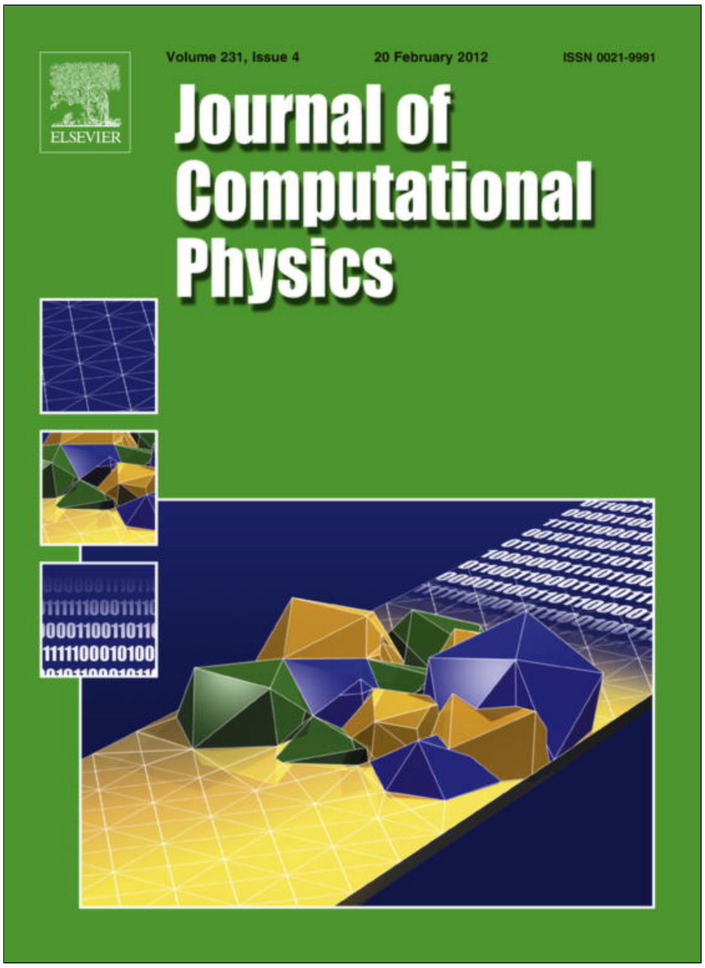
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Wave propagation in locally perturbed periodic media (case with absorption): Numerical aspects

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ABSTRACT

We are interested in the numerical simulation of wave propagation in media which are a local perturbation of an infinite periodic one. The question of finding artificial boundary conditions to reduce the actual numerical computations to a neighborhood of the perturbation via a DtN operator was already developed in [1] at the continuous level. We deal in this article with the numerical aspects associated to the discretization of the problem. In particular, we describe the construction of discrete DtN operators that relies on the numerical solution of local cell problems, non stationary Ricatti equations and the discretization of non standard integral equations in Floquet variables.

1. Introduction and model problem

Periodic media play a major role in applications, in particular in optics for micro and nano-technology [2–5]. 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 [4,6]. 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 coupling techniques between volumic methods and integral representations or integral equation techniques [7–10],
(ii) 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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(iii) the local radiation conditions at finite distance [11,12], constructed as a local approximation of the exact non local condition at various orders with respect to a small parameter, typically the inverse of the frequency.

Methods (i) and (ii) are exact (up to numerical approximation). The method (iiii) 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 [13] 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 [14,15]).

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 localized modes (non trivial solutions 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 [16–18] for existence results). The supercell method analyzed [19] 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 fast with respect to the size of the truncated domain. The notion of DtN maps already appears for instance, in [20] for the diffraction problem by periodic gratings or in [21] 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 [22], 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 Ricatti equation. In a second paper [1], we proposed an extension of the above work to the case where the unperturbed media is periodic in the two directions. We presented the conceptual aspects of the method for the construction of the DtN operator and we exposed the main theoretical issues and results. The chapter [23] of the e-book "Wave Propagation in Periodic Media (volume 1)" is devoted to a general presentation of the method of [1,24] adapted to the case of a RtR (for Robin-to-Robin) boundary condition: instead of relating the Dirichlet and the Neumann traces of the solution, we want to relate two different Robin traces of the solution. From the numerical point of view, one of the interest of RtR operators is that, contrary to DtN operators for instance, they are bounded operators with bounded inverse and their discretization leads to well-conditioned matrices.

We tackle, here, the discretization of the method explained in [1], especially the computation of the DtN operator. For the sake of conciseness of the presentation, we shall restrict ourselves to the exposition of the main ideas and results, to give some validation of the method and to illustrate it through numerical results. On the other hand, for the sake of rigor, we have chosen to make precise the functional framework inside which the arguments we shall develop can be completely justified. However, most theorems will be stated without proofs. The reader can find these proofs together additional details in [22,1,24].

Let us also mention that, as in [1], we consider the case where the propagation medium is slightly absorbing, the absorption being quantified by a small positive parameter $\varepsilon > 0$ (see the model problem (P). The challenging question of studying the limit case when ε tends to 0 (i.e. the limiting absorption principle) 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 [22,24] for the case of periodic waveguides. A forthcoming article will deal with the a numerical limiting absorption principle for the locally perturbed periodic media. The propagation model we consider is a simple 2D ($\mathbf{x} = (x, y)$) harmonic scalar wave problem with absorption:

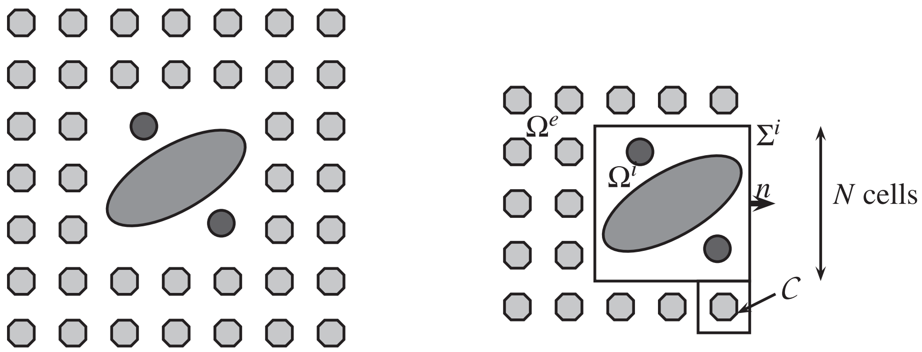
$$-\Delta u(\mathbf{x}) - \rho(\mathbf{x})(\omega^2 + \imath\varepsilon\omega)u(\mathbf{x}) = f(\mathbf{x}). \qquad \text{(P)}$$

where $\varepsilon > 0$ is a (small) physical parameter, that represents a (slight) absorption in the medium.

Moreover, we suppose that (see Fig. 1 for some notation):

(i) The local perturbation to the periodicity in the domain of propagation $\Omega = \mathbb{R}^2$ is contained inside the bounded region Ω^i. In $\Omega^e = \Omega \backslash \Omega^i$ the periodicity is along the x and y directions with the same period L. We denote by $\mathcal{C}$ the reference unit periodicity cell

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



(a) The domain of propagation Ω. (b) Some notation

Fig. 1. The domain of propagation Ω and notation.

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:

$$\Omega^i = \left]-\frac{NL}{2},\frac{NL}{2}\right[^2.$$

For the sake of presentation, we will suppose that $N = 1$ here. However the generalization is straightforward and presented in [1]. The boundary of Ω^i is denoted by $\Sigma^i = \partial\Omega^i$. See Fig. 1(b) for notation.

(ii) The function ρ is supposed to coincide with a periodic function outside Ω^i. More precisely, we suppose that there exists a function ρ_p such that

$$0 < \rho_- = \inf_{\mathbf{x}\in\Omega} \rho(\mathbf{x}) \leqslant \rho_+ = \sup_{\mathbf{x}\in\Omega} \rho(\mathbf{x}) < +\infty,$$

$$\mathrm{Supp}(\rho - \rho_p) \subset \Omega^i \quad \text{where } \rho_p(x \pm L, y \pm L) = \rho_p(x,y), \quad \forall (x,y) \in \Omega.$$

(iii) The support of the source f is contained in Ω^i.

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 $L^2(\Omega)$.

Remark 1 (*Extension*). 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.

In [1], we have characterized the restriction of the solution u to Ω^i as the solution of (P) in Ω^i with boundary conditions of the form:

$$\partial_{\mathbf{n}^i} u + \Lambda u = 0 \quad \text{on } \Sigma^i, \tag{1}$$

where $\mathbf{n}^i$ is the exterior normal to Ω^i and

$$\Lambda \in \mathcal{L}(\mathcal{D},\mathcal{N})$$

where $\mathcal{D}$ (resp. $\mathcal{N}$) is the space of Dirichlet (resp. Neumann) data on Σ_i:

$$\mathcal{D} := H^{1/2}(\Sigma^i), \quad \mathcal{N} := H^{-1/2}(\Sigma^i), \tag{2}$$

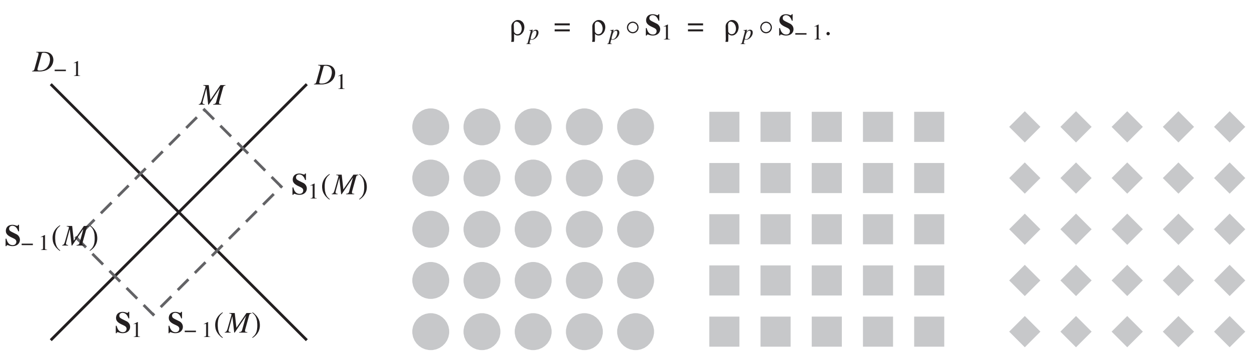
is a transparent DtN operator. In [1], we have also provided a method for the construction of this operator (see Section 2 of this paper for a recap). Our goal is to explain how to compute in practice an approximation of the DtN operator and then the solution of (P).

For the sake of simplicity, we shall restrict ourselves to doubly symmetric media (see however the appendix B of [1] for the extension to the general case) which correspond to the following assumptions (see Fig. 2(b) for examples of periodic functions with double symmetry).

(H1) the periodicity cell $\mathcal{C}$ and the boundary Σ^i present a double symmetry: is invariant by the symmetries with respect to $D_1 = \{(x,y) : x = y\}$ ($\mathbf{S}_1$) and $D_1 = \{(x,y) : x = -y\}$ $\mathbf{S}_{-1}$ (see Fig. 2(a)).

(H2) the restriction of ρ_p to $\mathcal{C}$ is with double symmetry i.e.

$$\rho_p = \rho_p \circ \mathbf{S}_1 = \rho_p \circ \mathbf{S}_{-1}.$$



(a) The symmetries (b) Functions with double symmetry (the grey represent the value 1 and the white one 2)

Fig. 2. Double symmetry: definitions and examples.

This article is organized as follows. We will remind in Section 2 all what is needed from [1] to understand the present paper. Section 3 deals with the discretization of the problem and the numerical methods used for the resolution of the various discrete problems. It contains in particular an appropriate discretization of a non-classical operator valued integral equation (one of the most original part of the article). Section 4 is devoted to numerical results and Section 5 to give some conclusions and perspectives.

2. Resolution of the Helmholtz problem with absorption in a locally perturbed periodic plane: a recap of the main results from [1]

Instead of solving (P) which is posed in the infinite domain $\Omega = \mathbb{R}^2$, a classical idea is to characterize the restriction of the solution to Ω^i as the solution of the following problem posed in Ω^i

$$\left| \begin{array}{ll} -\Delta u^i - \rho(\omega^2 + \imath\varepsilon\omega)u^i = f & \text{in } \Omega^i, \\ \partial_{\mathbf{n}^i} u^i + \Lambda u^i = 0 & \text{on } \Sigma^i, \end{array} \right. \tag{P^i}$$

where $\mathbf{n}^i$ is the exterior normal to Ω^i and Λ is the DtN operator defined by

$$\begin{array}{l} \Lambda : H^{1/2}(\Sigma^i) \to H^{-1/2}(\Sigma^i), \\ \varphi \mapsto \Lambda\varphi = -\partial_{\mathbf{n}^i} u^e(\varphi)|_{\Sigma^i}, \end{array}$$

where $u^e(\varphi) \in H^1(\Delta, \Omega^e) = \{u \in H^1(\Omega^e),\ \Delta u \in L^2(\Omega^e)\}$ is the unique solution of the problem posed on Ω^e with Dirichlet conditions

$$\left| \begin{array}{ll} -\Delta u^e - \rho_p(\mathbf{x})(\omega^2 + \imath\varepsilon\omega)u^e = 0 & \text{in } \Omega^e, \\ u^e = \varphi & \text{on } \Sigma^i. \end{array} \right. \tag{P^e}$$

The notation $u^e(\varphi)$ indicates the dependence of the solution to (P^e) on the Dirichlet boundary data.

The whole problem can then be solved in three main steps:

1. the construction of Λ (see Sections 2.1, 2.2 and 2.3);
2. the resolution of the interior problem;
3. the reconstruction of the solution in the whole domain (see Section 2.5).

2.1. Bloch diagonalization of the DtN operator in doubly symmetric media

As a real function can be decomposed as the sum of an odd and en even function, a function defined in a set with double symmetry (Σ^i or Ω^e) can be decomposed as the sum of four functions, each one being symmetric and/or antisymmetric with respect to D_1 or D_{-1}. More precisely, for $H = H^1(\Delta, \Omega^e)$, $H^{1/2}(\Sigma^i)$ or $H^{-1/2}(\Sigma^i)$ we have

$$H = H_{(s,s)} \oplus H_{(s,a)} \oplus H_{(a,s)} \oplus H_{(a,a)}, \tag{3}$$

where, given $\varepsilon_s = 1$ and $\varepsilon_a = -1$,

$$\forall (p,q) \in \{s,a\}^2, \quad H_{(p,q)} = \left\{ v \in H,\ v = \varepsilon_p v \circ \mathbf{S}_1 = \varepsilon_q v \circ \mathbf{S}_{-1} \right\}$$

if $H = H^{1/2}(\Sigma^i)$ or $H = H^1(\Omega^e, \Delta)$ and

$$\forall (p,q) \in \{s,a\}^2, \quad H^{-1/2}_{(p,q)}(\Sigma^i) = \left\{ \partial_{\mathbf{n}^i} u|_{\Sigma^i},\ u \in H^1_{(p,q)}(\Omega^e, \Delta) \right\}.$$

To shorten the notation, we shall set, according to (2):

$$\mathcal{D}_{(p,q)} := H^{1/2}_{(p,q)}(\Sigma^i), \quad \mathcal{N}_{(p,q)} := H^{-1/2}_{(p,q)}(\Sigma^i).$$

Clearly, it suffices then to compute $\Lambda\varphi$ for φ in each $\mathcal{D}_{(p,q)}$ to fully characterize Λ.

At this stage, we have not used the hypothesis (H1) and (H2). Actually, because of the symmetry property of the media and the domain and the properties of the Laplacian, the Theorem 10 and 12 of [1] states that if the Dirichlet data φ is symmetric (or antisymmetric) with respect to D_1 (or D_{-1}) then the exterior solution $u^e(\varphi)$ remains symmetric (or antisymmetric) with respect to D_1 (or D_{-1}). In other words

$$\forall (p,q) \in \{s,a\}^2, \quad \varphi \in \mathcal{D}_{(p,q)} \Rightarrow u^e(\varphi) \in H^1_{(p,q)}(\Omega^e, \Delta)$$

and by definition of the space $\mathcal{N}_{(p,q)}$, we conclude that

$$\forall (p,q) \in \{s,a\}^2, \quad \Lambda\left(\mathcal{D}_{(p,q)}\right) \subset \mathcal{N}_{(p,q)}.$$

Therefore, if we note

$$\forall (p,q) \in \{s,a\}^2, \quad \Lambda_{(p,q)} = \Lambda\big|_{\mathcal{D}_{(p,q)}} \in \mathcal{L}\left(\mathcal{D}_{(p,q)}, \mathcal{N}_{(p,q)}\right), \tag{4}$$

the operator Λ can be written in a diagonal form:

$$\Lambda = \begin{bmatrix} \Lambda_{(s,s)} & 0 & 0 & 0 \\ 0 & \Lambda_{(s,a)} & 0 & 0 \\ 0 & 0 & \Lambda_{(a,s)} & 0 \\ 0 & 0 & 0 & \Lambda_{(a,a)} \end{bmatrix}. \tag{5}$$

2.2. A constructive method for the DtN operator $\Lambda_{(p,q)}$

In the following, see Fig. 3, Σ_0 will denote the vertical right side of Σ_i. Note that, by symmetry, any element of $\mathcal{D}_{(p,q)}$ is completely determined by its restriction to Σ_0. We shall also set

$$\widetilde{\Sigma} = \widetilde{\Sigma}^- \cup \Sigma_0 \cup \widetilde{\Sigma}^+ \quad \text{(that can be identified to the } y \text{ real line)},$$

where $\widetilde{\Sigma}^+$ and $\widetilde{\Sigma}^-$ are the two vertical half-lines in Fig. 3. An essential technical tool is the partial Floquet–Bloch transform in the y-variable, whose definition is recalled in Appendix A. It will be denoted $\mathcal{F}_y$. Let us simply mention here that $\mathcal{F}_y$ transforms a function of $y \in \mathbb{R}$ into a function of $(y, k_y) \in \mathbb{K}$ (k_y is by definition the dual variable of y) where $\mathbb{K}$ denotes the rectangle

$$\mathbb{K} = \Sigma_0 \times]-\pi/L, \pi/L[.$$

We give below, without any justifications (which can be found in [1,24]) a decomposition of the operator $\Lambda_{(p,q)}$ that will be used for the numerical justification. This decomposition involves the introduction of new operators that will be defined in Section 2.3. Some useful explanations about this decomposition will be however given in Section 2.4.

