pi}{4}}\sqrt{\frac{2}{\Delta t}}\left(\widetilde{\mathbb{E}^n}\exp\left(iq\Delta t\frac{|\zeta^s|^2}{2}\right)\sum_{k=1}^{n}\beta_{n+1-k}\overline{\mathbb{E}^k}v^k\right)\\ &-i\frac{q}{4}\partial_{\mathbf{n}}(|\zeta^s|^2)\left(\frac{\Delta t}{2}\zeta^s + \Delta t\widetilde{\mathbb{E}^n}\exp\left(iq\Delta t\frac{|\zeta^s|^2}{2}\right)\sum_{k=1}^{n}\overline{\mathbb{E}^k}v^k\right). \end{aligned}$$

The notations $\mathbb{E}^p$ and $\widetilde{\mathbb{E}^{p-1}}$ are the quantities defined by

$$\begin{aligned} \mathbb{E}^p = \exp(i\mathbb{U}^p) &= \exp\left(iq\Delta t\sum_{l=1}^{p-1}\left|u^l\right|^2\right)\exp\left(iq\frac{\Delta t}{2}\left|u^p\right|^2\right)\\ &= \widetilde{\mathbb{E}^{p-1}}\exp\left(iq\frac{\Delta t}{2}\left|u^p\right|^2\right), \end{aligned} \tag{5.5}$$

setting $\mathbb{E}^0 = 1$ and $\mathbb{E}^1 = \exp(i\mathbb{U}^1)$.

The Crank-Nicolson scheme (5.3) coupled to (5.4) remains nonlocal in time since we have to deal with convolution terms. In this direction, $\mathrm{NLABC}_{2,m}^M$ are computationally more efficient since they are based on the Padé approximants and are therefore local in time. For example, $\mathrm{NLABC}_{2,m}^4$ reads

$$\begin{aligned} \partial_{\mathbf{n}}\zeta^{s+1} = i\sum_{k=0}^{m}a_k^m\zeta^{s+1} - i\sum_{k=1}^{m}a_k^m d_k^m\left(\frac{\phi_k^s+\varphi_k^n}{2}\right)\\ -\operatorname{sg}(\partial_{\mathbf{n}}q|\zeta^s|^2)\frac{\sqrt{|\partial_{\mathbf{n}}q|\zeta^s|^2|}}{2}\left(\frac{\chi^s+\psi^n}{2}\right), \end{aligned} \tag{5.6}$$

with

$$\phi_k^s = \left(\frac{i}{\Delta t} + q\frac{|\zeta^s|^2}{2} + \frac{d_k^m}{2}\right)^{-1}\left(\zeta^s + \varphi_k^n\left(\frac{i}{\Delta t} - q\frac{|\zeta^s|^2}{2} - \frac{d_k^m}{2}\right)\right),$$

where $\varphi_k^0 = 0$, $\forall k$, $\phi_k^0 = \varphi_k^n$ and

$$\chi^s = \left(\frac{i}{\Delta t} + q\frac{|\zeta^s|^2}{2}\right)^{-1}\left(\frac{\sqrt{|\partial_{\mathbf{n}} q|\zeta^s|^2|}}{2}\zeta^s + \left(\frac{i}{\Delta t} - q\frac{|\zeta^s|^2}{2}\right)\psi^n\right)$$

where $\psi^0 = 0$ and $\chi^0 = \psi^n$. When the convergence assumption

$$\|\zeta^{s+1} - \zeta^s\|_{L^2} \leq \varepsilon$$

is reached, one affects $\varphi_k^{n+1} = \phi_k^s$ and $\psi^{n+1} = \chi^s$.

6 Numerical examples

The aim of this section is to provide some test cases to validate our approach. We perform some experiments for Schrödinger equations with both variable potentials and nonlinearities. For each situation, we use a variational formulation of the semi-discrete time problem with n_h linear finite elements (with spatial size h) and integrate the ABCs in the corresponding scheme as a Fourier-Robin boundary condition. This leads to a tridiagonal banded matrix. The solution to the associated linear system is then simple and is realized by a direct LU solver.

