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The numerical solution of an inverse periodic transmission problem

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Abstract

We consider the inverse problem of recovering a 2D periodic structure from scattered waves measured above and below the structure. We discuss convergence and implementation of an optimization method for solving the inverse TE transmission problem, following an approach first developed by Kirsch and Kress for acoustic obstacle scattering. The convergence analysis includes the case of Lipschitz grating profiles and relies on variational methods and solvability properties of periodic boundary integral equations. Numerical results for exact and noisy data demonstrate the practicability of the inversion algorithm.

1 Introduction

The reconstruction of the shape of periodic structures from measurements of scattered electromagnetic waves is a problem of great practical importance for instance in modern diffractive optics [2], [21]. Direct scattering problems for diffraction gratings and corresponding optimal design problems were extensively studied using variational methods or integral equation methods by several authors; see, e.g., [3], [6], [9], [11], [20].

We assume the grating to be periodic in one direction and constant in the other, and consider the TE mode of polarization for the diffraction by a periodic interface between two materials. This corresponds to a two–dimensional quasi–periodic transmission problem for the Helmholtz equation. In Section 2 we will give the variational formulation of the direct transmission problem and recall an existence and uniqueness result.

The goal of this paper is the investigation of an optimization method applied to the inverse transmission problem of reconstructing the periodic interface. Here the grating is illuminated by an incident monochromatic plane wave, and data of the scattered field are taken on two lines lying above and below the grating profile, respectively. 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. We refer to [7] for an overview on inverse scattering problems in general (nonperiodic) structures.

For the reconstruction of perfectly reflecting periodic interfaces leading to the inverse Dirichlet problem, several inversion algorithms based on analytic continuation [15], iterative regularization [14], linear sampling [1], and the Kirsch–Kress optimization method [5], [4] became recently available. The latter approach was originally developed for acoustic obstacle scattering [17], [7], [23] and avoids the solution of direct diffraction problems. Its implementation for the inverse periodic Dirichlet problem turned out to be rather easy, and a mathematical foundation in the practically important case of nonsmooth grating profiles could be given [13].

In Sections 3–5 we introduce and analyze the profile reconstruction method for our inverse transmission problem. As in [13], [5], this method splits the inverse problem into a linear ill–posed part to reconstruct the scattered field and a nonlinear well–posed part to find the profile curve. The minimization of the Tikhonov functional for the linear problem and the defect minimization of the transmission conditions are then combined into one cost functional. Much effort will be spent on proving a convergence result in the general case of Lipschitz grating profiles, extending the variational approach of [13] for the perfectly reflecting case. However, in the transmission case, it is harder to establish convergence of the cost functional; see Section 4 for a crucial density result which is based on (nontrivial) continuity and solvability properties of layer potentials on periodic Lipschitz graphs.

The implementation of the reconstruction algorithm as a two–step method will be discussed in Section 6. Similar to [4], two unknown density functions are first computed from near–field data measured above and below the grating structure, which allows us to represent the scattered and transmitted fields as single layer potentials. Then these density functions are used as inputs to a nonlinear least squares problem, which determines the unknown profile as a curve where the associated transmission conditions are fulfilled. After discretization, the least squares problem is solved iteratively by the Gauss–Newton method. Finally, numerical results for smooth grating profiles with exact and noisy data are reported.

An alternative reconstruction method based on finite element and optimization techniques for the inverse periodic transmission problem is presented in [10].

2 Direct diffraction problem

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

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

with $f \in C^{0,1}_{per}$, i.e., f is a periodic Lipschitz function of period 2π. Assume that the regions above and below Λ_f

$$G^\pm := \{x \in \mathbb{R}^2 : x_2 \gtrless f(x_1)\,,\ x_1 \in \mathbb{R}\}$$

are filled with materials whose indices of refraction (or wave numbers) $k^\pm$ satisfy

$$k^\pm > 0\,,\ \operatorname{Re} k^- > 0\,,\ \operatorname{Im} k^- \geq 0\,. \tag{2.1}$$

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 diffracted field v^{sc} in the TE (transverse electric) mode satisfies the Helmholtz equations

$$\Delta v^{sc} + (k^{\pm})^2 v^{sc} = 0 \quad \text{in} \quad G^{\pm}\,, \tag{2.2}$$

together with the transmission conditions

$$[v]_\Lambda = [\partial_\nu v]_\Lambda = 0 \tag{2.3}$$

for the total field v given by

$$v = v^{sc} + v^{in} \quad \text{in} \quad G^+\,,\; v = v^{sc} \quad \text{in} \quad G^-\,.$$

Here ν denotes the unit normal to Λ pointing from G^+ to G^-, and $[v]_\Lambda$ stands for the jump across Λ:

$$[v]_\Lambda(x) = r^- v(x) - r^+ v(x) := \lim_{h\to+0} \{v(x + h\nu(x)) - v(x - h\nu(x))\}\,,\; x \in \Lambda\,. \tag{2.4}$$

Moreover, v is assumed to be α-quasiperiodic

$$v(x_1 + 2\pi, x_2) = \exp(2i\alpha\pi) v(x_1, x_2)\,, \tag{2.5}$$

and we require that v satisfies radiation conditions as $x_2 \to \pm\infty$, i.e., the scattered field can be expanded as infinite sums of plane waves

$$v^{sc}(x) = \sum_{n\in\mathbb{Z}} A_n^{\pm} \exp\{i(n + \alpha)x_1 \pm i\beta_n^{\pm} x_2\}\,, \qquad x_2 > \max(f) \quad \text{resp.} \quad x_2 < \min(f)\,, \tag{2.6}$$

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

$$\beta_n(\alpha, k) := (k^2 - (n + \alpha)^2)^{1/2}\,,\; 0 \le \arg \beta_n(\alpha, k) < \pi\,. \tag{2.7}$$

Since $\beta_n^{\pm}$ are real for at most finitely many indices, we observe that only a finite number of plane waves in the sums (2.6) propagate into the far field, with the remaining evanescent waves decaying exponentially as $x_2 \to \pm\infty$.

The transmission problem (2.2), (2.3), (2.5), (2.6) admits a variational formulation in a bounded periodic cell in $\mathbb{R}^2$, enforcing the transmission and radiation conditions (cf. [3], [9], [11]). Introduce artificial boundaries

$$\Gamma^{\pm} := \{(x_1, b^{\pm}) : 0 \le x_1 \le 2\pi\}\,,\; b^+ > \max(f)\,,\; b^- < \min(f)\,,$$

and the bounded domain

$$\Omega := (0, 2\pi) \times (b^-, b^+)\,.$$

The function $u := \exp(-i\alpha x_1)v$, which is 2π-periodic in x_1, satisfies the Helmholtz equation

$$(\Delta_\alpha + k^2)u = 0 \quad \text{in} \quad \Omega\,, \quad \text{with} \quad k = k^{\pm} \quad \text{in} \quad \Omega^{\pm} := \Omega \cap G^{\pm}\,, \tag{2.8}$$

where we use the notation

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

and the corresponding transmission conditions $[u]_\Lambda = [\partial_\nu u]_\Lambda = 0$ are included. The radiation conditions (2.6) are equivalent to the nonlocal boundary conditions

$$\partial_\nu u|_{\Gamma^+} + T^+ u = -2i\beta\exp(-i\beta b^+) =: g^+\,,\ \partial_\nu u|_{\Gamma^-} + T^- u = 0\,, \tag{2.9}$$

