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Unconditionally stable discretization schemes of non-reflecting boundary conditions for the one-dimensional Schrödinger equation

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Abstract

This paper addresses the problem of the construction of stable approximation schemes for the one-dimensional linear Schrödinger equation set in an unbounded domain. After a study of the initial boundary-value problem in a bounded domain with a transparent boundary condition, some unconditionally stable discretization schemes are developed for this kind of problem. The main difficulty is linked to the involvement of a fractional integral operator defining the transparent operator. The proposed semi-discretization of this operator yields with a very different point of view the one proposed by Yevick, Friese and Schmidt [J. Comput. Phys. 168 (2001) 433]. Two possible choices of transparent boundary conditions based on the Dirichlet–Neumann (DN) and Neumann–Dirichlet (ND) operators are presented. To preserve the stability of the fully discrete scheme, conform Galerkin finite element methods are employed for the spatial discretization. Finally, some numerical tests are performed to study the respective accuracy of the different schemes.

1. Introduction

In this paper, we address the problem of the numerical approximation of a dispersive wave u solution to the Schrödinger equation defined in an unbounded domain. More concretely, we consider the following linear equation:

$$\begin{aligned} &(\mathrm{i}\partial_t + \partial_x^2)u = V(x,t)u, \quad x \in \mathbb{R}, \ \ t > 0, \\ &u(x,0) = u_0(x), \end{aligned} \tag{1}$$

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where V designates a given potential, and for the sake of conciseness, we assume that u_0 is a compactly supported datum. This model equation arises in many practical domains of physical and technological interest. For instance, this equation can be constructed from an approximation of the two-dimensional Helmholtz equation in a preferred direction. Then, this is the so-called standard Parabolic Equations (PE) [16].

The solution to Eq. (1) is defined on the whole domain $\Omega = \{(x,t) \in \mathbb{R}^2 : t > 0\}$ and must vanish for $x \to \pm\infty$. However, from a practical point of view, the infinite domain of propagation has to be truncated to next use a well-adapted discretization scheme for Eq. (1). To this end, let us split the initial domain Ω into three regions. We designate by $\Omega_i = \{(x,t) \in \mathbb{R}^2 : x_l \leqslant x \leqslant x_r,\ t > 0\}$ the interior domain where one wishes to compute an approximate solution. To simplify the problem, we suppose that the support $\widetilde{\Omega}$ of u_0 is embedded in Ω_i. As recently noticed by Arnold and Ehrhardt [5], this restriction is not so cumbersome as it *a priori* seems and may be avoided. Finally, two other complementary regions can be defined by $\Omega_l = \{(x,t) \in \mathbb{R}^2 : x < x_l,\ t > 0\}$ and $\Omega_r = \{(x,t) \in \mathbb{R}^2 : x > x_r,\ t > 0\}$ for, respectively, the left and right half-spaces (see Fig. 1).

The essential difficulty consists now to write a boundary condition such that no spurious reflection arises at the fictive boundary $\Gamma = \{x_l\} \cup \{x_r\}$. In the case of a Schrödinger equation with a vanishing potential ($V = 0$), this non-reflecting boundary condition is given by the Dirichlet–Neumann (DN) pseudodifferential operator on Γ

$$\partial_{\mathbf{n}} u(x,t) + \frac{e^{-i\pi/4}}{\sqrt{\pi}} \partial_t \int_0^t \frac{u(x,s)}{\sqrt{t-s}}\, ds = 0 \quad \text{on } \Gamma,\ t > 0$$

or yet

$$\partial_{\mathbf{n}} u(x,t) + e^{-i\pi/4} D_t^{1/2} u(x,t) = 0 \quad \text{on } \Gamma,\ t > 0, \tag{2}$$

where $D_t^{1/2}$ is the fractional derivative operator [13] of order 1/2 and $\mathbf{n}$ stands for the outwardly directed unit normal vector to the computational bounded domain Ω_i. This condition may be directly derived in the one-dimensional case by an explicit calculation based on the Laplace transform. Moreover, a generalization of this condition can be developed in the two-dimensional case for a regular curved boundary Γ [1]. As a consequence, the boundary-value problem to approximate is now given by

$$\begin{aligned} &(i\partial_t + \partial_x^2) u = 0 \quad \text{in } \Omega_i \times \mathbb{R}, \\ &\partial_{\mathbf{n}} u + e^{-i\pi/4} D_t^{1/2} u = 0 \quad \text{on } \Gamma \times \mathbb{R}, \\ &u(x,0) = u_0. \end{aligned}$$

The main difficulty of the numerical approximation is now linked to the presence in the boundary condition of a convolution operator which can lead to a loss of stability of the interior scheme if an unsuitable discretization is employed (see [6,17]).

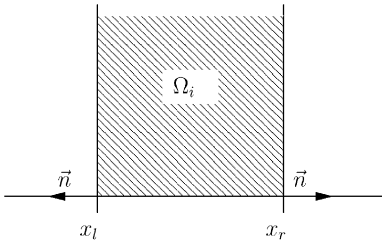

Fig. 1. The computational domain $\Omega_i \times \mathbb{R}^{*+}$ and the left and right half-spaces.

A first possible approach essentially developed by Arnold and Ehrhardt [3–5,10] consists in writing an exact discrete transparent operator directly from the fully discretized Schrödinger equation by using, e.g., a Crank–Nicolson scheme. Hence, the resulting discrete system has the same property of unconditional stability as the initial Crank–Nicolson scheme on the whole space. However, even if the approach leads to accurate numerical results, it seems quite difficult to extend it to two-dimensional curved boundaries. Moreover, the involvement of varying potentials is not straightforward. Finally, this approach requires the use of a uniform discretization which can be a strong restriction in some applications. A second approach introduced by Schmidt et al. [18–20] consists to choose a semi-discrete scheme of the Schrödinger equation and to explicit the associated non-local transparent boundary condition. This method has been widely developed and has proved to be efficient. Furthermore, the resulting scheme is unconditionally stable. However, the possibility of its extension to two-dimensional surfaces not seems so obvious. At last, a third direction (and also the older one) has been introduced by Mayfield [17] and next by Baskakov and Popov [6] in the beginning of the nineties. This technique consists in applying a suitable numerical quadrature formula to the continuous fractional operator defined by Eq. (2). Unfortunately, the resulting schemes have proved to be stable under some suitable conditions. Recently, in [12], Friese et al. have proposed some unconditionally stable and accurate discretization schemes for the transparent operator. The interest of their approach is that it can be extended to the two-dimensional case since it is constructed on the basis of the continuous problem. This is the approach considered in the present paper. Finally, we can notice that other approaches can be used to truncate the computational domain as, e.g., by using some local artificial boundary conditions based on paraxial approximations of the transparent operator [9,11,15,21] or also to adapt the method of Bérenger Perfectly Matching Layer (PML) [7] to the paraxial equation [8].

The plan of the paper is the following. In Section 2, we study the well-posedness of the Schrödinger equation with a non-vanishing potential and the associated transparent condition. In Section 3, we give a representation of the transparent boundary condition. The associated semi-discrete representation in the time domain is next derived by using the Fourier transform and the principle of images. We consider two possible choices of the transparent boundary condition which are a priori equivalent. They are based on the involvement of the Dirichlet–Neumann (DN) or Neumann–Dirichlet (ND) pseudodifferential operator. In particular, this approach allows us to make the connection between the proposed approximation of the transparent boundary condition for the DN operator and the discretization previously described in Friese et al. [12]. We next state the unconditionally stability of the resulting semi-discrete schemes. For the full discretization, we develop a classical Galerkin finite element approximation. Finally Section 4 is devoted to some numerical experiments showing the effectiveness of our approach. We also compare the two possible choices of transparent boundary conditions with most well-known discretizations of the transparent operator.

