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Diffraction by an acoustic grating perturbed by a bounded obstacle

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An original approach to solve 2D time harmonic diffraction problems involving locally perturbed gratings is proposed. The propagation medium is composed of a periodically stratified half-space and a homogeneous half-space containing a bounded obstacle. Using Fourier and Floquet transforms and integral representations, the diffraction problem is formulated as a coupled problem of Fredholm type with two unknowns: the trace of the diffracted field on the interface separating the two half-spaces on one hand, and the restriction of the diffracted field to a bounded domain surrounding the obstacle, on the other hand.

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1. Introduction

Diffraction gratings have known in the last decade a significant growth of interest. This phenomenon can be explained on one hand by the number of fields of application concerned by periodic structures (integrated optics, micro-electronics, coatings, etc.), and, on the other hand, by the technological progress achieved (especially by semiconductor industry) to realize small optical devices with complicated physical features. For an introduction to the electromagnetic theory of gratings, see the collection of articles in [14]. Besides the large number of papers from the engineering community, theoretical approaches and numerical methods have been proposed to formulate and simulate direct and inverse problems in gratings (see [9] and the references therein). In particular, variational (cf. [1,2,6]) and integral (cf. [13]) methods have been proposed. Some specific problems related to gratings have also been studied: non uniqueness for diffractive gratings in [3], singularities analysis for conical problems in [8].

Nevertheless, the problem that is usually studied in the literature concerns the diffraction of an incident plane wave by a perfect grating (i.e., a perfectly periodic structure). The diffracted field is then known to be quasi-periodic, and this property naturally leads to a formulation of the problem in one elementary cell of the grating. This new problem can then be treated, for instance, using a variational approach or an integral method. In this paper, our concern is to answer the following question: what happens if the grating is not anymore perfect (for instance if it contains a bounded obstacle), or if the incident field is not a plane wave? In both cases, we loose the quasi-periodicity property of the diffracted field and the problem can not anymore be set in one cell of the grating. In fact, no general answer to this question is known in the literature, and even setting the problem is an open question (especially concerning the radiation condition). Let us emphasize here that "locally perturbed gratings" are of great interest for the applications, since they can model the defaults present in a grating. In some cases, the periodicity of the grating can even be perturbed on purpose to realize structures which are able to trap specific modes (one can, for instance, think of removing the conductor in one cell of a conductors grating).

In this paper, we present an original method to derive a rigorous formulation of the diffraction problem for some perturbed gratings. Furthermore, the formulation obtained is variational and thus naturally leads to a numerical approximation of the diffracted field by a Galerkin method. The approach we propose has been introduced for the first time in [4] to solve problems of (open or closed) 2D wave-guides junctions.

Before giving the main ideas of this approach, let us precise the kind of geometries we will deal with in this paper. We consider a 2D grating located in a half space, periodic in one direction, say y, and invariant in the other one, say x. The other half-space is asssumed to be an homogeneous medium containing a bounded obstacle. Figure 1 gives an example of such structures (the grating is constituted of a stratified medium in the vertical direction y). When illuminated by a plane wave, the total field at any point of the space can be decomposed into two parts: a quasi-periodic one (corresponding to the sum of the incident plane wave and the field associated to its diffraction by the grating without obstacle) and a non quasi periodic part φ due to the presence of the obstacle. Our aim is to determine this contribution φ, which can be seen as the field diffracted by the obstacle when illuminated by the quasi-periodic part.

To achieve this, the method we propose is based on the following observation: if the trace u of the diffracted field φ on the fictitious interface Σ (see figure 1) separating the "elementary" media (the grating and the homogeneous medium) is known, then φ can be easily recovered in each medium. Indeed, we will show that the diffracted field can be explicitely derived in terms of its trace u on Σ using suitable functional transforms in each medium (Fourier transform for the homogeneous medium and Floquet transform for the periodic one). Solving the complete diffraction problem amounts then to determine this unknown trace u on Σ, and this is simply done by matching the normal derivatives of the representations obtained for the diffracted field on both sides of Σ.

The outline of the paper is the following: in section 2, we introduce the notations for the geometry and set the diffraction problem. In section 3, we present Floquet transform and then formally derive a representation of the diffracted field in terms of its trace on Σ. In section 4, we deal with the homegeneous medium containing the obstacle and

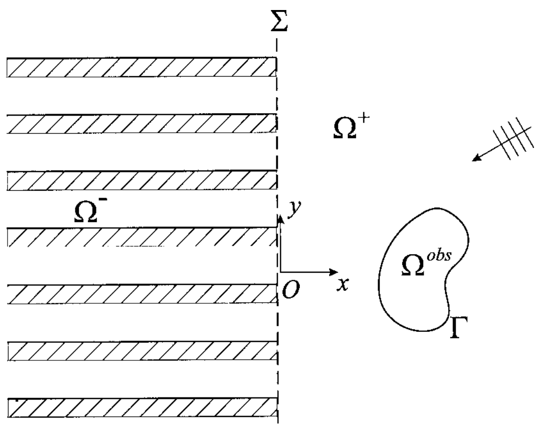

Figure 1. The perturbed grating.

derive a formal representation of the diffracted field in terms of u. Because of the presence of the obstacle, this representation also involves another unknown: the restriction of the diffracted field φ to a bounded domain Ω' surrounding the obstacle. In section 5, the normal derivatives of the formal representations obtained in sections 3 and 4 are derived and matched. Solving the diffraction problem amounts then to solve a pseudodifferential equation on Σ coupled to a boundary value problem set in the bounded domain Ω'. A weak formulation of this coupled problem is given. Section 6 is devoted to the rigorous analysis of this weak formulation. In particular, the question of the suitable functional framework in which this variational formulation should be set is investigated. Finally, section 7 deals with the well-posedness of this varitional formulation. In particular, it is proved that Fredholm alternative holds for the diffraction problem under some conditions on the spectrum of the grating.

2. Problem setting

Let (O, x, y) be an orthonormal system of coordinates in $\mathbb{R}^2$ and consider the two dimensional grating given in figure 1.

The half space $\{x > 0\}$ is supposed to be an homogeneous medium of celerity c^+ that contains a bounded obstacle Ω^{obs} of boundary Γ. We denote by Ω^+ the subdomain of the half space $\{x > 0\}$ located outside the obstacle: $\Omega^+ = \{x > 0\}\backslash\overline{\Omega^{\mathrm{obs}}}$.

The half space $\Omega^- = \{x < 0\}$ is assumed to be invariant in the x direction and periodic in the y direction with period 1. The unit cell $\mathbb{R}^- \times (0, 1)$ of this grating is characterized by a celerity $y \to c^-(y)$ where $c^- \in L^\infty(\mathbb{R})$ is a given periodic function of period 1. Finally, we denote by $\Omega = \mathbb{R}^2\backslash\overline{\Omega^{\mathrm{obs}}}$ the domain of propagation and by ν its outgoing unit normal on $\Gamma = \partial\Omega^{\mathrm{obs}}$.

When illuminated by a plane wave, the total field is constituted of a quasi-periodic part (the sum of incident plane wave and the field corresponding to its diffraction by the grating without obstacle) and a non-quasi-periodic part φ due to the presence of the obstacle. This contribution φ can be seen as the field diffracted by the obstacle when illuminated by the quasi-periodic part.

So let $\psi_{\mathrm{inc}}(x, y, t) = \varphi_{\mathrm{inc}}(x, y)\,\mathrm{e}^{-\mathrm{i}\omega t}$ be the quasi-periodic solution of the diffraction problem of a plane wave by the unperturbed grating (i.e., without obstacle). Then, the diffracted field $\varphi(x, y)$ by the perturbed grating (i.e., with obstacle) is an outgoing solution of the following diffraction problem

$$\begin{cases} \Delta\varphi + k^2\varphi = 0 & (\Omega) \\ \partial_\nu\varphi = g & (\Gamma) \end{cases} \tag{1}$$

with $g = -\,\partial_\nu\varphi_{\mathrm{inc}}$ and

$$k(x, y) = \begin{cases} k^+ & \text{for } x > 0, \\ k^-(y) & \text{for } x < 0, \end{cases}$$

where $k^+ = \omega/c^+$ and $k^-(y)$ is the periodic function with period 1 defined by $k^-(y) = \omega/c^-(y)$.

3. Representation in Ω^-

We begin this section by a short presentation of Floquet transform that will be used to derive an explicit representation of the diffracted field in Ω^- in terms of its trace u on Σ.

3.1. Floquet transform

The analysis of wave propagation in cristals is based on the so-called Floquet theory. This theory, which deals with differential operators with periodic coefficients, has given rise to several studies since the sixties (especially Schrödinger equation for periodic potentials, cf. [15,16]). For an exhaustive bibliography, one can see [11] and the references therein. The main tool in this theory is known as Floquet transform (or Bloch transform), which plays in the case of periodic differential equations the role played by Fourier transform for differential equations in strips. In this section, we give a brief presentation of this functional transform and sum up those of its properties used throughout the paper.

Let f be a function defined on $\mathbb{R}$ and consider the quantity $\sum_{n\in\mathbb{Z}} f(x+n)\,\mathrm{e}^{\mathrm{i}n\theta}$ for $x, \theta \in \mathbb{R}$. For $f \in \mathcal{S}(\mathbb{R})$, this series converges for any $(x, \theta) \in \mathbb{R}^2$ and its limit defines a function $\mathcal{F}f$ of (x, θ):

$$\mathcal{F}f(x, \theta) = \sum_{n\in\mathbb{Z}} f(x+n)\mathrm{e}^{\mathrm{i}n\theta}. \tag{2}$$

First, note that this function is completely determined by its values for $(x, \theta) \in [0, 1] \times [0, 2\pi]$, since for every $x, \theta \in \mathbb{R}$ we have

$$\mathcal{F}f(x, \theta + 2\pi) = \mathcal{F}f(x, \theta), \qquad \mathcal{F}f(x+1, \theta) = \mathrm{e}^{-\mathrm{i}\theta}\mathcal{F}f(x, \theta).$$

In other words, $\mathcal{F}f(x,\cdot)$ is 2π-periodic, while $\mathcal{F}f(\cdot,\theta)$ is "quasi-periodic". Furthermore, if (2) is seen as a Fourier series expansion of $\theta \to \mathcal{F}f(x,\theta)$, one obtains immediately the following inversion formula

$$f(x+n) = \frac{1}{2\pi}\int_0^{2\pi} \mathcal{F}f(x,\theta)\mathrm{e}^{-\mathrm{i}n\theta}\,\mathrm{d}\theta, \quad \forall x \in [0,1],\ \forall n \in \mathbb{Z}.$$

Thanks to the next proposition, the functional transform $\mathcal{F}$ can be extended from $\mathcal{S}(\mathbb{R})$ to $L^2(\mathbb{R})$.

Proposition 1. For every $f \in \mathcal{S}(\mathbb{R})$, we have

$$\|\mathcal{F}f\|_{L^2((0,2\pi),L^2(0,1))} = \sqrt{2\pi}\,\|f\|_{L^2(\mathbb{R})}.$$

The application $\mathcal{F}: f \to \mathcal{F}f$ can thus be uniquely extended from $\mathcal{S}(\mathbb{R})$ to $L^2(\mathbb{R})$ as an unitary operator fom $L^2(\mathbb{R})$ onto the space $L^2((0,2\pi), L^2(0,1))$.