where $T^\pm$ is the periodic pseudodifferential operator (of order 1)

$$T^\pm u = T(\alpha, k^\pm)u := -\sum_{n\in\mathbb{Z}} i\beta_n(\alpha, k^\pm)\hat{u}_n^\pm \exp(inx_1) \tag{2.10}$$

and $\hat{u}_n^\pm$ are the Fourier coefficients of $u(x_1, b^\pm)$. The operator $T^\pm$ is bounded from $H^s_{per}(\Gamma^\pm)$ into $H^{s-1}_{per}(\Gamma^\pm)$ for any $s \in \mathbb{R}$, where H^s_{per} stands for the 2π-periodic Sobolev space of order s. For $s \geq 0$ let $H^s_{per}(\Omega)$ 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 (2.8), (2.9): Determine $u \in H^1_{per}(\Omega)$ such that

$$\begin{aligned} B(u,\varphi) &:= \int_\Omega (\nabla_\alpha u \cdot \overline{\nabla_\alpha \varphi} - k^2 u\overline{\varphi}) + \int_{\Gamma^+} (T^+u)\overline{\varphi} + \int_{\Gamma^-} (T^-u)\overline{\varphi} \\ &= \int_{\Gamma^+} g^+\overline{\varphi}\,,\ \forall \varphi \in H^1_{per}(\Omega)\,. \end{aligned} \tag{2.11}$$

Since the operators $T^\pm : H^{1/2}_{per}(\Gamma^\pm) \to H^{-1/2}_{per}(\Gamma^\pm)$ are continuous, the sesquilinear form B generates a continuous linear operator $\mathcal{B}$ acting from $H^1_{per}(\Omega)$ into its dual $H^1_{per}(\Omega)'$, with respect to the pairing $(u, \varphi) \to \int_\Omega u\overline{\varphi}$, via

$$(\mathcal{B}u, \varphi) = B(u, \varphi)\,,\ u, \varphi \in H^1_{per}(\Omega)\,. \tag{2.12}$$

We recall the following existence and uniqueness result, which is a special case of [3, Thm.3.5].

Theorem 2.1 *If the grating profile Λ is given by a periodic Lipschitz graph and the refractive index k satisfies (2.1), then the operator $\mathcal{B}$ defined by (2.12) is invertible from $H^1_{per}(\Omega)$ onto $H^1_{per}(\Omega)'$. In particular, the variational problem (2.11) or, equivalently, problem (2.8), (2.9) has a unique solution $u \in H^1_{per}(\Omega)$.*

To prove this result, one first verifies that the form B defined in (2.11) is strongly elliptic over $H^1_{per}(\Omega)$; see also [11]. Thus $\mathcal{B}$ defined in (2.12) is a Fredholm operator of index 0 from $H^1_{per}(\Omega)$ into its dual. For $\operatorname{Im} k^- > 0$, the uniqueness follows using a simple integration by parts. In the case $k^- > 0$, the uniqueness is obtained by applying a periodic version of the Rellich identity and the fact that the x_2 component of the normal ν does not change sign on Λ. For the periodic Dirichlet problem, we refer to [13]. The proof for the TE transmission problem is simpler, since its solution always belongs to $H^2_{per}(\Omega)$ by the elliptic regularity of the operator $\Delta_\alpha + k^2$.

3 Inverse problem and reconstruction method

Our goal in this paper is to study the *inverse problem* or the *profile reconstruction problem.*

(IP): Given the solution u to (2.8), (2.9), determine the profile function f from the traces of the scattered field

$$u_b := (u_b^+, u_b^-)\,,\; u_b^\pm := u^{sc}|_{\Gamma^\pm} = \sum_{n\in\mathbb{Z}} A_n^\pm \exp(inx_1 \pm i\beta_n^\pm b^\pm) \tag{3.1}$$

on the horizontal lines $x_2 = b^\pm$, where $u^{sc} := \exp(-i\alpha x_1)v^{sc}$.

Thus all Rayleigh coefficients $A_n^\pm$ are assumed to be known, and (IP) also involves near field measurements since the evanescent waves cannot be measured far away from the grating profile. Since (IP) is nonlinear and severely ill-posed, it is quite natural to apply regularization and optimization techniques.

Suppose that we have the a priori information about our reconstruction problem that the unknown profile Λ_f lies between the horizontal lines

$$\Gamma_1^\pm = \{(x_1, a^\pm) : 0 \le x_1 \le 2\pi\}\,,\; b^- < a^- < a^+ < b^+\,.$$

For simplicity, we further exclude resonances by assuming

$$\beta_n^\pm \neq 0 \quad \text{for all} \quad n \in \mathbb{Z} \tag{3.2}$$

in the sequel. Then the free space 2π-periodic Green function of the operator $\Delta_\alpha + (k^\pm)^2$ takes the form (cf. [20], [6])

$$\mathcal{G}^\pm(x,y) = \frac{i}{4\pi}\sum_{n\in\mathbb{Z}} \frac{1}{\beta_n^\pm} \exp\{in(x_1 - y_1) + i\beta_n^\pm|x_2 - y_2|\}\,,\; x \neq y\,, \tag{3.3}$$

with $\beta_n^\pm = \beta_n(\alpha, k^\pm)$. We try to represent the scattered field u^{sc} above Γ_1^- resp. below Γ_1^+ as single layer potentials

$$\begin{aligned} u^{sc}(x) = S^\pm\varphi^\pm(x) &:= \int_0^{2\pi} \mathcal{G}^\pm(x_1, x_2, t, a^\mp)\varphi^\pm(t)dt \\ &= \frac{i}{2}\sum_{n\in\mathbb{Z}} \frac{c_n^\pm}{\beta_n^\pm}\exp(inx_1 + i\beta_n^\pm|x_2 - a^\mp|)\,, \\ &\quad \text{for} \quad x_2 > a^- \quad \text{resp.} \quad x_2 < a^+\,, \end{aligned} \tag{3.4}$$

with unknown density functions

$$\varphi^\pm(t) = \sum_{n\in\mathbb{Z}} c_n^\pm \exp(int) \in X := L^2(0, 2\pi)\,.$$

Introduce the linear operators $S_b^\pm : X \to X$ by

$$S_b^\pm\psi(t) := S^\pm\psi(t, b^\pm)\,,\; t \in (0, 2\pi)\,. \tag{3.5}$$

Note that $S_b^{\pm}\varphi^{\pm}$ approximates the output of the scattered field on $\Gamma^{\pm}$, whereas

$$S^{\pm}\varphi^{\pm} \circ f(t) := S^{\pm}\varphi^{\pm}(t, f(t)) \, , \; t \in (0, 2\pi) \, ,$$

represent approximations of u^{sc} on the profile Λ_f. In the following we identify the space $L^2(\Lambda_f)$ with X via

$$\|u \circ f\|_X = \left(\int_0^{2\pi} |u(t, f(t))|^2 dt \right)^{1/2} \, , \; u \in L^2(\Lambda_f) \, ,$$

which is a uniformly equivalent norm when f varies in an admissible set of profile functions. Since the operators $S_b^{\pm} : X \to X$ are compact with exponentially decreasing singular values, the determination of the density $\varphi = (\varphi^+, \varphi^-)$ from the first kind equation