2. Study of the initial-boundary-value problem

Let us recall that for a vanishing potential the non-reflecting DN boundary condition is given by the non-local pseudodifferential equation

$$\partial_{\mathbf{n}} u(x,t) + \mathrm{e}^{-\mathrm{i}\pi/4} D_t^{1/2} u(x,t) = 0 \quad \text{on } \Gamma \times \mathbb{R}.$$

Its definition involves the Dirichlet–Neumann operator $-\mathrm{e}^{-\mathrm{i}\pi/4} D_t^{1/2}$ which is a convolution pseudodifferential operator. Another possible choice would be to rather consider the pseudoinverse operator of the previous operator, the so-called Neumann–Dirichlet (ND) operator. They are a priori equivalent from a continuous point of view. This operator is given by $-\mathrm{e}^{\mathrm{i}\pi/4} I_t^{1/2}$, where $I_t^{1/2}$ designates the fractional integral operator of order $-1/2$ given by

$$I_t^{1/2} v(x,t) = \frac{1}{\sqrt{\pi}} \int_0^t \frac{v(x,s)}{\sqrt{t-s}}\, \mathrm{d}s,$$

for a distribution v. Then, the new non-reflecting ND boundary condition is now

$$u(x,t) + \mathrm{e}^{\mathrm{i}\pi/4} I_t^{1/2} \partial_{\mathbf{n}} u(x,t) = 0 \quad \text{on } \Gamma. \tag{3}$$

In a spirit of conciseness, let us now focus our study on the ND operator. Similar details may be directly transposed to the DN operator. We now assume that V varies according to both the time and space variables in the computational domain $\Omega_i \times \mathbb{R}$. We moreover supposed that it only depends on the time variable in the exterior domains $\Omega_{\mathrm{l,r}} \times \mathbb{R}$. Therefore, we have $V_{\mathrm{l,r}}(t) = V(x,t)|_{\Omega_{\mathrm{l,r}}}$. In the unbounded regions, the potential may be eliminated by setting $\varphi_{\mathrm{l,r}} = \mathrm{e}^{\mathrm{i}\mathscr{V}_{\mathrm{l,r}}(t)} u_{\mathrm{l,r}}(x,t)$ as a new unknown, for $(x,t) \in \Omega_{\mathrm{l,r}} \times \mathbb{R}$, with $u_{\mathrm{l,r}} = u|_{\Omega_{\mathrm{l,r}}}$ on $\Omega_{\mathrm{l,r}} \times \mathbb{R}$. The dephasing function $\mathscr{V}_{\mathrm{l,r}}$ is explicitly given by

$$\mathscr{V}_{\mathrm{l,r}}(t) = \int_0^t V_{\mathrm{l,r}}(s)\, \mathrm{d}s \quad \forall t > 0.$$

In quantum mechanics, this modification is better known under the name of gauge change. As a consequence the transparent ND condition can be rewritten as

$$\varphi_{\mathrm{l,r}} + \mathrm{e}^{\mathrm{i}\pi/4} I_t^{1/2} \partial_{\mathbf{n}} \varphi_{\mathrm{l,r}} = 0 \quad \text{on } \Gamma.$$

Coming back to the initial unknown u, we deduce the transparent ND condition

$$u_{\mathrm{l,r}} + \mathrm{e}^{\mathrm{i}(\pi/4 - \mathscr{V}_{\mathrm{l,r}}(t))} I_t^{1/2} (\mathrm{e}^{\mathrm{i}\mathscr{V}_{\mathrm{l,r}}(t)} \partial_{\mathbf{n}} u_{\mathrm{l,r}}) = 0 \quad \text{on } \Gamma.$$

Coupled to the Schrödinger equation in Ω_i and to the initial condition on u, we can then determinate the solution u for a problem with a potential. The assumption about the x independence of the potential in the exterior regions is physically acceptable for homogeneous exterior media. Finally, let us remark that if V is simply a constant, the reconstruction is straightforward. Indeed, function $\mathscr{V}_{\mathrm{l,r}}$ can be computed by a direct integration and only acts as a simple multiplication.

Remark. In the case where an incident wave u^{inc} is prescribed at an endpoint of Ω_i, the transparent boundary condition is applied to the wave $u - u^{\mathrm{inc}}$ [3].

Hence the ND initial-boundary-value problem is given by

$$\begin{aligned} &(\mathrm{i}\partial_t + \partial_x^2) u(x,t) = V(x,t) u(x,t) \quad \text{in } \Omega_i, \\ &u_{\mathrm{l,r}} + \mathrm{e}^{\mathrm{i}(\pi/4 - \mathscr{V}_{\mathrm{l,r}}(t))} I_t^{1/2} (\mathrm{e}^{\mathrm{i}\mathscr{V}_{\mathrm{l,r}}(t)} \partial_{\mathbf{n}} u_{\mathrm{l,r}}) = 0 \quad \text{on } \Gamma, \\ &u(x,0) = u_0. \end{aligned} \tag{4}$$

Classically, the density $\|u\|_{L^2(\mathbb{R})}$ is decreasing for system (1) in the whole space if $\mathrm{Im}(V) < 0$. In the case of a bounded domain, this should also be the case for the $L^2(\Omega_i)$-norm of the approximate solution. More precisely, the following result holds.

Theorem 1. *Let us assume that potential $V \in \mathscr{C}(\mathbb{R}_t^+, L^\infty(\mathbb{C}))$ satisfies*: $\mathrm{Im}(V(x,t)) \leqslant 0$, *for $x \in \Omega_i$ and $\forall t \geqslant 0$. Let $u(x,t)$ be a solution to the initial-boundary-value problem* (4). *Then, $u \in \mathscr{C}(\mathbb{R}_t^+, H^1(\Omega_i))$ and fulfils the following energy inequality*

$$\|u(t)\|_{L^2(\Omega_i)} \leqslant \|u_0\|_{L^2(\Omega_i)} \quad \forall t > 0 \quad \textit{and} \quad u_0 \in H^1(\Omega_i).$$

Remark. The uniqueness of the solution to the boundary-value problem directly results from the above inequality. An identical result may be obtained when the DN condition is considered instead of the ND condition. Finally, the assumption about the negativeness of the imaginary part of the potential is physically realistic. Indeed, in the framework of the PE methods, it reflects the fact that the wave propagates in a dissipative medium, i.e., with a positive conductivity [16].

Proof. Let us multiply the Schrödinger equation by the test function $-\mathrm{i}\overline{u}$, where $\overline{u}$ designates the complex conjugate of u. Integrating according to the space variable and next considering the real part of the resulting expression, we get

$$\mathrm{Re}\left(\int_{\Omega_i}(\partial_t u + \mathrm{e}^{-\mathrm{i}\pi/2}(\partial_x^2 u - V(x,t)u))\overline{u}\,\mathrm{d}x\right) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_i}|u|^2(x,t)\,\mathrm{d}x - \int_{\Omega_i}\mathrm{Im}(V(x,t))|u|^2(x,t)\,\mathrm{d}x + \sum_{\gamma=\mathrm{l,r}}\mathrm{Re}(\mathrm{e}^{-\mathrm{i}\pi/2}\partial_{\mathbf{n}}u(x_\gamma,t)\overline{u}(x_\gamma,t)). \tag{5}$$

Now let us integrate this last relation on the interval $[0,t]$. On one hand, we deduce the following identity for the first quantity appearing in the right-hand side of Eq. (5)

$$\int_0^t \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_i}|u|^2(x,s)\,\mathrm{d}x\,\mathrm{d}s = \|u\|^2_{L^2(\Omega_i)}(t) - \|u_0\|^2_{L^2(\Omega_i)}.$$

On the other hand, the positiveness of the second quantity is clear from the assumption on the potential. Let us replace now the trace of the solution on the boundary Γ by the expression obtained with the help of the transparent condition (3). Then we get for any time $t > 0$

$$\mathrm{Re}\left(\int_0^t \mathrm{e}^{\mathrm{i}\pi/4}\mathrm{e}^{\mathrm{i}\gamma_{\mathrm{l,r}}(s)}\partial_x u(x_{\mathrm{l,r}},s)I_s^{1/2}(\overline{\mathrm{e}^{\mathrm{i}\gamma_{\mathrm{l,r}}(s)}\partial_x u(x_{\mathrm{l,r}},s)})\,\mathrm{d}s\right). \tag{6}$$

Adaptating the arguments given by Arnold and Ehrhardt [5] for the operator $\mathrm{e}^{\mathrm{i}\pi/4}D_s^{1/2}$, we can prove that the operator $\mathrm{e}^{\mathrm{i}\pi/4}I_s^{1/2}$ is a positive operator in the sense of operators with memory. More precisely, we have the following result.

