Exact Boundary Conditions for Periodic Waveguides Containing a Local Perturbation

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Abstract. We consider the solution of the Helmholtz equation $-\Delta u(\mathbf{x}) - n(\mathbf{x})^2 \omega^2 u(\mathbf{x}) = f(\mathbf{x})$, $\mathbf{x} = (x,y)$, in a domain Ω which is infinite in x and bounded in y. We assume that $f(\mathbf{x})$ is supported in $\Omega^0 := \{\mathbf{x} \in \Omega \,|\, a^- < x < a^+\}$ and that $n(\mathbf{x})$ is x-periodic in $\Omega \backslash \Omega^0$. We show how to obtain exact boundary conditions on the vertical segments, $\Gamma^- := \{\mathbf{x} \in \Omega \,|\, x = a^-\}$ and $\Gamma^+ := \{\mathbf{x} \in \Omega \,|\, x = a^+\}$, that will enable us to find the solution on $\Omega^0 \cup \Gamma^+ \cup \Gamma^-$. Then the solution can be extended in Ω in a straightforward manner from the values on Γ^- and Γ^+. The exact boundary conditions as well as the extension operators are computed by solving local problems on a single periodicity cell.

Key words: Exact boundary conditions; periodic media; Dirichlet to Neumann maps.

1 Introduction

Periodic media play a major role in applications, in particular in optics for micro and nano-technology. From the point of view of applications, one of the main interesting features is the possibility offered by such media of selecting ranges of frequencies for which waves can or cannot propagate. Mathematically, this property is linked to the gap structure of the spectrum of the underlying differential operator appearing in the model. For a complete, mathematically oriented presentation, we refer the reader to [14, 15].

There is a need for efficient numerical methods for computing the propagation of waves inside such structures. In real applications, the media are not perfectly periodic but differ from periodic media only in bounded regions (which are small with respect to the total size of the propagation domain). In this case, a natural idea is to reduce the pure numerical computations to these regions and to try to take advantage of the periodic structure of

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the problem outside: this is particularly of interest when the periodic regions contain a large number of periodicity cells.

This paper is a contribution to the construction of such methods in a particular situation. We are interested in propagation media which are a local perturbation of an infinite (or very large) periodic waveguide, namely an infinite structure which is periodic in one privileged direction (the propagation direction) and bounded in the other transverse variables (one says that one has a closed waveguide, as opposed to open waveguides as considered in [23], for instance). Physically the perturbation may be a defect or simply a junction. We investigate the question of finding artificial (but exact) boundary conditions to reduce the numerical computation to a neighborhood of this perturbation.

In the case of "classical" waveguides, which are invariant in the propagation direction, (in some sense, periodic with any period), the usual approach consists in applying Dirichlet to Neumann conditions [10, 16] : using the separation of variables, the solution in the semi-infinite waveguide can be written as the superposition of guided modes, that are exponentially varying along the waveguide direction. As a consequence, one can write explicitly a diagonal form of the DtN map in an appropriate (orthonormal) basis. An alternative approach has been proposed recently which uses the method of Perfectly Match Layer (see [2] for the application to waveguides), which does not easily extend to periodic waveguides.

We investigate in this paper the generalization of the DtN approach to periodic waveguides, which is complicated by the fact that separation of variables can no longer be used. However, the notion of guided modes has a natural extension: the notion of Floquet modes. By revisiting the Floquet-Bloch theory [13], we propose a method for constructing DtN operators by solving local problems on a single periodicity cell. This is closely connected to operator-valued Riccati equations (here, of stationary nature), a topic which is already present in many problems concerning artificial boundary conditions (see, for instance, [5, 11]). It appears also that our method is similar to the matrix transfer approach developed for ordinary equations with periodic coefficients [17]. However, except in the 1D case ([8, 19]), this theory cannot be applied directly to our problem due to the fact that the Cauchy problem for the Helmholtz equation is ill-posed in higher dimensions.

In this first paper, our goal is to present the essential ideas and the main theoretical foundations of our method, explain how we can implement it numerically, and present the first numerical results. We expect to give a more complete theory in a subsequent article.

It seems that there are very few works in this direction in the mathematical literature. Most of the existing work is devoted to the determination of the band gap structure of periodic media. The notion of DtN maps did appear, for instance, in the works by T. Abboud [1] for diffraction problems by periodic gratings and by J. Tausch [23] for periodic open waveguides, but it was used to deal with the unboundedness of the propagation medium in the direction(s) transverse to the periodicity direction(s), a much more standard situation than the one we consider in this paper.
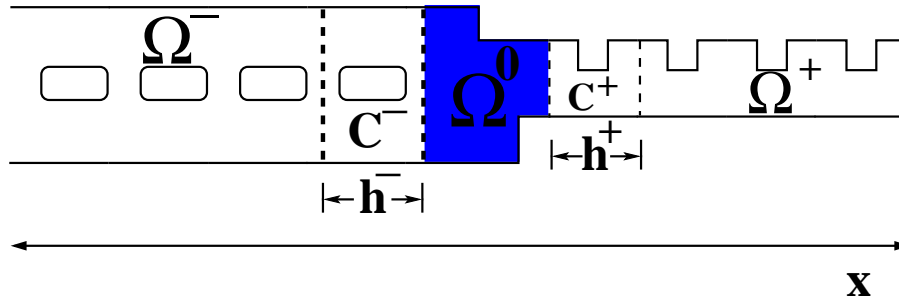
Figure 1: Outside the bounded region Ω^0, the geometry as well as the material properties of the waveguide are periodic to the left and to the right. The cells over one period are denoted C^- and C^+, respectively.

2 Model problem

The model problem that we consider in this paper is that of a 2D periodic waveguide, which allows us to consider a scalar model, but the treatment of the 3D case (where the periodicity is in one direction and the domain bounded in the other two directions) would be similar in principle. We shall assume that the geometry as well as the material properties of the waveguide are x-periodic except in a bounded region (see Fig. 1).
The propagation model is a simple 2D ($\mathbf{x} = (x, y)$) scalar model:

$$n(\mathbf{x})^2 \, \frac{\partial^2 U(\mathbf{x}, t)}{\partial t^2} - \Delta U(\mathbf{x}, t) = F(\mathbf{x}, t).$$

This model holds in electromagnetism when the 2D model is seen as the cross section of a 3D one, invariant in the z direction. In the case of the transverse electric polarization, U represents the z-component of the electric field and $n(\mathbf{x}) \in L^\infty$ is the index of refraction of the medium. Moreover, we suppose that:

$$0 < n_- = \inf_{\mathbf{x} \in \Omega} n(\mathbf{x}) \le n_+ = \sup_{\mathbf{x} \in \Omega} n(\mathbf{x}) < +\infty.$$

We assume that the source term $F(\mathbf{x}, t) = f(\mathbf{x}) \, e^{-\imath \omega t}$ is time-harmonic with frequency $\omega > 0$, and look for the time-harmonic solution $U(\mathbf{x}, t) = u(\mathbf{x}) \, e^{-\imath \omega t}$ where u satisfies the Helmholtz equation:

$$-\Delta u(\mathbf{x}) - n(\mathbf{x})^2 \, \omega^2 \, u(\mathbf{x}) = f(\mathbf{x}). \qquad (2.1)$$

The domain of propagation Ω is bounded in the y direction, infinite in the x direction, and periodic outside a bounded region $\Omega^0 = \Omega \cap \{\, a^- < x < a^+ \}$ that also contains the support of f. The two infinite periodic sub-domains $\Omega^\pm = \Omega \cap \{\pm x > \pm a^\pm\}$ are of the form:

$$\Omega^\pm = \bigcup_{j=0}^{\infty} \left\{ C^\pm \pm (jh^\pm, 0) \right\},$$

where the unit periodicity cells are

$$C^\pm = \Omega \cap \{\, \pm a^\pm \le \pm x \le \pm a^\pm + h^\pm \}.$$

The function $n(\mathbf{x})$ is "x-periodic" as well:

$$n(x,y) = n(x \pm h^{\pm}, y), \ (x,y) \in \Omega^{\pm}.$$

The boundary condition on $\partial\Omega$ (which we suppose to be piecewise C^1 and Lipschitz continuous) can be Dirichlet (this would be consistent with the perfectly conducting boundary condition in electromagnetism), Neumann, or any combination, but they need to be compatible with the periodicity of equation (2.1) in Ω^- and Ω^+. In the following, for the simplicity of the exposition (in particular from the functional analytic point of view) we will consider homogeneous Neumann boundary conditions on $\partial\Omega \bigcap \partial\Omega^-$ and $\partial\Omega \bigcap \partial\Omega^+$ without mentioning it again. However, all that we shall say can easily be extended to the other boundary conditions mentioned above.

Our objective is to characterize the restriction of u to Ω^0 as the solution of (2.1) in Ω^0 that satisfies the boundary conditions on the "Ω^0-part" of $\partial\Omega$, and in addition, satisfies boundary conditions of the form

$$\pm\frac{\partial u}{\partial x} + \Lambda^{\pm} u = 0 \qquad (2.2)$$

on the two "vertical" boundaries $\Gamma^{\pm} = \Omega \cap \{x = a^{\pm}\}$.

The proper definition of $\Lambda^{\pm}$ is linked, of course, to the question of defining (uniquely) the good physical solution of (2.1). This question is not so obvious and may even be controversial for physicist (see for instance [3,19]). We use the limiting absorption principle ([21]) and look for the solution u as the limit (in a sense to be determined), as ε goes to 0, of the unique H^1 solution of

$$-\Delta u_{\varepsilon}(\mathbf{x}) - n(\mathbf{x})^2 \left(\omega^2 + \imath\varepsilon\right) u_{\varepsilon}(\mathbf{x}) = f(\mathbf{x}), \quad \varepsilon > 0. \qquad (2.3)$$

The operators $\Lambda^{\pm}$ should be the limit of the corresponding operators in the transparent, or "exact" (in the sense that they are satisfied by the exact solution) boundary conditions associated with u_{ε}, which are of the form

$$\pm\frac{\partial u_{\varepsilon}}{\partial x} + \Lambda_{\varepsilon}^{\pm} u_{\varepsilon} = 0. \qquad (2.4)$$

Finally, due to the periodicity of (2.3) in $\Omega\backslash\Omega^0$, we know from the Floquet-Bloch theory that there exists two extension operators which will extend the solution u_{ε} from the data on Γ^- and Γ^+ to all of Ω^- and Ω^+. The limits of the extension operators for u_{ε} will define the extension operators for u. The limiting process for u_{ε} and the associated operators requires further theoretical justification. In this paper we shall explain how to find u_{ε} for a fixed ε, and give preliminary numerical results on finding the limit, as ε goes to 0, of the various operators involved. In a later paper we hope to give a more complete theory.

This paper is organized as follows. In Section 3 we give analytical results on the structure of u_{ε}. In Sections 4-6 we describe the computation of $\Lambda_{\varepsilon}^{\pm}$ via the solution of local problems, as well as the procedure used to compute the limit operators $\Lambda^{\pm}$. In the

process, we also obtain the extension operators for u. In Section 7 we show numerical examples. Section 8 contains the conclusions. In the Appendix we connect, for the case of an infinitely periodic waveguide without defect, the construction of the transparent boundary condition to the familiar notion of outgoing waves.

3   Structure of the solution u_ε

For simplicity, we shall restrict ourselves to the construction of the boundary condition on Γ^+. Note that, by periodicity, all the "vertical" interfaces $\Gamma_j^+ = \Gamma^+ + (jh^+, 0)$ can be identified to $\Gamma^+(= \Gamma_0^+)$ and all the cells $C_j^+ = C^+ + (jh^+, 0)$ to $C^+(= C_0^+)$.

It is well-known that the Helmholtz equation with absorption in (2.3), posed on the infinite domain Ω, has a unique H^1 solution, u_ε. In Theorem 3.1 we give a basic result about the structure of u_ε in a part of the domain, namely, in the "half-guide" Ω^+.