6.1 Linear Schrödinger equation with variable potential

We consider the initial gaussian datum $u_0(x) = e^{ik_0x - x^2}$, where k_0 designates the wave number fixed to $k_0 = 10$ in our simulations. This choice, like for the nonlinear Schrödinger equation, is related to the fact that our ABCs are derived under a high frequency hypothesis. We present here one kind of potential: $V(x,t) = 5xt$ (more examples are available in [5]). The computational domain is $\Omega =]-5;10[$. The final time of computation is $T = 2.5$. The spatial step size is $h = 2.5 \times 10^{-3}$ for the linear finite element method and the time step is $\Delta t = 10^{-4}$. We present in Figure 6.1 the quantity $\log_{10}(|u(x,t)|)$ in the domain Ω_T. We begin by reporting the reference solution (top left) computed on a larger domain to avoid any effect related to spurious reflection at the boundary. Next, we present (top) the solutions using ABC_1^2 and ABC_1^4 which show that increasing the order of the boundary conditions yields smaller undesired back reflections. Finally, we compare the effect of the localization based

on the Padé approximation of order m for the second-order ABC and strategy 2. We choose $m = 20$ ($\mathrm{ABC}^2_{2,20}$) and $m = 50$ ($\mathrm{ABC}^2_{2,50}$) terms. To get an equivalent precision to ABC^2_1, $m = 50$ is required. However, we note here that this leads to a negligible additional cost compared to $m = 20$. We also see on the right bottom picture that the precision of ABC^4_2 is conserved for $\mathrm{ABC}^4_{2,50}$. All these simulations show that the proposed ABCs have increasing accuracy according to the order M, with similar accuracy for the same order when a localization process is applied.

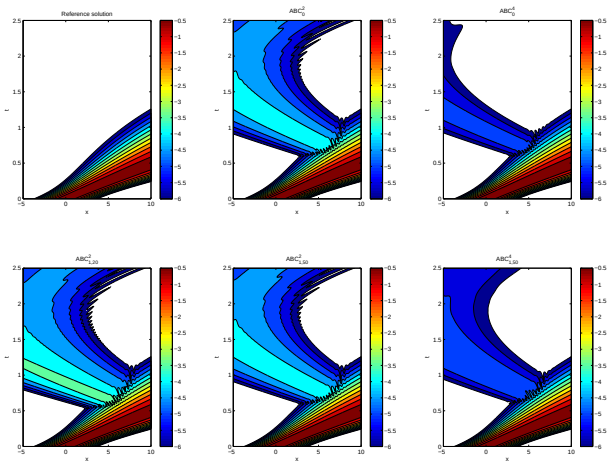

Figure 6.1: $\log_{10}$ representation of the amplitude of the computed solutions for $V(x,t) = 5xt$. From left to right, top: reference solution, ABC^2_1, ABC^4_1; bottom: $\mathrm{ABC}^2_{2,20}$, $\mathrm{ABC}^2_{2,50}$, $\mathrm{ABC}^4_{2,50}$.

6.2 Nonlinear Schrödinger equation

The one-dimensional cubic nonlinear Schrödinger equation is integrable by using the inverse scattering theory [25]. This approach yields the so-called exact *soliton* solution given by

$$u_{\mathrm{ex}}(x,t) = \sqrt{\frac{2a}{q}}\mathrm{sech}(\sqrt{a}(x-ct))\exp(i\frac{c}{2}(x-ct))\exp(i(a+\frac{c^2}{4})t).$$

From now on, we fix the focusing parameter q to 1. The real parameter a, equals to 2 here, characterizes the amplitude of the wavefield. Finally, c is the velocity of the soliton. Like in the previous subsection, since the derivation of the nonlinear artificial boundary conditions has been constructed under a high-frequency assumption ($|\tau|$ large), we take $c = 15$. All along the computations, we consider $\varepsilon = 10^{-6}$ in the fixed-point algorithm. The numerical parameters are $\Delta t = 10^{-3}$ for a final

time $T = 2$. The finite computational spatial domain is $\Omega =]-10, 10[$ discretized with $n_h = 4000$ equally spaced points ($h = 0.5 \times 10^{-2}$). Concerning the Padé approximation, we choose $m = 50$ since this is an optimal choice for the potential test cases.