Theorem 2. *Let $\phi \in H^{-1/4}(0,t)$ a function extended to zero for all time $s > t$. Then, we get the inequality*

$$Re\left(\int_0^\infty \mathrm{e}^{\mathrm{i}\pi/4}\overline{\phi(s)}I_s^{1/2}(\phi)(s)\,\mathrm{d}s\right) \geqslant 0.$$

Finally, the application of this last theorem to the function $\phi = \overline{\mathrm{e}^{\mathrm{i}\gamma_{\mathrm{l,r}}(s)}\partial_x u(x_{\mathrm{l,r}},s)}$ provides the positiveness of the quantities (6). This ends the proof. □

3. Construction and study of the discrete model

For the sake of conciseness, let us consider the following simplified boundary-value problem where we choose only one fictive point at x_r and a vanishing potential for the ND transparent operator

$$\begin{aligned}&(\mathrm{i}\partial_t + \partial_x^2)u = 0, \text{ for } x < x_\mathrm{r},\ t > 0,\\ &u(x_\mathrm{r},t) + \mathrm{e}^{\mathrm{i}\pi/4}I_t^{1/2}\partial_{\mathbf{n}}u(x_\mathrm{r},t) = 0,\\ &u(x,0) = u_0(x).\end{aligned}$$

Let us now construct a function v following the so-called image principle [14]. In the right unbounded domain Ω_{r}, we set $v(x,t) = u(x,t)_{|\Omega_{\mathrm{r}}}$, where u is solution to the Schrödinger equation in the whole space. In order to define a distribution on the entire space and to use a Green's integral representation of the solution, we extend v by reflection according to the point x_{r} by setting $v(x,t) = u(2x_{\mathrm{r}} - x, t)$, if $x < x_{\mathrm{r}}$. If we assume that u_0 is compactly supported in Ω_i, then $v(x,0) = 0$ on $\mathbb{R}$. Moreover, in the sense of distributions, we have: $\partial_t v = \partial_t u$. We can see that function v is continuous at x_{r} whereas its spatial derivative has a jump: $\partial_x^2 v = \partial_x^2 u + [\partial_x u(x_{\mathrm{r}}, t)]\delta_{x_{\mathrm{r}}}$, where $\delta_{x_{\mathrm{r}}}$ designates the Dirac delta function at point x_{r} and $[\varphi]$ is the jump of a distribution φ across the fictive boundary $\{x = x_{\mathrm{r}}\}$. Hence, function v satisfies the system of equations

$$\begin{aligned} &(\mathrm{i}\partial_t + \partial_x^2)v = 2\partial_{\mathbf{n}} u(x_{\mathrm{r}}, t)\delta_{x_{\mathrm{r}}}, \quad (x,t) \in \mathbb{R} \times \mathbb{R}^{*+}, \\ &v(x,0) = 0, \quad x \in \mathbb{R}. \end{aligned} \tag{7}$$

Function v is then solution to a Schrödinger equation on $\mathbb{R}$, with a vanishing initial datum and a measure source term.

Now, let us define S as the Schrödinger group which satisfies $S(t)(f) = G(x,t) *_x f$, where G is the Green's kernel given by

$$G(x,t) = \frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{2\sqrt{\pi}\sqrt{t}} \exp\left(-\frac{|x|^2}{4\mathrm{i}t}\right). \tag{8}$$

Solution v to (7) can be written as

$$v(x,t) = S(t)v(x,0) - 2\mathrm{i}\int_0^t S(t-s)\partial_{\mathbf{n}} u(x_{\mathrm{r}}, s)\delta_{x_{\mathrm{r}}}\,\mathrm{d}s.$$

By an explicit writing of the above formulation we get

$$\begin{aligned} v(x,t) &= S(t)v(x,0) - 2i\int_0^t \int_y G(x-y, t-s)\partial_{\mathbf{n}} u(x_{\mathrm{r}}, s)\delta_{x_{\mathrm{r}}}(y)\,\mathrm{d}y\,\mathrm{d}s \\ &= S(t)v(x,0) - 2\mathrm{i}\int_0^t G(x - x_{\mathrm{r}}, t-s)\partial_{\mathbf{n}} u(x_{\mathrm{r}}, s)\,\mathrm{d}s. \end{aligned} \tag{9}$$

Since we have $v(x,0) = 0$, we deduce that

$$v(x_{\mathrm{r}}, t) = -\mathrm{e}^{\mathrm{i}\pi/4} I_t^{1/2}\partial_{\mathbf{n}} u(x_{\mathrm{r}}, t) = u(x_{\mathrm{r}}, t).$$

3.1. Semi-discrete representation of the ND transparent boundary condition for the Crank–Nicolson scheme

The solution to the Cauchy system (7) directly gives the Dirichlet datum $u(x_{\mathrm{r}}, t)$ at the boundary $x = x_{\mathrm{r}}$ and leads to the expected boundary condition. Now we want to compute a solution v to (7). We are dealing with a linear Schrödinger equation with a measure source term. Obviously, no explicit solution is a priori known. Therefore, we seek a numerical approximate solution which allows to estimate the solution at (x_{r}, t). Concerning the time discretization of this equation, many possibilities can be used. Maybe the most common scheme used to solve our initial problem is the Crank–Nicolson scheme. It is well-known for its property of conservation of the L^2-norm on the whole space. Moreover, this is a second-order scheme for

the semi-discretization in time. This is also this choice which will be considered for the interior discretization of the Schrödinger equation and as a consequence, for solving problem (7). To describe the method, let us introduce the following classical notations.

For a time step δt, we introduce the sequence of discretization points: $t^{n+1} = (n+1)\delta t$. Let us denote by v^n and u^n the respective approximations of v and u at time $t = t^n$. The Crank–Nicolson method applied to system (7) consists in writing the following semi-discrete time discretization scheme

$$\begin{aligned} &\mathrm{i}\frac{v^{n+1}-v^n}{\delta t} + \partial_x^2\left(\frac{v^{n+1}+v^n}{2}\right) = 2\frac{\partial_{\mathbf{n}}u^{n+1}(x_\mathrm{r}) + \partial_{\mathbf{n}}u^n(x_\mathrm{r})}{2}\delta_{x_\mathrm{r}}, \\ &v^0 = u_0. \end{aligned} \tag{10}$$

Let us now give the expression of v^{n+1}. To this end, we compute the spatial Fourier transform of the first Eq. of system (10). We denote by $\widehat{v^n}$ the partial Fourier transform of v^n according to the space variable, where ξ is the covariable of x. A straightforward calculation yields

$$\widehat{v^{n+1}}(\xi) = \frac{\mathrm{i}+2\pi^2\xi^2\delta t}{\mathrm{i}-2\pi^2\xi^2\delta t}\widehat{v^n}(\xi) + \frac{2\delta t}{\mathrm{i}-2\pi^2\xi^2\delta t}\frac{\partial_{\mathbf{n}}u^{n+1}(x_\mathrm{r}) + \partial_{\mathbf{n}}u^n(x_\mathrm{r})}{2}\mathrm{e}^{-2\mathrm{i}\pi x_\mathrm{r}\xi}.$$

Let us now introduce the symbols

$$A(\xi) = \frac{\mathrm{i}+2\pi^2\xi^2\delta t}{\mathrm{i}-2\pi^2\xi^2\delta t} \quad \text{and} \quad B(\xi) = \frac{1}{\mathrm{i}-2\pi^2\xi^2\delta t}.$$

