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An inverse problem in periodic diffractive optics: Reconstruction of Lipschitz grating profiles

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Abstract

We consider the problem of recovering a two-dimensional periodic structure from scattered waves measured above the structure. Following an approach by Kirsch and Kress, this inverse problem is reformulated as a nonlinear optimization problem. We develop a theoretical basis for the reconstruction method in the case of an arbitrary Lipschitz grating profile. The convergence analysis is based on new perturbation and stability results for the forward problem.

1 Introduction

The problem of recovering a periodic structure from illuminating the structure by incident plane waves is of great practical importance in modern diffractive optics, e.g., in quality control and design of diffractive elements with prescribed far field patterns (see [3], [20]). The efficient numerical solution of inverse problems of this type is challenging due to the fact that they are both nonlinear and severely ill–posed in general. We refer to [9], [10] for an overview on inverse scattering problems in general (nonperiodic) structures. An introduction to electromagnetic scattering by periodic structures (diffraction gratings) can be found in [19].

In this paper we restrict ourselves to the two–dimensional Dirichlet problem for perfectly conducting gratings. Uniqueness results and local stability estimates were obtained in [2], [4], [13], [16], and a first result on global stability was proved in [5]. Ito and Reitich [14] proposed a conjugate gradient algorithm based on analytic continuation for the numerical solution of this problem, which appears to be efficient for sufficiently smooth profile curves. An alternative algorithm for the inverse Dirichlet problem was presented in [6], following an approach first developed by Kirsch and Kress [17] (see also [10], Chap. 5) for acoustic obstacle scattering.

In that method, the inverse problem is decomposed into the ill-posed linear problem of reconstructing the scattered wave from measurements above the grating structure and into the well-posed nonlinear problem of determining the unknown profile as the location of the zeros of the total field. The resulting optimization problem then leads to a nonlinear least squares problem which may be solved by using the Levenberg-Marquardt algorithm. The numerical performance of the optimization method, whose implementation turns out to be rather easy, is discussed in [6]. The goal of the present paper is to clarify its mathematical foundation in the practically important case of nonsmooth grating profiles. As in the case of acoustic obstacle scattering (cf. [22], [23] for smooth boundaries), it is surely possible to extend the results to the TE and TM transmission problems for diffraction gratings.

The paper is organized as follows. In Section 2 we will give mathematical formulations of the direct and inverse diffraction problems. Section 3 is devoted to the variational method for the direct problem with a Lipschitz grating profile and presents new perturbation and stability results which are needed in the convergence analysis of the reconstruction method. Theorem 3.1 extends, in particular, a result of Kirsch [15] on the continuous dependence of the variational solution on the boundary to perturbations of the profile in the C norm. Another main tool is a uniform L^2 estimate for the Neumann data of radiating solutions to the Helmholtz equation (Theorem 3.3). For the proof, which is postponed to the final section, we adapt Nečas' approach [18] of approximating the profile by smooth curves and applying a Rellich identity to our periodic boundary value problem. As a by–product we obtain uniqueness for the forward problem with an arbitrary Lipschitz profile. This result seems to be known; see [7, Chap. 5.2] where an integration by parts argument was used but not justified for nonsmooth boundaries.

In Sections 4 and 5, we introduce and analyze the profile reconstruction method. Most effort here will be spent on proving a convergence result in the general case of Lipschitz grating profiles.

2 Direct and inverse diffraction problems

Let the profile of the diffraction grating be described by the curve

$$\Lambda = \Lambda_f := \big\{(x_1, x_2) \in \mathbb{R}^2 : x_2 = f(x_1)\big\}$$

with $f \in C_p^{0,1}$, i.e., f is a periodic Lipschitz function of period 2π. The space below Λ is filled with some perfectly reflecting material. Let

$$\Omega_f := \{x \in \mathbb{R}^2 : x_2 > f(x_1)\,,\ x_1 \in \mathbb{R}\}$$

be filled with a material whose index of refraction (or wave number) k is a positive constant. Suppose further that a plane wave given by

$$v^{in}(x) = \exp(i\alpha x_1 - i\beta x_2)$$

is incident on Λ from the top, where $\alpha = k\sin\theta$, $\beta = k\cos\theta$, and $\theta \in (-\pi/2, \pi/2)$ is the incident angle. Then the scattered field in the TE (transverse electric) mode satisfies the Helmholtz equation with a Dirichlet boundary condition

$$(\Delta + k^2)v = 0 \quad \text{in} \quad \Omega_f\,, \quad v = -v^{in} \quad \text{on} \quad \Lambda_f\,. \tag{2.1}$$

Moreover, v is assumed to be α-quasiperiodic

$$v(x_1 + 2\pi, x_2) = \exp(2i\alpha\pi)v(x_1, x_2)\,, \tag{2.2}$$

and we require that v satisfies a radiation condition, i.e., the diffracted field can be expanded as an infinite sum of plane waves

$$v(x) = \sum_{n\in\mathbb{Z}} A_n \exp\{i(n+\alpha)x_1 + i\beta_n x_2\}\,, \quad x_2 > \|f\|_{C_p^0} := \max_{0\le t\le 2\pi} |f(t)|\,, \tag{2.3}$$

with the Rayleigh coefficients $A_n \in \mathbb{C}$. Here $\beta_n = \beta_n(\alpha, k)$ is defined by

$$\beta_n := \begin{cases} \left(k^2 - (n+\alpha)^2\right)^{1/2} & \text{if } \ |n+\alpha| \le k\,, \\ i\left((n+\alpha)^2 - k^2\right)^{1/2} & \text{if } \ |n+\alpha| > k\,. \end{cases} \tag{2.4}$$

Since β_n is real for at most a finite number of indices, we see that only a finite number of plane waves in the sum (2.3) propagate into the far field, with the remaining evanescent waves decaying exponentially as $x_2 \to \infty$.

