Construction of artificial boundary conditions for dispersive equations

1 Derivation of transparent boundary conditions (TBC) for linear dispersive equations

1.1 Introduction to dispersive equations

There appears to be no single precise definition of what exactly constitutes a wave. Various restrictive definitions can be given, but to cover the whole range of wave phenomena it seems preferable to be guided by the intuitive view that a wave is any recognizable signal that is transferred from one part of the medium to another with a recognizable velocity of propagation. One can distinguish two main classes of waves. The first is formulated mathematically in terms of hyperbolic partial differential equations, and such waves will be referred to as *hyperbolic*. The second class cannot be characterized as easily, but since it starts from the simplest cases of dispersive waves in linear problems, we shall refer to the whole class as *dispersive*. The classes are not exclusive. There is some overlap in that certain wave motions exhibit both types of behavior, and there are certain exceptions that fit neither. Concerning the *hyperbolic* equation, I refer to the lectures given by Prof. P. Noble.

The prototype for dispersive waves is based on a type of solution rather than a type of equation. A linear dispersive system is any system which admits solutions of the form

$$\varphi = A\exp(i\boldsymbol{\kappa}\cdot\mathbf{x} - i\omega t), \tag{1.1}$$

where the frequency ω is a definite real function of the wave number $\boldsymbol{\kappa}$ and the function $\omega(\boldsymbol{\kappa})$ is determined by the particular system, and A is the amplitude. To satisfy the equations, $\boldsymbol{\kappa}$ and ω have to be related by an equation

$$G(\omega, \boldsymbol{\kappa}) = 0.$$

Some of the typical examples of dispersive equations are the beam equation

$$\varphi_{tt} + \gamma^2\varphi_{xxxx} = 0, \text{ for which we require } \omega^2 - \gamma^2\kappa^4 = 0, \tag{1.2}$$

and the linear Korteweg-de Vries equation

$$\varphi_t + c_0\varphi_x + \nu\varphi_{xxx} = 0, \text{ for which we require } \omega = c_0\kappa - \nu\kappa^3. \tag{1.3}$$

The relation between ω and $\boldsymbol{\kappa}$ is called the **dispersion relation**, and as will become evident below, we can dispense with the equations once we know the dispersion relation; conversely, we can construct the equation from the dispersion relation.

We assume that the dispersion relation may be solved in the form of real roots

$$\omega = W(\boldsymbol{\kappa}). \tag{1.4}$$

There will be a number of such solutions, in general, with different functions $W(\boldsymbol{\kappa})$. We refer to these as different modes.

The actual solution is

$$\mathrm{Re}\varphi = |A|\cos(\boldsymbol{\kappa}\cdot\mathbf{x} - \omega t + \eta), \quad \eta = \arg A.$$

The quantity

$$\theta = \boldsymbol{\kappa}\cdot x - \omega t \tag{1.5}$$

is the *phase*.

Remark

θ determines the position on the cycle between a crest, where Reφ is maximum, and a trough, where Reφ is a minimum. In this plane wave solution, phase surfaces θ=constant are parallel planes. The gradient of θ in space is the wave number κ, whose direction is normal to the planes and whose magnitude κ is the average number of crests per 2π units of distance in that direction. The derivative with respect to t of θ is the **frequency** ω, that is to say the average number of crests per 2π units of time. The **wavelength** is $\lambda = 2\pi/k$ and the period is $\tau = 2\pi/\omega$.

The wave motion is recognized from (1.5). Any particular phase surface is moving with normal velocity ω/κ in the direction of $\boldsymbol{\kappa}$. We therefore introduce the **phase velocity**,

$$\boldsymbol{c} = \frac{\omega}{\kappa}\hat{\boldsymbol{\kappa}}, \tag{1.6}$$

where $\hat{\boldsymbol{\kappa}}$ is the unit vector in the $\boldsymbol{\kappa}$ direction. For any particular mode $\omega = W(\boldsymbol{\kappa})$, the phase velocity is a function of $\boldsymbol{\kappa}$. For the wave equation $\varphi_{tt} = c_0^2\Delta\varphi$, the dispersion relation gives $\omega = \pm c_0\kappa$ and $c = \pm c_0$: the phase velocity agrees with the usual propagation speed. In general, c is not independent of κ. Different wave numbers will lead to different phase speeds. This accounts for the term **dispersion**. The waves are usually said to be **dispersive** if this phase velocity is not a constant but depends on κ.

The heat equation $\varphi_t = \Delta\varphi$ has solutions (1.1) with $\omega = -i\kappa^2$, but the solutions are not wavelike. To eliminate the unwanted cases, we restrict the term **dispersive** to those cases for which

$$W(\boldsymbol{\kappa}) \text{ is real}, \quad \text{and determinant} \left|\frac{\partial^2 W}{\partial\kappa_i\partial\kappa_j}\right| \neq 0. \tag{1.7}$$

For one dimensional problems, the second condition is just $W''(\kappa) \neq 0$.

Correspondence Between Equation and Dispersion Relation.
A single linear equation with constant coefficients may be written

$$P\left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right)\varphi = 0,$$

where P is a polynomial. We have a direct correspondence between the equation and the dispersion relation through the correspondence

$$\frac{\partial}{\partial t} \leftrightarrow -i\omega, \quad \frac{\partial}{\partial x_j} \leftrightarrow i\kappa_j.$$

The dispersion relation must be

$$P(-i\omega, i\kappa_1, i\kappa_2, i\kappa_3) = 0.$$

For example, if we consider the dispersion relation

$$\hbar\omega = \frac{\hbar^2\kappa^2}{2m},$$

we obtain the Schrödinger equation

$$i\hbar\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\varphi. \tag{1.8}$$

As we said, a linear dispersive system is any system which admits solutions of the form (1.1). For linear problems, solutions more general are obtained by superposition to form Fourier integrals, such as

$$\varphi = \int_{-\infty}^{\infty} F(\boldsymbol{\kappa})\exp(i\boldsymbol{\kappa}\cdot x - iW(\boldsymbol{\kappa})t)\,d\boldsymbol{\kappa}. \tag{1.9}$$

The solution in (1.9) is a superposition of wavetrains of different wave numbers, each traveling with its own phase velocity

$$c(\boldsymbol{\kappa}) = \frac{W(\boldsymbol{\kappa})}{\kappa}\hat{\boldsymbol{\kappa}}. \tag{1.10}$$

As time evolves, these different component modes "disperse" with the result that a single concentrated hump, for example, disperses into a whole oscillatory train. The key concept that comes out of the analysis is that of the *group velocity* defined as

$$C(\kappa) = \nabla_{\hat{\boldsymbol{\kappa}}}\omega. \tag{1.11}$$

In one dimensional problem, $C(\kappa) = \omega'(\kappa)$.

The oscillatory train arising from (1.9) does not have constant wave-length; the whole range of wave numbers κ is still present. The different values of wave number propagate through this oscillatory train and the speed of propagation is the group velocity (1.11). In a similar sense it is found that energy also propagates with the group velocity.

It is desirable to find direct ways of deriving the group velocity and its properties without the intermediary of the Fourier analysis. Assume that the nonuniform oscillatory wave is described approximately in the form

$$\varphi = a\cos\theta,$$

where a and θ are functions of x and t. The function $\theta(x,t)$ if the "phase" and $a(x,t)$ is the amplitude. The special uniform wavetrain has

$$a = \text{constant}, \quad \theta = \kappa x - \omega t, \quad \omega = W(\kappa).$$

In the more general case, we define a local wave number $\kappa(x,t)$ and a local frequency $\omega(x,t)$ by

$$\kappa(x,t) = \frac{\partial\theta}{\partial x}, \quad \omega(x,t) = -\frac{\partial\theta}{\partial t}.$$

Assume now that these are still related by the dispersion relation $\omega = W(\kappa)$. This is then an equation for θ

$$\frac{\partial\theta}{\partial t} + W\left(\frac{\partial\theta}{\partial x}\right) = 0,$$

and its solution determines the kinematic properties of the wavetrain. It is more convenient to eliminate θ to obtain

$$\frac{\partial \kappa}{\partial t} + \frac{\partial \omega}{\partial x} = 0,$$

or again

$$\frac{\partial \kappa}{\partial t} + C(\kappa)\frac{\partial \kappa}{\partial x} = 0,$$

where $C(\kappa)$ is the group velocity. This equation for κ is just the simplest nonlinear hyperbolic equation. It may be interpreted as a wave equation for the propagation of κ with speed $C(\kappa)$. The group velocity $C(\kappa)$ is the propagation velocity for the wave number κ. In this rather subtle way, hyperbolic phenomena are hidden in dispersive waves.

As a conclusion, "dispersion" will refer to the fact that different frequencies in this equation will tend to propagate at different velocities, thus dispersing the solution over time. This is in contrast to transport equations, which move all frequencies with the same velocity (and is thus a degenerate case of a dispersive equation), or dissipative equations such as the heat equation, in which frequencies do not propagate but instead simply attenuate to zero. The wave equation is partly dispersive - the frequency of a wave determines the direction of propagation, but not the speed;

As we have seen, the Schrödinger and the Korteweg-de Vries equations are dispersive. A more general definition for the linear dispersive equations are given by

Definition 1.1 *A constant-coefficient linear dispersive PDE takes the form*

$$\partial_t u(t,x) = Lu(t,x); \quad u(0,x) = u_0(x) \tag{1.12}$$

where $u : \mathbb{R} \times \mathbb{R}^d \to V$ takes values in the Hilbert space V, and L is skew-adjoint constant coefficient differential operator in space, thus taking the form

$$Lu(x) := \sum_{|\alpha| \leq k} c_\alpha \partial_x^\alpha u(x),$$

where $k \geq 1$ is an integer (the order of the differential operator), $\alpha = (\alpha_1, \cdots, \alpha_d) \in \mathbb{Z}_+^d$ ranges over all multi-indices with $|\alpha| := \alpha_1 + \cdots + \alpha_d$ less than or equal to k, ∂_x^α is the partial derivative

$$\partial_x^\alpha := (\frac{\partial}{\partial x_1})^{\alpha_1} \cdots (\frac{\partial}{\partial x_d})^{\alpha_d},$$

and $c_\alpha \in \mathbb{C}$ are coefficients that do not depend on x.

We recall that T is skew-adjoint operator if $T^* = -T$ or also if iT is self-adjoint (T is self adjoint if $T^* = T$). If one considers the Schrödinger equation (1.8) or the Airy equation (linearized version if KdV)

$$\partial_t u + \partial_{xxx} u = 0, \tag{1.13}$$

on can easily check that the operator L is skew-adjoint.

We can also write $L = ih(D)$, where D is the frequency operator

$$D := \frac{1}{i}\nabla = (\frac{1}{i}\partial_{x_1}, \cdots, \partial_{x_d}),$$

and h is the polynomial

$$h(\xi_1, \cdots, \xi_d) = \sum_{|\alpha| \leq k} i^{|\alpha|-1} c_\alpha \xi_1^{\alpha_1} \cdots \xi_d^{\alpha_d}.$$

Since L is skew-adjoint, one has $< Lu(x), v(x) >_V = - < u(x), Lv(x) >_V$ for all test functions u, v; this is equivalent to requiring that coefficients of the polynomial h be self-adjoint, so in the scalar case we require h to be real-valued. We refer to the polynomial h as *the dispersion relation* of the equation (1.12). For the Schrödinger equation (1.8), one has $h(\xi) = -\frac{\hbar}{2m}|\xi|^2$ and for the Airy equation (2.16), $h(\xi) = \xi^3$.

The constant-coefficient dispersive equations have a number of symmetries. All are invariant under time translation $u(t,x) \to u(t-t_0, x)$ and spatial translation $u(t,x) \to u(t, x-x_0)$. Several also enjoy a scaling symmetry: the equation is invariant under the scaling $u(t,x) \to u(\frac{t}{\lambda^k}, \frac{x}{\lambda})$ for any $\lambda > 0$ where k is the degree operator. There is also usually a time reversal symmetry, though the precise nature of the symmetry varies. For instance, for the Schrödinger and the Airy equations one takes $u(t,x) \to u(-t,-x)$. The Schrödinger equation also has a very useful Galilean invariance. The solution u solves (1.8) if and only if

$$\tilde{u}(t,x) := e^{imx\cdot v/\hbar} e^{imt|v|^2/2\hbar} u(t, x - vt)$$

solves (1.8) too. Finally, the Schrödinger equation also enjoys the pseudo-conformal symmetry. Let us define

$$v(t,x) := \frac{1}{(it)^{d/2}} \overline{u(\frac{1}{t}, \frac{x}{t})} e^{i|x|^2/2t},$$

with the convention

$$v(0,x) = \frac{1}{(2\pi)^{d/2}} \overline{\hat{u}_0(x)}.$$

Then one has

$$(i\partial_t v + \frac{1}{2}\Delta v)(t,x) = \frac{1}{t^2} \frac{1}{(it)^{d/2}} \overline{(i\partial_t u + \frac{1}{2}\Delta u)(\frac{1}{t}, \frac{x}{t})} e^{i|x|^2/2t}$$

for $t \neq 0$. In particular, if u solves (1.8) with $\hbar = m = 1$, the v also solves the Schrödinger equation.

The spatial Fourier transform, and the closely related spacetime Fourier transform, is an exceptionally well-suited tool to analyze constant coefficient linear dispersive equations. This is ultimately due to the invariance of these equations under translations in either space or time. One hint that the Fourier transform will be useful for solving equations comes from the simple observation that given any frequency $\xi_0 \in \mathbb{R}^d$, the plane wave $e^{ix\cdot\xi_0 + ith(\xi_0)}$ solves the equation with $L = ih(D)$. From the principle of superposition for linear equations, we thus see that we can construct solutions as superpositions of plane waves. Let us restrict our attention to the Schwartz space $\mathcal{S}_x(\mathbb{R}^d)$ (space of functions all of whose derivatives are rapidly decreasing). If $u \in C^1_{l,loc}\mathcal{S}_x(\mathbb{R}^d)$ of (1.12), we conclude

$$\partial_t \widehat{u(t)}(\xi) = ih(\xi)\widehat{u(t)}(\xi)$$

wihch has the unique solution

$$\widehat{u(t)}(\xi) = e^{ith(\xi)}\widehat{u_0}(\xi).$$

Since $h(\xi)$ is real and $\widehat{u_0}$ is Schwartz, the function $e^{ith(\xi)}\widehat{u_0}(\xi)$ is then also Schwartz for any $t \in \mathbb{R}$. We may thus apply the Fourier inversion formula and obtain the solution

$$u(t,x) = \int_{\mathbb{R}^d} e^{ith(\xi)+ix\cdot\xi}\widehat{u_0}(\xi)\, d\xi;$$

because of this, we shall let $e^{tL} = e^{ith(D)}$ denote the linear propagator

$$e^{tL}u_0(x) := \int_{\mathbb{R}^d} e^{ith(\xi)+ix\cdot\xi}\widehat{u_0}(\xi)\, d\xi;$$

This propagator is defined initially for Schwartz functions, but can be extended by standard density arguments to other spaces. For instance, Plancherel's theorem allows one to extend e^{tL} to be defined on the Lebesgue space $L^2_x(\mathbb{R}^d)$. It is clear that e^{tL} is a unitary operator on these spaces, and in particular on $L^2_x(\mathbb{R}^d)$

$$\|e^{tL}f\|_{L^2_x(\mathbb{R}^d)} = \|f\|_{L^2_x(\mathbb{R}^d)}.$$

This identity is very important. It says that the L^2-norm is a conserved quantity. The dispersive equations are known to have many preserved quantities.
For free linear Schrödinger equation, one has

$$e^{tL}\varphi(x) = \frac{1}{(4\pi it)^{d/2}}\int_{\mathbb{R}^d} e^{i|x-y|^2/4t}\varphi(y)\, dy.$$

Therefore, e^{Lt} sends L^1 to L^∞ since for all $\varphi \in L^1$, we get

$$|e^{Lt}\varphi|_{L^\infty} \leq Ct^{-d/2}|\varphi|_{L^1}.$$

As a more general result, we have: Let p, p' two integer with $2 \leq p \leq +\infty$ and $\frac{1}{p} + \frac{1}{p'} = 1$, then $\exists C > 0$ s.t. forall $\varphi \in L^{p'}(\mathbb{R}^d)$ and $t > 0$, $e^{tL}\varphi \in L^p(\mathbb{R}^d)$ and

$$\|e^{tL}\varphi\|_{L^p} \leq C\, t^{-d(1/2-1/p)}\|\varphi\|_{L^{p'}}.$$

For Schrödinger equation $i\partial_t u + \Delta u = 0$, we can give an explicit formula for the linear propagator. We have

$$e^{tL}u_0(x) = \frac{1}{(4\pi it)^{d/2}}\int_{\mathbb{R}^d} e^{i|x-y|^2/4t}u_0(y)\, dy.$$

Therefore, e^{tL} sends L^1 into L^∞ since we have

$$\|e^t L\varphi\|_{L^\infty} \leq Ct^{-d/2}\|\varphi\|_{L^1}.$$

1.2 Usual models: Schrödinger and linear Korteweg-de Vries equations

The dispersive equations that we will focuss on are the Schrödinger and Korteweg-de Vries equations. The nonlinear version of these equations could be derived in the context of water waves. The KdV equation is interesting to describe long waves in water of relatively shallow depth. On the opposite, the Schrödinger equation describes the long wave with an infinite depth. The last equation also arises in the context of cold atoms and more specifically to describe the state of matter denoted as Bose-Einstein condensates for which a collection of

"frozen" atoms can be described by a super wave function.
We recall that the KdV equation reads

$$\begin{cases} \partial_t \varphi(t,x) + \varphi \partial_x \varphi(t,x) + \partial_{xxx} \varphi(t,x) = 0, & (t,x) \in \mathbb{R}^+ \times \mathbb{R}, \\ \varphi(0,x) = \varphi_0(x), & x \in \mathbb{R}. \end{cases} \tag{1.14}$$

The cubic nonlinear Schrödinger equation that we could be interested in is given by

$$\begin{cases} i\partial_t u(t,x) = -\Delta u(t,x) + V(x)u(t,x) + \lambda |u(t,x)|^2 u(t,x), & (t,x) \in \mathbb{R}^+ \times \mathbb{R}^d, \\ u(0,x) = u_0(x), & x \in \mathbb{R}^d, \end{cases} \tag{1.15}$$

where $u(t,x)$ is the wave function depending on the time t. The function $V(x)$ is a real interaction potential function, and the operator $\Delta = \sum_{i=1}^d \partial_{x_i}^2$ is the Laplace operator. The constant λ is a real parameter. As initial condition, we impose that the function $u(t,x)$ at time $t = 0$ is equal to a given function u_0.