The passage from φ to $\Lambda_{(p,q)}\varphi$ can be decomposed into three steps:

$$\Lambda_{(p,q)} : \varphi(y) \underset{D_{(p,q)}}{\mapsto} \hat{\psi}_{(p,q)}(y, k_y) \underset{\Lambda^H}{\mapsto} \hat{\theta}_{(p,q)}(y, k_y) \underset{R_{(p,q)}}{\mapsto} \Lambda_{(p,q)}\varphi(y),$$

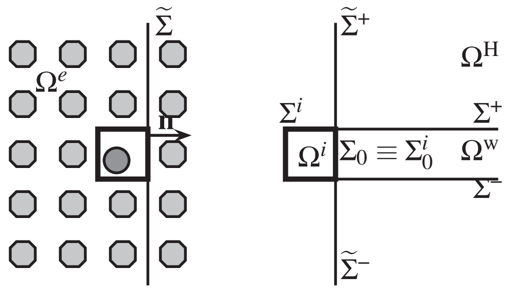


Fig. 3. 2D-plane medium.

which corresponds to the following factorization of $\Lambda_{(p,q)}$

$$\Lambda_{(p,q)} = \widehat{R}_{(p,q)} \circ \widehat{\Lambda}^H \circ \widehat{D}_{(p,q)} \tag{6}$$

into the product of three operators

$$\widehat{D}_{(p,q)} \in \mathcal{L}\left(\mathcal{D}_{(p,q)}, \mathcal{D}_{QP}\right), \quad \widehat{\Lambda}^H \in \mathcal{L}(\mathcal{D}_{QP}, \mathcal{N}_{QP}), \quad \widehat{R}_{(p,q)} \in \mathcal{L}\left(\mathcal{N}_{QP}, \mathcal{N}_{(p,q)}\right), \tag{7}$$

where the intermediate spaces $\mathcal{D}_{QP} := \mathcal{F}_y\left(H^{1/2}(\widetilde{\Sigma})\right)$ and $\mathcal{N}_{QP} = \mathcal{F}_y\left(H^{-1/2}(\widetilde{\Sigma})\right)$ are spaces of (generalized) functions on $\mathbb{K}$, that are described in more detail in Appendix A and satisfy

$$\mathcal{D}_{QP} \subset L^2(\mathbb{K}) \subset \mathcal{N}_{QP}, \quad \mathcal{N}_{QP} \text{ is the dual space of } \mathcal{D}_{QP}.$$

The three steps of (6) consist of (see Fig. 4)

(1) $\hat{\psi}_{(p,q)} = \widehat{D}_{(p,q)}\varphi \in \mathcal{D}_{QP}$ is the unique solution of the integral equation in $\hat{\psi}$:

$$\left|\begin{array}{ll} \text{(i)} & \hat{\psi}(\cdot, k_x) - \frac{L}{2\pi}\int_{-\pi/L}^{\pi/L} \mathbf{K}_{(p,q)}(k_x, k_y)\hat{\psi}(\cdot; k_y) : dk_y = 0, \\ \text{(ii)} & \sqrt{\frac{L}{2\pi}}\int_{-\pi/L}^{\pi/L} \hat{\psi}(\cdot, k_x) : dk_x = \varphi|_{\Sigma_0}, \end{array}\right. \tag{$\mathrm{E}_{(p,q)}(\varphi)$}$$

where the data appears in the affine constraint (ii) and where the kernel $\mathbf{K}_{(p,q)}(k_x,k_y)$ is for each (k_x,k_y) an operator defined in Section 2.3.3.

(2) $\hat{\theta}_{(p,q)} = \widehat{\Lambda}^H \hat{\psi}_{(p,q)} \in \mathcal{N}_{QP}$ is given by the expression:

$$\forall k_y \in]-\pi/L, \pi/L[, \quad \hat{\theta}_{(p,q)}(\cdot, k_y) = \Lambda^{\mathrm{w}}(k_y)\left[\hat{\psi}_{(p,q)}(\cdot, k_y)\right], \tag{8}$$

where $\Lambda^{\mathrm{w}}(k_y)$ is for each k_y the DtN operator for a periodic half waveguide problem with k_y-quasi periodic conditions (see Section 2.3.2).

(3) $\Lambda_{(p,q)}\varphi = \widehat{R}_{(p,q)}\hat{\theta}_{(p,q)} \in \mathcal{N}_{(p,q)}$ is first defined via its restriction to Σ_0:

$$\Lambda_{(p,q)}\varphi|_{\Sigma_0} = \widehat{R}_{(p,q)}\hat{\theta}_{(p,q)} := \sqrt{\frac{L}{2\pi}}\int_{-\pi/L}^{\pi/L} \hat{\theta}_{(p,q)}(\cdot, k_y)dk_y \tag{9}$$

and reconstructed over all Σ^i according to the (p,q) symmetries.

2.3. Construction of the operators $\mathbf{K}_{(p,q)}(k_x,k_y)$ and $\Lambda^{\mathrm{w}}(k_y)$

We describe in this section the definition and properties of the operators involved in the steps (1) and (2) of the above decomposition algorithm. A basic ingredient is the resolution of local problems posed only on a periodicity cell ([1]) that we present in the next subsection.

We refer to Fig. 5 for the notation used in this section. Note that we use the same notation Σ_0 for the left vertical side of $\mathcal{C}$ and the right vertical side of Σ_i (see section S) which can be both identified to a segment of length L. The definition of the spaces $H^{\pm 1/2}_{k_y}(\Sigma_0)$ of k_y-quasi-periodic $H^{\pm 1/2}$ functions on Σ_0 is given in the appendix.

2.3.1. Elementary cell problems

For $k_y \in]-\pi/L,\pi/L[$ and $\hat{\psi} \in H^{1/2}_{k_y}(\Sigma_0)$ (see appendix for the definition), let

$$e^0(k_y;\hat{\psi}) \quad \text{and} \quad e^1(k_y;\hat{\psi})$$

be the unique solutions in $H^1(\mathcal{C})$ of the following elementary cell problems:

$$-\Delta e^\ell - \rho_p(\omega^2 + \imath\varepsilon\omega)e^\ell = 0, \quad \text{in } \mathcal{C} \tag{10}$$

satisfying k_y quasi-periodic boundary conditions on Σ_1^+ and Σ_1^-:

$$e^\ell|_{\Sigma_1^+} = e^{\imath k_y L}e^\ell|_{\Sigma_1^-}, \quad \text{and} \quad (\partial_y e^\ell)|_{\Sigma_1^+} = e^{\imath k_y L}\cdot(\partial_y e^\ell)|_{\Sigma_1^-}, \tag{11}$$

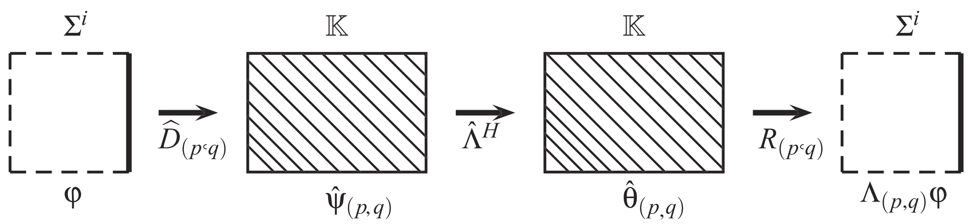


Fig. 4. Factorization of $\Lambda_{(p,q)}$ (see (6)).

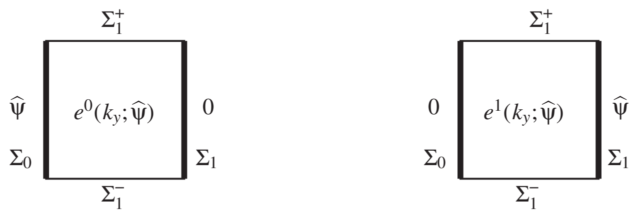


Fig. 5. The functions $e^j(k_y;\hat{\psi}_{k_y}),\ j=0,1$.

and non homogeneous Dirichlet conditions on Σ_0 and Σ_1:

$$e^0|_{\Sigma_0}=\hat{\psi} \quad \text{and} \quad e^0|_{\Sigma_1}=0, \qquad e^1|_{\Sigma_0}=0 \quad \text{and} \quad e^1|_{\Sigma_1}=\hat{\psi}. \tag{12}$$

We define then the four local DtN operators

$$T^{ij}(k_y)\in\mathcal{L}\Big(H^{1/2}_{k_y}(\Sigma_0),H^{-1/2}_{k_y}(\Sigma_0)\Big),\quad (i,j)\in\{0,1\}^2$$

as follows (Σ_1 being implicitly identified to Σ_0)

$$\left|\begin{array}{l} T^{00}(k_y)\hat{\psi}=-\partial_x e^0(k_y;\hat{\psi})\Big|_{\Sigma_0},\quad T^{01}(k_y)\hat{\psi}=\partial_x e^0(k_y;\hat{\psi})\Big|_{\Sigma_1},\\ T^{10}(k_y)\hat{\psi}=-\partial_x e^1(k_y;\hat{\psi})\Big|_{\Sigma_0},\quad T^{11}(k_y)\hat{\psi}=\partial_x e^1(k_y;\hat{\psi})\Big|_{\Sigma_1}, \end{array}\right. \tag{13}$$

We also define four local DtD operators

$$D^{\ell,\pm}(k_y)\in\mathcal{L}\Big(H^{1/2}_{k_y}(\Sigma_0),H^{1/2}_{k_y}(\Sigma_0)\Big),\quad \ell\in\{0,1\}$$

by taking the traces of $e^\ell(k_y;\hat{\psi})$ on $\Sigma_1^\pm$. Formally

$$D^{\ell,\pm}(k_y)\hat{\psi}\equiv e^\ell(k_y;\hat{\psi})\Big|_{\Sigma_1^\pm}. \tag{14}$$

The above equality being understood modulo the identification of Σ_0 with $\Sigma_1^\pm$ and an orientation of $\Sigma_1^\pm$ illustrated by Fig. 6. More precisely, (14) means (Σ_0 being implicitly identified to $]-L/2,L/2[$)

$$\left|\begin{array}{l} \Big[D^{\ell,-}(k_y)\hat{\psi}\Big](y)=\Big[e^\ell(k_y;\hat{\psi})\Big](L-y,-L/2),\\ \Big[D^{\ell,+}(k_y)\hat{\psi}\Big](y)=\Big[e^\ell(k_y;\hat{\psi})\Big](y,L/2). \end{array}\right. \tag{15}$$

2.3.2. Characterization of the half-waveguide DtN operator $\Lambda^w(k_y)$

The construction of the operator

$$\Lambda^w(k_y)\in\mathcal{L}\Big(H^{1/2}_{k_y}(\Sigma_0),H^{-1/2}_{k_y}(\Sigma_0)\Big)$$

is based on the determination of propagation operators $P(k_y)$ (see [1] for more details). For each k_y, the operator $P(k_y)$ is characterized as the unique compact operator (the notation $\mathcal{K}(H)$ holds for the space of compact operators in an Hilbert space H)

$$P(k_y)\in\mathcal{K}\Big(H^{1/2}_{k_y}(\Sigma_0)\Big)$$

whose spectral radius satisfies the condition

$$\rho(P(k_y))<1$$

and which solves the stationary Riccati equation:

$$T^{10}(k_y)P(k_y)^2+\Big(T^{00}(k_y)+T^{11}(k_y)\Big)P(k_y)+T^{01}(k_y)=0, \tag{16}$$

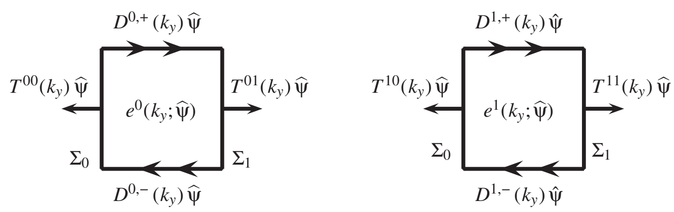


Fig. 6. The local DtN operators $T^{ij}_{k_y}$ and the local DtD operators $D^{\ell,\pm}(k_y)$.

where the operators $T^{ij}(k_y)$ are the local DtN operators defined in (13).

Then $\Lambda^{\mathrm{w}}(k_y)$ is given by

$$\Lambda^{\mathrm{w}}(k_y) = T^{00}(k_y) + T^{10}(k_y)P(k_y). \tag{17}$$

2.3.3. Definition of the kernels $\mathbf{K}_{(p,q)}$

For each (k_x, k_y) the kernel $\mathbf{K}_{(p,q)}(k_x, k_y)$ is defined by, setting $\varepsilon_s = 1$ and $\varepsilon_a = -1$,

$$\left| \begin{array}{l} \mathbf{K}_{(p,q)}(k_x, k_y) \in \mathcal{L}\left(H^{1/2}_{k_y}(\Sigma_0), H^{1/2}_{k_x}(\Sigma_0)\right), \\ \mathbf{K}_{(p,q)}(k_x, k_y) = \mathbf{I} + \varepsilon_p \mathbf{K}^{+}(k_x, k_y) + \varepsilon_q \mathbf{K}^{-}(k_x, k_y), \end{array} \right. \tag{18}$$

where

$$\mathbf{K}^{\pm}(k_x, k_y) = e^{\mp \imath L k_x}\left(D^{0,\pm}(k_y) + D^{1,\pm}(k_y)P(k_y)\right)\left(\mathbf{I} - P(k_y)e^{\mp \imath L k_x}\right)^{-1},$$

where the operators $D^{\ell,\pm}(k_y)$ are the local DtD operators defined in (14).

Let us remark that the operator $\mathbf{I} - P(k_y)e^{\mp \imath L k_x}$ is invertible since the spectral radius of $P(k_y)$ is strictly less than 1 (which is moreover true uniformly in k_y-see [1,24] for more details).

2.4. More details on the factorization

The key idea given in [1] to obtain the factorization (6) is another factorization of $\Lambda_{(p,q)}$ in (1) as

$$\Lambda_{(p,q)} = D_{(p,q)} \circ \Lambda^{H} \circ R_{(p,q)}, \tag{19}$$

where

- $D_{(p,q)} \in \mathcal{L}\left(\mathcal{D}_{(p,q)}, H^{1/2}(\widetilde{\Sigma})\right)$ is a Dirichlet to Dirichlet operator defined as

  $$D_{(p,q)}\varphi = u^{e}(\varphi)|_{\widetilde{\Sigma}},$$

  where $u^{e}(\varphi)$ is the solution of (P^{e}). It can be seen as an extension operator from Σ_0 to $\widetilde{\Sigma}$ since $u^{e}(\varphi) = \varphi$ on Σ^{i}.

- $\Lambda^{\mathrm{H}} \in \mathcal{L}\left(H^{1/2}(\widetilde{\Sigma}), H^{-1/2}(\widetilde{\Sigma})\right)$ is the halfspace DtN operator:

  $$\Lambda^{\mathrm{H}}\psi = -\partial_x u^{\mathrm{H}}(\psi)|_{\widetilde{\Sigma}},$$

  where $u^{\mathrm{H}} := u^{\mathrm{H}}(\psi)$ is the solution of the halfspace problem in Ω^{H}

  $$\left| \begin{array}{ll} -\Delta u^{\mathrm{H}} - \rho_p(\omega^2 + \imath\varepsilon\omega)u^{\mathrm{H}} = 0 & \text{in } \Omega^{\mathrm{H}}, \\ u^{\mathrm{H}} = \psi & \text{on } \widetilde{\Sigma}, \end{array} \right. \tag{P^{H}}$$

- $R_{(p,q)} \in \mathcal{L}\left(H^{-1/2}(\widetilde{\Sigma}), \mathcal{N}_{(p,q)}\right)$ is simply the restriction extension operator on Σ_0:

  $$R_{(p,q)}\theta|_{\Sigma_0} = \theta|_{\Sigma_0} \tag{20}$$

  and is extended to all Σ^{i} according to the (p,q) symmetries.

To obtain the factorization (19) it suffices to remark that, by construction of $D_{(p,q)}$

$$u^{e}(\varphi)|_{\Omega^{\mathrm{H}}} = u^{\mathrm{H}}(D_{(p,q)}\varphi). \tag{21}$$

The link between the two factorizations (6) and (19) is simply related to the introduction of the Floquet–Bloch transform as an intermediate operator, which is useful from the computational point of view. More precisely we have:

$$\widehat{D}_{(p,q)} = \mathcal{F}_y D_{(p,q)}, \quad \widehat{\Lambda}^{\mathrm{H}} = \mathcal{F}_y \Lambda^{\mathrm{H}} \mathcal{F}_y^{-1}, \quad \widehat{R}_{(p,q)} = R_{(p,q)}\mathcal{F}_y^{-1}. \tag{22}$$

The link between Λ^{H} and $\widehat{\Lambda}^{\mathrm{H}}$ is obtained by applying the partial Floquet–Bloch transform in y to the solution of the half-space problem (P_{H}), which reduces it to a family (indexed by k_y) of half-waveguide problems with k_y-quasi-periodic conditions. This establishes the link between the half-space DtN operator and the half-waveguide DtN operators $\Lambda^{\mathrm{w}}(k_y)$ defined in section, through the formula (8).

If one denotes $\hat{\theta}$ the Floquet–Bloch transform of θ, (9) is nothing but (20) expressed in terms of Floquet–Bloch transforms. This enlightens the last equality of (22).

Much less trivial is the link between $D_{(p,q)}$ and $\widehat{D}_{(p,q)}$ (and thus the integral equation and the kernels). Let us give the main ideas in the symmetric case $(p,q) = (s,s)$ which is simpler to explain. The key point is the obtention of an equation that characterizes $D_{(s,s)}\varphi$ for a given doubly symmetric function φ. To get this equation it is useful to introduce the broken line Σ represented in Fig. 7, that can be trivially identified to the straight line $\widetilde{\Sigma}$. Reminding that the solution $u^e(\varphi)$ of the exterior problem is doubly symmetric, we have

$$u^e(\varphi)|_{\widetilde{\Sigma}} = u^e(\varphi)|_{\Sigma} \quad \text{(modulo the identification of } \Sigma \text{ with } \widetilde{\Sigma})$$

namely, using (21) and the boundary condition in (P_H) (with $\psi = D_{(s,s)}\varphi$)

$$D_{(s,s)}\varphi|_{\widetilde{\Sigma}} = u^H(D_{(s,s)}\varphi)|_{\Sigma}, \tag{23}$$

which is a homogeneous linear equation in $D_{(s,s)}\varphi$ that we can complete with the affine constraint

$$D_{(s,s)}\varphi|_{\Sigma^0}, = \varphi|_{\Sigma^0}, \tag{24}$$

which expresses nothing but $u^e(\varphi) = \varphi$ on Σ_0.

Which is less obvious, but true, is that (23), (24) characterize $D_{(s,s)}\varphi$.

Finally, denoting $\psi = D_{(s,s)}\varphi$ and $\hat{\psi}$ denotes its Fourier–Bloch transform, we obtain, by applying the Fourier–Bloch transform to (23), (24) (this is a more involved computation detailed in [1,24]), the equation $(\mathcal{E}_{(s,s)}(\varphi))$ with the kernel $\mathbf{K}_{(s,s)}$ given by (18). More precisely (23) leads to (i) and (24) to (ii).