The Dirichlet problem (2.1)–(2.3) admits a variational formulation in a bounded periodic cell in $\mathbb{R}^2$, enforcing the radiation condition (cf. [2], [15]). Introduce an artificial boundary

$$\Gamma := \{(x_1, b) : 0 \le x_1 \le 2\pi\}\,, \quad b > \|f\|_{C_p^0}\,,$$

and the bounded domain

$$\Omega = \Omega_{f,b} := \{x \in \mathbb{R}^2 : f(x_1) < x_2 < b\,,\ 0 < x_1 < 2\pi\}\,.$$

The function $u := \exp(-i\alpha x_1)(v + v^{in})$, which is 2π-periodic in x_1, satisfies the boundary value problem

$$\Delta_\alpha u + k^2 u = 0 \quad \text{in} \quad \Omega\,, \quad u|_\Lambda = 0\,, \tag{2.5}$$

where we use the notation

$$\nabla_\alpha := \nabla + i(\alpha, 0)\,, \quad \Delta_\alpha := \nabla_\alpha \cdot \nabla_\alpha = \Delta + 2i\alpha\partial_1 - \alpha^2\,.$$

The radiation condition is equivalent to the nonlocal boundary condition

$$\partial_\nu u|_\Gamma + Tu = -2i\beta \exp(-i\beta b) =: g_0\,, \tag{2.6}$$

where ν denotes the exterior normal and T is the periodic pseudodifferential operator (of order 1)

$$Tu = T(\alpha, k)u := -\sum_{n\in\mathbb{Z}} i\beta_n \hat{u}_n e^{inx_1}\,, \quad \hat{u}_n := \frac{1}{2\pi}\int_0^{2\pi} u(x_1, b)e^{-inx_1}\mathrm{d}x_1\,. \tag{2.7}$$

The operator T is continuous from $H_p^s(\Gamma)$ to $H_p^{s-1}(\Gamma)$ for any $s \in \mathbb{R}$, where $H_p^s(\Gamma)$ stands for the 2π-periodic Sobolev space of order s. For $s \ge 0$ let $H_p^s(\Omega)$ denote the Sobolev space of functions on Ω which are 2π-periodic in x_1. Integrating by parts then leads to the variational formulation of the direct diffraction problem (2.5)–(2.6): Determine $u \in V$ such that

$$\begin{aligned} B(u,\varphi) = B(u,\varphi;\Omega) &:= \int_\Omega (\nabla_\alpha u \cdot \overline{\nabla_\alpha \varphi} - k^2 u\bar{\varphi}) + \int_\Gamma (Tu)\bar{\varphi} \\ &= \int_\Gamma g_0\bar{\varphi}\,, \quad \forall \varphi \in V\,. \end{aligned} \tag{2.8}$$

Here V denotes the energy space

$$V = V(\Omega) := \left\{ u \in H_p^1(\Omega) : u|_\Lambda = 0 \right\} .$$

The *inverse problem* or the *profile reconstruction problem* can be stated as follows: Suppose that $u \in V$ solves the diffraction problem (2.8). Determine the profile function f by the knowledge of the trace $u|_\Gamma$ of u.

Note that this problem also involves near field measurements since the evanescent waves cannot be measured far away from the grating profile.

3 Stability and perturbation results for the direct problem

For the reader's convenience, we first recall some properties of the sesquilinear form B defined in (2.8); see [12] in the case of the TE and TM transmission problems. In the following the energy space $V(\Omega)$ is equipped with the norm

$$\|u\|_V = \left(\int_\Omega |\nabla_\alpha u|^2 \right)^{1/2} ,$$

which is equivalent to the norm in $H^1(\Omega)$ because of $u|_\Lambda = 0$ and Friedrichs' inequality; see [18, Thm. 1.1.9].

1) Since $T : H_p^{1/2}(\Gamma) \to H_p^{-1/2}(\Gamma)$ is continuous, the form B generates a continuous linear operator

$$\mathcal{B} : V(\Omega) \to V(\Omega)' .$$

Here V' denotes the dual space of V with respect to the duality $(\cdot,\cdot)_\Omega$ extending the $L^2(\Omega)$ scalar product.

2) Setting $\mathcal{U} := \{n \in \mathbb{Z} : |n+\alpha| < k\}$, we have

$$\begin{aligned} B(u,u) = & \int_\Omega (|\nabla_\alpha u|^2 - k^2|u|^2) + \sum_{n\in\mathcal{U}} (-2i\pi)(k^2 - (n+\alpha)^2)^{1/2} |\hat{u}_n|^2 \\ & + \sum_{n\in\mathbb{Z}\setminus\mathcal{U}} 2\pi((n+\alpha)^2 - k^2)^{1/2}|\hat{u}_n|^2 , \quad u \in V . \end{aligned} \tag{3.1}$$

Defining

$$A(u,\varphi) := \int_\Omega \nabla_\alpha u \cdot \overline{\nabla_\alpha \varphi} + \int_\Gamma (Tu)\bar{\varphi} , \quad K(u,\varphi) := -k^2 \int_\Omega u\bar{\varphi} , \tag{3.2}$$

we then obtain $B = A + K$ and from (3.1)

$$\mathrm{Re}\left\{e^{i\pi/4} A(u,u)\right\} \geq c \int_\Omega |\nabla_\alpha u|^2 = c\,\|u\|_V^2 , \quad u \in V , \tag{3.3}$$

where c does not depend on u and k. Note that the form K is compact over V.

3) The operator $\mathcal{B} : V \to V'$ takes the form $\mathcal{B} = \mathcal{A} + \mathcal{K}$ with a compact operator $\mathcal{K}$ of norm $\leq ck^2$ and a coercive operator $\mathcal{A}$ satisfying

$$\mathrm{Re}\,\{e^{i\pi/4}(\mathcal{A}u, u)_\Omega\} \geq c\|u\|_V^2\,, \;\; u \in V\,, \tag{3.4}$$

where c is independent of k and u.

Hence the operator $\mathcal{B}$ is always invertible if k is sufficiently small. For arbitrary $k > 0$, it is invertible provided the homogeneous problem (2.8) (i.e., $g_0 := 0$) has only the trivial solution. The latter is always true for C^2 profiles; see [15]. We will generalize this result to arbitrary Lipschitz profiles using an approach of Nečas [18, Chap. 5]. For this and later purposes, we need the following results on the uniform boundedness of the norm of the inverse operator $\mathcal{B}^{-1}$ and on the continuous dependence of the solution to (2.8) on the grating profile.