Both of the equations have preserved quantities. As we saw before, they both preserved the mass (L^2 norm). A second way of derivation exists. We present it on the nonlinear Schrödinger equation. It consists in multiplying the equation (1.15) by $\overline{u}$ and to integrate over x. Since $u \in L^2(\mathbb{R}^d)$, we can assume that u decays at infinity.

$$i \int_{\mathbb{R}^d} u_t \overline{u}\, dx = \int_{\mathbb{R}^d} \nabla u \cdot \nabla \overline{u} dx + \int_{\mathbb{R}^d} V(x)|u|^2 + \lambda |u|^4 dx.$$

We have

$$\mathrm{Re}(u_t \overline{u}) = \frac{1}{2} \partial_t |u|^2 (t,x).$$

Taking the imaginery part of the result, we have

$$\frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} |u|^2 dx = 0,$$

and so the L^2 norm is conserved. In the same way, if we multiply the equation (1.15) by $\overline{\partial_t u}$ and integrate over $\mathbb{R}^d$, we get

$$i \int_{\mathbb{R}^d} |u_t|^2\, dx = \int_{\mathbb{R}^d} \nabla u \cdot \nabla \overline{u_t}\, dx + \int_{\mathbb{R}^d} (V(x) + \lambda |u|^2) u \overline{u_t}\, dx.$$

Taking the real part of the equation leads to

$$\frac{1}{2} \frac{d}{dt} \left(\int_{\mathbb{R}^d} |\nabla u|^2\, dx + \int_{\mathbb{R}^d} V(x)|u|^2 + \frac{\lambda}{2} |u|^4\, dx \right) = 0.$$

The energy is conserved and be the sum of a kinetic part and a potential energy.

The both equations are set on the undounded domain $\mathbb{R}$ (we restrict ourselves here to the one dimensional case to introduce the concept). If one wants to solve such a whole space evolution problem numerically, one has to restrict the computational (interior) domain $\Omega_{int} = \{(x,t) \in]x_l, x_r[\times \mathbb{R}^+\}$ by introducing artificial boundary conditions. Artificial boundary conditions are constructed with the objective to approximate the exact solution of the whole–space problem, restricted to Ω_{int}. Such BCs are called *absorbing boundary conditions* (ABCs)

if they yield a well–posed initial boundary value problem (IBVP), where some "energy" is absorbed at the boundary. If this approximate solution actually coincides on Ω_{int} with the exact solution of the whole–space problem, one refers to these BCs as *transparent boundary conditions* (TBCs).

The aim of this series of lectures is to present different ways to get such artificial boundary conditions.

1.3 Derivation of TBC for linear wave equation and generalization for previous models

In order to present the derivation of transparent boundary conditions for dispersive equation, we begin by considering the homogeneous one dimensional wave equation

$$(\mathcal{P}) \quad \begin{cases} \partial_t^2\psi - \partial_x^2\psi = 0\,, & (x,t) \in \mathbb{R}_x \times [0;T]\,, \\ \psi(x,0) = \psi_0(x)\,, & x \in \mathbb{R}_x\,, \\ \partial_t\psi(x,0) = \psi_1(x)\,, & x \in \mathbb{R}_x\,, \end{cases} \tag{1.16}$$

where we assume that the initial data ψ_0 and ψ_1 satisfy $\mathrm{supp}(\psi_{0,1}) \subset B(0,R)$. The solution of (1.16) is given as

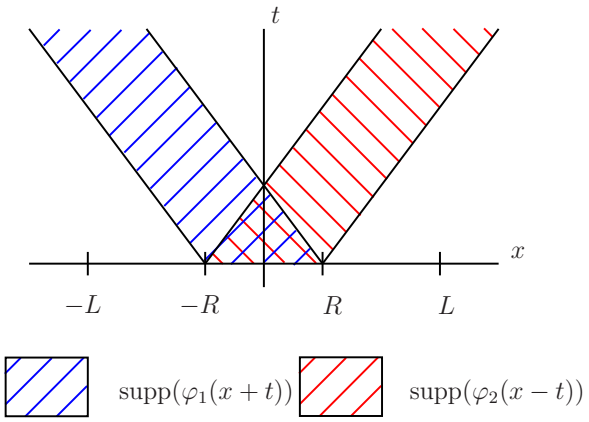
$$\psi(x,t) = \frac{1}{2}(\psi_0(x+t) + \psi_0(x-t)) + \frac{1}{2}\int_{x-t}^{x+t} \psi_1(y)dy.$$

One can see that we can rewrite it as the superposition of two waves, one propagated to the left direction and the other one to the right, with velocity 1

$$\psi(x,t) = \varphi_1(x+t) + \varphi_2(x-t)\,,$$

with

$$\begin{aligned} 2\varphi_1(x) &= \psi_0(x) + \int_{-\infty}^{x} \psi_1(y)dy\,, \\ 2\varphi_2(x) &= \psi_0(x) - \int_{-\infty}^{x} \psi_1(y)dy\,. \end{aligned}$$



Comme on le voit sur la figure ci-dessus, for any $t > 0$ and $\forall |x| > R$, the supports of the two waves are disjoint. Therefore, we have

$x=-L$	$x=L$
$\psi(x,t)=\varphi_1(x+t)$	$\psi(x,t)=\varphi_2(x-t)$
$\partial_x\psi=\partial_t\psi$	$\partial_x\psi=-\partial_t\psi$

Then, on $x=\pm L$, the *Neumann* datum is expressed in function of the *Dirichlet* one

$$\partial_{\mathbf{n}}\psi+\partial_t\psi=0$$

where $\mathbf{n}$ denotes the outwardly unit normal vector to $\Omega=(-L,L)$.

The problem $(\mathcal{P})$ is thus transformed in $(\mathcal{P}_{\text{app}})$

$$(\mathcal{P}_{\text{app}})\quad\begin{cases}\partial_t^2\psi^{\text{a}}-\partial_x^2\psi^{\text{a}}=0\,, & (x,t)\in\Omega\times[0;T]\,,\\ \psi^{\text{a}}(x,0)=\psi_0(x)\,, & x\in\Omega\,,\\ \partial_t\psi^{\text{a}}(x,0)=\psi_1(x)\,, & x\in\Omega\,,\\ \partial_{\mathbf{n}}\psi^{\text{a}}+\partial_t\psi^{\text{a}}=0\,, & (x,t)\in\Gamma\times[0;T]\,,\end{cases}$$

where $\Gamma=\{-L,L\}$. Since the relation that gives the boundary conditions, we have

$$\psi_{|\Omega}(x,t)=\psi^{\text{a}}(x,t)\,,\quad (x,t)\in\Omega\times[0;T]\,.$$

The BCs do not perturb the solution. Therefore, we have got **Transparent Boundary Conditions (TBC)**.

It is interesting to see that we can recover the TBC thanks to the use of Laplace transform. The Laplace transformation with respect to the time variable t is defined by

$$\mathscr{L}\{f\}(\omega)=\hat{f}(\omega)=\int_0^\infty f(t)e^{-\omega t}dt=\lim_{\tilde{t}\to\infty}\int_0^{\tilde{t}}f(t)e^{-\omega t}dt. \tag{1.17}$$

The variable $\omega=\sigma+i\tau$ is the frequency and is also known as the time covariable. We assume that in (1.17) the function $f(t)$ is defined for all positive t in the range $(0,\infty)$, and, most importantly, that the integral is convergent. A necessary condition for convergence is that

$$\sigma>\gamma,\quad \text{where } \gamma \text{ is a positive constant}$$

and $f(t)$ satisfies

$$|f(t)|=O(e^{\gamma t}) \text{ as } t\to\infty. \tag{1.18}$$

This condition implies that the function $f(t)$ is smaller in magnitude than the term $e^{-\omega t}$ for large t ($>t_0$, say) and, unless $f(t)$ has some singularity for $t<t_0$, the integral in (1.17) is convergent. Because of the restrictions imposed by (1.18) it is clear that a function such as $\exp(t^2)$ cannot have a Laplace transform since no value of the constant γ can be found for which $|e^{t^2}|<e^{\gamma t}$, for large t. As examples, we have

$$\mathscr{L}\{1\}=\int_0^\infty e^{-\omega t}dt=1/\omega,\quad (\text{Re}(\omega)>0).$$

$$\begin{aligned}\mathscr{L}\{t\}\ &=\int_0^\infty e^{-\omega t}tdt=\left(\frac{-te^{-\omega t}}{\omega}\right)\Big|_0^\infty+\int_0^\infty(e^{-\omega t}/\omega)dt,\\ &=(1/\omega)\int_0^\infty e^{-\omega t}dt=1/\omega^2.\end{aligned}$$

The Laplace transform is linear

$$\mathscr{L}\{f(t)+g(t)\}=\hat{f}(\omega)+\hat{g}(\omega)$$

and

$$\mathscr{L}\{\kappa f(t)\}=\kappa\hat{f}(\omega),\quad \kappa \text{ a constant.}$$

For our applications of Laplace transforms, we need to find the transform of f', the derivative of f or of higher derivatives of f. Assume that f is differentiable and continuous and $O(e^{\gamma t})$ as $t\to\infty$. Further, if we introduce a finite number of points $t_1,t_2,\cdots,t_n$ in any finite interval $[0,T]$, we have

$$\int_0^T e^{-\omega t}f'(t)dt=\int_0^{t_1}e^{-\omega t}f'(t)dt+\int_{t_1}^{t_2}e^{-\omega t}f'(t)dt+\cdots+\int_{t_n}^{T}e^{-\omega t}f'(t)dt.$$

Integrating by parts a typical term on the right hand side is

$$\begin{aligned}\int_{t_r}^{t_r+1}e^{-\omega t}f'(t)dt &= e^{-\omega t}f(t)\Big|_{t_r}^{t_{r+1}}+\omega\int_{t_r}^{t_r+1}e^{-\omega t}f(t)dt,\\ &= e^{-\omega t_{r+1}}f(t_{r+1^-})-e^{-\omega t_r}f(t_{r^+})+\omega\int_{t_r}^{t_r+1}e^{-\omega t}f(t)dt,\end{aligned}$$

where

$$f(a^-)=\lim_{\epsilon\to 0}f(a-\epsilon),\quad f(a^+)=\lim_{\epsilon\to 0}f(a+\epsilon),\quad \epsilon>0.$$

Since $f(t)$ is continuous at each t_i, we find

$$\int_0^T e^{-\omega t}f'(t)dt=e^{-\omega T}f(T)-f(0^+)+\omega\int_0^T e^{-\omega t}f(t)dt.$$

Letting $T\to\infty$, we obtain the result

$$\mathscr{L}\{f'(t)\}=\omega\hat{f}(\omega)-f(0^+). \tag{1.19}$$

In a similar way, if we assume that f' is continuous and differentiable and f'' is continuous except at a finite number of points in any finite interval $(0,T)$ then

$$\mathscr{L}\{f''(t)\}=\omega^2\hat{f}(\omega)-\omega f(0^+)-f'(0^+). \tag{1.20}$$

This result can be extended to higher derivatives to yield

$$\mathscr{L}\{f^{(n)}(t)\}=\omega^n\hat{f}(\omega)-\omega^{(n-1)}f(0^+)-\omega^{(n-2)}f'(0^+)-\cdots-f^{(n-1)}(0^+).$$

An other interesting feature concerns the Laplace transformation of a convolution product. One has

$$\mathscr{L}\{f*g\}(\omega)=\mathscr{L}\{f\}(\omega)\mathscr{L}\{g\}(\omega)$$

Finally, the inverse Laplace transformation is given as follows. The inverse of the Laplace transformation is given by the Bromwich integral

$$\mathscr{L}^{-1}\{\hat{f}\{(t)=\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}e^{st}\hat{f}(s)\,ds,$$

where γ is a vertical contour in the complex plane chosen such that all singularities of $\hat{f}(s)$ are to the left of it. We present a collection of used inverse Laplace–transformation rules

$$\begin{aligned}
\mathscr{L}^{-1}\left\{\frac{1}{\sqrt{\omega}}\right\} &= \frac{1}{\sqrt{\pi}}t^{-1/2},\\
\mathscr{L}^{-1}\left\{\hat{f}(\omega+\sigma)\right\} &= f(t)e^{-\sigma t},\\
\mathscr{L}^{-1}\left\{s\hat{f}(\omega+\sigma)\right\} &= \frac{d}{dt}\left\{f(t)e^{-\sigma t}\right\}, \quad \text{if } f(0)=0.
\end{aligned}$$

If we come back to the derivation of the TBCs for the wave equation, we have

$$\mathscr{L}(u)(\omega,x) = \hat{u}(\omega,x) = \int_0^\infty u(t,x)e^{-\omega t}dt$$

and

$$\begin{aligned}
\mathscr{L}(\partial_t u)(\omega,x) &= \omega\hat{u}(\omega,x) - u(x,0)\,,\\
\mathscr{L}(\partial_t^2 u)(\omega,x) &= \omega^2\hat{u}(\omega,x) - \omega u(0,x) - \partial_t u(0,x)\,.
\end{aligned}$$

Since we have $\mathrm{supp}(\psi_{0,1}) \subset B(0,R) := \Omega$, we can see the problem (P) as a transmission problem splitted in an interior problem

$$\begin{cases}
(\partial_t^2 - \partial_x^2)v = 0, & x\in\Omega,\ t>0,\\
\partial_x v = \partial_x w, & x\in\Gamma,\ t>0,\\
v(x,0) = \psi_0(x), & x\in\Omega,\\
\partial_t v(x,0) = \psi_1(x), & x\in\Omega,
\end{cases}$$

and an exterior one

$$\begin{cases}
(\partial_t - \partial_x^2)w = 0, & x\in\overline{\Omega}, t>0,\\
w(x,t) = v(x,t), & x=\pm L,\ t>0,\\
w(x,0) = 0, & x\in\overline{\Omega},\\
\partial_t w(x,0) = 0, & x\in\overline{\Omega}.
\end{cases}$$

We consider the exterior problem, and more specifically the right part of it, *ie* $x > R$. Since the initial data for the exterior problem are zeros, we can apply the Laplace transform and the equation is transformed as

$$\omega^2\hat{w} - \partial_x^2\hat{w} = 0.$$

The solution is given by

$$\hat{w}(\omega,s) = A^+(\omega)e^{\omega\, x} + A^-(\omega)e^{-\omega\, x}.$$

Since $\mathrm{Re}(\omega) > 0$, in order to the solution to not blow up as $x\to\infty$, we have to ask $A^+ = 0$. The solution is therefore

$$\hat{w}(\omega,s) = e^{-\omega\,(x-R)}\mathscr{L}(w(\cdot,R))(\omega).$$

Taking derivative

$$\partial_x\hat{w}(\omega,s)|_{x=R} = -\omega\,\hat{w}(s,\omega)|_{x=R}$$

We inverse the Laplace tranform and we get

$$\partial_x w(t,x)|_{x=R} = -\partial_t w(t,x)|_{x=R}.$$

Thus, by continuity at the boundary, we obtain the TBC for v

$$\partial_{\mathbf{n}} v + \partial_t v = 0.$$

We can apply the same technique to the linear Schrödinger equation

$$\begin{cases} i\partial_t u + \partial_x^2 u = 0, & (t,x) \in \mathbb{R}^+ \times \mathbb{R}, \\ u(0,x) = u_0(x), & x \in \mathbb{R}. \end{cases} \tag{1.21}$$

As for the wave equation, we split (1.21) into interior and exterior problems

$$\begin{cases} (i\partial_t + \partial_x^2)v = 0, & x \in \Omega,\ t > 0, \\ \partial_x v = \partial_x w, & x \in \Sigma,\ t > 0, \\ v(x,0) = \psi_0(x), & x \in \Omega. \end{cases}$$

and

$$\begin{cases} (i\partial_t + \partial_x^2)w = 0, & x \in \overline{\Omega}, t > 0, \\ w(x,t) = v(x,t), & x = x_{l,r},\ t > 0, \\ \lim\limits_{|x|\to+\infty} w(x,t) = 0, & t > 0, \\ w(x,0) = 0, & x \in \overline{\Omega}. \end{cases}$$

We apply the Laplace transform to the exterior problem on Ω_r

$$i\partial_t w + \partial_x^2 w = 0 \quad \longrightarrow \quad i\omega\hat{w} + \partial_x^2 \hat{w} = 0.$$

Before giving the solutions, we have to define the complex fractional power function. We introduce the function

$$\log_0 : \mathbb{C}\backslash]-\infty, 0] \to \mathbb{C}, \quad \log_0(z) = \ln(|z|) + i\mathrm{Arg}(z),$$

where $\mathrm{Arg}(z) \in]-\pi, \pi[$ denotes the principal determination of the argument. We define the analytic function z^α as

$$z^\alpha = e^{\alpha \log_0(z)}, \quad z \in \mathbb{C}\backslash]-\infty, 0[.$$

For example, we have

$$z^{1/2} = e^{\frac{1}{2}\ln(\sqrt{x^2+y^2})} e^{i\mathrm{Arg}(z)/2}, \quad z = x + iy.$$

The solutions are given by

$$\hat{w}(x,\omega) = A^+(\omega) e^{\sqrt{-i\omega}\, x} + A^-(\omega) e^{-\sqrt{-i\omega}\, x}.$$

Since $\omega = \sigma + i\tau$ and $\sigma > 0$, we obtain

$$\log_0(-i\omega) = \ln(\sqrt{\sigma^2 + \omega^2}) + i\mathrm{Arg}(-i\omega).$$

Since $-\pi/2 < \mathrm{Arg}(\omega) < \pi/2$, we have $-\pi < \mathrm{Arg}(-i\omega) < 0$. Therefore

$$\sqrt{-i\omega} = e^{\frac{1}{2}\ln(\sqrt{\sigma^2+\omega^2})} e^{i\frac{\mathrm{Arg}(-i\omega)}{2}}$$

with

$$-\pi/2 < \frac{\mathrm{Arg}(-i\omega)}{2} < 0.$$

Therefore, $\mathrm{Re}(\sqrt{-i\omega}) > 0$. We ask that $w \in L^2(\Omega_r)$ to select the outgoing wave which leads to ask $A^+ = 0$. We therefore have

$$\hat{w}(x,\omega) = e^{-\sqrt[+]{-i\omega}\,(x - x_r)} \mathcal{L}(v(x_r,\cdot))(\omega),$$

then, taking derivative and using continuity $\partial_x v = \partial_x w$ at the boundary

$$\begin{aligned}\partial_x \hat{v}(x,\omega)|_{x=x_r} &= -\sqrt[+]{-i\omega}\,\hat{v}(x,\omega)|_{x=x_r} \\ &= -e^{-i\pi/4}\omega \frac{\hat{v}(x,\omega)|_{x=x_r}}{\sqrt{\omega}}\end{aligned}$$

The inverse Laplace transform leads to

$$\partial_x v(x,t)|_{x=x_r} = -e^{-i\pi/4}\partial_t\left(\frac{1}{\sqrt{\pi}}\int_0^t \frac{v(x,s)|_{x=x_r}}{\sqrt{t-s}}ds\right) = -e^{-i\pi/4}\partial_t^{1/2} v(x_r,t).$$

The exact boundary condition on x_r is therefore given by

$$\partial_x v(x,t)|_{x=x_r} = -e^{-i\pi/4}\partial_t^{1/2} v(x_r,t)$$

where we have define the fractional derivative operator of order $1/2$

$$\partial_t^{1/2} f(x,t) = \frac{1}{\sqrt{\pi}}\,\partial_t \int_0^t \frac{f(x,s)|_{x=x_r}}{\sqrt{t-s}}\,ds.$$

We can perform the same computation on the left part of the domain and we get finally the transparent boundary condition for the linear Schrödinger equation

$$\partial_{\mathbf{n}} v + e^{-i\pi/4}\partial_t^{1/2} v = 0, \quad \text{on } \Sigma \times [0;T].$$

The computation of the solution to (1.21) is therefore replaced by

$$(S_{\text{app}}) \quad \begin{cases} i\partial_t \psi + \Delta\psi = 0, & (x,t) \in \Omega_T \\ \partial_{\mathbf{n}}\psi + e^{-i\pi/4}\partial_t^{1/2}\psi = 0, & \text{on } \Sigma_T, \\ \psi(x,0) = \psi_0(x), & x \in \Omega_T \end{cases}$$

where $\partial_{\mathbf{n}}$ is the outwardly directed normal derivative.
We remark that we could also write the transparent boundary condition as

$$\psi(x,t) + e^{i\pi/4} I_t^{1/2}\partial_{\mathbf{n}}\psi = 0, \quad x \in \Sigma_T,$$

where

$$I_t^{1/2} f = \frac{1}{\sqrt{\pi}}\int_0^t \frac{f(x,s)}{\sqrt{t-s}}\,ds.$$

We summarize the procedure to derive the continuous TBC:

1. Split original problem into coupled equations: interior and exterior problems.
2. Apply a Laplace transformation (1.17) in time t.
3. Solve the ordinary differential equations in x.
4. Allow only "outgoing" waves by selecting the decaying solution as $x \to \pm\infty$.
5. Match Dirichlet and Neumann values at $x = x_l$, $x = x_r$.
6. Apply the inverse Laplace transformation.