Theorem 3.1. *There exist two linear operators,*

$$\mathcal{R}_\varepsilon^+ \in \mathcal{L}(H^{\frac{1}{2}}(\Gamma^+)) \quad and \quad \mathcal{S}_\varepsilon^+ \in \mathcal{L}(H^{\frac{1}{2}}(\Gamma^+), H^1(C^+)),$$

such that $\mathcal{R}_\varepsilon^+$ is compact, injective, and

$$\rho(\mathcal{R}_\varepsilon^+) < 1,$$

where $\rho(\mathcal{R}_\varepsilon^+)$ denotes the spectral radius of $\mathcal{R}_\varepsilon^+$, and such that, if we define $\varphi := u_\varepsilon|_{\Gamma^+}$, then for any $j \geq 0$,

$$u_\varepsilon|_{C_j^+} = \mathcal{S}_\varepsilon^+ \circ (\mathcal{R}_\varepsilon^+)^j \, \varphi. \tag{3.1}$$

As a consequence of this theorem, once we have the operator $\mathcal{S}_\varepsilon^+$, Λ_ε^+, the Dirichlet-to-Neumann operator on Γ^+, can be obtained via

$$\Lambda_\varepsilon^+(\varphi) = -\frac{\partial}{\partial x} \left(\mathcal{S}_\varepsilon^+ \varphi \right) \Big|_{\Gamma^+}. \tag{3.2}$$

Then the boundary conditions in (2.4) will enable us to solve for the restriction of u_ε on Ω^0. In addition, once we have the operators $\mathcal{R}_\varepsilon^+$ and $\mathcal{S}_\varepsilon^+$, we only need the trace of u_ε on Γ^+ to be able to extend the solution to all of Ω^+.

We summarize in Algorithm 1.

Algorithm 1 Construction of u_ε from $\mathcal{S}_\varepsilon^+$, $\mathcal{R}_\varepsilon^+$, Λ_ε^+, and $\mathcal{S}_\varepsilon^-$, $\mathcal{R}_\varepsilon^-$, Λ_ε^-.

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  1. Solve (2.3) in Ω^0 subject to

$$\begin{cases} \dfrac{\partial u_\varepsilon}{\partial x} + \Lambda_\varepsilon^+ u_\varepsilon = 0, & \mathbf{x} \in \Gamma^+, \\[2mm] -\dfrac{\partial u_\varepsilon}{\partial x} + \Lambda_\varepsilon^- u_\varepsilon = 0, & \mathbf{x} \in \Gamma^-. \end{cases} \tag{3.3}$$

  2. Extend the solution: $j = 0, 1, 2, \cdots$

$$\begin{cases} u_\varepsilon|_{C_j^+} = \mathcal{S}_\varepsilon^+ \circ (\mathcal{R}_\varepsilon^+)^j (u_\varepsilon|_{\Gamma^+}), \\[2mm] u_\varepsilon|_{C_j^-} = \mathcal{S}_\varepsilon^- \circ (\mathcal{R}_\varepsilon^-)^j (u_\varepsilon|_{\Gamma^-}). \end{cases} \tag{3.4}$$

We will describe later how we propose to efficiently compute these operators; for now we proceed with the proof of Theorem 3.1.

Proof. We define the "half-guide problem":

$$\begin{cases} -\Delta u_\varepsilon^+(\varphi) - n(\mathbf{x})^2 \, (\omega^2 + \imath\varepsilon) \, u_\varepsilon^+(\varphi) = 0, & \text{in } \Omega^+, \\[2mm] u_\varepsilon^+(\varphi) = \varphi, & \text{on } \Gamma^+. \end{cases} \tag{3.5}$$

For any $\varphi \in H^{\frac{1}{2}}(\Gamma^+)$, the solution $u_\varepsilon^+(\varphi) \in H^1(\Omega^+)$ exists and is unique. By construction $u_\varepsilon^+(\varphi)$ coincides with u_ε on $\overline{\Omega^+}$. We will define the operators $\mathcal{S}_\varepsilon^+$ and $\mathcal{R}_\varepsilon^+$ to be its restriction to the first cell and its further boundary, respectively:

$$\mathcal{S}_\varepsilon^+ \varphi := u_\varepsilon^+(\varphi)\big|_{C^+}, \tag{3.6}$$

$$\mathcal{R}_\varepsilon^+ \varphi := u_\varepsilon^+(\varphi)\big|_{\Gamma_1^+}. \tag{3.7}$$

Clearly, the extension equation (3.1) is satisfied for $j = 0$. Looking at the translation of $u_\varepsilon^+ = u_\varepsilon^+(\varphi)$ by one period,

$$\tilde{u}_\varepsilon^+(x, y) := u_\varepsilon^+(x + h^+, y), \tag{3.8}$$

we see that $\tilde{u}_\varepsilon^+$ is also in $H^1(\Omega^+)$ and that it satisfies the PDE,

$$\begin{aligned} &-\triangle \tilde{u}_\varepsilon^+(x, y) - n(x, y)^2 \, (\omega^2 + \imath\varepsilon) \, \tilde{u}_\varepsilon^+(x, y) \\ &\quad = -\triangle u_\varepsilon^+(x + h^+, y) - n(x + h^+, y)^2 \, (\omega^2 + \imath\varepsilon) \, u_\varepsilon^+(x + h^+, y) = 0, \end{aligned}$$

for all $(x, y) \in \Omega^+$, as well as the boundary condition:

$$\tilde{u}_\varepsilon^+ \big|_{\Gamma^+} = \mathcal{R}_\varepsilon^+ \varphi.$$

By the uniqueness of the solution to (3.5), we have

$$\tilde{u}_\varepsilon^+\big|_{C^+} = \mathcal{S}_\varepsilon^+ \circ \mathcal{R}_\varepsilon^+ \varphi. \tag{3.9}$$

Finally,

$$u_\varepsilon^+\big|_{C_1^+} = \tilde{u}_\varepsilon^+\big|_{C^+} = \mathcal{S}_\varepsilon^+ \circ \mathcal{R}_\varepsilon^+ \varphi.$$

Hence, we have shown that (3.1) holds for $j = 1$. For $j > 1$, we proceed by induction.

From interior elliptic regularity for u_ε, we deduce that the operator $\mathcal{R}_\varepsilon^+$ is regularizing. More precisely, taking into account the regularity assumptions about n and $\partial\Omega$, we know that there exists a neighborhood $\mathcal{V}^+$ of Γ_1^+ and some $\delta > 0$ such that

$$u_\varepsilon \in H^{1+\delta}(\Omega \cap \mathcal{V}^+) \quad \text{and} \quad \|u_\varepsilon\|_{H^{1+\delta}(\Omega \cap \mathcal{V}^+)} \leq C(\mathcal{V}^+) \, \|\varphi\|_{H^{\frac{1}{2}}(\Gamma^+)}.$$

As a consequence:

$$\mathcal{R}_\varepsilon^+ \in \mathcal{L}(H^{\frac{1}{2}}(\Gamma^+), H^{\frac{1}{2}+\delta}(\Gamma^+)).$$

The compactness of $\mathcal{R}_\varepsilon^+$ follows immediately.

For the injectivity of $\mathcal{R}_\varepsilon^+$, we use an argument of unique continuation. Indeed, let us take a function φ such that $\mathcal{R}_\varepsilon^+ \varphi = 0$. We restrict the problem to the domain $\Omega_1^+ = \Omega^+ \cap \{x \geq a^+ + h^+\}$ with the boundary condition :

$$u_\varepsilon^+ \big|_{\Gamma_1^+} = \mathcal{R}_\varepsilon^+ \varphi = 0.$$

By uniqueness of the solution, we deduce that $u_\varepsilon^+ = 0$ in Ω_1^+. Hence, by an argument of unique continuation, the restriction of u_ε^+ to C^+ is zero, in particular, its value on Γ^+ : $\varphi = 0$.

To show that the spectral radius of $\mathcal{R}_\varepsilon^+$ is < 1, we proceed by contradiction. Suppose its spectral radius is ≥ 1, then there exists an eigenvalue λ_0 such that $|\lambda_0| \geq 1$. Let φ_0 be the associated eigenfunction, then $\mathcal{R}_\varepsilon^+ \varphi_0 = \lambda_0 \, \varphi_0$. From (3.1) we obtain

$$u_\varepsilon^+(\varphi_0)|_{C_j^+} = \mathcal{S}_\varepsilon^+ \circ (\mathcal{R}_\varepsilon^+)^j \varphi = \lambda_0^j \mathcal{S}_\varepsilon^+ \varphi,$$

thus the L^2 norm of $u_\varepsilon^+(\varphi_0)$ is

$$\sum_{j=0}^\infty \int_{C_j^+} |u_\varepsilon^+(\varphi_0)|^2 = \sum_{j=0}^\infty \int_{C_j^+} |\lambda_0|^{2j} |\mathcal{S}_\varepsilon^+ \varphi|^2 = +\infty.$$

This contradicts the fact that $u_\varepsilon^+(\varphi)$ is in $L^2(\Omega^+)$. $\qquad \square$

Remark 3.1. The definitions of the operators in (3.6), (3.7), and (3.2) and their counterparts in Ω^- are not yet of any practical use since (3.5) and its counterpart in Ω^- are still posed in an unbounded domain.

4   Characterization of operators via local problems

In practice, we need to compute the operators, $\mathcal{S}_\varepsilon^+$, $\mathcal{R}_\varepsilon^+$, Λ_ε^+, and their counterparts in Ω^- by solving "local" problems. In this section we show how to do so for the operators in Ω^+. We introduce $u_{\varepsilon,\ell}^+(\varphi)$, $\ell = 0, 1$, the solutions of two problems posed on a single periodicity cell C^+:

$$-\Delta u_{\varepsilon,\ell}^+(\varphi) - n(\mathbf{x})^2 \, (\omega^2 + \imath\varepsilon) \, u_{\varepsilon,\ell}^+(\varphi) = 0, \quad \text{in } C^+, \tag{4.1}$$

subject to non-homogeneous Dirichlet conditions on Γ^+ and Γ_1^+:

$$\begin{cases} u_{\varepsilon,0}^+(\varphi) = \varphi \quad \text{on } \Gamma^+, \quad u_{\varepsilon,0}^+(\varphi) = 0 \quad \text{on } \Gamma_1^+, \\[2mm] u_{\varepsilon,1}^+(\varphi) = 0 \quad \text{on } \Gamma^+, \quad u_{\varepsilon,1}^+(\varphi) = \varphi \quad \text{on } \Gamma_1^+. \end{cases} \tag{4.2}$$

We define four DtN-like operators,

$$\begin{aligned} \mathcal{T}_{00}^+(\varepsilon) \, \varphi &= - \frac{\partial}{\partial x} u_{\varepsilon,0}^+(\varphi) \Big|_{\Gamma^+}, \quad \mathcal{T}_{01}^+(\varepsilon) \, \varphi = \frac{\partial}{\partial x} u_{\varepsilon,0}^+(\varphi) \Big|_{\Gamma_1^+}, \\[2mm] \mathcal{T}_{10}^+(\varepsilon) \, \varphi &= - \frac{\partial}{\partial x} u_{\varepsilon,1}^+(\varphi) \Big|_{\Gamma^+}, \quad \mathcal{T}_{11}^+(\varepsilon) \, \varphi = \frac{\partial}{\partial x} u_{\varepsilon,1}^+(\varphi) \Big|_{\Gamma_1^+}, \end{aligned} \tag{4.3}$$

which, after identification between Γ^+ and Γ_1^+, we consider as bounded operators in $\mathcal{L}(H^{\frac{1}{2}}(\Gamma^+), H^{-\frac{1}{2}}(\Gamma^+))$.

It is easy to see that the restrictions to $H^1(\Gamma^+)$ of these operators define unbounded operators in $L^2(\Gamma^+)$, which we will still denote by $\mathcal{T}_{pq}^+(\varepsilon)$ for simplicity, and they have the following properties. (In what follows, if A denotes a closed operator in $L^2(\Gamma^+)$, A^* denotes its adjoint and $\overline{A}$ its complex conjugate).

Lemma 4.1. *The following relationships hold:*

$$\begin{aligned} \left[\mathcal{T}_{00}^+(\varepsilon)\right]^* &= \overline{\mathcal{T}_{00}^+(\varepsilon)}, \qquad \left[\mathcal{T}_{11}^+(\varepsilon)\right]^* = \overline{\mathcal{T}_{11}^+(\varepsilon)}, \\[2mm] \left[\mathcal{T}_{01}^+(\varepsilon)\right]^* &= \overline{\mathcal{T}_{10}^+(\varepsilon)}, \qquad \left[\mathcal{T}_{10}^+(\varepsilon)\right]^* = \overline{\mathcal{T}_{01}^+(\varepsilon)}. \end{aligned} \tag{4.4}$$

Moreover, the operators $\mathcal{T}_{pq}^+(\varepsilon)$ are all injective, and so is the operator

$$\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon) \; .$$

Proof. The equalities in (4.4) follow directly from Green's formula. The injectivity of $\mathcal{T}_{00}^+(\varepsilon)$ and $\mathcal{T}_{11}^+(\varepsilon)$ is proved directly using Lax-Milgram's lemma. The injectivity of $\mathcal{T}_{01}^+(\varepsilon)$ and $\mathcal{T}_{10}^+(\varepsilon)$ relies on a unique continuation argument. The details are left to the reader.