Under the previous notations, we have

$$\widehat{v^{n+1}}(\xi) = A(\xi)\widehat{v^n}(\xi) + 2\delta t B(\xi)\frac{\partial_{\mathbf{n}}u^{n+1}(x_\mathrm{r}) + \partial_{\mathbf{n}}u^n(x_\mathrm{r})}{2}\mathrm{e}^{-2\mathrm{i}\pi x_\mathrm{r}\xi}.$$

A successive application of the above formula yields

$$\widehat{v^{n+1}}(\xi) = A^{n+1}(\xi)\widehat{v^0}(\xi) + 2\delta t\sum_{k=0}^{n} B(\xi)A^k(\xi)\frac{\partial_{\mathbf{n}}u^{n+1-k}(x_\mathrm{r}) + \partial_{\mathbf{n}}u^{n-k}(x_\mathrm{r})}{2}\mathrm{e}^{-2\mathrm{i}\pi x_\mathrm{r}\xi}.$$

If we consider the first term appearing in the right-hand side of the above equation, we remark that it corresponds via an inverse Fourier transform to a convolution term exactly as in the continuous case in Eq. (9). If we now evaluate this expression at point x_r and next we apply the inverse Fourier transform according to ξ, we get the expression of $v^{n+1}(x_\mathrm{r})$

$$v^{n+1}(x_\mathrm{r}) = 2\delta t\left(\sum_{k=0}^{n}\int_{\mathbb{R}} BA^k(\xi)\,\mathrm{d}\xi\right)\frac{\partial_{\mathbf{n}}u^{n+1-k}(x_\mathrm{r}) + \partial_{\mathbf{n}}u^{n-k}(x_\mathrm{r})}{2}.$$

A simple calculation shows that the inverse Fourier transform of the symbols can be rewritten as

$$I_k = \int_{\mathbb{R}} BA^k(\xi)\,\mathrm{d}\xi = -\frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\pi\sqrt{2\delta t}}\int_{\mathbb{R}}\frac{(1-x^2)^k}{(1+x^2)^{k+1}}\,\mathrm{d}x, \quad k \geqslant 0.$$

In fact, each integral I_k may be explicitly computed

$$I_0 = -\frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{2\delta t}},$$

$$I_{2p+1} = 0 \quad \text{if } p \geqslant 1,$$

$$I_{2p} = -\frac{e^{i\pi/4}}{\sqrt{2\delta t}} \prod_{j=1}^{p} \frac{2j-1}{2j} \quad \text{if } p \geqslant 1.$$

Let us remark that we have the following recursive formula

$$I_{2p} = \frac{2p-1}{2p} I_{2(p-1)}.$$

Finally, we obtain the expression of v^{n+1} for the Crank–Nicolson scheme

$$v^{n+1}(x_r) = -e^{i\pi/4}\sqrt{2\delta t} \sum_{k=0}^{n} \gamma_k \left(\frac{\partial_{\mathbf{n}} u^{n+1-k}(x_r) + \partial_{\mathbf{n}} u^{n-k}(x_r)}{2} \right),$$

where the sequence of coefficients $(\gamma_k)_{k\in\mathbb{N}}$ is given by the relations

$$\gamma_k = \begin{cases} 1 & \text{if } k = 0, \\ 0 & \text{if } k = 2p+1, \\ \prod_{j=1}^{p} \frac{2j-1}{2j} = \frac{2p-1}{2p}\gamma_{2(p-1)} & \text{if } k = 2p. \end{cases}$$

As a consequence, we have the following semi-discretization in time of the non-reflecting ND boundary condition (3) for the Crank–Nicolson scheme

$$\begin{aligned} u^{n+1}(x_r) + e^{i\pi/4}\sqrt{\frac{\delta t}{2}}\partial_{\mathbf{n}} u^{n+1}(x_r) = &-e^{i\pi/4}\sqrt{\frac{\delta t}{2}}\partial_{\mathbf{n}} u^{n}(x_r) \\ &- e^{i\pi/4}\sqrt{2\delta t} \sum_{k=2}^{n} \gamma_k \left(\frac{\partial_{\mathbf{n}} u^{n+1-k}(x_r) + \partial_{\mathbf{n}} u^{n-k}(x_r)}{2} \right). \end{aligned} \tag{11}$$

This condition can also be rewritten in the following form

$$u^{n+1}(x_r) = -e^{i\pi/4} \frac{\sqrt{2\delta t}}{2} \sum_{k=0}^{n+1} \alpha_k \partial_{\mathbf{n}} u^{n+1-k}(x_r),$$

setting

$$(\alpha_0, \alpha_1, \ldots) = \left(1, 1, \frac{1}{2}, \frac{1}{2}, \frac{3}{8}, \frac{3}{8}, \ldots\right). \tag{12}$$

This is another derivation of the approximation obtained by Friese–Schmidt–Yevick [12] for the discretization of the transparent condition. The proof of the equivalence between these two relations is based on a splitting of the formula (11) according to the parity of n and next using some reorderings.

3.2. Stability of the ND semi-discrete scheme

We have proved in Section 2 that the solution $u(x,t)$ to (4) satisfies the following inequality

$$\|u(t)\|_{L^2(\Omega_i)} \leqslant \|u_0\|_{L^2(\Omega_i)} \quad \forall t > 0. \tag{13}$$

So, we seek to extend this property to the semi-discrete version of the continuous problem by using the Crank–Nicolson scheme and the associated representation of the ND transparent condition. Only the approximation of the boundary condition can prevent the $L^2(\Omega_i)$-norm to decrease. The approach of Mayfield [17] and Baskakov and Popov [6] is limited since this property is no longer fulfilled for a fixed value of the time step δt. Their semi-discrete scheme is conditionally stable. The stability is preserved here by using the semi-discrete representation of the ND transparent boundary condition. More precisely, we have the following result.

Theorem 3. *The semi-discrete Crank–Nicolson scheme for the Schrödinger equation associated with the representation* (11) *of the ND transparent boundary condition is given by the system*

$$\mathrm{i}\frac{u^{n+1}-u^n}{\delta t}+\partial_x^2\left(\frac{u^{n+1}+u^n}{2}\right)=0 \quad \forall x\in\Omega_i, \tag{14a}$$

$$\begin{aligned} &u^{n+1}(x_\gamma)=-\mathrm{e}^{\mathrm{i}\pi/4}\frac{\sqrt{2\delta t}}{2}\sum_{k=0}^{n+1}\alpha_k\partial_{\mathbf{n}}u^{n+1-k}(x_\gamma) \quad \text{for } \gamma=\mathrm{l},\mathrm{r},\ \ t>0,\\ &u^0=u_0 \quad \forall x\in\Omega_i, \end{aligned} \tag{14}$$

where $(\alpha_k)_{k\in\mathbb{N}}$ *is the sequence given by relation* (12). *This scheme is unconditionally stable in the sense of the* $\|.\|_{L^2(\Omega_i)}$*-norm. Moreover, we have the energy inequality*

$$\|u^{N+1}\|_{L^2(\Omega_i)}<\|u_0\|_{L^2(\Omega_i)} \quad \forall N\geqslant 0. \tag{15}$$

Remark. The inequality (15) is the semi-discrete version of (13).