If we now consider the linear Schrödinger equation with a potential $V(x)$ which is constant outside of Ω, equal to $V_{l,r}$ on $\Omega_{l,r}$. The Laplace transformation of the equation (on Ω_r) reads

$$i\omega\widehat{w} + \partial_x^2\widehat{w} = V_r\widehat{w}, \quad x \in \Omega_r. \tag{1.22}$$

The solution to this ordinary differential equation can be written as

$$\hat{w}(x,\omega) = A^+(\omega)e^{\sqrt[+]{-i\omega+V_r}\,x} + A^-(\omega)e^{-\sqrt[+]{-i\omega+V_r}\,x}, \quad x > x_r, \tag{1.23}$$

However, since the solution must be in $L^2(\Omega_r)$, the coefficient A^+ must vanish. Using the Dirichlet data at the artificial boundary yields

$$\hat{w}(x,\omega) = e^{-\sqrt[+]{-i\omega+V_r}\,(x-x_r)}\mathscr{L}(v(x_r,\cdot))(\omega),$$

and hence

$$\partial_x\hat{v}(x,\omega)|_{x=x_r} = -\sqrt[+]{-i\omega+V_r}\,\hat{v}(x,\omega+V)|_{x=x_r}. \tag{1.24}$$

The analogous condition at the left boundary is

$$-\partial_x\hat{v}(x,\omega)|_{x=x_l} = -\sqrt[+]{-i\omega+V_l}\,\hat{v}(x,\omega+V)|_{x=x_l}.$$

Inserting its inverse Laplace transformation yields

$$\begin{aligned}
(i\partial_t + \partial_x^2)v &= V(x,t)v, \quad (x,t) \in \Omega \times \mathbb{R}^+,\\
\partial_{\mathbf{n}}v(x,t) &= \mathcal{L}^{-1}(-\sqrt[+]{-i\cdot+V_{l,r}}\,\hat{v}(x,\cdot))(t)\\
&= \int_0^t f(t-\tau)v(x,\tau)\,d\tau, \quad x = x_{l,r},\ t > 0,\\
v(x,0) &= u^I(x), \quad x \in \Omega,
\end{aligned} \tag{1.25}$$

where $\mathcal{L}(f)(\omega) = F(\omega) = -\sqrt[+]{-i\omega+V_{l,r}}$.

Remark

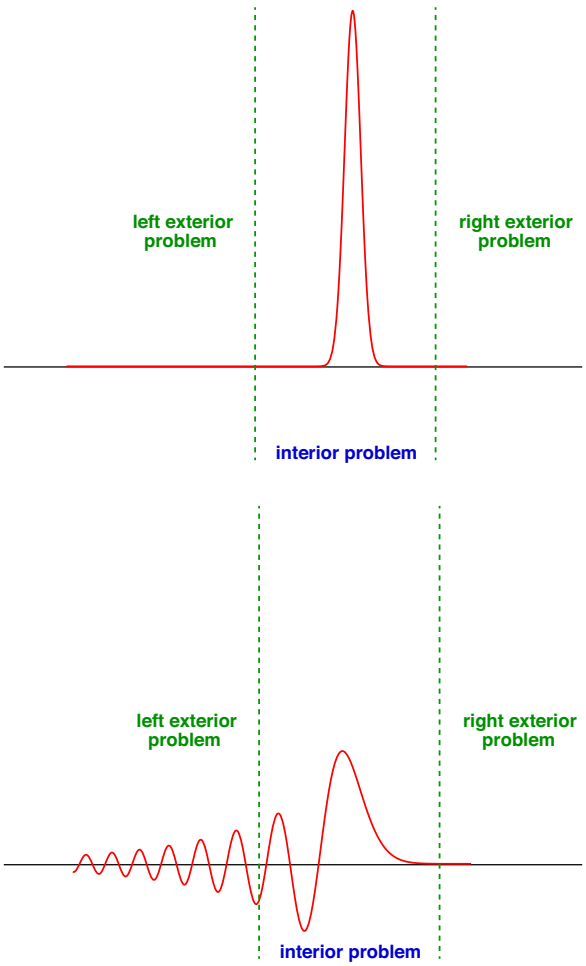
(Time-dependent exterior potential). Consider the Schrödinger equation with exterior potentials that only depend on time, i.e., $V(x,t)|_{\Omega_{l,r}} = V_{l,r}(t)$. The following gauge change in the linear Schrödinger equation with potential for the unknown u then reduces this case to zero exterior potential for unknown ψ:

$$\psi_{l,r} = e^{i\nu_{l,r}(t)}u_{l,r}, \quad \text{with } \nu_{l,r} = \int_0^t V_{l,r}(s)ds,\ \forall t > 0.$$

The resulting TBC is then given by

$$\partial_{\mathbf{n}}u + e^{-i(\pi/4-V_{l,r}(t))}\partial_t^{1/2}(e^{-iV_{l,r}(t))}u) = 0, \quad x = x_{l,r}.$$

We now would like to deal with the Airy equation (2.16). Even if the idea of the derivation is similar, we have to take care about the type of sollution. Indeed, as we can see on the following figures, the behaviour of the solution implies that the boundary conditions at left and right boundaries are different



We have two exterior and one interior problems. They are respectively given by

$$\begin{cases} (\partial_t + \partial_x^3)u = 0, & x < x_\ell,\ t > 0, \\ u(x,0) = 0, & x < x_\ell, \\ u(x_\ell, t) = v(x_\ell, t), & t > 0, \\ \partial_x u(x_\ell, t) = \partial_x v(x_\ell, t), & t > 0, \\ \partial_x^2 u(x_\ell, t) = \partial_x^2 v(x_\ell, t), & t > 0, \\ u \to 0, & x \to -\infty, \end{cases}$$

$$\begin{cases} (\partial_t + \partial_x^3)v = 0, & x \in [x_\ell, x_r],\ t > 0, \\ v(x,0) = v_0(x), & x \in [x_\ell, x_r], \\ v(x_\ell, t) = u(x_\ell, t),\ v(x_r, t) = w(x_r, t), & t > 0, \\ \partial_x v(x_\ell, t) = \partial_x u(x_\ell, t),\ \partial_x v(x_r, t) = \partial_x w(x_r, t), & t > 0, \\ \partial_x^2 v(x_\ell, t) = \partial_x^2 u(x_\ell, t),\ \partial_x^2 v(x_r, t) = \partial_x^2 w(x_r, t), & t > 0, \end{cases}$$

and

$$\begin{cases} (\partial_t + \partial_x^3)w = 0, & x > x_r,\ t > 0, \\ w(x,0) = 0, & x < x_r, \\ w(x_r,t) = v(x_r,t), & t > 0, \\ \partial_x w(x_r,t) = \partial_x v(x_r,t), & t > 0, \\ \partial_x^2 w(x_r,t) = \partial_x^2 v(x_r,t), & t > 0, \\ w \to 0, & x \to \infty, \end{cases}$$

Let us begin by applying the Laplace transform w.r.t time to the exterior Airy equation for w. This gives

$$\partial_t w + \partial_x^3 w = 0 \quad \longrightarrow \quad \omega\hat{w} + \partial_x^3 \hat{w} = 0.$$

The solutions are given by

$$\hat{w}(x,\omega) = A(\omega)e^{\lambda_1(\omega)x} + B(\omega)e^{\lambda_2(\omega)x} + C(\omega)e^{\lambda_3(\omega)x}$$

with

$$\lambda_1(\omega) = -\sqrt[3]{\omega}, \quad \lambda_2(\omega) = j\lambda_1, \quad \lambda_3(\omega) = j^2\lambda_1,$$

with $j = e^{2i\pi/3}$. We recall that

$$\sqrt[3]{\omega} = e^{\frac{1}{3}\ln(\sqrt{\sigma^2+\omega^2})}e^{i\frac{\mathrm{Arg}(\omega)}{3}}$$

Since $\mathrm{Re}(\omega) > 0$, we have $-\pi/6 < \mathrm{Arg}(\sqrt[3]{\omega}) \leq \pi/6$ and

$$\mathrm{Arg}(\lambda_1) \in]-\pi, -5\pi/6[\cup]5\pi/6, \pi[.$$

Multiplying by j or j^2 makes a rotation of angle $\pm 2\pi/3$ and we therefore have the inequalities $\mathrm{Re}\,\lambda_1(\omega) < 0$, $\mathrm{Re}\,\lambda_2(\omega) > 0$, $\mathrm{Re}\,\lambda_3(\omega) > 0$.

One has to determine the variables A, B and C. Since one asks $w \to 0$ as $x \to \infty$, we have to select $B = C = 0$ and $w(x,\omega) = A(\omega)e^{\lambda_1(\omega)x}$. We use the continuity relation $w(x_r,t) = v(x_r,t)$ to get

$$w(x,\omega) = \mathscr{L}\{v(x_r,\cdot)\}(\omega)e^{\lambda_1(x-x_r)}.$$

In order to satisfy the continuity of the first and second order derivatives, two relations are remaining: $\partial_x w(x_r,t) = \partial_x v(x_r,t)$ and $\partial_x^2 w(x_r,t) = \partial_x^2 v(x_r,t)$. But

$$\partial_x \hat{w}(x,\omega) = \lambda_1 \mathscr{L}\{v(x_r,\cdot)\}(\omega)e^{\lambda_1(x-x_r)}$$

and

$$\partial_x^2 \hat{w}(x,\omega) = \lambda_1^2 \mathscr{L}\{v(x_r,\cdot)\}(\omega)e^{\lambda_1(x-x_r)}.$$

This implies

$$\begin{aligned} \partial_x \mathscr{L}\{v(x_r,\cdot)\}(\omega) &= \lambda_1 \mathscr{L}\{v(x_r,\cdot)\}(\omega), \\ \partial_x^2 \mathscr{L}\{v(x_r,\cdot)\}(\omega) &= \lambda_1^2 \mathscr{L}\{v(x_r,\cdot)\}(\omega). \end{aligned}$$

Since we have $\hat{v} = \partial_x \hat{v}/\lambda_1$ and $\hat{v} = \partial_x \hat{v}/\lambda_1^2$, we replace the first relation by the following which is equivalent

$$\partial_x \hat{v} = \frac{\partial_x^2 \hat{v}}{\lambda_1}, \quad x = x_r.$$

Applying the inverse Laplace transform, we obtain

$$v(x_r,t) - I_t^{2/3}\partial_x^2 v(x_r,t) = 0,$$
$$\partial_x v(x_r,t) + I_t^{1/3}\partial_x^2 v(x_r,t) = 0,$$

where $I_t^{(\alpha)}$ is the fractional integral operator or order α defined by

$$I_t^{(\alpha)}(h) = \frac{1}{\Gamma(\alpha)}\int_0^t (t-s)^{\alpha-1}h(s)\,ds, \quad t \geq 0,\ \alpha > 0. \tag{1.26}$$

The boundary condition for $x = x_\ell$ remains to be determined. We proceed as before. This time, one has

$$\hat{u}(x,\omega) = B(\omega)e^{\lambda_2(\omega)x} + C(\omega)e^{\lambda_3(\omega)x}.$$

We need two relations to determine B and C. We have

$$\partial_x\hat{u}(x,\omega) = \lambda_2 B e^{\lambda_2 x} + \lambda_3 C e^{\lambda_3 x}.$$

Using these two relations at point $x = x_\ell$ and the continuity relation at interface, we get

$$\hat{v}(x_\ell,\omega) = Be^{\lambda_2 x_\ell} + Ce^{\lambda_3 x_\ell}$$

and

$$\partial_x\hat{v}(x_\ell,\omega) = \lambda_2 Be^{\lambda_2 x_\ell} + \lambda_3 Ce^{\lambda_3 x_\ell}.$$

After computation we find

$$B = \frac{\lambda_3\hat{v} - \partial_x\hat{v}}{\lambda_3 - \lambda_2}e^{-\lambda_2 x_\ell} = \beta e^{-\lambda_2 x_\ell}, \quad C = \frac{\partial_x\hat{v} - \lambda_2\hat{v}}{\lambda_3 - \lambda_2}e^{-\lambda_3 x_\ell} = \gamma e^{-\lambda_3 x_\ell}.$$

We therefore have

$$\hat{u}(x,\omega) = \beta e^{\lambda_2(x-x\ell)} + \gamma e^{\lambda_3(x-x\ell)},$$
$$\partial_x\hat{u}(x,\omega) = \lambda_2\beta e^{\lambda_2(x-x\ell)} + \lambda_3\gamma e^{\lambda_3(x-x\ell)}.$$

We can now use the last relation concerning the continuity of the second order derivative to find the resulting boundary condition. We have

$$\partial_x^2\hat{v}(x_\ell,\omega) = \partial_x^2\hat{w}(x_\ell,\omega) = \lambda^2\beta + \lambda^3\gamma = (\lambda_2+\lambda_3)\partial_x\hat{v} - \lambda_2\lambda_3\hat{v}.$$

But $\lambda_1 + \lambda_2 + \lambda_3 = 0$ since $1 + j + j^2 = 0$ and $\lambda_2\lambda_3 = j^3\lambda_1^2$. Therefore, we have

$$\hat{v}(x_\ell,\omega) + \frac{1}{\lambda_1}\partial_X\hat{v}(x_\ell,\omega) + \frac{1}{\lambda_1^2}\partial_x^2\hat{v}(x_\ell,\omega) = 0.$$

Applying the inverse Laplace transform, we obtain

$$v(x_\ell,t) - I_t^{1/3}\partial_x v(x_\ell,t) + I_t^{2/3}\partial_x^2 v(x_\ell,t) = 0.$$

The computation of the solution to the initial Airy equation is replaced by

$$(A_{\text{app}}) \quad \begin{cases} u_t + u_{xxx} = 0, & (x,t) \in [x_\ell, x_r]\times(0,T) \\ u - I_t^{1/3}u_x + I_t^{2/3}u_{xx} = 0, & x = x_\ell,\ t > 0, \\ u - I_t^{2/3}u_{xx} = 0, & x = x_r,\ t > 0, \\ u_x + I_t^{1/3}u_{xx} = 0, & x = x_r,\ t > 0, \\ u(x,0) = u_0(x), & x \in [x_\ell, x_r] \end{cases}$$

We can also propose an other derivation of the TBCs for the Airy equation

$$\partial_t u + \partial_x^3 u = 0.$$

If we set $v = \partial_x u$ and $w = \partial_x v = \partial_x^2 u$, then

$$\partial_x w = \partial_x^3 u = -\partial_t u.$$

The Airy equation then can also be written

$$\partial_x \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -\partial_t & 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix}. \tag{1.27}$$

Applying the Laplace transform leads to

$$\partial_x \begin{pmatrix} \hat{u} \\ \hat{v} \\ \hat{w} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -\omega & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{u} \\ \hat{v} \\ \hat{w} \end{pmatrix}. \tag{1.28}$$

Let $\hat{U} = \begin{pmatrix} \hat{u} \\ \hat{v} \\ \hat{w} \end{pmatrix}$ and $A_0 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -\omega & 0 & 0 \end{pmatrix}$. We obtain

$$\partial_x \hat{U} = A_0 \hat{U}.$$

The eigenvalues of A_0 are given by the roots of the characteristic polynomial $\lambda^3 + \omega = 0$. We get

$$\lambda_k = -j^{k-1}\omega^{1/3}, \quad j = e^{2i\pi/3}, \quad k = 1, 2, 3,$$

with

$$\mathrm{Re}(\lambda_1) < 0, \quad \mathrm{Re}(\lambda_2) > 0 \quad \mathrm{Re}(\lambda_3) > 0.$$

The associated eigenvectors are given by $X_k = \begin{pmatrix} 1 \\ \lambda_k \\ \lambda_k^2 \end{pmatrix}$, and the change of basis matrix is

$$P_0 = \begin{pmatrix} 1 & 1 & 1 \\ \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_1^2 & \lambda_2^2 & \lambda_3^2 \end{pmatrix}.$$

We thus obtain

$$A_0 = P_0\, D_0\, P_0^{-1}, \quad D_0 = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

and the differential system becomes

$$\partial_x \hat{U} = P_0\, D_0\, P_0^{-1} \hat{U}.$$

Let $\bar{U} = P_0^{-1}\hat{U} = \begin{pmatrix} \bar{u} \\ \bar{v} \\ \bar{w} \end{pmatrix}$ which leads to $\partial_x \bar{U} = D_0 \bar{U}$. This system can be easyly integrated and we find

$$\begin{aligned} \bar{u}(\omega, x) &= A\, e^{\lambda_1 x}, \\ \bar{v}(\omega, x) &= B\, e^{\lambda_2 x}, \\ \bar{w}(\omega, x) &= C\, e^{\lambda_3 x}. \end{aligned}$$

Thus,

$$\hat{U} = \begin{pmatrix} A\, e^{\lambda_1 x} + B\, e^{\lambda_2 x} + C\, e^{\lambda_3 x} \\ \lambda_1 A\, e^{\lambda_1 x} + \lambda_2 B\, e^{\lambda_2 x} + \lambda_3 C\, e^{\lambda_3 x} \\ \lambda_1^2 A\, e^{\lambda_1 x} + \lambda_2^2 B\, e^{\lambda_2 x} + \lambda_3^2 C\, e^{\lambda_3 x} \end{pmatrix}.$$

Behavior when $x \to +\infty$ It is clear that

$$\lim_{x \to +\infty} e^{\lambda_1 x} = 0 \quad \text{et} \quad \lim_{x \to +\infty} e^{\lambda_{2,3} x} = \infty.$$

The fields B and C must be cancelled. We ask to $\hat{U}$ to belong to the eigenspace E_1 associated to the eigenvalue λ_1. For this, we ask

$$\hat{U} \wedge X_1 = 0.$$

which gives

$$\begin{aligned} \lambda_1^2 \partial_x \hat{u} - \lambda_1 \partial_x^2 \hat{u} &= 0 \\ \partial_x^2 \hat{u} - \lambda_1^2 \hat{u} &= 0 \\ \lambda_1 \hat{u} - \partial_x \hat{u} &= 0. \end{aligned}$$

Only two of these relations are useful. Usign the fact that $\partial_x \hat{u} = \hat{v}$ and $\partial_x^2 \hat{u} = \hat{w}$, $\hat{u}$ must satisfty two right boundary conditions

$$\begin{aligned} \partial_x^2 \hat{u} &= \lambda_1^2 \hat{u}, \\ \partial_x \hat{u} &= \lambda_1 \hat{u}. \end{aligned} \tag{1.29}$$

Behavior when $x \to -\infty$ This time, we have

$$\lim_{x \to -\infty} e^{\lambda_1 x} = \infty \quad \text{et} \quad \lim_{x \to -\infty} e^{\lambda_{2,3} x} = 0.$$

We would like to avoid the A field. We aks to $\hat{U}$ to belong to $E_2 \cup E_3$. An orthogonal vector to $E_2 \cup E_3$ is given by $X_2 \wedge X_3$. If we would like to belong to $E_2 \cup E_3$, we have to be orthogonal to $X_2 \wedge X_3$, which is equivalent to

$$\begin{pmatrix} \hat{u} \\ \hat{v} \\ \hat{w} \end{pmatrix} \cdot (X_2 \wedge X_3) = 0.$$

This is translated to the relation

$$\lambda_2 \lambda_3 \hat{u} - (\lambda_2 + \lambda_3) \partial_x \hat{u} + \partial_x^2 \hat{u} = 0.$$

But, $\lambda_2 \lambda_3 = \lambda_1^2$ and $\lambda_2 + \lambda_3 = -\lambda_1$, the equation becomes

$$\partial_x^2 \hat{u} + \lambda_1 \partial_x \hat{u} + \lambda_1^2 \hat{u} = 0. \tag{1.30}$$

We therefore recover the previous absorbing boundary conditions.