Finally, let φ be in the kernel of the operator $\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon)$, we set:

$$v_\varepsilon = u_{\varepsilon,0}^+(\varphi) + u_{\varepsilon,1}^+(\varphi).$$

Since $\quad -\Delta v_\varepsilon - n(\mathbf{x})^2 \, (\omega^2 + \imath\varepsilon) \, v_\varepsilon = 0$, in C^+, we get (multiply the equation by $\overline{v}_\varepsilon$, integrate over C^+ and use $\mathcal{T}_{00}^+(\varepsilon) \, \varphi + \mathcal{T}_{11}^+(\varepsilon) \, \varphi = 0$):

$$\int_{C^+} \left(|\nabla v_\varepsilon|^2 - n(\mathbf{x})^2 \, (\omega^2 + \imath\varepsilon) \, |v_\varepsilon|^2 \right) d\mathbf{x} = (\mathcal{T}_{01}^+(\varepsilon)\varphi, \varphi)_{L^2(\Gamma^+)} + (\mathcal{T}_{10}^+(\varepsilon)\varphi, \varphi)_{L^2(\Gamma^+)} \, .$$

We use (4.4) (second line) and take the imaginary part of the above identity to obtain:

$$\varepsilon \int_{C^+} |v_\varepsilon|^2 \, d\mathbf{x} = 0 \quad \Longrightarrow \quad v_\varepsilon = 0 \quad \Longrightarrow \quad \varphi = 0.$$

This concludes the proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Remark 4.1. One easily sees that the operators $\mathcal{T}_{00}^+(\varepsilon), \mathcal{T}_{11}^+(\varepsilon)$, and $\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon)$ are of Fredholm type. Thus, from Lemma 4.1, they are isomorphisms from $H^1(\Gamma^+)$ onto $L^2(\Gamma^+)$.

We now characterize the operator $\mathcal{R}_\varepsilon^+$ as the solution of a quadratic characteristic equation (a stationary Riccati equation) subject to a constraint. The operators $\mathcal{T}_{pq}^+(\varepsilon)$ appear as coefficients of the characteristic equation.

Theorem 4.1. *The operator $\mathcal{R}_\varepsilon^+ \in \mathcal{L}(H^{\frac{1}{2}}(\Gamma^+))$ is the unique compact operator which solves the characteristic equation (in $\mathcal{L}(H^{\frac{1}{2}}(\Gamma^+), H^{-\frac{1}{2}}(\Gamma^+)$, the unknown being the operator $\mathcal{R}$)*

$$\mathcal{T}(\varepsilon, \mathcal{R}) := \mathcal{T}_{10}^+(\varepsilon) \, \mathcal{R}^2 + \left(\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon) \right) \mathcal{R} + \mathcal{T}_{01}^+(\varepsilon) = 0 \tag{4.5}$$

and satisfies the condition

$$\rho(\mathcal{R}) < 1. \tag{4.6}$$

Proof. We have shown that $\rho(\mathcal{R}_\varepsilon^+) < 1$ in Theorem 3.1. Now we show that $\mathcal{R}_\varepsilon^+$ satisfies (4.5). Again, let $u_\varepsilon^+(\varphi)$ be the unique $H^1(\Omega^+)$ solution to (3.5). Since any solution of (4.1) with specified Dirichlet data on Γ^+ and Γ_1^+ is a linear combination of the basic solutions $u_{\varepsilon,\ell}^+, \ell = 0, 1$, the restriction of $u_\varepsilon^+(\varphi)$ on C^+ is the sum

$$u_\varepsilon^+(\varphi)\big|_{C^+} = u_{\varepsilon,0}^+(\varphi) + u_{\varepsilon,1}^+(\mathcal{R}_\varepsilon^+\varphi). \tag{4.7}$$

Combining with the extension equation (3.1), we obtain

$$\mathcal{S}_\varepsilon^+\varphi = u_{\varepsilon,0}^+(\varphi) + u_{\varepsilon,1}^+(\mathcal{R}_\varepsilon^+\varphi). \tag{4.8}$$

Equation (3.5) implies the continuity of $\dfrac{\partial u_\varepsilon^+(\varphi)}{\partial x}$ at the Γ_j^+'s, namely

$$\lim_{x \to (a^+ + (j+1)h^+)^-} \frac{\partial u_\varepsilon^+(\varphi)}{\partial x} = \lim_{x \to (a^+ + (j+1)h^+)^+} \frac{\partial u_\varepsilon^+(\varphi)}{\partial x}, \quad j = 0, 1, 2, \cdots$$

which, due to (3.1), is equivalent to

$$\frac{\partial \mathcal{S}_\varepsilon^+ \circ (\mathcal{R}_\varepsilon^+)^j \varphi}{\partial x}\bigg|_{\Gamma_1^+} = \frac{\partial \mathcal{S}_\varepsilon^+ \circ \mathcal{R}_\varepsilon^+ (\mathcal{R}_\varepsilon^+)^j \varphi}{\partial x}\bigg|_{\Gamma^+}, \tag{4.9}$$

for all $\varphi \in L^2(\Gamma^+)$. Inserting the quantities in (4.8) into (4.9), we obtain

$$\mathcal{T}_{01}^+(\varepsilon)\,\varphi + \mathcal{T}_{11}^+(\varepsilon)\mathcal{R}_\varepsilon^+ \varphi = -\mathcal{T}_{00}^+(\varepsilon)\mathcal{R}_\varepsilon^+ \varphi - \mathcal{T}_{10}^+(\varepsilon)(\mathcal{R}_\varepsilon^+)^2\varphi.$$

Reciprocally, if $\mathcal{R}$ is a compact operator with spectral radius $\rho(\mathcal{R}) < 1$ which satisfies (4.5), then the function defined by

$$\tilde{u}_\varepsilon^+(\varphi)\big|_{C_j^+} := u_{\varepsilon,0}^+\left(\mathcal{R}^j\varphi\right) + u_{\varepsilon,1}^+\left(\mathcal{R}^{j+1}\varphi\right), \quad j = 0, 1, 2, \cdots$$

satisfies (3.5) in each C_j^+, is continuous and has continuous normal derivatives across the Γ_j^+'s. Moreover, the fact that $\rho(\mathcal{R}) < 1$ implies that $\tilde{u}_\varepsilon^+(\varphi)$ belongs to $H^1(\Omega^+)$. Indeed, the property (see [24]):

$$\lim_{n \to +\infty} \|\mathcal{R}^n\|_{\mathcal{L}(H^{\frac{1}{2}}(\Gamma^+))}^{1/n} = \rho(\mathcal{R}) \tag{4.10}$$

implies that, for some $\rho_* \in \left(\,\rho(\mathcal{R}), 1\,\right)$ and j large enough:

$$\|\mathcal{R}^j\|_{\mathcal{L}(H^{\frac{1}{2}}(\Gamma^+))} \le \rho_*^j,$$

so that, setting $C_\varepsilon = \|\mathcal{S}_\varepsilon^+\|_{\mathcal{L}(H^{\frac{1}{2}}(\Gamma^+), H^1(C^+))}$:

$$\|\tilde{u}_\varepsilon^+(\varphi)\|_{H^1(C_j^+)} \le C_\varepsilon\,\rho_*^j\,\|\varphi)\|_{H^{\frac{1}{2}}(\Gamma^+)}.$$

Thus, $\tilde{u}_\varepsilon^+(\varphi)$ is none other than $u_\varepsilon^+(\varphi)$, which shows that $\mathcal{R} = \mathcal{R}_\varepsilon^+$. $\qquad\square$

Finally, in terms of quantities available from the solution of local problems in C^+, we have the following formulae for Λ_ε^+ and $\mathcal{S}_\varepsilon^+$:

$$\begin{aligned}
\Lambda_\varepsilon^+ &= \mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{10}^+(\varepsilon)\,\mathcal{R}_\varepsilon^+, \\
\mathcal{S}_\varepsilon^+ &= u_{\varepsilon,0}^+ + u_{\varepsilon,1}^+\mathcal{R}_\varepsilon^+.
\end{aligned} \tag{4.11}$$

Remark 4.2. If one removes the condition about the spectral radius, it is clear that the equation (4.5) has an infinity of solutions.

5   Solution of the characteristic equation for $\mathcal{R}_\varepsilon^+$.

Both Λ_ε^+ and $\mathcal{S}_\varepsilon^+$ depend on the operator $\mathcal{R}_\varepsilon^+$ (see (4.11)) and in this section we talk about how to compute it.

Section 5.1 describes computing the eigenvalues and the associated eigenfunctions of $\mathcal{R}_\varepsilon^+$. The eigenvalues and eigenfunctions completely define the operator $\mathcal{R}_\varepsilon^+$ only if the eigenfunctions form a complete set of $H^{\frac{1}{2}}(\Gamma^+)$. We do not have a proof of this (see Remark 5.1). Nevertheless, we believe that it is instructive from both an analytical and a numerical point of view to proceed with a spectral analysis of $\mathcal{R}_\varepsilon^+$.

In Section 5.2 we describe a Newton's method to solve (4.5) subject to the constraint in (4.6).

5.1   Via a spectral decomposition

A priori, to take into account the constraint about the spectral radius, a natural way to characterize the operator $\mathcal{R}_\varepsilon^+$ is to determine the eigenvalues and associated eigenfunctions. From Theorem 4.1, and defining $\mathcal{T}(\varepsilon, \lambda)$ by replacing $\mathcal{R}$ by λ in (4.5), we deduce that a number $\lambda \in C$ is an eigenvalue of $\mathcal{R}_\varepsilon^+$ with the corresponding eigenfunction φ if and only if it solves

$$\mathcal{T}(\varepsilon, \lambda)\varphi = 0, \quad \varphi \neq 0, \tag{5.1}$$

subject to the constraint

$$|\lambda| < 1. \tag{5.2}$$

Of course, the solutions λ and φ of (5.1)-(5.2) are functions of ε: $\lambda = \lambda(\varepsilon)$, $\varphi = \varphi(\varepsilon)$.

Remark 5.1. The eigenvalues and eigenfunctions completely define the operator $\mathcal{R}_\varepsilon^+$ only if the eigenfunctions form a complete set of $H^{\frac{1}{2}}(\Gamma^+)$. In the quasi-1D case, namely when:

$$\Omega^+ = (a^+, +\infty) \times (0, L), \quad n(x,y) = n(x) \text{ in } \Omega^+, \tag{5.3}$$

one can show that the operator $\mathcal{R}_\varepsilon^+$ is normal and thus diagonalizable in an orthonormal basis (here the basis $\{w_n(y) = \sqrt{2/L}\sin(n\pi y/L)\}$). Our numerical results show that this property is lost in general. Our conjecture is that the generalized eigenfunctions of $\mathcal{R}_\varepsilon^+$ form a complete set of $L^2(\Gamma^+)$ (an equivalent of Jordan's theorem in infinite dimension) but this remains an open question.

Using the properties of the operators $\mathcal{T}_{\varepsilon,pq}^+$ it is easy to prove the following structural property:

Theorem 5.1. *For any $\lambda \neq 0$, one has the property:*

$$Ker \; \mathcal{T}(\varepsilon, \lambda) \neq 0 \quad \Longleftrightarrow \quad Ker \; \mathcal{T}(\varepsilon, 1/\lambda) \neq 0.$$

Proof. From the definition of $\mathcal{T}(\varepsilon, \lambda)$, we get that

$$\overline{\lambda}^2 \; \mathcal{T}(\varepsilon, 1/\lambda)^* = \overline{\mathcal{T}(\varepsilon, \lambda)}.$$

From classical results about adjoint operators, one deduces that 0 is in the spectrum of $\mathcal{T}(\varepsilon, \lambda)$ if and only if it belongs to the spectrum of $\mathcal{T}(\varepsilon, 1/\lambda)$. Finally it remains to remark that 0 belongs to the spectrum of $\mathcal{T}(\varepsilon, \lambda)$ if and only if 0 is an eigenvalue of $\mathcal{T}(\varepsilon, \lambda)$. To see that, it suffices to write:

$$\mathcal{T}(\varepsilon, \lambda) = \lambda \left(\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon) \right) \; [\; I + C(\varepsilon, \lambda) \;],$$

where $C(\varepsilon, \lambda) = \left(\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon) \right)^{-1} \left(\lambda^{-1} \; \mathcal{T}_{01}^+(\varepsilon) + \lambda \; \mathcal{T}_{10}^+(\varepsilon) \right)$ is compact, and use Fredholm's alternative. $\qquad\square$

In other words, this result means that the solutions of the quadratic eigenvalue problem (5.1) come in pairs, $(\lambda, 1/\lambda)$. From each pair we choose λ (and the associated φ), with $|\lambda| < 1$, and discard $1/\lambda$.

