

Exact boundary conditions for time-harmonic wave propagation in locally perturbed periodic media

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ABSTRACT

We consider the solution of the Helmholtz equation with absorption $-\Delta u(\mathbf{x}) - n(\mathbf{x})^2(\omega^2 + i\varepsilon)u(\mathbf{x}) = f(\mathbf{x})$, $\mathbf{x} = (x, y)$, in a 2D periodic medium $\Omega = \mathbb{R}^2$. We assume that $f(\mathbf{x})$ is supported in a bounded domain Ω^i and that $n(\mathbf{x})$ is periodic in the two directions in $\Omega^e = \Omega \setminus \Omega^i$. We show how to obtain exact boundary conditions on the boundary of Ω^i , Σ_S that will enable us to find the solution on Ω^i . Then the solution can be extended in Ω in a straightforward manner from the values on Σ_S . The particular case of medium with symmetries is exposed. The exact boundary conditions are found by solving a family of waveguide problems.

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1. Introduction

Periodic media play a major role in applications, in particular in optics for micro and nano-technology [14,16,19,24]. 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 [19,20]. 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 the problem outside: this is particularly of interest when the periodic regions contain a large number of periodicity cells.

In the case where the unperturbed medium is homogeneous (in some sense, a periodic medium with an arbitrarily small period), this is a very old problematic. Various methods can be used to restrict the computation around the perturbation. A first class of methods consists in applying an artificial boundary condition which is transparent or approximately transparent. Let us cite:

- (i) the local radiation condition at finite distance [2,6],
- (ii) coupling techniques between volumic methods and integral representation or integral equation technique [10,13,15,21],
- (iii) the DtN approaches which consists in computing exactly the Dirichlet-to-Neumann operator associated to the exterior medium, provided that the geometry of the boundary is properly chosen (typically a circle in 2D).

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Methods (ii) and (iii) are exact (up to numerical approximation). The method (i) is approximate and its accuracy improves where the order of the condition increases or the artificial boundary goes to infinity. However, none of these methods can be applied or extended directly to general exterior periodic media because they use the homogeneous nature of the exterior medium (explicit formulas are used for the solution of the exterior problem in (i), (ii) and (iii), the knowledge of the Green function is used in case (ii) and separation of variables is used in case (iii)).

The second approach consists in surrounding the computational domain by an absorbing layer in which the PML technique [3] is applied. Physically the method can be interpreted as letting an incident wave from the computational domain enters the layer without reflexion and absorbs the wave inside the layer preventing it to come back in the computational domain. This principle is not adapted a priori to periodic media for which a wave leaving the computational domain will interact with heterogeneities of the medium up to infinity. That is why the standard PML technique cannot work in this case (see however the pole condition techniques that can be seen as a generalization of the PML method in the case of non-homogeneous media [11,12]).

It seems that there are very few works in the same spirit in the mathematical literature for the case of periodic perturbed media. A problem similar that have some similarities with the one we consider in this paper is the numerical computation of the localized modes (non-trivial solution of the propagation model in the absence of any source term) that may appear for specific frequencies due to the presence of a local perturbation of the periodic media (see [7–9] for existence results). The supercell method analyzed [25] has similarities with the radiation condition at finite distance (i): it consists in making computations in a bounded domain of large size, the resulting solution converging to the true solution when the size goes to infinity. Note however that in this case as the localized modes are exponentially decreasing, this convergence is exponentially.

The notion of DtN maps already appears for instance, in the works of T. Abboud [1] for the diffraction problem by periodic gratings or of J. Tausch [26] for periodic open waveguides. However in these two cases the DtN map is used to deal with the unboundedness of the propagation medium in the direction(s) transverse to the periodicity direction(s).

In a first paper [17], we treated the case of locally perturbed periodic waveguide: typically the unperturbed propagation medium is bounded in one direction and periodic in the other. We proposed a numerical method for determining DtN operators by solving local cell problems an operator valued stationary Riccati equation. In this paper we proposed an extension of the above work to the case where the unperturbed media is periodic in the two directions.

This article is devoted to the presentation of the conceptual aspects of our method and the exposition of the main theoretical issues. The numerical aspects are under way and will be treated in a forthcoming paper. Let us also mention that, in order to avoid mathematical difficulties, we consider the case where the propagation medium is slightly absorbing, the absorption being quantified by a small positive parameter $\varepsilon > 0$ (see Section 2). The challenging question of studying the limit case when ε tends to 0 (i.e. the limiting absorption principle, see Remark 2) is still an open question to our knowledge. However the method that we present here can be formally extended to non-absorbing media by using the heuristics proposed in [17] for the case of periodic waveguides.

2. The model problem

The model problem that we consider in this paper is the propagation of a time harmonic scalar wave in a 2D periodic medium, $\Omega = \mathbb{R}^2$, with a local perturbation. More precisely, we shall assume that the geometry as well as the material properties of the plane are x and y -periodic except in a bounded region (see Fig. 1). The propagation model we consider is a simple 2D $(\mathbf{x} = (x, y))$ scalar model:

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

where η is a physical parameter, typically small, that represents a slight absorption in the medium. We shall assume that $\eta > 0$. See Remark 2 for the limit case $\eta \rightarrow 0$.

This model can be used for instance in electromagnetism: the 2D model is then 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 refractive index of the medium. Moreover, we suppose that:

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

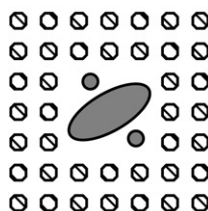


Fig. 1. The domain of propagation Ω .

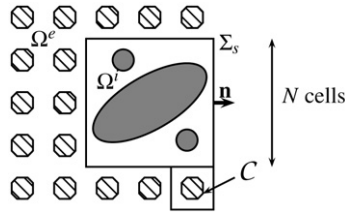


Fig. 2. Geometry and notation.

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

$$-\Delta u(\mathbf{x}) - n(\mathbf{x})^2(\omega^2 + i\varepsilon)u(\mathbf{x}) = f(\mathbf{x}) \tag{P}$$

with $\varepsilon = \eta\omega$. It is well known that this problem admits a unique solution in $H^1(\Delta, \Omega)$, the closed subspace of functions in $H^1(\Omega)$ whose Laplacian is in $L^2(\Omega)$.

The domain of propagation Ω is infinite in the two directions x and y and periodic outside a bounded region Ω^i (i for interior domain) (see Fig. 2). The exterior domain Ω^e is: $\Omega^e = \Omega \setminus \Omega^i$. The basic periodicity cell is denoted C :

$$C = \left] -\frac{L}{2}, \frac{L}{2} \right[^2.$$

In the sequel for the simplicity of the exposition, we will consider that the periodicity is the same in the x and y directions. L is the period.

The region Ω^i is a square, contains the defect, which is represented in three possible ways: a local source term f , a compact perturbation of the refraction index n and/or geometrical defects. In the following, Ω^i is chosen in such a way that the size of each edge is a multiple of the period of the medium:

$$\Omega^i = \left] -\frac{L}{2}, \frac{(2N-1)L}{2} \right[^2.$$

For the sake of presentation, we will suppose that $N = 1$ here. However the generalization is straightforward (see Appendix A).

The function n is supposed to coincide with a periodic function outside Ω^i . More precisely, we suppose that there exists a L -periodic function n_p , i.e.,

$$\forall (j, k) \in \mathbb{Z}^2, \quad \forall (x, y) \in \Omega \Rightarrow n_p(x, y) = n_p(x + jL, y + kL),$$

such that: $\text{Supp}(n - n_p) \subset \Omega^i$.

Our goal is to characterize the restriction of the solution u to Ω^i as the solution of (2) in Ω^i with boundary conditions of the form:

$$\frac{\partial u}{\partial \mathbf{n}} + \Lambda u = 0 \quad \text{on } \Sigma_S = \partial\Omega^i, \tag{1}$$

where $\Lambda \in \mathcal{L}(H^{1/2}(\Sigma_S), H^{-1/2}(\Sigma_S))$.

Remark 1. Considering that a constant medium is a particular periodic medium, our method thus provides as a by product a way to obtain exact DtN boundary conditions for an homogeneous exterior medium with an artificial boundary chosen along a square (and not a circle as is done usually).

Remark 2. The presence of the absorption term in (P) guarantees the well-posedness of the Helmholtz equation (existence and uniqueness of the solution u in \mathbb{R}^2). A natural question is to understand what happens as η or ε goes to 0: do the solutions of (P) have a limit? This is the limiting absorption principle. This question is linked, of course, to the question of (uniquely) defining the proper physical solution of:

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

This question is far from being obvious and is actually controversial for physicists (see for instance [4,23]).

In the case of periodic waveguides, this question was partially addressed in [17]. To our knowledge, in the general 2D case, this is still an open question, and, in this article, we will concentrate on the case with (possibly arbitrarily small) absorption.

This article is organized as follows. We will successively consider three particular situations of increasing complexity, each case using the solution from the previous one. Sections 3 and 4 provide intermediate results for Section 5, which is the main section of the article. In these two sections, we treat the construction of an exact DtN operator for problems that are simpler than the one we present in Section 2 but whose resolution is useful for the resolution of the full problem. In Section 3, we explain how to modify the method of [17] for the resolution of the locally perturbed waveguide to handle quasi-periodic conditions. Section 4 treats the construction of the DtN operator associated to a periodic halfspace: this operator can be characterized by mean of a half waveguide DtN operators. Section 5 deals with the resolution of the model problem. It contains the original aspects of the method (as compared to [17]). The key idea is to factorize the operator A in (1) as the product of A^H , the DtN operator associated to a periodic halfspace and a Dirichlet-to-Dirichlet operator. This new operator is characterized through an equation that we derive and for which well-posedness is proven. We provide an equation for this new operator for which we show an existence and uniqueness result. From the practical view point, it should be emphasized that the numerical resolution of this equation only requires the solution of local cell-problems, the same that are used for the computation of A^H . We give some conclusions and perspectives in Section 6. In Appendix B, we explain how to extend the method to the more general case of a medium without any symmetries.

Remark 3. The method developed in this article can be easily extended to more general elliptic operator $u \mapsto \nabla \cdot (\mu \nabla u)$ where μ is a compact perturbation of a periodic function.

The domain Ω can also be more complex, containing for example a periodic set of holes. In this case we have simply to ensure that the boundary conditions at the holes are compatible with the periodicity of the problem.

3. The periodic half waveguide problem

In this section we explain how to construct the DtN operator A^W associated to a periodic half-guide Ω^W :

$$\Omega^W = \bigcup_{n=0}^{+\infty} \{C + (n+1)L, 0\}.$$

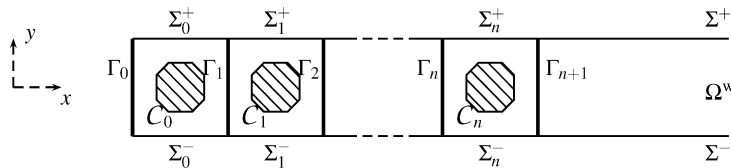


Fig. 3. Notation in the case of a half guide.

Note that by periodicity, all the “vertical” interfaces $\Gamma_n = \Gamma_0 + (nL, 0)$ can be identified to $\Gamma (= \Gamma_0) \sim [-L/2, L/2]$ and all the cells $C_n = C_0 + (nL, 0)$ to $C (= C_0)$. See Fig. 3.

3.1. Presentation of the problem

For a fixed $k \in [-\pi/L, \pi/L]$, we define the “half-guide problem”:

$$\begin{cases} -\Delta u^W(k; \varphi) - n(\mathbf{x})^2(\omega^2 + i\varepsilon)u^W(k; \varphi) = 0, & \text{in } \Omega^W, \\ u^W(k; \varphi) = \varphi, & \text{on } \Gamma_0, \\ u^W(k; \varphi)|_{\Sigma^+} = e^{ikL}u^W(k; \varphi)|_{\Sigma^-}, \\ \frac{\partial}{\partial y}u^W(k; \varphi)|_{\Sigma^+} = e^{ikL}\frac{\partial}{\partial y}u^W(k; \varphi)|_{\Sigma^-}. \end{cases} \quad (\mathcal{P}^W)$$

Let us begin with some functional analysis. Let us introduce the space:

$$C_k^\infty(\Omega^W) = \{u \in C^\infty(\Omega^W), u|_{\Sigma^+} = e^{ikL}u|_{\Sigma^-}\}.$$

We note $H_k^1(\Omega^W)$ the closure of $C_k^\infty(\Omega^W)$ in $H^1(\Omega^W)$ and $H_k^1(\Delta, \Omega^W)$ the closed subspace of functions in $H_k^1(\Omega^W)$ with Laplacian in $L^2(\Omega^W)$. We shall define the subspace $H_k^{1/2}(\Gamma)$ of $H^{1/2}(\Gamma)$ by:

$$H_k^{1/2}(\Gamma) = \{u|_\Gamma, u \in H_k^1(\Omega^W)\}.$$

Remark 4. $H_k^{1/2}(\Gamma)$ can also be defined as:

$$H_k^{1/2}(\Gamma) = \{\varphi \in H^{1/2}(\Gamma), \tilde{\varphi} \in H^{1/2}(\mathbb{R})\},$$

where $\tilde{\varphi}$ is the quasi-periodic extension of φ in \mathbb{R} , that means:

$$\forall m \in Z, \forall y \in \Gamma, \tilde{\varphi}(y + mL) = e^{ikmL}\varphi(y).$$

It can also be defined by (by a straightforward adaptation of the results of [22])

$$H_k^{1/2}(\Gamma) = \left\{ \varphi \in H^{1/2}(\Gamma), \int_{\Gamma} \frac{|\varphi(y) - e^{ikL}\varphi(-y)|^2}{y - L/2} dy < +\infty \right\}.$$

We will define $H_k^{-1/2}(\Gamma)$ as the dual of $H_k^{1/2}(\Gamma)$.