Proof. Let $f \in \mathcal{S}(\mathbb{R})$. Then, applying Fubini's theorem and Parseval's identity, one easily obtains that

$$\begin{aligned}
&\|\mathcal{F}f\|^2_{L^2((0,2\pi),L^2(0,1))}\\
&\quad = \int_0^{2\pi}\int_0^1 \left|\mathcal{F}f(x,\theta)\right|^2 \mathrm{d}x\,\mathrm{d}\theta = \int_0^1\int_0^{2\pi} \left|\sum_{n\in\mathbb{Z}} f(x+n)\mathrm{e}^{\mathrm{i}n\theta}\right|^2 \mathrm{d}\theta\,\mathrm{d}x\\
&\quad = 2\pi\int_0^1 \sum_{n\in\mathbb{Z}} \left|f(x+n)\right|^2 \mathrm{d}x = 2\pi\sum_{n\in\mathbb{Z}}\int_n^{n+1} \left|f(y)\right|^2 \mathrm{d}y = 2\pi\|f\|^2_{L^2(\mathbb{R})}.
\end{aligned}$$

The extension of $\mathcal{F}: f \mapsto \mathcal{F}f$ from $\mathcal{S}(\mathbb{R})$ to $L^2(\mathbb{R})$ as a unitary operator from $L^2(\mathbb{R})$ onto the space $L^2((0,2\pi), L^2(0,1))$ follows then from the density of $\mathcal{S}(\mathbb{R})$ in $L^2(\mathbb{R})$. Furthermore, this application defines an isomorphism. Indeed, $\mathcal{F}$ is clearly injective. To prove its surjectivity, let F be in $L^2((0,2\pi), L^2(0,1))$ and consider for almost every fixed x in $(0,1)$ the Fourier series expansion of $F(x,\cdot)$ in $L^2(0,2\pi)$, namely,

$$F(x,\theta) = \sum_{n\in\mathbb{Z}} c_n(x)\mathrm{e}^{\mathrm{i}n\theta}.$$

Define then the function $x \mapsto f(x)$ such that

$$f(x+n) = c_n(x), \quad \forall x \in (0,1),\ \forall n \in \mathbb{Z}.$$

We have

$$\begin{aligned}
\int_{\mathbb{R}} |f|^2 &= \int_0^1 \sum_{n\in\mathbb{Z}} \left|f(x+n)\right|^2 \mathrm{d}x = \int_0^1 \sum_{n\in\mathbb{Z}} \left|c_n(x)\right|^2 \mathrm{d}x\\
&= \int_0^1\int_0^{2\pi} \left|F(x,\theta)\right|^2 \mathrm{d}x\frac{\mathrm{d}\theta}{2\pi} < +\infty,
\end{aligned}$$

and thus $f \in L^2(\mathbb{R})$. Furthermore, by construction, we have $\mathcal{F}f = F$, and the theorem is proved. □

This proof also provides the inversion formula for Floquet transform, stating that f can be recovered from its Floquet transform $\mathcal{F}f$ on every interval $(n, n+1)$, $n \in \mathbb{Z}$ as follows:

Proposition 2. For every $f \in L^2(\mathbb{R})$, the following inverse formula holds for almost every $x \in (0,1)$

$$f(x+n) = \frac{1}{2\pi}\int_0^{2\pi} \mathcal{F}f(x,\theta)\mathrm{e}^{-\mathrm{i}n\theta}\,\mathrm{d}\theta, \quad \forall n \in \mathbb{Z}.$$

Remark 3. In fact, we can more generally define the Floquet transform $\mathcal{F}f$ of any function $f \in H^s(\mathbb{R})$, for $s \geqslant 0$, as a function with values in $L^2((0,2\pi), H^s(0,1))$, since the following equation holds for any $f \in \mathcal{S}(\mathbb{R})$ (and thus for any $f \in H^s(\mathbb{R})$ by density):

$$\|\mathcal{F}f\|_{L^2((0,2\pi),H^s(0,1))} = \sqrt{2\pi}\,\|f\|_{H^s(\mathbb{R})}.$$

To conclude this brief outline, let us emphasize some links between Floquet transform, Fourier series and Fourier transform.

We have already noticed that $\mathcal{F}f$ can be seen as the Fourier series expansion with respect to θ of the function-valued application $\theta \to \mathcal{F}f(\cdot,\theta)$. In particular, one can show that $\mathcal{F}$ defines an isomorphism from

$$\mathcal{L}^2(\mathbb{R}) = \left\{ f \in L^2_{\mathrm{loc}}(\mathbb{R});\ \sum_{n\in\mathbb{Z}} \|f\|_{L^2(n,n+1)} < +\infty \right\}$$

onto the space $\mathcal{E}$ of Fourier series in θ that converge normally in $L^2(0,1)$ and satisfy the quasi-periodicity condition.

On the other hand, since $\mathcal{F}f(\cdot,\theta)$ is quasi-periodic for a fixed θ, the function $x \to \mathrm{e}^{\mathrm{i}\theta x}\mathcal{F}f(x,\theta)$ is periodic of period 1. Writing the Fourier series expansion of this function, one gets the following expansion of $\mathcal{F}f(x,\theta)$

$$\mathcal{F}f(x,\theta) = \sum_{n\in\mathbb{Z}} \mathcal{F}_n(\theta)\mathrm{e}^{\mathrm{i}\theta_n x},$$

where we have set

$$\begin{cases} \theta_n = 2n\pi - \theta \\ \mathcal{F}_n(\theta) = \displaystyle\int_0^1 \mathcal{F}f(x,\theta)\mathrm{e}^{-\mathrm{i}\theta_n x}\,\mathrm{d}x. \end{cases}$$

In fact, the coefficients $\mathcal{F}_n(\theta)$ are directly related to the Fourier transform $\hat{f}$ of f. Indeed, we have

$$\begin{aligned}
\mathcal{F}_n(\theta) &= \int_0^1 \left(\sum_{p\in\mathbb{Z}} f(x+p)\mathrm{e}^{\mathrm{i}p\theta}\right)\mathrm{e}^{-\mathrm{i}\theta_n x}\,\mathrm{d}x = \sum_{p\in\mathbb{Z}} \int_0^1 f(x+p)\mathrm{e}^{\mathrm{i}p\theta}\,\mathrm{e}^{-\mathrm{i}\theta_n x}\,\mathrm{d}x \\
&= \sum_{p\in\mathbb{Z}} \int_p^{p+1} f(y)\mathrm{e}^{\mathrm{i}p(\theta+\theta_n)}\,\mathrm{e}^{-\mathrm{i}\theta_n y}\,\mathrm{d}y = \sum_{p\in\mathbb{Z}} \int_p^{p+1} f(y)\mathrm{e}^{-\mathrm{i}\theta_n y}\,\mathrm{d}y \\
&= \int_{\mathbb{R}} f(y)\mathrm{e}^{-\mathrm{i}\theta_n y}\,\mathrm{d}y.
\end{aligned}$$

In other words, we have $\mathcal{F}_n(\theta) = \sqrt{2\pi}\,\hat{f}(\theta_n) = \sqrt{2\pi}\,\hat{f}(2n\pi - \theta)$.

3.2. *Formal representation of the diffracted field in Ω^-*

Assuming that $u = \varphi_{|\Sigma}$ is known, we are now going to derive a formal representation of the diffracted field $\varphi^- = \varphi_{|\Omega^-}$ in Ω^- in terms of u. First, recall that φ^- is an outgoing solution of the following diffraction problem

$$\begin{cases} \Delta\varphi^- + \left(k^-\right)^2\varphi^- = 0 & (\Omega^-) \\ \varphi^- = u & (\Sigma). \end{cases} \tag{3}$$

We proceed as follows: first, taking the Floquet transform of this problem in the y direction will lead us to solve a family of boundary-value problems $(\mathcal{P}_\theta)_{\theta\in(0,2\pi)}$ (with θ denoting Floquet parameter) satisfied by the Floquet transform of φ^-. Each problem $(\mathcal{P}_\theta)$ is set in the unit cell $(x, y) \in \mathbb{R}\times(0,1)$ and involves quasi-periodic boundary conditions on the boundaries $y = 0$ and $y = 1$. Using the spectral decomposition of an auxialiary 1D operator A_θ, $(\mathcal{P}_\theta)$ is solved using a method of separation of variables. Finally, φ^- is recovered from its Floquet transform thanks to the inverse formula given in proposition 2.

Let us now precise these different steps.

For almost every $x \in \mathbb{R}^-$, let $\widetilde{\varphi}_\theta(x, y)$ denote the Floquet transform of the function $y \to \varphi(x, y)$ evaluated at the point (y, θ):

$$\widetilde{\varphi}_\theta(x, y) = \sum_{n\in\mathbb{Z}} \varphi^-(x, y+n)\mathrm{e}^{\mathrm{i}n\theta}.$$

Taking advantage of the periodicity and quasi-periodicity properties of $\widetilde{\varphi}_\theta(x, y)$ with respect to θ and y, it suffices to study $\widetilde{\varphi}_\theta(x, y)$ for $(y, \theta) \in (0,1)\times(0,2\pi)$. Moreover, we have $\mathcal{F}\Delta = \Delta\mathcal{F}$ and thanks to the periodicity of $y \to k^-(y)$, we can write that $\mathcal{F}((k^-)^2\varphi) = (k^-)^2\mathcal{F}\varphi$. Consequently, taking the Floquet transform of (3) with respect to y shows that for almost every $\theta \in (0, 2\pi)$, $\widetilde{\varphi}_\theta$ solves the following quasi-periodic problem set in the unit cell $\mathbb{R}^- \times (0, 1)$:

$$\begin{cases} \Delta\widetilde{\varphi}_\theta(x,y) + \big(k^-(y)\big)^2\widetilde{\varphi}_\theta(x,y) = 0 & \text{for } (x,y) \in \mathbb{R}^- \times (0,1), \\ \widetilde{\varphi}_\theta(0,y) = \tilde{u}_\theta(y) & \text{for } y \in (0,1), \\ \widetilde{\varphi}_\theta(x,1) = \mathrm{e}^{-\mathrm{i}\theta}\widetilde{\varphi}_\theta(x,0) & \text{for } x \in \mathbb{R}^-, \\ \partial_y\widetilde{\varphi}_\theta(x,1) = \mathrm{e}^{-\mathrm{i}\theta}\partial_y\widetilde{\varphi}_\theta(x,0) & \text{for } x \in \mathbb{R}^-, \end{cases} \qquad (\mathcal{P}_\theta)$$

where $\tilde{u}_\theta(y) = \sum_{n\in\mathbb{Z}} u(y+n)\mathrm{e}^{\mathrm{i}n\theta}$ is the Floquet transform of u.

To solve this problem, we introduce for almost every $\theta \in (0, 2\pi)$ the one-dimensional operator A_θ of domain

$$D(A_\theta) = \big\{v \in H^2(0,1);\ v(1) = \mathrm{e}^{-\mathrm{i}\theta}v(0),\ v'(1) = \mathrm{e}^{-\mathrm{i}\theta}v'(0)\big\}$$

and defined by

$$A_\theta v = -v'' - \big(k^-(y)\big)^2 v.$$

This second order ordinary differential operator with quasi-periodic boundary conditions has been extensively studied in the framework of Schrödinger equation with periodic potentials (see [15], for instance). The properties of A_θ needed in this paper are collected in the appendix. In particular, it is seen there that A_θ is a self-adjoint operator with compact resolvant. Consequently, its spectrum is constituted of a sequence $(\lambda_p(\theta))_{p\geqslant 1}$ of eigenvalues tending to $+\infty$. One can in addition show that these eigenvalues are simple for $\theta \in]0, \pi[\cup]\pi, 2\pi[$. Finally, there exists an orthonormal basis $(\psi_p^\theta)_{p\geqslant 1}$ of $L^2(0,1)$ constituted of eigenvectors of A_θ.