Before the statement of the proof of the above result, we make the assumption that $u^0(x_{\mathrm{l,r}})=\partial_{\mathbf{n}}u^0(x_{\mathrm{l,r}})=0$. This hypothesis is not restrictive since the support of the initial datum is embedded into the computational domain. Then we have at each endpoint of the domain

$$\sum_{k=0}^{n}\gamma_k\partial_{\mathbf{n}}\left(\frac{u^{n+1-k}+u^{n-k}}{2}\right)=\frac{1}{2}\sum_{k=0}^{n+1}\gamma_k\partial_{\mathbf{n}}u^{n+1-k}+\frac{1}{2}\sum_{k=0}^{n}\gamma_k\partial_{\mathbf{n}}u^{n-k}. \tag{16}$$

Let us introduce the discrete time convolution denoted by $\bigstar$ and defined by

$$f_n\bigstar g^n=\sum_{k=0}^{n}f_kg^{n-k},$$

where f and g are two sequences defined by $f=(f_k)_{k\in\mathbb{N}}$ and $g=(g^k)_{k\in\mathbb{N}}$. This allows us to rewrite relation (16) under the form

$$\sum_{k=0}^{n}\gamma_k\partial_{\mathbf{n}}\left(\frac{u^{n+1-k}+u^{n-k}}{2}\right)=\frac{(\gamma_{n+1}\bigstar\partial_{\mathbf{n}}u^{n+1})+(\gamma_n\bigstar\partial_{\mathbf{n}}u^n)}{2}.$$

Proof. Let us multiply Eq. (14a) by $-\mathrm{i}\overline{u^{n+1/2}}$, integrate by parts on the domain Ω_i and take the imaginary part of the resulting equation. Then, after some simplifications and summing on the indices n such that $0\leqslant n\leqslant N$, we get

$$\frac{1}{2\delta t}(\|u^{N+1}\|^2_{L^2(\Omega_i)} - \|u^0\|^2_{L^2(\Omega_i)}) + \sum_{\gamma=\mathrm{l,r}} A^\gamma = 0, \tag{17}$$

where we have set

$$A^\gamma = \sum_{n=0}^{N} A_n^\gamma = \sum_{n=0}^{N} \mathrm{Re}(-\mathrm{i}\partial_x u^{n+1/2}(x_\gamma)\overline{u^{n+1/2}(x_\gamma)}), \quad \gamma = \mathrm{l,r}.$$

We now have to precise the sign of A_n^γ. In order to determinate this sign, we proceed as Arnold and Ehrhardt [5] by using the $\mathscr{Z}$-transform of a signal $(f_n)_{n\in\mathbb{N}}$ which is defined by

$$\mathscr{Z}(f_n) = \sum_{n=0}^{\infty} f_n z^{-n} = \widehat{f}(z), \quad |z| > R\widehat{f},$$

where $R\widehat{f}$ is the convergence radius of the series $\widehat{f}$. Let us briefly recall some classical properties of this discrete transform. We have the two shift relations

$$\mathscr{Z}(f_{n+1}) = z\widehat{f}(z) - zf_0 \quad \text{and} \quad \mathscr{Z}(f_{n+1} \pm f_n) = (z \pm 1)\widehat{f}(z) - zf_0.$$

If, $\widehat{f}(z)$ and $\widehat{g}(z)$ are defined for, respectively, $|z| > R\widehat{f}$ and $|z| > R\widehat{g}$, then, the $\mathscr{Z}$-transform of the discrete convolution operation $f_n \bigstar g_n$ exists in the following sense

$$\mathscr{Z}(f_n \bigstar g_n) = \widehat{f}(z)\widehat{g}(z), \quad |z| > \max(R\widehat{f}, R\widehat{g}).$$

Finally, if $R\widehat{f}R\widehat{g} < 1$, then $\mathscr{Z}(f_n\overline{g}_n)$ exists for $|z| > R\widehat{f}R\widehat{g}$ and we have

$$\sum_{n=0}^{\infty} f_n\overline{g_n} = \mathscr{Z}(f_n\overline{g_n})(z=1) = \frac{1}{2\pi}\int_0^{2\pi} \widehat{f}(r\mathrm{e}^{\mathrm{i}\varphi})\overline{\widehat{g}\left(\frac{\mathrm{e}^{\mathrm{i}\varphi}}{r}\right)}\,\mathrm{d}\varphi, \tag{18}$$

where the integration path is the circle defined by $R\widehat{f} < r < 1/R\widehat{g}$. Furthermore, if the two radii fulfil $R\widehat{f} < 1$ and $R\widehat{g} < 1$, then $r = 1$ and (18) is satisfied for $r = 1$.

Each term A_n^γ involves the value of $u^{n+1/2}$ at boundary points x_γ. This value is provided using the ND transparent condition which is given by

$$u^{n+1}(x_\gamma) = -\mathrm{e}^{\mathrm{i}\pi/4}\frac{\sqrt{2\delta t}}{2}\alpha_{n+1} \bigstar \partial_{\mathbf{n}} u^{n+1}(x_\gamma).$$

To suitably use the $\mathscr{Z}$-transform, we need to extend the finite sequence $(u^n)_{0\leqslant n\leqslant N}$ to an infinite sequence without modifying the quantities to estimate. To this end, we introduce the new sequence $(v_n^N)_{n\in\mathbb{N}}$ defined by

$$v_n^N = \begin{cases} u^n & \text{if } n \leqslant N+1, \\ (-1)^k u^{N+1} n & \text{if } n = N+1+k,\ k > 0. \end{cases}$$

We can then define the complex-valued sequences $(f_n^\gamma)_n$ and $(g_n^\gamma)_n$

$$f_n^\gamma = \frac{(\alpha_{n+1} \bigstar \partial_x v_{n+1}^N(x_\gamma)) + (\alpha_n \bigstar \partial_x v_n^N(x_\gamma))}{2}, \quad \gamma = \mathrm{l,r},\ \ 0 \leqslant n \leqslant N,$$

and

$$g_n^\gamma = \partial_x v_{n+1/2}^N(x_\gamma), \quad \gamma = \mathrm{l}, \mathrm{r}, \ \ 0 \leqslant n \leqslant N.$$

An immediate calculation shows that we have

$$\overline{u^{n+1/2}(x_\gamma)} = -\mathrm{e}^{-\mathrm{i}\pi/4}\frac{\sqrt{2\delta t}}{2}\overline{f_n^\gamma} \quad \text{and} \quad \partial_x u^{n+1/2}(x_\gamma) = g_n^\gamma \ \text{ if } n \leqslant N.$$

Consequently, we have the new expression of A^γ for $n \leqslant N$

$$A^\gamma = \delta t \frac{\sqrt{2\delta t}}{2}\mathrm{Re}\left(\mathrm{e}^{\mathrm{i}\pi/4}\sum_{n=0}^{N}\overline{f_n^\gamma}g_n^\gamma\right), \quad \gamma = \mathrm{l}, \mathrm{r}.$$

Using results on $\mathscr{Z}$-transform, we have the relation

$$\widehat{g_n^\gamma}(z) = \frac{z+1}{2}\mathscr{Z}(\partial_x v_n^N(x_\gamma)) - \frac{z}{2}\partial_x v_0^N(x_\gamma) = \frac{z+1}{2}\mathscr{Z}(\partial_x v_n^N(x_\gamma)),$$

since $\partial_x v_0^N(x_\gamma) = 0$. The above function is analytic on $|z| > 0$ since this is also the case for $\mathscr{Z}(\partial_x v_n^N(x_\gamma))$. Moreover, we have

$$\widehat{f_n^\gamma}(z) = \frac{z+1}{2}\mathscr{Z}(\alpha_n)\mathscr{Z}(\partial_x v_n^N(x_\gamma)).$$

From the definition of the sequence $(\alpha_n)_{n\in\mathbb{N}}$, we can assert that

$$\mathscr{Z}(\alpha_n) = \sum_{n=0}^{\infty}\alpha_n z^{-n} = \mathrm{i}\sqrt{\frac{1+z}{1-z}},$$

which is analytic for $|z| > 1$. Consequently this proves that $\widehat{f_n^\gamma}$ is also analytic on $|z| > 1$. As a consequence the application of relation (18) (for $r = 1$) implies that

$$\sum_{n=0}^{\infty}\overline{f_n^\gamma}g_n^\gamma = \sum_{n=0}^{\infty}\left|\frac{z+1}{2}\right|^2\left|\mathscr{Z}(\partial_x v_n^N(x_\gamma))\right|^2\overline{\mathscr{Z}(\alpha_n)} = \frac{1}{2\pi}\int_0^{2\pi}\left|\frac{z+1}{2}\right|^2_{|z=\mathrm{e}^{\mathrm{i}\varphi}}\left|\mathscr{Z}(\partial_x v_n^N(x_\gamma))\right|^2_{|z=\mathrm{e}^{\mathrm{i}\varphi}}\overline{\mathscr{Z}(\alpha_n)_{|z=\mathrm{e}^{\mathrm{i}\varphi}}}\mathrm{d}\varphi,$$

where the integral is well-defined. After some simplifications we obtain the expression of A^γ

$$A^\gamma = \frac{\sqrt{2\delta t}}{4\pi}\mathrm{Re}\left(\mathrm{e}^{\mathrm{i}\pi/4}\int_0^{2\pi}\left[\left|\frac{z+1}{2}\right|^2\left|\mathscr{Z}(\partial_x v_n^N(x_\gamma))\right|^2\overline{\sqrt{\frac{1+z}{1-z}}}\right]_{|z=\mathrm{e}^{\mathrm{i}\varphi}}\mathrm{d}\varphi\right).$$