5.2   Via a modified Newton's method

One can also solve directly the quadratic equation (4.5), using a Newton's algorithm, for instance. The difficulty is to take into account the constraint about the spectral radius. That is why we propose a heuristic modified Newton's algorithm where a projection step is applied at each step of the algorithm.

To formulate properly this algorithm, we denote by $K(H^{\frac{1}{2}}(\Gamma^+))$ the space of compact operators in $H^{\frac{1}{2}}(\Gamma^+)$ and introduce the function (which is well defined due to the invertibility of $\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon)$):

$$F_\varepsilon(R) = \mathcal{R} + \left(\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon)\right)^{-1} \left[\mathcal{T}_{10}^+(\varepsilon)\,\mathcal{R}^2 + \mathcal{T}_{01}^+(\varepsilon)\right]$$

which is a differentiable map from $K(H^{\frac{1}{2}}(\Gamma^+))$ in $K(H^{\frac{1}{2}}(\Gamma^+))$ with:

$$DF_\varepsilon(\mathcal{R}) \cdot H = H + \left(\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon)\right)^{-1} \mathcal{T}_{10}^+(\varepsilon)\,[\,H\,\mathcal{R} + \mathcal{R}\,H\,].$$

Note that (4.5) is nothing but $F_\varepsilon(\mathcal{R}_\varepsilon^+) = 0$.

The algorithm we suggest consists in constructing, from an initial guess $\mathcal{R}_{\varepsilon,0}^+ \in K(H^{\frac{1}{2}}(\Gamma^+))$, (0, for example), the sequence $\mathcal{R}_{\varepsilon,n}^+$ defined by:

- Compute $\delta R_{\varepsilon,n+1}^+$ solution of:

$$\delta\mathcal{R}_{\varepsilon,n+1}^+ + \left(\mathcal{T}_{00}^+(\varepsilon) + \mathcal{T}_{11}^+(\varepsilon)\right)^{-1} \mathcal{T}_{10}^+(\varepsilon)\left[\,\mathcal{R}_{\varepsilon,n}^+\,\delta\mathcal{R}_{\varepsilon,n+1}^+ + \delta\mathcal{R}_{\varepsilon,n+1}^+\,\mathcal{R}_{\varepsilon,n}^+\,\right]$$
$$= F_\varepsilon(\mathcal{R}_{\varepsilon,n}^+); \tag{5.4}$$

- Compute $\tilde{\mathcal{R}}_{\varepsilon,n+1}^+ = \mathcal{R}_{\varepsilon,n}^+ - \delta\mathcal{R}_{\varepsilon,n+1}^+$;

- Choose $\begin{cases} \mathcal{R}_{\varepsilon,n+1}^+ = \tilde{\mathcal{R}}_{\varepsilon,n+1}^+ & \text{if } \rho(\tilde{\mathcal{R}}_{\varepsilon,n+1}^+) \leq 1, \\ \mathcal{R}_{\varepsilon,n+1}^+ = \tilde{\mathcal{R}}_{\varepsilon,n+1}^+/\rho(\tilde{\mathcal{R}}_{\varepsilon,n+1}^+) & \text{if } \rho(\tilde{\mathcal{R}}_{\varepsilon,n+1}^+) > 1; \end{cases}$

- Stop the algorithm when:

$$\frac{\|\delta R_{\varepsilon,n+1}^+\|}{\|\mathcal{R}_{\varepsilon,n}^+\|} \quad \text{is small enough.}$$

Indeed, the solution $\mathcal{R}_\varepsilon^+$ is expected to be the limit of the sequence $\mathcal{R}_{\varepsilon,n}^+$.

6   About the limiting absorption process

In the previous sections we have shown how to construct the boundary conditions in (2.4) associated with the Helmholtz equation with absorption (2.3). In particular, we have shown that the restriction of the unique H^1 solution u_ε of (2.3), posed on Ω, is indeed the

same as what we obtain by solving (2.3) on Ω^0 subject to the boundary condition (2.4). In fact, we can recover u_ε on as large a region of Ω as we like by using the extension formula (3.1).

Now we return to the solution of the original Helmholtz equation (2.1) and the boundary conditions (2.2). Equation (2.1), posed on the infinite domain Ω, is not in itself sufficient to allow us to define a "reasonable" solution. An additional criterion needs to be found which can be thought of as equivalent to an outgoing condition for a standard waveguide or the radiation condition for the scattering problem. In those two cases, the Helmholtz equation posed on an infinite domain plus the additional criterion give rise to a unique solution (under reasonable assumptions) which also makes "physical" sense, meaning that such a solution can be observed in the real world.

The notion of a "physical" solution in a periodic waveguide is much less intuitive and we do not have a simple physical interpretation of it, in contrast to the case of a standard waveguide where the "physical" solution contains "outgoing", as opposed to "incoming", waves (this is the well-known outgoing condition [10]). Instead, we chose to rely on the limit absorption principle, namely, we would like to impose an additional criterion so that the solution to (2.1) exists, is unique, and is the limit, in some sense to be determined, as ε (> 0) goes to 0, of u_ε.

We have seen that the procedure involving the operators $\mathcal{R}_\varepsilon^+$, Λ_ε^+, and $\mathcal{S}_\varepsilon^+$ (and their counterparts in Ω^-) can reproduce u_ε on Ω. We want to do something similar for the problem without absorption. In other words, we want to compute, by solving local problems as well as a constrained quadratic equation, the analogous operators $\mathcal{R}^+$, Λ^+, and $\mathcal{S}^+$ (and their counterparts in Ω^-) and use the analogous procedure, solution of the boundary value problem on Ω^0 and extension, to produce a solution of (2.1), which is also the limit of u_ε.

One is led to ask the following questions: If we formally take the limits of the local problems (4.1)-(4.2) and the constrained quadratic equation (4.5)-(4.6), as well as the definitions (4.3), (4.11) does that give rise to well-defined operators $\mathcal{R}^+$, Λ^+, and $\mathcal{S}^+$? Are they the limits of $\mathcal{R}_\varepsilon^+$, Λ_ε^+, and $\mathcal{S}_\varepsilon^+$? Do $\mathcal{R}^+$, Λ^+, and $\mathcal{S}^+$ (and their counterparts in Ω^-) lead to a solution of (2.1)? Is this solution the limit of u_ε? And most basically, do the limits of $\mathcal{R}_\varepsilon^+$, Λ_ε^+, $\mathcal{S}_\varepsilon^+$ (and their counterparts in Ω^-), and u_ε, exist?

Unfortunately, at this point, we are not able to answer these questions except in a few greatly simplified cases, for example, when the problem can be reduced to a 1D problem (that means that the index of refraction n depends only on x or on y). Our conjecture is that, for almost every frequency ω, u_ε has a limit. We say almost every frequency because there are frequencies which, a priori, we need to exclude from consideration. For example, for standard waveguides, there may be frequencies ω for which it is not possible to define a outgoing solution [25]. We believe a similar thing is true for periodic waveguides. However, we also believe that the set of such frequencies is discrete.

Supposing that u_ε, as well as $\mathcal{R}_\varepsilon^+$, Λ_ε^+, $\mathcal{S}_\varepsilon^+$, have a limit, we propose several possible ways of defining the operators $\mathcal{R}^+$, Λ^+, and $\mathcal{S}^+$ based on heuristic arguments that they should be the limits of $\mathcal{R}_\varepsilon^+$, Λ_ε^+, and $\mathcal{S}_\varepsilon^+$, respectively.

First we speak about Λ^+ and $\mathcal{S}^+$. We denote by u_0^+ and u_1^+ the solutions of local problems (4.1)-(4.2) where we have substituted $\varepsilon = 0$. We denote by $\mathcal{T}_{pq}^+$ the DtN-like operators acting on u_0^+ and u_1^+ following the formulae in (4.3). We propose to define Λ^+, and $\mathcal{S}^+$ using these quantities in a similar manner to (4.11). In Lemma 6.1 we show that that there is no ambiguity in these definitions, under the assumption that the operator $\mathcal{R}^+$ can be defined. The question of the definition of $\mathcal{R}^+$ is left to Sections 6.1-6.3.

For Lemma 6.1 to hold, we exclude, a priori, some critical values of ω^2, namely:

(a) ω^2 is not an eigenvalue of the operator $-n^{-2}\Delta$ in C^+ with Dirichlet conditions on Γ_0^+ and Γ_1^+,

(b) ω^2 is not an eigenvalue of the operator $-n^{-2}\Delta$ in C^+ with Neumann conditions on Γ_0^+ and Γ_1^+.

The restrictions (a) and (b) are not essential. Typically, they correspond to the exclusion of interior eigenvalues for classical integral equations for obstacle scattering [6, 18]. They resulted from our having chosen, for the simplicity of presentation, Dirichlet conditions in the definitions of the local problems, (see Equation (4.2)), and can be avoided by considering other operators constructed with boundary conditions of mixed type.

The proof of Lemma 6.1 is straightforward and the details are omitted.

Lemma 6.1. *Assume that* (a) *holds then the following is true:*

$$\begin{cases} u_0^+ = \lim_{\varepsilon \to 0} u_{\varepsilon,0}^+ \\ u_1^+ = \lim_{\varepsilon \to 0} u_{\varepsilon,1}^+ \end{cases} \quad and \quad \mathcal{T}_{pq}^+ = \lim_{\varepsilon \to 0} \mathcal{T}_{pq}^+(\varepsilon), \quad (in \ \mathcal{L}(H^{1/2}(\Gamma^+))).$$

Moreover, one has the following properties:

- $\mathcal{T}_{00}^+$ *and* $\mathcal{T}_{11}^+$ *are self-adjoint operators,*
- $\mathcal{T}_{01}^+$ *is the adjoint of* $\mathcal{T}_{10}^+$ *(and reciprocally).*
- *If* (b) *holds, the operators* $\mathcal{T}_{00}^+$, $\mathcal{T}_{11}^+$, *and* $\mathcal{T}_{00}^+ + \mathcal{T}_{11}^+$ *are isomorphisms.*

6.1 An equation for $\mathcal{R}^+$

In this section we speak about the construction of the operator $\mathcal{R}^+$.

We conjecture that $\mathcal{R}_\varepsilon^+$ approaches, at least in some weak sense, some limit compact operator $\mathcal{R}^+$. Then, passing to the limit in (4.5), $\mathcal{R}^+$ should be solution of the characteristic equation:

$$\mathcal{T}(\mathcal{R}) := \mathcal{T}_{10}^+ \, \mathcal{R}^2 + \left(\mathcal{T}_{00}^+ + \mathcal{T}_{11}^+ \right) \mathcal{R} + \mathcal{T}_{01}^+ = 0. \tag{6.1}$$

Moreover, the constraint in (4.6) becomes, in the limit,

$$\rho(\mathcal{R}^+) \le 1. \tag{6.2}$$

However, (6.1)-(6.2) are not sufficient for determining $\mathcal{R}^+$ uniquely; an additional criterion needs to be found. In the following two sections, we develop heuristically, for the periodic half-guide problem, several possible ways of defining an operator $\mathcal{R}^+$, which satisfies (6.1)-(6.2) and which we hope to be the limit of $\mathcal{R}_\varepsilon^+$.

6.2   Towards the characterization of $\mathcal{R}^+$

In this section we characterize the eigenvalues and eigenvectors of $\mathcal{R}^+$. (We are not yet able to prove that $\mathcal{R}^+$ is diagonalizable).

We can show easily that $\mathcal{R}_\varepsilon^+$ depends continuously on ε and using [22], we can show that the eigenvalues $\lambda(\varepsilon)$ of $\mathcal{R}_\varepsilon^+$ depend continuously on ε too. So if $\mathcal{R}^+$ is the limit of $\mathcal{R}_\varepsilon^+$, the eigenvalues $\mathcal{R}^+$ should be the limits of the eigenvalues of $\mathcal{R}_\varepsilon^+$. Suppose $\lambda \in \mathbb{C}$ is an eigenvalue of $\mathcal{R}^+$ with the corresponding eigenfunction φ, then they satisfy

$$\mathcal{T}(\lambda)\varphi = 0, \quad \varphi \neq 0, \tag{6.3}$$

subject to the constraint

$$|\lambda| \leq 1. \tag{6.4}$$

We have defined $\mathcal{T}(\lambda)$ by replacing $\mathcal{R}$ by λ in (6.1).