Now, we are going to see that problem $(\mathcal{P}_\theta)$ can be solved by decomposing $\tilde{u}_\theta$ in this basis $(\psi_p^\theta)_{p\geqslant 1}$. More precisely, if

$$\tilde{u}_\theta(y) = \sum_{p\geqslant 1}\big(\tilde{u}_\theta, \psi_p^\theta\big)_{L^2(0,1)}\psi_p^\theta(y)$$

then by linearity, the solution $\widetilde{\varphi}_\theta$ of $(\mathcal{P}_\theta)$ simply reads

$$\widetilde{\varphi}_\theta(x,y) = \sum_{p\geqslant 1}\big(\tilde{u}_\theta, \psi_p^\theta\big)_{L^2(0,1)}\widetilde{\varphi}_\theta^p(x,y), \tag{5}$$

where the function $\widetilde{\varphi}_\theta^p$ solves the following problem

$$\begin{cases} \Delta\widetilde{\varphi}_\theta^p(x,y) + (k^-(y))^2\widetilde{\varphi}_\theta^p(x,y) = 0 & \text{for } (x,y) \in \mathbb{R}^- \times (0,1), \\ \widetilde{\varphi}_\theta^p(0,y) = \psi_p^\theta(y) & \text{for } y \in (0,1), \\ \widetilde{\varphi}_\theta^p(x,1) = \mathrm{e}^{-\mathrm{i}\theta}\widetilde{\varphi}_\theta^p(x,0) & \text{for } x \in \mathbb{R}^-, \\ \partial_y\widetilde{\varphi}_\theta^p(x,1) = \mathrm{e}^{-\mathrm{i}\theta}\partial_y\widetilde{\varphi}_\theta^p(x,0) & \text{for } x \in \mathbb{R}^-. \end{cases} \qquad (\mathcal{P}_\theta^p)$$

In other words, solving $(\mathcal{P}_\theta)$ amounts to solve a countable set of elementary problems $(\mathcal{P}_\theta^p)_{p\geqslant 1}$ associated to the right-hand sides ψ_p^θ. Each problem $(\mathcal{P}_\theta^p)$ is elementary in the sense that its solution can be found explicitely using a method of separation of variables. Indeed, let us seek for a solution $\widetilde{\varphi}_\theta^p$ of $(\mathcal{P}_\theta^p)$ of the form

$$\widetilde{\varphi}_\theta^p(x, y) = S_\theta^p(x)\psi_p^\theta(y). \tag{6}$$

Then, S_θ^p satisfies $(S_\theta^p)'' = \lambda S_\theta^p$ for $x \in \mathbb{R}^-$ and $S_\theta^p(0) = 1$. Keeping only the outgoing solutions, we get:

$$S_\theta^p(x) = \mathrm{e}^{\sqrt[c]{\lambda_p(\theta)}x}, \tag{7}$$

where the complex square root $\sqrt[c]{\lambda_p(\theta)}$ is defined by

$$\sqrt[c]{\lambda_p(\theta)} = \begin{cases} \sqrt{\lambda_p(\theta)} & \text{for } \lambda_p(\theta) \geqslant 0, \\ -\mathrm{i}\sqrt{-\lambda_p(\theta)} & \text{for } \lambda_p(\theta) \leqslant 0. \end{cases} \tag{8}$$

Remark 4. Let

$$\mathcal{I}_\theta^- = \{p \geqslant 1, \lambda_p(\theta) \leqslant 0\} \quad \text{and} \quad \mathcal{I}_\theta^+ = \{p \geqslant 1, \lambda_p(\theta) > 0\}.$$

$\mathcal{I}_\theta^-$ is a finite set corresponding to waves propagating in the x direction towards $-\infty$ since their dependence with respect to (x, t) is of the form: $\mathrm{e}^{-\mathrm{i}(\omega t + \sqrt{|\lambda_p(\theta)|}x)}$. On the contrary, the countable set $\mathcal{I}_\theta^+$ corresponds to evanescent waves decreasing exponentially when $x \to -\infty$.

In both cases, we are dealing with waves transporting energy in the x direction towards $-\infty$ (with or without attenuation) and this is why it is natural to call them "outgoing". Nevertheless, a rigorous justification of this convention requires the proof of a "limiting absorption" result (cf. [7]) that would be beyond the scope of this paper.

Summing up (5)–(7), the solution $\widetilde{\varphi}_\theta$ of $(\mathcal{P}_\theta)$ reads for almost every $\theta \in (0, 2\pi)$:

$$\forall (x, y) \in \mathbb{R}^- \times (0, 1)\colon \quad \widetilde{\varphi}_\theta(x, y) = \sum_{p \geqslant 1} \big(\tilde{u}_\theta, \psi_p^\theta\big)_{L^2(0,1)} \mathrm{e}^{\sqrt[c]{\lambda_p(\theta)}x} \psi_p^\theta(y). \tag{9}$$

The diffracted field φ^- in Ω^- can be easily recovered in every cell $\mathbb{R}^- \times (n, n+1)$ thanks to the inversion formula

$$\varphi^-(x, y + n) = \frac{1}{2\pi} \int_0^{2\pi} \widetilde{\varphi}_\theta(x, y) \mathrm{e}^{-\mathrm{i}n\theta} \, \mathrm{d}\theta, \quad \forall x \in \mathbb{R}^-, \ \forall y \in (0, 1).$$

4. Representation in Ω^+

The diffracted field $\varphi^+ = \varphi_{|\Omega^+}$ in the homogeneous medium $\Omega^+ = \{x > 0\}\backslash\overline{\Omega^{\text{obs}}}$ solves the following diffraction problem

$$\begin{cases} \Delta\varphi^+ + \left(k^+\right)^2\varphi^+ = 0 & (\Omega^+) \\ \varphi^+ = u & (\Sigma) \\ \partial_\nu\varphi^+ = g & (\Gamma), \end{cases}$$

where $g = -\,\partial_\nu\varphi_{\text{inc}}$.

In this section, we derive a formal representation of $\varphi^+ = \varphi_{|\Omega^+}$ in terms of the trace u. To achieve this, we first deal with the case of the unperturbed medium by removing the obstacle. This simplification allows us to use Fourier transform in the y direction and get an explicit representation φ^∞ of the "unperturbed" diffracted field. The second step is to determine the perturbation $\varphi^{\text{obs}} = \varphi^+ - \varphi^\infty$ induced by the presence of the obstacle. It is proved that φ^{obs} solves a classical diffraction problem set in the unbounded domain Ω^+. Among the several methods that can be used to solve this problem, we have chosen to use the one coupling a variational formulation with an integral representation (cf. [12]).

4.1. Problem without obstacle

Let us consider in this section the case of an unperturbed medium (without obstacle) $\Omega^\infty = \{x > 0\}$ and let φ^∞ denote the outgoing solution of the diffraction problem

$$\begin{cases} \Delta\varphi^\infty + \left(k^+\right)^2\varphi^\infty = 0 & (\Omega^\infty) \\ \varphi^\infty = u & (\Sigma). \end{cases} \tag{10}$$

Freezing the variable x and taking the Fourier transform of this problem with respect to y, we see that $\widehat{\varphi^\infty}(x,\xi) = (1/\sqrt{2\pi})\int_{-\infty}^{+\infty}\varphi(x,y)\,\mathrm{e}^{-\mathrm{i}\xi y}\,\mathrm{d}y$ of $\varphi(x,\cdot)$ satisfies

$$\begin{cases} \dfrac{\mathrm{d}^2}{\mathrm{d}x^2}\widehat{\varphi^\infty}(x,\xi) + \left(\left(k^+\right)^2 - \xi^2\right)\widehat{\varphi^\infty}(x,\xi) = 0 & (x,\xi) \in \mathbb{R}^+ \times \mathbb{R}, \\ \widehat{\varphi^\infty}(0,\xi) = \hat{u}(\xi) & \xi \in \mathbb{R}. \end{cases}$$

Keeping only the outgoing solutions, we see that $\widehat{\varphi^\infty}$ is necessarily given by

$$\widehat{\varphi^\infty}(x,\xi) = \hat{u}(\xi)\mathrm{e}^{-\sqrt[c]{\xi^2-(k^+)^2}\,x}, \tag{11}$$

where the complex square root $\sqrt[c]{\xi^2 - (k^+)^2}$ is defined by

$$\sqrt[c]{\xi^2 - \left(k^+\right)^2} = \begin{cases} \sqrt{\xi^2 - \left(k^+\right)^2} & \text{for } \xi^2 \geqslant \left(k^+\right)^2, \\ -\mathrm{i}\sqrt{\left(k^+\right)^2 - \xi^2} & \text{for } \xi^2 \leqslant \left(k^+\right)^2. \end{cases} \tag{12}$$

Once again, one can note here that the case $\xi^2 \geqslant (k^+)^2$ corresponds to evanescent waves, while $\xi^2 \leqslant (k^+)^2$ corresponds to waves propagating in the direction of the positive values of x.

Summing up, the diffracted field φ^∞ for the unperturbed case is simply given by

$$\varphi^\infty(x, y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \hat{u}(\xi) \mathrm{e}^{\,c\!\!+\!\sqrt{\xi^2-(k^+)^2}x} \mathrm{e}^{\mathrm{i}\xi y}\, \mathrm{d}\xi. \tag{13}$$

4.2. *Problem with obstacle*

Let us now consider the case where Ω^∞ contains the obstacle Ω^{obs} of boundary Γ. Recall that the diffracted field φ^+ in $\Omega^+ = \Omega^\infty \backslash \overline{\Omega^{\mathrm{obs}}}$ satisfies

$$\begin{cases} \Delta\varphi^+ + (k^+)^2\varphi^+ = 0 & (\Omega^+) \\ \varphi^+ = u & (\Sigma) \\ \partial_\nu \varphi^+ = g & (\Gamma). \end{cases}$$

Comparing this problem and (10), we see that the contribution of the obstacle $\varphi^{\mathrm{obs}} = \varphi^+ - \varphi^\infty$ in the diffracted field φ^+ is an outgoing solution of the following diffraction problem

$$\begin{cases} \Delta\varphi^{\mathrm{obs}} + (k^+)^2\varphi^{\mathrm{obs}} = 0 & (\Omega^+) \\ \varphi^{\mathrm{obs}} = 0 & (\Sigma) \\ \partial_\nu \varphi^{\mathrm{obs}} = g - \partial_\nu \varphi^\infty & (\Gamma). \end{cases} \tag{14}$$

In order to solve this classical diffraction problem, we are going to reduce it to a problem set in a bounded domain using the integral representation of φ^{obs}.

More precisely, let $G(\mathbf{x}, \mathbf{y})$ denote for $(\mathbf{x}, \mathbf{y}) \in \Omega^\infty \times \Omega^\infty$ the outgoing fundamental solution of Helmholtz operator $\Delta + (k^+)^2$ in the half-space $\Omega^\infty = \mathbb{R}^+ \times \mathbb{R}$ satisfying the homogeneous Dirichlet boundary condition on $\Sigma = \partial\Omega^\infty = \{0\} \times \mathbb{R}$.

Remark 5. This fundamental solution $G(\mathbf{x}, \mathbf{y})$ can be deduced from Helmholtz outgoing (i.e., satisfying Sommerfeld radiation condition) Green's function in $\mathbb{R}^2$ given by

$$\mathcal{G}(\mathbf{x}, \mathbf{y}) = \frac{1}{4\mathrm{i}} H_0^1\big(k^+|\mathbf{x} - \mathbf{y}|\big).$$

Indeed, by symmetry, we have

$$G(\mathbf{x}, \mathbf{y}) = \mathcal{G}(\mathbf{x}, \mathbf{y}) - \mathcal{G}\big(\mathbf{x}', \mathbf{y}\big),$$

where $\mathbf{x}'$ denotes the symmetric point of $\mathbf{x}$ with respect to Σ.