$$S_b\varphi := (S_b^+\varphi^+, S_b^-\varphi^-) = (u_b^+, u_b^-) =: u_b$$

is a severely ill-posed problem. We may solve its Tikhonov regularized version

$$\gamma\varphi + S_b^* S_b \varphi = S_b^* u_b \tag{3.6}$$

with regularization parameter $\gamma > 0$. Given the solution of (3.6) and the corresponding approximation of the scattered field, we can then seek the profile Λ_f of the grating by minimizing the defect

$$\|u^{in} + S^+\varphi^+ - S^-\varphi^-\|_{L^2(\Lambda_f)} + \|\partial_\nu (u^{in} + S^+\varphi^+ - S^-\varphi^-)\|_{L^2(\Lambda_f)} \, , \; f \in \mathcal{M} \tag{3.7}$$

of the transmission conditions over a class $\mathcal{M}$ of admissible profiles. In the following we choose $\mathcal{M}$ to be a subset of $C^{0,1}_{per}$ such that

$$a^- < \min(f) \, , \; \max(f) < a^+ \, , \; \|f\|_{C^{0,1}_{per}} \leq c \tag{3.8}$$

for all $f \in \mathcal{M}$ and some $c > 0$. Note that $\mathcal{M}$ is then compact with respect to the convergence $f_n \to f$ given by

$$\max|f - f_n| \to 0 \quad \text{as} \quad n \to \infty \, , \quad \text{and} \quad \sup_{n \in \mathbb{N}} \|f_n\|_{C^{0,1}_{per}} < \infty \, . \tag{3.9}$$

For the reformulation of the inverse transmission problem (IP) as an optimization problem, we now combine the minimization of the Tikhonov functional for (3.6) and the defect minimization (3.8) into the following cost functional:

$$\begin{aligned} F(\varphi, f; \gamma) :=& \|S_b\varphi - u_b\|^2_{X\times X} + \gamma\|\varphi\|^2_{X\times X} + \varrho_1 \|(u^{in} + S^+\varphi^+ - S^-\varphi^-) \circ f\|^2_X \\ &+ \varrho_2 \|\partial_\nu (u^{in} + S^+\varphi^+ - S^-\varphi^-) \circ f\|^2_X \, . \end{aligned} \tag{3.10}$$

Here, $\gamma > 0$ is again the regularization parameter, and $\varrho_1, \varrho_2 > 0$ are coupling parameters which have to be chosen appropriately for the numerical implementation. For theoretical purposes, we may assume $\varrho_1 = \varrho_2 = 1$ in the sequel.

Our reconstruction method, which was first introduced by Kirsch and Kress [17], [7] in the case of acoustic scattering by sound-soft obstacles, consists in solving the following optimization problem. We also refer to Zinn [23] who studied the transmission boundary conditions for obstacles with C^2 boundaries.

(OP): Find $\varphi \in X \times X$ and $f \in \mathcal{M}$ such that

$$F(\varphi, f; \gamma) = m(\gamma) := \inf\{F(\psi, g; \gamma) : \psi \in X \times X\,,\; g \in \mathcal{M}\}\,.$$

The existence of a minimizer is guaranteed by the following theorem.

Theorem 3.1 *For each $\gamma > 0$, the problem* (OP) *has a solution.*

Here we need not assume that u_b is an exact output of the scattered field. The proof is analogous to that of [13, Thm.4.2] in the case of the inverse periodic Dirichlet problem and will be omitted. The following convergence result extends [13, Thm.4.3] to the inverse transmission problem.

Theorem 3.2 *Let u_b be the exact pattern of the scattered field u^{sc} on the horizontal lines $x_2 = b^{\pm}$ corresponding to some profile function $f \in \mathcal{M}$. Then we have:*

(i) $\lim_{\gamma\to 0} m(\gamma) = 0$, *i.e., convergence of the cost functional.*

(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) in the sense of (3.9), and every limit point f^* of (f_n) represents a profile function such that the total field u satisfies $[u]_{\Lambda^*} = [\partial_\nu u]_{\Lambda^*} = 0$ on $\Lambda^* = \Lambda_{f^*}$.*

The proof of Theorem 3.2 will be given in Section 5.

Remark 3.1 If we have the a priori information that our inverse problem (IP) has at most one solution, then from Theorem 3.2 (ii) we obtain convergence of the total sequence (f_n) to f. Presently the uniqueness for (IP) is only known if $\operatorname{Im} k^- > 0$ (see [10]); uniqueness results with a single wave number for the inverse periodic Dirichlet problem can be found in [12].

For $k^- > 0$ we can try to achieve uniqueness and more accurate reconstructions by replacing the cost functional (3.10) by a sum corresponding to several incident waves with different wavelengths and/or incident angles, and the preceding theorems carry over to this case.

Remark 3.2 If condition (3.2) is violated, i.e. Rayleigh frequencies do occur, we may replace the approximations (3.4) of the scattered field through a single layer potential by

$$S^{\pm}\varphi^{\pm}(x) = \sum_{n\in\mathbb{Z}} c_n^{\pm} \exp(inx_1 + i\beta_n^{\pm}|x_2 - a^{\mp}|)\,.$$

Then the above results remain valid; compare [13] for the inverse Dirichlet problem.

4 A density result and solvability of periodic boundary integral equations

To prove Theorem 3.2, we need the following crucial density result which justifies the ansatz (3.4) and the choice of the cost functional (3.10). Its proof is based on continuity and solvability properties of boundary integral operators on periodic Lipschitz graphs.

Theorem 4.1 *Let $f \in \mathcal{M}$. For all $\varepsilon > 0$ and $(\chi, \psi) \in L^2(\Lambda) \times L^2(\Lambda)$, $\Lambda = \Lambda_f$, there exist $\varphi^\pm \in L^2(0, 2\pi)$ such that*

$$\|S^+\varphi^+ - S^-\varphi^- - \chi\|_{L^2(\Lambda)} + \|\partial_\nu(S^+\varphi^+ - S^-\varphi^-) - \psi\|_{L^2(\Lambda)} < \varepsilon \,.$$

Proof. Introduce the sets

$$\mathfrak{W} := \{(w|_\Lambda, \partial_\nu w|_\Lambda) : w \in W\} \,, \; W := \text{span}\,\{e_n^+, e_n^- : n \in \mathbb{Z}\} \,,$$

where $e_n^\pm(x) := \exp(inx_1 \pm i\beta_n^\pm x_2)$. It is sufficient to show (cf. (3.4)) that the set $\mathfrak{W}$ is dense in $L^2(\Lambda) \times L^2(\Lambda)$. Then it remains to verify that the orthogonality relations

$$\int_\Lambda (\chi w + \psi \partial_\nu w) ds = 0 \quad \forall w \in W \,, \quad \text{with} \quad \chi, \psi \in L^2(\Lambda) \,, \tag{4.1}$$

imply $\chi = \psi = 0$. Let $\mathcal{H}^\pm$ be the free space 2π-periodic Green function of the operator $\Delta_{-\alpha} + (k^\pm)^2$, i.e., we replace $\beta_n^\pm = \beta_n(\alpha, k^\pm)$ in (3.3) by $\beta_n(-\alpha, k^\pm) = \beta_{-n}(\alpha, k^\pm)$ (cf. (2.7)). For $\chi, \psi \in L^2(\Lambda)$ the corresponding single and double layer potentials on Λ are defined by