Since the application $z \mapsto (1+z)/(1-z)$ is a homography from $D(0,1)$ onto $\{\mathrm{Re}(z) \geqslant 0\}$ and which map $C(0,1)$ onto $\mathrm{i}\mathbb{R}$, we have

$$\arg\left(\mathrm{e}^{\mathrm{i}\pi/4}\left[\overline{\sqrt{\frac{1+z}{1-z}}}\right]_{|z=\mathrm{e}^{\mathrm{i}\varphi}}\right) \in \left[0, \frac{\pi}{2}\right].$$

As a consequence, using (17), we concluded that the following inequality holds:

$$\|u^{N+1}\|_2 < \|u_0\|_2 \quad \forall N \geqslant 0.$$

This yields the $L^2(\Omega_i)$-stability of solution to (14), ending hence the proof. □

Remark. All the results developed in the case of a vanishing potential can be easily extended if a potential V satisfying the assumptions given in Section 2 is involved.

3.3. Semi-discrete formulation using the DN transparent boundary condition

In all the preceding Sections, we have focus our study on the case where one considers the ND transparent boundary condition. From a continuous point of view, it is equivalent to choose the DN or ND operator. A natural question is how to suitably derive the semi-discrete approximation of the DN transparent operator. In fact, its determination can be very easily stated by the previous analysis. Indeed, during the proof of the stability result, we have shown that the application of a $\mathscr{Z}$-transform to the ND transparent condition leads to

$$\mathscr{Z}(u^n(x_\gamma)) = -e^{i\pi/4}\frac{\sqrt{2\delta t}}{2}\mathscr{Z}(\alpha_n \bigstar \partial_x u^n(x_\gamma)).$$

Now using the convolution formula, we get

$$\mathscr{Z}(\alpha_n \bigstar \partial_x u^n(x_\gamma)) = \mathscr{Z}(\alpha_n)\mathscr{Z}(\partial_x u^n(x_\gamma)).$$

Combining the two above formula straightforwardly yields the deconvolution of the ND transparent operator

$$\mathscr{Z}(\partial_x u^n(x_\gamma)) = \frac{-e^{-i\pi/4}\sqrt{2/\delta t}}{\mathscr{Z}(\alpha_n)}\mathscr{Z}(u^n(x_\gamma)).$$

As a consequence, since

$$\frac{1}{\mathscr{Z}(\alpha_n)} = \frac{1}{i}\sqrt{\frac{1-z}{1+z}},$$

we deduce the semi-discrete form of the associated DN transparent boundary condition by using once again the convolution formula and the inverse $\mathscr{Z}$-transform of the signal

$$\partial_x u^n(x_\gamma) = -e^{-i\pi/4}\sqrt{\frac{2}{\delta t}}\sum_{k=0}^{n}\beta_k u^{n-k}(x_\gamma). \tag{19}$$

The sequence of coefficients $(\beta_k)_{k\geqslant 0}$ defining the new semi-discrete convolution operator are given by

$$\beta_k = (-1)^k\alpha_k, \quad k \in \mathbb{N}. \tag{20}$$

Under the above notations, we can state the stability of the semi-discrete Crank–Nicolson scheme for the semi-discretization (19) of the DN transparent boundary condition.

Theorem 4. *The semi-discrete Crank–Nicolson scheme for the Schrödinger equation associated with the representation* (19) *of the DN transparent boundary condition is given by the system*

$$\mathrm{i}\frac{u^{n+1}-u^n}{\delta t}+\partial_x^2\left(\frac{u^{n+1}+u^n}{2}\right)=0 \quad \forall x\in\Omega_i,$$

$$\partial_{\mathbf{n}}u^{n+1}(x_\gamma)=-\mathrm{e}^{-\mathrm{i}\pi/4}\sqrt{\frac{2}{\delta t}}\sum_{k=0}^{n+1}\beta_k u^{n+1-k}(x_\gamma) \quad \text{for } \gamma=\mathrm{l},\mathrm{r},\ \ t>0,$$

$$u^0=u_0 \quad \forall x\in\Omega_i,$$

where the set of coefficients $(\beta_k)_{k\in\mathbb{N}}$ *is given by relation* (20). *Then, this scheme is unconditionally stable in the sense of the* $\|\cdot\|_{L^2(\Omega_i)}$*-norm. Moreover, we have the energy inequality*

$$\|u^{N+1}\|_{L^2(\Omega_i)}<\|u_0\|_{L^2(\Omega_i)} \quad \forall N\geqslant 0.$$

We do not detail here the proof of the Theorem which is very similar to the one presented for the ND transparent boundary condition.

3.4. Finite element approximation

As seen above, the time semi-discrete schemes are unconditionally stable. This property is preserved at the fully discrete level by considering a conform finite element subspace for the spatial discretization of the variational formulation. The implementation of the DN transparent boundary condition does not present any difficulty since it naturally appears in the weak formulation. The ND transparent condition is implemented in the variational formulation as a Fourier–Robin-type boundary condition. More precisely, we consider the following weak formulation

$$\int_{\Omega_i}\mathrm{i}\frac{u^{n+1}-u^n}{\delta t}\varphi\,\mathrm{d}\Omega_i-\frac{1}{2}\int_{\Omega_i}\partial_x u^{n+1/2}\partial_x\varphi\,\mathrm{d}\Omega_i+[\partial_x u^{n+1/2}\varphi]_{x_\mathrm{r}}^{x_\mathrm{l}}=0, \tag{21}$$

where we have define the mean value $u^{n+1/2}$ by the relation

$$u^{n+1/2}=\frac{u^{n+1}+u^n}{2},$$

and where φ is a sufficiently smooth function. From relation (11), the transparent condition allows us to express the mean normal derivative at the endpoints of the computational domain by

$$\partial_{\mathbf{n}}u^{n+1/2}(x_\mathrm{r})=-\frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{\sqrt{2\delta t}}u^{n+1}(x_\mathrm{r})-\sum_{k=2}^{n}\gamma_k\left(\frac{\partial_{\mathbf{n}}u^{n+1-k}(x_\mathrm{r})+\partial_{\mathbf{n}}u^{n-k}(x_\mathrm{r})}{2}\right).$$

This expression is therefore considered as a Fourier–Robin boundary condition and is introduced in the variational Eq. (21). The spatial discretization is based upon linear or quadratic Lagrange finite element for a uniform grid of points $(x_j)_{0\leqslant j\leqslant J}$. Hence, we have: $x_j=x_\mathrm{l}+j\delta x$ for a step $\delta x=(x_\mathrm{r}-x_\mathrm{l})/J$. We denote by DN_1 and DN_2 the linear and quadratic finite element approximations for the DN transparent boundary condition. The approximation of problem ND requires more attention. Indeed, the computation of normal derivatives in Section 3.4 can lead to the loss of one order of convergence of the finite element method. To highlight this phenomenon, we implement some finite element methods of order i on the interval $[x_1,x_{J-1}]$ and j on $[x_0,x_1]\cup[x_{J-1},x_J]$. These methods are designated by $\mathrm{ND}_{i,j}$.