The integral representation formula (cf. [5]) of φ^{obs} reads with these notations

$$\forall \mathbf{x} \in \Omega^+: \quad \varphi^{\mathrm{obs}}(\mathbf{x}) = \int_\Gamma \big[\partial_{\nu_\mathbf{y}} G(\mathbf{x}, \mathbf{y})\varphi^{\mathrm{obs}}(\mathbf{y}) - G(\mathbf{x}, \mathbf{y})\partial_{\nu_\mathbf{y}}\varphi^{\mathrm{obs}}(\mathbf{y})\big]\, \mathrm{d}\gamma_\mathbf{y},$$

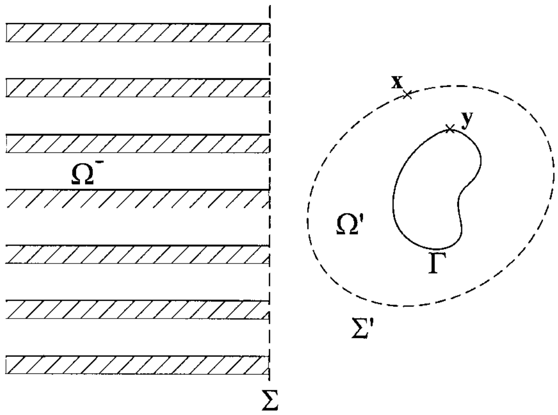

Figure 2. The bounded domain surrouding the obstacle.

where $\nu_{\mathbf{y}}$ denotes the unit outgoing normal of Ω^+ at the the point $\mathbf{y} \in \Gamma$. Since φ^{obs} satisfies on Γ:

$$\partial_\nu \varphi^{\text{obs}} = g - \partial_\nu \varphi^\infty,$$

this integral representation also reads for any $\mathbf{x} \in \Omega^+$:

$$\varphi^{\text{obs}}(\mathbf{x}) = \int_\Gamma \partial_{\nu_{\mathbf{y}}} G(\mathbf{x}, \mathbf{y}) \varphi^{\text{obs}}(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} - \int_\Gamma G(\mathbf{x}, \mathbf{y}) \big(g - \partial_{\nu_{\mathbf{y}}} \varphi^\infty\big)(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}}. \tag{15}$$

Now, we are going to use this integral representation to derive an equivalent formulation of (14) which is set in a bounded domain containing the obstacle. Let $\Omega' \subset \Omega^+$ be such a domain and assume that its boundary $\partial\Omega' = \Gamma \cup \Sigma'$ satisfies $\Sigma' \cap \Gamma = \emptyset$ and $\Sigma' \cap \Sigma = \emptyset$ (as in figure 2).

Then, it is clear that $\varphi' = \varphi^{\text{obs}}_{|\Omega'}$ satisfies

$$\Delta\varphi' + \big(k^+\big)^2 \varphi' = 0 \quad \text{in } \big(\Omega'\big) \quad \text{and} \quad \partial_\nu \varphi' = g - \partial_\nu \varphi^\infty \quad \text{on } (\Gamma).$$

To get a boundary value problem for φ' set in Ω', we need to complete these equations by a boundary condition on the fictitious boundary Σ'. A possible condition is given by the integral representation (15), namely,

$$\forall \mathbf{x} \in \Sigma' : \quad \varphi'(\mathbf{x}) = \int_\Gamma \partial_{\nu_{\mathbf{y}}} G(\mathbf{x}, \mathbf{y}) \varphi'(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} - \int_\Gamma G(\mathbf{x}, \mathbf{y}) \big(g - \partial_{\nu_{\mathbf{y}}} \varphi^\infty\big)(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}}.$$

Unfortunately, this choice gives rise to (non physical) irregular frequencies (i.e., frequencies k^+ for which problem (14) and the problem set in the bounded domain Ω' are not equivalent). To avoid this situtation, one can use (as in [12]) a slighlty different boundary condition on Σ', namely, a Robin boundary condition:

$$D\varphi'(\mathbf{x}) = \int_\Gamma \partial_{\nu_{\mathbf{y}}} DG(\mathbf{x}, \mathbf{y}) \varphi'(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} - \int_\Gamma DG(\mathbf{x}, \mathbf{y}) \big(g - \partial_{\nu_{\mathbf{y}}} \varphi^\infty\big)(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}}, \tag{16}$$

where we have set $Df(\mathbf{x}) = (\partial_{\nu_{\mathbf{x}}} + \mathrm{i}) f(x)$.

Remark 6. Note that for $(\mathbf{x}, \mathbf{y}) \in \Sigma' \times \Gamma$, the fundamental solution $G(\mathbf{x}, \mathbf{y})$ is infinitely differentiable and the quantity $DG(\mathbf{x}, \mathbf{y})$ is thus perfectly defined.

It is well known (see [12]) that this boundary condition is a transparent boundary condition for all frequencies and the following equivalence result holds.

Proposition 7. (i) If φ is an outgoing solution of the diffraction problem (14), then $\varphi' = \varphi^{\text{obs}}_{|\Omega'}$ solves the following boundary value problem in Ω'

$$\begin{cases} \Delta\varphi' + (k^+)^2\varphi' = 0 & (\Omega') \\ \partial_\nu\varphi' = g - \partial_\nu\varphi^\infty & (\Gamma) \\ D\varphi'(\mathbf{x}) = \displaystyle\int_\Gamma \partial_{\nu_\mathbf{y}} DG(\mathbf{x}, \mathbf{y})\varphi'(\mathbf{y})\,\mathrm{d}\gamma_\mathbf{y} & \\ \qquad - \displaystyle\int_\Gamma DG(\mathbf{x}, \mathbf{y})\big(g - \partial_{\nu_\mathbf{y}}\varphi^\infty\big)(\mathbf{y})\,\mathrm{d}\gamma_\mathbf{y} & (\Sigma'), \end{cases} \tag{17}$$

where $D = \partial_\nu + \mathrm{i}$.

(ii) Conversely, if φ' solves (17), then the solution φ^{obs} of (14) is given at any point $\mathbf{x} \in \Omega^+$ by the integral representation formula

$$\varphi^{\text{obs}}(\mathbf{x}) = \int_\Gamma \partial_{\nu_\mathbf{y}} G(\mathbf{x}, \mathbf{y})\varphi'(\mathbf{y})\,\mathrm{d}\gamma_\mathbf{y} - \int_\Gamma G(\mathbf{x}, \mathbf{y})\big(g - \partial_{\nu_\mathbf{y}}\varphi^\infty\big)(\mathbf{y})\,\mathrm{d}\gamma_\mathbf{y}.$$

Let us conclude this section by giving the variational formulation of problem (17) that we will need in the next section. Using Green's formula, one easily gets from (17) that for any $\psi \in H^1(\Omega')$, we have

$$\int_{\Omega'} \big(\nabla\varphi' \cdot \overline{\nabla\psi} - (k^+)^2\varphi'\overline{\psi}\big) - \int_\Gamma \big(g - \partial_\nu\varphi^\infty\big)\overline{\psi} - \int_{\Sigma'} (D - \mathrm{i})\varphi'\overline{\psi} = 0, \quad \forall\psi \in H^1(\Omega').$$

where we have used the relation $\partial_\nu = D - \mathrm{i}$ on Σ'. Thanks to the transparent boundary condition (16) on Σ', we finally get the following variational formulation for (17)

$$\begin{aligned} &\int_{\Omega'} \nabla\varphi' \cdot \overline{\nabla\psi} - \int_{\Omega'} (k^+)^2\varphi'\overline{\psi} + \mathrm{i}\int_{\Sigma'} \varphi'\overline{\psi} + \int_\Gamma \partial_\nu\varphi^\infty\,\overline{\psi} \\ &\quad - \int_{\Sigma'} \left(\int_\Gamma \partial_{\nu_\mathbf{y}} DG(\mathbf{x}, \mathbf{y})\varphi'(\mathbf{y})\,\mathrm{d}\gamma_\mathbf{y}\right)\overline{\psi(\mathbf{x})}\,\mathrm{d}\gamma_\mathbf{x} \\ &\quad - \int_{\Sigma'} \left(\int_\Gamma DG(\mathbf{x}, \mathbf{y})\partial_\nu\varphi^\infty(\mathbf{y})\,\mathrm{d}\gamma_\mathbf{y}\right)\overline{\psi(\mathbf{x})}\,\mathrm{d}\gamma_\mathbf{x} \\ &= \int_\Gamma g\overline{\psi} - \int_{\Sigma'} \left(\int_\Gamma DG(\mathbf{x}, \mathbf{y})g(\mathbf{y})\,\mathrm{d}\gamma_\mathbf{y}\right)\overline{\psi(\mathbf{x})}\,\mathrm{d}\gamma_\mathbf{x}, \quad \forall\psi \in H^1(\Omega'). \end{aligned} \tag{18}$$

5. Formal derivation of the problem

As it has been already precised in the introduction, the method proposed in this paper to deal with bounded obstacles in diffraction gratings is to transform the diffraction problem (1) into a one-dimensional problem whose unknown is the trace u of the diffracted field φ on the fictitious boundary Σ. In sections 3 and 4, we have seen that $\varphi^{\pm} = \varphi_{|\Omega^{\pm}}$ are totally determined by the trace u. We are thus lead to derive a problem satisfied by $u = \varphi_{|\Sigma}$. To achieve this, we simply match the normal derivatives $\partial_{\nu^+}\varphi^+$ and $\partial_{\nu^-}\varphi^-$ of φ^+ and φ^- across Σ ($\nu^{\pm}$ denotes here the unit outgoing normal to $\Omega^{\pm}$). In other words, $u = \varphi_{|\Sigma}$ solves the following problem

$$\langle \partial_{\nu^-}\varphi^-, v\rangle_{\Sigma} + \langle \partial_{\nu^+}\varphi^+, v\rangle_{\Sigma} = 0, \quad \forall v \in \mathcal{D}(\Sigma).$$

As we are going to see now, using the representations of $\varphi^{\pm}$ derived in sections 3 and 4, these duality products can be explicitely formulated in terms of u.