$$V^\pm\chi(x) := \int_\Lambda \mathcal{H}^\pm(x,y)\chi(y) ds(y) \,, \; K^\pm\psi(x) := \int_\Lambda \partial_{\nu(y)}\mathcal{H}^\pm(x,y)\psi(y) ds(y) \,, \quad x \in \Omega\backslash\Lambda \,, \tag{4.2}$$

and for $\sigma \in [-1/2, 1/2]$ the operators

$$V^\pm : H_{per}^{-1/2+\sigma}(\Lambda) \to H_{per}^{1+\sigma}(\Omega) \,, \; K^\pm : H_{per}^{1/2+\sigma}(\Lambda) \to H_{per}^{1+\sigma}(\Omega^+ \cup \Omega^-) \tag{4.3}$$

are continuous. Recall from (2.8) that Λ divides the rectangle Ω into the upper domain Ω^+ and the lower domain Ω^-. Moreover, the following jump relations hold:

$$[V^\pm\chi]_\Lambda = 0 \,, \quad [\partial_\nu V^\pm \chi]_\Lambda = -\chi \,, \; \chi \in L^2(\Lambda) \,; \tag{4.4}$$

$$[K^\pm\psi]_\Lambda = \psi \,, \; [\partial_\nu K^\pm \psi]_\Lambda = 0 \,, \; \psi \in H^1_{per}(\Lambda) \,. \tag{4.5}$$

While the continuity properties (4.3) for $\sigma \in (-1/2, 1/2)$ and the relations (4.4), (4.5) follow by adapting Costabel's elementary approach [8] to the periodic Helmholtz equation, the endpoint results for $\sigma = \pm 1/2$ rely on Calderon's Theorem on the L^2 continuity of the Cauchy integral on Lipschitz curves. We refer to [22], [16] in the case of the Laplace operator and to [18] for the Helmholtz operator on Lipschitz domains.

To prove that (4.1) implies $\chi = \psi = 0$, we introduce the functions

$$\begin{aligned} U^{\pm}(x) &:= -V^{\pm}\chi(x) + K^{\pm}\psi(x)\,,\ x \in \Omega\backslash\Lambda\,; \\ U(x) &:= U^{\pm}(x)\,,\ x \in \Omega^{\pm}\,. \end{aligned} \tag{4.6}$$

From the orthogonality relations (4.1) and the form of the Green function $\mathcal{H}^{+}$ (cf. (3.3) with $\beta_n^{+} = \beta_{-n}(\alpha, k^{+})$), we obtain that $U^{+}(x) = 0$ if $x_2 < \min(f)$, hence $U^{+}(x) = 0$, $x \in \Omega^{-}$, by analytic continuation. Analogously, from (4.1) we have $U^{-}(x) = 0$, $x \in \Omega^{+}$.

Furthermore, from (4.3), (4.6) and the relation $U^{+} = 0$ in Ω^{-}, and recalling the definition of the restriction operators $r^{\pm}$ in (2.4), we observe that $\psi \in L^2(\Lambda)$ satisfies the boundary integral equation

$$r^{-}K^{+}\psi = r^{-}V^{+}\chi \in H^1_{per}(\Lambda) \tag{4.7}$$

on Λ. As a consequence of Theorem 4.2 below, we then obtain $\psi \in H^1_{per}(\Lambda)$, which implies

$$U|_{\Omega^{\pm}} = U^{\pm} \in H^1_{per}(\Omega^{\pm}) \tag{4.8}$$

using (4.3) again. Moreover, from $U^{\pm} = 0$ in $\Omega^{\mp}$ and the jump relations (4.4), (4.5), we have

$$\begin{aligned} [U]_{\Lambda} &= r^{-}U^{-} - r^{+}U^{+} = r^{-}(K^{-}\psi - V^{-}\chi) - r^{+}(K^{+}\psi - V^{+}\chi) \\ &= [K^{-}\psi]_{\Lambda} - [V^{-}\chi]_{\Lambda} - [K^{+}\psi]_{\Lambda} + [V^{+}\chi]_{\Lambda} = \psi - \psi = 0\,, \\ [\partial_\nu U]_{\Lambda} &= r^{-}\partial_\nu(K^{-}\psi - V^{-}\chi) - r^{+}\partial_\nu(K^{+}\psi - V^{-}\chi) \\ &= [\partial_\nu K^{-}\psi]_{\Lambda} - [\partial_\nu V^{-}\chi]_{\Lambda} - [\partial_\nu K^{+}\psi]_{\Lambda} + [\partial_\nu V^{+}\chi]_{\Lambda} = \chi - \chi = 0\,. \end{aligned}$$

Together with (4.8), this implies that $U \in H^1_{per}(\Omega)$ satisfies the homogeneous version of problem (2.8), (2.9) (i.e., $g^{+} = 0$), giving $U = 0$ in Ω by Theorem 2.1 and then $\chi = \psi = 0$ by applying the jump relations (4.4), (4.5) again. □

To prove the above (nontrivial) regularity result for equation (4.7), we now study the mapping properties of boundary integral operators on the Lipschitz graph $\Lambda = \Lambda_f$. Setting $V = V^{+}$, $K = K^{+}$ in the sequel, we introduce the direct values on Λ of these layer potentials:

$$\begin{aligned} \mathcal{V}\psi(x) &:= \int_{\Lambda} \mathcal{H}^{+}(x,y)\psi(y)ds(y)\,, \\ \mathcal{K}\psi(x) &:= p.v. \int_{\Lambda} \partial_{\nu(y)}\mathcal{H}^{+}(x,y)\psi(y)ds(y)\,,\ x \in \Lambda\,. \end{aligned}$$

The dual operator of $\mathcal{K}$ with respect to the pairing $(\psi, \chi) \to \int_{\Lambda} \psi\chi ds$ is given by

$$\mathcal{K}^{*}\psi(x) = p.v. \int_{\Lambda} \partial_{\nu(x)}\mathcal{G}^{+}(x,y)\psi(y)ds(y)\,,\ x \in \Lambda\,,$$

where $\mathcal{G}^+$ is the (periodic) Green function of $\Delta_\alpha + (k^+)^2$; recall that $\mathcal{H}^+$ corresponds to $\Delta_{-\alpha} + (k^+)^2$. Then we have the continuity of the operators

$$\begin{aligned} &\mathcal{V} : H_{per}^{-1/2+\sigma}(\Lambda) \to H_{per}^{1/2+\sigma}(\Lambda)\,,\ \mathcal{K} : H_{per}^{1/2+\sigma}(\Lambda) \to H_{per}^{1/2+\sigma}(\Lambda)\,, \\ &\mathcal{K}^* : H_{per}^{-1/2+\sigma}(\Lambda) \to H_{per}^{-1/2+\sigma}(\Lambda)\,,\ \sigma \in [-1/2, 1/2]\,, \end{aligned} \tag{4.9}$$

and the jump relations

$$r^\pm K\psi = \left(\mp\frac{1}{2} + \mathcal{K}\right)\psi\,,\ r^\pm V\psi = \left(\mp\frac{1}{2} + \mathcal{K}^*\right)\psi\,,\ \psi \in L^2(\Lambda)\,; \tag{4.10}$$

we again refer to [22], [16], [18] for the case of (nonperiodic) Dirichlet and Helmholtz operators. The periodic case can then be treated using the fact that

$$\mathcal{H}^+(x,y) - \frac{1}{2\pi}\log\frac{1}{|x-y|}\,, \quad \text{for} \quad |x_1 - y_1| < \pi\,,$$

is a C^1 function; see [20], [6].