Stability properties We focus here on the Schrödinger equation. Equivalent relations can be estalished for the Airy equation. Stability properties that we can hope to obtain with boundary conditions are based on the following lemma. In this lemma, we see that the symmetry of operators plays a crucial role, as evidenced by the proof.

Lemma 1.1 *Let $\varphi \in H^{1/4}(0,T)$ and $\psi \in L^2(0,T)$ two functions extended by zero for times $s > T$. We have the following properties*

$$\Re\left(e^{i\pi/4}\int_0^{+\infty} \overline{\varphi}\ \partial_t^{1/2}\varphi\, dt\right) \geq 0, \tag{1.31}$$

and

$$\Re\left(\int_0^{+\infty} \overline{\psi}\, I_t\, \psi\, dt\right) = 0. \tag{1.32}$$

The proof of this lemma is based on the Plancherel identity for the Laplace transform

Lemma 1.2 *Let f and g two functions with their respective Laplace transform F and G. We have*

$$\int_0^{+\infty} f(x)\,\overline{g(x)}\,dx = \frac{1}{2i\pi}\int_{-i\infty}^{+i\infty} F(v)\,\overline{G(v)}\,dv = \frac{1}{2\pi}\int_{-\infty}^{+\infty} F(iv)\,\overline{G(iv)}\,dv. \tag{1.33}$$

Proof

We apply the Plancerel's indentity for the Laplace transform to φ and $\partial_t^{1/2}\varphi$ using $\mathscr{L}(\partial_t^{1/2}u)(\omega) = \sqrt{\omega}\,\mathscr{L}(u)(\omega)$. On a

$$\begin{aligned}
\int_0^{+\infty} \overline{\varphi(s)}\,\partial_s^{1/2}\varphi(s)\,ds &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \overline{\mathscr{L}(\varphi)(iv)}\,\mathscr{L}(\partial_s^{1/2}\varphi)(iv)\,dv \\
&= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \overline{\mathscr{L}(\varphi)}(iv)\,\sqrt{iv}\,\mathscr{L}(\varphi)(iv)\,dv \\
&= \frac{1}{2\pi}\int_0^{+\infty} |\mathscr{L}(\varphi)(iv)|^2\, e^{i\pi/4}\sqrt{v}\,dv + \frac{1}{2\pi}\int_{-\infty}^{0} |\mathscr{L}(\varphi)(iv)|^2\, e^{-i\pi/4}\sqrt{-v}\,dv.
\end{aligned}$$

Therefore, we obtain

$$e^{i\pi/4}\int_0^{+\infty} \overline{\varphi(s)}\,\partial_s^{1/2}\varphi(s)\,ds = \frac{i}{2\pi}\int_0^{+\infty} |\mathscr{L}(\varphi)(iv)|^2\,\sqrt{v}\,dv + \frac{1}{2\pi}\int_{-\infty}^{0} |\mathscr{L}(\varphi)(iv)|^2\,\sqrt{-v}\,dv.$$

But, the two integrals that appear in the r.h.s are both two positive real numbers. The r.h.s is thus the sum of an element from $i\mathbb{R}^+$ and an element from $\mathbb{R}^+$; specifically, it has a positive real part which gives (1.31).

For the second inequality, we have

$$\begin{aligned}
\int_0^{+\infty} \overline{\psi(s)}\, I_s\psi(s)\,ds &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \overline{\mathscr{L}(\psi(iv))}\,\mathscr{L}(I_s\psi)(iv)\,dv \\
&= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \overline{\mathscr{L}(\psi(iv))}\,\frac{\mathscr{L}(\psi)(iv)}{iv}\,dv \\
&= \frac{-i}{2\pi}\int_{-\infty}^{+\infty} |\mathscr{L}(\psi)(iv)|^2\,\frac{1}{v}\,dv.
\end{aligned}$$

The second term is pure imaginary, the equality (1.32) is proved, which finish the proof of lemma 1.1.

□

We now turn to the discussion of the well–posedness of the problem (S_{app}). The existence of a solution to the 1D Schrödinger equation with the TBCs is clear from the used construction. For regular enough initial data, e.g. $u_0 \in H^1(x_\ell, x_r)$, the whole–space solution $u(x,t)$ will satisfy the TBCs at least in a weak sense. It remains to check the uniqueness of the solution, i.e. whether the TBC gives rise to spurious solutions. We would like to prove uniform boundedness of $\|u(\cdot,t)\|_{L^2(x_\ell,x_r)}$. We multiply the Schrödinger equation $iu_t + u_{xx} = 0$ by $\overline{u}$:

$$\overline{u}u_t = i\overline{u}u_{xx}, \quad x_\ell < x < x_r,\ t > 0.$$

Integrating by parts on $x_\ell < x < x_r$, and taking the real part gives

$$\begin{aligned}
\partial_t \int_{x_\ell}^{x_r} |u(x,t)|^2\, dx &= = \mathrm{Re}\{\, i\overline{u}(x,t)u_x(x,t)|_{x=x_\ell}^{x=x_r}\,, \\
&= -\sqrt{\frac{2}{\pi}}\mathrm{Re}\left\{ e^{i\pi/4}\overline{u}(x_r,t)\frac{d}{dt}\int_0^t \frac{u(x_r,s)}{\sqrt{t-s}}\, ds \right\} \\
&\quad -\sqrt{\frac{2}{\pi}}\mathrm{Re}\left\{ e^{i\pi/4}\overline{u}(x_\ell,t)\frac{d}{dt}\int_0^t \frac{u(x_\ell,s)}{\sqrt{t-s}}\, ds \right\}.
\end{aligned}$$

Now integrating in time and applying Lemma (1.1) yields the estimate

$$\|u(\cdot,t)\|_{L^2(x_\ell,x_r)} \le \|u_0(\cdot,t)\|_{L^2(x_\ell,x_r)}, \quad t > 0. \tag{1.34}$$

This implies uniqueness of the solution to the Schrödinger IBVP. Equation (1.34) reflects the fact that some of the initial mass or particle density $n(x,t) = |u(x,t)|^2$ leaves the computational domain $[x_\ell, x_r]$ during the evolution. In the whole–space problem, $\|u(t)\|_{L^2(\mathbb{R})}$ is of course conserved.

2 Numerical approximations of TBC

2.1 Approximation of linear Schrödinger equation and linear KdV models, usual schemes

Let us denote by $(t_n)_{0\le n\le N}$ a uniform subdivision of the time interval $[0,T]$ given by $t_n = n\Delta t$ with the temporal step size $\Delta t = T/N$:

$$0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = T.$$

We also define $(x_j)_{0\le j\le J}$ a uniform subdivision of $[a,b]$ given by $x_j = a + j\Delta x$ with the spatial step size $\Delta x = (b-a)/J$:

$$a = x_0 < x_1 < \cdots < x_{J-1} < x_J = b.$$

We consider the problem (1.21) discretized uniformly in time with the step size Δt by an A-stable multi-step method, and denote by u^n the approximation to $u(x, n\Delta t)$:

$$\frac{i}{\Delta t}\sum_{j=0}^{K} \alpha_j u^{n-j} = \sum_{j=0}^{K} \beta_j \left(-\partial_x^2\right) u^{n-j}, \quad n \ge K. \tag{2.1}$$

For example, the usual Crank-Nicolson scheme and the implicit Euler scheme are defined for $k = 1$ and $(\alpha_0, \alpha_1, \beta_0, \beta_1) = (1, -1, 1/2, 1/2)$ and $(\alpha_0, \alpha_1, \beta_0, \beta_1) = (1, -1, 1, 0)$ respectively.

Example

The *trapezoidal rule* discretization is given by

$$\begin{aligned} & i\frac{u^{n+1}-u^n}{\Delta t} = -\partial_x^2 \frac{u^{n+1}+u^n}{2}, \quad x \in \mathbb{R}, \forall n \in \mathbb{N}_0, \\ & \lim_{|x|\to\infty} u^n(x) = 0, \quad \forall n \in \mathbb{N}_0, \\ & u^0 = u^I(x) \quad \text{given for } x \in \mathbb{R}. \end{aligned} \tag{2.2}$$

This method is also known as the Crank-Nicolson scheme. For the Airy equation, we can also consider the usual Crank-Nicolson scheme.

We recall below what is an A-stable method. This notion is related to the numerical computation of solutions to ordinary differential equation. We consider the ODE $y'(t) = ky(t)$ with $k \in \mathbb{C}$. The solution is given by $y(t) = Ce^{kt}$ and $\lim_{t\to\infty} y(t) = 0$ if $\mathrm{Re}(k) < 0$. On the numerical side, the solution could be written $y^{n+1} = \phi(k\Delta t)y^n$ or again $y^n = (\phi(k\Delta t))^n y^0$. The function ϕ is called stability function and the condition $\lim_{n\to\infty} y^n = 0$ is

$$|\phi(k\Delta t)| < 1.$$

Thus, we say that the numerical method with stability function ϕ is A-stable if

$$S := \{z \in \mathbb{C} |\, |\phi(z)| < 1\} \supset \mathbb{C}^- := \{z \in \mathbb{C} | \mathrm{Re}(z) < 0\}.$$

An other definition could be to show that

$$\begin{array}{rccl} \phi: & \mathbb{C}^- & \to & B(0,1) = \{z \in \mathbb{C},\ |z| < 1\} \\ & z & \mapsto & \phi(z). \end{array}$$

The standard Euler scheme is not A-stable. The Crank-Nicolson satisfies the previous relation and is therefore A-stable. Indeed, we have $y^{n+1} = \phi(k\Delta t)y^n$ with

$$\phi(z) = \frac{1+z/2}{1-z/2}.$$

Thus, in order to have $|\phi(z)| \leq 1$, we must have $\mathrm{Re}(z) < 0$ and we get $S = \mathbb{C}^-$.

Usually, the function ϕ can be writtent as an homography

$$\begin{array}{rccl} f: & \mathbb{C}\backslash\{-d/c\} & \to & \mathbb{C} \\ & z & \mapsto & \dfrac{az+b}{cz+d}, \quad ad-bc \neq 0 \end{array}$$

An homography could be seen as the composition of translation, homothetic transformation and inversion. Therefore, an homography transform a complex circle of a complex line in a complex circle of a complex line. Since ϕ is an homography, its inverse is also an homography given by

$$\phi^{-1}(z) = \frac{dz-b}{a-cz}.$$

We can show that $\phi^{-1}(z) = \delta(z)$ where

$$\delta(z) = \left(\sum_{j=0}^{K} \alpha_j z^{K-j}\right) \Big/ \left(\sum_{j=0}^{K} \beta_j z^{K-j}\right)$$

is the *generating function of the time integration scheme*. Therefore, we have

$$\delta \ : \ B(0,1) \longrightarrow \mathbb{C}^{-}.$$

Since ϕ and δ are homographies (map circle or line to cirle or line), we have

$$\delta \ : \ \{z \in \mathbb{C}, \ |z| > 1\} \longrightarrow \mathbb{C}^{+}.$$

2.2 Approximation of fractional integral and derivative operators

Analogously to the first step (1) of the procedure to derive the continuous TBC, we split the problem into interior and exterior problems (with respective solutions v^n and w^n). Instead of applying the Laplace transformation w.r.t. t to equation (1.21), we apply a $\mathscr{Z}$-transformation to (2.1). The $\mathscr{Z}$-transformation which is the discrete analogue of the Laplace-transformation.

Definition 2.1 ($\mathscr{Z}$-transformation) *The formal connection between a sequence and a complex function given by the correspondence*

$$\mathscr{Z}\{f_n\} = \hat{f}(z) := \sum_{n=0}^{\infty} f_n \, z^{-n}, \quad z \in \mathbb{C}, \quad |z| > R_{\hat{f}}, \tag{2.3}$$

is called $\mathscr{Z}$-transformation. The function $\hat{f}(z)$ is called $\mathscr{Z}$-transformation of the sequence $\{f_n\}$, $n = 0, 1, \cdots$ and $R_{\hat{f}} \geq 0$ denotes the radius of convergence.

The $\mathscr{Z}$-transformation of a sequence (u^n) is defined by

$$\mathscr{Z}(u^n) = \hat{u}(z) := \sum_{n=0}^{\infty} u^n \, z^{-n}, \quad z \in \mathbb{C}, \quad |z| > R(\mathscr{Z}(u^n)), \tag{2.4}$$

where $R(\mathscr{Z}(u^n))$ is the radius of convergence of the Laurent series $\mathscr{Z}(u^n)$.

The discrete analogue of the Differentiation Theorem for the Laplace transformation is the *shifting theorem*:

Theorem 2.1 (Shifting Theorem) *If the sequence $\{f_n\}$ is exponentially bounded, i.e., there exist $C > 0$ and c_0 such that*

$$|f_n| \leq C \, e^{c_0 n}, \qquad n = 0, 1, \cdots,$$

then the $\mathscr{Z}$-transformation $\hat{f}(z)$ is given by the Laurent series (2.3) *and for the shifted sequence $\{g_n\}$ with $g_n = f_{n+1}$ holds*

$$\mathscr{Z}\{f_{n+1}\} = z\hat{f}(z) - z f_0. \tag{2.5}$$

The initial values enter into the transformation of the shifted sequence. As a useful consequence of the shifting theorem we have:

$$\mathscr{Z}\{f_{n+1} \pm f_n\} = (z \pm 1)\hat{f}(z) - z f_0. \tag{2.6}$$

The discrete convolution $f_n * g_n$ of two sequences $\{f_n\}$, $\{g_n\}$, $n = 0, 1, \cdots$ is defined by $\sum_{k=0}^{n} f_k \, g_{n-k}$. For the $\mathscr{Z}$-transformation of a convolution of two sequences we formulate the following theorem:

Theorem 2.2 (Convolution Theorem) *If $\hat{f}(z) = \mathscr{Z}\{f_n\}$ exists for $|z| > R_{\hat{f}} \geq 0$ and $\hat{g}(z) = \mathscr{Z}\{g_n\}$ for $|z| > R_{\hat{g}} \geq 0$, then there also exists $\mathscr{Z}\{f_n * g_n\}$ for $|z| > \max(R_{\hat{f}}, R_{\hat{g}})$ with*

$$\mathscr{Z}\{f_n * g_n\} = \hat{f}(z)\,\hat{g}(z). \tag{2.7}$$

Note that (2.7) is nothing else but an expression for the Cauchy product of two power series. Finally, we present the *inverse $\mathscr{Z}$-transformation* which is essential for formulating the discrete TBCs in physical space.

Theorem 2.3 (Inverse $\mathscr{Z}$-transformation) *If $\{f_n\}$ is an exponentially bounded sequence and $\hat{f}(z)$ the corresponding $\mathscr{Z}$-transformation then the inverse $\mathscr{Z}$-transformation is given by*

$$f_n = \mathscr{Z}^{-1}\left\{\hat{f}(z)\right\} = \frac{1}{2\pi i}\oint_{\mathcal{C}} \hat{f}(z)\, z^{n-1} dz, \qquad n = 0, 1, \cdots, \tag{2.8}$$

where $\mathcal{C}$ denotes a circle around the origin with sufficiently large radius.

The most important formula is the *inverse $\mathscr{Z}$-transformation of a product*:

$$\mathscr{Z}^{-1}\left\{\hat{f}(z)\,\hat{g}(z)\right\} = f_n * g_n = \sum_{k=0}^{n} f_k\, g_{n-k}. \tag{2.9}$$

The $\mathcal{Z}$-transformation of (2.1) yields the second order ordinary differential equation:

$$\left(\partial_x^2 + i\frac{\delta(z)}{\Delta t} - V_r\right)\hat{w}(z) = 0, \quad x > x_r, \tag{2.10}$$

where

$$\delta(z) = \left(\sum_{j=0}^{K} \alpha_j z^{K-j}\right) \Big/ \left(\sum_{j=0}^{K} \beta_j z^{K-j}\right)$$

is the *generating function of the time integration scheme*. On top of the standard assumption $\mathrm{supp}(u^I) \subset [x_l, x_r]$ we made here the following assumption on the start-up procedure for the multi-step method (2.1):

$$\mathrm{supp}(u^j) \subset [x_l, x_r], \quad 0 \leq j \leq K-1.$$

The *generating function* for the Crank-Nicolson method is $\delta(z) = 2(z-1)/(z+1)$, and for the implicit Euler scheme $\delta(z) = (z-1)/z$.