Now we would like to determine which solutions of (6.3)-(6.4) are eigenvalues of $\mathcal{R}^+$. Clearly, a solution of (6.3) with $|\lambda| < 1$ is an eigenvalue of $\mathcal{R}^+$. What is not clear is when a solution of (6.3) satisfies exactly $|\lambda| = 1$.

First we show that the solutions of (6.3) comes in pairs of $(\lambda, 1/\lambda)$, just as in Theorem 5.1 where we showed this for $\varepsilon > 0$.

Theorem 6.1. *For any $\lambda \neq 0$, one has the property :*

$$Ker \; \mathcal{T}(\lambda) \neq 0 \quad \Longleftrightarrow \quad Ker \; \mathcal{T}(1/\lambda) \neq 0.$$

If there are solutions on the unit circle, then according to Theorem 6.1, there are necessarily an even number of them and these solutions come in pairs of $(\lambda, \overline{\lambda})$. This suggests that when there are N pairs of this type, the characteristic equation (6.1) admits 2^N solutions with spectral radius ≤ 1. (This can be proven rigorously in the quasi-1D case; see Remark 5.1). Only one of these solutions is $\mathcal{R}^+$. In terms of eigenvalues, in each pair, since

$$\{\lambda, \overline{\lambda}\} = \lim_{\varepsilon \to 0}\{\lambda(\varepsilon), \lambda(\varepsilon)^{-1}\} \quad \text{with} |\lambda(\varepsilon)| < 1,$$

only one element of the pair is an eigenvalue of $\mathcal{R}^+$. The problem is to determine which one.

A first heuristic approach consists in computing the eigenvalues $\{\lambda_i(\varepsilon)\}$ of the operator $\mathcal{R}_\varepsilon^+$ for a small ε and choosing among the pair $(\lambda_i, \overline{\lambda_i})$ the one closer to $\lambda_i(\varepsilon)$. However, it can happen, in terms of numerical implementation, when there are multiple pairs on the unit circle and when ε is not small enough, one can have trouble determining which $\lambda(\varepsilon)$ goes with which pair $(\lambda, \overline{\lambda})$. In this case one can try to make a determination based on the eigenvectors.

A more rigorous approach consists in looking at the solutions $\lambda(\varepsilon)$ of (5.1) as functions of ε, and looking at the derivative values $\frac{\partial\lambda}{\partial\varepsilon}(0)$. Let λ with $|\lambda| = 1$ be a solution of (6.3). It is an eigenvalue of $\mathcal{R}^+$ if and only if there exists a solution $\lambda(\varepsilon)$ of (5.1)-(5.2) such that:

$$\lambda = \lim_{\varepsilon \to 0} \lambda(\varepsilon). \tag{6.5}$$

Let us make the first assumption (that we conjecture to be generically satisfied):

(H1) λ is a solution of (6.3) with multiplicity one, namely,
dim Ker $\mathcal{T}(\lambda) = 1$.

From [12], we know that the function $\lambda(\varepsilon)$ is differentiable and we make the second assumption:

(H2) $\mathrm{Re}\left(\dfrac{\partial \lambda}{\partial \varepsilon}(0)\,\overline{\lambda}\right) \neq 0.$

(This second assumption asserts the movement of $\lambda(\varepsilon)$ is not tangential to the unit circle at λ.)

We now give a condition for ensuring that λ is an eigenvalue of $\mathcal{R}^+$, which is the content of the following lemma.

Lemma 6.2. *Assume that λ, with $|\lambda| = 1$, is a complex number that satisfies (6.5) as well as assumptions* (H1) *and* (H2). *Then λ is an eigenvalue of the operator $\mathcal{R}^+$ if and only if*

$$Re\left(\frac{\partial \lambda}{\partial \varepsilon}(0)\,\overline{\lambda}\right) < 0. \tag{6.6}$$

Proof. Simply remark that

$$\frac{\partial}{\partial \varepsilon}\left(|\lambda(\varepsilon)|^2\right)(0) = 2\,\mathrm{Re}\,\left(\frac{\partial \lambda}{\partial \varepsilon}(0)\,\overline{\lambda(0)}\right).$$

This will lead to (6.6).   □

Remark 6.1. In the limit case $\mathrm{Re}(\frac{\partial \lambda}{\partial \varepsilon}(0)\,\overline{\lambda}) = 0$, one would need to look at, at least, $\frac{\partial^2 \lambda}{\partial \varepsilon^2}(0)$ in order to obtain a conclusion. We have not considered this case because it occurs very rarely in practice.

Remark 6.2. Considering that

$$\frac{\partial}{\partial \varepsilon}\left(\frac{1}{|\lambda(\varepsilon)|^2}\right)(0) = -2\,\mathrm{Re}\,\left(\frac{\partial \lambda}{\partial \varepsilon}(0)\,\overline{\lambda(0)}\right),$$

it is easy to see that if the term on the right is not equal to 0, exact one element of the pair, $(\lambda, 1/\lambda)$, $|\lambda| = 1$, satisfies the condition in (6.6).

The condition (6.6) will provide an effective criterion if we are able to give a computable expression for $\frac{\partial \lambda}{\partial \varepsilon}(0)$. To get such an expression, we first determine the operators $\frac{\partial \mathcal{T}_{pq}^+}{\partial \varepsilon}(0)$. It is straightforward to see that these operators are defined by:

$$\frac{\partial \mathcal{T}_{00}^+}{\partial \varepsilon}(0)\,\varphi = -\left.\frac{\partial}{\partial x}\tilde{u}_0^+(\varphi)\right|_{\Gamma^+}, \quad \frac{\partial \mathcal{T}_{01}^+}{\partial \varepsilon}(0)\,\varphi = \left.\frac{\partial}{\partial x}\tilde{u}_0^+(\varphi)\right|_{\Gamma_1^+},$$

$$\frac{\partial \mathcal{T}_{10}^+}{\partial \varepsilon}(0)\,\varphi = -\left.\frac{\partial}{\partial x}\tilde{u}_1^+(\varphi)\right|_{\Gamma^+}, \quad \frac{\partial \mathcal{T}_{11}^+}{\partial \varepsilon}(0)\,\varphi = \left.\frac{\partial}{\partial x}\tilde{u}_1^+(\varphi)\right|_{\Gamma_1^+},$$

where $\tilde{u}_j^+(\varphi)$, $j = 0, 1$, are solutions of

$$\begin{cases} -\triangle \tilde{u}_j^+(\varphi) - n(\mathbf{x})^2 \, \omega^2 \, \tilde{u}_j^+(\varphi) = \imath \, n(\mathbf{x})^2 \, u_j^+(\varphi), \quad \text{in } C^+, \\ \\ \tilde{u}_j^+(\varphi) = 0 \quad \text{on } \Gamma^+ \text{ and } \Gamma_1^+. \end{cases} \tag{6.7}$$

Theorem 6.2. *Let λ be given by (6.5) and $\varphi \in Ker\, \mathcal{T}(\lambda)$. Then*

$$\frac{\partial \lambda}{\partial \varepsilon}(0) \;=\; -\frac{A(\lambda, \varphi)}{B(\lambda, \varphi)},$$

with

$$\begin{cases} A(\lambda, \varphi) &= \left(\left[\lambda^2 \dfrac{\partial \mathcal{T}_{10}^+}{\partial \varepsilon}(0) + \lambda \left(\dfrac{\partial \mathcal{T}_{11}^+}{\partial \varepsilon}(0) + \dfrac{\partial \mathcal{T}_{00}^+}{\partial \varepsilon}(0) \right) + \dfrac{\partial \mathcal{T}_{01}^+}{\partial \varepsilon}(0) \right] \varphi, \; \varphi \right), \\ \\ B(\lambda, \varphi) &= \left(\left[2\lambda \mathcal{T}_{10}^+ + \mathcal{T}_{11}^+ + \mathcal{T}_{00}^+ \right] \varphi, \; \varphi \right). \end{cases}$$

where $(\cdot, \cdot)$ is the scalar product of $L^2(\Gamma^+)$.

Proof. By definition of $\lambda(\varepsilon)$, there exists $\varphi(\varepsilon)$ differentiable [12] satisfying

$$\Big(\varphi(\varepsilon), \varphi(\varepsilon) \Big) = 1, \quad \text{and} \quad \varphi = \lim_{\varepsilon \to 0} \varphi(\varepsilon),$$

such that

$$\mathcal{T}(\varepsilon, \lambda(\varepsilon)) \, \varphi(\varepsilon) = 0.$$

We differentiate this equality with respect to ε, evaluate the result for $\varepsilon = 0$ and take the scalar product with φ. We get:

$$\left(\frac{\partial \mathcal{T}}{\partial \varepsilon}(0, \lambda) \, \varphi, \varphi \right) + \frac{\partial \lambda}{\partial \varepsilon}(0) \left(\frac{\partial \mathcal{T}}{\partial \lambda}(0, \lambda) \, \varphi, \varphi \right) + \left(\mathcal{T}(0, \lambda) \, \frac{\partial \varphi}{\partial \varepsilon}(0), \varphi \right) \;=\; 0.$$

Using Lemma 6.1, one sees that

$$[\mathcal{T}(0, \lambda)]^* = \overline{\lambda^2} \, \mathcal{T}(1/\overline{\lambda}) = \overline{\lambda^2} \, \mathcal{T}(\lambda), \quad \text{since } |\lambda| = 1.$$

Consequently,

$$\left(\mathcal{T}(0, \lambda) \, \frac{\partial \varphi}{\partial \varepsilon}(0), \varphi \right) = \overline{\lambda}^2 \left(\frac{\partial \varphi}{\partial \varepsilon}(0), \mathcal{T}(0, \lambda) \, \varphi \right) = 0.$$

One concludes since $\left(\dfrac{\partial \mathcal{T}}{\partial \varepsilon}(0, \lambda) \, \varphi, \varphi \right) = A(\lambda, \varphi)$ and $\left(\dfrac{\partial \mathcal{T}}{\partial \lambda}(0, \lambda) \, \varphi, \varphi \right) = B(\lambda, \varphi)$. $\qquad \square$

Remark 6.3. We show in the Appendix how the condition in (6.6) can be related to the sign of the group velocity of the so-called propagating Floquet modes. These are particular solutions of the Helmholtz equation in an infinite periodic waveguide of the form :

$$u(x, y) = e^{\imath \theta x} u_p(x, y),$$

where $\lambda = e^{\imath \theta}$ and u_p is periodic in x. One recovers in this way the more traditional notion of outgoing modes (see [19]).

6.3   About the resolution of the characteristic equation

As in the case with absorption, we propose two different methods to determine $\mathcal{R}^+$:

(i) via a spectral decomposition. We determine the eigenfunctions and eigenvalues of
$\mathcal{R}^+$ by solving the quadratic eigenvalue problem (6.3), and for selecting the good
eigenvalues of modulus one :

    (a) either we apply the heuristic idea exploiting the proximity of the eigenvalues of
$\mathcal{R}_\varepsilon^+$ for ε small enough. This requires an additional resolution of the character-
istic equation;

    (b) or the criterion in (6.6) of Lemma 6.2. This requires the determination of the
operators $\frac{\partial}{\partial\varepsilon}\mathcal{T}_{pq}^+$, $p,q = 0,1$, through the resolution of the boundary problems
(6.7).

(ii) combine the modified Newton's algorithm as explained in Section 5.2 with a contin-
uation method with respect to ε. In practice, this will consist in:

    (a) computing the solution $\mathcal{R}_\varepsilon$ of (4.5)-(4.6) for ε small enough;

    (b) applying the modified Newton algorithm to the limit equation starting from
$\mathcal{R}_\varepsilon^+$ as an initial guess.

The second method has the advantage of avoiding any diagonalization process which is
costly from the computation point of view and is harder to justify.

7   Numerical results

Since we do not have actual "physical solutions" to the problem of wave propagation in
an infinite periodic waveguide containing a local perturbation, we cannot say for certain
that the solution we obtain by following the procedure described in the previous sections
is indeed the "good" solution. Hence, we make comparisons to check self-consistency in
all the numerical examples.

In particular, we compare the spectral decomposition approach and the modified New-
ton's method to see that they produce the same $\mathcal{R}^+$. However, from a practical point of
view, we think that using the modified Newton's algorithm and continuation with respect
to ε is preferable to the spectral approach because it avoids any diagonalization procedure.
The spectral approach also suffers from some uncertainty in terms of

- when one checks the closeness of $(\lambda,\overline{\lambda})$ to $\lambda(\varepsilon)$, how to choose the size of ε;
- when one checks the sign of $\mathrm{Re}\left(\frac{\partial\lambda}{\partial\varepsilon}(0)\,\overline{\lambda}\right)$, what to do when it is very close to 0.