2.5. Algorithm for the computation of the solution

2.5.1. Algorithm for the construction of the DtN operator Λ

1. Resolution of the cell problems
   (i) For each k_y, solve the cell problems (10)–(12) and compute the local DtN operators $T^{ij}(k_y)$ as well as the local DtD operators $D^{\ell,\pm}(k_y)$ (see (13) and (14)).
   (ii) For each k_y, determine of the propagation operator $P(k_y)$ solving the stationary Riccati equation (16).
2. Construction of $\Lambda_{(p,q)}$ for each $(p,q) \in \{s,a\}^2$
   (i) Build the operator $\widehat{D}_{(p,q)}$ by solving $(E_{(p,q)}(\varphi))$ for each $\varphi \in H^{1/2}_{(p,q)}(\Sigma^i)$.
   (ii) Construct $\widehat{\Lambda}^{\mathrm{H}}$ using (8).
   (iii) Construct $\Lambda_{(p,q)}$ using (6).
3. Determination of the DtN operator Λ from (5).

2.5.2. Algorithm for the numerical computation of the solution

Once the DtN operator Λ is computed, the interior problem (P^i) with the exact boundary conditions can be solved.

As a by-product, the methods allows to compute the solution u of (P) outside the bounded region Ω^i, and defined, thanks to the solutions of the interior and exterior problems, by

$$\left| \begin{array}{ll} u = u^i, & \text{in } \Omega^i, \\ u = u^e(\varphi^i), & \text{in } \Omega^e, \text{ with } \varphi^i = u^i|_{\Sigma^i}, \end{array} \right.$$

where u^i is the solution of (P^i) and u^e is the solution of (P^e). Indeed, it suffices to use the following algorithm of reconstruction using essentially the solution u^H of halfspace problems (P_H) and the DtD operators $D_{(p,q)}$ involved in the characterization of Λ (see Section 2.4).

1. Thanks to the decomposition (3) of Section 2.1, φ^i can be decomposed by

$$\varphi^i = \sum_{(p,q)\in\{s,a\}^2} \varphi^i_{(p,q)} \quad \text{with } \forall (p,q) \in \{s,a\}^2, \quad \varphi^i_{(p,q)} \in H^{1/2}_{(p,q)}(\Sigma^i).$$

2. We build $\hat{\psi}_{(p,q)} = \widehat{D}_{(p,q)}\varphi^i_{(p,q)}$ and by definition of the DtD operator $D_{(p,q)}$,

$$\forall (p,q) \in \{s,a\}^2, \quad \mathcal{F}_y\left(u^e\left(\varphi^i_{(p,q)}\right)\Big|_{\widetilde{\Sigma}}\right) = \hat{\psi}_{(p,q)}.$$

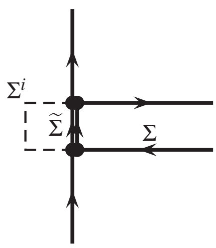


Fig. 7. Identification of $\widetilde{\Sigma}$ with Σ.

3. The restriction of the exterior solution $u^{\rm e}(\varphi^i_{(p,q)})$ in the right halfspace $\Omega^{\rm H}$

$$u^{\rm H}_{(p,q)} = u^{\rm e}\left(\varphi^i_{(p,q)}\right)\Big|_{\Omega^{\rm H}}, \quad \text{where } \Omega^{\rm H} = \bigcup_{\substack{m\in\mathbb{Z}\\ n\in\mathbb{N}^*}} \mathcal{C}_{nm} \text{ and } \mathcal{C}_{nm} = \Omega^i + (nL, mL)$$

can be computed semi-analytically (see [1] for details): $\forall n \in \mathbb{N}^*,\ \forall m \in \mathbb{Z}$

$$u^{\rm e}\left(\varphi^i_{(p,q)}\right)\Big|_{\mathcal{C}_{nm}} = \sqrt{\frac{L}{2\pi}}\int_{-\pi/L}^{\pi/L}\left[e^0\left(k_y; P(k_y)^{n-1}\hat{\psi}(\cdot,k_y)\right) + e^1\left(k_y; P(k_y)^n\hat{\psi}(\cdot,k_y)\right)\right]e^{\imath m k_y L}\,dk_y.$$

4. By symmetry arguments, we build

$$\forall (p,q)\in\{s,a\}^2, \quad u^e(\varphi^i_{(p,q)}) = \left|\begin{array}{ll} u^{\rm H}_{(p,q)} & \text{in } \Omega^{\rm H},\\ \varepsilon_p S_1\left(u^{\rm H}_{(p,q)}\right) & \text{in } S_1\Omega^{\rm H},\\ \varepsilon_q S_{-1}\left(u^{\rm H}_{(p,q)}\right) & \text{in } S_{-1}\Omega^{\rm H},\\ \varepsilon_p\varepsilon_q S_1\circ S_{-1}\left(u^{\rm H}_{(p,q)}\right) & \text{in } S_1\circ S_{-1}\Omega^{\rm H},\end{array}\right.$$

where we have posed $u^{\rm H}_{(p,q)} = u^{\rm e}\left(\varphi^i_{(p,q)}\right)\Big|_{\Omega_{\rm H}},\ \varepsilon_s = 1,\ \varepsilon_a = -1$ and where S_1 and S_{-1} are the symmetries defined in Section 1 (in (H1)).

5. By linearity, we have finally

$$u^e(\varphi^i) = \sum_{(p,q)\in\{s,a\}^2} u^e(\varphi^i_{(p,q)}).$$

At this stage, we have described the computational algorithm at the continuous level. In practice, we have to work in a discrete setting via a numerical approximation process. This is the objective of the next section.

3. Discretization for the computation of Λ

We propose in this section to construct a discrete version of the transparent DtN operator Λ in which the spaces $\mathcal{D}$ and $\mathcal{N}$ of Dirichlet and Neumann data (cf. (2)) are replaced by finite dimensional spaces. We start from a 1D mesh $\mathcal{T}_h(\Sigma_0)$ of Σ_0, with step size h (typically a uniform mesh) devoted to tend to 0. Next, we extend this mesh by symmetry across the lines $D_{\pm 1}$ into a mesh $\mathcal{T}_h(\Sigma^i)$ of Σ^i. Given an integer $m \geqslant 0$, we choose:

$$\mathcal{D}^h = \mathcal{N}^h \equiv L^2_h(\Sigma^i) := \left\{\varphi_h \in L^2(\Sigma^i)/\forall \mathcal{S}\in\mathcal{T}_h(\Sigma^i),\ \varphi_h|_{\mathcal{S}}\in\mathcal{P}_m\right\},$$

where $\mathcal{P}_m$ denotes the space of $1D$ polynomials of degree less or equal to m. This choice will lead to a nonconforming approximation in the sense that $\mathcal{D}^h \not\subset \mathcal{D}$ but presents the (practical) advantage that linear operators from $\mathcal{D}^h$ to $\mathcal{N}^h$ can be manipulated as square matrices.

The construction of the discrete DtN operator will involve an additional approximation parameter linked to the discretization of the Floquet variable:

$$\Delta k = 2\pi/NL,$$

where N is an integer devoted to tend to $+\infty$. We shall use the letter $\mathbf{h}$ to summarize the two approximation parameters

$$\mathbf{h} = (h, \Delta k).$$

We shall construct the discrete DtN operator as an operator

$$\Lambda^{\mathbf{h}} \in \mathcal{L}(\mathcal{D}^h, \mathcal{N}^h).$$

Other approximation choices are possible. The one we make here is well adapted to the use of mixed finite elements for the discretization of the interior problem ($\mathrm{P}^{\rm i}$). According to (4) and (5), we shall search $\Lambda^{\mathbf{h}}$ in diagonal form with diagonal blocks

$$\Lambda^{\mathbf{h}}_{(p,q)} \in \mathcal{L}\left(\mathcal{D}^h_{(p,q)}, \mathcal{N}^h_{(p,q)}\right), \quad (p,q)\in\{a,s\}^2,$$

where the spaces

$$\mathcal{D}^h_{(p,q)} = \mathcal{N}^h_{(p,q)} \equiv L^2_h(\Sigma^i)\cap L^2_{(p,q)}(\Sigma^i) \tag{25}$$

are all isomorphic, due to symmetry, to

$$L^2_h(\Sigma_0) := \left\{\varphi_h \in L^2(\Sigma_0)/\forall \mathcal{S}\in\mathcal{T}_h(\Sigma_0),\ \varphi_h|_{\mathcal{S}}\in P_m\right\}$$

namely the spaces of restrictions to Σ_0 of functions in $L^2_h(\Sigma^i)$.

According to (6) and (7), we look for $\Lambda^{\mathbf{h}}_{(p,q)}$ in the form

$$\Lambda^{\mathbf{h}}_{(p,q)} = \widehat{R}^{\mathbf{h}}_{(p,q)} \circ \widehat{\Lambda}^H_{\mathbf{h}} \circ \widehat{D}^{\mathbf{h}}_{(p,q)}, \tag{26}$$

$$\widehat{D}^{\mathbf{h}}_{(p,q)} \in \mathcal{L}\left(\mathcal{D}^h_{(p,q)}, \mathcal{D}^{\mathbf{h}}_{QP}\right), \quad \widehat{\Lambda}^H_{\mathbf{h}} \in \mathcal{L}\left(\mathcal{D}^{\mathbf{h}}_{QP}, \mathcal{N}^{\mathbf{h}}_{QP}\right), \quad \widehat{R}^{\mathbf{h}}_{(p,q)} \in \mathcal{L}\left(\mathcal{N}^{\mathbf{h}}_{QP}, \mathcal{N}^h_{(p,q)}\right), \tag{27}$$

where $\mathcal{D}^{\mathbf{h}}_{QP}$ and $\mathcal{N}^{\mathbf{h}}_{QP}$ are finite dimension approximation spaces for $\mathcal{D}_{QP}$ and $\mathcal{N}_{QP}$.

According to the definition of $\mathcal{D}_{QP}$ and $\mathcal{N}_{QP}$ (see the appendix), their discretization relies on discrete approximation of the spaces

$$H^{1/2}_{k_y}(\Sigma_0) \quad \text{and} \quad H^{-1/2}_{k_y}(\Sigma_0)$$

that also appear in the definition of the waveguide DtN operators $\Lambda^w(k_y)$. Consistently with (25), we choose the same approximation space, namely $L^2_h(\Sigma_0)$. This leads to

$$\mathcal{D}^{\mathbf{h}}_{QP} = \mathcal{N}^{\mathbf{h}}_{QP} \equiv L^2_{\mathbf{h}}(\mathbb{K}) \subset L^2(\mathbb{K}), \tag{28}$$

where $q \geqslant 0$ denoting a given integer, and reminding that $N = 2\pi/(L\Delta k)$

$$L^2_{\mathbf{h}}(\mathbb{K}) = \text{span}\left\{\varphi_h(y)\,\hat{\psi}_N(k_y),\ \varphi_h \in L^2_h(\Sigma_0),\ \hat{\psi}_h \in L^2_N\left(-\frac{\pi}{L},\frac{\pi}{L}\right)\right\},$$

where we use a uniform mesh $k_l = l\Delta k, 0 \leqslant l \leqslant N$ for the discretization of k_y and

$$L^2_N\left(-\frac{\pi}{L},\frac{\pi}{L}\right) = \left\{\hat{\psi}_N \in L^2\left(-\frac{\pi}{L},\frac{\pi}{L}\right)/\forall l \leqslant N,\ \hat{\psi}_N|_{[k_l,k_{l+1}]} \in \mathcal{P}_q\right\}.$$

Note that $L^2_{\mathbf{h}}(\mathbb{K})$ is naturally generated by tensor products basis functions (see (50)).

Again, this corresponds to a non conforming approximation for $\mathcal{D}_{QP}$. In particular, the k_y quasi-periodicity, that appears for instance in the waveguide problems, is not taken in the approximation spaces but in the weak formulations of the problems, which has many practical advantages.

Concerning the various discrete operators appearing in (26)

- The operator $\widehat{R}^{\mathbf{h}}_{(p,q)}$ is nothing but the restriction of $\widehat{R}_{(p,q)}$ to $\mathcal{N}^{\mathbf{h}}_{QP} \subset \mathcal{N}_{QP}$. Then it suffices to apply the formula (9) and no approximation process is involved. Note that the piecewise polynomial dependence in y is preserved by k_y-integration and that the integral appearing in (9) can be computed exactly thanks to the piecewise polynomial dependence in k_y.
- The operator $\widehat{\Lambda}^H_{\mathbf{h}}$ is defined by a Galerkin approach to Eq. (8).

More precisely, for any $\psi_{\mathbf{h}} \in L^2_{\mathbf{h}}(\mathbb{K}),\ \widehat{\Lambda}^H_{\mathbf{h}}\psi_{\mathbf{h}} \in L^2_{\mathbf{h}}(\mathbb{K})$ is defined as

$$\int_{\mathbb{K}} \left(\widehat{\Lambda}^H_{\mathbf{h}}\psi_{\mathbf{h}}\right)(\cdot,k_y)\tilde{\psi}_{\mathbf{h}}(\cdot,k_y)\,dy\,dk_y = \int_{\mathbb{K}} \Lambda^{\mathrm{w}}_h(k_y)\left[\hat{\psi}_{\mathbf{h}}(\cdot,k_y)\right]\tilde{\psi}_{\mathbf{h}}(\cdot,k_y)\,dy\,dk_y, \quad \forall\tilde{\psi}_{\mathbf{h}} \in L^2_{\mathbf{h}}(\mathbb{K}), \tag{29}$$

where $\Lambda^{\mathrm{w}}_h(k_y) \in \mathcal{L}(L^2_h(\Sigma_0))$ is a discrete equivalent of the DtN waveguide operator $\Lambda^{\mathrm{w}}(k_y)$ and given, according to (17) by

$$\Lambda^{\mathrm{w}}_h(k_y) = T^{00}_h(k_y) + T^{10}_h(k_y)P_h(k_y).$$

In the above formula the operators $T^{ij}_h(k_y)$ (resp. $P_h(k_y)$) belong to $\mathcal{L}\left(L^2_h(\Sigma_0)\right)$ and are discrete equivalents of the local DtN operators $T^{ij}(k_y)$ – see Section 3.1.1 – (resp. the propagator $P(k_y)$ – see Section 3.1.2). Their construction relies on a numerical approximation of the local cell problems (10)–(12) and the Riccati Eq. (16). This will be explained in Section 3.1.
Note that, in practice, due to the piecewise polynomial nature (in k_y) of functions in $L^2_{\mathbf{h}}(\mathbb{K})$, the left hand side of (29) can be evaluated using appropriate quadrature formulas (depending on the degree q) inside each segment $[k_l, k_{l+1}]$. For the right hand side, since the dependency in k_y of $\Lambda^{\mathrm{w}}_h(k_y)$ is not known analytically (and certainly not polynomial) the integral in k_y has to be approximated using the same quadrature approach as for the left hand side. This only requires to evaluate $\Lambda^{\mathrm{w}}_h(k_y)$ only for discrete values of k_y corresponding to the quadrature points. We shall not come back in detail to this aspect of the approximation process (see however the Section 3.2.2 where similar techniques have to be applied).
- For each (p,q), the operator

$$\widehat{D}^{\mathbf{h}}_{(p,q)} \in \mathcal{L}\left(\mathcal{D}^h_{(p,q)}, \mathcal{D}^{\mathbf{h}}_{QP}\right)$$

will be defined via a numerical discretization of the problems defining $(E_{(p,q)}(\varphi))$ for a given φ. This implies in particular to construct discrete equivalents

$$\mathbf{K}^h_{(p,q)}(k_y,k_y) \in \mathcal{L}\left(L^2_h(\Sigma_0)\right)$$

of the operators $\mathbf{K}_{(p,q)}(k_y,k_y)$ using the formula (18). This requires then to construct discrete equivalent

$$D^{\ell,\pm}_h(k_y) \in \mathcal{L}\left(L^2_h(\Sigma_0)\right)$$

of the DtD operators $D^{\ell,\pm}(k_y)$ which also relies on the numerical approximation of the local cell problems (10)–(12) (see (14)). This will be explained in Sections 3.1 and 3.2.2.

The essential difficulties and computationally involved steps of our approach are thus concentrated in the numerical approximation of the local cell problems (10)–(12) (and the related construction of the discrete local DtN and DtD operators), the construction of the discrete propagator and finally the numerical approximation of the problems $(E_{(p,q)}(\varphi))$.