The semi-discrete TBC is obtained by solving the differential equation (2.10) (Step (3)). Its general solution is:

$$\hat{w}(x, z) = A^+(z) e^{i\sqrt[+]{i\frac{\delta(z)}{\Delta t}}\,x} + A^-(z) e^{-i\sqrt[+]{i\frac{\delta(z)}{\Delta t}}\,x}, \quad x > x_r. \tag{2.11}$$

In order for u^n to lie in $L^2(]x_r, \infty[)$, A^- must vanish. This is due to the fact that δ maps $\{|z| > 1\}$ into the right half-plane $\{\Re(z) > 0\}$ (due to A-stability), and hence

$$\Re\left(-i\sqrt[+]{i\frac{\delta(z)}{\Delta t}}\right) > 0, \quad \forall |z| > 1. \tag{2.12}$$

Differentiating $\hat{w}(x,z)$ w.r.t. x leads to

$$\mathscr{Z}(\partial_x w^n)(z) = i\sqrt[+]{i\frac{\delta(z)}{\Delta t}}\,\mathscr{Z}(w^n)(z), \tag{2.13}$$

at $x = x_r$. An inverse $\mathscr{Z}$-transformation yields an expression for $\partial_x w^n(x_r)$ in terms of $w^k(x_r)$, $0 \le k \le n$. The resulting TBC is a discrete temporal convolution which depends on the generating function δ.

Resuming Example 2.1 we finally obtain for the interior problem

$$\begin{aligned} &i\frac{v^{n+1}-v^n}{\Delta t} = -\partial_x^2\frac{v^{n+1}+v^n}{2}, \quad x\in\Omega, \forall n\in\mathbb{N}_0,\\ &v^0(x) = u^I(x), \quad x\in\Omega,\\ &\partial_{\mathbf{n}} v^{n+1} = \sum_{k=0}^{n+1}\psi_k^{(l,r)} v^{n+1-k}, \quad \text{at } x = x_l, x_r, \end{aligned} \tag{2.14}$$

where the weights $\psi_n^{(l,r)}$ are given by

$$\hat{\psi}(z) = \mathscr{Z}(\psi_n^{(l,r)})(z) = i\sqrt[+]{i\frac{\delta(z)}{\Delta t}}\,.$$

The weights ψ_n can be obtained either analytically or numerically, depending on δ. In case of the trapezoidal rule, we have

$$\delta(z) = 2\frac{z-1}{z+1}.$$

Performing a series expansion of $\hat{\psi}(z)$ for the Crank-Nicolson scheme, we have

$$\hat{\psi}(z) = -e^{i\pi/4}\sqrt{\frac{2}{\Delta t}}\left(1 - z + \frac{1}{2}z^2 - \frac{1}{2}z^3 + \frac{3}{8}z^4 - \frac{3}{8}z^5 + ...\right).$$

Therefore, one gets explicitly the coefficients

$$\begin{aligned} &\psi_k = -e^{-\frac{i\pi}{4}}\sqrt{\frac{2}{\Delta t}}(-1)^k\tilde{\psi}_k, \quad k\in\mathbb{N}_0,\\ &(\tilde{\psi}_0,\,\tilde{\psi}_1,\tilde{\psi}_2,\tilde{\psi}_3,\tilde{\psi}_4,\tilde{\psi}_5,\cdots) = \left(1,1,\frac{1}{2},\frac{1}{2},\frac{1\cdot 3}{2\cdot 4},\frac{1\cdot 3}{2\cdot 4},\cdots\right). \end{aligned} \tag{2.15}$$

We present the derivation of the coefficient for the Airy equation with more details. We perform the computations for the Crank-Nicolson scheme.

We consider the Airy equation

$$\partial_t u + \partial_x^3 u = 0, \tag{2.16}$$

the Crank Nicolson scheme becomes

$$\frac{u^{n+1}-u^n}{\Delta t} + \partial_x^3\left(\frac{u^{n+1}+u^n}{2}\right) = 0, \tag{2.17}$$

where $u^n(x)$ is an approximation of $u(t_n,x)$, $t_n = n\Delta t$. We recall that the $\mathscr{Z}$ transform is a sequence $(f_n)_n$ given by

$$\mathscr{Z}\{f_n\}(z) = \hat{f}(z) = \sum_{k=0}^{\infty} f_k z^{-k}, \quad |z| > R_f.$$

One of the important properties is that $\mathcal{Z}\{f_{n+1}\}(z) = z\mathcal{Z}\{f_n\}(z)$. Then, the $\mathcal{Z}$ transform applied to (2.19) leads to

$$\partial_x^3 \hat{u} + \delta(z)\hat{u} = 0, \quad \delta(z) = \frac{2}{\Delta t}\frac{z-1}{z+1}.$$

The roots of the characteristic equation are $\lambda_k = -(\delta(z))^{1/3} j^{k-1}$, $k = 1, 2, 3$. Following the procedure we have to derive the transparent boundary conditions for (2.16), we deduce the transparent boundary conditions for (2.19)

$$\begin{array}{ll} x \to -\infty & \partial_x^2 \hat{u} + \lambda_1 \partial_x \hat{u} + \lambda^1 \hat{u} = 0, \\ x \to +\infty & \partial_x \hat{u} = \lambda_1 \hat{u}, \\ & \partial_x^2 \hat{u} = \lambda_1^2 \hat{u}. \end{array} \tag{2.18}$$

The challenge is therfore to compute the inverse $\mathcal{Z}$ transform of $\lambda_1^l \hat{u}$, $l = 1, 2$. For this point, we know that

$$\lambda_1 = -(\delta(z))^{1/3} = -\left(\frac{2}{\Delta t}\right)^{1/3}\left(\frac{z-1}{z+1}\right)^{1/3} = -\left(\frac{2}{\Delta t}\right)^{1/3}\left(\frac{1-1/z}{1+1/z}\right)^{1/3}, \quad |z| > 1.$$

Approximation of $\partial_t^{1/3}$ We make a power serie expansion of λ_1. We have

$$\left(1 - \frac{1}{z}\right)^{1/3} = \sum_{k=0}^{\infty} \alpha_k^{(1)} z^{-k}, \quad \alpha_0 = 1, \ \alpha_n^{(1)} = -\frac{1/3 - n + 1}{n}\alpha_{n-1}^{(1)}$$

and

$$\left(1 + \frac{1}{z}\right)^{-1/3} = \sum_{k=0}^{\infty} \beta_k^{(1)} z^{-k}, \quad \beta_0^{(1)} = 1, \ \beta_n^{(1)} = \frac{-1/3 - n + 1}{n}\beta_{n-1}^{(1)}.$$

Then, we deduce

$$\left(\frac{1-1/z}{1+1/z}\right)^{1/3} = \sum_{k=0}^{\infty} \alpha_k^{(1)} z^{-k} \sum_{k=0}^{\infty} \beta_k^{(1)} z^{-k} = \sum_{k=0}^{\infty} a_k^{(1)} z^{-k}.$$

If we consider the boundary condition $\partial_x \hat{u} = \lambda_1 \hat{u}$, we have

$$\mathcal{Z}^{-1}\left(\partial_x \hat{u} = -\left(\frac{2}{\Delta t}\right)^{1/3} \underbrace{\sum_{k=0}^{\infty} a_k^{(1)} z^{-k}}_{\mathcal{Z}\{a_n^{(1)}\}} \underbrace{\hat{u}}_{\mathcal{Z}\{u^n\}}\right)$$

This gives

$$\partial_x u^n = -\left(\frac{2}{\Delta t}\right)^{1/3} \sum_{k=0}^{n} a_k^{(1)} u^{n-k} \Longleftrightarrow \partial_x u = -\partial_t^{1/3} u$$

and

$$\partial_t^{1/3} u(t_n, \cdot) \approx \left(\frac{2}{\Delta t}\right)^{1/3} \sum_{k=0}^{n} a_k^{(1)} u^{n-k}(\cdot).$$

Approximation of $\partial_t^{2/3}$ We make a power serie expansion of λ_1^2. We have

$$\left(1-\frac{1}{z}\right)^{2/3}=\sum_{k=0}^{\infty}\alpha_k^{(2)}z^{-k},\quad \alpha_0=1,\ \alpha_n^{(2)}=-\frac{2/3-n+1}{n}\alpha_{n-1}^{(2)}$$

and

$$\left(1+\frac{1}{z}\right)^{-2/3}=\sum_{k=0}^{\infty}\beta_k^{(2)}z^{-k},\quad \beta_0^{(2)}=1,\ \beta_n^{(2)}=\frac{-2/3-n+1}{n}\beta_{n-1}^{(2)}.$$

Then, we deduce

$$\left(\frac{1-1/z}{1+1/z}\right)^{2/3}=\sum_{k=0}^{\infty}\alpha_k^{(2)}z^{-k}\sum_{k=0}^{\infty}\beta_k^{(2)}z^{-k}=\sum_{k=0}^{\infty}a_k^{(2)}z^{-k}.$$

If we consider the boundary condition $\partial_x^2\hat{u}=\lambda_1^2\hat{u}$, we have

$$\mathcal{Z}^{-1}\left(\partial_x^2\hat{u}=\left(\frac{2}{\Delta t}\right)^{2/3}\underbrace{\sum_{k=0}^{\infty}a_k^{(2)}z^{-k}}_{\mathcal{Z}\{a_n^{(2)}\}}\underbrace{\hat{u}}_{\mathcal{Z}\{u^n\}}\right)$$

This gives

$$\partial_x^2u^n=\left(\frac{2}{\Delta t}\right)^{2/3}\sum_{k=0}^{n}a_k^{(2)}u^{n-k}\Longleftrightarrow\partial_x^2u=\partial_t^{2/3}u$$

and

$$\partial_t^{2/3}u(t_n,\cdot)\approx\left(\frac{2}{\Delta t}\right)^{2/3}\sum_{k=0}^{n}a_k^{(2)}u^{n-k}(\cdot).$$

Approximation de $I_t^{1/3}$ et $I_t^{2/3}$ To build this approximation, it is sufficient to see that $\partial_x^2\hat{u}=\lambda_1^2\hat{u}$ reads also $\hat{u}=\lambda_1^{-2}\partial_x^2\hat{u}$ which leads to $u=I_t^{2/3}\partial_x^2u$. Thereby, we have

$$\begin{aligned}\hat{u}=\lambda_1^{-2}\partial_x^2\hat{u}\ &\longleftrightarrow\ u=I_t^{2/3}\partial_x^2u\\ \hat{u}=\lambda_1^{-1}\partial_x\hat{u}\ &\longleftrightarrow\ u=-I_t^{1/3}\partial_xu.\end{aligned}$$

One make power series expansion of λ_1^{-1} and λ_1^{-2}. We obtain

$$I_t^{1/3}(u(t_n))\approx-\left(\frac{2}{\Delta t}\right)^{-1/3}\sum_{k=0}^{n}b_k^{(1)}u^{n-k}$$

et

$$I_t^{2/3}(u(t_n))\approx\left(\frac{2}{\Delta t}\right)^{-2/3}\sum_{k=0}^{n}b_k^{(2)}u^{n-k}.$$

Conclusion

$$\partial_t^{1/3} u(t_n) = -Op(\lambda_0) u(t_n) \approx \theta \sum_{k=0}^{n} a_k^{(1)} u^{n-k},$$
$$\partial_t^{2/3} u(t_n) = Op(\lambda_0^2) u(t_n) \approx \theta^2 \sum_{k=0}^{n} a_k^{(2)} u^{n-k},$$
$$I_t^{1/3} u(t_n) = -Op(\lambda_0^{-1}) u(t_n) \approx \theta^{-1} \sum_{k=0}^{n} b_k^{(1)} u^{n-k},$$
$$I_t^{2/3} u(t_n) = Op(\lambda_0^{-2}) u(t_n) \approx \theta^{-2} \sum_{k=0}^{n} b_k^{(2)} u^{n-k},$$

with $\theta = (2/\Delta t)^{1/3}$.

2.3 Derivation of TBC from fully discrete numerical scheme

A combination of temporally and spatially discrete TBCs yields fully discrete TBCs for problem (1.21). While one could use here any spatial discretization (that is regular in the exterior domain), we consider here the example of second order finite differences, i.e.,

$$\begin{aligned} & i\frac{u_j^{n+1} - u_j^n}{\Delta t} = -D_x^2 \frac{u_j^{n+1} + u_j^n}{2}, \quad j \in \mathbb{Z}, \quad n \in \mathbb{N}_0, \\ & \lim_{|j|\to\infty} u_j^n = 0, \quad n \in \mathbb{N}_0, \\ & u_j^0 = u^I(j\Delta x), \quad j \in \mathbb{Z}, \end{aligned} \tag{2.19}$$

where D_x^2 denotes the standard second order difference quotient

$$D_x^2 u_j = \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2} \tag{2.20}$$

and $x_j = x_l + j\Delta x$, $j \in \mathbb{Z}$ is a uniform grid. The right artificial boundary is located at $x_J = x_l + J\Delta x = x_r$ and the left boundary at $x_0 = x_l$. Again we apply the $\mathcal{Z}$-transformation (2.4) and obtain, as a discrete analogue of (2.10) in the right exterior domain:

$$\left(D_x^2 + i\frac{\delta(z)}{\Delta t} - V_r \right) \hat{w}_j(z) = 0, \quad j > J. \tag{2.21}$$

This is a *second-order difference equation with constant coefficients* which reads explicitly

$$\hat{w}_{j+1}(z) - 2\left(1 - \frac{\Delta x^2}{2}\left(i\frac{\delta(z)}{\Delta t}\right)\right)\hat{w}_j(z) + \hat{w}_{j-1}(z) = 0, \quad j > J. \tag{2.22}$$

Its general solution takes the form

$$\hat{w}_j(z) = A^+(z)\chi^{j-J}(z) + A^-(z)\chi^{-(j-J)}(z), \quad j \geq J-1, \tag{2.23}$$

where $\chi(z)$ and $\chi(z)^{-1}$ are the roots of the quadratic equation

$$X^2 - 2\left(1 - \frac{\Delta x^2}{2}\left(i\frac{\delta(z)}{\Delta t}\right)\right)X + 1 = 0. \tag{2.24}$$

In order to have decaying solutions $\hat{w}_j(z)$ outside of the computational domain (i.e., for $j \to \infty$) we have to choose the branch of the square root such that $|\chi(z)| > 1$.

Finally we obtain the $\mathscr{Z}$-transformed right discrete TBC:

$$\hat{u}_{J-1}(z) = \chi^{-1}(z)\hat{u}_J(z). \tag{2.25}$$

The transformed boundary kernel $\chi(z)$ is calculated as

$$\chi(z) = 1 - \frac{\Delta x^2}{2}\left(i\frac{\delta(z)}{\Delta t}\right) + \sqrt[+]{\frac{\Delta x^2}{2}\left(i\frac{\delta(z)}{\Delta t}\right)\left(\frac{\Delta x^2}{2}\left(i\frac{\delta(z)}{\Delta t}\right) - 2\right)}. \tag{2.26}$$

The inverse $\mathscr{Z}$-transform of χ then defines the convolution coefficients for the discrete TBCs:

$$(\chi_n) := \mathscr{Z}^{-1}(\chi(z)), \quad n \in \mathbb{N}_0.$$

Since the magnitude of χ_n does not decay as $n \to \infty$ (χ_n behaves like $const \cdot (-1)^n$ for large n), it is more convenient to use a modified formulation of the discrete TBCs. We introduce

$$\hat{s}(z) := \frac{z+1}{z}\hat{\chi}(z), \text{ and } (s_n) = \mathscr{Z}^{-1}\{\hat{s}(z)\}, \tag{2.27}$$

which satisfy

$$s_0 = \chi_0, \quad s_n = \chi_n + \chi_{n-1} = \mathcal{O}\left(n^{-\frac{3}{2}}\right), \quad n \in \mathbb{N}. \tag{2.28}$$

The corresponding Laurent series of $\hat{s}(z)$ converges (and is continuous) for $|z| \geq 1$ because of the decay (2.28).

In physical space the right discrete TBC (written as DtN map) then reads:

$$u_J^n - u_{J-1}^n = -\sum_{k=1}^{n} s_{n-k}u_J^k + u_{J-1}^{n-1}, \quad n \in \mathbb{N}, \tag{2.29}$$

with the explicitly calculated convolution weights:

$$\begin{aligned} s_n &= (-iR)\,\delta_n^0 + (1+iR)\,\delta_n^1 + \gamma\, e^{-in\varphi}\frac{P_n(\mu) - P_{n-2}(\mu)}{2n-1}, \\ \varphi &= \arctan\frac{2}{R}, \quad \mu = \frac{R^2}{\sqrt{R^2\,(R^2+4)}}, \\ R &= \frac{\Delta x^2}{\Delta t} \quad \gamma = i\sqrt[4]{R^2\,(R^2+4)}\, e^{i\varphi/2}. \end{aligned} \tag{2.30}$$

Here P_n denotes the Legendre polynomials ($P_{-1} \equiv P_{-2} \equiv 0$), and δ_n^k is the Kronecker symbol.

In order to formulate the discrete TBC as in (2.25) it is necessary that the discrete initial condition vanishes at the two adjacent (spatial) grid points appearing in (2.25). Here, we chose to formulate the discrete TBC at the boundary of the computational interval and one grid point in the *interior*. Hence we have assumed that the initial condition satisfies

$$u_0^0 = u_1^0 = 0, \quad u_{J-1}^0 = u_J^0 = 0.$$

However, without any change to our subsequent analysis one could also prescribe the discrete TBC at $j = -1$, 0 and at $j = J$, $J+1$, respectively.

3 Derivation of absorbing boundary conditions (ABC) for Schrödinger equation with x-dependent potential, numerical approximations

We recall that if u is solution to

$$\begin{cases} i\partial_t u + \partial_x^2 u + V(t)\, u = 0, & (x,t) \in \mathbb{R} \times \mathbb{R}^+, \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{3.1}$$

then, denoting

$$\mathcal{V}_{\ell,r}(t) = \int_0^t V_{\ell,r}(\varrho)\, d\varrho, \tag{3.2}$$

the TBC associated to (3.1) is given by

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}_{\ell,r}}\, \partial_t^{1/2} \left(e^{-i\mathcal{V}_{\ell,r}} u \right) = 0, \quad \text{on } \Sigma_T \tag{3.3}$$

where $\Sigma_T = \partial\Omega \times [0,T]$. $\partial\Omega$ denotes the boundary of the computational domain. The complementary domains are respectively Ω_ℓ and Ω_r such that $\mathbb{R} = \Omega_l \cup \Omega \cup \Omega_r$.

In order to obtain this result, we introduce the gauge change

$$v(x,t) = e^{-i\mathcal{V}(t)} u(x,t). \tag{3.4}$$

We deduce that

$$i\partial_t u + \partial_x^2 u + V(t)u = \left(i\partial_t v + \partial_x^2 v \right)\, e^{i\mathcal{V}}.$$

Consequently, v is solution to the free Schrödinger equation

$$i\partial_t v + \partial_x^2 v = 0,\ (x,t) \in \Omega_r \times \mathbb{R}^+.$$

Since the TBC for v is

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

we get

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

We would like to extend this kind of results to the more general case $V(x,t)$. In order to make this extension, we assume that the potential are repulsive. The attractive case is not interesting when dealing with TBC. Indeed, is confines the solutions in a "compact" set (not completely true) and usual homgeneous Dirichlet boundary conditions can be used.