The "Newton plus continuation" approach is more automatic. Of course, one must also
choose ε to be small enough so that the Newton's method converges to the "good" solution
of (5.1).

7.1 Discretization and implementation issues

We introduce a regular (for simplicity) 1D mesh of Γ^+ made of N equal segments of length $k > 0$ and approximate $L^2(\Gamma^+)$ by the subspace L^2_k of piecewise constant functions on this mesh. The approximate operators $\mathcal{T}^{+,k}_{\varepsilon,pq}$, $\mathcal{R}^{+,k}_{\varepsilon}$, and $\Lambda^{+,k}_{\varepsilon}$ will be constructed as operators in $\mathcal{L}(L^2_k)$ and thus are represented by $N \times N$ matrices.

For solving the cell problems (4.1)-(4.2) (we have $2N$ problems of this type), we first rewrite (4.1) as a (∇, div) first order system, use $H(\mathrm{div}) \times L^2$ mixed formulation [4] and discretize the resulting variational problem with the lowest order Raviart-Thomas mixed finite elements [20] on a "periodic" mesh of C^+ (i.e. the "traces" of this mesh on Γ^+ and Γ^+_1 coïncide with the 1D mesh introduced above). The advantage of such a choice is that both the traces of the scalar unknown and of its normal derivative are degrees of freedom of the method and both belong to L^2_k, so that the operators $\mathcal{T}^{+,k}_{\varepsilon,pq}$ are naturally in $\mathcal{L}(L^2_k)$.

To determine $\mathcal{R}^{+,k}_{\varepsilon}$, we use the discrete version of one of the two methods presented in Section 5. For the finite dimensional version of the Newton method presented in 5.2, we have implemented Bartels-Stewart method as explained in [9].

In practice, the limit absorption operators $\mathcal{T}^{+,k}_{pq}$ are found by the procedure described above, i.e., by solving $2N$ variational problems (4.1)-(4.2) on C^+, but with $\varepsilon = 0$. To obtain $\mathcal{R}^{+,k}$, we use one of the two methods proposed in the section 6.3. Once $\mathcal{R}^{+,k}$ is available, $\mathcal{S}^{+,k}$ and $\Lambda^{+,k}$ can be computed via (4.11).

7.2 A one-dimensional example

We begin with a one-dimensional example, shown in Figs. 2, 3, 4, and 5. In this case, the method used to solve the cell problems is a finite difference method.

The profiles of $n(x)^2$ and $f(x)$ are shown in Fig. 2(a). To begin, we make the choice $\Omega^0 = (-0.5, 0.5)$, $h^- = 1$, $h^+ = 1$, and $\omega = 5$.

The operators $R^{\pm,k}$ in this case are just complex numbers. In Fig. 3(a) we plot the two roots of the quadratic equation associated with $R^{-,k}$ (marked by a square and a cross). They both lie exactly on the unit circle. Then we solve the quadratic equation associated with $R^{-,k}_{\varepsilon}$, with $\varepsilon = 0.1$. The root which is < 1, i.e., $R^{-,k}_{\varepsilon}$, is plotted inside the unit circle (marked by a diamond). As a result, $R^{-,k}$ is chosen to be the root in the lower half complex plane (marked by the square), since this root is closer to $R^{-,k}_{\varepsilon}$. In Fig. 3(b), we show that $R^{+,k}$ is also chosen to be the complex number on the unit circle that is in the lower half complex plane.

We can also calculate, as described in the Section 6.2, the derivative with respect to ε of the two roots and choose the one for which the condition in (6.6) holds, that is, the one whose derivative is directed towards the interior of the unit circle. This is illustrated in Figs. 4(a) and 4(b).

In Fig. 2(b) we show that the solution (dashed) for $\omega = 5$, $h^- = 1$, and $h^+ = 1$, obtained by using $\Omega^0 = (-1.5, 1.5)$, is identical to that (solid) obtained by using the smaller interval $\Omega^0 = (-0.5, 0.5)$.

(a) $n(x)^2$ and $f(x)$ (b) $\Omega^0 = (-1.5, 1.5)$ and $\Omega^0 = (-0.5, 0.5)$
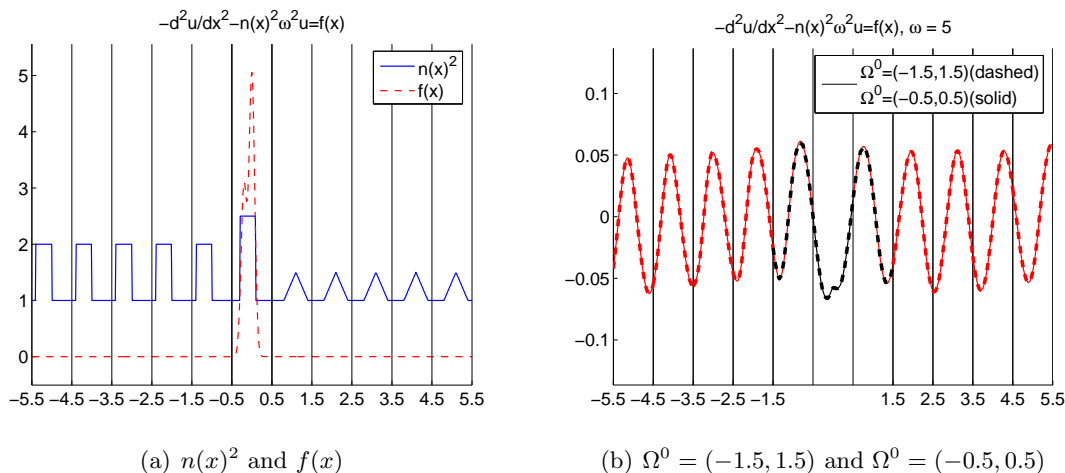
Figure 2: One dimensional example. In Fig. 2(b) we show the solution (dashed) using $\Omega^0 = (-1.5, 1.5)$ superimposed on the solution (solid) using $\Omega^0 = (-0.5, 0.5)$. They are identical.
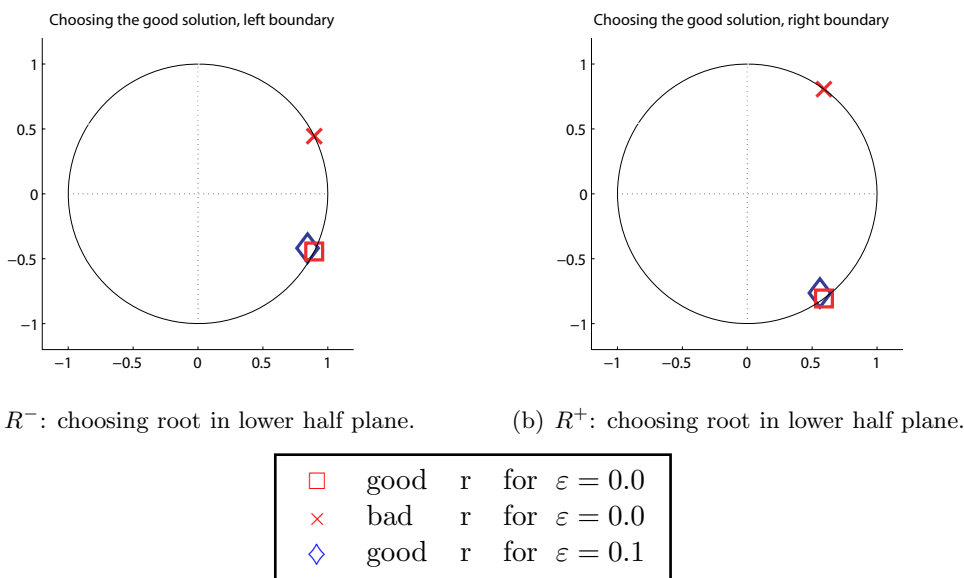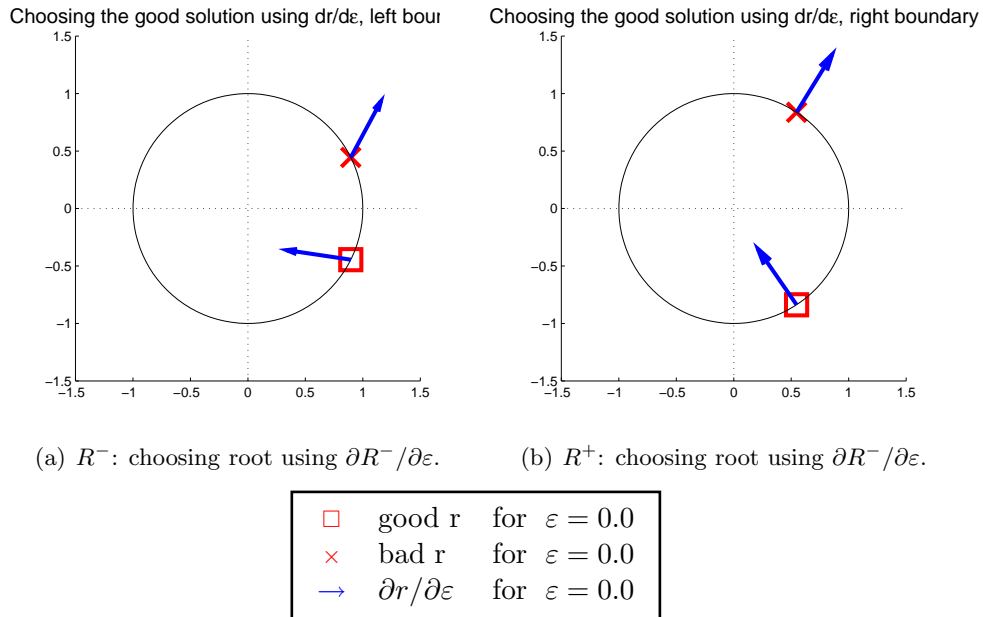

(a) R^-: choosing root in lower half plane.   (b) R^+: choosing root in lower half plane.

□	good	r	for	$\varepsilon = 0.0$
×	bad	r	for	$\varepsilon = 0.0$
◇	good	r	for	$\varepsilon = 0.1$

Figure 3: One dimensional example: $R^\pm$ are chosen to be the roots (squares, on unit circle) in the lower half plane because they are closer to $R_\varepsilon^\pm$ (diamonds, inside the unit circle).
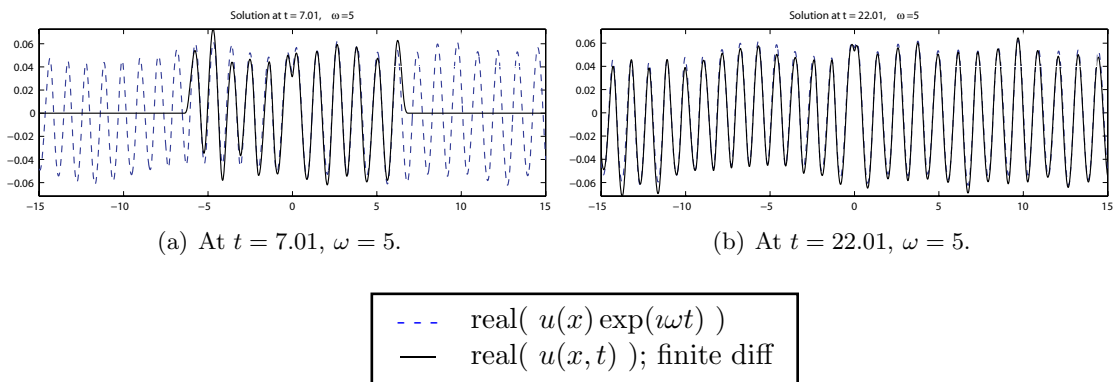
Then we tested the validity of our frequency domain solution using the limiting amplitude principle [7], whereby if $u(x,t)$ is the solution to the time domain problem,

$$n(x)^2 \frac{\partial^2 \bar{u}(x,t)}{\partial t^2} - \frac{\partial^2 \bar{u}(x,t)}{\partial x^2} = f(x) \, e^{-i\omega t}, \tag{7.1}$$

Choosing the good solution using dr/dε, left boun   Choosing the good solution using dr/dε, right boundary

(a) R^-: choosing root using $\partial R^-/\partial\varepsilon$.   (b) R^+: choosing root using $\partial R^-/\partial\varepsilon$.

□	good r	for	$\varepsilon = 0.0$
×	bad r	for	$\varepsilon = 0.0$
→	$\partial r/\partial\varepsilon$	for	$\varepsilon = 0.0$

Figure 4: One dimensional example: the same result is obtained using criterion (6.6).

Solution at t = 7.01, ω = 5   Solution at t = 22.01, ω = 5

(a) At $t = 7.01$, $\omega = 5$.   (b) At $t = 22.01$, $\omega = 5$.

