

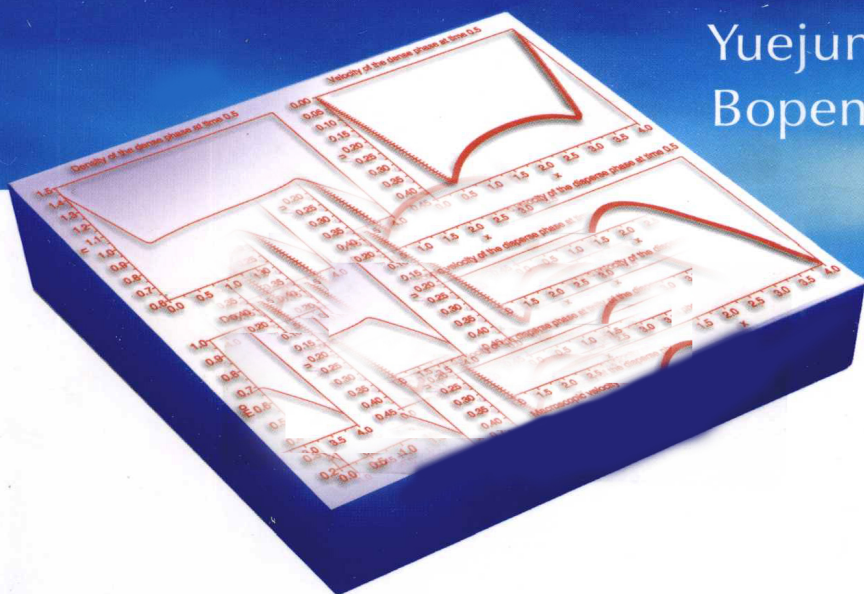
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Some Problems on Nonlinear Hyperbolic Equations and Applications

非线性双曲型方程的一些问题与应用

Tatsien Li
Yuejun Peng
Bopeng Rao

editors



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高等教育出版社·北京
HIGHER EDUCATION PRESS BEIJING

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Preface

This book is a collection of manuscripts from lectures given in the French-Chinese Summer Institute on Applied Mathematics, which was held at the School of Mathematical Sciences of Fudan University from September 1 to September 21, 2008. This Institute was mainly sponsored by the Centre National de Recherche Scientifique (CNRS) and the National Natural Science Foundation of China (NSFC). The activities were organized by the Institut Sino-Français de Mathématiques Appliquées (ISFMA). There were more than 70 participants, including graduate students, postdoctors and junior faculty members from universities and research institutions in China and France.

This volume is entitled *Some Problems on Nonlinear Hyperbolic Equations and Applications*. The volume is composed of two parts: Mathematical and Numerical Analysis for Strongly Nonlinear Plasma Models and Exact Controllability and Observability for Quasilinear Hyperbolic Systems and Applications, which represent two subjects of the Institute. These topics are important not only for industrial applications but also for the theory of partial differential equations itself.

The main propose of the Institute was to present recent progress and results obtained in the domains related to both subjects and to organize discussions for studying important problems by sustainable collaborations. We hope that this experience will be useful for the activities of the French-Chinese collaboration in the future.

During the activities of the Institute, more than 30 lectures of 50 minutes each were delivered. The speakers gave their presentation without attaching much importance to the details of proofs but rather to difficulties encountered, to open problems and possible ways to be exploited. Each lecture was followed by a free discussion of 30 minutes, so that the participants were able to clarify the situation of each problem and to find interesting subjects to be cooperated in the future. Three mini-courses of 3×1.5 hours each were given by Jean-Michel Coron (Université Paris 6, France), Vilmos Komornik (Université Louis Pasteur de Strasbourg, France) on the control theory and by Thierry Goudon (INRIA Lille-Nord Europe, France) on the mathematical theory for plasmas. The mini-course notes were prepared for all the students before the activities of the Institute. Moreover, in the middle and before the end of the Institute, we organized two sessions of general discussion on the open problems for future investigations by collaboration.

The editors would like to express their sincere thanks to all the authors in this volume for their contributions and to all the participants in the Summer Institute. Liqiang Lu, Zhiqiang Wang and Chunlian Zhou deserve our special thanks for their prompt and effective assistance to make the Institute run smoothly. The editors are grateful to the Centre National de Recherche Scientifique (CNRS), the Consulate General of France in Shanghai, the French Embassy in Beijing, the Institut Sino-Français de Mathématiques Appliquées (ISFMA), the National Natural Science Foundation of China (NSFC) and the School of Mathematical Sciences of Fudan University for their help and support. Finally, the editors wish to thank Tianfu Zhao (Senior Editor, Higher Education Press) and Chunlian Zhou for their patience and professional assistance.