Let us first consider the term $\langle \partial_{\nu^-}\varphi^-, v\rangle_{\Sigma}$. From the isometry property of Floquet transform (see proposition 1), we get

$$\langle \partial_{\nu^-}\varphi^-, v\rangle_{\Sigma} = \int_{\mathbb{R}} \partial_x \varphi^-(0, y)\overline{v(y)}\,\mathrm{d}y = \frac{1}{2\pi}\int_0^{2\pi}\int_0^1 \partial_x \widetilde{\varphi}_\theta(0, y)\overline{\tilde{v}_\theta(y)}\,\mathrm{d}y\,\mathrm{d}\theta,$$

where $\widetilde{\varphi}_\theta(x, y)$ and $\tilde{v}_\theta(y)$ denote respectively the Floquet transforms (in the y direction) of $\varphi(x, y)$ and $v(y)$. Since $\widetilde{\varphi}_\theta(x, y)$ is given explicitely by (9), one gets

$$\partial_x \widetilde{\varphi}_\theta(0, y) = \sum_{p\geqslant 1} \sqrt[c]{\lambda_p(\theta)}\big(\tilde{u}_\theta, \psi_p^\theta\big)_{L^2(0,1)}\psi_p^\theta(y).$$

We can thus write that

$$\langle \partial_{\nu^-}\varphi^-, v\rangle_{\Sigma} = \frac{1}{2\pi}\int_0^{2\pi} \sum_{p\geqslant 1} \sqrt[c]{\lambda_p(\theta)}\big(\tilde{u}_\theta, \psi_p^\theta\big)_{L^2(0,1)}\overline{\big(\tilde{v}_\theta, \psi_p^\theta\big)_{L^2(0,1)}}\,\mathrm{d}\theta.$$

To derive now the expression of $\langle \partial_{\nu^+}\varphi^+, v\rangle_{\Sigma}$, recall first that $\varphi^+ = \varphi^\infty + \varphi^{\mathrm{obs}}$, where φ^∞ represents the diffracted field without the obstacle and φ^{obs} the perturbation due to the obstacle. On one hand, Parseval's identity shows that

$$\langle \partial_{\nu^+}\varphi^\infty, v\rangle_{\Sigma} = -\int_{\mathbb{R}} \partial_x \varphi^\infty(0, y)\overline{v}(y)\,\mathrm{d}y = -\int_{\mathbb{R}} \partial_x \widehat{\varphi^\infty}(0, \xi)\overline{\hat{v}(\xi)}\,\mathrm{d}\xi,$$

where $\widehat{\varphi^\infty}(x, \xi)$ and $\hat{v}(\xi)$ denote respectively the Fourier transforms (in the y direction) of $\varphi^\infty(x, y)$ and $v(y)$. Since $\widehat{\varphi^\infty}(x, \xi)$ is given by (11), we have

$$\langle \partial_{\nu^+}\varphi^\infty, v\rangle_{\Sigma} = \int_{\mathbb{R}} \sqrt[c]{\xi^2 - \big(k^+\big)^2}\,\hat{u}(\xi)\overline{\hat{v}(\xi)}\,\mathrm{d}\xi.$$

On the other hand, it follows from the expression φ^{obs} given in proposition 7 (part (ii)) that

$$\langle \partial_{\nu^+}\varphi^{\mathrm{obs}}, v\rangle_{\Sigma} = -\int_{\Sigma} \partial_{\nu^+_{\mathbf{x}}}\varphi^{\mathrm{obs}}(\mathbf{x})\overline{v(\mathbf{x})}\,\mathrm{d}\gamma_{\mathbf{x}}$$

$$= -\int_\Sigma \left(\int_\Gamma \partial_{\nu_{\mathbf{x}}^+} \partial_{\nu_{\mathbf{y}}} G(\mathbf{x}, \mathbf{y}) \varphi'(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{v(\mathbf{x})} \, \mathrm{d}\gamma_{\mathbf{x}} + \int_\Sigma \left(\int_\Gamma \partial_{\nu_{\mathbf{x}}^+} G(\mathbf{x}, \mathbf{y}) \big(g - \partial_{\nu_{\mathbf{y}}} \varphi^\infty \big)(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{v(\mathbf{x})} \, \mathrm{d}\gamma_{\mathbf{x}}.$$

Summing up these results, the weak fomulation of the equation: $\partial_{\nu^-}\varphi^- + \partial_{\nu^+}\varphi^+ = 0$ reads

$$a^-(u, v) + a^+(u, v) + a^\infty(u, v) + c_1\big(\varphi', v\big) = l_1(v), \quad \forall v \in \mathcal{D}(\Sigma). \tag{19}$$

with

$$\begin{aligned} a^-(u, v) &= \frac{1}{2\pi} \int_0^{2\pi} \sum_{p \geqslant 1} \sqrt[c]{\lambda_p(\theta)} \big(\tilde{u}_\theta, \psi_p^\theta \big)_{L^2(0,1)} \overline{\big(\tilde{v}_\theta, \psi_p^\theta \big)_{L^2(0,1)}} \, \mathrm{d}\theta, \\ a^+(u, v) &= \int_{\mathbb{R}} \sqrt[c]{\xi^2 - \big(k^+\big)^2} \hat{u}(\xi) \overline{\hat{v}(\xi)} \, \mathrm{d}\xi, \\ a^\infty(u, v) &= -\int_\Sigma \left(\int_\Gamma \partial_{\nu_{\mathbf{x}}^+} G(\mathbf{x}, \mathbf{y}) \partial_{\nu_{\mathbf{y}}} \varphi^\infty(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{v(\mathbf{x})} \, \mathrm{d}\gamma_{\mathbf{x}}, \\ c_1\big(\varphi', v\big) &= \int_\Sigma \left(\int_\Gamma \partial_{\nu_{\mathbf{x}}^+} \partial_{\nu_{\mathbf{y}}} G(\mathbf{x}, \mathbf{y}) \varphi'(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{v(\mathbf{x})} \, \mathrm{d}\gamma_{\mathbf{x}}, \\ l_1(v) &= -\int_\Sigma \left(\int_\Gamma \partial_{\nu_{\mathbf{x}}^+} G(\mathbf{x}, \mathbf{y}) g(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{v(\mathbf{x})} \, \mathrm{d}\gamma_{\mathbf{x}}, \end{aligned} \tag{20}$$

where φ^∞ given by (13) depends linearly on u, φ' solves (17) and the square roots $\sqrt[c]{\lambda_p(\theta)}$ and $\sqrt[c]{\xi^2 - (k^+)^2}$ are respectively defined in (8) and (12).

Let us emphasize here that problem (19) is a coupled problem in (u, φ') since φ' solves a boundary problem (namely (17)) where u plays the role of a source term, through the function φ^∞. This is why (19) needs to be completed by the variational formulation (18) in $H^1(\Omega')$ of problem (17), which reads

$$b\big(\varphi', \psi\big) + c_2(u, \psi) = l_2(\psi), \quad \forall \psi \in H^1\big(\Omega'\big) \tag{21}$$

with

$$\begin{aligned} b\big(\varphi', \psi\big) &= \int_{\Omega'} \nabla\varphi' \cdot \overline{\nabla\psi} - \int_{\Omega'} \big(k^+\big)^2 \varphi' \overline{\psi} + \mathrm{i} \int_{\Sigma'} \varphi' \overline{\psi} \\ &\quad - \int_{\Sigma'} \left(\int_\Gamma \partial_{\nu_{\mathbf{y}}} DG(\mathbf{x}, \mathbf{y}) \varphi'(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{\psi(\mathbf{x})} \, \mathrm{d}\gamma_{\mathbf{x}}, \\ c_2(u, \psi) &= \int_\Gamma \partial_\nu \varphi^\infty \, \overline{\psi} - \int_{\Sigma'} \left(\int_\Gamma DG(\mathbf{x}, \mathbf{y}) \partial_\nu \varphi^\infty(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{\psi(\mathbf{x})} \, \mathrm{d}\gamma_{\mathbf{x}}, \\ l_2(\psi) &= \int_\Gamma g \overline{\psi} - \int_{\Sigma'} \left(\int_\Gamma DG(\mathbf{x}, \mathbf{y}) g(\mathbf{y}) \, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{\psi(\mathbf{x})} \, \mathrm{d}\gamma_{\mathbf{x}}. \end{aligned} \tag{22}$$

6. Variational formulation and functional framework

In the previous section, we obtained a variational formulation of the problem satisfied by the couple of unknowns $(u, \varphi') = (\varphi_{|\Sigma}, \varphi_{|\Omega'})$, that reads

$$\begin{cases} a^-(u, v) + a^+(u, v) + a^\infty(u, v) + c_1(\varphi', v) = l_1(v), \\ b(\varphi', \psi) + c_2(u, \psi) = l_2(\psi) \end{cases} \tag{23}$$

for any $(v, \psi) \in \mathcal{D}(\Sigma) \times H^1(\Omega')$ (the different terms of this formulation are defined in (20) and (22)).

Let us now study the functional framework in which this variational formulation should be set. The appropriate functional space for the unknown φ' is clearly $H^1(\Omega')$. On the contrary, the choice of a suitable functional space for the trace u is far from being obvious. To achieve this, a very precise and attentive description of the "energy" spaces V^- and V^+ respectively associated to the bilinear forms $a^-(\cdot,\cdot)$ and $a^+(\cdot,\cdot)$ is needed. In fact, we are going to see that these spaces are isomorphic (respectively, through Floquet and Fourier transforms) to some weighted L^2 spaces. The main difficulty in the analysis of these weighted spaces comes from the fact that the weights they involve (namely, $\sqrt{|\lambda_p(\theta)|}$ for V^- and $\sqrt{|\xi^2 - (k^+)^2|}$ for V^+) can vanish.

The space V^+ has been studied in detail in [4]. Its main properties are summarized in the next theorem.

Theorem 8. Let $F^{-1}_{\xi\to y}$ denote the usual inverse Fourier transform

$$F^{-1}_{\xi\to y}(\hat{v})(y) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{v}(\xi) e^{iy\xi} \, d\xi.$$

Then, the functional space

$$V^+ = F^{-1}_{\xi\to y}\left\{\hat{v} \in \mathcal{S}'(\mathbb{R});\ \int_{\mathbb{R}} \sqrt{\left|\xi^2 - (k^+)^2\right|}\left|\hat{v}(\xi)\right|^2 d\xi < +\infty\right\} \tag{24}$$

is well defined and constitutes a Hilbert space when equipped with the norm

$$\|v\|_{V^+} = \left(\int_{\mathbb{R}} \sqrt{\left|\xi^2 - (k^+)^2\right|}\left|\hat{v}(\xi)\right|^2 d\xi\right)^{1/2}, \tag{25}$$

where $\hat{v} = F_{y\to\xi}(v)$ denotes the Fourier transform of v.

Proof. Let Φ^+ denote the application

$$\Phi^+ : \hat{f} \to \hat{v}(\xi) = \hat{f}(\xi) / \sqrt[4]{\left|\xi^2 - (k^+)^2\right|}.$$

This application defines an isomorphism from $L^2(\mathbb{R})$ onto the space

$$\widehat{V}^+ = \left\{\hat{v};\ \int_{\mathbb{R}} \sqrt{\left|\xi^2 - (k^+)^2\right|}\left|\hat{v}(\xi)\right|^2 d\xi < +\infty\right\}.$$

Furthermore, $\Phi^+ : L^2(\mathbb{R}) \to \widehat{V}^+$ is an isometry if $\widehat{V}^+$ is equipped with the norm

$$\|\hat{v}\|_{\widehat{V}^+} = \left(\int_{\mathbb{R}} \sqrt{\left|\xi^2 - \left(k^+\right)^2\right|}\left|\hat{v}(\xi)\right|^2 \mathrm{d}\xi\right)^{1/2}.$$

Consequently, $(\widehat{V}^+, \|\cdot\|_{\widehat{V}^+})$ is a Hilbert space. To conclude, let us show that the elements of $\widehat{V}^+$ are tempered distributions (and this will allow us to set $V^+ = F^{-1}_{\xi\to y}(\widehat{V}^+)$). To achieve this, we prove that $\widehat{V}^+ \subset L^1_{\mathrm{loc}}(\mathbb{R})$. Indeed, for any compact $K \subset \mathbb{R}$, Cauchy–Schwartz inequality shows that for any $\hat{v} \in \widehat{V}^+$:

$$\int_K \left|\hat{v}(\xi)\right| \mathrm{d}\xi = \int_K \frac{|\hat{f}(\xi)|\,\mathrm{d}\xi}{\sqrt[4]{|\xi^2 - (k^+)^2|}} \leqslant \|\hat{f}\|_{L^2(\mathbb{R})} \int_K \frac{\mathrm{d}\xi}{\sqrt{|\xi^2 - (k^+)^2|}} < +\infty.$$

Consequently, $V^+ = F^{-1}_{\xi\to y}(\widehat{V}^+)$ is well defined and constitutes a Hilbert space when equipped with the norm $\|v\|_{V^+} = \|\hat{v}\|_{\widehat{V}^+}$. □

For V^-, the same kind of results can be shown using Floquet transform instead of Fourier transform. Nevertheless, some additional conditions are needed to ensure the summability of the discrete weights $\sqrt{|\lambda_p(\theta)|}$ with respect to θ. More precisely, the following result holds.