Definition 3.1 *We will say that a potential $V : \mathbb{R} \times \mathbb{R}^+$ is repulsive if, inside the computational domain Ω, it satisfies $V_{|\Omega} \in C\left(\mathbb{R}^+, L^\infty(\Omega)\right)$ and if, in the outside domains $\Omega_{\ell,r}$, it satisfies the condition to belong to $C^\infty(\Omega_{\ell,r} \times \mathbb{R}^+)$ and s.t.*

$$x\partial_x V(x,t) > 0, \quad \forall (x,t) \in \Omega_{\ell,r} \times \mathbb{R}^+. \tag{3.5}$$

For example, we will consider the harmonic repulsive potential $V(x) = \beta^2 x^2$.

3.1 (Fourier) Pseudodifferential operators

We consider here the pseudodifferential calculus based on Fourier transform. For a function g belonging to $L^1(\mathbb{R})$, we note $\mathscr{F}(g)$ or $\hat{g}$ its Fourier transform:

$$\hat{g}(\tau) = \frac{1}{2\pi}\int_{\mathbb{R}} g(t)\, e^{-it\tau} dt, \quad \text{for } \tau \in \mathbb{R}.$$

Let τ be the Fourier covariable of t, and ξ the covariable of x. When it is well defined, the inverse Fourier transform of g is given by

$$\mathscr{F}^{-1}(g)(t) = \int_{\mathbb{R}} g(\tau)\, e^{it\tau}\, d\tau \quad \text{for } t \in \mathbb{R},$$

and if g and $\hat{g}$ are integrable, we have the relation $g = \mathscr{F}^{-1}(\hat{g})$.

A pseudodifferential operator w.r.t time $P(x,t,\partial_t)$ is defined by its total symbol $p(x,t,\tau)$ in Fourier space

$$P(x,t,\partial_t)u(x,t) = \mathscr{F}_t^{-1}\Big(p(x,t,\tau)\,\hat{u}(x,\tau)\Big) = \int_{\mathbb{R}} p(x,t,\tau)\,\hat{u}(x,\tau)\, e^{it\tau}\, d\tau, \tag{3.6}$$

where $\mathscr{F}_t$ denotes the partial Fourier transform w.r.t time. We only give below the properties we will use next. Let α be a real number and Ξ an open set of $\mathbb{R}$. Then, the class of symbols $S^\alpha(\Xi\times\Xi)$ denotes the vector space of functions C^∞ $a(x,t,\tau)$ in $\Xi\times\Xi\times\mathbb{R}$ such that for all $K \subseteq \Xi\times\Xi$ and for all indices β, δ, γ, there exists a constant $C_{\beta,\delta,\gamma}(K)$ s.t.

$$|\partial_\tau^\beta \partial_t^\delta \partial_x^\gamma a(x,t,\tau)| \le C_{\beta,\delta,\gamma}(K)(1+|\tau|)^{\alpha-\beta}, \tag{3.7}$$

for all $(x,t) \in K$ and $\tau \in \mathbb{R}$. In the framework of the Schrödinger equation, we will note the class of symbols S^α_S instead of S^α. To a pseudodifferential operator, one associates the notion of derivative thanks to the following definition l'indique la définition suivante.

Definition 3.2 *A function $f(x,t,\tau)$ is said to be* homogeneous of order m *if and only if, for all $\mu > 0$, one has*

$$f(x,t,\mu\tau) = \mu^m\, f(x,t,\tau). \tag{3.8}$$

Them we say that the pseudodifferential operator $P = P(x,t,\partial_t)$ is classic, homogeneous of order M, $M \in \mathbb{Z}/2$, if its total symbol, denoted by $p = \sigma(P)$, admits an asymptotic expansion in homogeneous symbols $\{p_{M-j/2}\}_{j=0}^{+\infty}$ which write

$$p(x,t,\tau) \sim \sum_{j=0}^{+\infty} p_{M-j/2}(x,t,\tau), \tag{3.9}$$

where each function $p_{M-j/2}$ is homogeneous of order $2M-j$, for $j \in \mathbb{N}$. Considering the asymptotic behavior in τ of the definition (3.7) in classes of symbols, the expansion (3.9) also corresponds to an asymptotic expansion in high-frequency in τ. The meaning of the symbol $\sim$ is the following:

$$\forall \widetilde{m} \in \mathbb{N}, \quad p - \sum_{j=0}^{\widetilde{m}} p_{M-j/2} \in S_S^{M-(\widetilde{m}+1)/2}. \tag{3.10}$$

A symbol p satisfying the above property is denoted $p \in S_S^M$ and the associated operator $P = Op(p)$ define by the inverse Fourier transform, $P \in OPS_S^M$. The class $OPS_S^{-\infty}$ corresponds

to the intersection of all classes OPS_S^M for $M \in \mathbb{Z}$. Then, for P and Q two pseudodifferential operator of respective symbols p and q, and $M \in \mathbb{Z}/2$, we will write

$$P = Q \mod OPS_S^M \tag{3.11}$$

or equivalently

$$p = q \mod S_S^M \tag{3.12}$$

if the difference of the symbols satisfies

$$p - q \in S_S^M.$$

One of the keypoint of pseudodifferential calculus is that it allows to manipulate symbols of operators at algebraic level instead operators themselves at functional level, which gives useful calculus rules, for example for the composition of two integro-differential opertors with variables coefficients (i.e. the ones with symbols which are not polynomial w.r.t to τ).

3.2 Examples

Let us consider the case of an operator $A(x,t)$, which consists in the multiplication by a regular function $a(x,t)$. To determine the symbol of A, one writes, using the definition of Fourier transform

$$A\,u(x,t) = a(x,t)\,u(x,t) = a(x,t)\int_{\mathbb{R}} \hat{u}(x,\tau)e^{it\tau}\,d\tau = \int_{\mathbb{R}} a(x,t)\hat{u}(x,\tau)e^{it\tau}\,d\tau,$$

because the function $a(x,t)$ is independent of the Fourier variable τ. Thanks to the definition (3.6), this means that the operator A has symbol $\sigma(A) = a(x,t)$.

For the derivative operator w.r.t to time ∂_t, one has

$$\partial_t u(x,t) = \partial_t \int_{\mathbb{R}} \hat{u}(x,\tau)e^{it\tau}\,d\tau = \int_{\mathbb{R}} \hat{u}(x,\tau)\,\partial_t\left(e^{it\tau}\right)\,d\tau = \int_{\mathbb{R}} \hat{u}(x,\tau)\,i\tau\,e^{it\tau}\,d\tau.$$

The symbol of ∂_t is thus $\sigma(\partial_t) = i\tau$. Dealing with the integration w.r.t time operator, denoted I_t, we have

$$I_t u(x,t) = I_t \int_{\mathbb{R}} \hat{u}(x,\tau)e^{it\tau}\,d\tau = \int_{\mathbb{R}} \hat{u}(x,\tau)I_t\left(e^{it\tau}\right)\,d\tau = \int_{\mathbb{R}} \hat{u}(x,\tau)\frac{1}{i\tau}e^{it\tau}\,d\tau,$$

therefore $\sigma(I_t) = \dfrac{1}{i\tau}$.

In the previous examples, we have met differential or integral operator with integer power. Let us now consider fractional integro-differential operators. For example, we have the fractional integral operator of order $\alpha/2$, $I_t^{\alpha/2}$ defined for $\alpha \in \mathbb{N}$ by the relation

$$I_t^{\alpha/2} f(x,t) = \frac{1}{\Gamma(\alpha/2)}\int_0^t (t-s)^{\alpha/2-1} f(x,s)\,ds \tag{3.13}$$

where Γ denotes the usual special function, and more specifically the half order integral operator

$$I_t^{1/2} f(x,t) = \frac{1}{\sqrt{\pi}}\int_0^t \frac{f(x,s)}{\sqrt{t-s}}\,ds. \tag{3.14}$$

The operator I_t^α has symbol $\left(\frac{1}{i\tau}\right)^{\alpha/2}$. Moreover, the half order fractional derivative operator $\partial_t^{1/2}$ is given by

$$\partial_t^{1/2} f(t) = \frac{1}{\sqrt{\pi}}\,\partial_t \int_0^t \frac{f(s)}{\sqrt{t-s}}\,ds, \tag{3.15}$$

and its symbol is $\sqrt{i\tau}$. Following the previous notations, we have the links

$$Op\left(-i\sqrt{-\tau}\right) = e^{-i\pi/4}\partial_t^{1/2} \quad \text{et} \quad Op\left(\frac{1}{\tau}\right) = iI_t. \tag{3.16}$$

The table 1 presents the symbols of some useful differential and pseudodifferential operators.

Operator	Symbol	Order
∂_t	$i\tau$	1
$\partial_t^{1/2}$	$\sqrt{i\tau} = e^{-i\pi/4}\sqrt{-\tau}$	1/2
$\partial_t^{\alpha/2}$	$(i)^{\alpha/2}\sqrt{\tau}^{\alpha}$	$\alpha/2$

Operator	Symbol	Order
I_t	$\frac{1}{i\tau}$	1
$I_t^{1/2}$	$\frac{1}{\sqrt{i\tau}} = \frac{e^{i\pi/4}}{\sqrt{-\tau}}$	$-1/2$
$I_t^{\alpha/2}$	$\frac{1}{(i\tau)^{\alpha/2}}$	$-\alpha/2$

Table 1: Table of some pseudodifferential operator and their associated symbols.

3.3 Introduction to symbolic calculus

The interest of pseudodifferential operators is to allow to manipulate only associated symbols instead to direct operators. Indeed, every operation on operator such as composition, derivative, multiplication, can be easyly translated to the symbolic level.

Property 3.1 *(Composition) Let A and B two pseudodifferential operators with respective total symbols $\sigma(A)$ and $\sigma(B)$. Then, the composed operator, denoted AB, has the symbol:*

$$\sigma(AB) \sim \sum_{\alpha=0}^{+\infty} \frac{(-i)^\alpha}{\alpha!}\,\partial_\tau^\alpha \sigma(A)\,\partial_t^\alpha \sigma(B). \tag{3.17}$$

Moreover, if A is of order m and B is of order n, their composition AB is of order $m+n$.

As a consequence, when one multiplies a pseudodifferential operator by a regular function $a(x,t)$, the symbol of the new operator is itself multiplied by this function $a(x,t)$:

$$\sigma\Big(a(x,t)P(x,t,\tau)\Big) = a(x,t)\sigma(P). \tag{3.18}$$

Indeed, the multiplication by a function can be seen as the composition of an operator of degree 0 and symbol $a(x,t)$. The order of the new operator is preserved.

The effect of the derivative on a pseudodifferential operator on its symbol is summarized in the next proposition.

Property 3.2 *(Derivative) Let $P(x,t,\partial_t)$ a pseudodifférentiel differential opérateur of symbol $p(x,t,\tau)$ and order m. Then, we have*

$$\begin{aligned} \partial_x P &= Op\left(\partial_x p\right) + P\partial_x, \\ \sigma(\partial_x P) &= \partial_x p + \sigma(P\partial_x). \end{aligned} \tag{3.19}$$

Moreover, for $\alpha \in \mathbb{N}$ and if the derivatives are not zero, $\partial_x^\alpha P$ and $\partial_t^\alpha P$ are of order m, and $\partial_\tau^\alpha P$ is of order $m-\alpha$.

3.4 Construct of ABC at symbolic level

3.4.1 Two strategies

Two strategies are available to compute an artificial boundary condition adapted to the problem

$$\begin{cases} i\partial_t u + \partial_x^2 u + V\, u = 0, \quad (x,t) \in \mathbb{R} \times \mathbb{R}^+, \\ u(x,0) = u_0(x), \quad x \in \mathbb{R}, \end{cases} \tag{3.20}$$

where u_0 is an initial datum with compact support in the computational domain $\Omega :=]x_\ell, x_r[$ and V is a space and time dependent potential.

The more direct method consists in constructing an artificial boundary condition directly on the equation (3.20) of unknown u. An other method follows the approach used when $V = V(t)$. Indeed for a time dependent potential, the change of unknown $v = e^{-i\mathcal{V}}u$ with $\mathcal{V}(t) = \int_0^t V(s)\,ds$ allows to reduve the initial problem to the problem without potential for which the transparent boundary condition is known. We transpose this measure to the case of any potential $V(x,t)$ defining the phase function

$$\mathcal{V}(x,t) = \int_0^t V(x,s)\,ds, \tag{3.21}$$

and the new unknown

$$v(x,t) = e^{-i\mathcal{V}(x,t)}u(x,t), \tag{3.22}$$

where u is the exact solution to (3.20). Writting, $u = e^{i\mathcal{V}}v$, we deduce the relations

$$\begin{aligned} i\partial_t u &= (i\partial_t v - Vv)e^{i\mathcal{V}}, \\ \partial_x u &= (\partial_x v + i\partial_x \mathcal{V} v)e^{i\mathcal{V}}, \\ \partial_x^2 u &= \left(\partial_x^2 v + 2i(\partial_x \mathcal{V})\partial_x v + i(\partial_x^2 \mathcal{V})v - (\partial_x \mathcal{V})^2 v\right) e^{i\mathcal{V}}. \end{aligned}$$

The new unknown v is therefore solution to the Schrödinger equation with variables coefficients

$$i\partial_t v + \partial_x^2 v + f\,\partial_x v + g\,v = 0, \quad x \in \mathbb{R}, t > 0, \tag{3.23}$$

for which the coefficients are the functions of x and t given by

$$f = 2i\partial_x \mathcal{V} \quad \text{et} \quad g = i\partial_x^2 \mathcal{V} - (\partial_x \mathcal{V})^2. \tag{3.24}$$

Thus, we have to seek a boundary condition, exact or approximated, for the unknown v and the equation (3.23). We will come back next to u by making a reverse change of variable $v = e^{-i\mathcal{V}}u$.

We can unify these two strategies by considering the seek for an artificial boundary condition for the following problem

$$\begin{cases} i\partial_t w + \partial_x^2 w + A\partial_x w + Bw = 0, \quad (x,t) \in \Omega_T, \\ w(x,0) = w_0(x), \quad x \in \Omega, \end{cases} \tag{3.25}$$

with, in the case of Gauge change: $w = v = e^{-i\mathcal{V}}u$, $A = f = 2i\partial_x\mathcal{V}$, $B = g = i\partial_x^2\mathcal{V} - (\partial_x\mathcal{V})^2$, and the phase function $\mathcal{V}$ defined by (3.21), and in the case of the direct method: $w = u$, $A = 0$ and $B = V$. In the following, we will study the construct of an ABC for the problem (3.25), without distinguishing the considered strategy.

3.4.2 Asymptotic expansion in homogeneous symbol of the Dirichlet-to-Neumann map

On note $L = L(x,t,\partial_x,\partial_t)$ l'opérateur de Schrödinger associé au système (3.25)

$$L(x,t,\partial_x,\partial_t)w = i\partial_t w + \partial_x^2 w + A\partial_x w + Bw = 0. \tag{3.26}$$

Comme nous cherchons à construire une approximation de l'opérateur DtN sur la frontière, il faut exprimer l'opérateur de trace normale ∂_x (en se plaçant au point x_r) comme une fonction de l'opérateur de trace, au travers d'un opérateur Λ^+ qui fait intervenir des dérivées (fractionnaires) en temps de w, ainsi que l'effet du potentiel et de ses variations en (x,t). Ceci peut être réalisé de manière approchée grâce à une factorisation de type Nirenberg de l'opérateur L

Theorem 3.1 *Soit L l'opérateur de Schrödinger à coefficients variables défini par la relation (3.26). Il existe deux opérateurs pseudodifférentiels classiques inhomogènes $\Lambda^\pm = \Lambda^\pm(x,t,\partial_t) \in OPS_S^{1/2}$, réguliers par rapport à la variable d'espace x, et tels que*

$$L(x,t,\partial_x,\partial_t) = (\partial_x + i\Lambda^-)(\partial_x + i\Lambda^+) + R, \tag{3.27}$$

où R est un opérateur régularisant de $OPS_S^{-\infty}$. De plus, le symbole total $\lambda^\pm = \sigma(\Lambda^\pm)$ de $\Lambda^\pm$ admet un développement asymptotique en symboles homogènes

$$\sigma(\Lambda^\pm) = \lambda^\pm \sim \sum_{j=0}^{+\infty} \lambda^\pm_{1/2-j/2}. \tag{3.28}$$

En l'absence de condition aux limites sur Σ_T, une partie de la solution de $Lw = 0$ est réfléchie à l'intérieur du domaine à la traversée de la frontière Σ. Les opérateurs $\Lambda^\pm$ traduisent cette séparation de l'onde solution entre partie réfléchie et partie transmise. L'opérateur Λ^+ est associé à la partie sortante de la solution. Lorsque R est nul, écrire la relation

$$(\partial_x + i\Lambda^+)w = 0 \tag{3.29}$$

revient ainsi à écrire la condition pour que la solution soit uniquement sortante, qui est donc la condition transparente de ce problème. En toute généralité, on identifie les opérateurs à R près, et la condition (3.29) est la première condition aux limites approchée associée au problème.

Afin d'écrire la condition approchée associée au problème (3.26), il faut identifier l'opérateur pseudodifférentiel Λ^+. Celui-ci est entièrement décrit par son symbole total λ^+, lui-même développable en symboles homogènes $\lambda^+_{1/2-j/2}$, $j \in \mathbb{N}$. En explicitant ce développement asymptotique, on sera capable d'approcher Λ^+ et d'écrire la condition aux limites associée. Pour cela,

on développe le membre de droite de (3.27) en vue d'identifier ces termes avec ceux de (3.26), en fonction de leur ordre de dérivation en espace. On a, d'une part, d'après (3.27)

$$L = (\partial_x + i\Lambda^-)(\partial_x + i\Lambda^+) + R = \partial_x^2 + i\partial_x\Lambda^+ + i\Lambda^-\partial_x - \Lambda^-\Lambda^+ + R,$$

où R est un opérateur régularisant de $OPS_S^{-\infty}$. On utilise la propriété (3.19) pour exprimer $\partial_x\Lambda^+ = Op\left(\partial_x\lambda^+\right) + \Lambda^+\partial_x$. D'où l'équation

$$L = \partial_x^2 + i\left(Op\left(\partial_x\lambda^+\right) + \Lambda^+\partial_x\right) + i\Lambda^-\partial_x - \Lambda^-\Lambda^+ + R.$$

Finalement, en ordonnant les termes selon ∂_x, nous obtenons

$$L = \partial_x^2 + i(\Lambda^- + \Lambda^+)\,\partial_x + i\,Op\left(\partial_x\lambda^+\right) - \Lambda^-\Lambda^+ + R. \tag{3.30}$$

Par ailleurs, d'après (3.26), l'opérateur L est égal à

$$L = \partial_x^2 + A\partial_x + i\partial_t + B. \tag{3.31}$$

L'identification, à un opérateur de $\mathrm{OPS}_S^{-\infty}$ près, et sous la condition haute-fréquence en τ, des opérateurs mis en jeu dans (3.30) et dans (3.31) conduit au système d'opérateurs

$$\begin{cases} i(\Lambda^- + \Lambda^+) = A, \\ iOp\left(\partial_x\lambda^+\right) - \Lambda^-\Lambda^+ = i\partial_t + B. \end{cases} \tag{3.32}$$

Ce système d'équations sur des opérateurs pseudodifférentiels est transcrit en un système d'équations sur les symboles associés. On note $a = \sigma(A)$ et $b = \sigma(B)$ les symboles de A et B respectivement. Comme les opérateurs A et B sont d'ordre 0 en temps, ils coïncident avec leur symbole, donc on peut identifier a et A, b et B. L'opérateur $iOp\left(\partial_x\lambda^+\right)$ a pour symbole $i\partial_x\lambda^+$, l'opérateur $i\partial_t$ a pour symbole $-\tau$. Quant au symbole de la composée $\Lambda^-\Lambda^+$, il est donné par la formule (3.17). On obtient finalement le système suivant

$$i(\lambda^- + \lambda^+) = a, \tag{3.33a}$$

$$i\partial_x\lambda^+ - \sum_{\alpha=0}^{\infty} \frac{(-i)^\alpha}{\alpha!}\,\partial_\tau^\alpha\lambda^-\,\partial_t^\alpha\lambda^+ \sim -\tau + b. \tag{3.33b}$$

L'utilisation du développement asymptotique (3.28) de λ^+ permettra de résoudre le système (3.33) en déterminant les symboles successifs $\lambda^+_{1/2-j/2}$.