We now establish a result on the invertibility and the Fredholm property of the above boundary integral operators.

Theorem 4.2 *Let $\Lambda = \Lambda_f$ be given by a periodic Lipschitz graph. Then, for each $k^+ > 0$ and $\alpha = k^+ \sin\theta$, we have:*

(i) $\mathcal{V}$ is an invertible operator from $L^2(\Lambda)$ onto $H^1_{per}(\Lambda)$;

(ii) $\pm\frac{1}{2}I + \mathcal{K}$ are Fredholm operators with index zero on $L^2(\Lambda)$ and $H^1_{per}(\Lambda)$.

Assertion (ii) immediately gives the regularity property needed in the proof of Theorem 4.1: Note that (4.7) takes the form

$$\left(\frac{1}{2} + \mathcal{K}\right)\psi = g\,,\ g \in H^1_{per}(\Lambda)\,,\ \psi \in L^2(\Lambda)\,,$$

and since $\frac{1}{2}I + \mathcal{K}$ is Fredholm with the same index on both $L^2(\Lambda)$ and $H^1_{per}(\Lambda)$, we obtain $\psi \in H^1_{per}(\Lambda)$.

To prove Theorem 4.2, one can proceed as in [16, Chap.2.2] where the Laplace equation in unbounded domains given by Lipschitz graphs was treated. Since the spectral theory in the periodic case is somewhat different from that for the Helmholtz operator in a bounded domain and its exterior (cf. [18]), we prefer to give an outline of the proof.

Proof of Theorem 4.2. (i) Let $\psi \in L^2(\Lambda)$ and consider the function $u = V\psi \in H^1_{per}(\Omega)$. Then $u^\pm = u|_{\Omega^\pm}$ is a radiating solution of the Helmholtz equation $\Delta_{-\alpha}u + (k^+)^2 u = 0$ in $\Omega^\pm$. Applying (the periodic version of) the Rellich identity gives

$$\int_\Lambda \left(\partial_2 u^\pm \overline{\partial_{\nu,\alpha} u^\pm} + \partial_1 u^\pm \overline{\partial_{\tau,\alpha} u} + \nu_2(k^+)|u|^2\right) ds = 0\,, \tag{4.11}$$

with the weighted normal and tangential derivatives

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

see [3], [13]. Note that $r^+u^+ = r^-u^- = u|_\Lambda$. Since $-\nu_2$ is bounded from below by a positive constant, from (4.11) we easily obtain the inequalities

$$\begin{aligned} \|\partial_\tau u\|_{L^2(\Lambda)} &\le c\left(\|\partial_\nu u^\pm\|_{L^2(\Lambda)} + \|u\|_{L^2(\Lambda)}\right) \, , \\ \|\partial_\nu u^\pm\|_{L^2(\Lambda)} &\le c\|\partial_\tau u\|_{L^2(\Lambda)} \, , \; u = V\psi \, , \; \psi \in L^2(\Lambda) \, , \end{aligned} \tag{4.12}$$

with $c > 0$ depending only on the Lipschitz constant of Λ. For a Lipschitz graph, (4.11) and (4.12) can be justified by approximating Λ with the graphs of smooth functions and then passing to the limit; see [22], [13] for details.

(4.12) and the jump relations (4.10) imply the estimate

$$\begin{aligned} \|\mathcal{V}\psi\|_{H^1_{per}(\Lambda)} &\ge \|r^\pm\partial_\tau V\psi\|_{L^2(\Lambda)} \ge c\|r^\pm\partial_\nu V\psi\|_{L^2(\Lambda)} \\ &= c\left\|\left(\pm\frac{1}{2} + \mathcal{K}^*\right)\psi\right\|_{L^2(\Lambda)} \, , \end{aligned}$$

which gives

$$\|\mathcal{V}\psi\|_{H^1_{per}(\Lambda)} \ge c\|\psi\|_{L^2(\Lambda)} \quad \forall \psi \in L^2(\Lambda) \, .$$

Thus the operator $\mathcal{V} : L^2(\Lambda) \to H^1_{per}(\Lambda)$ is one-to-one with closed image. To finish the proof of (i), we now exploit the following homotopy argument. For $0 \le t \le 1$, consider the Lipschitz graph corresponding to tf and the corresponding operator $\mathcal{V}_t$. Then $\mathcal{V}_0$ corresponds to the operator on the x_1 axis, which is clearly invertible (cf. formula (3.4) with $a^- = 0$), and $\mathcal{V}_t$ is one-to-one with closed image and continuous in norm as a function of t. Consequently, the stability of the index implies that $\mathcal{V} = \mathcal{V}_1$ is invertible.

(ii) From (4.12) and the jump relations (4.10), we also obtain

$$\left\|\left(\pm\frac{1}{2} + \mathcal{K}^*\right)\psi\right\|_{L^2(\Lambda)} \le c\left(\left\|\left(\mp\frac{1}{2} + \mathcal{K}^*\right)\psi\right\|_{L^2(\Lambda)} + \|\mathcal{V}\psi\|_{L^2(\Lambda)}\right) \, ,$$

where c only depends on the Lipschitz constant of Λ. Therefore we have the estimates

$$\left\|\left(\pm\frac{1}{2} + \mathcal{K}^*\right)\psi\right\|_{L^2(\Lambda)} + \|\mathcal{V}\psi\|_{L^2(\Lambda)} \ge c\,\|\psi\|_{L^2(\Lambda)} \, ,$$

where the operator $\mathcal{V}$ is compact on $L^2(\Lambda)$. Hence $\pm\frac{1}{2}\,I + \mathcal{K}^*$ is a semi-Fredholm operator with finite dimensional null space on $L^2(\Lambda)$. Applying the above homotopy argument to the corresponding operators $\mathcal{V}_t$, $\mathcal{K}_t^*$, $0 \le t \le 1$, and noticing that $\mathcal{K}_0^* = 0$, we observe that $\pm\frac{1}{2}\,I + \mathcal{K}^*$ is Fredholm with index zero on $L^2(\Lambda)$, and so is $\pm\frac{1}{2}\,I + \mathcal{K}$ by duality. Finally, using the identity

$$\mathcal{V}\left(\frac{1}{2}\,I + \mathcal{K}^*\right)\psi = \left(\frac{1}{2}\,I + \mathcal{K}\right)\mathcal{V}\psi \, , \; \psi \in L^2(\Lambda)$$

which follows from Green's formula, and the invertiblity of $\mathcal{V}$, we see that $\pm\frac{1}{2}\,I + \mathcal{K}$ is also Fredholm with index zero on $H^1_{per}(\Lambda)$. This completes the proof of (ii). □

Remark 4.1 It can be proved similarly to [18, Sec.8] that $\pm\frac{1}{2}I + \mathcal{K}$ is invertible on $L^2(\Lambda)$ and $H^1_{per}(\Lambda)$ if and only if the homogeneous periodic Neumann problem for $\Lambda_\alpha + (k^+)^2$ in $\Omega^\pm$ has only the trivial solution. Note that the periodic Dirichlet problem is always uniquely solvable if Λ is given by a Lipschitz graph [13].