Theorem 9. Let $\mathcal{F}^{-1}_{(y,\theta)\to y}$ denote the inverse Floquet transform given by proposition 2

$$\mathcal{F}^{-1}_{(y,\theta)\to y}\big(\tilde{v}\big)(y+n) = \frac{1}{2\pi}\int_0^{2\pi} \tilde{v}(y,\theta)\mathrm{e}^{-\mathrm{i}n\theta}\,\mathrm{d}\theta, \quad \forall n \in \mathbb{Z},\ \forall y \in (0,1).$$

If one of the two following conditions holds

(A): $\forall\theta \in [0, 2\pi]$, $\lambda = 0$ is not an eigenvalue of A_θ,

(B): $\exists\theta^* \in [0, 2\pi]$ and $p^* \in \mathbb{N}^*$ such that $\lambda_{p^*}(\theta^*) = 0$ is a simple eigenvalue of A_{θ^*},

then the functional space

$$V^- = \mathcal{F}^{-1}_{(y,\theta)\to y}\left\{\tilde{v}(y,\theta) = \sum_{p\geqslant 1} \tilde{v}^p_\theta \psi^\theta_p(y);\ \int_0^{2\pi} \sum_{p\geqslant 1} \sqrt{\left|\lambda_p(\theta)\right|}\left|\tilde{v}^p_\theta\right|^2 \mathrm{d}\theta < +\infty\right\} \tag{26}$$

is well defined and constitutes a Hilbert space when equipped with the norm

$$\|v\|_{V^-} = \left(\frac{1}{2\pi}\int_0^{2\pi} \sum_{p\geqslant 1} \sqrt{\left|\lambda_p(\theta)\right|}\left|\tilde{v}^p_\theta\right|^2 \mathrm{d}\theta\right)^{1/2}, \tag{27}$$

where $\tilde{v}(y,\theta) = \sum_{p\geqslant 1} \tilde{v}^p_\theta \psi^\theta_p(y) = \mathcal{F}_{y\to(y,\theta)} v$ denotes the Floquet transform of v.

Proof. Let Φ^- be the application associating to $\tilde{f}(y,\theta) = \sum_{p\geqslant 1} \tilde{f}_\theta^p \psi_p^\theta(y)$ the function $\tilde{v}(y,\theta) = \sum_{p\geqslant 1} \tilde{v}_\theta^p \psi_p^\theta(y)$ such that $\tilde{v}_\theta^p = \tilde{f}_\theta^p / \sqrt[4]{|\lambda_p(\theta)|}$, $\forall p \geqslant 1$, $\forall \theta \in [0,1]$. Then, the Hilbert space

$$L^2\big((0,2\pi), L^2(0,1)\big) = \left\{ \tilde{f}(y,\theta) = \sum_{p\geqslant 1} \tilde{f}_\theta^p \psi_p^\theta(y);\ \int_0^{2\pi} \sum_{p\geqslant 1} \left| f_\theta^p \right|^2 \mathrm{d}\theta < +\infty \right\}$$

is obviously isometric by Φ^- to the functional space

$$\widetilde{V}^- = \left\{ \tilde{v}(y,\theta) = \sum_{p\geqslant 1} \tilde{v}_\theta^p \psi_p^\theta(y;\ \int_0^{2\pi} \sum_{p\geqslant 1} \sqrt{\left|\lambda_p(\theta)\right|} \left|\tilde{v}_\theta^p\right|^2 \mathrm{d}\theta < +\infty \right\}$$

if these spaces are equipped with the appropriate norms. Thus, $(\widetilde{V}^-, \|\cdot\|_{\widetilde{V}^-})$ is a Hilbert space. To conclude, it remains to check that we can take the inverse Floquet transform of this space. Let $\tilde{v}(y,\theta) = \sum_{p\geqslant 1} \tilde{v}_\theta^p \psi_p^\theta(y)$ belongs to $\widetilde{V}^-$. To show that the inverse formula can be used, it suffices to verify that the integrals

$$c_n(y) = \frac{1}{2\pi} \int_0^{2\pi} \tilde{v}(y,\theta) \mathrm{e}^{-\mathrm{i}n\theta}\, \mathrm{d}\theta$$

defining the restrictions of $v = F^{-1}_{\xi\to y}(\tilde{v})$ to $[n, n+1]$ exist for any $n \in \mathbb{Z}$ and almost every $y \in (0,1)$. Using Fubini theorem, we are going to prove that under condition (A) or condition (B), the function $\theta \mapsto \tilde{v}(y,\theta)$ belongs to $L^1(0,2\pi)$ for almost every $y \in (0,1)$.

We have

$$\int_0^1 \left(\int_0^{2\pi} \left|\tilde{v}(y,\theta)\right| \mathrm{d}\theta \right) \mathrm{d}y = \int_0^{2\pi} \left(\int_0^1 \left|\tilde{v}(y,\theta)\right| \mathrm{d}y \right) \mathrm{d}\theta.$$

Let us first deal with the case where condition (A) is satisfied. Cauchy–Schwartz inequality shows that

$$\int_0^1 \left|\tilde{v}(y,\theta)\right| \mathrm{d}y \leqslant \left(\int_0^1 \left|\tilde{v}(y,\theta)\right|^2 \mathrm{d}y \right)^{1/2} = \left(\sum_{p\geqslant 1} \left|\tilde{v}_\theta^p\right|^2 \right)^{1/2}$$

and thus

$$\int_0^1 \left(\int_0^{2\pi} \left|\tilde{v}(y,\theta)\right| \mathrm{d}\theta \right) \mathrm{d}y \leqslant \int_0^{2\pi} \left(\sum_{p\geqslant 1} \left|\tilde{v}_\theta^p\right|^2 \right)^{1/2} \mathrm{d}\theta \leqslant \sqrt{2\pi} \int_0^{2\pi} \sum_{p\geqslant 1} \left|\tilde{v}_\theta^p\right|^2 \mathrm{d}\theta.$$

Condition (A) implies then that

$$\int_0^1 \left(\int_0^{2\pi} \left|\tilde{v}(y,\theta)\right| \mathrm{d}\theta \right) \mathrm{d}y \leqslant \frac{\sqrt{2\pi}}{\sqrt{\eta}} \int_0^{2\pi} \sum_{p\geqslant 1} \sqrt{\left|\lambda_p(\theta)\right|} \left|\tilde{v}_\theta^p\right|^2 \mathrm{d}\theta < +\infty$$

for some constant $\eta > 0$.

Consequently, $(y,\theta) \mapsto \tilde{v}(y,\theta) \in L^1((0,1)\times(0,2\pi))$, and Fubini's theorem shows then that $\theta \mapsto \tilde{v}(y,\theta)$ belongs to $L^1(0,2\pi)$ for almost every $y \in (0,1)$. The integrals $c_n(y) = (1/2\pi)\int_0^{2\pi} \tilde{v}(y,\theta)\mathrm{e}^{-\mathrm{i}n\theta}\,\mathrm{d}\theta$ are thus well defined and the theorem is proved under condition (A).

Assume now that condition (B) is satisfied and let us show that $\tilde{v}$ still belongs to $L^1((0,1)\times(0,2\pi))$. Write that

$$\tilde{v}(y,\theta) = \sum_{p\geqslant 1} \tilde{v}_\theta^p \psi_p^\theta(y) = \tilde{v}_\theta^{p^*}\psi_{p^*}^\theta(y) + \sum_{p\neq p^*} \tilde{v}_\theta^p \psi_p^\theta(y).$$

The terms corresponding to $p \neq p^*$ can be treated as previously (i.e., under condition (A)) since the weights $\lambda_p(\theta)$ do not vanish for $p \neq p^*$. For the term $p = p^*$, the key point is that $\lambda_{p^*}(\theta) \sim (\mathrm{d}\lambda_{p^*}/\mathrm{d}\theta(\theta^*)(\theta-\theta^*)$ in the neighborhood of $\theta = \theta^*$ if $\lambda_{p^*}(\theta^*) = 0$ is a simple eigenvalue of A_{θ^*}. Indeed, using the regularity of the eigenvectors with respect to θ, we can write that

$$\int_0^{2\pi}\left(\int_0^1 \left|\tilde{v}_\theta^{p^*}\psi_{p^*}^\theta(y)\right|\mathrm{d}y\right)\mathrm{d}\theta \leqslant C^*\int_0^{2\pi}\left|\tilde{v}_\theta^{p^*}\right|\mathrm{d}\theta = C^*\int_0^{2\pi}\frac{\sqrt[4]{\lambda_{p^*}(\theta)}|\tilde{v}_\theta^{p^*}|}{\sqrt[4]{\lambda_{p^*}(\theta)}}\,\mathrm{d}\theta$$
$$\leqslant C^*\left(\int_0^{2\pi}\frac{\mathrm{d}\theta}{\sqrt{\lambda_{p^*}(\theta)}}\right)\left(\int_0^{2\pi}\sqrt{\lambda_{p^*}(\theta)}\left|\tilde{v}_\theta^{p^*}\right|^2\mathrm{d}\theta\right).$$

To conclude, just note that this last quantity is finite since $\tilde{v} \in \widetilde{V}^-$ and since the singularity of $1/\sqrt{\lambda_{p^*}(\theta)}$ is of the form $1/\sqrt{|\theta-\theta^*|}$. Consequently, $\tilde{v} \in L^1((0,1)\times(0,2\pi))$ and the theorem is proved. □

Remark 10. (i) Conditions (A) and (B) are not very strong. Indeed, the spectrum σ of the operator $\mathcal{A} = \int_\oplus^{(0,2\pi)} A_\theta$ has a band-gap structure (cf. [15]): $\sigma = \bigcup_{p\geqslant 1} I_p$, where I_p denotes the interval:

$$I_p = \left[\inf_{\theta\in(0,2\pi)}\lambda_p(\theta), \sup_{\theta\in(0,2\pi)}\lambda_p(\theta)\right].$$

Consequently, condition (A) is satisfied as soon as 0 belongs to a gap of the spectrum. On the other hand, even if $0 \in \sigma$, then the cases where 0 is not simple are quite exceptional. Indeed, the eigenvalues of A_θ are simple for $\theta \in]0,\pi[\,\cup\,]\pi,2\pi[$ (see proposition A.2 of the appendix or [15] for more details). In other words, (B) is not satisfied only if 0 is an eigenvalue of A_0 or A_π, these operators corresponding respectively to periodic and antiperiodic boundary conditions.

(ii) If $\lambda_{p^*}(\theta^*) = 0$ is a multiple eigenvalue of A_θ, then the singularities allowed by the correponding weight $\sqrt{|\lambda_{p^*}(\theta)|}$ are not necessarily integrable and V^- might be undefined.

The natural functional space in which the trace u of the diffracted field should be sought is thus $V = V^+ \cap V^-$ (V^+ and V^- are defined by (24) and (26)), equipped with the norm $\|\cdot\|_V = (\|\cdot\|_{V^+}^2 + \|\cdot\|_{V^-}^2)^{1/2}$ (where the norms on V^+ and V^- are given by (25) and (27)). We are now going to study the properties of this functional space. In particular, the question that arises is to compare V to the "usual" trace space $H^{1/2}(\mathbb{R})$. For V^+, this question has been answered in [4]: the only difference between the functions of V^+ and $H^{1/2}(\mathbb{R})$ comes from their behavior at infinity since the following result holds.