3.4.3 Détermination du symbole principal en fonction de la stratégie

C'est une question délicate. Nous ne justifierons pas ici ce choix. Nous utiliserons

1. Méthode directe, et symbole principal $\lambda^+_{1/2} = -\sqrt{-\tau + V}$
2. Changement de jauge $v = e^{-i\mathcal{V}}u$, et symbole principal $\lambda^+_{1/2} = -\sqrt{-\tau}$

3.4.4 Calcul de l'asymptotique en fonction du symbole principal

Considérons tout d'abord la première stratégie, aussi appelée changement de jauge. On a vu que dans ce cas, le symbole principal est donné par $\lambda^+_{1/2} = -\sqrt{-\tau}$, et les coefficients a et b valent $a = 2i\partial_x\mathcal{V}$, $b = i\partial_x^2\mathcal{V} - (\partial_x\mathcal{V})^2$. Pour déterminer le deuxième symbole λ^+_0, on résout l'équation (3.33b) dans laquelle on identifie les termes d'ordre 1/2. On obtient

$$i\partial_x\lambda^+_{1/2} + ia\lambda^+_{1/2} + 2\lambda^+_{1/2}\lambda^+_0 = 0,$$

d'où

$$\lambda^+_0 = -\frac{i}{2}a - \frac{i\partial_x\lambda^+_{1/2}}{2\lambda^+_{1/2}} = \partial_x\mathcal{V}.$$

On poursuit en identifiant les termes d'ordre 0 afin d'accéder à $\lambda^+_{-1/2}$

$$\begin{aligned} 2\lambda^+_{1/2}\lambda^+_{-1/2} &= b - i\partial_x\lambda^+_0 - ia\lambda^+_0 - \lambda^+_0\lambda^+_0 + i\partial_\tau\lambda^+_{1/2}\partial_t\lambda^+_{1/2} \\ &= i\partial_x^2\mathcal{V} - (\partial_x\mathcal{V})^2 - i\partial_x^2\mathcal{V} + 2(\partial_x\mathcal{V})^2 - (\partial_x\mathcal{V})^2, \end{aligned}$$

et donc $\lambda^+_{-1/2} = 0$. Pour finir, les termes d'ordre $-1/2$ donnent accès à λ^+_{-1}.

$$i\partial_x\lambda^+_{-1/2} + ia\lambda^+_{-1/2} + 2\lambda^+_{1/2}\lambda^+_{-1} + 2\lambda^+_0\lambda^+_{-1/2} - i\partial_\tau\lambda^+_{1/2}\partial_t\lambda^+_0 - i\partial_\tau\lambda^+_0\partial_t\lambda^+_{1/2} = 0,$$

d'où

$$\lambda^+_{-1} = \frac{i\partial_\tau\lambda^+_{1/2}\partial_t\lambda^+_0}{2\lambda^+_{1/2}} = \frac{i\partial_x V}{4\tau}.$$

La proposition suivante résume ces résultats.

Property 3.3 *Si le symbole principal est déterminé par le choix $\lambda^+_{1/2} = -\sqrt{-\tau}$ pour $a = 2i\partial_x\mathcal{V}$ et $b = i\partial_x^2\mathcal{V} - (\partial_x\mathcal{V})^2$, alors les trois termes suivants dans le développement asymptotique symbolique de λ^+ sont donnés par*

$$\lambda^+_0 = \partial_x\mathcal{V}, \quad \lambda^+_{-1/2} = 0 \quad \textit{et} \quad \lambda^+_{-1} = \frac{i\partial_x V}{4\tau}. \tag{3.34}$$

Cette situation sera appelée stratégie 1, ou changement de jauge.

On étudie ensuite la deuxième stratégie, appelée méthode directe. Le principe est le même que dans la stratégie de changement de jauge, mais on travaille désormais avec des symboles inhomogènes, ce qui rend plus délicate l'identification des termes d'un ordre fixé. Nous pouvons cependant mener les calculs et obtenons

Property 3.4 *Si le symbole principal est déterminé par $\lambda^+_{1/2} = -\sqrt{-\tau + V}$ pour $a = 0$ et $b = V$, alors les trois termes suivants dans le développement asymptotique de λ^+ sont*

$$\lambda^+_0 = 0, \quad \lambda^+_{-1/2} = 0, \quad \textit{et} \quad \lambda^+_{-1} = \frac{-i}{4}\frac{\partial_x V}{-\tau + V}. \tag{3.35}$$

Cette situation sera appelée stratégie 2, ou méthode directe.

3.5 Interprétation des symboles et choix de la condition

Le développement asymptotique de λ^+ nous donne accès au symbole principal de l'opérateur de Dirichlet-to-Neumann, puis à ses symboles secondaires. Chacun de ces symboles est en fait le symbole principal d'un opérateur qui reste à déterminer. Or pour un symbole $p(x,t,\tau)$ donné, il n'y a pas unicité de l'opérateur $P(x,t,\partial_t)$ dont p est le symbole principal. Il y aura donc plusieurs possibilités pour interpréter l'opérateur associé à chacun des symboles du développement de λ^+.

Considérons pour commencer la première stratégie. Le symbole principal $\lambda^+_{1/2} = -\sqrt{-\tau}$ est naturellement interprété comme $-e^{i\pi/4}\partial_t^{1/2}$. Le symbole $\lambda^+_0 = \partial_x\mathcal{V}$ est celui de l'opérateur de multiplication $\partial_x\mathcal{V}$. Le troisième symbole, $\lambda^+_{-1/2}$, est nul. Enfin, le dernier symbole étudié est

$$\lambda^+_{-1} = \frac{i\partial_x V}{4\tau}.$$

Le symbole $\frac{1}{i\tau}$ est associé à I_t, on peut donc voir λ^+_{-1} comme le symbole principal de l'opérateur A_{-1} défini par

$$A_{-1}v = -\frac{\partial_x V}{4} I_t v.$$

Dans ce cas, λ^+_{-1} est à la fois le symbole principal et le symbole total de A_{-1}. Cependant, avec ce choix, la condition aux limites sur $u = ve^{i\mathcal{V}}$ comporterait un terme de la forme

$$-i\frac{\partial_x V}{4} e^{i\mathcal{V}}\, I_t\left(e^{-i\mathcal{V}}u\right),$$

qui ne correspond pas à un opérateur symétrique car, sauf cas trivial, $\partial_x V$ n'est pas constant. Il faut donc s'arranger pour symétriser le terme $\partial_x V$. Cela n'est possible que si $\partial_x V$, et donc le potentiel V, est un potentiel réel (on verra plus loin que pour la preuve de stabilité, il faudra de plus supposer que le signe de $\partial_x V$ ne dépend pas du temps). Dans ce cas, on sépare $\partial_x V$ en son signe et sa valeur absolue, et on symétrise cette dernière, ce qui s'écrit

$$\partial_x V = \mathrm{sg}(\partial_x V)|\partial_x V| = \mathrm{sg}(\partial_x V)\sqrt{|\partial_x V|}\sqrt{|\partial_x V|}, \tag{3.36}$$

où sg désigne la fonction signe

$$\text{pour } x \in \mathbb{R}, \quad \mathrm{sg}(x) = \begin{cases} 1 & \text{si } x > 0, \\ 0 & \text{si } x = 0, \\ -1 & \text{si } x < 0. \end{cases}$$

On note que l'écriture (3.36) n'est complètement symétrique que si le terme $\mathrm{sg}(\partial_x V)$ est une constante, du moins par rapport au temps (puisque la condition aux limites est écrite en un point $x_{\ell,r}$ fixé). C'est néanmoins une hypothèse qui reste facilement vérifiable pour un potentiel donné, et qui en pratique sera très souvent vérifiée. Finalement, l'écriture symétrique de λ^+_{-1} est

$$\lambda^+_{-1} = \frac{1}{4}\,\mathrm{sg}(\partial_x V)\sqrt{|\partial_x V|}\,\frac{i}{\tau}\,\sqrt{|\partial_x V|},$$

qu'on interprète alors naturellement comme le symbole principal de B_{-1} défini par

$$B_{-1}v = -\frac{1}{4}\,\mathrm{sg}(\partial_x V)\sqrt{|\partial_x V|}\; I_t\left(\sqrt{|\partial_x V|}v\right).$$

En effet, l'opérateur B_{-1}, tout comme A_{-1} a pour symbole principal λ^+_{-1}, comme l'indique la proposition qui suit.

Property 3.5 *Soit $V = V(x,t)$ un potentiel réel. Soient A_{-1} et B_{-1} les opérateurs définis par*

$$A_{-1}w = -\frac{\partial_x V}{4}\, I_t\, w, \tag{3.37}$$

$$B_{-1}w = -\operatorname{sg}(\partial_x V)\frac{\sqrt{|\partial_x V|}}{2}\, I_t\left(\frac{\sqrt{|\partial_x V|}}{2} w\right). \tag{3.38}$$

Alors, les deux opérateurs A_{-1} et B_{-1} ont pour symbole principal λ^+_{-1}. De plus, on a l'approximation

$$A_{-1} = B_{-1} \mod OPS^{-2}_S. \tag{3.39}$$

On peut donc considérer que $Op\left(\lambda^+_{-1}\right) = A_{-1}$, ou que $Op\left(\lambda^+_{-1}\right) = B_{-1} \bmod \mathrm{OPS}^{-2}_S$. Parmi ces deux opérateurs, B_{-1} est symétrique et A_{-1} ne l'est pas. C'est donc B_{-1} qu'on choisira par la suite. L'interprétation de λ^+_{-1} en tant que symbole principal d'un opérateur est finalement

$$Op\left(\lambda^+_{-1}\right) v = -\operatorname{sg}(\partial_{\mathbf{n}} V)\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, I_t\left(\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, v\right), \tag{3.40}$$

bien que cette égalité ne soit vraie qu'à un opérateur d'ordre -2 près. Cet abus d'interprétation est justifié par la proposition 3.5 et la recherche de symétrie, dans l'optique du lemme 1.1.

3.6 Retour aux conditions artificielles

Comme on l'a vu à la suite du théorème 3.1, la condition exacte traduisant le fait que la solution est sortante s'écrit, sur la nouvelle inconnue v

$$\partial_{\mathbf{n}} v + i\Lambda^+ v = 0, \qquad \text{sur } \Sigma_T, \tag{3.41}$$

où le symbole de l'opérateur Λ^+ est développable en symboles homogènes

$$\sigma(\Lambda^+) = \lambda^+ \sim \sum_{j=0}^{+\infty} \lambda^+_{1/2-j/2}.$$

On approche Λ^+ en tronquant le développement asymptotique de λ^+. Si on ne garde que les M premiers termes $(\lambda^+_{1/2-j/2})_{0\le j\le M-1}$, la condition approchée d'ordre M s'écrit

$$\partial_{\mathbf{n}} v_M + i\sum_{j=0}^{M-1} Op\left(\lambda^+_{1/2-j/2}\right) v_M = 0, \quad \text{sur } \Sigma_T,$$

où v_M est alors solution approchée du problème (3.25). On effectue le changement de variable inverse $v = e^{-i\mathcal{V}}u$ pour exprimer la condition approchée sur u_M

$$\partial_{\mathbf{n}} u_M - i(\partial_x \mathcal{V})\, u_M + ie^{i\mathcal{V}} \sum_{j=0}^{M-1} Op\left(\lambda^+_{1/2-j/2}\right)\left(e^{-i\mathcal{V}} u_M\right) = 0, \quad \text{sur } \Sigma_T. \tag{3.42}$$

On adoptera les notations compactes

$$\partial_{\mathbf{n}} u + \Lambda^M_p(x,t,\partial_t)\, u = 0, \quad \text{sur } \Sigma_T, \tag{3.43}$$

où l'indice $p = 1$ (respectivement $p = 2$) fait référence à la stratégie du changement de jauge (respectivement à la stratégie de la méthode directe), et où l'entier M est le nombre de symboles homogènes retenus dans le développement asymptotique de λ^+.

En accord avec l'interprétation des symboles que nous venons de voir pour le changement de jauge, nous avons la proposition suivante

Property 3.6 *La méthode du changement de jauge ($p = 1$) conduit aux conditions artificielles d'ordre M suivantes*

$$\partial_{\mathbf{n}} u + \Lambda_1^M u = 0, \quad \text{sur } \Sigma_T, \tag{3.44}$$

où les opérateurs Λ_1^M sont donnés par

$$\Lambda_1^2(x,t,\partial_t)\, u = e^{-i\pi/4} e^{i\mathcal{V}(x,t)} \partial_t^{1/2} \left(e^{-i\mathcal{V}(x,t)} u \right), \tag{3.45}$$

et

$$\Lambda_1^4(x,t,\partial_t)\, u = \Lambda_1^2(x,t,\partial_t)\, u - i\,\mathrm{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{i\mathcal{V}(x,t)} I_t \left(\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{-i\mathcal{V}(x,t)} u \right). \tag{3.46}$$

Dans la suite, on désigne par ABC_1^M la condition aux limites (3.44)*.*

3.7 L'autre choix : $\mathbf{ABC}_2^M$

Considérons maintenant l'autre choix pour la condition artificielle, reposant sur la méthode directe. Dans ce cas, les symboles sont donnés par la proposition 3.4, et on obtient les conditions artificielles décrites ci-après.

Property 3.7 *La méthode directe $p = 2$ conduit aux conditions artificielles d'ordre M suivantes*

$$\partial_{\mathbf{n}} u + \Lambda_2^M u = 0, \quad \text{sur } \Sigma_T, \tag{3.47}$$

avec

$$\Lambda_2^2(x,t,\partial_t)\, u = Op\left(-i\sqrt{-\tau + V} \right) u, \tag{3.48}$$

et

$$\Lambda_2^4(x,t,\partial_t)\, u = \Lambda_2^2(x,t,\partial_t)\, u + \frac{1}{4} Op\left(\frac{\partial_x V}{-\tau + V} \right) u. \tag{3.49}$$

La condition aux limites (3.47) *sera désignée par ABC_2^M dans la suite.*

3.8 Le cas $V = V(x)$: relations entre les ABC

Le cas $V = V(x)$ est particulier, dans le sens où les deux stratégies étudiées précédemment se rejoignent. Ce résultat repose sur le lemme suivant

Lemma 3.1 *Si a est un symbole de S^m indépendant de t, et $V(x,t) = V(x)$, alors on a l'égalité*

$$Op\left(a(\tau - V(x))\right) u = e^{itV} Op\left(a(\tau)\right) \left(e^{-itV} u(x,t) \right). \tag{3.50}$$

Proof

Par définition, l'opérateur pseudodifférentiel associé au symbole $a(\tau - V(x))$ est donné par transformée de Fourier inverse

$$Op\left(a(\tau - V(x))\right) u = \mathscr{F}_t^{-1}\Big(a(\tau - V(x)) \mathscr{F}_t(u) \Big) = \int_{\mathbb{R}} a(\tau - V(x))\, \mathscr{F}_t(u)(x,\tau) e^{it\tau} d\tau.$$

On effectue dans l'intégrale le changement de variable $\rho = \tau - V(x)$ pour obtenir

$$Op\left(a(\tau - V(x))\right) u = \int_{\mathbb{R}} a(\rho)\, \mathscr{F}_t(u)(x, \rho + V(x))\, e^{it\rho} e^{itV(x)} d\rho.$$

En utilisant les propriétés de translation de la transformée de Fourier, on simplifie cette expression

$$Op\left(a(\tau - V(x))\right) u = e^{itV(x)} \int_{\mathbb{R}} a(\rho)\, \mathscr{F}_t(t \mapsto e^{-itV(x)} u(x,t))(x,\rho)\, e^{it\rho} d\rho.$$

On reconnaît l'opérateur associé au symbole $a(\rho)$ et appliqué à la fonction $e^{-itV(x)}u(x,t)$

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

On a bien montré l'égalité (3.50).

□

Corollary 3.1 *Si le potentiel V est indépendant du temps, alors les conditions aux limites artificielles ABC_1^M et ABC_2^M sont équivalentes, pour $M = 2, 4$, avec $\mathcal{V}$ qui est défini par $\mathcal{V}(x,t) = tV(x)$.*

3.9 Discrétisation des ABC basée sur les convolutions discrètes

Nous pouvons maintenant passer à l'étude de la discrétisation des conditions aux limites. Considérons pour commencer les conditions ABC_1^M. D'après la proposition 3.6, on a :

$$\mathrm{ABC}_1^2 : \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left(e^{-i\mathcal{V}} u\right) = 0, \tag{3.51}$$

$$\mathrm{ABC}_1^4 : \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left(e^{-i\mathcal{V}} u\right) - i\,\mathrm{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{i\mathcal{V}} I_t \left(\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{-i\mathcal{V}} u\right) = 0. \tag{3.52}$$

On considère également les opérateurs associés Λ_1^2 et Λ_1^4

$$\Lambda_1^2(x,t,\partial_t)\, u = e^{-i\pi/4} e^{i\mathcal{V}(x,t)} \partial_t^{1/2} \left(e^{-i\mathcal{V}(x,t)} u\right),$$

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

On utilise la forme symétrique de la condition ABC_1^4, ce qui est crucial dans le cas $V = V(x,t)$.

Les semi-discrétisations des conditions ABC_1^M sont données dans la proposition suivante.