Tatsien Li, Yuejun Peng, Bopeng Rao

April 2010

Contents

Part I Mathematical and Numerical Analyses of Strongly Nonlinear Plasma Models

Xavier Antoine, Pauline Klein, Christophe Besse

Open Boundary Conditions and Computational Schemes for Schrödinger Equations with General Potentials and Nonlinearities 3

Christophe Besse, Saja Borghol, Jean-Paul Dudon, Thierry Goudon, Ingrid Lacroix-Violet

On Hydrodynamic Models for LEO Spacecraft Charging 35

Mihai Bostan

Asymptotic Regimes for Plasma Physics with Strong Magnetic Fields 56

Li Chen

The Zero-Electron-Mass Limit in the Hydrodynamic Model (Euler-Poisson System) 86

Thierry Goudon, Pauline Lafitte, Mathias Rousset

Modeling and Simulation of Fluid-Particles Flows 100

Feimin Huang, Hailiang Li, Akitaka Matsumura, Shinji Odanaka

Well-Posedness and Stability of Quantum Hydrodynamics for Semiconductors in \mathbb{R}^3 131

Zhongyi Huang, Shi Jin, Peter A. Markowich, Christof Sparber

Bloch Decomposition-Based Method for High Frequency Waves in Periodic Media 161

Ingrid Lacroix-Violet

Some Results of the Euler-Poisson System for Plasmas and Semiconductors	189
---	-----

Zheng Li, Yaguang Wang

Behavior of Discontinuities in Thermoelasticity with Second Sound	213
---	-----

Shu Wang, Ke Wang, Jianwei Yang

The Convergence of Euler-Poisson System to the Incompressible Euler Equations	225
---	-----

Jiang Xu, Wen-An Yong

On the Relaxation-time Limits in Bipolar Hydrodynamic Models for Semiconductors	258
---	-----

Part II Exact Controllability and Observability for Quasilinear Hyperbolic Systems and Applications

Sylvain Ervedoza

Observability in Arbitrary Small Time for Discrete Approximations of Conservative Systems	283
---	-----

Xiaoyu Fu

Logarithmic Decay of Hyperbolic Equations with Arbitrary Small Boundary Damping	310
---	-----

Olivier Glass

A Remark on the Controllability of a System of Conservation Laws in the Context of Entropy Solutions	332
--	-----

Vilmos Komornik

Introduction to the Control of PDE's	344
--	-----

Tatsien Li, Bopeng Rao

Exact Controllability and Exact Observability for Quasilinear Hyperbolic Systems: Known Results and Open Problems	374
---	-----

Kim Dang Phung

Waves, Damped Wave and Observation 386

Jean-Pierre Puel

Control Problems for Fluid Equations 413

Qiong Zhang

Global Existence of a Degenerate Kirchhoff System with Boundary
Dissipation 426

Xu Zhang

Remarks on the Controllability of Some Quasilinear Equations ... 437

Open Boundary Conditions and Computational Schemes for Schrödinger Equations with General Potentials and Nonlinearities

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Abstract

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

1 Introduction

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

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

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

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

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

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

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

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

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

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

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

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

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

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

with

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

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

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

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

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

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

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

2 Open boundary conditions for linear Schrödinger equations

2.1 The constant coefficients case: derivation of the TBC

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

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

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

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

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

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

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

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

This splitting of the spatial domain \mathbb{R} into interior and exterior problems is explained in Fig. 2.1. It shows the basic idea for constructing the TBC. The Transparent Boundary Condition is obtained by applying the Laplace transformation \mathcal{L} with respect to the time t to the exterior problems (2.4). The Laplace transform is defined through the relation $\hat{w}(s) := \mathcal{L}(w)(s) := \int_{\mathbb{R}_+} w(t)e^{-st}dt$, where $s = \sigma + i\tau$ is the time covariable with $\sigma > 0$.