4. Numerical results

For the numerical purpose, we consider the linear Schrödinger equation with a vanishing potential. It is well-known that an explicit exact solution is given by

$$u(x,t) = \sqrt{\frac{\mathrm{i}}{-4t+\mathrm{i}}}\exp\left(\frac{-\mathrm{i}x^2 - k_0 x + k_0^2 t}{-4t+\mathrm{i}}\right).$$

This represents a Gaussian beam travelling with a wave number k_0.

For the numerical simulations, we consider the computational domain $\Omega_i =]-5,5[$ and a fixed frequency $k_0 = 8$ (see Fig. 1).

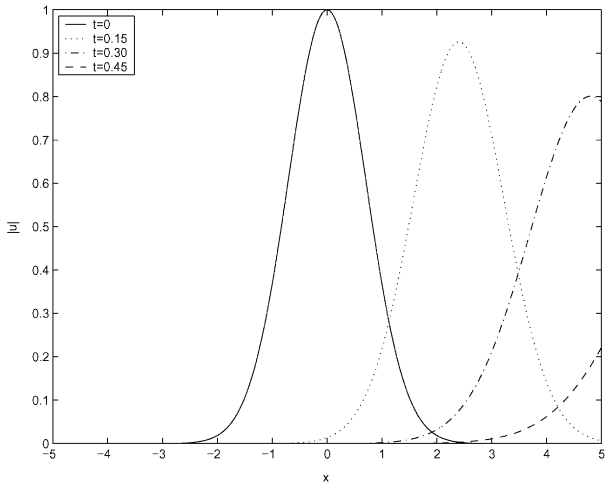

Fig. 2. Representation of the evolution of the solution at different times t for the DN_1 scheme.

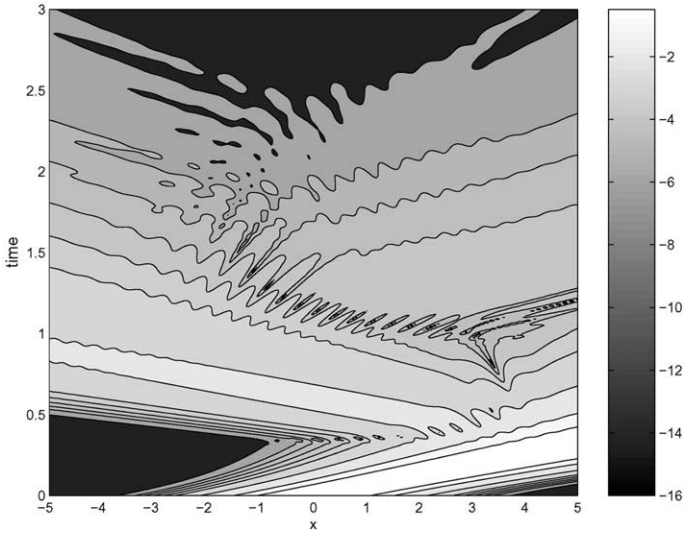

Fig. 3. Contour of the $\log_{10}(|u|)$ for the Baskakov–Popov method.

The first numerical experiment given on Fig. 2 consists in the representation of the evolution of the solution at different times $t = 0$, $t = 0.15$, $t = 0.30$ and $t = 0.45$ for the DN_1 scheme. The spatial domain Ω_i is discretized by using $J = 1024$ fixed intervals. This choice is motivated by the necessity to reproduce the oscillating behavior of the underlying solution by taking approximately 10 points per wavelength. Moreover we consider a time step $\delta t = 10^{-3}$.

In order to perform an exhaustive study of the proposed schemes, we compare the conditions $ND_{1,1}$, $ND_{1,2}$, $ND_{2,2}$, DN_1 and DN_2 to the classical schemes of Baskakov and Popov [6] and Arnold and Ehrhardt [5]. To bring to the fore the unphysical numerical reflections link to the different methods, we plot the

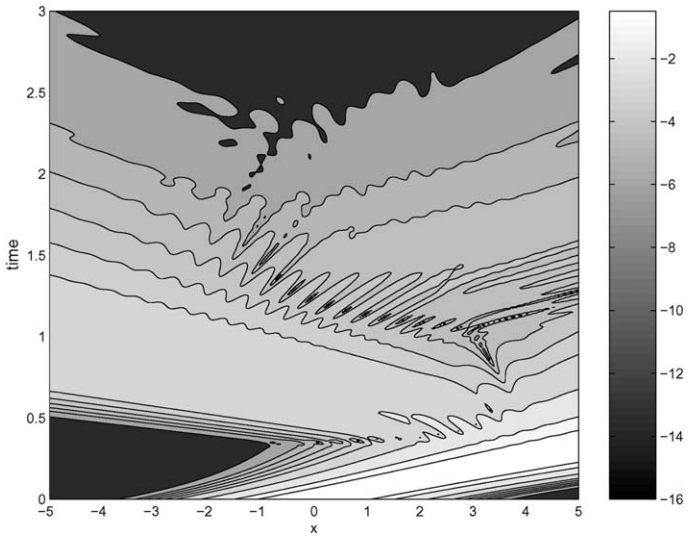

Fig. 4. Contour of the $\log_{10}(|u|)$ for the $ND_{1,1}$ method.

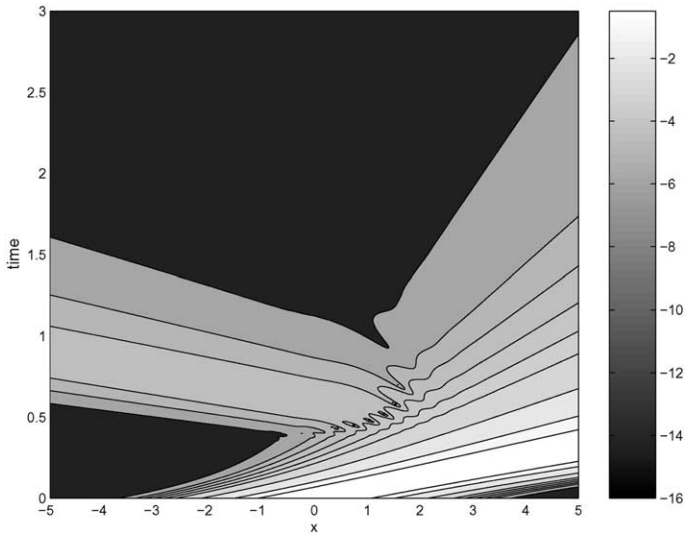

Fig. 5. Contour of the $\log_{10}(|u|)$ for the $ND_{1,2}$ method.

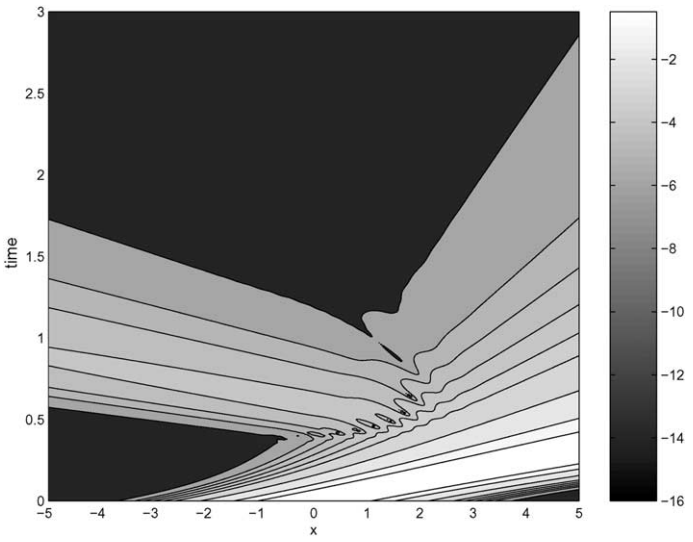

Fig. 6. Contour of the $\log_{10}(|u|)$ for the $ND_{2,2}$ method.