3.1. Discrete approximation of the DtN operator $\Lambda^w(k_y)$

3.1.1. Discretization of the local cell problems

The basic ingredient is the discretization of the local cell problem (10)–(12) (when $\hat{\psi}$ belongs to the discrete space $L^2_h(\mathcal{C})$, reason why we denote $\hat{\psi}_h$ in what follows). We first reformulate it as a first order system in

$$(e^\ell, \mathbf{g}^\ell) := \left(e^\ell(k_y,\hat{\psi}), \mathbf{g}^\ell(k_y,\hat{\psi})\right) \quad \text{with } \mathbf{g}^\ell := \nabla e^\ell$$

and use a classical mixed variational formulation of this problem in which e^ℓ is searched in $L^2(\mathcal{C})$ and $\mathbf{g}^\ell$ is searched in $H_{div}(\mathcal{C})$. As all of this is standard, we omit the details and will simply give the equations at the discrete level (cf (31)). For the discretization, we consider a doubly symmetric triangular mesh $\mathcal{T}_h(\mathcal{C})$ whose trace on $\partial\mathcal{C} \equiv \Sigma^i$ coincides with the 1D mesh $\mathcal{T}_h(\Sigma^i)$ (cf the beginning of Section 3). The approximate field e^h_ℓ will be searched in the space $L^2_h(\mathcal{C})$ of discontinuous functions which are piecewise polynomial functions of degree k and the approximate field $\mathbf{g}^\ell_h$ will be searched in a subspace of $H_{div,h}(\mathcal{C}) \subset H(\mathrm{div};\mathcal{C})$ constructed with Raviart–Thomas finite elements of degree m (we mean that m is the polynomial degree of the divergence of the vector fields, see [25,26] for more information) on the mesh $\mathcal{T}_h(\mathcal{C})$. The important property is the trace property (here $\mathbf{n}$ denotes the outgoing normal vector to Σ^i):

$$\left\{\tilde{\mathbf{g}}_h \cdot \mathbf{n},\ \tilde{\mathbf{g}}_h \in H_{div,h}(\mathcal{C})\right\} = L^2_h(\partial\mathcal{C}). \tag{30}$$

Our approximation space will be obtained by simply adding the k_y quasi-periodicity condition in the y-direction, namely, identifying Σ_1^+ and Σ_1^-

$$H^{k_y}_{div,h}(\mathcal{C}) = \left\{\tilde{\mathbf{g}}_h \in H_{div,h}(\mathcal{C}) / \tilde{\mathbf{g}}_h \cdot \mathbf{n}|_{\Sigma_1^+} = e^{ik_y}\tilde{\mathbf{g}}_h \cdot \mathbf{n}|_{\Sigma_1^-}\right\}.$$

The discrete variational problem reads

$$\begin{cases} \text{Find } (e^\ell_h, \mathbf{g}^\ell_h) \in L^2_h(\mathcal{C}) \times H^{k_y}_{div,h}(\mathcal{C}) \text{ such that} \\ \int_{\mathcal{C}} (\mathrm{div}\,\mathbf{g}^\ell_h + (\omega^2 + i\varepsilon\omega)e^\ell_h)\tilde{e}_h\,dx = 0, & \forall \tilde{e}_h \in L^2_h(\mathcal{C}), \\ \int_{\mathcal{C}} (\mathbf{g}^\ell_h \cdot \tilde{\mathbf{g}}_h + e^\ell_h\,\mathrm{div}\,\mathbf{g}^\ell_h)dx = \int_{\Sigma_\ell} \hat{\psi}_h \tilde{\mathbf{g}}_h \cdot \mathbf{n}\,d\sigma, & \forall \tilde{\mathbf{g}}_h \in H^{k_y}_{div,h}(\mathcal{C}). \end{cases} \tag{31}$$

We define the discrete local DtN operators T^{ij}_h

$$\left| \begin{array}{ll} T^{00}_h(k_y)\hat{\psi}_h = \mathbf{g}^0_h(k_y;\hat{\psi}_h)\cdot\mathbf{n}|_{\Sigma_0}, & T^{01}_h(k_y)\hat{\psi}_h = \mathbf{g}^0_h(k_y;\hat{\psi}_h)\cdot\mathbf{n}|_{\Sigma_1}, \\ T^{10}_h(k_y)\hat{\psi}_h = \mathbf{g}^1_h(k_y;\hat{\psi}_h)\cdot\mathbf{n}|_{\Sigma_0}, & T^{11}_h(k_y)\hat{\psi}_h = \mathbf{g}^1_h(k_y;\hat{\psi}_h)\cdot\mathbf{n}|_{\Sigma_1}, \end{array} \right.$$

Thanks to (30) and the definition of $L^2_h(\Sigma_0)$, one easily checks that:

$$T^{ij}_h(k_y) \in \mathcal{L}(L^2_h(\Sigma_0)), \quad (i,j) \in \{0,1\}^2.$$

To define the discrete equivalent of the DtD operators $D^{\ell,\pm}(k_y)$, according to (14), we need to take the traces of e^h_ℓ on the boundaries $\Sigma_1^\pm$. This can only be done in a weak sense.

More precisely, we define the trace of e^h_ℓ on $\partial\mathcal{C}$ by:

$$\forall \tilde{\mathbf{g}}_h \in H^{k_y}_{div,h}(\mathcal{C}), \quad \int_{\partial\mathcal{C}} (e^\ell_h|_{\partial\mathcal{C}})\tilde{\mathbf{g}}_h \cdot \mathbf{n}\,d\sigma = \int_{\mathcal{C}} (\mathbf{g}^\ell_h \cdot \tilde{\mathbf{g}}_h + e^\ell_h\,\mathrm{div}\,\mathbf{g}^\ell_h)dx,$$

which defines completely $e^\ell_h|_{\partial\mathcal{C}}$ thanks to (30). Then it suffices to define

$$D^{\ell,\pm}_h(k_y)\hat{\psi} \equiv e^\ell_h(k_y;\hat{\psi})\Big|_{\Sigma_1^\pm},$$

where the equality has to be understood in the sense of (15). By construction

$$D^{\ell,\pm}_h(k_y) \in \mathcal{L}\left(L^2_h(\Sigma_0)\right), \quad (i,j) \in \{0,1\}^2.$$

3.1.2. The operators $P_h(k_y)$ and $\Lambda^w_h(k_y)$

According to Section 2.3.2, a natural idea to define the discrete propagator $P_h(k_y)$ is to solve the following problem

$$\text{Find } P_h(k_y) \in \mathcal{L}\left(L^2_h(\Sigma_0)\right) \text{ such that } \rho\left(P_h(k_y)\right) < 1 \text{ and } \mathcal{T}_h(k_y, P_h(k_y)) = 0, \tag{32}$$

where

$$\forall X \in \mathcal{L}\Big(L_h^2(\Sigma_0)\Big), \quad \mathcal{T}_h(k_y, X) := T_h^{10}(k_y)X^2 + \Big(T_h^{00}(k_y) + T_h^{11}(k_y)\Big)X + T_h^{01}(k_y), \tag{33}$$

which does characterize $P_h(k_y)$ thanks to the following result.

Theorem 2. *The problem (32) admits a unique solution* $P_h(k_y) \in \mathcal{L}\Big(L_h^2(\Sigma_0)\Big)$.

We shall not give here the (long and tedious) proof of this result which follows the lines of the proof of the analogous existence and uniqueness for the continuous problem (cf. [22,24] for the details).

In practice, solving (32) amounts to solve a matrix quadratic equation with a nonlinear constraint on the spectral radius of the matrix. The numerical approach we propose consists in using a Newton's method, adequately modified to take care of the constraint about the spectral radius. That is why we have proposed a heuristic iterative algorithm where a "projection step" of the set of matrices with spectral radius less or equal than 1, is applied at each step of the algorithm. Starting from the initial guess $P_h^0(k_y) = 0$, the sequence $P_h^n(k_y)$ is defined inductively by:

- Compute $(\delta P)_h^{n+1} \in \mathcal{L}\Big(L_h^2(\Sigma_0)\Big)$ solution of the Lyapunov equation:

  $$T_h^{10}(k_y)\Big(P_h^n(k_y)(\delta P)_h^{n+1} + (\delta P)_h^{n+1}P_h^n(k_y)\Big) + \Big(T_h^{00}(k_y) + T_h^{11}(k_y)\Big)(\delta P)_h^{n+1} = \mathcal{T}_h(k_y, P_h^n(k_y)),$$

  where $\mathcal{T}_h$ is given by (33).
- Compute $\widetilde{P}_h^{n+1}(k_y) = P_h^n(k_y) - \delta P_h^{n+1}$ (this is the standard Newton's step),
- If $\rho\Big(\widetilde{P}_h^{n+1}(k_y)\Big) < 1$, keep

  $$P_h^{n+1}(k_y) = \widetilde{P}_h^{n+1}(k_y),$$

  if $\rho\Big(\widetilde{P}_h^{n+1}(k_y)\Big) \geqslant 1$, take (this is the projection step)

  $$P_h^{n+1}(k_y) = \widetilde{P}_h^{n+1}(k_y) \Big/ \rho\Big(\widetilde{P}_h^{n+1}(k_y)\Big).$$

The solution $P_h(k_y)$ is expected to be the limit of the sequence $P_h^n(k_y)$. In practice, we stop the algorithm when $\|\delta P_h^{n+1}\| / \|P_h^n(k_y)\|$ is small enough.

Remark 3. In practice, it appears that the standard Newton's method always converges to a solution of the equation $\mathcal{T}_h(k_y, X) = 0$ but the projection step appears essential to catch the good solution, namely the solution of (32).

Remark 4 (*Other method to solve (32)*). To solve (32), one can also think about using a spectral approach: that means looking for the eigenvalues and eigenvectors of $P_h(k_y)$. That leads to the resolution of a matrix quadratic eigenvalue problem. See [22] for more details.

Once, $P_h(k_y)$ is determined, the approximation of the DtN operator $\Lambda_h^{\mathrm{w}}(k_y)$ is obtained by

$$\Lambda_h^{\mathrm{w}}(k_y) = T_h^{00}(k_y) + T_h^{10}(k_y)P_h(k_y) \in \mathcal{L}\Big(L_h^2(\Sigma_0)\Big).$$

3.2. Approximation of the extension operators

In this section, we explain how we construct the discrete extension operators

$$\widehat{D}^{\mathbf{h}}_{(p,q)} \in \mathcal{L}\Big(\mathcal{D}^h_{(p,q)}, \mathcal{D}^{\mathbf{h}}_{QP}\Big)$$

appearing in (26) and (27) as discrete equivalents of the continuous operators $\widehat{D}_{(p,q)}$.

More precisely, we need to explain how to compute

$$\widehat{D}^{\mathbf{h}}_{(p,q)}\varphi_h \in \mathcal{D}^{\mathbf{h}}_{QP}, \quad \text{for any } \varphi_h \in \mathcal{D}^h_{(p,q)}.$$

This will be done by discretizing the problem $(E_{(p,q)}(\varphi))$ that defines $\widehat{D}_{(p,q)}\varphi$.

This discretization process will be described in sub Section 3.2.2. This process will rely on a variational formulation of the problem, which is the object of Section 3.2.1.

3.2.1. Variational formulation of the affine equation $(E_{(p,q)}(\varphi))$

The main issue in this section is to explain and justify how we treat the affine constraint $(E_{(p,q)}(\varphi)$-(ii)). Numerically, we wish to apply a Galerkin procedure to approximate the problem $(E_{(p,q)}(\varphi))$ whose solution is

$$\hat{\psi} = \hat{\psi}_{(p,q)} := \widehat{D}_{(p,q)}\varphi \in \mathcal{D}_{\mathrm{QP}}.$$

We would like to look for the unknown function in a vector space which amounts to make the condition $(E_{(p,q)}(\varphi)$-(ii)) homogeneous. To do so, we introduce a function satisfying

$$\hat{\psi}(\varphi) \in \mathcal{D}_{\mathrm{QP}}, \quad \text{such that } \sqrt{\frac{L}{2\pi}}\int_{-\pi/L}^{\pi/L}\left[\hat{\psi}(\varphi)\right](\cdot,k_x)dk_x = \varphi|_{\Sigma_0}, \tag{34}$$

In practice to find such function, it is equivalent to take the FBT of a function in $H^{1/2}(\widetilde{\Sigma})$ which is any extension of the restriction of φ on Σ_0:

$$\hat{\psi}(\varphi) = \mathcal{F}_y(\psi(\varphi)) \quad \text{with } \psi(\varphi) \in H^{1/2}(\widetilde{\Sigma}) \text{ and } \psi(\varphi)|_{\Sigma_0} = \varphi|_{\Sigma_0}.$$

Introducing the new unknown

$$\hat{\psi}^0 = \hat{\psi} - \hat{\psi}(\varphi) \quad \left(\Rightarrow \widehat{D}_{(p,q)}\varphi = \hat{\psi}^0 + \hat{\psi}(\varphi)\right), \tag{35}$$

we easily see that it is the unique solution to the problem:

$$\left|\begin{array}{l} \text{Find} \quad \hat{\psi}^0 \in \mathcal{D}_{\mathrm{QP}} \text{ such that} \\ \text{(i)} \quad \hat{\psi}^0(\cdot,k_x) - \frac{L}{2\pi}\int_{-\pi/L}^{\pi/L}\mathbf{K}_{(p,q)}(k_x,k_y)\hat{\psi}^0(\cdot;k_y)dk_y = [\hat{g}(\varphi)](\cdot,k_x), \\ \text{(ii)} \quad \sqrt{\frac{L}{2\pi}}\int_{-\pi/L}^{\pi/L}\hat{\psi}^0(\cdot,k_x)dk_x = 0 \end{array}\right. \tag{36}$$

with $\hat{g}(\varphi) \in \mathcal{D}_{\mathrm{QP}}$ given by

$$[\hat{g}(\varphi)](\cdot,k_x) = -\left[\left[\hat{\psi}(\varphi)\right](\cdot,k_x) - \frac{L}{2\pi}\int_{-\pi/L}^{\pi/L}\mathbf{K}_{(p,q)}(k_x,k_y)\left[\hat{\psi}(\varphi)\right](\cdot,k_y)dk_y\right]. \tag{37}$$

To write a variational formulation of (36), it is useful to introduce the space

$$\mathcal{D}_{QP}^0 := \left\{\hat{\psi}^0 \in \mathcal{D}_{QP}, \int_{-\pi/L}^{\pi/L}\hat{\psi}^0(\cdot,k)dk = 0\right\}. \tag{38}$$

In what follows, we shall denote the duality product between $\mathcal{D}_{QP}$ and $\mathcal{N}_{QP}$

$$\langle\hat{\psi},\hat{\theta}\rangle_{QP} := \int_{-\pi/L}^{\pi/L}\left\langle\hat{\psi}(\cdot;k_x);\hat{\theta}(\cdot;k_x)\right\rangle_{k_x}dk_x,$$

where the duality product $\langle\cdot,\cdot\rangle_{k_x}$ is the one between $H_{k_x}^{1/2}(\Sigma_0)$ and $H_{k_x}^{-1/2}(\Sigma_0)$. This duality product simply extends the standard inner product in $H = L^2(\mathbb{K})$.

We choose to solve by a Galerkin method the problem (36) which is, obviously, equivalent to the variational problem (simply take the duality product of the equality (36)(i) with any test function $\hat{\theta} \in \mathcal{N}_{QP}$):

$$\left\{\begin{array}{l} \text{Find } \hat{\psi}^0 \in \mathcal{D}_{QP}^0, \text{ such that for all } \hat{\theta} \in \mathcal{N}_{QP} \\ a_{(p,q)}(\hat{\psi}^0,\hat{\theta}) = \left\langle\hat{g}(\varphi),\hat{\theta}\right\rangle_{QP}, \end{array}\right. , \tag{39}$$

where we have introduced the bilinear form on $\mathcal{D}_{QP} \times \mathcal{N}_{QP}$

$$a_{(p,q)}(\hat{\psi},\hat{\theta}) := \langle\hat{\psi},\hat{\theta}\rangle_{QP} - \frac{L}{2\pi}\int_{-\pi/L}^{\pi/L}\int_{-\pi/L}^{\pi/L}\left\langle\mathbf{K}_{(p,q)}(k_x,k_y)\hat{\psi}(\cdot;k_y),\hat{\theta}(\cdot;k_x)\right\rangle_{k_x}dk_y\,dk_x. \tag{40}$$

Let us point out here a difficulty for the discretization of (39). Even if one uses the same space $\mathcal{D}_{QP}^{\mathbf{h}} \equiv \mathcal{N}_{QP}^{\mathbf{h}}$ (cf. (28)) as approximation spaces for $\mathcal{D}_{QP}$ and $\mathcal{N}_{QP}$, the (discrete) approximate solution should be searched in a subspace including the constraint (36) (ii), namely $\mathcal{D}_{QP}^{0,\mathbf{h}} \subset \mathcal{D}_{QP}^{\mathbf{h}}$. Therefore, since the test functions do not satisfy such a constraint, the naive discretization of (39) would lead to a rectangular linear system with more equations than unknowns! This is not a true difficulty because the right hand side is a particular one. In fact, to overcome this apparent difficulty, we show that it is possible to restrict at the continuous level, the space of test functions to the space

$$\mathcal{N}_{QP}^0 := \left\{\hat{\psi}^0 \in \mathcal{N}_{QP}, \int_{-\pi/L}^{\pi/L}\hat{\psi}^0(\cdot,k)dk = 0\right\}. \tag{41}$$

Remark 5. By definition of the inverse FBT (see Proposition 12), we have

$$\mathcal{D}_{QP}^0 = \mathcal{F}_y\left\{\psi \in H^{\frac{1}{2}}(\widetilde{\Sigma}),\ \psi \equiv 0 \text{ on } \Sigma_0\right\}, \quad \mathcal{N}_{QP}^0 = \mathcal{F}_y\left\{\psi \in H^{-\frac{1}{2}}(\widetilde{\Sigma}),\ \psi \equiv 0 \text{ on } \Sigma_0\right\}.$$

Proposition 6 (Variational formulation). *The problem* (36) (or (39)) *is equivalent to the variational problem*

$$\begin{cases} \text{Find } \hat{\psi}^0 \in \mathcal{D}^0_{QP}, \text{ such that for all } \hat{\theta}^0 \in \mathcal{N}^0_{QP} \\ a_{(p,q)}(\hat{\psi}^0, \hat{\theta}^0) = \langle \hat{g}(\varphi), \hat{\theta}^0 \rangle_{QP}. \end{cases} \tag{42}$$

Proof. Since $\mathcal{N}^0_{QP} \subset \mathcal{N}_{QP}$, the solution $\hat{\psi}^0$ of (36) (or (39)) is also a solution of (42). To conclude, it suffices to show the uniqueness of the solution of (42), namely to prove that

$$a_{(p,q)}(\hat{\psi}^0, \hat{\theta}^0) = 0, \quad \forall \hat{\theta}^0 \in \mathcal{N}^0_{QP} \quad \text{and} \quad \hat{\psi}^0 \in \mathcal{D}^0_{QP} \Rightarrow \hat{\psi}^0 = 0. \tag{43}$$

We shall restrict ourselves to give the proof in the case: $(p,q) = (s,s)$.

For conciseness, it is useful to introduce the operator $\widehat{D}^{\mathrm{H}}_{(s,s)} \in \mathcal{L}(\mathcal{D}_{QP})$ defined by

$$\forall \hat{\psi} \in \mathcal{D}_{QP}, \quad \widehat{D}^{\mathrm{H}}_{(s,s)} \hat{\psi}(\cdot; k_x) = \frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} \mathbf{K}_{(s,s)}(k_x, k_y) \hat{\psi}(\cdot; k_y) dk_y,$$

so that, $a_{(p,q)}(\hat{\psi}^0, \hat{\theta}^0) = 0, \ \forall \hat{\theta}^0 \in \mathcal{N}^0_{QP}$ can be simply rewritten

$$\left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}^0, \hat{\theta}^0 \right\rangle_{QP} = 0, \quad \forall \hat{\theta}^0 \in \mathcal{N}^0_{QP}. \tag{44}$$

The result (43) is a consequence of the following two properties (see the proof below):

$(^*)$ $\mathrm{Ker}\left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(p,q)} \right) \cap \mathcal{D}^0_{QP} = \{0\}$.

$(^{**})$ $\left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}, \hat{\theta}^0 \right\rangle_{QP} = 0, \quad \forall \hat{\theta}^0 \in \mathcal{N}^0_{QP} \Rightarrow \hat{\psi} \in \mathrm{Ker}\left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(p,q)} \right)$.

Indeed, by hypothesis and $(^{**})$, $\hat{\psi}^0 \in \mathrm{Ker}\left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(p,q)} \right) \cap \mathcal{D}^0_{QP}$ which yields $\hat{\psi}^0 = 0$ by $(^*)$.