Proposition 11. The embeddings $H^{1/2}(\mathbb{R}) \hookrightarrow V^+ \hookrightarrow H^{1/2}_{\text{loc}}(\mathbb{R})$ are continuous. Moreover, any function $v \in V^+$ can be written as $v = v_1 + v_2$, where $v_1 \in H^{1/2}(\mathbb{R})$ and $v_2 \in \mathcal{C}^\infty(\mathbb{R})$ satisfies $\lim_{y\to+\infty} v_2(y) = 0$.

As one can expect, the same kind of result can be proved for V^-:

Proposition 12. If condition (A) of theorem 9 is satified, then $V^- = H^{1/2}(\mathbb{R})$. If condition (B) of theorem 9 is satisfied, the embeddings $H^{1/2}(\mathbb{R}) \hookrightarrow V^- \hookrightarrow H^{1/2}_{\text{loc}}(\mathbb{R})$ are continuous.

Proof. As it has been stated in section 3.1, the norm of any function $v \in H^{1/2}(\mathbb{R})$ can be estimated from the norm of its Floquet transform in $L^2((0,2\pi), H^{1/2}(0,1))$, since

$$\|v\|_{H^{1/2}(\mathbb{R})} = \frac{1}{\sqrt{2\pi}} \|\tilde{v}\|_{L^2((0,2\pi),H^{1/2}(0,1))},$$

where $\tilde{v} = \sum_{p\geqslant 1} \tilde{v}^p_\theta \psi^\theta_p(y)$ denotes the Floquet transform of v. On the other hand, using the characterization of $H^{1/2}(0,1)$ based on the spectral decomposition of A_θ given in the appendix (cf. proposition A.3), we see that

$$\|v\|^2_{H^{1/2}(\mathbb{R})} = \frac{1}{2\pi} \|\tilde{v}\|^2_{L^2((0,2\pi),H^{1/2}(0,1))} = \frac{1}{2\pi} \int_0^{2\pi} = \sum_{p\geqslant 1} \sqrt{\lambda_p(\theta)+\kappa} \left|\tilde{v}^p_\theta\right|^2 \mathrm{d}\theta,$$

where the constant κ satisfies $\kappa > \|k^-\|^2_\infty$ (to ensure the coercivity of $A_\theta + \kappa$).

Consequently, if (A) is satisfied, the weights $\sqrt{|\lambda_p(\theta)|}$ never vanish and the norms $\|\cdot\|_{H^{1/2}(\mathbb{R})}$ and $\|\cdot\|_{V^-}$ are then clearly equivalent, showing that $V^- = H^{1/2}(\mathbb{R})$.

If (B) is satisfied, the embedding $H^{1/2}(\mathbb{R}) \hookrightarrow V^-$ is clearly continuous since

$$\|v\|^2_{V^-} = \frac{1}{2\pi} \int_0^{2\pi} \sum_{p\geqslant 1} \sqrt{\left|\lambda_p(\theta)\right|} \left|\tilde{v}^p_\theta\right|^2 \mathrm{d}\theta \leqslant \|v\|^2_{H^{1/2}(\mathbb{R})}.$$

To prove the last embedding, write (with the notations of theorem 9) that

$$\tilde{v}(y,\theta) = \sum_{p\geqslant 1} \tilde{v}^p_\theta \psi^\theta_p(y) = \tilde{v}^{p^*}_\theta \psi^\theta_{p^*}(y) + \sum_{p\neq p^*} \tilde{v}^p_\theta \psi^\theta_p(y).$$

The term $\sum_{p\neq p^*} \tilde{v}^p_\theta \psi^\theta_p(y)$ clearly defines the Floquet transform of a function $v_1 \in H^{1/2}(\mathbb{R})$ since the weights $\lambda_p(\theta)$ do not vanish for $p \neq p^*$. Let us show that the term $\tilde{v}_\theta^{p^*}\psi_{p^*}^\theta(y)$ defines the Floquet transform of a function $v_2 \in H^{1/2}_{\mathrm{loc}}(\mathbb{R})$. For any fixed $n \in \mathbb{Z}$, we have

$$v_2(y+n) = \frac{1}{2\pi}\int_0^{2\pi} \tilde{v}_\theta^{p^*}\psi_{p^*}^\theta(y)\,\mathrm{e}^{-\mathrm{i}n\theta}\,\mathrm{d}\theta, \quad \forall y \in (0,1).$$

For almost every $\theta \in (0,2\pi)$, $\psi_{p^*}^\theta : y \to \psi_{p^*}^\theta(y)$ belongs to $H^2(0,1)$ and is thus in $\mathcal{C}^1([0,1])$. Furthermore, since $\|\psi_{p^*}^\theta\|_{L^2(0,1)} = 1$, $\forall\theta \in [0,2\pi]$, the function $\psi_{p^*}^\theta$ is also bounded in $H^2(0,1)$ independently of θ by some positive constant C^* (the first derivative is bounded from the variational formulation of the eigenvalue problem solved by $\psi_{p^*}^\theta$, while the second derivative is bounded since $(\psi_{p^*}^\theta)'' = -(k^-)^2\psi_{p^*}^\theta$). Thus, for almost every $y \in (0,1)$ and $\theta \in (0,2\pi)$, we have

$$\left|\tilde{v}_\theta^{p^*}\frac{\mathrm{d}\psi_{p^*}^\theta}{\mathrm{d}y}(y)\,\mathrm{e}^{-\mathrm{i}n\theta}\right| \leqslant C^*\left|\tilde{v}_\theta^{p^*}\right|.$$

Since

$$\int_0^{2\pi}\left|\tilde{v}_\theta^{p^*}\right|\mathrm{d}\theta \leqslant \left(\int_0^{2\pi}\frac{\mathrm{d}\theta}{\sqrt{\lambda_{p^*}(\theta)}}\right)\left(\int_0^{2\pi}\sqrt{\lambda_{p^*}(\theta)}\left|\tilde{v}_\theta^{p^*}\right|^2\mathrm{d}\theta\right),$$

the function $\theta \to \tilde{v}_\theta^{p^*}$ belongs to $L^1(0,2\pi)$ and thus v_2 is differentiable for almost every $y \in (n,n+1)$ by Lebesgue domination theorem and its derivative is bounded. Thus, $\mathrm{d}v_2/\mathrm{d}y \in L^2(n,n+1)$ and consequently $v_2 \in H^{1/2}_{\mathrm{loc}}(\mathbb{R})$.

This proves that V^- is included in $H^{1/2}_{\mathrm{loc}}(\mathbb{R})$ and also the continuity of the embedding $V^- \hookrightarrow H^{1/2}_{\mathrm{loc}}(\mathbb{R})$. □

We can now state this useful result concerning the space $V = V^+ \cap V^-$.

Theorem 13. Under condition (A) of theorem 9, we have $V = H^{1/2}(\mathbb{R})$. If condition (B) of theorem 9 is satisfied, $(V, \|\cdot\|_V)$ is a Hilbert space and the embeddings $H^{1/2}(\mathbb{R}) \hookrightarrow V \hookrightarrow H^{1/2}_{\mathrm{loc}}(\mathbb{R})$ are continuous.

Proof. If (A) is satisfied, the result follows immediately from propositions 11 and 12. If (B) is satisfied, let v_n be a Cauchy sequence in V. Then, v_n converges in V^+ to a limit v^+ and in V^- to a limit v^-. To conclude that $v^+ = v^-$ (and thus that v_n converges to this common limit in V), one simply uses the fact that the embeddings of V^+ and V^- into $H^{1/2}(K)$ are continuous for any compact $K \subset \mathbb{R}$. Finally, thanks to propositions 11 and 12, the continuity of the embeddings is obvious. □

Remark 14. Since V^+ and V^- are included in $H^{1/2}(\mathbb{R})$, so is $V = V^+ \cap V^-$. The question that naturally arises now is to know if the opposite inclusion holds, or, in other words, to know if $V = H^{1/2}(\mathbb{R})$. This is still an open question.

Thus, the rigorous variational formulation of our problem reads

$$\begin{cases} \text{Find } (u, \varphi') \in V \times H^1(\Omega') \text{ such that } \forall (v, \psi) \in V \times H^1(\Omega'): \\ a^-(u, v) + a^+(u, v) + a^\infty(u, v) + c_1(\varphi', v) = l_1(v), \\ b(\varphi', \psi) + c_2(u, \psi) = l_2(\psi). \end{cases} \tag{28}$$

The next section is devoted to the study of the well-posedness of this weak formulation.

7. Fredholm alternative

The aim of this section is to prove the main result of the paper, which can be stated as follows:

Theorem 14. Assume that $\Sigma \cap \Gamma = \emptyset$ and $\Sigma' \cap \Gamma = \emptyset$. If condition (A) or (B) of theorem 9 is satisfied, Fredholm alternative holds for the variational formulation (28).

Proof. Recall that the linear and bilinear forms appearing in (28) are defined in (20) and (22).

First, note that $a^-(\cdot,\cdot) + a^+(\cdot,\cdot)$ is obviously continuous and coercive on $V \times V$. On the other hand, the bilinear form $b(\cdot,\cdot)$ can be written as $b = b_1 + b_2$, where

$$\begin{aligned} b_1(\varphi', \psi) &= \int_{\Omega'} \nabla\varphi' \cdot \overline{\nabla\psi} + \int_{\Omega'} \varphi'\overline{\psi}, \\ b_2(\varphi', \psi) &= -\int_{\Omega'} \left(1 + (k^+)^2\right)\varphi'\overline{\psi} + \mathrm{i}\int_{\Sigma'} \varphi'\overline{\psi}\,\overline{\psi(\mathbf{x})}\,\mathrm{d}\gamma_{\mathbf{x}} \\ &\quad - \int_{\Sigma'} \left(\int_\Gamma \partial_{\nu_{\mathbf{y}}} DG(\mathbf{x}, \mathbf{y})\varphi'(\mathbf{y})\,\mathrm{d}\gamma_{\mathbf{y}} \right). \end{aligned}$$

Thus, $b_1(\cdot,\cdot)$ is clearly coercive on $H^1(\Omega') \times H^1(\Omega')$.

Consequently, the theorem will be proved if we show that the remaining forms ($a^\infty(\cdot,\cdot)$, $b_2(\cdot,\cdot)$ and the coupling terms $c_1(\cdot,\cdot)$ and $c_2(\cdot,\cdot)$) are associated to compact operators. Actually, this is mainly due to the fact that the boundary of the obstacle Γ does not intersect the boundaries Σ and Σ'.

Let us first detail the proof for the term $b_2(\cdot,\cdot)$.

The integrals

$$\int_{\Omega'} \left(1 + (k^+)^2\right)\varphi'\overline{\psi} \quad \text{and} \quad \int_{\Sigma'} \varphi'\overline{\psi}$$

are clearly associated to compact operators defined on $H^1(\Omega')$ thanks to the compact embedding of $H^1(\Omega')$ in $L^2(\Omega')$ and the continuity of the trace operator. For the term

$$\int_{\Sigma'} \left(\int_\Gamma \partial_{\nu_{\mathbf{y}}} DG(\mathbf{x}, \mathbf{y})\varphi'(\mathbf{y})\,\mathrm{d}\gamma_{\mathbf{y}} \right) \overline{\psi(\mathbf{x})}\,\mathrm{d}\gamma_{\mathbf{x}},$$

one has just to note that the kernel $\partial_{\nu_{\mathbf{y}}} DG(\mathbf{x}, \mathbf{y})$ is infinitely differentiable for $(\mathbf{x}, \mathbf{y}) \in \Sigma' \times \Gamma$ as soon as $\Sigma' \cap \Gamma = \emptyset$. Thus, using Cauchy–Schwartz inequality, we have

$$\left| \int_{\Sigma'} \left(\int_{\Gamma} \partial_{\nu_{\mathbf{y}}} DG(\mathbf{x}, \mathbf{y}) \varphi'(\mathbf{y})\, \mathrm{d}\gamma_{\mathbf{y}} \right) \overline{\psi(\mathbf{x})}\, \mathrm{d}\gamma_{\mathbf{x}} \right| \leqslant C \|\varphi'\|_{L^2(\Gamma)} \|\psi\|_{L^2(\Sigma')},$$

where $C = \sup_{(\mathbf{x},\mathbf{y}) \in \Sigma' \times \Gamma} |\partial_{\nu_{\mathbf{y}}} DG(\mathbf{x}, \mathbf{y})| > 0$.