THEOREM 3.1. *Assume for $f \in C_p^{0,1}$ that the solution u of* (2.8) *is unique, and that $f_n, n \in \mathbb{N}$, is a sequence of Lipschitz profile functions such that $\|f_n - f\|_{C_p^0} \to 0$ as $n \to \infty$. Then:*

(i) The operators $\mathcal{B}_n : V(\Omega_n) \to V(\Omega_n)'$ generated by the sesquilinear forms $B(\cdot,\cdot;\Omega_n)$, $\Omega_n = \Omega_{f_n,b}$, are invertible for any sufficiently large n and satisfy the stability estimate

$$\|\mathcal{B}_n^{-1}\|_{V(\Omega_n)' \to V(\Omega_n)} \leq c\,, \quad \forall n \geq n_0\,. \tag{3.5}$$

(ii) For an arbitrary domain G with $\bar{G} \subset \bar{\Omega}\backslash\Lambda$, the (unique) solutions u_n of the perturbed forward problems converge to u in the norm of $H^1(G)$.

Remark 3.2. If $\Omega_n \subset \Omega$ for all n, then we have $u_n \to u$ in $V(\Omega)$ which is a consequence of the weak convergence $u_n \rightharpoonup u$ in $V(\Omega)$ (cf. the proof of Theorem 3.1 in Section 6) and the decomposition of B into a coercive form and a compact one. If additionally k is small, then this is a special case of [18, Thm. 3.6.7] and follows directly from the coerciveness of the form B.

The next theorem shows that the first assumption of Theorem 3.1 can be omitted, and it is also crucial for proving convergence of our reconstruction method.

THEOREM 3.3. *For any $h \in L^2(\Omega)$ the boundary value problem*

$$(\Delta_\alpha + k^2)u = h \quad in \quad \Omega\,, \quad u|_\Lambda = 0\,, \quad \partial_\nu u|_\Gamma + Tu = 0 \tag{3.6}$$

has a unique solution $u \in V(\Omega)$ satisfying the estimate

$$\|\partial_\nu u\|_{L^2(\Lambda)} \leq c\|h\|_{L^2(\Omega)}\,, \tag{3.7}$$

where c only depends on $\|f\|_{C_p^{0,1}}$ and $\|\mathcal{B}^{-1}\|_{V' \to V}$.

Note that a solution $u \in V(\Omega)$ of (3.6) satisfies $\partial_\nu u|_\Lambda \in H_p^{-1/2}(\Lambda)$, where the trace is defined by the relation

$$\int_\Lambda (\partial_\nu u)\bar{\varphi} = B(u,\varphi;\Omega) + \int_\Omega h\bar{\varphi}\,, \quad \forall \varphi \in H_p^1(\Omega)\,; \tag{3.8}$$

see [11]. Thus Theorem 3.3 says that the trace even exists in the L^2 sense.

In particular, we have

Corollary 3.4. *For $f \in C_p^{0,1}$, the direct diffraction problem* (2.5) *and* (2.6) *possesses a unique solution $u \in V(\Omega)$.*

The proof of Theorems 3.1 and 3.3 will be given in Section 6.

4 An optimization method for the inverse problem

We now study an optimization method for determining the profile function f from the output of the total field

$$u_b := u|_\Gamma = u^{in}|_\Gamma + \sum_{n\in\mathbb{Z}} A_n \exp(inx_1 + i\beta_n b)\,, \tag{4.1}$$

where $u^{in} = \exp(-i\beta x_2)$ and all Rayleigh coefficients A_n are assumed to be known. Suppose that we have the a priori information about our inverse diffraction problem that, without loss of generality, the unknown profile Λ_f lies below Γ and above the line $\Gamma_0 := \{(x_1, 0) : 0 \le x_1 \le 2\pi\}$. We try to represent the scattered field $u^{sc} = u - u^{in}$ in the form

$$u^{sc}(x) = S\varphi(x) := \sum_{n\in\mathbb{Z}} c_n \exp(inx_1 + i\beta_n x_2)\,, \tag{4.2}$$

where

$$\varphi(x) = \sum_{n\in\mathbb{Z}} c_n \exp(inx_1) \in L^2(\Gamma_0)$$

is an unknown density function. Introduce the linear operators

$$S_b\varphi(x) := S\varphi(x_1, b)\,,\ x \in \Gamma\,; \quad S_f\varphi(x) := S\varphi(x_1, f(x_1))\,,\ x \in \Lambda_f\,, \tag{4.3}$$

where $f \in C_p^{0,1}$ is fixed. Note that $S_b\varphi$ approximates the output of the scattered field on Γ, whereas $S_f\varphi$ (which is nonlinear with respect to f) represents an approximation of u^{sc} on the profile Λ_f. Obviously, the operator $S_b : L^2(\Gamma_0) \to L^2(\Gamma)$ is compact with exponentially decreasing singular values. Hence the determination of the density φ from the first kind equation

$$S_b\varphi = u_b - u^{in}|_\Gamma \tag{4.4}$$

is a severely ill-posed problem. To reformulate the inverse diffraction problem as an optimization method, we then combine Tikhonov's regularization for equation (4.4) with the minimization of the defect

$$\|u^{in} + S_f\varphi\|_{L^2(\Lambda_f)}\,, \quad f \in \mathcal{M}$$

of the Dirichlet boundary condition over a class $\mathcal{M}$ of admissible curves Λ_f.

Definition 4.1. Let f and f_n ($n \in \mathbb{N}$) be Lipschitz profile functions. We shall write $f_n \to f$ if

$$\|f_n - f\|_{C_p^0} \to 0 \quad \text{as} \quad n \to \infty \quad \text{and} \quad \sup_{n\in\mathbb{N}} \|f_n\|_{C_p^{0,1}} < \infty\,. \tag{4.5}$$

In the sequel we choose $\mathcal{M}$ to be a compact set of $C_p^{0,1}$ with respect to the convergence introduced above and such that

$$0 < \inf\left\{\|f\|_{C_p^0} : f \in \mathcal{M}\right\}, \quad \sup\left\{\|f\|_{C_p^0} : f \in \mathcal{M}\right\} < b\,.$$

Examples of compact sets are, e.g., given by the following:

1) $\{f \in C_p^{1,\lambda} : \|f\|_{C_p^{1,\lambda}} \le c\}$ for some $\lambda > 0$, with the norm in $C_p^{1,\lambda}$ defined by

$$\|f\|_{C_p^{1,\lambda}} := \|f\|_{C_p^0} + \|f'\|_{C_p^0} + \sup_{0\le t<\tau\le 2\pi}\{(\tau - t)^{-\lambda}|f'(\tau) - f'(t)|\},$$

2) $\{f = c_1 f_1 + \cdots + c_N f_N : \sum |c_i| \le c\}$ where N is fixed and $f_1, ..., f_N$ are fixed Lipschitz functions,

3) set of continuous piecewise linear functions where the number of corner points is bounded together with the slope of the segments.