Finally, the restriction to $H_k^1(\Delta, \Omega^w)$ of the trace application γ_1 defined by:

$$\forall u \in H^1(\Delta, \Omega^w), \gamma_1 u = -\frac{\partial u}{\partial x} \Big|_{\Gamma},$$

is a continuous application from $H_k^1(\Delta, \Omega^w)$ onto $H_k^{-1/2}(\Gamma)$.

Let us first state without proof (see [5]), the standard existence and uniqueness result for (\mathcal{P}^w) :

Theorem 1. *Let $k \in [-\pi/L, \pi/L]$. For any $\varphi \in H_k^{1/2}(\Gamma)$, (\mathcal{P}^w) admits a unique solution $u^w(k; \varphi)$ in $H_k^1(\Delta, \Omega^w)$.*

According to Theorem 1, for every $k \in [-\pi/L, \pi/L]$, we can define the DtN operator $\Lambda^w(k) \in \mathcal{L}(H_k^{1/2}(\Gamma), H_k^{-1/2}(\Gamma))$ by:

$$\forall \varphi \in H_k^{1/2}(\Gamma), \Lambda^w(k)\varphi = -\frac{\partial}{\partial x} u^w(k; \varphi) \Big|_{\Gamma_0},$$

where $u^w(k; \varphi)$ is the solution of (\mathcal{P}^w) .

We develop next the method for (numerically) computing the operator Λ^w . For this, we adapt the method developed in [17] where Dirichlet boundary conditions were considered instead of quasi-periodic conditions. We shall restrict ourselves to presenting the main steps of the method and state without proofs the main related results. For more details, we refer the reader to [17].

Thanks to the periodicity, the construction of $u^w(k; \cdot)$ in Ω^w and $\Lambda^w(k)$ for every k is reduced to the knowledge of two linear operators,

$$\mathcal{R}(k) \in \mathcal{L}(H_k^{1/2}(\Gamma)) \quad \text{and} \quad \mathcal{S}(k) \in \mathcal{L}(H_k^{1/2}(\Gamma), H^1(\mathcal{C})),$$

defined by:

$$\mathcal{S}(k)\varphi := u^w(k; \varphi)|_{\mathcal{C}_0}, \tag{3}$$

$$\mathcal{R}(k)\varphi := u^w(k; \varphi)|_{\Gamma_1}. \tag{4}$$

The important properties of $\mathcal{R}(k)$ are summarized in the following theorem.

Theorem 2. *For every $k \in [-\pi/L, \pi/L]$, $\mathcal{R}(k)$ is compact, injective and its spectral radius is strictly less than 1.*

Using the definition of $\mathcal{S}(k)$ and $\mathcal{R}(k)$ (expressions (3) and (4)) and the periodicity of the problem, we deduce the following characterization of $u^w(k; \cdot)$.

Theorem 3. *The solution $u^w(k; \cdot)$ of problem (\mathcal{P}^w) is characterized by*

$$\forall j \geq 0, u^w(k; \varphi)|_{\mathcal{C}_j} := \mathcal{S}(k) \circ (\mathcal{R}(k))^j \varphi. \tag{5}$$

As a consequence of the definition of $\mathcal{S}(k)$, $\Lambda^w(k)$ is also characterized by:

$$\Lambda^w(k)\varphi := -\frac{\partial}{\partial x} (\mathcal{S}(k)\varphi) \Big|_{\Gamma_0}. \tag{6}$$

At this stage, the definitions of $\mathcal{R}(k)$ and $\mathcal{S}(k)$ rely on u^w which is the solution of a problem posed in unbounded domain. We shall see in the following section how to determine these operators by solely solving local problems.

3.2. Characterization of operators via local problems

Let $e_\ell(k; \varphi)$, $\ell = 0, 1$, be the solutions of two problems posed on a single periodicity cell \mathcal{C} :

$$-\Delta e_\ell(k; \varphi) - n(\mathbf{x})^2(\omega^2 + i\varepsilon)e_\ell(k; \varphi) = 0, \quad \text{in } \mathcal{C}, \tag{7}$$

satisfying both quasi-periodic conditions on Σ_0^+ and Σ_0^- :

$$\begin{cases} e_\ell(k; \varphi)|_{\Sigma_0^+} = e^{i k L} e_\ell(k; \varphi)|_{\Sigma_0^-}, \\ \frac{\partial}{\partial y} e_\ell(k; \varphi)|_{\Sigma_0^+} = e^{i k L} \frac{\partial}{\partial y} e_\ell(k; \varphi)|_{\Sigma_0^-} \end{cases} \tag{8}$$

subject to non-homogeneous Dirichlet conditions on Γ_0 and Γ_1 :

$$e_0(k; \varphi) = \varphi \quad \text{on } \Gamma_0, \quad e_0(k; \varphi) = 0 \quad \text{on } \Gamma_1, \tag{9}$$

$$e_1(k; \varphi) = 0 \quad \text{on } \Gamma_0, \quad e_1(k; \varphi) = \varphi \quad \text{on } \Gamma_1. \tag{10}$$

We define four DtN-like operators,

$$\begin{aligned} \mathcal{T}_{00}(k)\varphi &= -\frac{\partial}{\partial x} e_0(k; \varphi) \Big|_{\Gamma_0}, & \mathcal{T}_{01}(k)\varphi &= \frac{\partial}{\partial x} e_0(k; \varphi) \Big|_{\Gamma_1}, \\ \mathcal{T}_{10}(k)\varphi &= -\frac{\partial}{\partial x} e_1(k; \varphi) \Big|_{\Gamma_0}, & \mathcal{T}_{11}(k)\varphi &= \frac{\partial}{\partial x} e_1(k; \varphi) \Big|_{\Gamma_1}, \end{aligned} \tag{11}$$

which, after identification between Γ_0 and Γ_1 , we consider as bounded operators in $\mathcal{L}(H_k^{1/2}(\Gamma), H_k^{-1/2}(\Gamma))$.

These four operators are sufficient to treat the waveguide problem. However to deal with the more general 2D case, we shall need 4 additional ‘‘Dirichlet-to-Dirichlet’’ operators

$$\mathcal{D}_0^\pm(k) \in \mathcal{L}(H_k^{1/2}(\Gamma), H^{1/2}(\Sigma_0^\pm)) \quad \text{and} \quad \mathcal{D}_1^\pm(k) \in \mathcal{L}(H_k^{1/2}(\Gamma), H^{1/2}(\Sigma_0^\pm))$$

that we defined below

$$\begin{aligned} \mathcal{D}_0^-(k)\varphi &= e_0(k; \varphi)|_{\Sigma_0^-}, & \mathcal{D}_0^+(k)\varphi &= e_0(k; \varphi)|_{\Sigma_0^+}, \\ \mathcal{D}_1^-(k)\varphi &= e_1(k; \varphi)|_{\Sigma_0^-}, & \mathcal{D}_1^+(k)\varphi &= e_1(k; \varphi)|_{\Sigma_0^+}, \end{aligned} \tag{12}$$

where (see Fig. 3):

$$\Sigma_0^\pm = \left[\frac{L}{2}, \frac{3L}{2} \right] \times \left\{ \pm \frac{L}{2} \right\} \quad \text{and} \quad \bar{\Sigma}_0^\pm = \left[\frac{3L}{2}, \frac{L}{2} \right] \times \left\{ -\frac{L}{2} \right\},$$

Remark 5. Note that the trace in Σ_0^+ is taken in the increasing x -direction whereas the one in Σ_0^- is taken in the decreasing x -direction. We will understand in Section 5.4 this nuance and why we have to introduce these four DtD operators.

Using linearity and periodicity of the problem, one can show easily that:

$$\begin{aligned} u^w(k, \varphi)|_{\mathcal{C}_0} &= e_0(k; \varphi) + e_1(k; \mathcal{R}(k)\varphi) \quad (= \mathcal{S}(k)\varphi), \\ u^w(k, \varphi)|_{\mathcal{C}_1} &= e_0(k; \mathcal{R}(k)\varphi) + e_1(k; \mathcal{R}(k)^2\varphi). \end{aligned} \tag{13}$$

Using the continuity of the derivative of u^w across Γ_1 , one can show the following theorem (see [17]):

Theorem 4. $\mathcal{R}(k)$ is the unique compact operator of $\mathcal{L}(H_k^{1/2}(\Gamma))$ whose spectral radius is strictly less than 1, which solves the following Riccati equation:

$$\text{Find } \mathcal{R} \in \mathcal{L}(H_k^{1/2}(\Gamma)), \quad \mathcal{T}_{10}(k)\mathcal{R}^2 + (\mathcal{T}_{00}(k) + \mathcal{T}_{11}(k))\mathcal{R} + \mathcal{T}_{01}(k) = 0.$$

Moreover, we have the following formulae for $\Lambda^w(k)$:

$$\Lambda^w(k) = \mathcal{T}_{00}(k) + \mathcal{T}_{10}(k)\mathcal{R}(k).$$

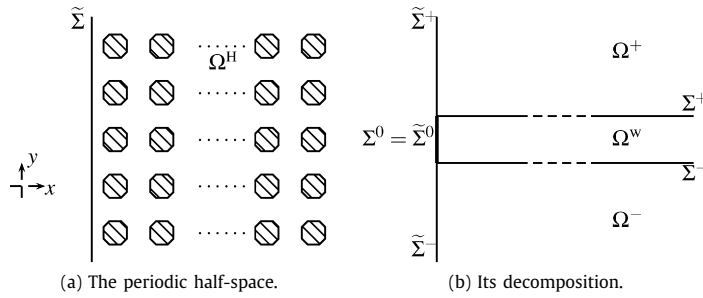


Fig. 4. Halfspace notation.

Thus, solving first cell problems and then this Ricatti-type equation, one can obtain the operator $\mathcal{R}(k)$. The operator $S(k)$ is then determined using (13). We can reconstruct $u^W(k, \cdot)$ in the whole guide Ω^W by (5) and in particular its trace on Σ^+ and $\tilde{\Sigma}^-$ by: $\forall j \geq 0$

$$\begin{cases} u^W(k; \varphi) = (D_0^+(k) + D_1^+(k)\mathcal{R}(k))\mathcal{R}(k)^j \varphi & \text{on } \Sigma_j^+ \equiv \left[\frac{L}{2} + jL, \frac{3L}{2} + jL \right], \\ u^W(k; \varphi) = (D_0^-(k) + D_1^-(k)\mathcal{R}(k))\mathcal{R}(k)^j \varphi & \text{on } \tilde{\Sigma}_j^- \equiv \left[\frac{3L}{2} + jL, \frac{L}{2} + jL \right]. \end{cases} \tag{14}$$

4. The half-space problem

4.1. Presentation of the problem

In this section, we present a method to characterize the DtN operator Λ^H of the periodic halfspace, defined by:

$$\begin{aligned} \Lambda^H : H^{1/2}(\tilde{\Sigma}) &\rightarrow H^{-1/2}(\tilde{\Sigma}) \\ \psi &\mapsto \Lambda^H \psi = \frac{\partial}{\partial x} u^H(\psi) \Big|_{\tilde{\Sigma}}, \end{aligned}$$

where $u^H(\psi) \in H^1(\Delta, \Omega^H)$ is the unique solution of:

$$\begin{cases} -\Delta u^H(\psi) - n(\mathbf{x})^2(\omega^2 + i\varepsilon)u^H(\psi) = 0, & \text{in } \Omega^H, \\ u^H(\psi) = \psi, & \text{on } \tilde{\Sigma}, \end{cases} \tag{P^H}$$

where $\Omega^H = [L/2, +\infty[\times \mathbb{R} = \Omega^+ \cup \Omega^W \cup \Omega^-$ and $\tilde{\Sigma} = \{L/2\} \times \mathbb{R} = \tilde{\Sigma}^+ \cup \tilde{\Sigma}^0 \cup \tilde{\Sigma}^-$ (see Fig. 4).

4.2. The Floquet–Bloch transformation: definition and properties

We first define the FB transform of smooth compactly supported functions.