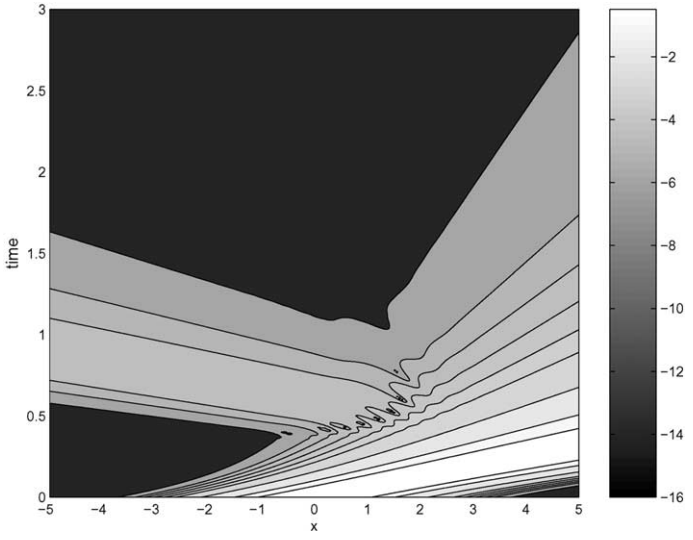

Fig. 7. Contour of the $\log_{10}(|u|)$ for the DN_1 method.

contour of $\log_{10}(|u|)$ on Figs. 3–9. This curves are presented according to their increasing accuracy. As it can be remarked on Fig. 3, the approach of Baskakov and Popov generates relatively important reflections with an amplitude of the order of 10^{-1}. The level of the reflected wave is sufficiently powerful to create a new reflected wave at the left fictive boundary. Moreover, this scheme is known to be conditionally stable [17].

Using condition $ND_{1,1}$ (cf. Fig. 4) lightly improves the approximation while keeping on being reflective. As precised in the previous section, the order of the finite element is increased by one on $[x_0, x_1] \cup [x_{J-1}, x_J]$. The $ND_{1,2}$ approximation leads to a visible improvement of the accuracy (cf. Fig. 5). This clearly indicates a loss of one order in the approximation when the normal derivatives in formula (3.4) are evaluated. This order

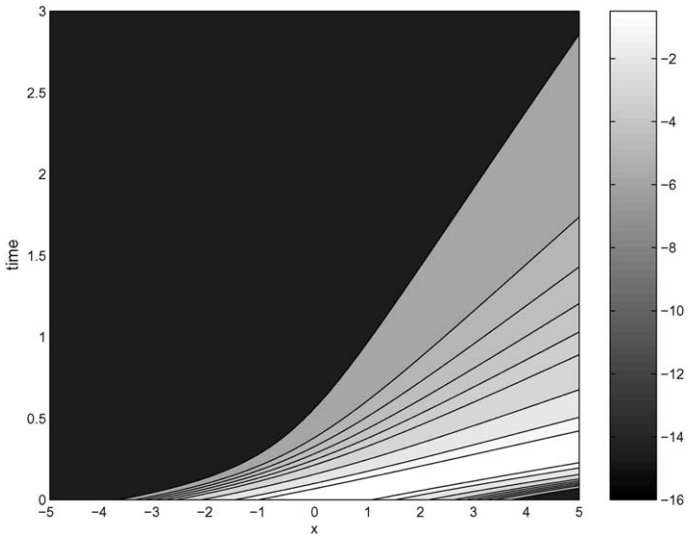

Fig. 8. Contour of the $\log_{10}(|u|)$ for the DN_2 method.

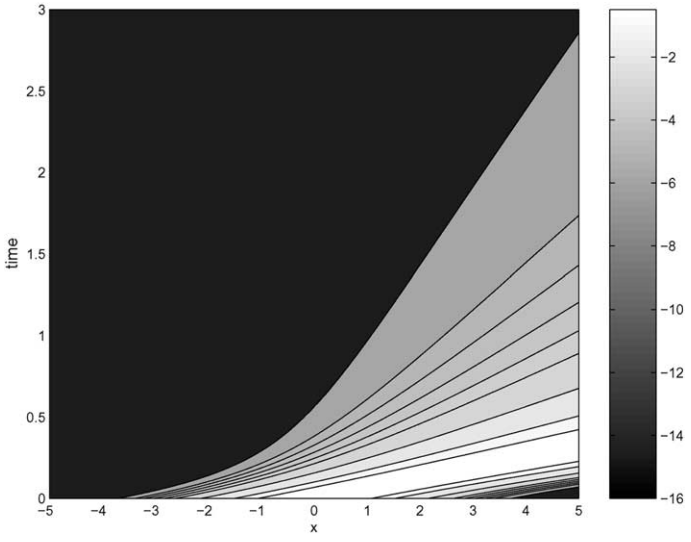

Fig. 9. Contour of the $\log_{10}(|u|)$ for the Arnold–Ehrhardt method.

is recovered simply by increasing the order of both the right and left boundary finite elements. Thereby, only two points are added to the initial mesh without increasing the computational cost of the $ND_{1,1}$ scheme. Moreover, no improvement arises when using $ND_{i,i}$ compared to $ND_{i-1,i}$ (cf. Fig. 6 where $i = 2$).

We see on Fig. 7 that the use of the DN_1 Dirichlet–Neumann operator yields really a much more accurate solution. Indeed, the reflected wave is only of the order of 10^{-5}. Therefore, the dispersive effects begin to be possibly observed. To increase the accuracy of the method, we consider in Fig. 8, a quadratic finite element approximation of the solution. This allows us to apparently avoid any spurious reflections. In fact, some very small reflected waves, here invisible, of the magnitude 10^{-10}–10^{-11} appear. Now, the effect of

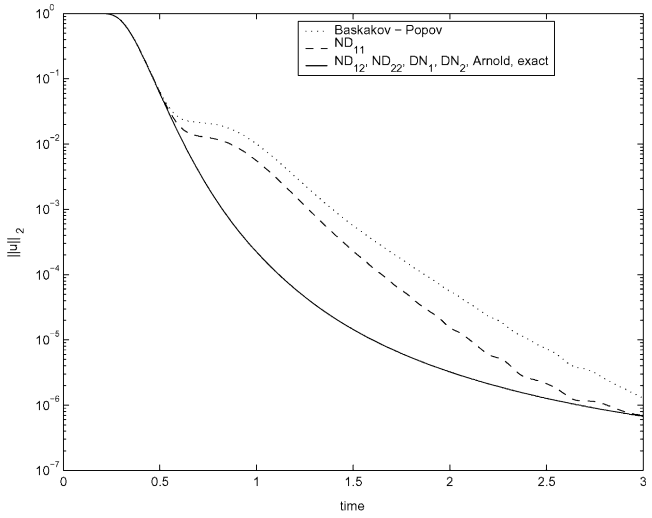

Fig. 10. Evolution of the remaining power in the computational domain.

the dispersion is precisely reproduced. Let us remark that this method has approximately the same computational cost as when using linear finite elements if we perform a mass lumping process. Since we are working with finite elements, it is possible to consider some adaptative meshes to compute the solution.

We represent on Fig. 9, the contour of the solution obtained with the Arnold–Ehrhardt approach. We observe no reflection in finite arithmetic precision. However, this approach has the drawback to fix the order of the approximation scheme and to only consider a uniform mesh. This can be restrictive for some practical applications.

Finally, we plot on Fig. 10 the remaining power in the computational domain, that is to say $\log_{10}(||u||_{L^2(\Omega_i)})$. Then, we remark that the approaches of Baskakov–Popov and $ND_{1,1}$ do not accurately reproduce the results obtained for the exact solution. In contrast, this is not the case of the other proposed schemes and Arnold–Ehrhardt methods.

5. Conclusion

In this paper, we have given a different point of view on the derivation of the transparent boundary conditions described in Friese–Schmidt–Yevick [12] for the one-dimensional Schrödinger equation. The resulting fully discrete schemes based on finite element methods have proved to be unconditionally stable. The extension to the two-dimensional framework using the transparent boundary conditions derived in [1] for general curved boundaries is actually under progress [2]. The new approach is useful to be extended to the two-dimensional case since it is a priori based on a direct approximation by a quadrature rule of the continuous transparent operator. This not seems to be the case for the quasi-exact approach of Arnold and Ehrhardt.

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