We define the cost functional F by

$$F(\varphi, f; \gamma) := \|u^{in} + S_b\varphi - u_b\|^2_{L^2(\Gamma)} + \gamma\|\varphi\|^2_{L^2(\Gamma_0)} + \rho\|u^{in} + S_f\varphi\|^2_{L^2(\Lambda_f)}\,. \tag{4.6}$$

Here $\gamma > 0$ denotes the regularization parameter, and $\rho > 0$ is a coupling parameter which has to be chosen appropriately for the numerical implementation. For theoretical purposes we may assume $\rho = 1$ in the following.

Our reconstruction method, which was first introduced by Kirsch and Kress [17] (see also [10, Chap. 5.4]) in the case of scattering by bounded obstacles with C^2 boundaries, now consists in solving the following optimization problem.
(**OP**): Find $\varphi \in L^2(\Gamma_0)$ and $f \in \mathcal{M}$ such that

$$F(\varphi, f; \gamma) = m(\gamma) := \inf\{F(\psi, g; \gamma) : \psi \in L^2(\Gamma_0)\,,\ g \in \mathcal{M}\}\,.$$

We shall prove the following theorems which are the analogues of Theorems 5.20–5.22 in [10].

THEOREM 4.2. *For each $\gamma > 0$ the problem* (OP) *has a solution.*

THEOREM 4.3. *Let u_b be the exact pattern of the total field on Γ which corresponds to some profile function $f \in \mathcal{M}$. Then we have:*

(i) $\lim_{\gamma\to 0} m(\gamma) = 0$.

(ii) Let (γ_n) be a null sequence and let (φ_n, f_n) be a corresponding sequence of solutions to (OP) *with regularization parameter γ_n. Then there exists a convergent subsequence of (f_n), and every limit point f^* of (f_n) represents a profile function such that the total field u vanishes on Λ_{f^*}.*

If we have the a priori information that our inverse problem has at most one solution (e.g., for sufficiently small wave number or height of the grating; see [5],

[13]), then from Theorem 4.3 (ii) we obtain convergence of the total sequence (f_n) to f. In the general case we can try to achieve uniqueness of the inverse problem and more accurate reconstructions by using more incident waves u_j^{in} $(j = 1, ..., N)$ with different wavelengths and/or incident angles. In fact, it was proved in [13] that the grating profile is uniquely determined by a finite number of wave numbers if some a priori information on the amplitude of the periodic structure is available. For the optimization method (OP) we then have to replace the cost functional (4.6) by a corresponding sum over j, and the results of the preceding theorems carry over to this case.

The proof of Theorems 4.2 and 4.3 will be given in the next section.

5 Proof of Theorems 4.2 and 4.3

To establish Theorem 4.2, which guarantees the existence of a minimizer of the cost functional (4.6), one can proceed similarly as in [10, Thm. 5.20]. We present the arguments for the convenience of the reader.

Proof of Theorem 4.2: Let (φ_n, f_n) be a minimizing sequence in $L^2(\Gamma_0) \times \mathcal{M}$, i.e.,

$$F(\varphi_n, f_n; \gamma_n) \to m(\gamma) \quad \text{as} \quad n \to \infty\,.$$

We can assume that $f_n \to f \in \mathcal{M}$ in the sense of Definition 4.1 since $\mathcal{M}$ is compact. From $\gamma > 0$ and

$$\gamma \|\varphi_n\|^2_{L^2(\Gamma_0)} \le F(\varphi_n, f_n; \gamma) \to m(\gamma)$$

we conclude that the sequence (φ_n) is bounded, hence some subsequence converges weakly, $\varphi_n \rightharpoonup \varphi$ in $L^2(\Gamma_0)$ as $n \to \infty$. Since the operators (cf. (4.2), (4.3))

$$S_b : L^2(\Gamma_0) \to L^2(\Gamma)\,, \quad S_f : L^2(\Gamma_0) \to L^2(\Lambda_f)$$

are compact, we obtain

$$S_b\varphi_n \to S_b\varphi \quad \text{in} \quad L^2(\Gamma)\,, \quad S_f\varphi_n \to S_f\varphi \quad \text{in} \quad L^2(\Lambda_f)\,, \quad n \to \infty\,.$$

We then deduce that

$$\|u^{in} + S_{f_n}\varphi_n\|^2_{L^2(\Lambda_n)} \to \|u^{in} + S_f\varphi\|^2_{L^2(\Lambda_f)}\,. \tag{5.1}$$

Here we used the fact that the last term in the estimate

$$\begin{aligned} &|S\varphi_n(x_1, f(x_1)) - S\varphi_n(x_1, f_n(x_1))|^2 \\ &\le \|\varphi_n\|^2_{L^2(\Gamma_0)} \sum_{j\in\mathbb{Z}} |\exp(i\beta_j f(x_1)) - \exp(i\beta_j f_n(x_1))|^2\,, \quad 0 \le x_1 \le 2\pi \end{aligned}$$

can be made as small as desired, uniformly in x_1, if n is chosen sufficiently large. To see this, estimate the sum over $|j| \ge J$ with J large enough and apply the mean value theorem and the relations (4.5) to the terms with $|j| \le J$.

The relation (5.1) now implies

$$\gamma\|\varphi_n\|^2_{L^2(\Gamma_0)} \to m(\gamma) - \|u^{in} + S_b\varphi - u_b\|^2_{L^2(\Gamma)} - \|u^{in} + S_f\varphi\|^2_{L^2(\Lambda_f)}$$
$$\leq \gamma\|\varphi\|^2_{L^2(\Gamma_0)}\,, \quad n \to \infty\,,$$

hence $\limsup_{n\to\infty}\|\varphi_n\| \leq \|\varphi\|$. On the other hand, from the weak convergence we have $\|\varphi\| \leq \liminf_{n\to\infty}\|\varphi_n\|$. Thus we have $\varphi_n \rightharpoonup \varphi$ in $L^2(\Gamma_0)$ and $\lim_{n\to\infty}\|\varphi_n\| = \|\varphi\|$, so that $\varphi_n \to \varphi$ in $L^2(\Gamma_0)$. Finally, by continuity

$$F(\varphi, f; \gamma) = \lim_{n\to\infty} F(\varphi_n, f_n; \gamma) = m(\gamma)\,. \quad \blacksquare$$

To prove our second theorem, we need the following lemmas. The first lemma shows that the range of the operator S_f is dense in $L^2(\Lambda_f)$ which justifies the ansatz (4.2) and the choice of the cost functional (4.6).