Definition 5. The Floquet–Bloch (FB) transform of period L is defined by (see [18]):

$$\begin{aligned} \mathcal{F} : C_0^\infty(\mathbb{R}) &\rightarrow L^2\left(\mathbb{K} = \left[-\frac{L}{2}; \frac{L}{2}\right] \times \left[-\frac{\pi}{L}; \frac{\pi}{L}\right]\right), \\ \psi(y) &\mapsto \mathcal{F}\psi(y; k) = \sqrt{\frac{L}{2\pi}} \sum_{n \in \mathbb{Z}} \psi(y + nL)e^{-inkL}, \end{aligned}$$

where $C_0^\infty(\mathbb{R})$ is the set of C^∞ -functions with compact support.

Remark 6. The sum in the definition of the FB transformation is finite because of the compact support of ψ .

Proposition 7 (Extension to $L^2(\mathbb{R})$). The FB transformation extends to an isometry between $L^2(\mathbb{R})$ and $L^2(\mathbb{K})$:

$$\forall (\psi, \phi) \in L^2(\mathbb{R}), \quad (\mathcal{F}\psi, \mathcal{F}\phi)_{L^2(\mathbb{K})} = (\psi, \phi)_{L^2(\mathbb{R})}.$$

Proof. We give a short proof for completeness. Note that for a fixed $y \in [-L/2; L/2]$, $k \rightarrow \mathcal{F}\psi(y; k)$ is the trigonometric series associated to the coefficients $(\psi(y + nL))$. The Plancherel theorem then ensures that

$$\int_{-\pi/L}^{\pi/L} |\mathcal{F}\psi(y; k)|^2 dk = \sum_{n \in \mathbb{Z}} |\psi(y + nL)|^2.$$

Integrating y between $-L/2$ and $L/2$ we obtain:

$$\int_{-L/2}^{L/2} \int_{-\pi/L}^{\pi/L} |\mathcal{F}\psi(y; k)|^2 dk dy = \int_{-\infty}^{+\infty} |\psi(y)|^2 dy.$$

This identity allows to extend uniquely the operator \mathcal{F} by density to an isometry from $L^2(\mathbb{R})$ to $L^2(\mathbb{K})$. \square

We shall use in the sequel the following properties of the FB transformation (the proofs are straightforward and left to the reader. See also [18]). These properties make the FB transformation a privileged tool for the analysis of linear PDEs with periodic coefficients.

Proposition 8 (Inversion formula). *We have:*

$$\forall y \in \left[-\frac{L}{2}; \frac{L}{2}\right], \forall n \in \mathbb{Z}, \quad \psi(y + nL) = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} \mathcal{F}\psi(y; k) e^{inLk} dk.$$

Proposition 9 (Main properties). *The FB transformation has the following properties*

(1) *it commutes with the differential operators, in the sense that*

$$\mathcal{F}\left(\frac{d\psi}{dy}\right) = \frac{\partial}{\partial y}(\mathcal{F}\psi).$$

(2) *It diagonalizes the translation operators*

$$(\tau_q\psi)(y) = \psi(y + qL) \Rightarrow \mathcal{F}(\tau_q\psi)(y; k) = e^{-iqkL} \mathcal{F}\psi(y; k), \quad (y, k) \in \mathbb{K}.$$

(3) *It commutes with the multiplication by a periodic function, in the sense that if μ is a L -periodic function*

$$\mathcal{F}(\mu\psi)(y; k) = \mu(y)\mathcal{F}\psi(y; k), \quad (y, k) \in \mathbb{K}.$$

(4) *it extends to the space $H^{1/2}(\mathbb{R})$ and*

$$\psi \in H^{1/2}(\mathbb{R}) \Rightarrow \forall k \in \left[-\frac{\pi}{L}, \frac{\pi}{L}\right], \quad \mathcal{F}\psi(\cdot; k) \in H_k^{1/2}\left(\left[-\frac{L}{2}, \frac{L}{2}\right]\right). \text{ It extends to the space } H^{-1/2}(\mathbb{R}) \text{ by duality.}$$

Let $\Omega^H = [L/2, +\infty[\times \mathbb{R}$. For a function of $u(x, y) \in L^2(\Omega^H)$, we shall denote by \mathcal{F}_y the FB transform applied in the y -direction. Then $\mathcal{F}_y u$ is a function of three variables $(x, y; k)$ such that

$$\forall x \in \mathbb{R}, \quad (\mathcal{F}_y u)(x, \cdot; \cdot) = \mathcal{F}[u(x, \cdot)].$$

According to Proposition 7 and Fubini’s theorem, we see that for each $k \in [-\pi/L, \pi/L]$, the function $\mathcal{F}_y u(\cdot, \cdot; k)$ is defined in the band $\Omega^W = [L/2, +\infty[\times [-L/2, L/2]$ and

$$k \mapsto \mathcal{F}_y u(\cdot, \cdot; k) \in L^2\left(\left[-\frac{\pi}{L}, \frac{\pi}{L}\right], L^2(\Omega^W)\right).$$

4.3. Solution of the halfspace problem

Let $u^H(\psi)$ be the solution of the problem (\mathcal{P}^H) and $\mathcal{F}_y(u^H(\psi))$ its FB transform in the y -direction. Then

$$\mathcal{F}_y(u^H(\psi)) \in L^2\left(\Omega^W \times \left[-\frac{\pi}{L}, \frac{\pi}{L}\right]\right).$$

The following theorem is an immediate consequence of the properties of the FB-transform (we refer to Proposition 9).

Theorem 6. *For every $k \in [-\pi/L, \pi/L]$, $\mathcal{F}_y u^H(\psi)(\cdot, k)$ is in $H^1(\Omega^W)$ and is the solution in Ω^W of the waveguide problem:*

$$\begin{cases} [-\Delta \mathcal{F}_y u^H(\psi) - n^2(\omega^2 + i\varepsilon) \mathcal{F}_y u^H(\psi)](\cdot; k) = 0, & \text{in } \Omega^W \\ \mathcal{F}_y u^H(\psi)(\cdot; k)|_{\Sigma^0} = \mathcal{F}_y \psi(y; k), \\ \mathcal{F}_y u^H(\psi)(\cdot; k)|_{\Sigma^+} = e^{ikL} \mathcal{F}_y u^H(\psi)(\cdot; k)|_{\Sigma^-}, \\ \partial_y \mathcal{F}_y u^H(\psi)(\cdot; k)|_{\Sigma^+} = e^{ikL} \partial_y \mathcal{F}_y u^H(\psi)(\cdot; k)|_{\Sigma^-}, \end{cases} \quad (\mathcal{P}_k^H)$$

where Σ^+ (resp. Σ^-) is the upper (resp. lower) boundary of Ω^W , Σ^0 is its left boundary ($= \Gamma_0$ in Section 3) (see Fig. 4 for the notations).

Using the method developed in Section 3, we can characterize and compute, for every $k \in [-\pi/L, \pi/L]$, the corresponding waveguide problem. In particular, the solution of (\mathcal{P}_k^H) is defined by:

$$\forall n \in \mathbb{N}, \quad \mathcal{F}_y u^H(\psi)(\cdot; k)|_{\mathcal{C}_n} = \mathcal{S}(k)\mathcal{R}(k)^n(\mathcal{F}_y \psi(\cdot; k)),$$

where $\mathcal{S}(k)$ and $\mathcal{R}(k)$ are defined in Section 3.

Using the inversion formula given in Proposition 8, we can reconstruct semi-analytically $u^H(\psi)$ in the whole domain Ω^H for any Dirichlet condition $\psi \in H^{1/2}(\tilde{\Sigma})$:

$$\forall (x, y) \in \Omega^W, \quad \forall n \in \mathbb{Z}, \quad u^H(\psi)(x, y + nL) = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} \mathcal{F}_y u^H(\psi)(x, y; k) e^{inkL} dk. \tag{15}$$

We can also define the operator $\hat{\Lambda}^H$ by:

$$\hat{\Lambda}^H : \prod_{k \in [-\pi/L, \pi/L]} H_k^{1/2}(\Sigma^0) \rightarrow \prod_{k \in [-\pi/L, \pi/L]} H_k^{-1/2}(\Sigma^0),$$

where

$$\prod_{k \in [-\pi/L, \pi/L]} H_k^{\pm 1/2}(\Sigma^0) = \left\{ \psi \in H^{\pm}(\mathbb{K}), \text{ a.e. } k \in \left[-\frac{\pi}{L}, \frac{\pi}{L}\right], \mathcal{F}_y \psi(\cdot; k) \in H_k^{\pm 1/2}(\Sigma^0) \right\}$$

and

$$\forall k, \quad (\hat{\Lambda}^H \psi)(\cdot, k) = \Lambda^W(k)\psi(\cdot; k).$$

We can show then the following theorem using Proposition 9, which expresses that Λ^H can be described in terms of a family of “waveguide” DtN operators and relates this section to Section 3.

Theorem 7. *The halfspace DtN operator Λ^H is given by:*

$$\Lambda^H = \mathcal{F}_y^{-1}[\Lambda^W(k)(\mathcal{F}_y \psi(\cdot; k))]. \tag{16}$$

5. The 2D plane problem

We shall restrict ourselves to a particular situation that makes the presentation of our method simpler. More precisely, we shall consider the case where

- (H1) the periodicity cell \mathcal{C} has double symmetry,
- (H2) the restriction of the function n to \mathcal{C} is a function with double symmetry.

The notion of double symmetry will be explained in Section 5.1.1. This situation is often met in the applications. We extend the method to more general situations in Appendix B.

Let us recall that the restriction of u , the solution of (\mathcal{P}) , to Ω^i is the solution of

$$\begin{cases} -\Delta u^i - n(\mathbf{x})^2(\omega^2 + \iota\varepsilon)u^i = 0, & \text{in } \Omega^i, \\ \frac{\partial u^i}{\partial \mathbf{n}} + \Lambda u^i = 0, & \text{on } \Sigma_S, \end{cases} \tag{\mathcal{P}^i}$$

where the DtN operator Λ is defined by

$$\Lambda : H^{1/2}(\Sigma_S) \rightarrow H^{-1/2}(\Sigma_S) \\ \phi \mapsto \Lambda \phi = \left. \frac{\partial}{\partial \mathbf{n}} u^e(\phi) \right|_{\Sigma_S},$$

where $u^e(\phi) \in H^1(\Delta, \Omega^e)$ is the unique solution of

$$\begin{cases} -\Delta u^e(\phi) - n(\mathbf{x})^2(\omega^2 + \iota\varepsilon)u^e(\phi) = 0, & \text{in } \Omega^e, \\ u^e(\phi) = \phi, & \text{on } \Sigma_S. \end{cases} \tag{\mathcal{P}^e}$$

See Fig. 5 for notations. Our goal is to derive a method for the computation of Λ by using the FB transformation as in Section 4 and to only solve local cell problems as in Section 3.

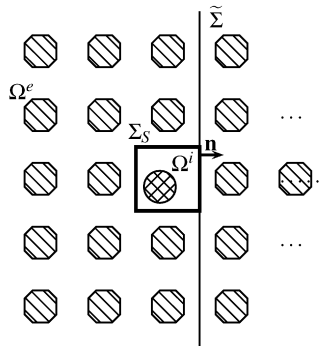


Fig. 5. 2D-plane medium.

5.1. Double symmetry and related results

5.1.1. Main definitions

Definition 8 (Double symmetry (1)). Let S_α be the symmetry with respect to the line $y = \alpha x$. A subset \mathcal{O} of \mathbb{R}^2 has double symmetry if it is invariant with respect to S_1 and S_{-1} .

Remark 10. If a domain \mathcal{O} of \mathbb{R}^2 has double symmetry, its boundary \mathcal{O} has too.

Definition 9 (Double symmetry (2)). Let \mathcal{O} be an open set with double symmetry and let a function n be defined from \mathcal{O} to \mathbb{R} or \mathbb{C} . The function n has double symmetry if:

$$n = n \circ S_1 = n \circ S_{-1}.$$

5.1.2. Functional spaces and trace theorems

The following properties of function spaces on a set having double symmetry are straight forward.

Proposition 11. Let \mathcal{O} (typically \mathcal{C} , Ω^i , Ω^e or Σ_S) be an open domain with double symmetry and $H^p(\mathcal{O})$, $p \geq 0$, the associated Sobolev space.