5 Proof of Theorem 3.2

With Theorem 4.1 at hand, the convergence proof for our reconstruction method uses similar ideas as in the case of the inverse Dirichlet problem [13], but is simpler due to the H^2 regularity of solutions to the direct problem.

Let $\Lambda = \Lambda_f$, $f \in \mathcal{M}$, $\mathcal{M}$ being an admissible set of Lipschitz profile functions, and consider the transmission problem

$$\begin{gathered}(\Delta_\alpha + k^2)w = 0 \quad \text{in} \quad \Omega^+ \cup \Omega^- \,, \quad [w]_\Lambda = g \,, \; [\partial_{\nu,\alpha} w]_\Lambda = h \,, \\ \partial_\nu w|_{\Gamma^+} + T(\alpha, k^+)w = 0 \,, \; \partial_\nu w|_{\Gamma^-} + T(\alpha, k^-)w = 0 \,,\end{gathered} \tag{5.1}$$

where $k = k^\pm$ in $\Omega^\pm$, $\partial_{\nu,\alpha} = \partial_\nu + i\alpha$, and the pseudodifferential operators $T(\alpha, k^\pm)$ on the horizontal lines $\Gamma^\pm$ are defined in (2.10). The following lemma shows that the traces on $\Gamma^\pm$ of a solution w to (5.1) depend continuously on the interface data g, h, uniformly with respect to $f \in \mathcal{M}$.

Lemma 5.1 *If $w \in H^2_{per}(\Omega^+ \cup \Omega^-)$ satisfies the problem (5.1), then the estimates*

$$\|w\|_{L^2(\Gamma^\pm)} \le c_1 \|w\|_{L^2(\Omega)} \le c \left(\|g\|_{L^2(\Lambda)} + \|h\|_{L^2(\Lambda)} \right) \tag{5.2}$$

hold, where c and c_1 do not depend on g, h and Λ_f.

Proof. Consider the problem

$$\begin{gathered}(\Delta_{-\alpha} + k^2)z = \bar{w} \quad \text{in} \quad \Omega \,, \\ \partial_\nu w|_{\Gamma^+} + T(-\alpha, k^+)w = 0 \,, \; \partial_\nu w|_{\Gamma^-} + T(-\alpha, k^-)w = 0 \,,\end{gathered} \tag{5.3}$$

which has a unique solution $z \in H^2_{per}(\Omega)$ by Theorem 2.1 and elliptic regularity. From (5.1), (5.3) and Green's formula we have

$$\begin{aligned}\int_\Omega |w|^2 &= \int_\Omega w(\Delta_{-\alpha} + k^2)z = \int_\Lambda ([w\partial_{\nu,-\alpha} z]_\Lambda - [z\partial_{\nu,\alpha} w]_\Lambda) \\ &= \int_\Lambda ([w]_\Lambda \partial_{\nu,-\alpha} z - z[\partial_{\nu,\alpha} w]_\Lambda) = \int_\Lambda (g\partial_{\nu,-\alpha} z - hz) \,,\end{aligned}$$

which implies the estimate

$$\|w\|^2_{L^2(\Omega)} \le \|g\|_{L^2(\Lambda)} \|\partial_{\nu,-\alpha} z\|_{L^2(\Lambda)} + \|h\|_{L^2(\Lambda)} \|z\|_{L^2(\Lambda)} \,. \tag{5.4}$$

Using the Rayleigh expansions of w in the rectangles $(0, 2\pi) \times (a^+, b^+)$, $(0, 2\pi) \times (b^-, a^-)$ and our assumption (3.8) on Λ_f, it is easy to verify the uniform bounds

$$\|w\|_{L^2(\Gamma^\pm)} \le c_1 \|w\|_{L^2(\Omega)} \,. \tag{5.5}$$

Then (5.2) follows from (5.4) and (5.5), provided the uniform estimate

$$\|\partial_\nu z\|_{L^2(\Lambda)} + \|z\|_{L^2(\Lambda)} \le c\|w\|_{L^2(\Omega)} \tag{5.6}$$

holds. To prove (5.6), we make use of the inequality

$$\|z\|_{H^1_{per}(\Omega)} \le c\|w\|_{L^2(\Omega)}\,, \tag{5.7}$$

where z is the solution of (5.3) and c is independent of w and the profile function f. This estimate follows from the fact that the operators

$$\mathcal{B}_f : H^1_{per}(\Omega) \to H^1_{per}(\Omega)'\,,\ f \in \mathcal{M}\,, \tag{5.8}$$

which correspond to (2.11), (2.12) and the interface Λ_f, are uniformly stable, i.e., $\mathcal{B}_f^{-1}$ is bounded in norm independent of f. The uniform stability follows from Theorem 2.1 (applied to (5.3)), and the compactness of the admissible set $\mathcal{M}$ and the continuity in norm of $\mathcal{B}_f$ with respect to the convergence of profile functions introduced in (3.9); see also [10, Thm.2.2] where a more general perturbation result was established.

Now, by invoking elliptic regularity, from (5.7) we obtain the uniform estimate

$$\begin{aligned}\|z\|_{H^2_{per}(\Omega)} &\le c\left(\|(\Delta_{-\alpha} + k^2)z\|_{L^2(\Omega)} + \|z\|_{L^2(\Omega)}\right)\\ &\le c\left(\|w\|_{L^2(\Omega)} + \|z\|_{L^2(\Omega)}\right) \le c\|w\|_{L^2(\Omega)}\,.\end{aligned}$$

To conclude the proof of (5.6), it remains to check that

$$\|z\|_{L^2(\Lambda)} + \|\partial_\nu z\|_{L^2(\Lambda)} \le c\|z\|_{H^2_{per}(\Omega)}\,,\ \Lambda = \Lambda_f\,,\ f \in \mathcal{M}\,. \tag{5.9}$$

As a consequence of Theorem 2.4.2 in [19] (or rather its proof) we have

$$\|z\|_{L^2(\Lambda)} \le c\|z\|_{H^1_{per}(\Omega)}\,,$$

where c only depends on the Lipschitz constant of Λ, and applying the last estimate also to ∇z finally gives the desired inequality (5.9). □

Proof of Theorem 3.2: (i) By Theorem 4.1, given $\varepsilon > 0$ there exist $\varphi^\pm \in X = L^2(0,2\pi)$ such that

$$\|(u^{in} + S^+\varphi^+ - S^-\varphi^-)\circ f\|_X + \|\partial_\nu(u^{in} + S^+\varphi^+ - S^-\varphi^-)\circ f\|_X < \varepsilon\,. \tag{5.10}$$

Let u denote the solution of the forward problem (2.8), (2.9). Then w defined by

$$w := u^{in} + S^+\varphi^+ - u \quad \text{in} \quad \Omega^+\,,\ w := S^-\varphi^- - u \quad \text{in} \quad \Omega^-$$

satisfies the transmission problem (5.1) with

$$g := (S^-\varphi^- - S^+\varphi^+ - u^{in})|_\Lambda\,,\ h := \partial_{\nu,\alpha}(S^-\varphi^- - S^+\varphi^+ - u^{in})|_\Lambda\,.$$

Combining (5.2) and (5.10), we arrive at

$$\begin{aligned}\|S_b\varphi - u\|_{X\times X} &\le c\left(\|S^+\varphi^+ + u^{in} - u\|_{L^2(\Gamma^+)} + \|S^-\varphi^- - u\|_{L^2(\Gamma^-)}\right)\\ &\le c\left(\|g\|_{L^2(\Lambda)} + \|h\|_{L^2(\Lambda)}\right) \le c\varepsilon\,,\end{aligned} \tag{5.11}$$

where c does not depend on ε. Thus we have from (3.10), (5.10) and (5.11)

$$F(\varphi, f; \gamma) \leq c\varepsilon^2 + \gamma\|\varphi\|^2_{X\times X} \to c\varepsilon^2 \,,\; \gamma \to 0\,,$$

which completes the proof of assertion (i).