Proof of $(^*)$. It is sufficient to observe that $(^*)$ is nothing but a rephrasing of the uniqueness result for equation $(E_{(p,q)}(\varphi))$. Indeed, writing that $\hat{\psi} \in \mathcal{D}_{QP}$ is a solution of $(E_{(p,q)}(\varphi))$ with $\varphi = 0$ can be rewritten as

$$\hat{\psi} - \widehat{D}^{\mathrm{H}}_{(p,q)} \hat{\psi} = 0 \quad \text{and} \quad \hat{\psi} \in \mathcal{D}^0_{QP}.$$

Proof of $(^{**})$. Let us suppose $\hat{\psi} \in \mathcal{D}_{QP}$ such that

$$\left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}, \hat{\theta}^0 \right\rangle_{QP} = 0, \quad \forall \hat{\theta}^0 \in \mathcal{N}^0_{QP}$$

We want to show that $\hat{\psi} \in \mathrm{Ker}\left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(p,q)} \right)$ which is equivalent to show, by duality, that

$$\left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}, \hat{\theta} \right\rangle_{QP} = 0, \quad \forall \hat{\theta} \in \mathcal{N}_{QP}$$

According to Remark 15,

$$\forall \hat{\theta} \in \mathcal{N}_{QP}, \quad (y, k_y) \mapsto \frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} \hat{\theta}(\cdot, k) dk \in \mathcal{N}_{QP}$$

and by definition of $\mathcal{N}_{QP}$ and $\mathcal{N}^0_{QP}$, we have

$$\forall \hat{\theta} \in \mathcal{N}_{QP}, \quad \hat{\theta} - \frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} \hat{\theta}(\cdot, k) dk \in \mathcal{N}^0_{QP} \tag{45}$$

Then, we have for any $\hat{\theta} \in \mathcal{N}_{QP}$,

$$\begin{aligned} \left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}, \hat{\theta} \right\rangle_{QP} &= \left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}, \hat{\theta} - \frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} \hat{\theta}(\cdot, k) dk \right\rangle_{QP} + \left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}, \frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} \hat{\theta}(\cdot, k) dk \right\rangle_{QP} \\ &= \left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}, \frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} \hat{\theta}(\cdot, k) dk \right\rangle_{QP} \quad (\text{by } (44) \text{ and } (45)). \end{aligned}$$

By definition of the Floquet Bloch Transform in $H^{-1/2}(\widetilde{\Sigma})$ applied to this last term and according to Remark 15

$$\left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi}, \hat{\theta} \right\rangle_{QP} = \left\langle \mathcal{F}_y^{-1} \left(\left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)} \right) \hat{\psi} \right), \mathcal{F}_y^{-1} \left(\frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} \hat{\theta}(\cdot, k) dk \right) \right\rangle_{\widetilde{\Sigma}} = \left\langle \psi - \mathcal{F}_y^{-1} \left(\widehat{D}^{\mathrm{H}}_{(s,s)} \hat{\psi} \right), \tilde{\theta}_{\Sigma_0} \right\rangle_{\widetilde{\Sigma}},$$

where $\langle \cdot, \cdot \rangle_{\widetilde{\Sigma}}$ is the duality product between $H^{1/2}(\widetilde{\Sigma})$ and $H^{-1/2}(\widetilde{\Sigma})$, $\psi = \mathcal{F}_y^{-1}(\hat{\psi})$, $\theta = \mathcal{F}_y^{-1}(\hat{\theta})$ and $\tilde{\theta}_{\Sigma_0} \in H^{-1/2}(\widetilde{\Sigma})$ is the extension by 0 of $\theta|_{\Sigma_0}$. Finally

$$\left\langle \left(\mathbf{I} - \widehat{D}^{\mathrm{H}}_{(s,s)}\right)\hat{\psi}, \hat{\theta} \right\rangle_{QP} = 0$$

since

$$\mathcal{F}_y^{-1}\left(\widehat{D}^{\mathrm{H}}_{(s,s)}\hat{\psi}\right)\Big|_{\Sigma_0} = \psi|_{\Sigma_0}.$$

Indeed, according to in Section 2.4 (see also [1,24]), we can show that

$$\forall \hat{\psi} \in \mathcal{D}_{QP}, \quad \psi = \mathcal{F}_y^{-1}(\hat{\psi}), \quad \mathcal{F}_y^{-1}\left(\widehat{D}^{\mathrm{H}}_{(s,s)}\hat{\psi}\right) = u^{\mathrm{H}}(\psi)|_{\Sigma},$$

where u^{H} is the solution of the halfspace problem $(\mathrm{P_H})$ which by definition satisfies

$$u^{\mathrm{H}}(\psi)|_{\Sigma_0} = \psi|_{\Sigma_0} \qquad \square$$

3.2.2. Construction of the discrete extension operator $\widehat{D}^{\mathbf{h}}_{(p,q)}$

We need to explain how to compute

$$\widehat{D}^{\mathbf{h}}_{(p,q)}\varphi_h \in \mathcal{D}^{\mathbf{h}}_{QP}$$

for any $\varphi_h \in \mathcal{D}_h$. According to (35), it will be defined as

$$\widehat{D}^{\mathbf{h}}_{(p,q)}\varphi_h = \hat{\psi}^0_{\mathbf{h}} + \hat{\psi}_{\mathbf{h}}(\varphi_h),$$

which is made in two steps.

Step 1: Construction of $\hat{\psi}_{\mathbf{h}}(\varphi_h)$.
Based on (34), we construct $\hat{\psi}_{\mathbf{h}}(\varphi_h)$ as the FBT of the trivial extension of φ_h by 0 outside Σ_0. As this extension has support in one period, $\hat{\psi}_{\mathbf{h}}(\varphi_h)$ only depends on the space variable, more precisely:

$$\left[\hat{\psi}_{\mathbf{h}}(\varphi_h)\right](\cdot, k_x) = \sqrt{\frac{L}{2\pi}}\varphi_h \tag{46}$$

Step 2: Construction of $\hat{\psi}^0_{\mathbf{h}}$.
This is obtained by solving a discrete equivalent of the variational problem (42) where φ is replaced by φ_h. First, we must construct a discrete approximation of $g(\varphi)$ appearing in the right hand side of (42). To do so, we approximate the formula (37) by using quadrature in the k_x variable. As it is natural this quadrature is based on the uniform mesh of step-size Δk of the interval [0,1] (see the beginning of Section 3) and a standard quadrature formula in each sub-interval $[k_l, k_{l+1}]$ in [0,1] deduced from the quadrature formula in [0,1]

$$\int_0^1 f(\tau)d\tau \equiv \sum_{r=1}^{M} \omega_r f(\tau_r), \quad 0 \leqslant \tau_1 < \cdots < \tau_M \leqslant 1, \tag{47}$$

where M defines the "order" of the quadrature formula, the ω_m's are the quadrature weights and the τ_m's are the reference quadrature points. This leads to introduce the quadrature points

$$k_l^r = k_l + \tau_r \Delta k, \quad l = 0, \ldots, N-1, \quad r = 1, \ldots, M.$$

Taking into account (46), this choice leads to define $\hat{g}_{\mathbf{h}}(\varphi_h)$ such that

$$[\hat{g}_{\mathbf{h}}(\varphi_h)](\cdot, k_x) = \sqrt{\frac{L}{2\pi}}\left(-1 + \frac{1}{N}\sum_{r=1}^{N}\sum_{l=1}^{M}\omega_l \mathbf{K}^h_{(p,q)}(k_x, k_l^r)\right)\varphi_h,$$

where the discrete kernels $\mathbf{K}^h_{(p,q)}(k_x, k_y) \in \mathcal{L}\left(L^2_h(\Sigma_0)\right)$ are constructed, consistently with formula (18) by, setting $\varepsilon_s = 1$ and $\varepsilon_a = -1$,

$$\mathbf{K}^h_{(p,q)}(k_x, k_y) = \mathbf{I} + \varepsilon_p \mathbf{K}^+_h(k_x, k_y) + \varepsilon_q \mathbf{K}^-_h(k_x, k_y) \tag{48}$$

with

$$\mathbf{K}^{\pm}_h(k_x, k_y) = e^{\mp \imath L k_x}\left(D_h^{0,\pm}(k_y) + D_h^{1,\pm}(k_y)P_h(k_y)\right)\left(\mathbf{I} - P_h(k_y)e^{\mp \imath L k_x}\right)^{-1},$$

where the operators $D_h^{\ell,\pm}(k_y)$ have been defined in Section 3.1.1 and the operators $P_h(k_y)$ in Section 3.1.2.

Remark 7. A natural choice for the quadrature formula (47) is to use the Gauss formula with M points. This is the choice that we have done in our computational code. Moreover, to be consistent with the polynomial order for the k_y-approximation, a natural choice for M is $M = q$ (even though q and M are *a priori* independent).

Next, according to (38), (41) and (28), we introduce the finite dimension spaces:

$$\mathcal{D}_{QP}^{\mathbf{h},\mathbf{0}} = \mathcal{N}_{QP}^{\mathbf{h},\mathbf{0}} = \left\{ \hat{\psi}_{\mathbf{h}} \in L^2_{\mathbf{h}}(\mathbb{K}) \Big/ \int_{-\pi/L}^{\pi/L} \hat{\psi}_h(\cdot,k)dk = 0 \right\}$$

as subspaces of the discrete spaces $\mathcal{D}_{QP}^{\mathbf{h}}$ and $\mathcal{N}_{QP}^{\mathbf{h}}$ introduced at the beginning of Section 3, and we solve the discrete variational problem

$$\begin{cases} \text{Find } \hat{\psi}^0_{\mathbf{h}} \in \mathcal{D}_{QP}^{\mathbf{h},\mathbf{0}}, \text{ such that for all } \hat{\theta}^0 \in \mathcal{N}_{QP}^{\mathbf{h},\mathbf{0}} \\ a^{\mathbf{h},M}_{(p,q)}\left(\hat{\psi}^0_{\mathbf{h}}, \hat{\theta}^0_{\mathbf{h}}\right) = \left\langle \hat{g}_{\mathbf{h}}(\varphi_h), \hat{\theta}^0_{\mathbf{h}} \right\rangle^{\mathbf{h}}_{QP}, \end{cases} \tag{49}$$

In (49), the discrete duality product $\langle\cdot,\cdot\rangle^{\mathbf{h}}_{QP}$ only differs from the continuous one, (which would be, in this case, the $L^2(\mathbb{K})$ inner product) through, again, the use of quadrature formulas

$$\left\langle \hat{\psi}_{\mathbf{h}}, \hat{\theta}_{\mathbf{h}} \right\rangle^{\mathbf{h}}_{QP} := \frac{2\pi}{NL} \sum_{r=1}^{N} \sum_{l=1}^{M} \omega_l \left(\hat{\psi}_h(\cdot,k_l^r), \hat{\theta}_h(\cdot,k_l^r) \right)_{L^2}.$$

The bilinear form $a^{\mathbf{h},M}_{(p,q)}(\cdot,\cdot)$ defined on $\mathcal{D}_{QP}^{\mathbf{h}} \times \mathcal{N}_{QP}^{\mathbf{h}}$ differs from $a_{(p,q)}(\cdot,\cdot)$ given by (40) because

- the integrals in k_x and k_y in (40) are replaced by quadrature formulas,
- the kernels $\mathbf{K}_{(p,q)}(k_x,k_y)$ are replaced by their discrete equivalents $\mathbf{K}^h_{(p,q)}(k_x,k_y)$.

More precisely $a^{\mathbf{h},M}_{(p,q)}(\cdot,\cdot)$ is defined by

$$\left| \begin{array}{l} a^{\mathbf{h},M}_{(p,q)}(\hat{\psi}_{\mathbf{h}}, \hat{\theta}_{\mathbf{h}}) := \frac{2\pi}{NL} \sum\limits_{r=1}^{N} \sum\limits_{l=1}^{M} \omega_l \left(\hat{\psi}_h(\cdot,k_l^r), \hat{\theta}_h(\cdot,k_l^r) \right)_{L^2} \\ \quad - \left(\frac{2\pi}{NL}\right)^2 \sum\limits_{r=1}^{N} \sum\limits_{s=1}^{N} \sum\limits_{l=1}^{M} \sum\limits_{m=1}^{M} \omega_l \omega_m \left(\mathbf{K}^h_{(p,q)}(k_l^r,k_m^s) \hat{\psi}_h(\cdot,k_l^r), \hat{\theta}_h(\cdot,k_m^s) \right)_{L^2} \end{array} \right.$$

Remark 8. Our conjecture is that the discrete problem (49) is well posed, at least if h is small enough and N large enough. This has been confirmed by our numerical experiments. However, this seems hard to prove. Let us nevertheless mention that if we consider a semi-discrete version (in which the space variable is discretized but where the dual variable k_y remains continuous, h being the only approximation parameter) of (42), one can prove the well-posedness for any h.

In practice, of course, (49) is transformed into a square linear system after expansion of the discrete unknown in a tensor product basis of the space $\mathcal{D}_{QP}^{\mathbf{h},\mathbf{0}}$, namely

$$\{w_i(y)v_j(k_y), 1 \leqslant i \leqslant N_h,\ 1 \leqslant j \leqslant qN-1\}, \tag{50}$$

where, if N_x denotes the number of segments in the mesh $\mathcal{T}_h(\Sigma_0)$, $N_h = (m+1)N_x$ is the dimension of $L^2_h(\Sigma_0)$ and

$$\{w_i(y), 1 \leqslant i \leqslant N_h\}$$

is a standard discontinuous finite element basis of $L^2_h(\Sigma_0)$ and where

$$\{v_j(k_y), 1 \leqslant j \leqslant qN-1\}$$

is a basis of the space of functions in $L^2(-\pi/L, \pi/L)$ with mean value 0.

Remark 9. The choice of the basis has no influence on the results but it can be done to make the assembling of the linear system easiest.

The resolution of the linear system requires the inversion of a full matrix whose size is $N_h(qN-1) \times N_h(qN-1)$. This step of the algorithm is the most costly in terms of the computational cost and the memory storage.

4. Numerical results

We give first in this section some relevant validations of the construction of the DtN operators and the determination of the solution of the whole problem. We show then numerical results for general periodic media.

Let us mention that for each quasi-period k_y, the construction of the half waveguide DtN operator have already been validated in [22]. First, a homogeneous half-waveguide problem, which is a particular periodic half-waveguide problem is used and the computed DtN operator is compared to the analytical DtN operator.

Moreover, the construction of the halfspace DtN operator and the solution of the halfspace problem have been validated in [24,27] which deals with the transmission and reflexion of an incident wave by a periodic halfspace. The computed DtN operator and the computed halfspace solution are compared to the analytical ones in the case of homogeneous media. The computed solution is compared to the solution computed using the FDTD method for a harmonic incident wave.

To validate the computation of the DtN operator, we need essentially to check the extension operators.

4.1. Validation of the computation of the extension operators

Since the resolution and the discretization of the integral Eq. (49) is not standard and its numerical analysis is not done, it seems essential to validate the computation of the extension operators $D_{(p,q)}$. The idea is to apply this resolution to a problem in an homogeneous media and use the analytical solution to compare the results.

Thus, noting that the first kind Hankel functions are the unique H^1 solutions of the Helmholtz equation with constant coefficients in the exterior domain Ω^e for a particular Dirichlet data on the boundary Σ^i, we should have by definition

$$\forall n \in \mathbb{N}, \quad u^e = \mathrm{H}_n^{(1)}\left(\sqrt{\rho_p(\omega^2 + \imath\varepsilon\omega)}\sqrt{x^2+y^2}\right), \quad u^e|_{\widetilde{\Sigma}} = D_{(s,s)}\left(u^e|_{\Sigma^i}\right)$$

because the Hankel function is with double symmetry if the point source is set on $(0,0)$. The numerical results are given for $n = 0$.

Let us take the coefficient $\rho_p = 1$, the frequency $\omega = 5$ and the period $L = 1$. This implies that

$$\Sigma_0^i = \{(0.5, y),\ y \in [-0.5, 0.5]\} \quad \text{and} \quad \widetilde{\Sigma} = \{(0.5, y),\ y \in \mathbb{R}\}.$$

We will make the absorption ε varying ($\varepsilon = 1, 0.5, 0.1, 0.05, 0.01$) in order to see the influence of the absorption in the precision of the discretization. In the following, we choose Raviart–Thomas finite elements of lowest degree ($m = 0$) for the discretization in space ($N_x = 60$), polynomials of degree 0 for the functions depending on the dual variables ($q = 0$ and $N = 60$) and a quadrature formula of order 1 (i.e. $M = 1$).