- - -	real($u(x)\exp(\imath\omega t)$)
——	real($u(x,t)$); finite diff

Figure 5: We illustrate the limiting amplitude principle by comparing $u(x,t)$(solid) and $u(x)e^{-\imath\omega t}$(dashed), $-100 \geq x \geq 100$. It is clear that $u(x,t)$ approaches $u(x)e^{-\imath\omega t}$ as t increases.

then we expect that (non uniformly in x)

$$\lim_{t\to+\infty} \bar{u}(x,t)\ e^{\imath\omega t} = u(x), \tag{7.2}$$

where $u(x)$ is the good physical solution of the frequency domain problem:

$$-\frac{d^2u(x)}{dx^2} - \omega^2 n(x)^2 u(x) = f(x).$$

We solved (7.1) using a simple finite difference scheme, with $f(x) = 3\exp(-100.(x + 0.2)^2).\chi_{[-0.5;0.5]}$, taking care to choose a computational domain large enough so that there

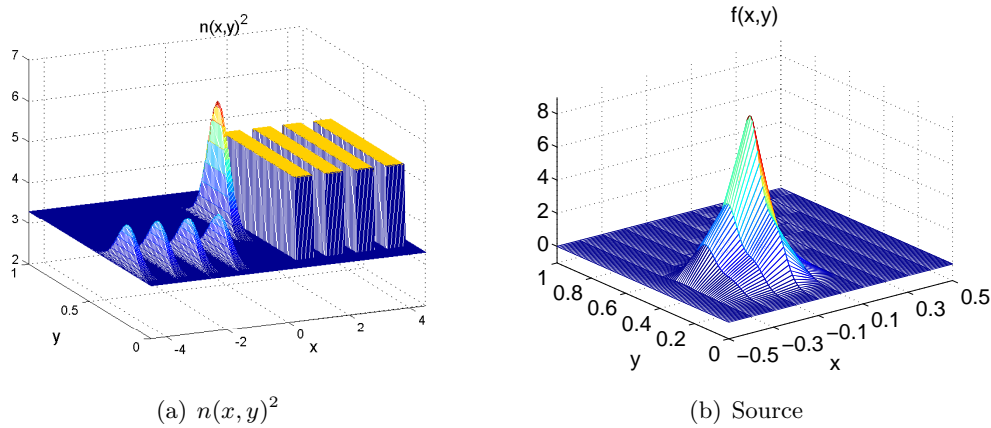(a) $n(x,y)^2$ (b) Source

Figure 6: A two dimensional example.

are no spurious reflections at the ends of the domain for the times we were considering. In Figs. 5(a) and 5(b) we show $u(x,t)$ and $u(x)e^{-i\omega t}$ at $t = 7.01$ and $t = 22.01$. It is clear that the time domain solution $u(x,t)$ is approaching the time-harmonic limit $u(x)e^{-i\omega t}$ as t increases.

7.3   The 2D case

In two dimensions, we have written a code using the lowest order rectangular Raviart-Thomas mixed finite elements.

7.3.1   A first 2D example

We present two-dimensional results for the example shown in Fig. 6, where $n(x,y)^2$ and $f(x,y)$ are displayed. The boundary conditions on $\partial\Omega$ are Neumann and we let $\omega = 15$. First, we choose the computational parameters to be $h^+ = h^- = 1$, $a^- = -0.5$, and $a^+ = 0.5$. The discretization step in the two directions (x and y) is $k = 0.0125$ (N=80). Note that this is a reasonable choice since the minimal wavelength of the solution is about 0.1. Moreover, we have checked that the solution we present here remains the same under mesh refinement.

In Figs. 7, 8, and 9, we illustrate how to choose the eigenvalues of the operators $R^{\pm,k}$. In Fig. 7(b), we show all the candidates for being the eigenvalues of $\mathcal{R}^{+,k}$ (circles in the complex plane) obtained by solving (6.3) with constraint (6.4). Note that there are a lot of eigenvalues which cluster around 0. In Fig. 7(a) we show the analogous picture for $\mathcal{R}^{-,k}$.

In Fig. 8(b), we solve (5.1)-(5.2) with $\varepsilon = 0.1$; the corresponding eigenvalues of $\mathcal{R}^{+,k}_{\varepsilon}$ are represented with diamonds. Most solutions of (5.1) whose norm is greater than 1 are also represented, by squares. We select the eigenvalues of $\mathcal{R}^{+,k}$, those marked by circles; the candidates marked by an $\times$ are eliminated. Fig. 8(a) shows the analogous picture for

(a) Eigenvalue candidates for $R^{-,k}$ (b) Eigenvalue candidates for $R^{+,k}$

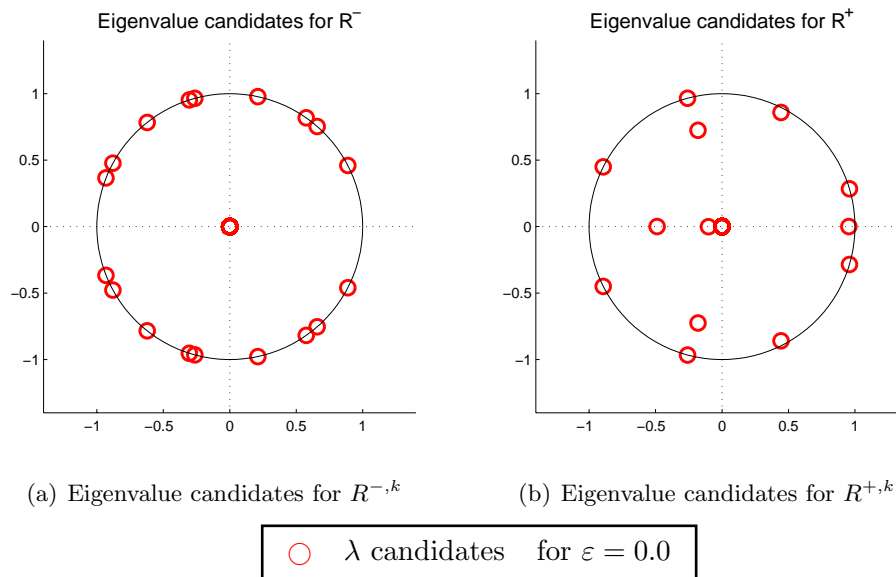○ λ candidates   for $\varepsilon = 0.0$

Figure 7: All the solutions of the quadratic eigenvalue problem associated with $\mathcal{R}^{\pm,k}$ are plotted as circles.

$\mathcal{R}_{\varepsilon}^{-,k}$ and $\mathcal{R}^{-,k}$. There two pairs whose real part is close to -0.3: we have distinguished between them by comparing the associated eigenvectors.

In the Figs. 9(a) and 9(b), we show how to choose the eigenvalues using criterion (6.6). We keep only the eigenvalue candidates whose derivative is directed towards the interior of the unit circle. First note that in Fig. 9(a) the difficulty present in the previous method for choosing within the pairs whose real part is close to -0.3 is removed by calculating the derivatives. However, also note that in Fig. 9(b) the derivatives of a pair $(\lambda, 1/\lambda)$ (the one whose real part is close to -0.8) are tangential to the unit circle: it is a case for which it is not possible to determine which eigenvalue we have to choose. However, this difficulty is not present in the previous method. Thus, the two methods of choosing the good eigenvalue candidates can be complementary.

We note here that the modified Newton's method plus continuation is automatic and produced the same result without the ambiguity concerning particular eigenvalues associated with the previous two methods.

In Fig. 10(a) we show the real part of the solution for this problem. We checked the validity of this result in two ways. First, we checked the convergence of the method by mesh refinement. Choosing as the reference solution the solution obtained on the finest mesh, we have been able to verify first order of convergence in the L^2 norm. Secondly, we changed the computational parameters associated with the location of the artificial boundary, this time, to $a^- = -2$ and $a^+ = 1$, and verified that the obtained solution is insensitive to this change (see Fig. 10(b)). The relative difference between the solutions arising from the two parameters choices is within 5×10^{-5}.
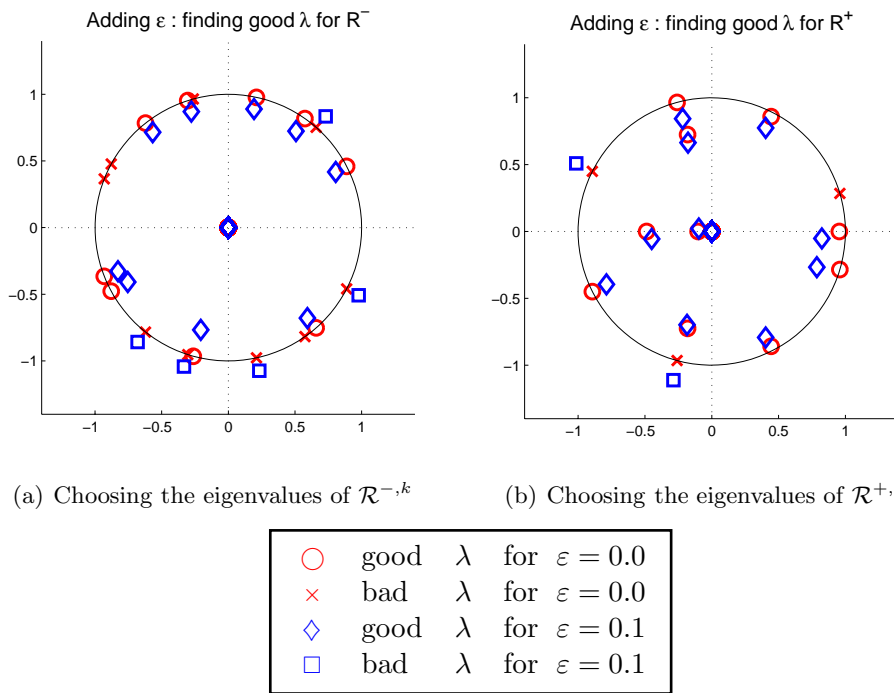
Adding ε : finding good λ for R⁻

Adding ε : finding good λ for R⁺

(a) Choosing the eigenvalues of $\mathcal{R}^{-,k}$

(b) Choosing the eigenvalues of $\mathcal{R}^{+,k}$

◯	good	λ	for	$\varepsilon = 0.0$
×	bad	λ	for	$\varepsilon = 0.0$
◇	good	λ	for	$\varepsilon = 0.1$
□	bad	λ	for	$\varepsilon = 0.1$

Figure 8: Choosing the eigenvalues of $R^{\pm,k}$. We see that of all the eigenvalue candidates which lie exactly on the unit circle, half are approached by an eigenvalue of $R_\varepsilon^{\pm,k}$. These are chosen to be the eigenvalues of $R^{\pm,k}$ and are marked by a circle. The rest, marked by an ×, are discarded.