Property 3.8 *Le schéma semi-discret de Crank-Nicolson pour le problème initial avec condition aux limites de type ABC_1^M est donné par*

$$\begin{cases} \dfrac{2i}{\Delta t} v^{n+1} + \partial_x^2 v^{n+1} + W^{n+1}\, v^{n+1} = \dfrac{2i}{\Delta t} u^n, \quad \textit{dans } \Omega, \\ \partial_{\mathbf{n}} v^{n+1} + \Lambda_{1,n+1}^M v^{n+1} = 0, \quad \textit{sur } \Sigma, \quad \textit{pour } M = 2 \textit{ ou } 4, \\ u^0 = u_0, \quad \textit{dans } \Omega, \end{cases} \tag{3.53}$$

pour $n = 0, ..., N-1$, où $v^{n+1} = \frac{u^{n+1}+u^n}{2}$, $W^{n+1} = \frac{V^{n+1}+V^n}{2}$, et les opérateurs semi-discrets $\Lambda_{1,n+1}^2$, $\Lambda_{1,n+1}^4$ sont définis par

$$\Lambda_{1,n+1}^2 v^{n+1} = e^{-i\pi/4} e^{i\mathscr{W}^{n+1}} \sqrt{\frac{2}{\Delta t}} \sum_{k=0}^{n+1} \beta_{n+1-k} e^{-i\mathscr{W}^k} v^k, \tag{3.54}$$

$$\Lambda_{1,n+1}^4 v^{n+1} = \Lambda_{1,n+1}^2 v^{n+1} - i\,\mathrm{sg}(\partial_{\mathbf{n}} W^{n+1}) \frac{\sqrt{|\partial_{\mathbf{n}} W^{n+1}|}}{2} e^{i\mathscr{W}^{n+1}} \frac{\Delta t}{2} \sum_{k=0}^{n+1} \gamma_{n+1-k} \frac{\sqrt{|\partial_{\mathbf{n}} W^k|}}{2} e^{-i\mathscr{W}^k} v^k. \tag{3.55}$$

Ici, $\mathscr{W}$ est défini par $\mathscr{W}^{n+1} = \frac{\mathcal{V}^{n+1}+\mathcal{V}^n}{2}$ et $\mathcal{V}$ est donné par (3.21).

3.10 Approximation des conditions ABC_2^M

Nous avons vu que les conditions ABC_1^M et ABC_2^M sont équivalentes dans le cas de potentiels indépendants du temps. Cela n'est plus vrai pour une fonction V qui dépend du temps. Dans une telle situation, le schéma développé précédemment peut être utilisé pour traiter le cas de ABC_1^M. Quant à ABC_2^M, la discrétisation des opérateurs pseudodifférentiels qui y sont impliqués n'est pas facile à obtenir. En particulier, les opérateurs dont le symbole est en racine carrée ne peuvent pas être exprimés en terme d'opérateurs fractionnaires en temps, car on n'a pas d'analogue au lemme 3.1 dans ce cas. Pour ces raisons, nous introduisons les approximations suivantes.

Lemma 3.2 *Nous avons les deux approximations suivantes :*

$$Op\left(\sqrt{-\tau+V}\right) = \sqrt{i\partial_t+V} \mod OPS_S^{-3/2}, \tag{3.56}$$

et

$$Op\left(\frac{\partial_x V}{4}\frac{1}{-\tau+V}\right) = \mathrm{sg}(\partial_{\mathbf{n}}V)\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}(i\partial_t+V)^{-1}\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2} \mod OPS_S^{-3}. \tag{3.57}$$

En conséquence du lemme 3.2, l'opérateur

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

est approché par

$$\widetilde{\Lambda_2^2}(x,t,\partial_t) = -i\sqrt{i\partial_t+V}, \tag{3.58}$$

et l'opérateur

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

est approché par

$$\widetilde{\Lambda_2^4}(x,t,\partial_t) = \widetilde{\Lambda_2^2}(x,t,\partial_t) + \mathrm{sg}(\partial_{\mathbf{n}}V)\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}(i\partial_t+V)^{-1}\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}, \tag{3.59}$$

les termes additionnels étant négligeables dans les deux cas. Les nouvelles conditions approchées $\widetilde{\mathrm{ABC}_2^M}$ sont finalement données par la proposition suivante.

Property 3.9 *Les conditions aux limites ABC_2^M données par la proposition 3.7 sont approchées par les conditions d'ordre M suivantes :*

$$\partial_{\mathbf{n}}u - i\sqrt{i\partial_t+V}u = 0, \tag{3.60}$$

pour la condition d'ordre deux, notée $\widetilde{ABC_2^2}$, et

$$\partial_{\mathbf{n}}u - i\sqrt{i\partial_t+V}u + \mathrm{sg}(\partial_{\mathbf{n}}V)\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}(i\partial_t+V)^{-1}\left(\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}u\right) = 0, \tag{3.61}$$

pour la condition d'ordre quatre, notée $\widetilde{ABC_2^4}$.

Ces approximations des conditions ABC_2^M faciliteront leur implémentation.

3.10.1 Approximants de Padé

On peut approcher de manière rationnelle la racine carrée grâce une approximation à m termes :

$$R_m(z) = a_0^m + \sum_{k=1}^{m} \frac{a_k^m z}{z + d_k^m} = \sum_{k=0}^{m} a_k^m - \sum_{k=1}^{m} \frac{a_k^m d_k^m}{z + d_k^m}, \tag{3.62}$$

où les coefficients a_k^m et d_k^m sont donnés par $a_0^m = 0$, et pour $1 \leq k \leq m$

$$a_k^m = \frac{1}{m \cos^2\left(\frac{(2k-1)\pi}{4m}\right)}, \quad d_k^m = \tan^2\left(\frac{(2k-1)\pi}{4m}\right). \tag{3.63}$$

Pour éviter la coupure sur la demi-droite $\mathbb{R}^-$, on peut utiliser des coefficients de Padé complexes liés à la technique de rotation de branche d'angle θ. La valeur optimale de θ est $\theta = \pi/4$. Avec la rotation de branche, $\sqrt{z}$ est approché par

$$\sqrt{z} \approx e^{i\theta/2} R_m(e^{-i\theta} z),$$

d'où

$$\sqrt{z} \approx \sum_{k=0}^{m} A_k^m - \sum_{k=1}^{m} \frac{A_k^m D_k^m}{z + D_k^m}$$

avec les nouveaux coefficients $A_0^m = 0$, et pour $1 \leq k \leq m$:

$$A_k^m = e^{i\theta/2} a_k^m = \frac{e^{i\theta/2}}{m \cos^2\left(\frac{(2k-1)\pi}{4m}\right)}, \quad D_k^m = e^{i\theta} d_k^m = e^{i\theta} \tan^2\left(\frac{(2k-1)\pi}{4m}\right). \tag{3.64}$$

3.10.2 Introduction des fonctions auxiliaires pour $\widetilde{ABC_2^M}$ et discrétisation

Commençons par étudier la condition d'ordre deux $\widetilde{\mathrm{ABC}_2^2}$. L'approche alternative aux convolutions discrètes consiste à approcher l'opérateur de racine carrée $i\partial_t + V$ par son approximant de Padé d'ordre m, défini par (3.62), et dont nous retiendrons la deuxième formulation. Rappelons que pour un nombre complexe z, cet approximant $R_m(z)$ est défini par

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

où les coefficients $(a_k^m)_{0 \leq k \leq m}$ et $(d_k^m)_{1 \leq k \leq m}$ sont donnés par (3.63) ou (3.64). Formellement, $\sqrt{i\partial_t + V}$ est alors approché par $R_m(i\partial_t + V)$, ce qui donne en remplaçant dans (3.60)

$$\partial_{\mathbf{n}} u - i \sum_{k=0}^{m} a_k^m \, u + i \sum_{k=1}^{m} a_k^m \, d_k^m (i\partial_t + V + d_k^m)^{-1} \, u = 0, \tag{3.65}$$

qui définit une condition aux limites artificielles d'ordre deux, désignée par $\mathrm{ABC}_{2,m}^2$ dans la suite. Pour réécrire cette condition sous une forme se prêtant à son implémentation numérique, il est classique d'introduire m fonctions auxiliaires φ_k, pour $1 \leq k \leq m$ comme suit :

$$\varphi_k = (i\partial_t + V + d_k^m)^{-1} \, u, \quad 1 \leq k \leq m. \tag{3.66}$$

Cette équation est constituée de deux équations différentielles du premier ordre en temps, portant sur la fonction φ_k, l'une au point x_ℓ et l'autre au point x_r

$$i\partial_t\varphi_k + V\varphi_k + d_k^m\varphi_k = u, \qquad \text{pour } 1 \le k \le m,\ \ x = x_{\ell,r}, \tag{3.67}$$

avec la condition initiale $\varphi_k(x,0) = 0$ en chacun des points $x = x_{\ell,r}$.

Finalement, la discrétisation de la condition aux limites $\mathrm{ABC}^2_{2,m}$ conduit à un système d'une équation et de m équations différentielles couplées, portant sur u et sur les m fonctions auxiliaires φ_k, $1 \le k \le m$

$$\begin{cases} \partial_{\mathbf{n}}u - i\displaystyle\sum_{k=0}^{m} a_k^m u + i\sum_{k=1}^{m} a_k^m\, d_k^m\, \varphi_k = 0, \quad x = x_{\ell,r}, \\ i\partial_t\varphi_k + V\varphi_k + d_k^m\varphi_k = u, \qquad 1 \le k \le m,\ x = x_{\ell,r}, \\ \varphi_k(x,0) = 0, \qquad 1 \le k \le m. \end{cases} \tag{3.68}$$

Considérons à présent la discrétisation du problème associé à cette condition. La discrétisation du système (3.68), en utilisant les fonctions $v^{n+1} = u^{n+1/2}$ et $W^{n+1} = V^{n+1/2}$, est la suivante

$$\begin{cases} \partial_{\mathbf{n}}v^{n+1} - i\displaystyle\sum_{k=0}^{m} a_k^m v^{n+1} + i\sum_{k=1}^{m} a_k^m d_k^m \varphi_k^{n+1/2} = 0, \quad x = x_{\ell,r}, \\ i\,\dfrac{\varphi_k^{n+1} - \varphi_k^n}{\Delta t} + W^{n+1}\varphi_k^{n+1/2} + d_k^m\varphi_k^{n+1/2} = v^{n+1}, \qquad 1 \le k \le m,\ x = x_{\ell,r}, \\ \varphi_k^0(x_{\ell,r}) = 0, \qquad 1 \le k \le m. \end{cases} \tag{3.69}$$

Si le système continu (3.68) couple les variables u et φ_k, dans le système discrétisé (3.69), les variables v^{n+1} et $\varphi_k^{n+1/2}$ peuvent être partiellement découplées. En effet, on peut tirer de la deuxième équation l'expression de $\varphi_k^{n+1/2}$ au point $x_{\ell,r}$ en fonction de φ_k^n et de v^{n+1}

$$\varphi_k^{n+1/2}(x_{\ell,r}) = \frac{1}{\frac{2i}{\Delta t} + W_{\ell,r}^{n+1} + d_k^m}\, v^{n+1}(x_{\ell,r}) + \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W_{\ell,r}^{n+1} + d_k^m}\, \varphi_k^n(x_{\ell,r}), \tag{3.70}$$

pour $1 \le k \le m$. Cette expression de $\varphi_k^{n+1/2}$ est réinjectée dans la première équation, de manière à exprimer $\partial_{\mathbf{n}}v^{n+1}$ en fonction de v^{n+1} et φ_k^n uniquement. On obtient, en $x = x_{\ell,r}$

$$\begin{aligned} \partial_{\mathbf{n}}v^{n+1} - i\left(\sum_{k=0}^{m} a_k^m\right) v^{n+1} + i\sum_{k=1}^{m} a_k^m d_k^m \frac{1}{\frac{2i}{\Delta t} + W^{n+1} + d_k^m}\, v^{n+1} \\ + i\sum_{k=1}^{m} a_k^m d_k^m \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W^{n+1} + d_k^m}\, \varphi_k^n = 0. \end{aligned} \tag{3.71}$$

L'équation (3.71) donne une condition aux limites artificielle locale inhomogène, de type Fourier-Robin, dans laquelle le second membre est actualisé grâce à (3.70).

Voyons à présent ce qu'il en est pour la condition d'ordre quatre donnée par (3.61). De même que pour la condition d'ordre deux, on note $\mathrm{ABC}^4_{2,m}$ la condition résultant de (3.61) après approximation du premier terme par m fonctions de Padé. Il faut ajouter au système (3.70)–(3.71) la discrétisation du terme

$$\mathrm{sg}(\partial_{\mathbf{n}}V)\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}(i\partial_t + V)^{-1}\left(\frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2}\, u\right).$$

Pour cela, on applique à nouveau le principe des fonctions auxiliaires. On introduit la fonction ψ définie par

$$\psi = (i\partial_t + V)^{-1} \left(\frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, u \right). \tag{3.72}$$

Avec cette définition, le terme correctif à ajouter dans la première équation de (3.68) s'écrit

$$\mathrm{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} \psi.$$

Quant à ψ, elle est solution d'une équation différentielle d'ordre un

$$i\partial_t \psi + V\psi = \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, u, \quad x = x_{\ell,r},$$

avec la condition initiale $\psi(x_{\ell,r}, 0) = 0$. Le système associé à $\mathrm{ABC}^4_{2,m}$ est finalement :

$$\begin{cases} \partial_{\mathbf{n}} u - i \sum_{k=0}^{m} a_k^m u + i \sum_{k=1}^{m} a_k^m\, d_k^m\, \varphi_k + \mathrm{sg}(\partial_{\mathbf{n}} V) \dfrac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} \psi = 0, \quad x = x_{\ell,r}, \\ i\partial_t \varphi_k + V\varphi_k + d_k^m \varphi_k = u, \qquad 1 \le k \le m,\ x = x_{\ell,r}, \\ i\partial_t \psi + V\psi = \dfrac{\sqrt{|\partial_{\mathbf{n}} V|}}{2}\, u, \qquad x = x_{\ell,r}, \\ \varphi_k(x_{\ell,r}, 0) = 0, \qquad 1 \le k \le m, \\ \psi(x_{\ell,r}, 0) = 0. \end{cases} \tag{3.73}$$

Pour conclure, étudions la discrétisation du système (3.73) associé à la condition d'ordre quatre. Sa discrétisation naturelle, en accord avec le schéma intérieur, est

$$\begin{cases} \partial_{\mathbf{n}} v^{n+1} - i \sum_{k=0}^{m} a_k^m v^{n+1} + i \sum_{k=1}^{m} a_k^m d_k^m \varphi_k^{n+1/2} + \mathrm{sg}(\partial_{\mathbf{n}} W^{n+1}) \dfrac{\sqrt{|\partial_{\mathbf{n}} W^{n+1}|}}{2} \psi^{n+1/2} = 0, \quad x = x_{\ell,r}, \\ i\, \dfrac{\varphi_k^{n+1} - \varphi_k^n}{\Delta t} + W^{n+1} \varphi_k^{n+1/2} + d_k^m \varphi_k^{n+1/2} = v^{n+1}, \qquad 1 \le k \le m,\ x = x_{\ell,r}, \\ i \dfrac{\psi^{n+1} - \psi^n}{\Delta t} + W^{n+1} \psi^{n+1/2} = \dfrac{\sqrt{|\partial_{\mathbf{n}} W^{n+1}|}}{2}\, v^{n+1}, \quad x = x_{\ell,r}, \\ \varphi_k^0(x_{\ell,r}) = 0, \quad \psi^0(x_{\ell,r}) = 0. \end{cases} \tag{3.74}$$

On découple le système (3.74) en procédant comme pour l'ordre deux. Les deuxième et troisième équations du système (3.74) permettent d'exprimer $\varphi_k^{n+1/2}$ en fonction de v^{n+1} et φ_k^n, d'une part, et $\psi^{n+1/2}$ en fonction de v^{n+1} et ψ^n, d'autre part. On réinjecte ensuite ces expressions dans la première équation afin d'exprimer $\partial_{\mathbf{n}} v^{n+1}$ en fonction de v^{n+1}, φ_k^n et ψ^n uniquement. L'équation de mise à jour de $\varphi_k^{n+1/2}$ est inchangée par rapport à (3.70). Pour les fonctions $\psi^{n+1/2}$, on obtient

$$\psi^{n+1/2}(x_{\ell,r}) = \frac{\sqrt{|\partial_{\mathbf{n}} W_{\ell,r}^{n+1}|}}{2} \frac{1}{\frac{2i}{\Delta t} + W_{\ell,r}^{n+1}}\, v^{n+1}(x_{\ell,r}) + \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W_{\ell,r}^{n+1}}\, \psi^n(x_{\ell,r}). \tag{3.75}$$

Finalement, la première équation de (3.74) devient, en $x = x_{\ell,r}$

$$\partial_{\mathbf{n}} v^{n+1} - i\left(\sum_{k=0}^{m} a_k^m\right) v^{n+1} + i\sum_{k=1}^{m} a_k^m d_k^m \frac{1}{\frac{2i}{\Delta t} + W^{n+1} + d_k^m} v^{n+1} + \frac{\partial_{\mathbf{n}} W^{n+1}}{4} \frac{1}{\frac{2i}{\Delta t} + W^{n+1}}\, v^{n+1}$$
$$+ i\sum_{k=1}^{m} a_k^m d_k^m \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W^{n+1} + d_k^m}\, \varphi_k^n + \mathrm{sg}(\partial_{\mathbf{n}} W^{n+1}) \frac{\sqrt{|\partial_{\mathbf{n}} W^{n+1}|}}{2} \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W^{n+1}} \psi^n = 0, \quad (3.76)$$

et le système complet semi-discrétisé pour $\mathrm{ABC}_{1,m}^4$ est

$$\begin{cases} \partial_{\mathbf{n}} v^{n+1} - i\left(\sum_{k=0}^{m} a_k^m\right) v^{n+1} + i\sum_{k=1}^{m} a_k^m d_k^m \frac{1}{\frac{2i}{\Delta t} + W^{n+1} + d_k^m} v^{n+1} + \frac{\partial_{\mathbf{n}} W^{n+1}}{4} \frac{1}{\frac{2i}{\Delta t} + W^{n+1}}\, v^{n+1} \\ \quad + i\sum_{k=1}^{m} a_k^m d_k^m \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W^{n+1} + d_k^m}\, \varphi_k^n + \mathrm{sg}(\partial_{\mathbf{n}} W^{n+1}) \frac{\sqrt{|\partial_{\mathbf{n}} W^{n+1}|}}{2} \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W^{n+1}} \psi^n = 0, \quad x = x_{\ell,r}, \\ \varphi_k^{n+1/2} = \frac{1}{\frac{2i}{\Delta t} + W^{n+1} + d_k^m} v^{n+1} + \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W^{n+1} + d_k^m}\, \varphi_k^n, \quad x = x_{\ell,r}, \quad 1 \le k \le m, \\ \psi^{n+1/2} = \frac{\sqrt{|\partial_{\mathbf{n}} W^{n+1}|}}{2} \frac{1}{\frac{2i}{\Delta t} + W^{n+1}}\, v^{n+1} + \frac{\frac{2i}{\Delta t}}{\frac{2i}{\Delta t} + W^{n+1}}\, \psi^n, \quad x = x_{\ell,r}, \\ \varphi_k^0(x_{\ell,r}) = \psi^0(x_{\ell,r}) = 0, \quad 1 \le k \le m, \end{cases} \quad (3.77)$$

pour $0 \le n \le N-1$.

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