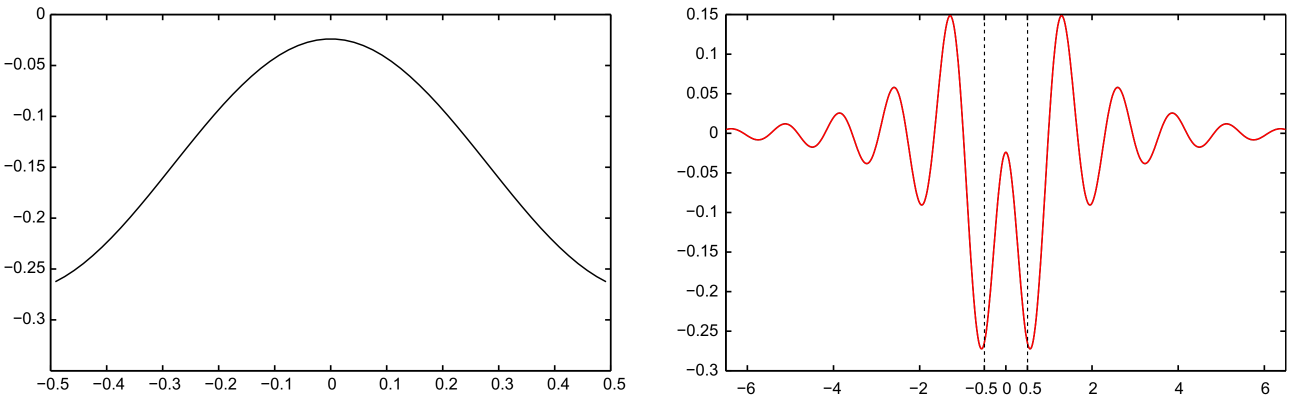
For the absorption $\varepsilon = 1$, the Fig. 8 represents on $[-6.5, 6.5]$ in black the Hankel function and in red its reconstruction using $\mathcal{F}_y^{-1}\left(\widehat{\mathrm{D}}^{\mathbf{h}}_{(s,s)}\varphi_h\right)$ (Fig. 8(b)), where φ_h is the projection on $\mathcal{V}_h$ of the restriction of the Hankel function on Σ^i (Fig. 8(a) shows this restriction on $\Sigma_0 \equiv [-0.5, 0.5]$). The relative error on the interval defined by

$$\frac{\left\|\mathcal{F}_y^{-1}\left(\widehat{\mathrm{D}}^{\mathbf{h}}_{(s,s)}\varphi_h\right) - D_{(s,s)}\varphi\right\|_{L^2([-6.5,6.5])}}{\|D_{(s,s)}\varphi\|_{L^2([-6.5,6.5])}} \tag{51}$$

is 0.11%. Fig. 9 shows the Hankel functions (in black) and its reconstruction (in red) for different values of ε ($\varepsilon = 0.5, 0.1, 0.05, 0.01$) in the case where the quadrature is still chosen of order 1 ($M = 1$). The errors are computed thanks to the relation (51). It seems that the approximation of $D_{(s,s)}$ computed with a quadrature of order 1 is deteriorating when ε goes to 0. The reason is that the approximation of the integral equation involves the one of the kernel defined by (48) and in particular of the terms

$$\left(\mathbf{I} - P_h(k_y)e^{\pm\imath L k_x}\right)^{-1}. \tag{52}$$

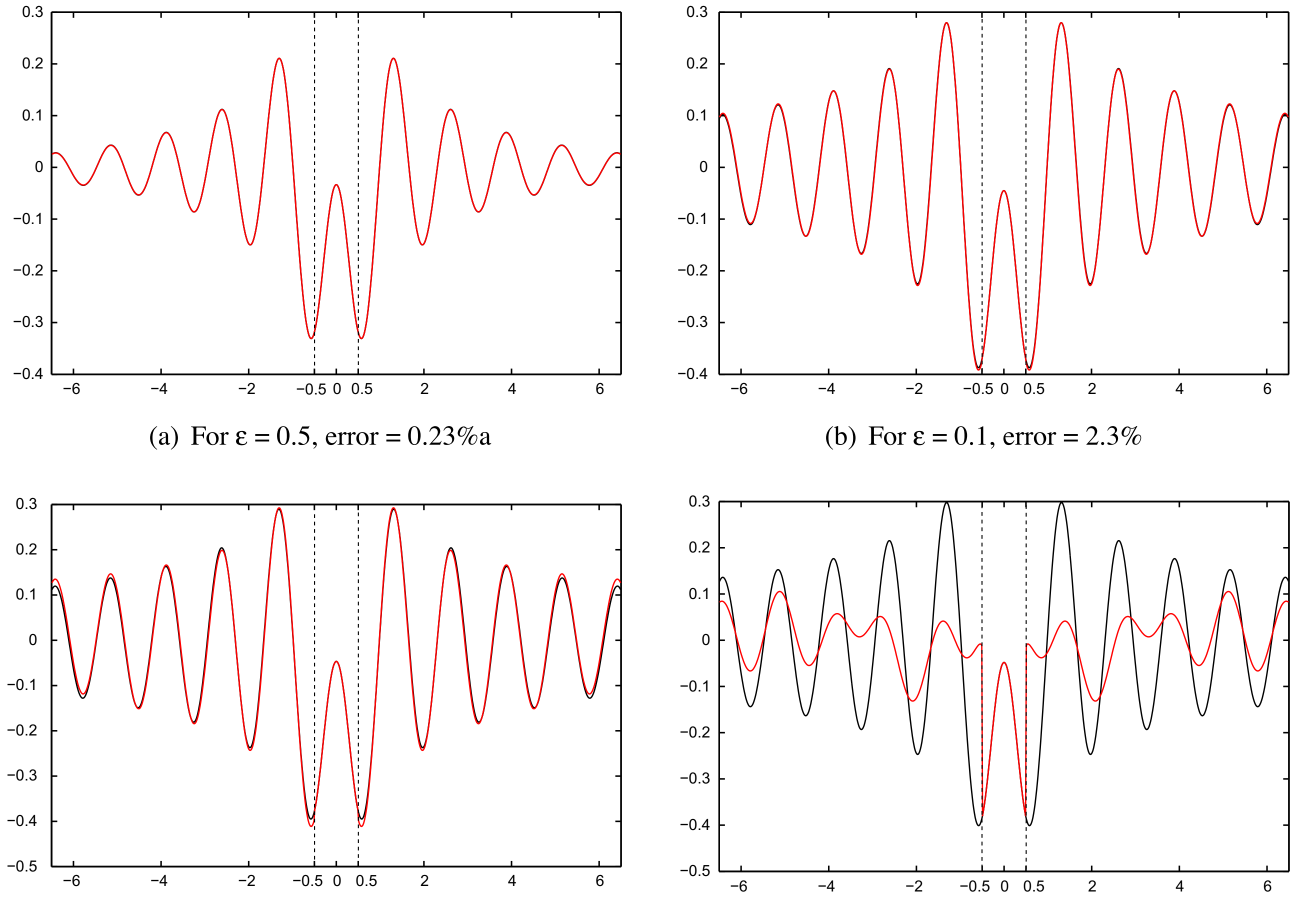
When ε goes to 0, it may exist some k_y for which one or more eigenvalues of $P_h(k_y)$ tend to 1 and then are close to some exp $(\imath\xi(k_y))$. Then the terms (52) may vary a lot around the points $(\pm\xi(k_y), k_y)$. We represent Fig. 10, for $\varepsilon = 0.01$, the norm in $\mathcal{L}(L^2(\Sigma^0))$, of $\mathbf{K}^h_{(s,s)}(k_x, k_y)$ with respect to (k_x, k_y) and note that it is almost singular around some curves.



(a) The restriction of the Hankel function to Σ_0^i

(b) The Hankel function (in black) and its reconstruction on $\widetilde{\Sigma}$ (in red)

Fig. 8. For $\varepsilon = 1$, the restriction of the Hankel function to $[-0.5, 0.5]$ (left) from which we compute its extension on $[-6.5, 6.5]$ (in red) and compare to the Hankel function (in black). $M = 1$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



(a) For ε = 0.5, error = 0.23%a

(b) For ε = 0.1, error = 2.3%

(c) For ε = 0.05, error = 9%

(d) For ε = 0.01, error = 60,4%

Fig. 9. The Hankel function (in black) and its extension (in red) on $[-6.5, 6.5]$ for different values of ε and for a quadrature of order $M = 1$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Remark 10. This curves are actually the intersection between the plane (ω^2) and the dispersion surfaces. We could show that the kernel acts like $1/\sqrt{k_x}$ for a fixed k_y. This point will be developed in an upcoming article which will give a numerical limiting absorption principle.

It is then difficult to account for the variations of the kernel approximating their integral by quadrature formula of lowest order. Fig. 11 shows the Hankel function and its reconstruction via the operator $\widehat{D}^{\mathbf{h}}_{(s,s)}$ for $\varepsilon = 0.01$ and for quadrature formula of increasing order $M = 2,3,4,5$. The approximation of the function is better when the quadrature increases. The absorption has an influence on the choice of the discretization: the better the quadrature formula the method must be enhanced for small value of the coefficient ε.

Finally it is possible to validate the computation of each operator $\widehat{D}^{\mathbf{h}}_{(p,q)},\ (p,q) \in \{s,a\}^2$ using linear combination of Hankel functions. Thus, if we denote

$$\forall (x,y) \in \Omega, \quad H_{x_0,y_0}(x,y) = \mathrm{H}_0^{(1)}\left(\sqrt{\rho_p(\omega^2 + \imath\varepsilon\omega)}\sqrt{(x-x_0)^2 + (y-y_0)^2}\right),$$

it is easy to see that

$$\forall (p,q) \in \{s,a\}^2, \quad u^e_{(p,q)} = H_{L/4,0} + \varepsilon_p H_{0,L/4} + \varepsilon_q H_{0,-L/4} + \varepsilon_p\varepsilon_q H_{-L/4,0} \in H^1_{(p,q)}(\Omega,\Delta)$$

is solution of a particular exterior problem and we have in particular

$$\forall (p,q) \in \{s,a\}^2, \quad u^e_{(p,q)}\Big|_{\widetilde{\Sigma}} = \widetilde{D}_{(p,q)}\left(u^e_{(p,q)}\Big|_{\Sigma^i}\right).$$

Fig. 12 shows each linear combination of Hankel functions and their reconstruction thanks to the computed extension operators, for $\varepsilon = 0.1$ and $M = 1$.

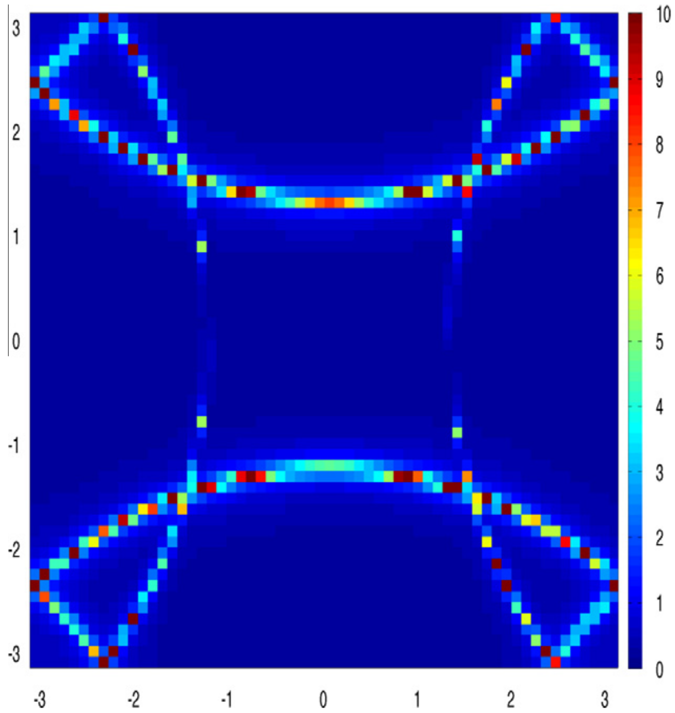


Fig. 10. Norm of the kernel $\mathbf{K}^h_{(s,s)}(k_x, k_y)$ with respect to (k_x,k_y) for $\varepsilon = 0.01$.

4.2. Validation of the whole algorithm

Considering again 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 a homogeneous exterior medium with an artificial boundary chosen along a square. Because usually the artificial boundary is a circle, it seems difficult to validate directly the DtN operator. However we validate it through the validation of the computed solution in the following. We will illustrate in the same time the reconstruction of the solution in the exterior domain described in Section 2.5.

The source f that we consider is given by

$$f(x,y) = 16\exp\left(-\frac{x^2+y^2}{0.2^2}\right)\chi_{[-0.5,0.5]^2} \tag{53}$$

the refraction index is $\rho = 1$ in the whole domain and the period is $L = 1$.Using the algorithm described previously, the DtN operator can be computed and the interior problem can be solved. We represent the interior solution Fig. 13 with $\omega = 5$ and $\varepsilon = 1$. Thus, even with a squared artificial boundary, we recover the revolution symmetry of the solution. Finally to build the solution everywhere, we use the algorithm presented in Section 2.5. Note that in this case, since the source is with double symmetry, φ^i is too: $\varphi^i = \varphi^i_{(s,s)}$. Then, thanks to the trace of u^i on Σ^i and applying the extension operator $D_{(s,s)}$ we compute the trace of the solution on $\widetilde{\Sigma}$. The resolution of the halfspace problem with this trace as Dirichlet data gives the restriction of the solution to the right halfspace Ω^H (Fig. 14(a)). Because the trace of u^i is doubly-symmetric, the solution is too and by symmetry we obtain restrictions of the solution to the above, below and left halfspaces (see Fig. 14(b) for the above halfspace). The restrictions corresponds in each quarter plane especially because the extension operator is solution of the integral equation and it is the only extension operator which allows this conformity. We can then build the solution everywhere (see Fig. 14(d)). Here again, we recover the revolution symmetry of the solution.

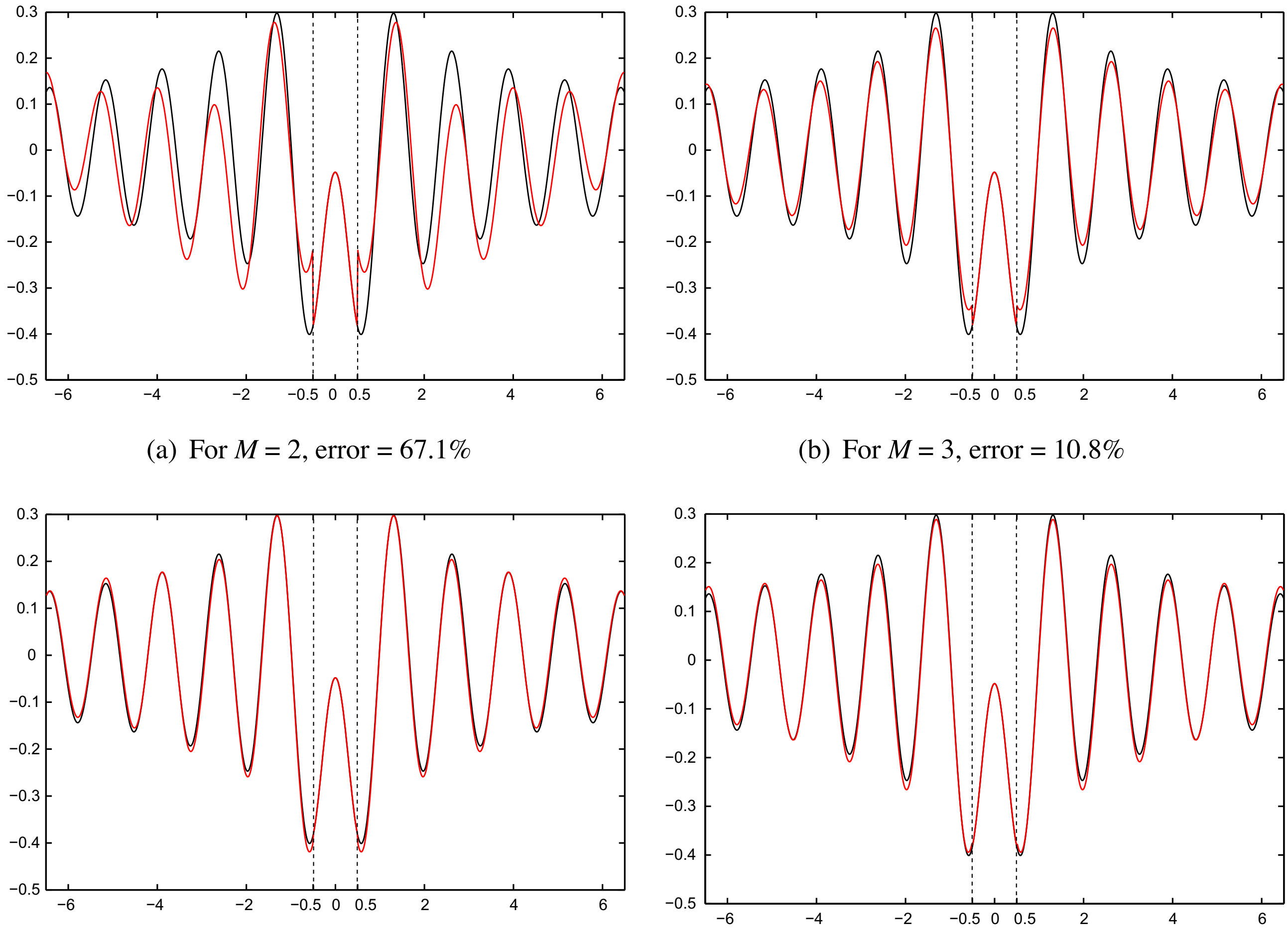
4.3. Application to periodic media

We can apply now our algorithm to a general periodic media, whose refraction index is given by (see Fig. 15(a))

$$\forall (x,y) \in [-0.5,0.5]^2, \forall n,\ m \in \mathbb{Z}^*,\ \rho(x+n, y+m) = 1 + 9\exp\left(-\frac{x^2+y^2}{0.2^2}\right) \quad \text{and } \rho(x,y) = 1 \tag{54}$$

the artificial boundary Σ^i is represented by a white line and the source is given by (53).

The period here is equal to 1. After computing the DtN operator, the interior problem can be solved and we represent the interior solution Fig. 16(a). We use finally the same algorithm as previously for the reconstruction of the solution outside Ω^i (see Fig. 16(b)).



(a) For $M = 2$, error = 67.1%

(b) For $M = 3$, error = 10.8%

(c) For $M = 4$, error = 8.1%t

(d) For $M = 5$, error = 7.1%

Fig. 11. The Hankel function (in black) and its extension (in red) on $[-6.5, 6.5]$ for $\varepsilon = 0.01$ and for quadrature formula of increasing order $M = 2, 3, 4, 5$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

4.3.1. Invariance with respect to the choice of Σ^i and $\mathcal{C}$

The solution of the whole problem has to be independent of the choice of the artificial boundary Σ^i and the periodicity cell $\mathcal{C}$. One easy way to validate the method is to change their size and check that the solution is the same. For the same media as previously, we choose a bigger boundary Σ^i as shown Fig. 15(b) with a white line. All the computations are done in a periodicity cell whose side is equal to 2. The new interior solution u^i is represented Fig. 17(a) and the solution is finally reconstructed in the region $[-6.5, 6.5]^2$ as shown in Fig. 17(b). We recover the solution computed in the previous section and shown Fig. 16(b).

4.3.2. Validation of the computation with the limiting amplitude principle

Now, we test the validity of our frequency domain solution conjecturing about the limiting amplitude principle, whereby if $U(\mathbf{x}, t)$ is the solution of the time domain problem

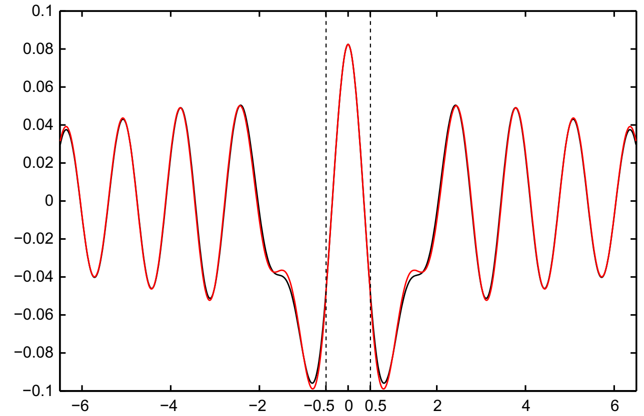
$$\rho(\mathbf{x})\left[\frac{\partial^2 U}{\partial t^2}(\mathbf{x}, t) - \varepsilon\frac{\partial U}{\partial t}(\mathbf{x}, t)\right] - \Delta U(\mathbf{x}, t) = f(\mathbf{x})\cos(\omega t) \tag{55}$$

then we expect that (uniformly in x)

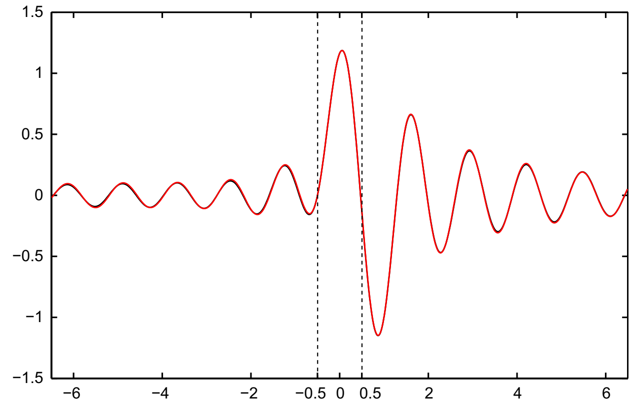
$$\lim_{t\to+\infty} U(\mathbf{x}, t) = \mathrm{Re}(u(x))\cos(\omega t) - \mathrm{Im}(u(x))\sin(\omega t)$$

where u is the good solution of the frequency domain problem (P).