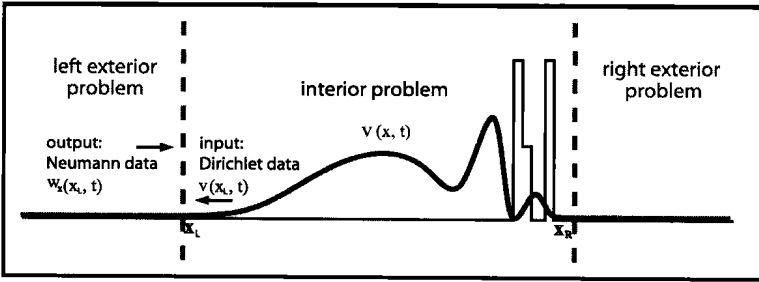


Figure 2.1 Domain decomposition for the construction of the TBC.

In the following, we focus on the derivation of the TBC at the right endpoint x_r . The Laplace transformation of (2.4) (on Ω_r) reads $is\hat{w} + \partial_x^2\hat{w} = 0$, $x \in \Omega_r$. The solution to this second-order ode with constant coefficients can be computed as $\hat{w}(x, s) = A^+(s)e^{\sqrt[4]{-is}x} + A^-(s)e^{-\sqrt[4]{-is}x}$, $x > x_r$, where the branch-cut of the square root $\sqrt[4]{\cdot}$ is taken such that the real part is positive. However, since the solution is an element of $L^2(\Omega_r)$, the coefficient A^+ must vanish. Using the Dirichlet data at the artificial boundary yields $\hat{w}(x, s) = e^{-\sqrt[4]{-is}(x-x_r)} \hat{w}(x, s)|_{x=x_r}$. Deriving $\hat{w}(x, s)$ with respect to x gives

$$\partial_x \hat{w}(x, s)|_{x=x_r} = -\sqrt[4]{-is} \hat{w}(x, s)|_{x=x_r}. \quad (2.5)$$

The analogous condition at the left boundary is $-\partial_x \hat{w}(x, s)|_{x=x_l} = -\sqrt[4]{-is} \hat{w}(x, s)|_{x=x_l}$. Applying an inverse Laplace transformation \mathcal{L}^{-1} is able to obtain an expression of the Neumann datum $\partial_x w(x_{l,r}, t)$ as a

function of the Dirichlet one. Since we have continuity of the traces on Σ_T , the boundary condition of Eq. (2.3) is into

$$\partial_{\mathbf{n}} v(x, t) = \mathcal{L}^{-1}(-\sqrt[4]{-i} \cdot \hat{v}(x, \cdot))(t) = \int_0^t f(t - \tau) v(x, \tau) d\tau, \quad \text{on } \Sigma_T, \quad (2.6)$$

where $\mathcal{L}(f)(s) = -\sqrt[4]{-is}$. By construction we have that u coincides with v on Ω , meaning that we have an exact or a Transparent Boundary Condition (TBC) given by the second equation of (2.6).

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

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

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

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

We recover the TBC on Σ_T with $\partial_{\mathbf{n}} v(x, t) = \mathcal{F}_t^{-1}(i\sqrt{-\cdot} \mathcal{F}_t v(x, \cdot))(t)$. This expression or its Laplace version $\partial_{\mathbf{n}} v(x, t) = \mathcal{L}^{-1}(-\sqrt[4]{-i} \cdot \hat{v}(x, \cdot))(t)$ can be simply written at points $x = x_{l,r}$ as follows:

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

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

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

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

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

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

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

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

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

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

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

The resulting TBC is then given by

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

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

$$\partial_n u(x, t) = \int_0^t f(t - \tau) u(x, \tau) d\tau, \quad \text{on } \Sigma_T, \quad (2.12)$$

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

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

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

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

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

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

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

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

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

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

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

$$\partial_n u(x, t) + ie^{iV_{l,r}t} Op(-\sqrt{-\tau}) (e^{-iV_{l,r}t} u)(x, t) = 0, \quad \text{on } \Sigma_T, \quad (2.14)$$

and

$$\partial_n u(x, t) + iOp\left(-\sqrt{-\tau + V_{l,r}}\right)(u)(x, t), \quad \text{on } \Sigma_T. \quad (2.15)$$

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

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

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

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

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

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

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

$$\partial_n \mathcal{F}_t u(x, \tau) = e^{-i\pi/3} \frac{\text{Ai}'((x - \tau)e^{-i\pi/3})}{\text{Ai}((x - \tau)e^{-i\pi/3})} \mathcal{F}_t u(x, \tau), \quad (2.17)$$

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

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

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

$$\partial_n u + iOp(-\sqrt{-\tau + x})(u) = 0, \quad \text{on } \Sigma_T. \quad (2.18)$$

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

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

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

At this point, some partial conclusions can be drawn:

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

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

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