LEMMA 5.1. *Let $f \in \mathcal{M}$, and introduce the set*

$$W := span\{\exp(inx_1 + i\beta_n x_2) : n \in \mathbb{Z}\}\,. \tag{5.2}$$

Then $W|_\Lambda$ is dense in $L^2(\Lambda)$ for any profile $\Lambda = \Lambda_f$.

Proof: For C^2 profiles, we refer to [16] in the case when the Rayleigh frequencies are excluded, i.e.,

$$\beta_n = \beta_n(\alpha, k) \neq 0 \quad \text{for all} \quad n \in \mathbb{Z}\,, \tag{5.3}$$

and to [1] in the general case. The arguments can be extended to Lipschitz profiles as follows.

If the condition (5.3) holds, then the free space 2π-periodic Green function of the operator $\Delta_\alpha + k^2$ takes the form (cf. [8], [21])

$$G(x,y) = \frac{i}{4\pi}\sum_{n\in\mathbb{Z}} \frac{1}{\beta_n}\exp\{in(x_1 - y_1) + i\beta_n|x_2 - y_2|\}\,, \quad x \neq y\,, \tag{5.4}$$

with $\beta_n = \beta_n(\alpha, k)$. It is sufficient to verify the lemma in the case that $\beta_n := \beta_n(-\alpha, k) = \beta_{-n}(\alpha, k)$ in (5.2). Suppose that $\psi \in L^2(\Lambda)$ satisfies

$$\int_\Lambda \psi(y)\exp\{iny_1 + i\beta_{-n}(\alpha, k)y_2\}\,\mathrm{d}s(y) = 0\,, \quad n \in \mathbb{Z}\,, \tag{5.5}$$

and consider the single layer potential

$$u(x) := \int_\Lambda G(x,y)\psi(y)\,\mathrm{d}s(y)\,, \quad x \in R\backslash\Lambda\,,$$

where R denotes the rectangle $(0, 2\pi)\times(0, b)$. The curve Λ divides R into the domain Ω and a lower subdomain Ω_1. Adapting Costabel's approach [11] to our periodic boundary value problem, we obtain that $u \in H^1_p(R)$ and that the jump of the normal derivative across Λ satisfies $[\partial_\nu u]_\Lambda = -\psi$ in the $H_p^{-1/2}(\Lambda)$ sense. Now (5.4) and (5.5) imply $u = 0$ in Ω_1 so that $u \in V(\Omega)$ solves the homogeneous diffraction problem in Ω. Therefore $u = 0$ in R. Here we used the uniqueness result of Section 3. By the jump relation we then have $\psi = 0$ which finishes the proof.

If some β_n vanishes, the nth term in (5.4) must be replaced by (cf. [21])

$$-(4\pi)^{-1}|x_2 - y_2| \exp(in(x_1 - y_1)) ,$$

and one can proceed similarly to deduce $\psi = 0$ from (5.5). ■

Let $\Lambda = \Lambda_f$, $f \in \mathcal{M}$, and consider the boundary value problem

$$(\Delta_\alpha + k^2)w = 0 \quad \text{in} \quad \Omega\,, \quad w|_\Lambda = h\,, \quad \partial_\nu w|_\Gamma + T(\alpha,k)w = 0\,. \tag{5.6}$$

The next lemma implies that the trace on Γ of a solution w to (5.6) depends continuously on the boundary data, uniformly with respect to $f \in \mathcal{M}$.

LEMMA 5.2. *If $w \in H^1_p(\Omega)$ solves the problem* (5.6), *then the estimate*

$$\|w\|_{L^2(\Gamma)} \le c_1 \|w\|_{L^2(\Omega)} \le c\|h\|_{L^2(\Lambda)} \tag{5.7}$$

holds, where the positive constants c and c_1 only depend on $\|f\|_{C^{0,1}_p}$ and the stability constant $\|\mathcal{B}^{-1}\|_{V'\to V}$.

Proof: Consider the problem

$$(\Delta_{-\alpha} + k^2)z = \bar{w} \quad \text{in} \quad \Omega\,, \quad z|_\Lambda = 0\,, \quad \partial_\nu z|_\Gamma + T(-\alpha,k)z = 0\,, \tag{5.8}$$

which has a unique solution $z \in V(\Omega)$ by Theorem 3.3. Using Green's formula we obtain from (5.6) and (5.8) that

$$\begin{aligned}\int_\Omega |w|^2 &= \int_\Omega w\,(\Delta_{-\alpha} + k^2)z = \int_{\partial\Omega} (w\,\partial_{\nu,-\alpha} z - z\,\partial_{\nu,\alpha} w)\\ &= \int_\Lambda w\,\partial_\nu z = \int_\Lambda h\,\partial_\nu z\,,\end{aligned}$$

where $\partial_{\nu,\alpha} := \partial_\nu + i\alpha\nu_1$. Applying estimate (3.7) to problem (5.8) now gives

$$\|w\|^2_{L^2(\Omega)} \le \|h\|_{L^2(\Lambda)}\,\|\partial_\nu z\|_{L^2(\Lambda)} \le c\,\|h\|_{L^2(\Lambda)}\,\|w\|_{L^2(\Omega)}\,,$$

hence the second inequality of (5.7). Using the Rayleigh expansion of w in a rectangle $\tilde{\Omega} = (0,2\pi) \times (b_1, b)$ lying above Λ, it is easy to check the bound

$$\|w\|_{L^2(\Gamma)} \le c\|w\|_{L^2(\tilde{\Omega})}\,,$$

where c only depends on b_1. This finishes the proof of (5.7). ■

Proof of Theorem 4.3: (i) By Lemma 5.1, given $\varepsilon > 0$ there exists $\varphi \in L^2(\Gamma_0)$ such that

$$\|S_f\varphi + u^{in}\|_{L^2(\Lambda)} \le \varepsilon\,, \quad \Lambda = \Lambda_f\,. \tag{5.9}$$