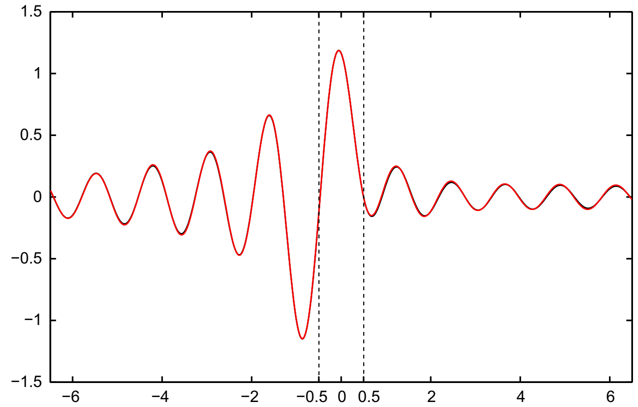
We solve (55) with (54) and (53) for $\omega = 5$ and $\varepsilon = 0.1$, using a very large domain of computation so the solution in our domain of observation is not affected, during the time of observation, by the presence of the external boundaries. In Fig. 18, we show the solution U for several times. If we focus on the particular times $t = N \times 2\pi/\omega$ (so that $\cos(\omega t) = 1$ and $\sin(\omega t) = 0$), it is clear that the time domain solution $U(x,t)$ is approaching the time-harmonic limit $u(x)$ (represented in Fig. 16(b)) as N increases.



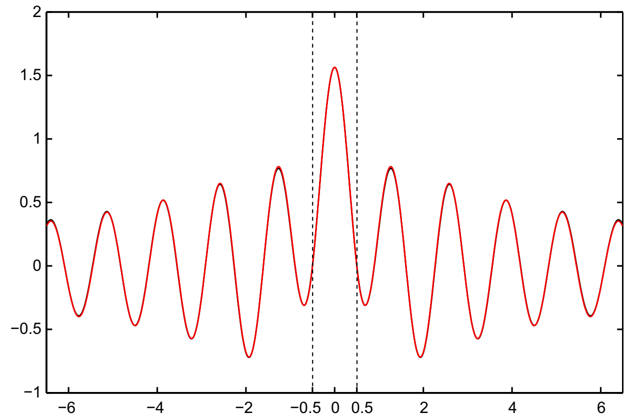
(a) Validation of $D^{h,N_k,q,M}_{(s,s)}$, error = 1.6%



(b) Validation of $D^{h,N_k,q,M}_{(s,a)}$, error = 1.5%



(c) Validation of $D^{h,N_k,q,M}_{(a,s)}$, error = 1.5%



(d) Validation of $D^{h,N_k,q,M}_{(a,a)}$, error = 3%

Fig. 12. Validation of each extension operator $D_{(p,q)}$.

5. Conclusions and perspectives

Our method is well established, rigorously justified and successfully tested in the case of absorbing media. A natural question is to understand what happens when the absorption ε goes to 0. This is the limiting absorption principle.

From a theoretical point of view, in the case of periodic waveguides, the construction of the DtN operator for the case without absorption has been already treated in [22,24]. To our knowledge, in the general 2D case, this raises new and challenging questions. However, a numerical procedure has been developped and has required specific developments (linked to the Remark 10) which corresponds to a numerical limiting absorption principle. This case will be treated in a forthcoming article.

Appendix A. Floquet Bloch Transform (FBT) and its properties

We recall the definition and more useful properties of the Floquet Bloch Transform (see [28] for a more complete exposition) of functions of one variable. This transform maps a function of $y \in \mathbb{R}$ into a function $(y, k_y) \in \mathbb{K} =]-L/2, L/2[\times] - \pi/L, \pi/L[$.

Definition 11. The FBT with period L defined by (see [28])

$$\begin{aligned}
&\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{K}),\\
&f(y) \to \hat{f}(y;k) = \sqrt{\frac{L}{2\pi}} \sum_{n\in\mathbb{Z}} f(y+nL)e^{-inkL}
\end{aligned}$$

is an isometry between $L^2(\mathbb{R})$ and $L^2(\mathbb{K})$:

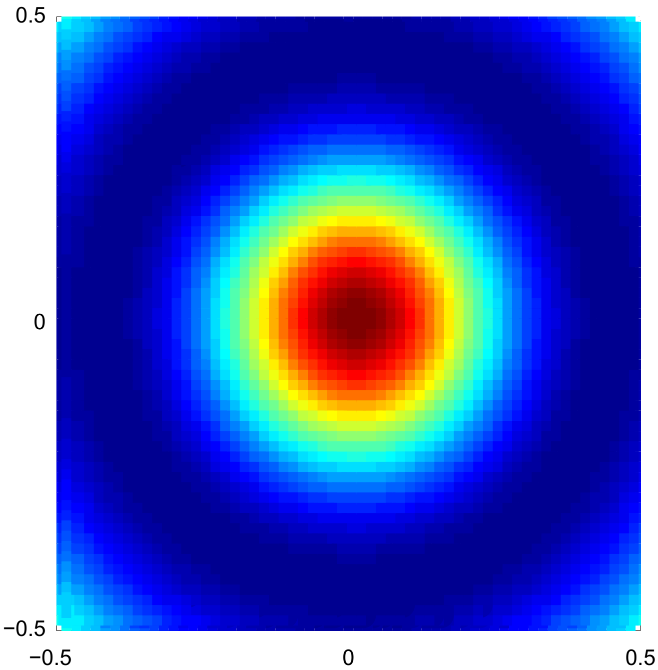


Fig. 13. The solution u^i of in Ω^i ($\mathrm{P^i}$) (computed thanks to the construction of DtN operator Λ).

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

The most important formula for us is the inversion formula:

Proposition 12. *The operator $\mathcal{F}$ is an isometric isomorphism from $L^2(\mathbb{R})$ into $L^2(\mathbb{K})$ whose inverse is given by*

$$\forall \hat{f} \in L^2(\mathbb{K}), \text{ a.e. } y \in [-L/2, L/2], \ \forall n \in \mathbb{Z}, \quad (\mathcal{F}^{-1}\hat{f})(y+nL) = \sqrt{\frac{L}{2\pi}} \int_{-\pi/L}^{\pi/L} \hat{f}(y;k) e^{inkL} dk.$$

Next we define the partial Floquet Bloch Transform in the y-direction in the halfspace Ω^{H}

$$\mathcal{F}_y : L^2(\Omega^{\mathrm{H}}) \to L^2(\Omega^{\mathrm{w}} \times]-\pi/L, \pi/L[)$$
$$u(x,y) \mapsto \mathcal{F}_y(x,y;k_y)$$

such that

$$\text{a.e. } x \in [L/2, +\infty[, (\mathcal{F}_y u)(x,\cdot;\cdot) = \mathcal{F}[u(x,\cdot)].$$

It is easy to see that $\mathcal{F}_y$ is an isomorphism from $L^2(\Omega^{\mathrm{H}})$ into $L^2(\Omega^{\mathrm{w}} \times]-\pi/L, \pi/L])$.

For the sequel, it is essential to know how the Floquet Bloch Transform can extend to every functional spaces appearing naturally in the study. We recall these results already developed and proven in [1,24]. We need first to introduce spaces of functions on the domain Ω^{w} of so-called k_y quasi-periodic functions (k_y) being a parameter in $]-\pi/L, \pi/L[$. We start from smooth quasi-periodic functions in Ω^{w}:

$$C^\infty_{k_y}(\Omega^{\mathrm{w}}) = \left\{ u = \tilde{u}|_{\Omega_w}, \ \tilde{u} \in C^\infty(\Omega^{\mathrm{H}}), \quad \tilde{u}(x, y+L) = e^{\imath k_y L} \tilde{u}(x,y) \right\}.$$

Let $H^1_{k_y}(\Omega^{\mathrm{w}})$ be the closure of $C^\infty_{k_y}(\Omega^{\mathrm{w}})$ in $H^1(\Omega^{\mathrm{w}})$.

$$H^1_{k_y}(\Omega^{\mathrm{w}}) = \left\{ u \in H^1(\Omega^{\mathrm{w}}), \ u|_{\Sigma^+} = e^{\imath k_y L} u|_{\Sigma^-} \right\},$$

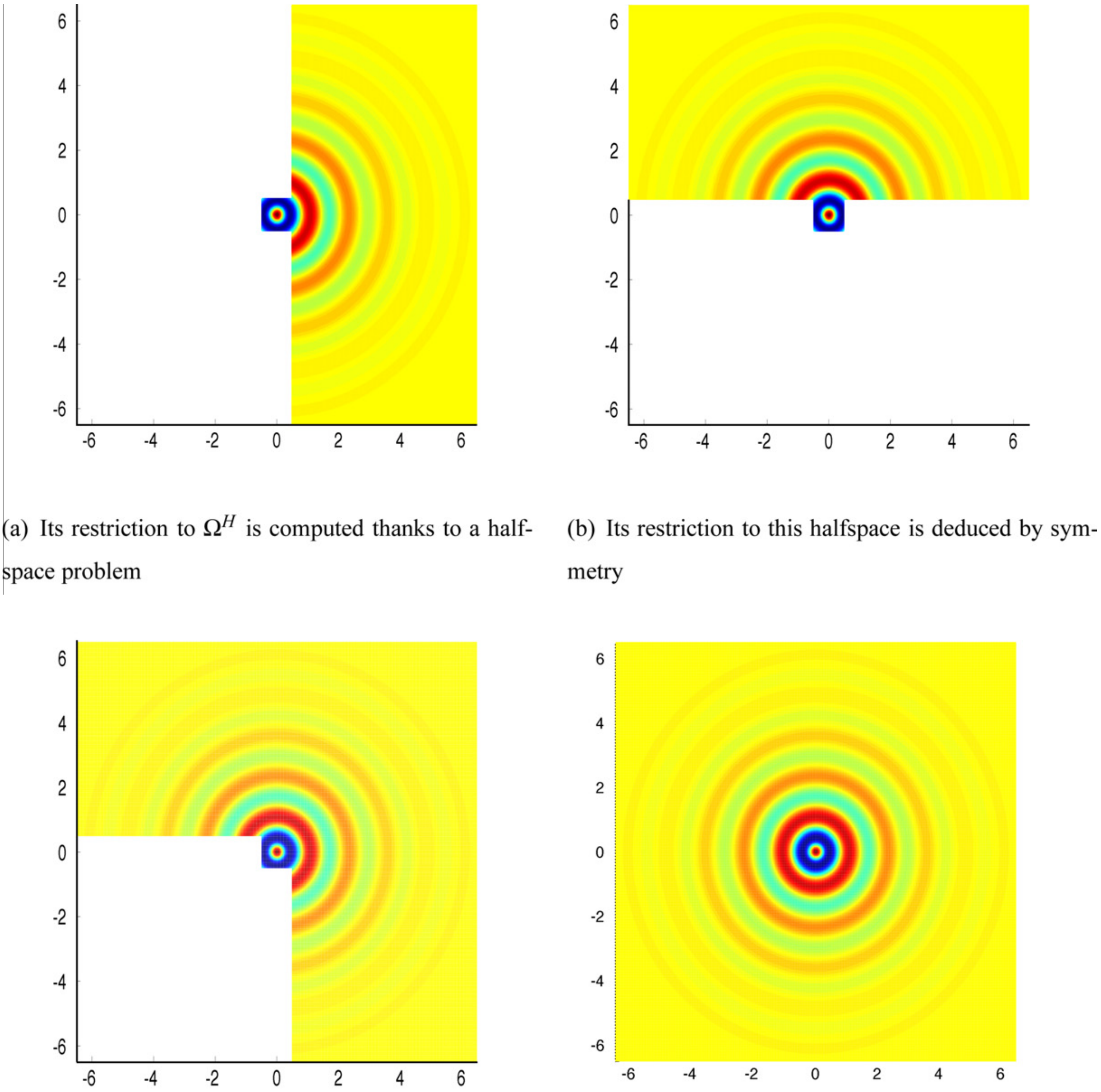
where in the last equality we have identified the spaces $H^{1/2}(\Sigma^+)$ and $H^{1/2}(\Sigma^-)$. Let $H^1_{k_y}(\Delta, \Omega^{\mathrm{w}})$ be the closure of $H^1(\Delta, \Omega^{\mathrm{w}}) = \{u \in H^1(\Omega^{\mathrm{w}}), \ \Delta u \in L^2(\Omega^{\mathrm{w}})\}$.

$$H^1_{k_y}(\Delta, \Omega^{\mathrm{w}}) = \left\{ u \in H^1(\Delta, \Omega^{\mathrm{w}}) \cap H^1_{k_y}(\Omega^{\mathrm{w}}), \ \left.\frac{\partial u}{\partial y}\right|_{\Sigma^+} = e^{\imath k_y L} \left.\frac{\partial u}{\partial y}\right|_{\Sigma^-} \right\},$$

where in the last equality we have identified the spaces $H^{1/2}_{00}(\Sigma^+)'$ and $H^{1/2}_{00}(\Sigma^-)'$.

The space $H^{1/2}_{k_y}(\Sigma_0)$ is defined by

$$H^{1/2}_{k_y}(\Sigma_0) = \gamma_0 \left(H^1_{k_y}(\Omega^{\mathrm{w}}) \right),$$



(a) Its restriction to Ω^H is computed thanks to a half-space problem

(b) Its restriction to this halfspace is deduced by symmetry

(c) The restrictions to the quarter plane corresponds thanks to $\mathcal{E}_{(s,s)}$

(d) The reconstruction of the solution

Fig. 14. The steps of reconstruction of the solution in $[-6.5, 6.5]^2$ in the case where the source is given by (53).

where $\gamma_0 \in \mathcal{L}(H^1(\Omega^{\mathrm{w}}), H^{1/2}(\Sigma_0))$ is the trace map on $\Sigma_0 : \forall u \in H^1(\Omega^{\mathrm{w}}),\ \gamma_0 u = u|_{\Sigma_0}$. $H^{1/2}_{k_y}(\Sigma_0)$ is then a dense subspace of $H^{1/2}(\Sigma_0)$ and the injection from $H^{1/2}_{k_y}(\Sigma_0)$ onto $H^{1/2}(\Sigma_0)$ is continuous.

We define $H^{-1/2}_{k_y}(\Sigma_0)$ as the dual of $H^{1/2}_{k_y}(\Sigma_0)$.

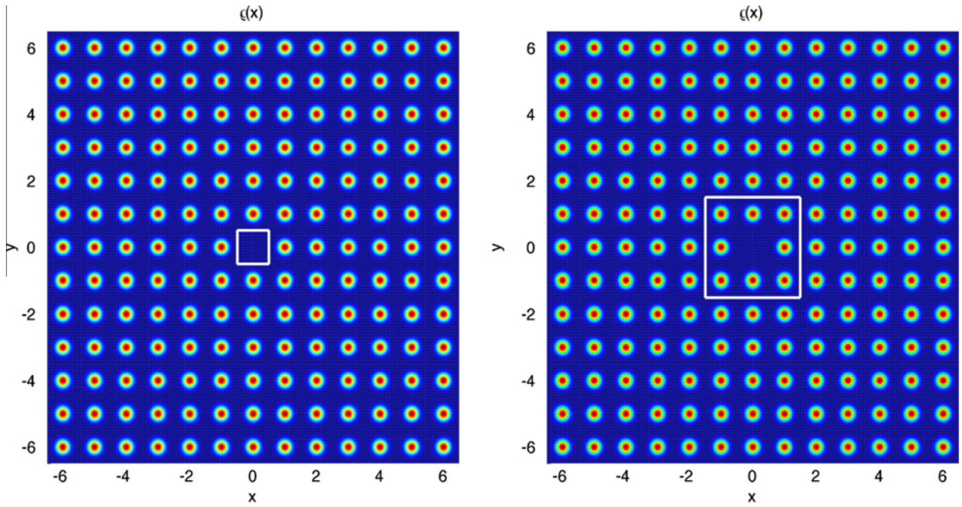
Finally, the trace application $\gamma_1 \in \mathcal{L}(H^1(\Delta, \Omega^{\mathrm{w}}), H^{1/2}_{(a,a)}(\Sigma_0)')$ defined by:

$$\forall u \in H^1(\Delta, \Omega^{\mathrm{w}}), \quad \gamma_1 u = \left.\frac{\partial u}{\partial x}\right|_{\Sigma_0}$$

is a continuous application from $H^1_{k_y}(\Delta, \Omega^{\mathrm{w}})$ onto $H^{-1/2}_{k_y}(\Sigma_0)$. Moreover, we can show that

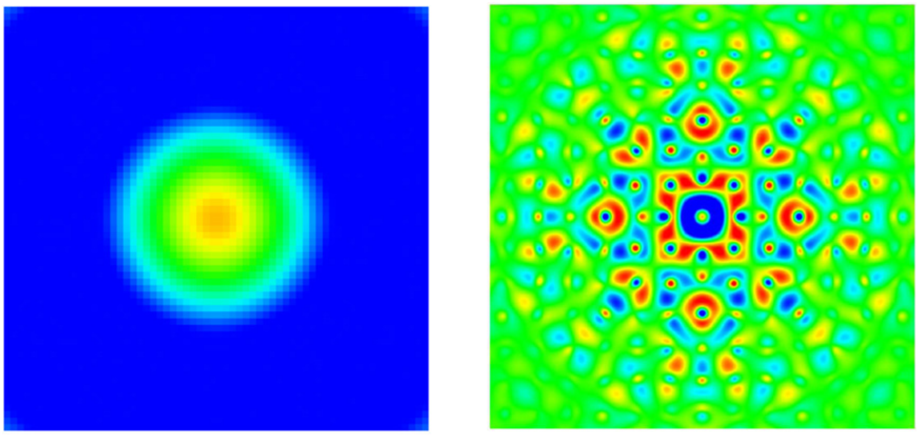
$$H^{-1/2}_{k_y}(\Sigma_0) = \gamma_1\left(H^1_{k_y}(\Delta, \Omega^{\mathrm{w}})\right).$$

We can now state the following results.