(ii) Let $(\varphi_n, f_n) \in X \times X \times \mathcal{M}$ be a sequencee of solutions to (OP) with regularization parameter $\gamma_n \to 0$. Let $f^* \in \mathcal{M}$ be a limit point of (f_n). Without loss of generality, we can assume that $f_n \to f^*$ $(n \to \infty)$ in the sense of (3.9); note that $\mathcal{M}$ is compact with respect to this convergence.

Furthermore, let $u_n, u^* \in H^2_{per}(\Omega)$ be the solutions of the forward problem (2.8), (2.9) corresponding to the profile functions f_n, f^*. Recall that $u_b = (u_b^+, u_b^-)$ is the exact output of the scattered field u^{sc} corresponding to some profile function $f \in \mathcal{M}$.

To prove Theorem 3.2 (ii), we show that

$$\|u_n - u^{in} - u_b^+\|^2_{L^2(\Gamma^+)} + \|u_n - u_b^-\|^2_{L^2(\Gamma^-)} \to 0\,,\; n \to \infty\,. \tag{5.12}$$

Since the convergence $f_n \to f$ and the uniform stability of the operators (5.8) imply $u_n \to u^*$ in $H^1_{per}(\Omega)$, relation (5.12) then gives

$$(u^* - u^{in})|_{\Gamma^*} = u_b^+ \,,\; u^*|_{\Gamma^-} = u_b^-\,. \tag{5.13}$$

Consequently, the total field u (which must coincide with u^* in Ω because of (5.13)) satisfies the transmission conditions $[u]_{\Lambda^*} = [\partial_\nu u]_{\Lambda^*} = 0$, where Λ^* corresponds to f^*. This completes the proof of assertion (ii).

It remains to verify (5.12). We note that $\varphi_n = (\varphi_n^+, \varphi_n^-) \in X \times X$ satisfies

$$F(\varphi_n, f_n; \gamma_n) = m(\gamma_n) \to 0\,,\; n \to \infty\,, \tag{5.14}$$

since f_n is optimal for the parameter γ_n. The left-hand side of (5.12) can obviously be estimated by the sum

$$\begin{aligned} &\|S^+\varphi_n^+ - u_b^+\|^2_{L^2(\Gamma^+)} + \|S^-\varphi_n^- - u_b^-\|^2_{L^2(\Gamma^-)} \\ &+ \|S^+\varphi_n^+ + u^{in} - u_n\|^2_{L^2(\Gamma^+)} + \|S^-\varphi_n^- - u_n\|^2_{L^2(\Gamma^-)}\,. \end{aligned} \tag{5.15}$$

We show that all terms in (5.15) can be uniformly bounded by $m(\gamma_n)$, which together with (5.14) then implies the desired relation (5.12). For the first two terms, this is clear by the definition of the cost functional. To obtain this bound for the last two terms in (5.15), we apply the second to last inequality of (5.11) where we replace $\varphi^\pm$ by $\varphi_n^\pm$ and consider the corresponding interface data g_n, h_n on the profile Λ_n corresponding to f_n. Note that the constant c in this inequality does not depend on $f \in \mathcal{M}$. Therefore, the mentioned terms of (5.15) can be uniformly estimated by

$$\|u^{in} + S^+\varphi_n^+ - S^-\varphi_n^-\|^2_{L^2(\Lambda_n)} + \|\partial_\nu(u^{in} + S^+\varphi_n^+ - S^-\varphi_n^-)\|^2_{L^2(\Lambda_n)} \leq cm(\gamma_n)\,.$$

This finishes the proof of the theorem. □

Remark 5.1 The above proof can be easily modified to give the following result on stability with respect to data errors for our reconstruction method. Assume additionally in Theorem 3.2 that we only have a sequence of measured data $u^\pm_{b,n}$ of noise level δ_n converging to zero, i.e.,

$$\|u^\pm_{b,n} - u^\pm_b\|^2_{L^2(\Gamma^\pm)} \le \delta_n\,, \quad \text{with} \quad \delta_n \to 0\,,\ n \to \infty\,.$$

Replace u_b in the cost functional (3.10) by $u_{b,n} = (u^+_{b,n}, u^-_{b,n})$ and consider the corresponding optimization problem (OP) (for $\gamma = \gamma_n$). Then for each n there exists a minimizer (φ_n, f_n) of (OP), and Theorem 3.2 remains valid.

6 Implementation as a two–step method and numerical results

Discretizing the optimization scheme (OP) based on the combined cost functional (3.10), we arrive at a finite dimensional nonlinear least squares problem which can be solved using a Levenberg-Marquardt algorithm. We refer to [5] in the case of the inverse Dirichlet problem. To reduce computational efforts, we here propose a two–step procedure as in [4].

Step 1. Let $u_b = (u^+_b, u^-_b)$ be the scattered field measured on the horizontal lines $x_2 = b^\pm$. Usually u_b is not given exactly, but perturbed by measurement errors. Let X again denote the Hilbert space $L^2(0, 2\pi)$ with scalar product $\langle\cdot,\cdot\rangle$, norm $\|\cdot\|$ and the orthonormal system $v_n(t) = \exp(int), n \in \mathbb{Z}$. We first solve the minimization problems

$$\|S^\pm_b \varphi^\pm - u^\pm_b\|^2 + \gamma\|\varphi^\pm\|^2 \to \inf_{\varphi^\pm \in X} \tag{6.1}$$

with regularization parameter $\gamma > 0$, which correspond to the Tikhonov regularization (3.6) for determining the density functions $\varphi^\pm$. Since the singular value decomposition of the first kind integral operators $S^\pm_b$ defined in (3.5) is known explicitly, the solutions $\varphi^\pm_\gamma$ can be represented as (cf. [4])

$$\varphi^\pm_\gamma = \sum_{n\in\mathbb{Z}} a^\pm_{n,\gamma} \langle u^\pm_b, v_n\rangle v_n\,, \tag{6.2}$$

where

$$a^\pm_{n,\gamma} = \begin{cases} \dfrac{-i(\beta^\pm_n)^{-1}\exp(\mp i\beta^\pm_n(b^\pm - a^\mp))}{(\beta^\pm_n)^{-2} + \gamma} & \text{if} \quad n \in \mathcal{U}^\pm \\[2ex] \dfrac{|\beta^\pm_n|^{-1}\exp(\mp|\beta^\pm_n|(b^\pm - a^\mp))}{|\beta^\pm_n|^{-2}\exp(\mp 2|\beta^\pm_n|(b^\pm - a^\mp)) + \gamma} & \text{if} \quad n \in \mathbb{Z}\backslash\mathcal{U}^\pm\,. \end{cases}$$

Here the finite index sets $\mathcal{U}^\pm := \{n \in \mathbb{Z} : |n+\alpha| < k^\pm\}$ correspond to the propagating modes of the scattered field as $x_2 \to \pm\infty$. One may expect fast convergence of these series so that only some finite section, say $|n| \le N$, will be necessary in the implementation. In our numerical examples N will be always chosen such that $\mathcal{U}^\pm \subseteq \{n \in \mathbb{Z} :\ |n| \le N\}$.