One has the following orthogonal decomposition:

$$H^p(\mathcal{O}) = H^p_{(s,s)}(\mathcal{O}) \oplus H^p_{(s,a)}(\mathcal{O}) \oplus H^p_{(a,s)}(\mathcal{O}) \oplus H^p_{(a,a)}(\mathcal{O}), \tag{17}$$

where

$$\begin{cases} v \in H^p_{(s,s)}(\mathcal{O}) \Leftrightarrow v = v \circ S_1 = v \circ S_{-1}, \\ v \in H^p_{(a,a)}(\mathcal{O}) \Leftrightarrow v = -v \circ S_1 = -v \circ S_{-1}, \\ v \in H^p_{(s,a)}(\mathcal{O}) \Leftrightarrow v = v \circ S_1 = -v \circ S_{-1}, \\ v \in H^p_{(a,s)}(\mathcal{O}) \Leftrightarrow v = -v \circ S_1 = v \circ S_{-1}. \end{cases}$$

Moreover the spaces $H^p_{(i,j)}(\mathcal{O})$, $(i, j) \in \{s, a\}^2$, are closed subspaces of $H^p(\mathcal{O})$ and orthogonal in $L^2(\mathcal{O})$.

Remark 12. To explain the notation, the indices s or a mean “symmetric” or “antisymmetric”, the first indice is with respect to S_1 and the second to S_{-1} . See Fig. 6 for an example for $p = 0$.

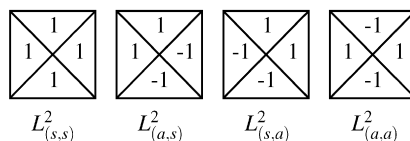


Fig. 6. Examples of functions of $L^2_{(i,j)}(\mathcal{O})$ with $\mathcal{O} = [-1, 1]^2$.

Let Ω be an open set of \mathbb{R}^2 with double symmetry (typically Ω^e). We see that for any $(i, j) \in \{s, a\}^2$, the restriction to $H^1_{(i,j)}(\Omega)$ of the trace application γ_0 defined by

$$\forall u \in H^1(\Omega), \quad \gamma_0 u = u|_{\partial\Omega}$$

is a continuous application from $H^1_{(i,j)}(\Omega)$ onto $H^{1/2}_{(i,j)}(\partial\Omega)$ (typically $\partial\Omega$ is Σ_S).

Finally we express in terms of function spaces the commutation of the Laplace operator with the symmetries $S_{\pm 1}$:

Theorem 10. Let Ω a subset of \mathbb{R}^2 with double symmetry. We recall that $H^1(\Delta; \Omega)$ is the space of functions in $H^1(\Omega)$ with Laplacian in $L^2(\Omega)$. We set:

$$\forall (i, j) \in \{s, a\}^2, \quad H^1_{(i,j)}(\Delta; \Omega) = H^1(\Delta; \Omega) \cap L^2_{(i,j)}(\Omega).$$

Then, for every (i, j) , the Laplace operator, Δ , maps $H^1_{(i,j)}(\Delta; \Omega)$ into $L^2_{(i,j)}(\Omega)$.

Observe that the decomposition (17) can be extended to the spaces $H^1(\Delta, \Omega)$ and $H^1_{(i,j)}(\Delta; \Omega)$.

We now aim at extending Proposition 11 to the Sobolev space $H^{-1/2}(\mathcal{O})$, where $\mathcal{O} = \partial\Omega$ (typically Σ_S) and Ω is an open set of \mathbb{R}^2 with double symmetry.

Definition 11. Let Ω be an open subset of \mathbb{R}^2 with double symmetry. We define the closed subspace $H^{-1/2}_{(i,j)}(\partial\Omega)$ of $H^{-1/2}(\partial\Omega)$ by

$$\forall (i, j) \in \{s, a\}^2, \quad H^{-1/2}_{(i,j)}(\partial\Omega) = \left\{ \gamma_1 u = \frac{\partial u}{\partial \mathbf{n}} \Big|_{\partial\Omega}, \quad u \in H^1_{(i,j)}(\Delta; \Omega) \right\},$$

Obviously, γ_1 is a continuous application from $H^1_{(i,j)}(\Delta; \Omega)$ onto $H^{-1/2}_{(i,j)}(\partial\Omega)$.

Using Proposition 11, Theorem 10 and Definition 11, we can prove the following proposition

Proposition 13. Let Ω be an open subset of \mathbb{R}^2 with double symmetry. We have

$$H^{-1/2}(\partial\Omega) = H^{-1/2}_{(s,s)}(\partial\Omega) \oplus H^{-1/2}_{(s,a)}(\partial\Omega) \oplus H^{-1/2}_{(a,s)}(\partial\Omega) \oplus H^{-1/2}_{(a,a)}(\partial\Omega), \tag{18}$$

where $H^{-1/2}_{(i,j)}(\partial\Omega)$ can be characterized as follows: given $v \in H^{-1/2}(\partial\Omega)$,

$$v \in H^{-1/2}_{(i,j)}(\partial\Omega) \iff \langle v, \phi \rangle_{\partial\Omega} = 0, \quad \forall \phi \in H^{1/2}_{(l,m)}(\partial\Omega), \quad (l, m) \neq (i, j). \tag{19}$$

Remark 14. Despite the notation, $H^{-1/2}_{(i,j)}(\partial\Omega)$ is strictly contained in $[H^{1/2}_{(i,j)}(\partial\Omega)]'$.

We shall now use these general properties of the spaces with double symmetry all along this section. We introduce restriction and extension operators for particular subsets of \mathbb{R}^2 which will be useful for the sequel, too.

Restriction and extension operators between Σ^0 and Σ_S (see Fig. 7). Let R be the restriction operator defined by

$$R : L^2(\Sigma_S) \rightarrow L^2(\Sigma^0), \\ \phi \mapsto \phi|_{\Sigma^0}.$$

For all $(i, j) \in \{s, a\}^2$, one check that R is an isomorphism from $L^2_{(i,j)}(\Sigma_S)$ onto $L^2(\Sigma^0)$, that we shall denote by $R_{(i,j)}$:

$$R_{(i,j)} : L^2_{(i,j)}(\Sigma_S) \rightarrow L^2(\Sigma^0).$$

Its inverse, $E_{(i,j)}$, is an extension operator, which can be given explicitly thanks to the symmetries setting $\varepsilon_s = 1$ and $\varepsilon_a = -1$:

$$\forall \phi \in L^2(\Sigma^0), \quad \begin{cases} E_{(i,j)}\phi|_{\Sigma^0} = \phi, \\ E_{(i,j)}\phi|_{S_1\Sigma^0} = \varepsilon_i\phi \circ S_1, \\ E_{(i,j)}\phi|_{S_{-1}\Sigma^0} = \varepsilon_j\phi \circ S_{-1}, \\ E_{(i,j)}\phi|_{S_1S_{-1}\Sigma^0} = \varepsilon_i\varepsilon_j\phi \circ S_1 \circ S_{-1}. \end{cases}$$

For each $(i, j) \in \{s, a\}^2$, we define the following spaces

$$H^{1/2}_{(i,j)}(\Sigma^0) = \{R_{(i,j)}\phi, \phi \in H^{1/2}_{(i,j)}(\Sigma_S)\} = \{\phi \in H^{1/2}(\Sigma^0), E_{(i,j)}\phi \in H^{1/2}_{(i,j)}(\Sigma_S)\}.$$

Then, from its definition, $R_{(i,j)}$ is an isomorphism from $H^{1/2}_{(i,j)}(\Sigma_S)$ onto $H^{1/2}_{(i,j)}(\Sigma^0)$.

The following proposition gives a more intrinsic characterization of these spaces.

Proposition 15. *We have*

$$\begin{aligned} H_{(s,s)}^{1/2}(\Sigma^0) &= H^{1/2}(\Sigma^0), \\ H_{(a,a)}^{1/2}(\Sigma^0) &= \{\phi \in H^{1/2}(\Sigma^0), (L^2/4 - y^2)^{-1/2}\phi(y) \in L^2(\Sigma^0)\}, \\ H_{(s,a)}^{1/2}(\Sigma^0) &= \{\phi \in H^{1/2}(\Sigma^0), (y + L/2)^{-1/2}\phi(y) \in L^2(\Sigma^0)\}, \\ H_{(a,s)}^{1/2}(\Sigma^0) &= \{\phi \in H^{1/2}(\Sigma^0), (L/2 - y)^{-1/2}\phi(y) \in L^2(\Sigma^0)\}. \end{aligned}$$

We now explain how to extend the restriction operator $R_{(i,j)}$ to $H_{(i,j)}^{-1/2}(\Sigma_S)$ (see Definition 11). This can be done by duality, noticing that we have $\forall(i, j) \in \{s, a\}^2$

$$\forall \phi \in L_{(i,j)}^2(\Sigma_S), \forall \psi \in L^2(\Sigma^0), \quad \langle R_{(i,j)}\phi, \psi \rangle_{\Sigma^0} = \frac{1}{4} \langle \phi, E_{(i,j)}\psi \rangle_{\Sigma_S}, \tag{20}$$

which suggests an extension of $R_{(i,j)}$ to $H_{(i,j)}^{-1/2}(\Sigma_S)$ by

$$\forall \phi \in H_{(i,j)}^{-1/2}(\Sigma_S), \forall \psi \in H_{(i,j)}^{1/2}(\Sigma^0), \quad \langle R_{(i,j)}\phi, \psi \rangle_{\Sigma^0} = \frac{1}{4} \langle \phi, E_{(i,j)}\psi \rangle_{\Sigma_S}. \tag{21}$$

We introduce the closed subspace of $[H_{(i,j)}^{1/2}(\Sigma^0)]'$:

$$H_{(i,j)}^{-1/2}(\Sigma^0) = R_{(i,j)}(H_{(i,j)}^{-1/2}(\Sigma_S)), \tag{22}$$

and conclude that $R_{(i,j)}$ is a linear continuous from $H_{(i,j)}^{-1/2}(\Sigma_S)$ onto $H_{(i,j)}^{-1/2}(\Sigma^0)$.

Analogously, $E_{(i,j)}$ can be extended to a linear continuous mapping from $H_{(i,j)}^{-1/2}(\Sigma^0)$ onto $H_{(i,j)}^{-1/2}(\Sigma_S)$, using:

$$\forall \psi \in H_{(i,j)}^{-1/2}(\Sigma^0), \forall \phi \in H_{(i,j)}^{1/2}(\Sigma_S), \quad \langle E_{(i,j)}\psi, \phi \rangle_{\Sigma_S} = 4 \langle \psi, R_{(i,j)}\phi \rangle_{\Sigma^0}. \tag{23}$$

5.2. Decomposition of the operator Λ

Using the definitions and properties of media and functions with double symmetries and considering Hypotheses (H1) and (H2), one can show the following theorem.

Theorem 12. *For any (i, j) , Λ maps $H_{(i,j)}^{1/2}(\Sigma_S)$ onto $H_{(i,j)}^{-1/2}(\Sigma_S)$ continuously.*

Proof. We make the proof for the case $(i, j) = (s, s)$. Generalization to the other cases are left to the reader.

Let ϕ be in $H_{(s,s)}^{1/2}(\Sigma_S)$. The open set Ω^e has double symmetry and the function n in Ω^e has too. Thus, because of Theorem 10, if u^e is solution of (\mathcal{P}^e) , $u^e \circ S_1$ and $u^e \circ S_{-1}$ are solutions too. From the uniqueness of the solution, $u^e(\phi)$ is then in $H_{(s,s)}^1(\Delta, \Omega^e)$.

Finally Definition 11 of the space $H_{(s,s)}^{-1/2}(\Sigma_S)$ yields the result. \square

Let us introduce

$$\forall(i, j) \in \{s, a\}, \quad \Lambda_{(i,j)} = \Lambda|_{H_{(i,j)}^{1/2}(\Sigma_S)} \in \mathcal{L}(H_{(i,j)}^{1/2}(\Sigma_S), H_{(i,j)}^{-1/2}(\Sigma_S)).$$

The decomposition of the spaces $H^{\pm 1/2}(\Sigma_S)$, given Proposition 11, leads to the following decomposition of Λ .

Proposition 16. *We have the diagonal decomposition*

$$\begin{aligned} \Lambda &= \bigoplus_{i,j} \Lambda_{(i,j)}, \quad \text{in the sense that } \forall \phi \in H^{1/2}(\Sigma_S), \quad \Lambda\phi = \sum_{i,j} \Lambda_{(i,j)}\phi_{(i,j)}, \\ \text{where } \phi &= \sum_{i,j} \phi_{(i,j)}, \quad \text{with } \forall(i, j) \in \{s, a\}^2, \phi_{(i,j)} \in H_{(i,j)}^{1/2}(\Sigma_S). \end{aligned}$$

5.3. Factorization of each DtN map $\Lambda_{(i,j)}$

We recall the following notation presented in Fig. 7:

$$\Omega^H = \Omega^- \cup \Omega^w \cup \Omega^+ \quad \text{and} \quad \tilde{\Sigma} = \tilde{\Sigma}^- \cup \tilde{\Sigma}^0 \cup \tilde{\Sigma}^+.$$

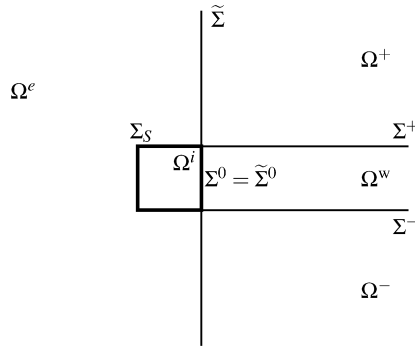


Fig. 7. 2D-plane notations.