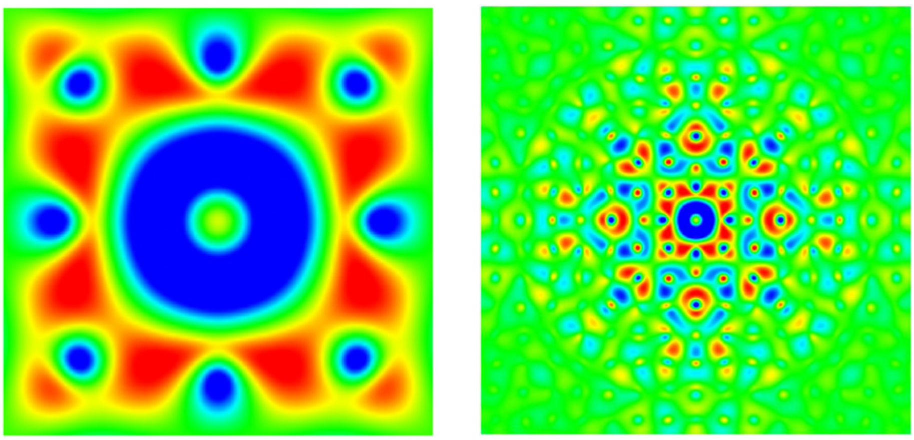
(a) $\Sigma^i = \partial\Omega^i$ with $\Omega^i = (-0.5, 0.5)^2$ (b) $\Sigma^i = \partial\Omega^i$ with $\Omega^i = (-1.5, 1.5)^2$

Fig. 15. The locally perturbed periodic media with two different location of the artificial boundary Σ^i.



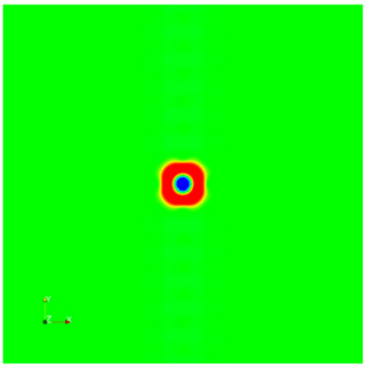
(a) The interior solution u^i (b) The global solution u

Fig. 16. The interior solution u^i in $\Omega^i = [-0.5, 0.5]^2$ and the global solution in the domain $[-6.5, 6.5]^2$ for $\omega = 10$ and $\varepsilon = 0.1$.

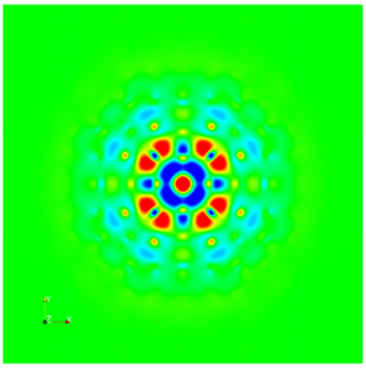


(a) The interior solution u^i (b) The global solution u

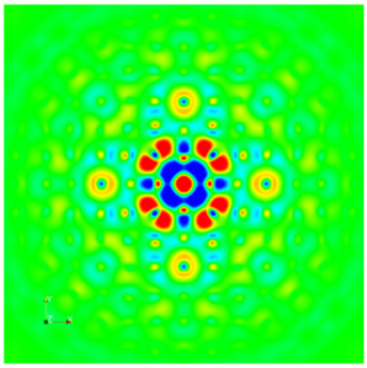
Fig. 17. The interior solution u^i in $\Omega^i = [-0.5, 1.5]^2$ and the global solution in the domain $[-6.5, 6.5]^2$ for $\omega = 10$ and $\varepsilon = 0.1$.



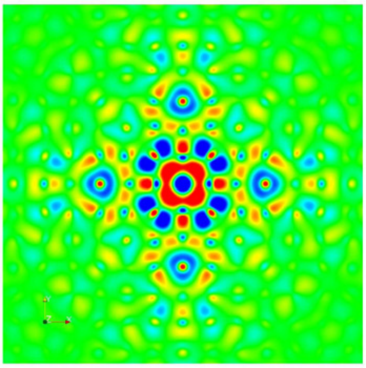
(a) Solution at $t = 0.5 * 2\pi/\omega$



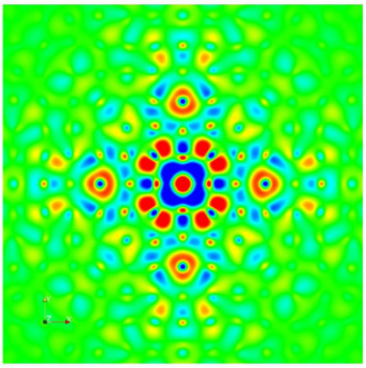
(b) Solution at $t = 5 * 2\pi/\omega$



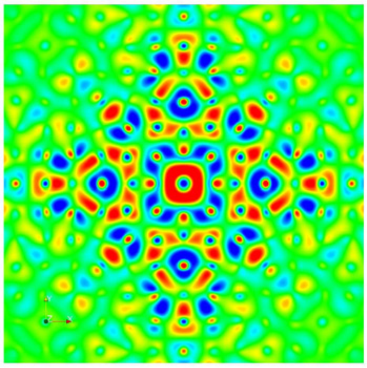
(c) Solution at $t = 10 * 2\pi/\omega$



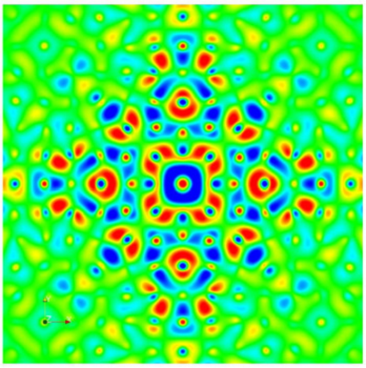
(d) Solution at $t = 22.5 * 2\pi/\omega$



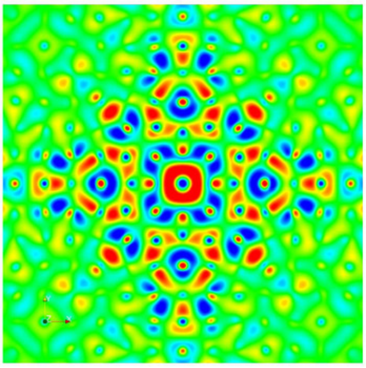
(e) Solution at $t = 30 * 2\pi/\omega$



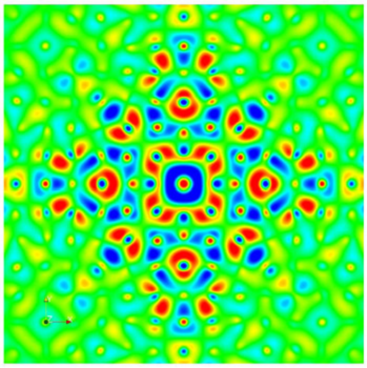
(f) Solution at $t = 35 * 2\pi/\omega$



(g) Solution at $t = 40 * 2\pi/\omega$



(h) Solution at $t = 42.5 * 2\pi/\omega$



(i) Solution at $t = 47 * 2\pi/\omega$

Fig. 18. The interior solution u^i in $\Omega^i = [-0.5, 1.5]^2$ and the global solution in the domain $[-6.5, 6.5]^2$ for $\omega = 10$ and $\varepsilon = 0.1$.

Theorem 13. *$\mathcal{F}_y$ is an isomorphism from $H^1(\Omega^H)$ into*

$$H^1_{\mathrm{QP}} = \left\{ \hat{u} \in L^2\left(-\frac{\pi}{L}, \frac{\pi}{L}; H^1(\Omega^{\mathrm{w}})\right) \Big/ \text{a.e. } k_y \in \left]-\frac{\pi}{L}, \frac{\pi}{L}\right[,\ \hat{u}(\cdot; k_y) \in H^1_{k_y}(\Omega^{\mathrm{w}}) \right\},$$

equipped with the norm of $L^2\left(-\frac{\pi}{L}, \frac{\pi}{L}; H^1(\Omega^{\mathrm{w}})\right)$.

$\mathcal{F}_y$ is an isomorphism from $H^1(\Delta, \Omega^H)$ into

$$H^1_{\mathrm{QP}}(\Delta) = \left\{ \hat{u} \in L^2\left(-\frac{\pi}{L}, \frac{\pi}{L}; H^1(\Delta; \Omega^{\mathrm{w}})\right) \Big/ \text{a.e. } k_y \in \left]-\frac{\pi}{L}, \frac{\pi}{L}\right[,\ \hat{u}(\cdot; k_y) \in H^1_{k_y}(\Delta, \Omega^{\mathrm{w}}) \right\}.$$

equipped with the norm of $L^2\left(-\frac{\pi}{L}, \frac{\pi}{L}; H^1(\Delta; \Omega^{\mathrm{w}})\right)$.

$\mathcal{F}_y$ is an isomorphism from $H^{1/2}(\widetilde{\Sigma})$ into

$$\mathcal{D}_{\mathrm{QP}} = \left\{ \hat{\psi} \in L^2\left(-\frac{\pi}{L}, \frac{\pi}{L}; H^{1/2}(\Sigma_0)\right) \Big/ \text{a.e. } k_y \in \left]-\frac{\pi}{L}, \frac{\pi}{L}\right[,\ \hat{\psi}(\cdot; k_y) \in H^{1/2}_{k_y}(\Sigma_0) \right\}.$$

equipped with the norm

$$\|\hat{\psi}\|^2_{\mathcal{D}_{QP}} = \int_{-\pi/L}^{\pi/L} \|\hat{\psi}(\cdot;k_y)\|^2_{H^{1/2}_{k_y}(\Sigma_0)}\,dk_y.$$

Finally, we can extend by duality the definition of $\mathcal{F}_y$ to the space $H^{-1/2}(\widetilde{\Sigma})$ introducing the dual of $\mathcal{D}_{QP}$:

$$\mathcal{N}_{QP} = \left\{\hat{\theta} \in L^2\left(-\frac{\pi}{L},\frac{\pi}{L};H^{1/2}_{00}(\Sigma_0)'\right)\Big/ \text{a.e. } k_y \in \left]-\frac{\pi}{L},\frac{\pi}{L}\right[,\ \hat{\theta}(\cdot;k_y) \in H^{-1/2}_{k_y}(\Sigma_0)\right\}.$$

Definition 14. Let θ be in $H^{-1/2}(\widetilde{\Sigma})$, the following application ($<\cdot,\cdot>_{\widetilde{\Sigma}}$ is the duality product between $H^{-1/2}(\widetilde{\Sigma})$ and $H^{1/2}(\widetilde{\Sigma})$)

$$\hat{\psi} \mapsto \langle \theta, \mathcal{F}_y^{-1}\hat{\psi}\rangle_{\widetilde{\Sigma}}$$

is a continuous linear application of $\mathcal{D}_{QP}$ because of Theorem 13. The theorem of Riesz representation implies then

$$\exists \hat{\theta} \in \mathcal{N}_{QP}, \quad \langle \hat{\theta}, \hat{\psi}\rangle_{QP} = \langle \theta, \psi\rangle_{\widetilde{\Sigma}},$$

where the first duality product is between $\mathcal{N}_{QP}$ and $\mathcal{D}_{QP}$. Finally, we define the FBT $\mathcal{F}_y$ in $H^{-1/2}(\widetilde{\Sigma})$ by

$$\forall \theta \in H^{-1/2}(\widetilde{\Sigma}), \quad \mathcal{F}_y\theta = \hat{\theta} \in \mathcal{N}_{QP},$$

which coincides with the classical definition in $L^2(\widetilde{\Sigma})$ (see Definition 11). Similarly, for any $\hat{\theta} \in \mathcal{N}_{QP}$, we define by duality $\mathcal{F}_y^{-1}\hat{\theta}$ in $H^{-1/2}(\widetilde{\Sigma})$.

Remark 15. Let us give some properties of the functions in $\mathcal{N}_{QP}$ which will be useful in Section 3.2.1.

For any $\hat{\theta} \in \mathcal{N}_{QP}$ (let us denote $\theta = \mathcal{F}_y^{-1}\hat{\theta} \in H^{1/2}(\widetilde{\Sigma})$), we could show that the function constant in k_y

$$(y,k_y) \mapsto \frac{L}{2\pi}\int_{-\pi/L}^{\pi/L} \hat{\theta}(y,k)dk$$

is also in the space $\mathcal{N}_{QP}$ as the Floquet-Bloch Transform of $\tilde{\theta}_{\Sigma_0} \in H^{-1/2}(\widetilde{\Sigma})$ which is the extension by 0 of $\theta|_{\Sigma_0}$:

$$\frac{L}{2\pi}\int_{-\pi/L}^{\pi/L} \hat{\theta}(\cdot,k)dk = \mathcal{F}_y\left(\tilde{\theta}_{\Sigma_0}\right).$$

Let us remark that this property is not true for any functions of $\hat{\psi} \in \mathcal{D}_{QP}$ because the extension by 0 of $\psi|_{\Sigma_0}$ for any $\psi \in H^{1/2}(\widetilde{\Sigma})$ is not necessarily in $H^{1/2}(\widetilde{\Sigma})$.

References

[1] S. Fliss, P. Joly, Exact boundary conditions for time-harmonic wave propagation in locally perturbed periodic media, Appl. Numer. Math. doi:10.1016/j.apnum.2008.12.013.
[2] J.D. Joannopoulos, R.D. Meade, J. Winn, Photonic Crystal – Molding the Flow of Light, Princeton Univeristy Press, 1995.
[3] S. Johnson, J.D. Joannopoulos, Photonic Crystal – The Road from Theory to Practice, Kluwer Acad. Publ., 2002.
[4] P. Kuchment, The Mathematics of Photonic Crystals, in: Mathematical Modeling in Optical Science, Frontiers in Applied Mathematics, vol. 22, SIAM, Philadelphia, 2001 (Chapter 7).
[5] K. Sakoda, Optical Properties of Photonic Crystals, Springer Verlag, Berlin, 2001.
[6] P. Kuchment, On some spectral problems of mathematical physics, in: Partial Differential Equations and Inverse Problems, vol. 362, Contemp. Math., Amer. Math. Soc., Providence, RI, 2004, pp. 241–276.
[7] C. Johnson, J.-C. Nédélec, On the coupling of boundary integral and finite element methods, Math. Comput. 35 (152) (1980) 1063–1079.
[8] V. Levillain, Coupling integral equation methods and finite volume elements for the resolution of time harmonic maxwell's equations in three dimensional heterogeneous medium, Technical report 222, Centre de Mathematiques appliquees, Ecole Polytechnique.
[9] C. Hazard, M. Lenoir, On the solution of time-harmonic scattering problems for Maxwell's equations, SIAM J. Math. Anal. 27 (6) (1996) 1597–1630.
[10] A. Jami, M. Lenoir, Formulation variationnelle pour le couplage entre une méthode d'éléments finis et une représentation intégrale, CR Acad. Sci. Paris Sér. A-B 285 (4) (1977) A269–A272.
[11] B. Engquist, A. Majda, Radiation boundary conditions for acoustic and elastic wave calculations, Comm. Pure Appl. Math. 32 (3) (1979) 314–358.
[12] A. Bayliss, E. Turkel, Radiation boundary conditions for wave-like equations, Comm. Pure Appl. Math. 33 (6) (1980) 707–725.
[13] J.-P. Berenger, A perfectly matched layer for the absorption of electromagnetic waves, J. Comput. Phys. 114 (2) (1994) 185–200.
[14] T. Hohage, F. Schmidt, L. Zschiedrich, Solving time-harmonic scattering problems based on the pole condition. I. Theory, SIAM J. Math. Anal. 35 (1) (2003) 183–210.
[15] T. Hohage, F. Schmidt, L. Zschiedrich, Solving time-harmonic scattering problems based on the pole condition. II: Convergence of the PML method, SIAM J. Math. Anal. 35 (3) (2003) 547–560.
[16] A. Figotin, A. Klein, Localized classical waves created by defects, J. Stat. Phys. 86 (1–2) (1997) 165–177.
[17] A. Figotin, A. Klein, Localization of light in lossless inhomogeneous dielectrics, J. Opt. Soc. Am. A 15 (5) (1998) 1423–1435.
[18] A. Figotin, A. Klein, Midgap defect modes in dielectric and acoustic media, SIAM J. Appl. Math. 58 (6) (1998) 1748–1773.
[19] S. Soussi, Convergence of the supercell method for defect modes calculations in photonic crystals, SIAM J. Numer. Anal. 43 (3) (2005) 1175–1201.
[20] T. Abboud, Electromagnetic waves in periodic media, in: Second International Conference on Mathematical and Numerical Aspects of Wave Propagation (Newark, DE, 1993), SIAM, Philadelphia, PA, 1993, pp. 1–9.
[21] J. Tausch, J. Butler, Floquet multipliers of periodic waveguides via Dirichlet-to-Neumann maps, J. Comput. Phys. 159 (1) (2000) 90–102.

[22] P. Joly, J.-R. Li, S. Fliss, Exact boundary conditions for periodic waveguides containing a local perturbation, Commun. Comput. Phys. 1 (6) (2006) 945–973.
[23] S. Fliss, P. Joly, J.-R. Li, Exact boundary conditions for wave propagation in periodic media containing a local perturbation, E-Book Series Progress in Computational Physics (PiCP), vol. 1, Bentham Science Publishers, 2009.
[24] S. Fliss, Etude mathTmatique et numTrique de la propagation des ondes dans des milieux pTriodiques localement perturbTs, Palaiseau, 2009.
[25] P.-A. Raviart, J.M. Thomas, A mixed finite element method for 2nd order elliptic problems, in: Mathematical Aspects of Finite Element Methods (Proc. Conf., Consiglio Naz. delle Ricerche (C.N.R.), Rome, 1975), Lecture Notes in Mathematics, vol. 606, Springer, Berlin, 1977, pp. 292–315.
[26] F. Brezzi, M. Fortin, Mixed and hybrid finite element methods, Springer Series in Computational Mathematics, vol. 15, Springer-Verlag, New York, 1991.
[27] S. Fliss, E. Cassan, D. Bernier, Computation of light refraction at the surface of a photonic crystal using dtn approach, J. Opt. Soc. Am. B 27 (7) (2010) 1492–1503, doi:10.1364/JOSAB.27.001492. <http://josab.osa.org/abstract.cfm?URI=josab-27-7-1492> .
[28] P. Kuchment, Floquet theory for partial differential equations, Operator Theory: Advances and Applications, vol. 60, Birkhäuser Verlag, Basel, 1993.