To focus on the spurious reflections link to the different methods, we plot the contour of $\log_{10}(|u|)$ on Figures 6.2-6.6. We see on Fig. 6.2 that the maximal reflection is approximately equal to 10^{-2} for an initial amplitude of 2 and the linear TBC (2.2). For Figures 6.3-6.6, the reflection attains a maximal value around 5×10^{-3}. The reflection occurring at the right boundary decreases according to the order M of the different conditions NLABC_1^M or $\mathrm{NLABC}_{2,m}^M$. Moreover, the most accurate results are obtained for the condition NLABC_4^2 with a minimal region of maximal reflection. Unlike the linear TBC, the reflection at the left boundary has an amplitude smaller than 10^{-4}.

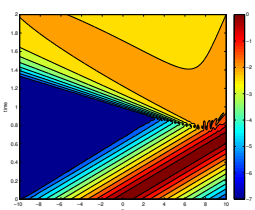

Figure 6.2: Contour plot of $\log_{10}(|u|)$ for the linear TBC (2.2).

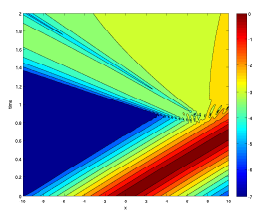

Figure 6.3: Contour plot for the boundary condition NLABC_1^2.

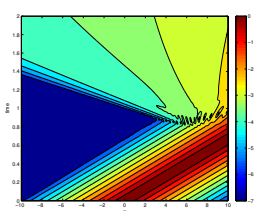

Figure 6.4: Contour plot for the boundary condition NLABC_1^4.

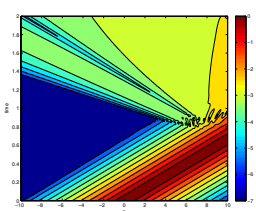

Figure 6.5: Contour plot for the boundary condition $\mathrm{NLABC}_{2,50}^2$.

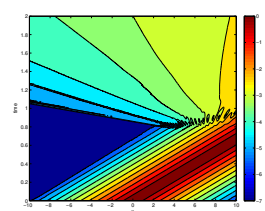

Figure 6.6: Contour plot for the boundary condition $\mathrm{NLABC}_{2,50}^4$.

To precise these results, we plot on figure 6.7 the relative error for the $L^2(\Omega)$-norm

$$\frac{\|u_{\mathrm{ex}} - u_{\mathrm{num}}\|_{L^2(\Omega)}}{\|u_{\mathrm{num}}\|_{L^2(\Omega)}},$$

where u_{num} denotes the numerical solution. For the linear TBC, the error is about 2% whereas the best result is obtained for the NLABC_1^4

condition for a final error of 0.2%. It is interesting to note that the ABCs NLABC_2^M with Padé approximations are very competitive. The relative error for NLABC_2^2 and $\mathrm{NLABC}_{2,50}^2$ are exactly the same, and $\mathrm{NLABC}_{2,50}^4$ is between NLABC_2^2 and NLABC_2^4 methods, the main difference is that methods based on Padé approximations are local in time and easy to implement. However, the fact that NLABC_2^4 and $\mathrm{NLABC}_{2,m}^4$ are not numerically equivalent requires further investigations. Indeed, for the variable potential cases, we obtained similar results while it is no longer the case here.

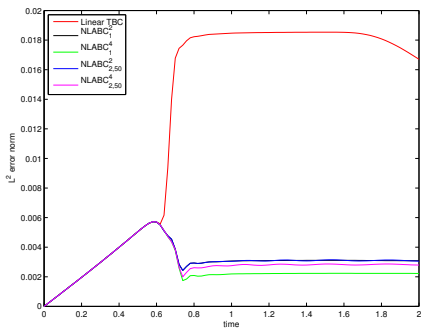

Figure 6.7: Relative error for the different linear and nonlinear ABCs.

7 Conclusion

We have introduced various constructions of Absorbing Boundary Conditions (ABCs) for the one-dimensional Schrödinger equation with time- and space-variable repulsive potentials and for the one-dimensional nonlinear cubic Schrödinger equation. They are derived with the help of general pseudodifferential techniques and applied to variable potentials and nonlinear equations. New accurate and efficient Absorbing Boundary Conditions for the nonlinear cubic Schrödinger equation are proposed. Numerical examples compare the different ABCs of various orders, showing that fourth-order ABCs yield accurate computations, and that Padé based approximations are accurate while they are also efficient. Further studies will include other nonlinearities as well as extensions to higher dimensions.

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