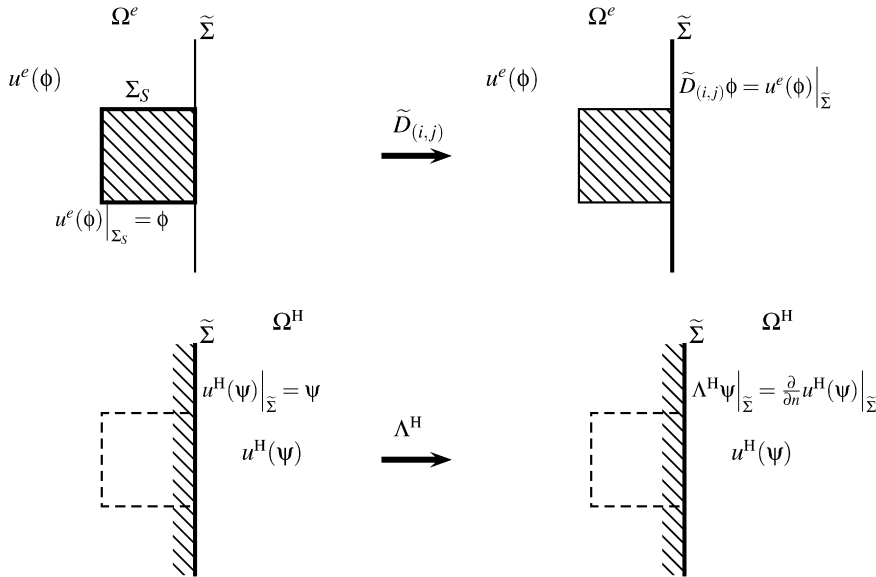


Fig. 8. Schematic decomposition of $\Lambda_{(i,j)} = E_{(i,j)} \circ \tilde{R} \circ \Lambda^H \circ \tilde{D}_{(i,j)}$.

Dirichlet-to-Dirichlet operators. Let \tilde{D} be the Dirichlet-to-Dirichlet (DtD) operator defined by:

$$\begin{aligned} \tilde{D} : H^{1/2}(\Sigma_S) &\rightarrow H^{1/2}(\tilde{\Sigma}), \\ \phi &\mapsto u^e(\phi)|_{\tilde{\Sigma}}, \end{aligned}$$

where $u^e(\phi)$ is the solution of the problem (\mathcal{P}^e) .

Let $H_{(i,j)}^{1/2}(\tilde{\Sigma})$ be the closed subspace of $H^{1/2}(\tilde{\Sigma})$ defined by

$$H_{(i,j)}^{1/2}(\tilde{\Sigma}) = \{ \psi \in H^{1/2}(\tilde{\Sigma}), \psi|_{\Sigma_0} \in H_{(i,j)}^{1/2}(\Sigma_0) \}.$$

We introduce for all $(i, j) \in \{s, a\}^2$ the DtD operators:

$$\tilde{D}_{(i,j)} = \tilde{D}|_{H_{(i,j)}^{1/2}(\Sigma_S)} \in \mathcal{L}(H_{(i,j)}^{1/2}(\Sigma_S), H_{(i,j)}^{1/2}(\tilde{\Sigma})).$$

The restriction operator. Let us denote

$$\tilde{R} : H^{-1/2}(\tilde{\Sigma}) \rightarrow [H_{(a,a)}^{1/2}(\Sigma^0)]'$$

the continuous extension of the restriction operator to Σ^0 from $L^2(\tilde{\Sigma})$ to $L^2(\Sigma^0)$. \tilde{R} is defined by duality as the adjoint of the zero extension of functions in $H_{(a,a)}^{1/2}(\Sigma^0)$ into $H^{1/2}(\tilde{\Sigma})$.

According to the schematic decomposition process of Fig. 8, we have the following theorem:

Theorem 13. The operator $\tilde{R} \circ \Lambda^H \circ \tilde{D}_{(i,j)}$ maps $H_{(i,j)}^{1/2}(\Sigma_S)$ into $H_{(i,j)}^{-1/2}(\Sigma^0)$ and

$$\Lambda_{(i,j)} = E_{(i,j)} \circ \tilde{R} \circ \Lambda^H \circ \tilde{D}_{(i,j)},$$

where

- $\tilde{D}_{(i,j)}$ is a Dirichlet-to-Dirichlet operator defined above,
- Λ^H is the halfspace DtN operator defined in Section 4,
- \tilde{R} is the restriction operator defined above,
- $E_{(i,j)}$ is the extension operator defined in Section 5.1.

Proof. Let $(i, j) \in \{s, a\}^2$ and ϕ be in $H^{1/2}_{(i,j)}(\Sigma_S)$. From the definition of $\tilde{D}_{(i,j)}$, $u^e(\phi)|_{\Omega^H}$ and $u^H(\tilde{D}_{(i,j)}\phi)$ satisfy the halfspace Helmholtz problem (\mathcal{P}^H) with the same Dirichlet condition on $\tilde{\Sigma}$, namely $\psi = \tilde{D}_{(i,j)}\phi$.

By uniqueness of the solution of (\mathcal{P}^H), we have

$$u^e(\phi)|_{\Omega^H} = u^H(\tilde{D}_{(i,j)}\phi)$$

and in particular, the traces of their normal derivatives on Σ_0 coincide, which can be written as (we omit the details of the rigorous proof which can be done using duality and symmetry arguments)

$$R_{(i,j)}\left(\frac{\partial}{\partial \mathbf{n}} u^e(\phi)|_{\Sigma_S}\right) = \tilde{R} \circ \Lambda^H \circ \tilde{D}_{(i,j)}\phi,$$

where $R_{(i,j)}$ is defined in Section 5.1.2. This relation proves the first part of the theorem. For the second part, we just use that $E_{(i,j)}$ is the inverse of $R_{(i,j)}$. \square

By Section 4 we know how to compute Λ^H with the help of the FB transformation. Thus, the determination of each DtN map $\Lambda_{(i,j)}$ is reduced to that of the DtD operator $\tilde{D}_{(i,j)}$. The computation of $\tilde{D}_{(i,j)}\phi$, for any given ϕ , a priori requires to compute the solutions u^e of the exterior problem (\mathcal{P}^e) defined in an unbounded domain. In the following section, we find another characterization of these operators which “avoids” the solution of the exterior problem.

5.4. Halfspace DtD operators

We introduce operators whose definitions rely on the solution of the halfspace problems (\mathcal{P}^H). These operators will be used in Section 5.5 to provide the new characterization of the operators $\tilde{D}_{(i,j)}$.

We decompose the boundary Σ of Ω^w according to Fig. 4:

$$\left\{ \begin{array}{l} \Sigma = \tilde{\Sigma}^- \cup \Sigma^0 \cup \Sigma^+ \\ \tilde{\Sigma}^- =]+\infty, \frac{L}{2}] \times \left\{-\frac{L}{2}\right\}, \quad \Sigma^0 = \left\{\frac{L}{2}\right\} \times \left[-\frac{L}{2}; \frac{L}{2}\right], \quad \Sigma^+ = \left[\frac{L}{2}, +\infty\right] \times \left\{\frac{L}{2}\right\}. \end{array} \right.$$

In the following we shall identify Σ and $\tilde{\Sigma}$ with \mathbb{R} , $\tilde{\Sigma}^-$ with $\tilde{\Sigma}^-$, Σ^0 with $\tilde{\Sigma}^0$ and, Σ^+ with $\tilde{\Sigma}^+$. We understand thanks to Fig. 9 why the point along the line Σ^- runs in the direction of decreasing values of x .

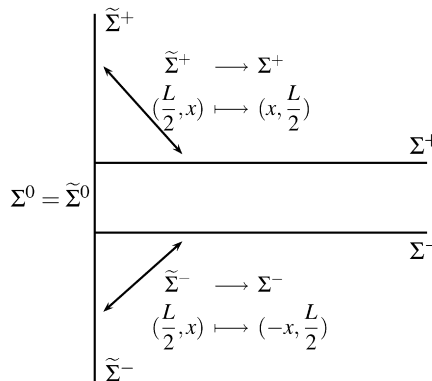


Fig. 9. Identification of $\tilde{\Sigma}$ and Σ .

Definition 14. We recall that u^H is the solution of (\mathcal{P}^H) . Let us introduce four half-space DtD operators:

$$\begin{aligned}
 D_{(s,s)}^H &: H^{1/2}(\tilde{\Sigma}) \longrightarrow H^{1/2}(\tilde{\Sigma}), & D_{(s,a)}^H &: H^{1/2}(\tilde{\Sigma}) \longrightarrow H^{1/2}(\tilde{\Sigma}), \\
 \psi \mapsto &\begin{cases} D_{(s,s)}^H \psi|_{\tilde{\Sigma}^-} \equiv +u^H(\psi)|_{\tilde{\Sigma}^-}, \\ D_{(s,s)}^H \psi|_{\tilde{\Sigma}^0} = \psi|_{\tilde{\Sigma}^0}, \\ D_{(s,s)}^H \psi|_{\tilde{\Sigma}^+} \equiv +u^H(\psi)|_{\Sigma^+}, \end{cases} & \psi \mapsto &\begin{cases} D_{(s,a)}^H \psi|_{\tilde{\Sigma}^-} \equiv -u^H(\psi)|_{\tilde{\Sigma}^-}, \\ D_{(s,a)}^H \psi|_{\tilde{\Sigma}^0} = \psi|_{\tilde{\Sigma}^0}, \\ D_{(s,a)}^H \psi|_{\tilde{\Sigma}^+} \equiv +u^H(\psi)|_{\Sigma^+}, \end{cases} \\
 D_{(a,s)}^H &: H^{1/2}(\tilde{\Sigma}) \longrightarrow H^{1/2}(\tilde{\Sigma}), & D_{(a,a)}^H &: H^{1/2}(\tilde{\Sigma}) \longrightarrow H^{1/2}(\tilde{\Sigma}), \\
 \psi \mapsto &\begin{cases} D_{(a,s)}^H \psi|_{\tilde{\Sigma}^-} \equiv +u^H(\psi)|_{\tilde{\Sigma}^-}, \\ D_{(a,s)}^H \psi|_{\tilde{\Sigma}^0} = \psi|_{\tilde{\Sigma}^0}, \\ D_{(a,s)}^H \psi|_{\tilde{\Sigma}^+} \equiv -u^H(\psi)|_{\Sigma^+}, \end{cases} & \psi \mapsto &\begin{cases} D_{(a,a)}^H \psi|_{\tilde{\Sigma}^-} \equiv -u^H(\psi)|_{\tilde{\Sigma}^-}, \\ D_{(a,a)}^H \psi|_{\tilde{\Sigma}^0} = \psi|_{\tilde{\Sigma}^0}, \\ D_{(a,a)}^H \psi|_{\tilde{\Sigma}^+} \equiv -u^H(\psi)|_{\Sigma^+}. \end{cases}
 \end{aligned}$$

Remark 17. A priori $D_{(i,j)}^H$ maps $H^{1/2}(\tilde{\Sigma})$ into $L^2(\tilde{\Sigma})$. However, because of Proposition 15, $D_{(i,j)}^H$ maps $H^{1/2}(\tilde{\Sigma})$ onto $H^{1/2}(\tilde{\Sigma})$.

Thanks to Section 4, we can give a semi-analytic expression for the operators $D_{(i,j)}^H$.

Proposition 18. $\forall (i, j) \in \{s, a\}^2, \forall \psi \in H^{1/2}(\tilde{\Sigma}), \forall k \in [-\pi/L, \pi/L]$,

$$\begin{aligned}
 \mathcal{F}_y(D_{(i,j)}^H \psi)(\cdot, k) &= +\varepsilon_j \frac{L}{2\pi} e^{iLk} \int_{-\pi/L}^{\pi/L} (D_0^-(\xi) + D_1^-(\xi)\mathcal{R}(\xi))(\mathbf{I} - \mathcal{R}(\xi)e^{iLk})^{-1} \mathcal{F}_y \psi(\cdot; \xi) d\xi + \sqrt{\frac{L}{2\pi}} \psi \Big|_{\tilde{\Sigma}^0} \\
 &\quad + \varepsilon_i \frac{L}{2\pi} e^{-iLk} \int_{-\pi/L}^{\pi/L} (D_0^+(\xi) + D_1^+(\xi)\mathcal{R}(\xi))(\mathbf{I} - \mathcal{R}(\xi)e^{-iLk})^{-1} \mathcal{F}_y \psi(\cdot; \xi) d\xi
 \end{aligned}$$

where $\varepsilon_s = 1$ and $\varepsilon_a = -1$.