If u denotes the solution of (2.5) and (2.6), then $w := S\varphi + u^{in} - u$ solves the problem (5.6) with $h := S_f\varphi + u^{in}|_\Lambda$. Lemma 5.2 together with (5.9) implies

$$\|S_b\varphi + u^{in} - u_b\|_{L^2(\Gamma)} \le c\|h\|_{L^2(\Lambda)} \le c\varepsilon\,.$$

Thus we obtain

$$F(\varphi, f; \gamma) \le (1+c^2)\varepsilon^2 + \gamma\|\varphi\|^2_{L^2(\Gamma_0)} \to (1+c^2)\varepsilon^2\,, \quad \gamma \to 0\,,$$

which finishes the proof of assertion (i).

(ii) The existence of a convergent subsequence $f_n \to f^*$ (in the sense of Definition 4.1) follows from the compactness of $\mathcal{M}$. Since f_n is optimal for the parameter γ_n, there exists $\varphi_n \in L^2(\Gamma_0)$ such that

$$F(\varphi_n, f_n; \gamma_n) = m(\gamma_n)\,, \quad n \in \mathbb{N}\,.$$

Note that $w_n := S\varphi_n + u^{in}$ solves the problem

$$(\Delta_\alpha + k^2)w_n = 0 \quad \text{in} \quad \Omega_n\,, \quad w_n|_{\Lambda_n} = h_n\,, \quad \partial_\nu w_n|_\Gamma + Tw_n = g_0\,,$$

where $h_n := (S\varphi_n + u^{in})|_{\Lambda_n}$ and the dependence of Ω and Λ on f_n is indicated by n. Furthermore, let $u_n \in V(\Omega_n)$ be the solution of the forward problem (2.5) and (2.6) corresponding to the profile function f_n. Then $v_n := w_n - u_n$ satisfies the boundary value problem

$$(\Delta_\alpha + k^2)v_n = 0 \quad \text{in} \quad \Omega_n\,, \quad v_n|_{\Lambda_n} = h_n\,, \quad \partial_\nu v_n|_\Gamma + Tv_n = 0\,. \tag{5.10}$$

Applying Lemma 5.2 to the problems (5.10), we get upon using Theorem 3.1 (i)

$$\|v_n\|_{L^2(\Gamma)} \le c\|h_n\|_{L^2(\Lambda_n)}\,, \quad n \in \mathbb{N}, \tag{5.11}$$

where c does not depend on n. Let u^* denote the solution of the direct problem (2.5) and (2.6) for the profile function f^*. Since $\|h_n\|_{L^2(\Lambda_n)} \to 0$ by Theorem 4.3 (i), it follows from (5.11) that $\|v_n\|_{L^2(\Gamma)} \to 0$ as $n \to \infty$. Moreover, applying Theorem 3.1 (ii) one obtains

$$\|w_n - u^*\|_{L^2(\Gamma)} \le \|v_n\|_{L^2(\Gamma)} + \|u_n - u^*\|_{L^2(\Gamma)} \to 0\,, \quad n \to \infty\,.$$

By Theorem 4.3 (i) we also have $\|w_n - u_b\|_{L^2(\Gamma)} \to 0$ so that $u_b = u^*|_\Gamma$. Together with $u^*|_{\Lambda_{f^*}} = 0$, this completes the proof of assertion (ii). ∎

6 Proof of Theorems 3.1 and 3.3

Proof of Theorem 3.1: (i) Consider the operators

$$\mathcal{B}_n = \mathcal{A}_n + \mathcal{K}_n : \ V(\Omega_n) \to V(\Omega_n)'$$

generated by the sesquilinear forms (2.8) and (3.2) on Ω_n. We prove the stability estimate (3.5) arguing by contradiction. If (3.5) were not true, there would exist a sequence $v_n \in V(\Omega_n)$ such that

$$\|v_n\|_{V(\Omega_n)} = 1 \quad \text{and} \quad \|\mathcal{B}_n v_n\|_{V(\Omega_n)'} \to 0\,, \quad n \to \infty\,. \tag{6.1}$$

Choose $\Omega_0 \supset \Omega$ such that $\Omega_n \subset \Omega_0$ ($n \geq n_0$), and extend v_n by zero to Ω_0. Then $v_n \rightharpoonup v$ in $V(\Omega_0)$ (for a subsequence). Since $v_n|_{\Lambda_n} = 0$ and $\|f_n - f\|_{C_p^0} \to 0$, we have $v = 0$ in $\Omega_0 \backslash \bar{\Omega}$, hence $v \in V(\Omega)$. Furthermore, for any C_p^∞ function φ with support in $\bar{\Omega}\backslash\Lambda$, we obtain

$$(\mathcal{B}_n v_n, \varphi)_{\Omega_n} \to (\mathcal{B} v, \varphi)_\Omega\,, \quad (\mathcal{B}_n v_n, \varphi)_{\Omega_n} \to 0\,, \quad n \to \infty\,.$$

Consequently, $(\mathcal{B}v, \varphi)_\Omega = 0$ for any $\varphi \in V(\Omega)$, which implies $v = 0$ since $\mathcal{B}$ is assumed to be invertible. Furthermore, we have

$$\|\mathcal{K}_n v_n\|_{V(\Omega_n)'} \leq \sup\left\{k^2 \left| \int_{\Omega_0} v_n \varphi \right| : \|\varphi\|_{V(\Omega_0)} \leq 1 \right\}\,. \tag{6.2}$$

Since $v_n \rightharpoonup 0$ in $V(\Omega_0)$ and the form K (defined on Ω_0) generates a compact operator of $V(\Omega_0)$ into $V(\Omega_0)'$, the inequality (6.2) then gives $\|\mathcal{K}_n v_n\|_{V(\Omega_n)'} \to 0$ which implies upon using (6.1)

$$\|\mathcal{A}_n v_n\|_{V(\Omega_n)'} \geq |(\mathcal{A}_n v_n, v_n)_{\Omega_n}| \to 0\,.$$

This is a contradiction since $\mathcal{A}_n$ is uniformly coercive with respect to n; note that the constant c in (3.3) does not depend on Λ.