Using ∂λ/∂ε : good λ whose norm is 1 for R⁻

Using ∂λ/∂ε : good λ whose norm is 1 for R⁺

(a) Choosing the eigenvalues of $\mathcal{R}^{-,k}$

(b) Choosing the eigenvalues of $\mathcal{R}^{+,k}$

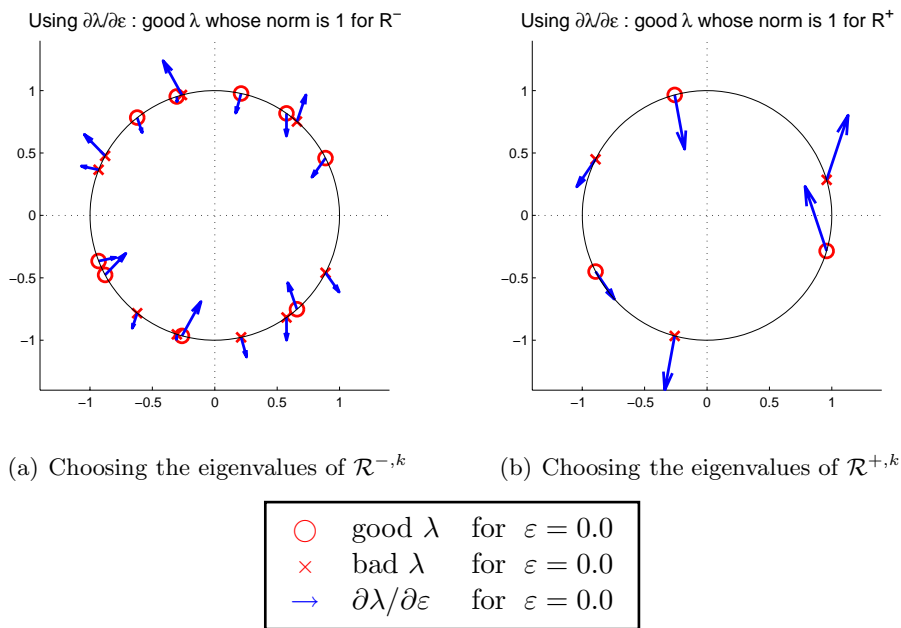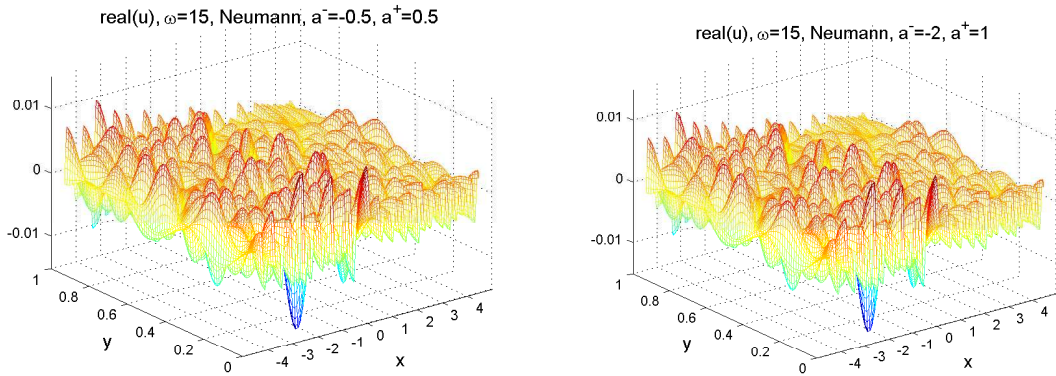| ◯	good λ	for	$\varepsilon = 0.0$
×	bad λ	for	$\varepsilon = 0.0$
→	$\partial\lambda/\partial\varepsilon$	for	$\varepsilon = 0.0$

Figure 9: Choosing the eigenvalues of $R^{\pm,k}$ using the condition (6.6), we keep the eigenvalues whose derivative is directed towards the interior of the unit circle.
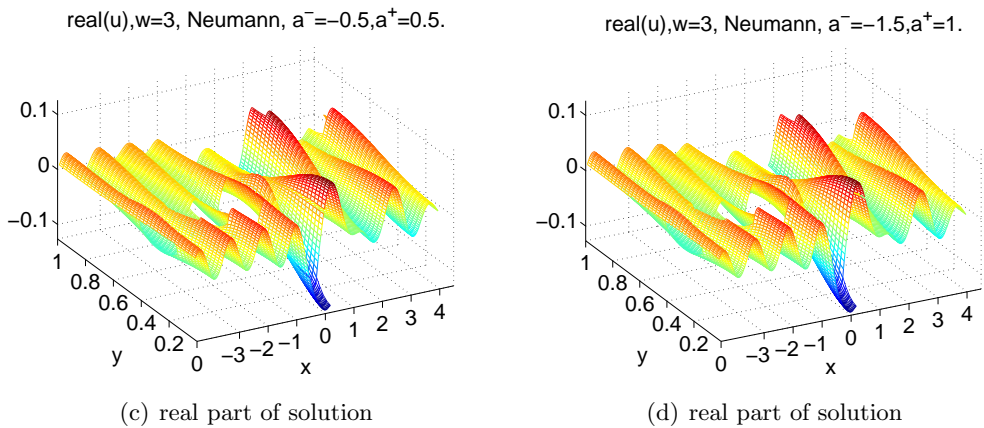
(a) Solution for $h^+ = h^- = 1, a^- = -0.5, a^+ = 0.5$ (b) Solution for $h^+ = h^- = 1, a^- = -2, a^+ = 1$

Figure 10: Real part of the solution for the example shown in Fig. 6, when solving (2.1) subject to homogeneous Neumann boundary conditions on $\partial\Omega$ and letting $\omega = 15$. Two choices of computational parameters yield identical solutions.
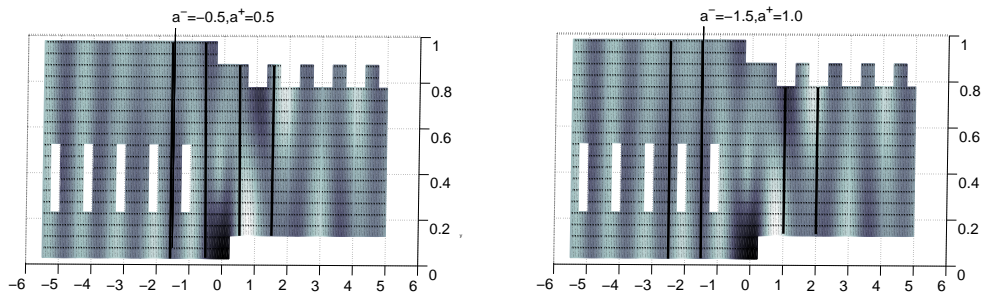
(a) $h^+ = h^- = 1$, $a^- = -0.5$, $a^+ = 0.5$ (b) $h^+ = h^- = 1$, $a^- = -1.5$, $a^+ = 1$

(c) real part of solution   (d) real part of solution

Figure 11: For the waveguide, using two sets of computational parameters, shown in Figs. 11(a) and 11(b), results in identical solutions.

7.4   A second 2D example

Now we consider a homogeneous waveguide ($n(x,y) = 1$), whose geometry is periodic and more complex. The reference cell C^- has a rectangular hole, Ω_0 is the transition domain, and the reference cell C^+ has an irregular upper boundary. We set $\omega = 5$ and solved with homogeneous Neumann conditions on $\partial\Omega$. The two sets of computational parameters we chose are $h^+ = h^- = 1$, $a^- = -0.5$, $a^+ = 0.5$, and $h^+ = h^- = 1$, $a^- = -1.5$, $a^+ = 1$, respectively. The exact geometries of these two choices are shown in Figs. 11(a) and 11(b). In Figs. 11(c) and 11(d) we show that changing the computational parameters does not change the solution we obtain.

8   Conclusions

In this paper we have described a method of constructing transparent boundary conditions for the problem of modeling wave propagation in a periodic closed waveguide which may contain a local perturbation. When the problem includes absorption, we have shown rigorously that the boundary conditions we construct are exact. We have made heuristic arguments for the case of the limit problem, when the absorption parameter goes to zero.

We have shown that the numerical procedure we propose works well in practice and checked our numerical results for self-consistency. We hope to be able to provide rigorous theoretical justification of our approach for the limit absorption case in a subsequent paper.

A   On the interpretation of the criterion of Lemma 6.2 as an outgoing condition

We consider the infinite periodic waveguide generated from the periodicity cell C_0^+:

$$\Omega_\infty^+ = \bigcup_{j=-\infty}^{+\infty} C_j^+.$$

We consider the Helmholtz equation

$$-\Delta u(\mathbf{x}) - n(\mathbf{x})^2\, \omega^2\, u(\mathbf{x}) = f(\mathbf{x}) \quad \text{in } \Omega_\infty^+. \tag{A.1}$$

Propagating Floquet modes are particular solutions of (A.1) of the form

$$u(x,y) = u_p(x,y)\, e^{\imath\theta x} \quad \left(\iff u(x,y)\, e^{-\imath\omega t} = u_p(x,y)\, e^{\imath(\theta x - \omega t)} \right), \tag{A.2}$$

where u_p is h^+-periodic function with respect to x and where $\theta \in [0, 2\pi]$ is by definition the wave number. The study of such solutions is closely related to the spectral theory of the unbounded (in L^2) self-adjoint operator A_p defined by:

$$D(A_p) = H^2(\Omega_\infty^+), \quad A_p = -\frac{1}{n(x,y)^2}\triangle.$$

The spectral theory of this operator is well known [13]. Introduce the reduced operators $A_p(\theta)$, $\theta \in [0, 2\pi]$ defined by:

$$
\begin{cases}
D(A_p(\theta)) = \left\{ u \in H^2(C^+),\ u|_{\Gamma_1} = e^{\imath\theta} u|_{\Gamma} \text{ and } \left.\dfrac{\partial u}{\partial x}\right|_{\Gamma_1} = e^{\imath\theta} \left.\dfrac{\partial u}{\partial x}\right|_{\Gamma} \right\}, \\[2mm]
A_p(\theta) = A_p|_{D(A_p(\theta))}.
\end{cases}
$$

Then the spectrum of A_p is given by:

$$
\sigma(A_p) = \bigcup_{\theta \in [0,2\pi]} \sigma(A_p(\theta)) \quad \text{where} \quad \sigma(A_p(\theta)) = \{\mu_n(\theta),\ n \geq 1\} \tag{A.3}
$$

and $0 \leq \mu_1(\theta) \leq \mu_2(\theta) \leq \ldots \leq \mu_n(\theta) \to +\infty$ are the eigenvalues of $A_p(\theta)$. Clearly, the operator $A_p(\theta)$ is well defined for $\theta \in \mathbb{C}$ and depends analytically on theta. Therefore, using well-known results from perturbation theory (see [12]), *each* eigenvalue $\mu_k(\theta)$ can be extended as an analytic function of θ in the neighborhood of the real axis in such way that the equality (A.3) holds for complex θ.

It is immediate that (A.2) is solution of (A.1) if and only if ω and θ are related by the following dispersion relation:

$$
\omega^2 = \mu_k(\theta) \quad \text{for some } k. \tag{A.4}
$$

If we impose $\omega > 0$, this gives:

$$
\omega = \mu_k(\theta)^{1/2},
$$

from which we define the good velocity of the mode (A.2), $v_k(\theta)$:

$$
v_k(\theta) = \frac{1}{2} \mu_k(\theta)^{-1/2} \mu_k'(\theta) \quad \left(\equiv \frac{\partial\omega}{\partial\theta}(\theta) \right). \tag{A.5}
$$

Next, we reinterpret the result of Lemma 6.2 in terms of the propagation of Floquet modes. Let $\lambda = e^{\imath\theta}$, $\theta \in [0, 2\pi]$ satisfy assumptions (6.5), (H1) and (H2). Obviously, there exists a function $\theta(\varepsilon) \in \mathbb{C}$ such that:

$$
\lambda(\varepsilon) = e^{\imath\theta(\varepsilon)} \text{ and } \lim_{\varepsilon \to 0} \theta(\varepsilon) = \theta. \tag{A.6}
$$

On the other hand, there exists an integer k such that:

$$
\omega^2 + i\varepsilon = \mu_k\big(\theta(\varepsilon)\big), \quad \text{for } \varepsilon \text{ small enough.} \tag{A.7}
$$

Indeed, by definition of $\lambda(\varepsilon)$, there exists $\varphi(\varepsilon) \in \operatorname{Ker} \mathcal{T}(\varepsilon, \lambda(\varepsilon))$. Let u_ε such that:

$$
u_\varepsilon = u_{\varepsilon,0}^+\big(\varphi(\varepsilon)\big) + u_{\varepsilon,1}^+\big(e^{\imath\theta(\varepsilon)}\varphi(\varepsilon)\big) \in H^1(C^+).
$$

By construction

$$
A_p\, u_\varepsilon = (\omega^2 + i\varepsilon)\, u_\varepsilon \quad \text{and} \quad u_{\varepsilon|\Gamma_1} = e^{\imath\theta(\varepsilon)}\, u_{\varepsilon|\Gamma_0},
$$

and moreover

$$\mathcal{T}(\varepsilon, \lambda(\varepsilon))\ \varphi(\varepsilon) = 0,$$

we then obtain

$$\left.\frac{\partial u_\varepsilon}{\partial x}\right|_{\Gamma_1} = e^{\imath\theta(\varepsilon)}\ \left.\frac{\partial u_\varepsilon}{\partial x}\right|_{\Gamma_0}.$$

Therefore, u_ε is an eigenfunction of $(A_p(\theta)$ with eigenvalue $\omega^2 + i\varepsilon$.

Let us differentiate (A.6) and (A.7) and take the results for $\varepsilon = 0$, we get

$$\frac{\partial\lambda}{\partial\varepsilon}(0) = \imath\ \theta'(0)\ \lambda \quad \text{and} \quad \mu'_k(\theta)\ \theta'(0) = \imath\ .$$

Consequently,

$$\left(\frac{\partial\lambda}{\partial\varepsilon}(0)\ \overline{\lambda}\right)^{-1} = -\mu'_k(\theta)\ . \tag{A.8}$$

Looking at (A.8) and (A.5), we have shown that $\lambda = e^{\imath\theta}$ satisfies the criterion (6.6) of Lemma 6.2 if and only if

$$v_k(\theta) > 0,$$

i.e., the group velocity of the Floquet mode of wave number θ is strictly positive.

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