The compactness of this term follows then from the compact embedding of $H^1(\Omega')$ in $H^{1/2+\varepsilon}(\Omega')$ and the continuity of the trace operator from $H^{1/2+\varepsilon}(\Omega')$ to $L^2(\Gamma)$.

The same arguments give the compactness of the term $c_1(\cdot,\cdot)$. For the remaining terms $a^\infty(\cdot,\cdot)$ and $c_2(\cdot,\cdot)$, an additional argument is needed since the dependence with respect to u is given there by the solution φ^∞ of (10). To overcome this difficulty, one has just to note that thanks to classical regularity results for elliptic operators, the application $u \mapsto \varphi^\infty$ is continuous from V to $H^m(K)$ for any $m \geqslant 1$ and any compact K of $\mathbb{R}^2_+$ as long as $K \cap \Sigma = \emptyset$. Consequently, the application $u \mapsto \partial_\nu \varphi^\infty$ is compact from V to $L^2(\Gamma)$ (since Γ does not intersect Σ) and thus $a^\infty(\cdot,\cdot)$ and $c_2(\cdot,\cdot)$ are associated to compact operators. □

8. Conclusion

In this paper, we have derived a mathematical formulation for a diffraction problem involving a locally perturbed grating. This formulation couples two unknowns: the trace u of the diffracted field φ on the fictitious interface Σ and the restriction φ' of φ to a bounded domain Ω' surrounding the obstacle. The equation satisfied by u involves Fourier and Floquet transforms and is thus non local. On the contrary, φ' solves a boundary value problem set in Ω' in which appears a integral representation formula. After a variational formulation of both problems is given, it is proved that Fredholm alternative holds for the diffraction problem under some conditions on the spectrum of the grating. This theoretical study should be completed by proving a limiting absorption principal, especially to justify the choice of the "outgoing" solutions.

Moreover, the approach proposed in this paper naturally leads to a numerical method to solve the diffraction problem by a Galerkin method. One should note here that the numerical implementation requires a special care. First, the fictitious interface Σ is unbounded. Secondly, the computation of the finite element matrices involves oscillating integrals.

Our method can be generalized to solve more general diffraction problems. For instance, problems involving two gratings (located on each side of Σ) having two different periods or diffraction problems with any incident waves can be treated using the approach developped in this paper. Some questions are nevertheless still open, like the question of the uniqueness of the solution for locally perturbed gratings.

Appendix

A.1. Spectral analysis of a differential operator with quasi-periodic boundary conditions

Let $k^-(y) \in L^\infty(\mathbb{R})$ be a periodic function of period 1. For $\theta \in [0, 2\pi]$, we consider the unbounded operator of $L^2(0,1)$ defined by

$$\begin{cases} D(A_\theta) = \{u \in H^2(0,1);\ u(1) = \mathrm{e}^{-\mathrm{i}\theta}u(0),\ u'(1) = \mathrm{e}^{-\mathrm{i}\theta}u'(0)\}, \\ A_\theta u = -u'' - \big(k^-(y)\big)^2 u. \end{cases} \tag{A.1}$$

The main properties of the operator A_θ are given by the two next propositions.

Proposition A.1. For every $\theta \in [0, 2\pi]$, A_θ is a self-adjoint operator with compact resolvant. Consequently, its spectrum is constituted of a sequence of eigenvalues $(\lambda_p(\theta))_{p\geqslant 1}$ such that $\lim_{p\to+\infty} \lambda_p(\theta) = +\infty$. Furthermore, there exists an orthonormal basis $(\psi_p^\theta)_{p\geqslant 1}$ of $L^2(0,1)$ constituted of eigenvectors of A_θ.

Proof. Indeed, A_θ is a symmetric operator, since for $u, v \in D(A_\theta)$, we have

$$(A_\theta u, v)_{L^2(0,1)} = (u, A_\theta v)_{L^2(0,1)} = \int_0^1 \Big(u'(y)\overline{v'(y)} - \big(k^-(y)\big)^2 u(y)\overline{v(y)}\Big)\,\mathrm{d}y.$$

The self-adjointness follows from the fact that $(A_\theta + \kappa I)$ is a coercive operator for $\kappa > \|k^-\|_\infty^2$, while the compactness of the resolvant is classically deduced from the embedding of $H^1(0,1)$ in $L^2(0,1)$. □

The next proposition recalls some classical results (see [15]) about the dependence of the eigenvalues $\lambda_p(\theta)$ with respect to θ.

Proposition A.2. We have

$$\lambda_p(\theta) = \lambda_p(2\pi - \theta), \quad \forall\theta \in [0, 2\pi].$$

For $\theta \in (0, \pi)$, the eigenvalues $\lambda_p(\theta)$ are simple, the function $\theta \mapsto \lambda_p(\theta)$ is analytic on $(0, \pi)$ and continuous at $\theta = 0$ and $\theta = \pi$. On the interval $[0, \pi]$, $\theta \mapsto \lambda_{2p+1}(\theta)$ is strictly increasing and $\theta \mapsto \lambda_{2p}(\theta)$ is strictly decreasing. Furthermore, we have

$$\begin{aligned} &\lambda_1(0) < \lambda_1(\pi) \leqslant \lambda_2(\pi) < \lambda_2(0) \leqslant \cdots \leqslant \lambda_{2p-1}(0) \\ &\quad < \lambda_{2p-1}(\pi) \leqslant \lambda_{2p}(\pi) < \lambda_{2p}(0) \leqslant \cdots . \end{aligned}$$

Let us conclude this section by studying the particular case where k^- is a piecewise constant function taking two values. Assume that

$$k^-(y) = \begin{cases} k_1^-, & 0 < y < \delta, \\ k_2^-, & \delta < y < 1. \end{cases}$$

For this particular potential, one can easily derive the dispersion relation for the eigenvalues $\lambda_p(\theta)$ and the explicit formulas for the eigenvectors $\psi_p^\theta(y)$. To achieve this, we notice that solving the eigenvalue problem $A_\theta\psi = \lambda\psi$ is equivalent to solve the following set of equations (with $\psi_1 = \psi_{|[0,\delta]}$ and $\psi_2 = \psi_{|[\delta,1]}$)

$$\begin{cases} \psi_1'' + \left((k_1^-)^2 + \lambda \right) \psi_1 = 0 & \text{for } 0 < y < \delta, \\ \psi_2'' + \left((k_2^-)^2 + \lambda \right) \psi_2 = 0 & \text{for } \delta < y < 1, \end{cases}$$

in addition to the transmission conditions and quasi-periodicity conditions

$$\begin{array}{ll} \psi_1(\delta) = \psi_2(\delta), & \psi_1'(\delta) = \psi_2'(\delta), \\ \psi_2(1) = \mathrm{e}^{-\mathrm{i}\theta} \psi_1(0), & \psi_2'(1) = \mathrm{e}^{-\mathrm{i}\theta} \psi_1'(0). \end{array}$$

Setting $\mu_i = \sqrt{(k_i^-)^2 + \lambda}$ for $i = 1, 2$ (where the square root satisfies $\mathrm{Re}\sqrt{z} \geqslant 0$), we have

$$\psi_i(y) = A_i \cos\bigl(\mu_i(y - \delta)\bigr) + B \sin\bigl(\mu_i(y - \delta)\bigr).$$

The transmission conditions for $y = \delta$ imply that $A_1 = A_2$ and $B_1 = B_2$. Set now

$$\begin{array}{ll} c_1 = \cos(\mu_1 \delta), & s_1 = \sin(\mu_1 \delta), \\ c_2 = \cos\bigl(\mu_2(1 - \delta)\bigr), & s_2 = \sin\bigl(\mu_2(1 - \delta)\bigr). \end{array}$$

The quasi-periodicity conditions read then

$$\begin{pmatrix} c_2 - \mathrm{e}^{-\mathrm{i}\theta} c_1 & s_2 + \mathrm{e}^{-\mathrm{i}\theta} s_1 \\ s_2 + \dfrac{\mu_1}{\mu_2} \mathrm{e}^{-\mathrm{i}\theta} s_1 & -c_2 + \dfrac{\mu_1}{\mu_2} \mathrm{e}^{-\mathrm{i}\theta} c_1 \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = 0.$$

Consequently, the eigenvalues are solutions of the following dispersion relation (expressing the fact that the matrix of this system has to be singular)

$$\mathrm{e}^{2\mathrm{i}\theta} - \left(1 + \frac{\mu_1}{\mu_2}\right)(c_2 c_1 - s_2 s_1) \mathrm{e}^{\mathrm{i}\theta} + \frac{\mu_1}{\mu_2} = 0.$$

A.2. Some results from interpolation theory

For $\kappa > \|k^-\|_\infty^2$, the operator $(A_\theta + \kappa)$, where A_θ is defined by (A.1), is a self-adjoint positive operator with compact resolvant. In addition, $(A_\theta + \kappa)$ is coercive on $H^1(0, 1)$ and its eigenvalues are $\lambda_p(\theta) + \kappa$, $p \geqslant 1$. Consequently, the operators $(A_\theta + \kappa)^s$ of $L^2(0, 1)$ can be easily defined for any $s \in [0, 1]$ by setting

$$\begin{cases} D\bigl((A_\theta + \kappa)^s\bigr) \\ \quad = \left\{ v = \sum_{p \geqslant 1} \bigl(v, \psi_p^\theta\bigr)_{L^2(0,1)} \psi_p^\theta, \ \sum_{p \geqslant 1} \bigl(\lambda_p(\theta) + \kappa\bigr)^{2s} \left| \bigl(v, \psi_p^\theta\bigr)_{L^2(0,1)} \right|^2 < +\infty \right\}, \\ (A_\theta + \kappa)^s v = \sum_{p \geqslant 1} \bigl(\lambda_p(\theta) + \kappa\bigr)^s \bigl(v, \psi_p^\theta\bigr)_{L^2(0,1)} \psi_p^\theta. \end{cases}$$

The interpolation theory (see [10]) shows that for $s \in [0, 1]$, we have

$$D\big((A_\theta + \kappa)^{s/2}\big) = \big[H^1(0, 1), L^2(0, 1)\big]_{1-s} = H^s(0, 1).$$

In particular, the following characterization of the Sobolev space $H^{1/2}(0, 1)$ holds:

Proposition A.3. Let κ be a positive constant satisfying $\kappa > \|k^-\|^2_\infty$. Then, we have

$$H^{1/2}(0, 1) = D\big((A_\theta + \kappa)^{1/4}\big)$$

or equivalently:

$$H^{1/2}(0, 1) = \left\{ v = \sum_{p\geqslant 1} \big(v, \psi_p^\theta\big)_{L^2(0,1)} \psi_p^\theta, \sum_{p\geqslant 1} \sqrt{\lambda_p(\theta) + \kappa} \left| \big(v, \psi_p^\theta\big)_{L^2(0,1)} \right|^2 < +\infty \right\}.$$

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