Proof. Let ψ be in $H^{1/2}(\tilde{\Sigma})$. We write the proof for $(i, j) = (s, s)$, the other cases follow similarly. In the case $n = 0$, expression (15) gives:

$$u^H(\psi)|_{\Sigma^\pm} = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} \mathcal{F}_y u^H(\psi)(\cdot; \xi)|_{\Sigma^\pm} d\xi.$$

We denote by $\tilde{\Sigma}_n^-$ and Σ_n^+ the following sequence of intervals of length L :

$$\forall n \in \mathbb{N}, \quad \begin{cases} \tilde{\Sigma}_n^- = \left] \frac{3L}{2} + nL, \frac{L}{2} + nL \right[\times \left\{ \frac{-L}{2} \right\}, \\ \Sigma_n^+ = \left] \frac{L}{2} + nL, \frac{L}{2} + nL \right[\times \left\{ \frac{L}{2} \right\}. \end{cases}$$

Using relation (14) in Section 3, we obtain

- On Σ^- : $\forall n \in \mathbb{N}$,

$$D_{(s,s)}^H \psi|_{\tilde{\Sigma}_n^-} = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} (D_0^-(\xi)\mathcal{R}(\xi)^n + D_1^-(\xi)\mathcal{R}(\xi)^{n+1}) \mathcal{F}_y \psi(\cdot; \xi) d\xi.$$

- On Σ^0 :

$$D_{(s,s)}^H \psi|_{\Sigma^0} = \psi|_{\Sigma^0}.$$

- On Σ^+ : $\forall n \in \mathbb{N}$,

$$D_{(s,s)}^H \psi|_{\Sigma_n^+} = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} (D_0^+(\xi)\mathcal{R}(\xi)^n + D_1^+(\xi)\mathcal{R}(\xi)^{n+1}) \mathcal{F}_y \psi(\cdot; \xi) d\xi.$$

We apply then the FB-transform to $D_{(s,s)}^H \psi$ using the identification $\Sigma \sim \mathbb{R}$,

$$\mathcal{F}_y(D_{(s,s)}^H \psi)(\cdot, k) = \sqrt{\frac{L}{2\pi}} \left(\sum_{n=-\infty}^0 D_{(s,s)}^H \psi|_{\tilde{\Sigma}_n^-} e^{i(n+1)kL} + D_{(s,s)}^H \psi|_{\Sigma^0} + \sum_{n=0}^{+\infty} D_{(s,s)}^H \psi|_{\Sigma_n^+} e^{-i(n+1)kL} \right).$$

By inverting the integrals over $[-\pi/L, \pi/L]$ and the sum over n , we are led to using the following formula (see Lemma 15 below for the justification)

$$\sum_{n \in \mathbb{N}} \mathcal{R}(\xi)^n e^{\pm i(n+1)Lk} = e^{\pm iLk} (\mathbf{I} - \mathcal{R}(\xi)e^{\pm iLk})^{-1}. \tag{24}$$

In fact for every ξ , $\mathcal{R}(\xi)$ is compact and its spectral radius is strictly less than 1, and then, for every k , the operators $\mathcal{R}(\xi)e^{\pm iLk}$ remains compact with a spectral radius strictly less than one. Therefore, for each ξ and k , $\mathbf{I} - \mathcal{R}(\xi)e^{\pm iLk}$ is invertible and the sum (24) converges uniformly in the norm of $\mathcal{L}(H^{1/2}(\Sigma^0))$. The inversion of the integral and the sum is then possible. \square

The justification of (24) relies on the following lemma which is a classical result for which we give a short proof.

Lemma 15. *Let E be a Hilbert space and $A \in \mathcal{L}(E)$ with a spectral radius $\rho(A) < 1$. Then the series $\sum A^n$ converges for the norm:*

$$\|A\| = \sup_{\substack{u \neq 0 \\ u \in E}} \frac{\|Au\|_E}{\|u\|_E}$$

and

$$\sum_{n \in \mathbb{N}} A^n = (I - A)^{-1}.$$

Proof. The property:

$$\lim_{n \rightarrow +\infty} \|A^n\|^{1/n} = \rho(A)$$

for the norm of $\mathcal{L}(H^{1/2}(\Sigma^0))$ ([27]), implies that for some $\rho_* \in]\rho(A), 1[$ and j large enough we have

$$\|A^j\| \leq \rho_*^j$$

which yields the absolute convergence of the series. \square

5.5. Characterization of $\tilde{D}_{(i,j)}$

$$\begin{aligned} \tilde{D}_{(i,j)} : H_{(i,j)}^{1/2}(\Sigma_S) &\rightarrow H_{(i,j)}^{1/2}(\tilde{\Sigma}), \\ \phi &\mapsto u^e(\phi)|_{\tilde{\Sigma}}. \end{aligned}$$

We first remark that $\tilde{D}_{(i,j)}$ belongs to the affine subspace:

$$\mathcal{L}_{\Sigma^0} = \{L \in \mathcal{L}(H^{1/2}(\Sigma_S), H^{1/2}(\tilde{\Sigma})), \forall \phi, L\phi|_{\Sigma^0} = \phi|_{\Sigma^0}\}.$$

Theorem 16. *For each $(i, j) \in \{s, a\}^2$, the operator $\tilde{D}_{(i,j)}$ is the unique solution of the problem*

$$\text{Find } \tilde{D} \in \mathcal{L}_{\Sigma^0}, \quad \tilde{D} = D_{(i,j)}^H \circ \tilde{D}. \tag{E}_{(i,j)}$$

Remark 19. Since \mathcal{L}_{Σ^0} is an affine subspace, problems $(\mathcal{E}_{(i,j)})$ are of affine nature, even though the equation is linear.

Proof. We give a proof for $\tilde{D}_{(s,s)}$. The extension to other $\tilde{D}_{(i,j)}$ is straightforward.

Existence. We prove that the operator $\tilde{D}_{(s,s)}$ is a solution of Problem $(\mathcal{E}_{(s,s)})$. We have already seen in the proof of Theorem 13 that

$$u^e(\phi)|_{\Omega^H} = u^H(\tilde{D}_{(s,s)}\phi).$$

Moreover, ϕ in $H_{(s,s)}^{1/2}(\Sigma_S)$ implies that $u^e(\phi)$ is in $H_{(s,s)}^1(\Omega^e)$ (see the proof Theorem 12). In particular:

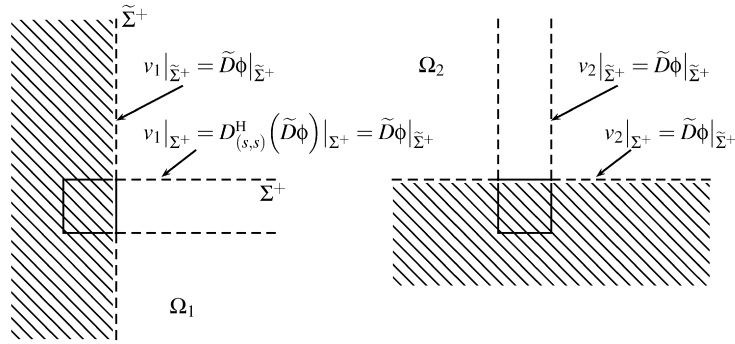


Fig. 10. Definition of v_1 and v_2 .

$$\begin{aligned} \tilde{\Sigma}^+ &= S_1 \Sigma^+ \Rightarrow u^e(\phi)|_{\tilde{\Sigma}^+} \equiv u^e(\phi)|_{\Sigma^+} = u^H(\tilde{D}_{(s,s)}\phi)|_{\Sigma^+}, \\ \tilde{\Sigma}^0 &= \Sigma^0 \Rightarrow u^e(\phi)|_{\tilde{\Sigma}^0} = u^e(\phi)|_{\Sigma^0} = \phi|_{\Sigma^0}, \\ \tilde{\Sigma}^- &= S_{-1} \Sigma^- \Rightarrow u^e(\phi)|_{\tilde{\Sigma}^-} \equiv u^e(\phi)|_{\Sigma^-} = u^H(\tilde{D}_{(s,s)}\phi)|_{\tilde{\Sigma}^-}. \end{aligned}$$

Using the definition of $D_{(s,s)}^H$, we obtain that $\tilde{D}_{(s,s)}$ satisfies $(\mathcal{E}_{(s,s)})$.

Uniqueness. Let \tilde{D} be an operator from $H_{(s,s)}^{1/2}(\Sigma_S)$ into $H_{(s,s)}^{1/2}(\tilde{\Sigma})$ such that:

$$\forall \phi \in H_{(s,s)}^{1/2}(\Sigma_S), \quad \tilde{D}\phi|_{\Sigma^0} = 0 \tag{25}$$

and which satisfies:

$$D_{(s,s)}^H \circ \tilde{D} - \tilde{D} = 0.$$

We prove that $\tilde{D} = 0$. Let $\phi \in H_{(s,s)}^{1/2}(\Sigma_S)$ and $v_1 = u^H(\tilde{D}\phi)$ defined in $\Omega^H \equiv \Omega_1$. We have in particular, thanks to (25):

$$v_1|_{\Sigma^0} = \tilde{D}\phi|_{\Sigma^0} = 0. \tag{26}$$

Now we build a function in the half-space $\Omega_2 = S_1\Omega_1$ by:

$$v_2 = v_1(S_1\mathbf{x}).$$

By a classical symmetry argument, since v_1 is solution of (\mathcal{P}^H) in Ω_1 , it is clear that v_2 is solution of:

$$-\Delta v_2 - n^2(\omega^2 + i\varepsilon)v_2 = 0, \quad \text{in } \Omega_2$$

while (26) yields:

$$v_2|_{S_1\Sigma^0} = 0. \tag{27}$$

We are going to show that v_1 and v_2 coincide in the quadrant $\Omega_1 \cap \Omega_2$: the reader will easily be convinced by looking at Fig. 10 that the difference $d_{12} = v_1 - v_2$ satisfies:

$$\begin{cases} -\Delta d_{12} - n^2(\omega^2 + i\varepsilon)d_{12} = 0, & \text{in } \Omega_1 \cap \Omega_2, \\ d_{12} = 0, & \text{on } \partial[\Omega_1 \cap \Omega_2]. \end{cases}$$

Thanks to a uniqueness argument for this Dirichlet problem, one concludes that $v_1 = v_2$ in $\Omega_1 \cap \Omega_2$.

With the same argument, we can construct for $j \in \{1, 2, 3, 4\}$, four functions v_j in the domains Ω_j ($\Omega_3 = S_{-1}\Omega_2$ and $\Omega_4 = S_{-1}\Omega_1$) which are solution of the Helmholtz equation in their respective domain and which coincide in their intersections:

$$\forall j \in \mathbb{Z}/4\mathbb{Z}, \quad v_{j+1} = v_j \quad \text{on } \Omega_j \cap \Omega_{j+1}. \tag{28}$$

Thus we can build a function $u^e \in H^1(\Omega^e)$ defined in the exterior domain Ω^e by:

$$u^e|_{\Omega_j} = v_j, \quad j \in \{1, 2, 3, 4\}.$$

Thanks to (28) and to the fact that v_j is the H^1 -solution of the Helmholtz equation in Ω_j , u^e is then a H^1 function which satisfies:

$$-\Delta u^e - n^2(\omega^2 + i\varepsilon)u^e = 0 \quad \text{in } \Omega^e$$

with the homogeneous Dirichlet condition

$$u^e = 0, \quad \text{on } \Sigma_S,$$

thanks to (26) and (27) and by symmetry.