(ii) For n sufficiently large, let $u_n \in V(\Omega_n) \subset V(\Omega_0)$ be the solution of the problem (2.8) for Ω_n. From (i) we obtain that $\|u_n\|_{V(\Omega_0)}$ is uniformly bounded and that $u_n \rightharpoonup u$ in $V(\Omega_0)$, where u is the solution of the forward problem for Ω extended by zero to Ω_0. Let $\psi \in C_0^\infty(\bar{\Omega}\backslash\Lambda)$ be 2π–periodic in x_1 and such that $\psi = 1$ on G. Then for all $n \geq n_0$

$$\|\mathcal{B}\psi(u_n - u)\|_{V(\Omega)'} \geq c\|\psi(u_n - u)\|_{V(\Omega)} \geq c\|u_n - u\|_{H^1(G)}\,. \tag{6.3}$$

It remains to show that the left side of (6.3) tends to zero as $n \to \infty$. For any $\varphi \in V(\Omega)$ we have

$$\begin{aligned}(\mathcal{B}\psi(u_n - u), \varphi)_\Omega \;=\; & B(u_n - u, \psi\varphi) \\ & + \int_\Omega \left\{\nabla_\alpha \psi (u_n - u) \cdot \overline{\nabla_\alpha \varphi} - \nabla_\alpha (u_n - u) \cdot \overline{\nabla_\alpha \psi \varphi}\right\}\,,\end{aligned}$$

where the first term on the right side vanishes. The last integral takes the form (note that $\psi = 1$ near Γ)

$$\begin{aligned}&\int_\Omega \left\{(u_n - u)\nabla\psi \cdot \overline{\nabla_\alpha \varphi} - \varphi \nabla_\alpha (u_n - u) \cdot \nabla\psi\right\} \\ &= \int_\Omega \left\{(u_n - u)\nabla\psi \cdot \overline{\nabla_\alpha \varphi} + (u_n - u)\overline{\nabla_\alpha \cdot \varphi \nabla\psi}\right\}\,.\end{aligned}$$

Since $u_n \to u$ in $L^2(\Omega_0)$, we then obtain

$$\begin{aligned}\|\mathcal{B}\psi(u_n - u)\|_{V(\Omega)'} &= \sup\left\{|(\mathcal{B}\psi(u_n-u),\varphi)_\Omega| : \|\varphi\|_{V(\Omega)} \le 1\right\} \\ &\le c\|u_n - u\|_{L^2(\Omega)} \to 0\end{aligned}$$

which completes the proof of assertion (ii). ∎

Proof of Theorem 3.3: Step 1. First we establish the uniform estimate (3.7) when $\Lambda = \Lambda_f$ is an infinitely smooth profile. A variational solution to (3.6) then satisfies $u \in H_p^2(\Omega) \cap V(\Omega)$, and integrating by parts we obtain

$$2 \operatorname{Re} \int_\Omega (\Delta_\alpha u + k^2 u)\, \partial_2 \bar{u} = \int_{\partial\Omega} \left(\partial_{\nu,\alpha} u\, \partial_2 \bar{u} + \partial_{\tau,\alpha} u\, \overline{\partial_{1,\alpha} u} + \nu_2 k^2 |u|^2\right), \tag{6.4}$$

where

$$\partial_{\nu,\alpha} := \nu_1 \partial_{1,\alpha} + \nu_2 \partial_2\,, \quad \partial_{\tau,\alpha} := -\nu_2 \partial_{1,\alpha} + \nu_1 \partial_2\,, \quad \partial_{1,\alpha} := \partial_1 + i\alpha\,.$$

On the segment Γ, the integral on the right hand side of (6.4) takes the form (cf. (2.4), (2.7))

$$\begin{aligned}\int_\Gamma (|Tu|^2 - |\partial_{1,\alpha} u|^2 + k^2|u|^2) &= 2\pi \sum_{n\in\mathbb{Z}} (|\beta_n|^2 + k^2 - (n+\alpha)^2)|\hat{u}_n|^2 \\ &= \sum_{n\in\mathcal{U}} 4\pi (k^2 - (n+\alpha)^2)|\hat{u}_n|^2\,,\end{aligned}$$

with the index set $\mathcal{U}$ defined in (3.1). Since $u|_\Lambda = 0$ and also $\partial_{\tau,\alpha} u|_\Lambda = 0$, we have from (3.6) and (6.4)

$$2 \operatorname{Re} \int_\Omega h\, \partial_2 \bar{u} = \int_\Lambda \nu_2 |\partial_\nu u|^2 + \sum_{n\in\mathcal{U}} 4\pi (k^2 - (n+\alpha)^2)|\hat{u}_n|^2\,. \tag{6.5}$$

This is just the analogue of the Rellich identity for our periodic diffraction problem; see [18, Chap. 5]. As in [15], it follows from (6.5) and the variational formulation that $h = 0$ implies $u = 0$. Hence (3.6) has a unique solution $u \in V(\Omega)$.

Furthermore, for a rectangle $\tilde{\Omega} = (0, 2\pi) \times (b_1, b) \subset \Omega$, we have the bound

$$|\hat{u}_n|^2 \le c\|u\|^2_{H_p^1(\tilde{\Omega})} \le c\|u\|^2_{V(\Omega)}\,, \quad n \in \mathcal{U}\,, \tag{6.6}$$

where c only depends on b_1. Moreover,

$$\|u\|_{V(\Omega)} \le \|\mathcal{B}^{-1}\|\, \|h\|_{V(\Omega)'} \le c\, \|\mathcal{B}^{-1}\|\, \|h\|_{L^2(\Omega)}\,, \tag{6.7}$$

where c depends on $\|f\|_{C_p^0}$. The last inequality of (6.7) follows by duality from the estimate $\|\varphi\|_{L^2(\Omega)} \le c\|\varphi\|_{V(\Omega)}$, which is a consequence of Friedrichs' inequality. Combining (6.5)–(6.7) gives the desired bound (3.7), with c only depending on $\|f\|_{C_p^{0,1}}$ and the stability constant $\|\mathcal{B}^{-1}\|$. Note that the exterior normal ν to Λ satisfies $-\nu_2 \ge C > 0$ on Λ, where C only depends on the Lipschitz constant of f.