By uniqueness of the solution in the exterior domain, we deduce $u^e = 0$ in Ω^e and in consequence:

$$\tilde{D}\phi|_{\tilde{\Sigma}^\pm} = u^e|_{\tilde{\Sigma}}$$

that means $\tilde{D} = 0$. \square

Actually the definition of $D_{(i,j)}^H$ (see Definition 14 and Proposition 18) is simpler in terms of FB-variables. The formulation in terms of FB-variables in this problem is thus more natural. More precisely, for every $(i, j) \in \{s, a\}^2$, for every function $\phi \in H_{(i,j)}^{1/2}(\Sigma^0)$, we compute

$$\tilde{D}_{(i,j)}\phi = \mathcal{F}_y^{-1}(\widehat{D_{ij}\phi}),$$

where $\hat{\psi}_{ij} = \widehat{D_{ij}\phi}$ is the unique solution of the “integral” problem:

Find $\hat{\psi} \in L^2(\mathbb{K})$, such that

$$\left\{ \begin{array}{l} \text{(i)} \quad \hat{\psi}(\cdot, k) - \int_{-\pi/L}^{\pi/L} K_{(i,j)}(\xi, k) \cdot \hat{\psi}(\cdot, \xi) d\xi = \sqrt{\frac{L}{2\pi}} \phi, \quad \forall k \in \left[-\frac{\pi}{L}; \frac{\pi}{L}\right], \\ \text{(ii)} \quad \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} \hat{\psi}(\cdot, k) dk = \phi. \end{array} \right. \tag{29}$$

where for each ξ and k , the kernel $K_{(i,j)}(\xi, k)$ is in $\mathcal{L}(H^{1/2}(\Sigma^0), H^{1/2}(\Sigma^0))$:

$$K_{(i,j)}(\xi, k) = \varepsilon_i \frac{L}{2\pi} e^{-iLk} (\mathcal{D}_0^+(\xi) + \mathcal{D}_1^+(\xi)\mathcal{R}(\xi)) (\mathbf{I} - \mathcal{R}(\xi)e^{-iLk})^{-1} + \varepsilon_j \frac{L}{2\pi} e^{iLk} (\mathcal{D}_0^-(\xi) + \mathcal{D}_1^-(\xi)\mathcal{R}(\xi)) (\mathbf{I} - \mathcal{R}(\xi)e^{iLk})^{-1},$$

The relation (29(ii)) expresses in terms of the FB-variables the condition:

$$\tilde{D}_{(i,j)}\phi|_{\Sigma^0} = \phi|_{\Sigma^0}.$$

6. Conclusions

In this article, we have described and analyzed a method for constructing the Dirichlet-to-Neumann operator Λ associated to the resolution of the exterior Helmholtz problem outside a square whose size is a multiple of the period L of the medium. From the numerical point of view, the main interest of the method lies in the fact that one only has to solve local cell problems. The numerical aspects of the problem will be treated elsewhere. The implementation of this method according to the decomposition Theorem 13 is based on the following algorithm:

- (1) Computation of Λ^H
 - (i) For each $k \in [-\pi/L, \pi/L]$, compute $\Lambda^W(k)$,
 - (ii) Computation Λ^H by recomposition using (16);
- (2) Computation of $\Lambda_{(i,j)}$ for each $(i, j) \in \{s, a\}^2$
 - (i) Compute $\tilde{D}_{(i,j)}$ by solving $(\mathcal{E}_{(i,j)})$,
 - (ii) apply the formula $\Lambda_{(i,j)} = E_{(i,j)} \circ \tilde{R} \circ \Lambda^H \circ \tilde{D}_{(i,j)}$.

In practice, this algorithm requires a discretization procedure with respect to the space variable $y \in]-L/2, L/2[$ (for the discretization of Σ^0) and with respect to the wave number $k \in]-\pi/L; \pi/L[$ (the dual variable). Moreover,

- Step 1(i) can be achieved along the same lines than the finite element method described in [17], two different values of k are decoupled,
- Step 1(ii) requires the construction of a discrete inverse FB-transform,
- Step 2(i) relies on the discretization of the integral equation (29(i)) which is non-local in y and k (this time, the problems for different k are coupled).

Other delicate question about the discretization in k (can one use a regular mesh in k or not?) or the way to properly take the constraint (29(ii)) into account have to be addressed.

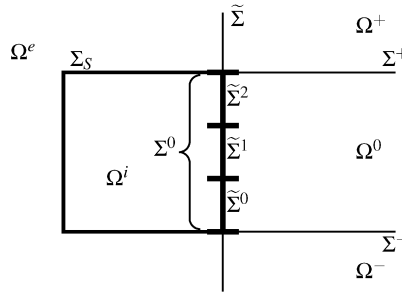


Fig. A.1. General notation.

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Appendix A. The extension of the method to $N > 1$

For the general case of larger defect, the reasoning is the same but the expression of the halfspace DtD operators $D_{(i,j)}^H$ change.

First let us give some new notation in Fig. A.1.

Here the size of the interior medium Ω^i is N times the size of a periodicity cell:

$$\Omega^i = \left] -\frac{L}{2}, \frac{(2N-1)L}{2} \right[.$$

Then

$$\Sigma^0 = \Sigma_S \cap \tilde{\Sigma} = \left] -\frac{L}{2}, \frac{(2N-1)L}{2} \right[= \bigcup_{l=0}^{N-1} \tilde{\Sigma}^l, \quad \text{where } \tilde{\Sigma}^l = \left] \frac{(2l-1)L}{2}, \frac{(2l+1)L}{2} \right[.$$

We recall the following notation:

$$\Sigma = \tilde{\Sigma}^- \cup \Sigma^0 \cup \Sigma^+, \quad \tilde{\Sigma} = \tilde{\Sigma}^- \cup \bigcup_{l=0}^{N-1} \tilde{\Sigma}^l \cup \tilde{\Sigma}^+,$$

where in particular

$$\tilde{\Sigma}^- = \left] +\infty, \frac{(2N-1)L}{2} \right[\times \left\{ -\frac{L}{2} \right\}, \quad \Sigma^+ = \left] \frac{(2N-1)L}{2}, +\infty \right[\times \left\{ \frac{(2N-1)L}{2} \right\}.$$

We still identify Σ and $\tilde{\Sigma}$ with \mathbb{R} , $\tilde{\Sigma}^-$ with $\tilde{\Sigma}^-$ and Σ^+ with $\tilde{\Sigma}^+$.

For this case, the decomposition of the operator Λ (Proposition 11) and the factorization of each $\Lambda_{(i,j)}$ (Theorem 13) still hold. The computation of Λ^H can obviously be done as in Section 4 working on the basic periodicity cell \mathcal{C} .

For the characterization of each $D_{(i,j)}$, we need to introduce the halfspace DtD operators $D_{(i,j)}^H$ whose expression depends on N . Let us recall the definition of these operators setting $\varepsilon_s = +1$ and $\varepsilon_a = -1$:

$$D_{(i,j)}^H : H_{(i,j)}^{1/2}(\tilde{\Sigma}) \longrightarrow H_{(i,j)}^{1/2}(\tilde{\Sigma}),$$

$$\psi \longmapsto \begin{cases} D_{(i,j)}^H \psi|_{\tilde{\Sigma}^-} \equiv \varepsilon_j u^H(\psi)|_{\tilde{\Sigma}^-}, \\ D_{(i,j)}^H \psi|_{\Sigma^0} = \psi|_{\Sigma^0}, \\ D_{(i,j)}^H \psi|_{\tilde{\Sigma}^+} \equiv \varepsilon_i u^H(\psi)|_{\Sigma^+}. \end{cases}$$

We give in the following proposition a more explicit definition for $D_{(i,j)}^H$ for the general case.

Proposition 20. $\forall (i, j) \in \{s, a\}^2, \forall \psi \in H_{(i,j)}^{1/2}(\tilde{\Sigma}), \forall k \in [-\frac{\pi}{L}, \frac{\pi}{L}]$,

$$\begin{aligned} \mathcal{F}_y(D_{(i,j)}^H \psi)(\cdot, k) &= \frac{\varepsilon_j L}{2\pi} e^{iLk} \int_{-\pi/L}^{\pi/L} (D_0^-(\xi) + D_1^-(\xi)\mathcal{R}(\xi))(\mathbf{I} - \mathcal{R}(\xi)e^{iLk})^{-1} \mathcal{F}_y \psi(\cdot; \xi) d\xi + \sqrt{\frac{L}{2\pi}} \sum_{l=0}^{N-1} \psi|_{\tilde{\Sigma}^l} e^{-iLlk} \\ &\quad + \frac{\varepsilon_i L}{2\pi} e^{-iNLk} \int_{-\pi/L}^{\pi/L} (D_0^+(\xi) + D_1^+(\xi)\mathcal{R}(\xi))(\mathbf{I} - \mathcal{R}(\xi)e^{-iLk})^{-1} \mathcal{F}_y \psi(\cdot; \xi) e^{i(N-1)\xi L} d\xi, \end{aligned}$$

where $\varepsilon_s = 1$ and $\varepsilon_a = -1$.

Proof. Let ψ be in $H^{1/2}(\tilde{\Sigma})$. We write the proof for $(i, j) = (s, s)$, the other cases follow similarly. In the case $n = 0$, expression (15) gives:

$$u^H(\psi)|_{\Sigma^-} = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} \mathcal{F}_y u^H(\psi)(\cdot; \xi)|_{y=-L/2} d\xi.$$

In the case $n = N - 1$, it gives:

$$u^H(\psi)|_{\Sigma^+} = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} \mathcal{F}_y u^H(\psi)(\cdot; \xi)|_{y=L/2} e^{i(N-1)\xi L} d\xi.$$

We denote $\tilde{\Sigma}_n^-$ and Σ_n^+ the following sequence of intervals of length L :

$$\forall n \in \mathbb{N}, \quad \begin{cases} \tilde{\Sigma}_n^- = \left[\frac{(2N-1)L + (n+1)L}{2}, \frac{(2N-1)L + nL}{2} \right] \times \left\{ \frac{-L}{2} \right\}, \\ \Sigma_n^+ = \left[\frac{(2N-1)L + nL}{2}, \frac{(2N-1)L + (n+1)L}{2} \right] \times \left\{ \frac{(2N-1)L}{2} \right\}, \end{cases}$$

and using relation (14) in Section 3, we obtain:

- On $\tilde{\Sigma}^-$: $\forall n \in \mathbb{N}$,

$$D_{(s,s)}^H \psi|_{\tilde{\Sigma}_n^-} = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} (D_0^-(\xi)\mathcal{R}(\xi)^n + D_1^-(\xi)\mathcal{R}(\xi)^{n+1}) \mathcal{F}_y \psi(\cdot; \xi) d\xi.$$

- On each $\tilde{\Sigma}^l$:

$$D_{(s,s)}^H \psi|_{\tilde{\Sigma}^l} = \psi|_{\tilde{\Sigma}^l}.$$

- On Σ^+ : $\forall n \in \mathbb{N}$,

$$D_{(s,s)}^H \psi|_{\Sigma_n^+} = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} (D_0^+(\xi)\mathcal{R}(\xi)^n + D_1^+(\xi)\mathcal{R}(\xi)^{n+1}) \mathcal{F}_y \psi(\cdot; \xi) e^{i(N-1)\xi L} d\xi.$$

We apply then the FB-transform to $D_{(s,s)}^H \psi$ using the identification $\Sigma \sim \mathbb{R}$,

$$\mathcal{F}_y(D_{(s,s)}^H \psi)(\cdot, k) = \sqrt{\frac{L}{2\pi}} \left(\sum_{n=0}^{+\infty} D_{(s,s)}^H \psi|_{\tilde{\Sigma}_n^-} e^{i(n+1)kL} + \sum_{l=0}^{N-1} D_{(s,s)}^H \psi|_{\tilde{\Sigma}^l} e^{-iLlk} + \sum_{n=0}^{+\infty} D_{(s,s)}^H \psi|_{\Sigma_n^+} e^{-i(n+N)kL} \right).$$

By inverting the integrals over $[-\pi/L, \pi/L]$ and the sum over n , we can use the same arguments as in Proposition 18 to conclude. \square

With this general expression of $D_{(i,j)}^H$, each $\tilde{D}_{(i,j)}$ is then the unique solution of $\mathcal{E}_{(i,j)}$. The formulation of these equations in terms of FB-variables is still again natural. More precisely for every $(i, j) \in \{s, a\}^2$, for every function $\phi \in H_{(i,j)}^{1/2}(\Sigma^0)$, we compute

$$\tilde{D}_{(i,j)} \phi = \mathcal{F}_y^{-1}(\widehat{D_{ij}\phi}),$$

where $\hat{\psi}_{ij} = \widehat{D_{ij}\psi}$ is the unique solution of the “integral” equation:

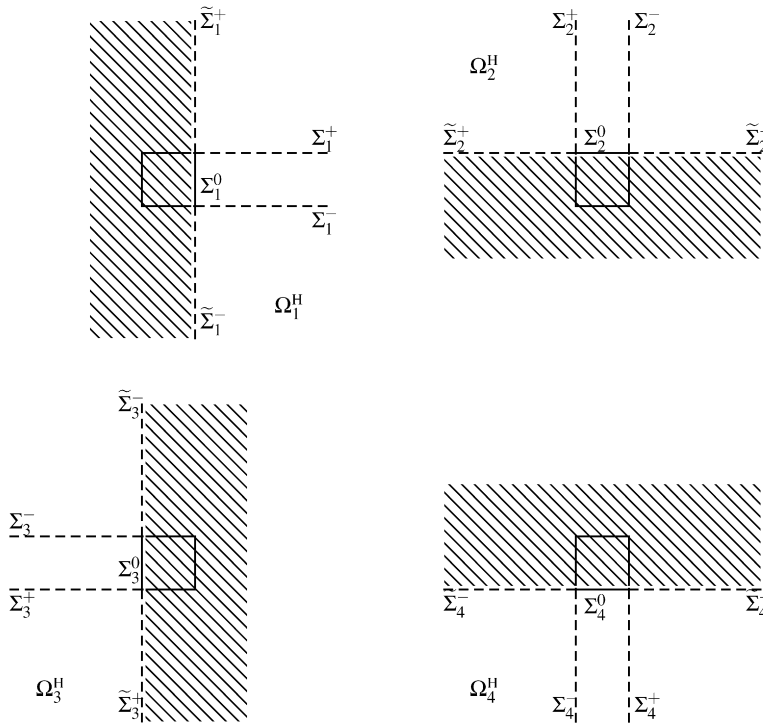


Fig. B.1. The four halfspaces $(\Omega_i^H)_i$.

Find $\hat{\psi} \in L^2(\mathbb{K})$, such that

$$\left\{ \begin{array}{l} \text{(i) } \hat{\psi}(\cdot, k) - \int_{-\pi/L}^{\pi/L} K_{(i,j)}(\xi, k) \cdot \hat{\psi}(\cdot, \xi) d\xi = \sqrt{\frac{L}{2\pi}} \sum_{l=0}^{N-1} \phi|_{\tilde{\Sigma}^l} e^{-iLk}, \quad \forall k \in \left[-\frac{\pi}{L}; \frac{\pi}{L}\right], \\ \text{(ii) } \forall l \in \{0, N-1\}, \quad \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} \hat{\psi}(\cdot, k) e^{iLk} dk = \phi|_{\tilde{\Sigma}^l}, \end{array} \right.$$

where for each ξ and k , the kernel $K_{(i,j)}(\xi, k)$ is in $\mathcal{L}(H^{1/2}(\Sigma^0), H^{1/2}(\Sigma^0))$:

$$K_{(i,j)}(\xi, k) = \varepsilon_i \frac{L}{2\pi} e^{-iNLk} (\mathcal{D}_0^+(\xi) + \mathcal{D}_1^+(\xi) \mathcal{R}(\xi)) (\mathbf{I} - \mathcal{R}(\xi) e^{-iLk})^{-1} e^{i(N-1)\xi L} + \varepsilon_j \frac{L}{2\pi} e^{iLk} (\mathcal{D}_0^-(\xi) + \mathcal{D}_1^-(\xi) \mathcal{R}(\xi)) (\mathbf{I} - \mathcal{R}(\xi) e^{iLk})^{-1}.$$

The relations (ii) express in terms of the FB-variables the N conditions:

$$\forall l \in \{0, N-1\}, \quad \tilde{D}_{(i,j)} \phi|_{\tilde{\Sigma}^l} = \phi|_{\tilde{\Sigma}^l} \Leftrightarrow \tilde{D}_{(i,j)} \phi|_{\Sigma^0} = \phi|_{\Sigma^0}.$$

Appendix B. On the generalization of the method to the media without any symmetry

We consider here media that do not exhibit any symmetry. For the simplicity of the presentation, we suppose however that the periodicity cell \mathcal{C} and the interior domain Ω^i are both squares.

All the operators introduced in Sections 3 and 4 can be used for they do not depend on the symmetry assumptions introduced in Section 5.

We provide a method to compute the operator Λ which extends the method developed in the main sections.

B.1. Four auxiliary halfspace problem

In Fig. B.1 we introduce four halfspaces $(\Omega_i^H)_i$ and their corresponding boundaries $(\tilde{\Sigma}_i)_i$ and $(\Sigma_i)_i$ defined by:

$$\left\{ \begin{array}{l} \tilde{\Sigma}_1 = \tilde{\Sigma}_1^- \cup \Sigma_1^0 \cup \tilde{\Sigma}_1^+, \\ \tilde{\Sigma}_2 = \tilde{\Sigma}_2^- \cup \Sigma_2^0 \cup \tilde{\Sigma}_2^+, \\ \tilde{\Sigma}_3 = \tilde{\Sigma}_3^- \cup \Sigma_3^0 \cup \tilde{\Sigma}_3^+, \\ \tilde{\Sigma}_4 = \tilde{\Sigma}_4^- \cup \Sigma_4^0 \cup \tilde{\Sigma}_4^+. \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} \Sigma_1 = \tilde{\Sigma}_1^- \cup \Sigma_1^0 \cup \Sigma_1^+, \\ \Sigma_2 = \tilde{\Sigma}_2^- \cup \Sigma_2^0 \cup \Sigma_2^+, \\ \Sigma_3 = \Sigma_3^- \cup \Sigma_3^0 \cup \Sigma_3^+, \\ \Sigma_4 = \Sigma_4^- \cup \Sigma_4^0 \cup \Sigma_4^+, \end{array} \right.$$

where the notation $\tilde{\Sigma}$ is used in case of taking the decreasing x or y- direction.

We have the following relations,

$$\tilde{\Sigma}_i^+ = \Sigma_{i+1}^- \quad \text{and} \quad \tilde{\Sigma}_i^- = \Sigma_{i-1}^+, \quad i \in \mathbb{Z}/4\mathbb{Z}.$$

For every $i = 1, \dots, 4$, for every $\psi \in H^{1/2}(\tilde{\Sigma})$, let $u_i^H(\psi)$ be the unique H^1 solution of the problem

$$\begin{cases} -\Delta u_i^H(\psi) - n(\mathbf{x})^2(\omega^2 + i\varepsilon)u_i^H(\psi) = 0, & \text{in } \Omega_i^H, \\ u_i^H(\psi) = \psi, & \text{on } \tilde{\Sigma}_i. \end{cases} \quad (\mathcal{P}_i^H)$$

We define the following DtN operator Λ_i^H

$$\Lambda_i^H : H^{1/2}(\tilde{\Sigma}_i) \rightarrow H^{-1/2}(\tilde{\Sigma}_i)$$

$$\psi \mapsto \Lambda_i^H \psi = -\frac{\partial}{\partial x} u_i^H(\psi) \Big|_{\tilde{\Sigma}_i}.$$

Now we have four independent halfspace problems to solve, using the method developed in Section 4.

Thanks to these resolutions we can determine four DtD operators $(D_i^H)_i$ defined by:

$$D_1^H : H^{1/2}(\tilde{\Sigma}_1) \longrightarrow H^{1/2}(\tilde{\Sigma}_1), \quad D_2^H : H^{1/2}(\tilde{\Sigma}_2) \longrightarrow H^{1/2}(\tilde{\Sigma}_2),$$

$$\psi \mapsto \begin{cases} D_1^H \psi|_{\tilde{\Sigma}_1^+} = u_1^H(\psi)|_{\Sigma_1^+}, \\ D_1^H \psi|_{\tilde{\Sigma}_1^0} = \psi|_{\tilde{\Sigma}_1^0}, \\ D_1^H \psi|_{\tilde{\Sigma}_1^-} = u_1^H(\psi)|_{\Sigma_1^-}, \end{cases} \quad \psi \mapsto \begin{cases} D_2^H \psi|_{\tilde{\Sigma}_2^+} = u_2^H(\psi)|_{\Sigma_2^+}, \\ D_2^H \psi|_{\tilde{\Sigma}_2^0} = \psi|_{\tilde{\Sigma}_2^0}, \\ D_2^H \psi|_{\tilde{\Sigma}_2^-} = u_2^H(\psi)|_{\Sigma_2^-}. \end{cases}$$

$$D_3^H : H^{1/2}(\tilde{\Sigma}_3) \longrightarrow H^{1/2}(\tilde{\Sigma}_3), \quad D_4^H : H^{1/2}(\tilde{\Sigma}_4) \longrightarrow H^{1/2}(\tilde{\Sigma}_4),$$

$$\psi \mapsto \begin{cases} D_3^H \psi|_{\tilde{\Sigma}_3^+} = u_3^H(\psi)|_{\Sigma_3^+}, \\ D_3^H \psi|_{\tilde{\Sigma}_3^0} = \psi|_{\tilde{\Sigma}_3^0}, \\ D_3^H \psi|_{\tilde{\Sigma}_3^-} = u_3^H(\psi)|_{\Sigma_3^-}, \end{cases} \quad \psi \mapsto \begin{cases} D_4^H \psi|_{\tilde{\Sigma}_4^+} = u_4^H(\psi)|_{\Sigma_4^+}, \\ D_4^H \psi|_{\tilde{\Sigma}_4^0} = \psi|_{\tilde{\Sigma}_4^0}, \\ D_4^H \psi|_{\tilde{\Sigma}_4^-} = u_4^H(\psi)|_{\Sigma_4^-}. \end{cases}$$

As in Proposition 18, we find a simple expression for the FB-transform of each D_i^H .

B.2. Determination of Λ

We note that $\Sigma_S = \bigcup_{i=1}^4 \Sigma_i^0$. We can show the following theorem according to the schematic decomposition process of Fig. 8:

Theorem 17. For every $\phi \in H^{1/2}(\Sigma_S)$, for every $i \in \{1, \dots, 4\}$, we have

$$\Lambda \phi|_{\Sigma_i^0} = \tilde{R}_i \circ \Lambda_i^H \circ \tilde{D}_i,$$

where

- \tilde{D}_i is a Dirichlet-to-Dirichlet operator defined by:

$$\tilde{D}_i : H^{1/2}(\Sigma_S) \rightarrow H^{1/2}(\tilde{\Sigma}_i),$$

$$\phi \mapsto u^e(\phi)|_{\tilde{\Sigma}_i},$$

where $u^e(\phi)$ is the solution of the problem (\mathcal{P}^e) ;

- Λ_i^H is the halfspace DtN operator defined in Section B.1;

- \tilde{R}_i is the restriction operator defined from $H^{-1/2}(\tilde{\Sigma}_i)$ into $[H_{00}^{1/2}(\Sigma_i^0)]'$ which is the continuous extension to Σ_i^0 of the restriction operator from $L^2(\tilde{\Sigma}_i)$ into $L^2(\Sigma_i^0)$.

Proof. The idea of the decomposition is the same idea as in the proof of Theorem 13. Here however, we have to guarantee that for every $\phi \in H^{1/2}(\Sigma_S)$, we can reconstruct a function $\Lambda\phi \in H^{-1/2}(\Sigma_S)$ thanks to $\tilde{R}_i \circ \Lambda_i^H \circ \tilde{D}_i\phi$ which belong to $H^{-1/2}(\Sigma_i)$ (i.e. $\tilde{R}_i \circ \Lambda_i^H \circ \tilde{D}_i\phi$ have to satisfy some conditions at the corners).

Let ϕ be in $H^{1/2}(\Sigma_S)$. For each $i \in \{1, \dots, 4\}$, by definition of \tilde{D}_i , $u^e(\phi)|_{\Omega_i^H}$ and $u_i^H(\tilde{D}_i\phi)$ satisfy the Helmholtz equation (\mathcal{P}_i^H) with the same Dirichlet condition in $\tilde{\Sigma}_i$, namely $\tilde{D}_i\phi$.

By uniqueness of the solution of (\mathcal{P}_i^H) , we have

$$u^e(\phi)|_{\Omega_i^H} = u_i^H(\tilde{D}_i\phi)$$

and in particular:

$$R_i\left(\frac{\partial}{\partial \mathbf{n}} u^e(\phi)\Big|_{\Sigma_S}\right) = \tilde{R}_i \circ \Lambda^H \circ \tilde{D}_i\phi,$$

where R_i is the restriction operator defined from $H^{-1/2}(\Sigma_S)$ into $[H_{00}^{1/2}(\Sigma_i^0)]'$ which the continuous extension to Σ_i^0 of the restriction from $L^2(\Sigma_S)$ into $L^2(\Sigma_i^0)$. If we recompose to a function of Σ_S , we obtain the Neumann trace of a $H^1(\Delta, \Omega^e)$ function. \square

Each Λ_i^H can be computed from the previous results. The determination of Λ is now reduced to that of the four DtD operators \tilde{D}_i . Each \tilde{D}_i is in the affine subspace:

$$\mathcal{L}_{\Sigma_i^0} = \{L \in \mathcal{L}(H^{1/2}(\Sigma_S), H^{1/2}(\tilde{\Sigma}_i)), \forall \phi \in H^{1/2}(\Sigma_S), L\phi|_{\Sigma_i^0} = \phi|_{\Sigma_i^0}\}.$$

With the same arguments as in the case with double symmetries, we can prove the following theorem.

Theorem 18. *The set of operators $(\tilde{D}_1, \tilde{D}_2, \tilde{D}_3, \tilde{D}_4)$ is the unique solution of the problem: Find $(\tilde{D}_1, \tilde{D}_2, \tilde{D}_3, \tilde{D}_4) \in \mathcal{L}_{\Sigma_1^0} \times \mathcal{L}_{\Sigma_2^0} \times \mathcal{L}_{\Sigma_3^0} \times \mathcal{L}_{\Sigma_4^0}, \forall i \in \mathbb{Z}/4\mathbb{Z}$,*

$$\begin{cases} \tilde{D}_i|_{\tilde{\Sigma}_i^+} = D_{i+1}^H \circ \tilde{D}_{i+1}|_{\Sigma_{i+1}^-}, \\ \tilde{D}_i|_{\tilde{\Sigma}_i^-} = D_{i-1}^H \circ \tilde{D}_{i-1}|_{\Sigma_{i-1}^+}. \end{cases} \quad (\mathcal{E})$$

Remark 21. The problem (\mathcal{E}) is of affine nature and is more involved than previously, especially because the equations satisfied by the four DtD operators are coupled.

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