Step 2. Now we consider the case when $f \in C_p^{0,1}$ and k is sufficiently small. Then $\mathcal{B} : V(\Omega) \to V(\Omega)'$ is invertible and (3.6) has a unique solution $u \in V(\Omega)$. Proceeding as in the proof of [18, Thm. 5.1.1], we choose C^∞ profiles $\Lambda_j = \Lambda_{f_j}$ such that $\Omega_j \subset \Omega$ for all n and

$$\|f_j - f\|_{C_p^0} \to 0\,, \quad \|f_j\|_{C_p^{0,1}} \leq c\,, \quad j \to \infty\,,$$

where c only depends on $\|f\|_{C_p^{0,1}}$. Let $u_j \in V(\Omega_j) \subset V(\Omega)$ be the solution of the problem (3.6) for Ω_j. Applying Theorem 3.1 (i) and the arguments used in Step 1, we obtain the uniform bound

$$\int_{\Lambda_j} |\partial_\nu u_j|^2 \leq c\|h\|^2_{L^2(\Omega)} \tag{6.8}$$

with c depending on $\|f\|_{C_p^{0,1}}$ and $\|\mathcal{B}^{-1}\|$.

In the following we identify the spaces $L^2(\Lambda_j)$ and $L^2(\Lambda)$ with $L^2(0, 2\pi)$ via the norm

$$\|v \circ f\|_{L^2(0,2\pi)} = \left(\int_0^{2\pi} |v(f(x_1))|^2 \,\mathrm{d}x_1\right)^{1/2}, \quad v \in L^2(\Lambda_f)\,,$$

which is a uniformly equivalent norm when f varies in a set of profile functions with uniformly bounded $C_p^{0,1}$ norm. From (6.8) we then get $\partial_\nu u_j \rightharpoonup v$ in $L^2(0, 2\pi)$ (for some subsequence). It remains to check that v coincides with the $H_p^{-1/2}$ trace of $\partial_\nu u$ on Λ.

By Remark 3.2 $u_j \to u$ in $V(\Omega)$, and Lemma 2.4.5 in [18] implies $\varphi|_{\Lambda_j} \to \varphi|_\Lambda$ in $L^2(0, 2\pi)$ for any $\varphi \in H_p^1(\Omega)$. Hence, passing to the limit in the identity

$$\int_{\Lambda_j} (\partial_\nu u_j)\bar{\varphi} = B(u_j, \varphi; \Omega) + \int_{\Omega_j} h\bar{\varphi}\,,\ \forall \varphi \in H_p^1(\Omega)\,,$$

we obtain (3.8) with v in place of $\partial_\nu u$, which finishes the proof.

Step 3. We finally consider the case of a Lipschitz profile and an arbitrary wave number $k > 0$. We only have to show that a solution $u \in V(\Omega)$ to the homogeneous problem (3.6) (with $h = 0$) must vanish in Ω. The estimate (3.7) for the inhomogeneous problem then follows as in Step 2. Consider the problem

$$\begin{aligned} (\Delta_\alpha + k_0^2)v = f := (k_0^2 - k^2)u \quad \text{in} \quad \Omega\,, \\ v|_\Lambda = 0\,, \quad \partial_\nu v|_\Gamma + T(\alpha, k)v = 0\,, \end{aligned} \tag{6.9}$$

where k_0 is chosen sufficiently small. Exactly as in Section 3 one verifies that the operator $\mathcal{B}_0 : V \to V'$ generated by the sesquilinear form

$$B_0(v, \varphi) := \int_\Omega (\nabla_\alpha v \cdot \overline{\nabla_\alpha \varphi} - k_0^2 v\bar{\varphi}) + \int_\Gamma \bar{\varphi} T(\alpha, k)v$$

is invertible. Hence $v = u$ is the unique solution of (6.9) in $V(\Omega)$. Denote by v_j the solution to problem (6.9) for Ω_j, where Λ is again approximated by a sequence of C^∞ profiles Λ_j. Arguing as in Step 2, one now obtains

$$\partial_\nu v_j|_{\Lambda_j} \rightharpoonup \partial_\nu u|_\Lambda \quad \text{in} \quad L^2(0, 2\pi)\,, \quad \text{as} \quad j \to \infty\,.$$

Rewriting the differential equation for v_j as

$$(\Delta_\alpha + k^2)v_j = h_j := (k_0^2 - k^2)(u - v_j)$$

and applying the Rellich identity (6.5), we have

$$2\,\mathrm{Re}\int_\Omega h_j\,\partial_2\bar{v}_j = \int_{\Lambda_j}\nu_2|\partial_\nu v_j|^2 + \sum_{n\in\mathcal{U}} 4\pi(k^2 - (n+\alpha)^2)|\hat{v}_{j,n}|^2\,, \tag{6.10}$$

where $\hat{v}_{j,n}$ are the Fourier coefficients of $v_j(x_1, b)$.

On the other hand, from the variational formulation we obtain

$$\int_\Omega(|\nabla_\alpha v_j|^2 - k^2|v_j|^2) + \int_\Gamma \bar{v}_j T(\alpha,k)v_j = -\int_\Omega h_j\bar{v}_j\,, \tag{6.11}$$

where the integral on Γ takes the form

$$-i2\pi\sum_{n\in\mathcal{U}}\beta_n|\hat{v}_{j,n}|^2 + 2\pi\sum_{n\in\mathbb{Z}\setminus\mathcal{U}}|\beta_n|^2|\hat{v}_{j,n}|^2\,.$$

Since $v_j \to u$ in $V(\Omega)$ by Theorem 3.1 and Remark 3.2 (applied to problem (6.9) instead of (2.5), (2.6), in which case the proof remains the same), one has $h_j \to 0$ in $L^2(\Omega)$ and it follows from (6.11) by taking imaginary parts that

$$\hat{v}_{j,n} \to 0\,,\quad n\in\mathcal{U}\,,\quad \text{as}\quad j\to\infty\,.$$

Then (6.10) implies

$$\|\partial_\nu u\|_{L^2(\Lambda)} \le \liminf_{j\to\infty}\|\partial_\nu v_j\|_{L^2(\Lambda_j)} = 0\,,$$

hence $u = \partial_\nu u = 0$ on Λ, which gives $u = 0$ in Ω and concludes the proof of the theorem. ∎

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