Step 2. Having computed the solutions $\varphi_\gamma^\pm \in X$ of (6.1) and the corresponding approximations (3.4) of the scattered field, we can then seek the profile function f of the grating by solving the minimization problem

$$\mathcal{F} := \|(u^{in} + S^+\varphi_\gamma^+ - S^-\varphi_\gamma^-) \circ f\|^2 + \|\partial_\nu(u^{in} + S^+\varphi_\gamma^+ - S^-\varphi_\gamma^-) \circ f\|^2 \to \inf_{f \in \mathcal{M}} \quad (6.3)$$

over a class of admissible profiles. Let us suppose that f depends smoothly on finitely many real parameters p_μ, $\mu = 1, ..., M$, and that after discretization the functional in (6.3) can be represented as

$$\mathcal{F} = \sum_{1 \le j \le K} r_j^2 \,,$$

where the real functions r_j depend smoothly on $p_1, \ldots, p_M$. From (6.3) we then obtain the finite dimensional least squares problem

$$\sum_{1 \le j \le K} r_j^2 \to \inf_{p \in \mathbb{R}^M} \quad (6.4)$$

which can be solved iteratively by a Gauss–Newton method. Note that the Jacobi matrix $J = (\partial r_j / \partial p_\mu)$ can be easily computed for several important classes of grating profiles; we refer to [4] for the perfectly reflecting case.

We do not have a convergence result for the two–step procedure. However the resulting algorithm is faster and gives results similar to those of the combined algorithm, even more accurate ones as our experience with the inverse Dirichlet problem shows [4].

In the following we restrict ourselves to Fourier gratings as one type of admissible sets of profile functions f. Let f be given as

$$f(t) = c_0 + 2 \sum_{1 \le \nu \le m} (c_\nu \cos(\nu t) + d_\nu \sin(\nu t)) \,,$$

where the number $M = 2m + 1$ of real parameters characterizing f is considered to be fixed. Let κ be a natural number and

$$s_j = \frac{2\pi}{\kappa}(j-1), \quad j = 1, ..., \kappa \,,$$

an equidistant partition of $[0, 2\pi]$. Then, using the trapezoidal rule to discretize the functional $\mathcal{F}$ in (6.3), we obtain a finite dimensional least squares problem (6.4) with $K = 2\kappa$.

Now we present some numerical examples using our method with exact and noisy data. The measured scattered field on the horizontal lines $x_2 = b^\pm$ is given at finite sets of equidistant points and is then perturbed by random errors:

$$u_b^\pm(s_j, b^\pm) + \delta\omega_j^\pm, \quad |\omega_j^\pm|^2 \le 1 \,. \quad (6.5)$$

Here δ is the noise level, and $\{s_j\}$ is the equidistant partition of $[0, 2\pi]$ introduced above. The values $u_b^\pm(s_j, b^\pm)$ were simulated using a finite element based direct solver, which is part of the program package DIPOG developed at the Weierstrass Institute (cf. www.wias-berlin.de/software). The Fourier coefficients of $u_b^\pm$ occurring in the first step of the algorithm (see (6.2)) are then also approximated using the trapezoidal rule:

$$\langle u_b^\pm, v_n \rangle \approx \frac{1}{\kappa} \sum_{j=1}^{\kappa} (u_b^\pm(s_j, b^\pm) + \delta\omega_j^\pm)\, v_n(s_j)\,.$$

We performed numerical experiments for the following two profile functions, chosen as in the examples discussed in [4] and [14] :

$$f_0(t) = 2 + \zeta(\cos(t) + \cos(2t) + \cos(3t))\,, \tag{6.6}$$

$$f_1(t) = 0.2e^{\sin(3t)} + 0.3e^{\sin(4t)}\,. \tag{6.7}$$

In the case (6.6), the parameter ζ can be considered as a measure of the profile steepness. As was found in [5], the reconstruction becomes worse when the steepness of the profile increases. In [5] we obtained satisfactory results for $\zeta \le 0.05\pi$. In [4] our improved algorithm allowed treating the case $\zeta \le 0.1\pi$. Here we considered the case $\zeta = 0.1\pi$, using unperturbed data taken at $b^+ = 3.577$, $b^- = 0.952$ for a single incoming wave with incident angle $\theta = 0$. The indices of refraction were chosen as $k^+ = 2.27$, $k^- = 4.45$. We used the regularization parameter $\gamma = 10^{-10}$ and updated 7 parameters in each of 400 Gauss–Newton iterations with step length 0.01. The results, which were stable with respect to large perturbations of the initial guess, are given in Table 1.

	c_0	c_1	c_2	c_3	d_1	d_2	d_3
target	2.00	.157	.157	.157	0	0	0
initial	1.80	.3	-.1	.0	.1	-.1	.1
initial	1.80	0	0	0	0	0	0
calcul	2.03	.162	.159	.098	.000	.000	.000

Table 1: Case (6.6) for $\zeta = 0.1\pi$

Instead of the profile function (6.7), we used its truncated Fourier series

$$f_1(t) = \langle f_1, v_0 \rangle + 2 \sum_{1 \le \nu \le 8} \big(\mathrm{Re}\,\{\langle f_1, v_\nu \rangle\} \cos(\nu t) + \mathrm{Im}\,\{\langle f_1, v_\nu \rangle\} \sin(\nu t)\big)\,,$$

which can be approximated by

$$0.633 + 2\big(-0.02715\cos(6t) - 0.0407\cos(8t) + 0.11303\sin(3t) + 0.1695\sin(4t)\big).$$

We considered the indices of refraction $k^+ = 4.54$, $k^- = 9.09$ and took a single incoming wave with $\theta = 0$. Then the index sets of the propagating modes are given by

$$\mathcal{U}^+ = \{n \in \mathbb{Z} : |n| \le 4\}\,, \quad \mathcal{U}^- = \{n \in \mathbb{Z} : |n| \le 9\}\,.$$

The measurements were taken at $x_2 = b^{\pm} = \pm 3$.

In the first step of the algorithm, we computed the density functions (6.2) by spectral cut–off with $N = 9$, where the propagating modes were used for the data on $x_2 = -3$, while 10 additional modes only appearing in the near field were taken into account for the data on $x_2 = 3$. The regularization parameter $\gamma = 10^{-7}$ was chosen to determine the density function corresponding to the reflected modes. Our numerical results presented in Table 2 turned out to be extremely robust with respect to the perturbed data (6.5). A reason for this might be that the measurements, taken far enough from the profile, could be considered as far field data for which an additional regularization is not necessary.

In the case of the perfectly reflecting profile (6.7) (see [4]), the computations were performed assuming a priori that all coefficients not appearing in the (unknown) target vanish, so that only 5 parameters had to be updated in the iterations. In the transmission case considered here, satisfactory results could be achieved by updating all 17 parameters. To reach stationarity, 800 iterations for $\lambda = .01$ were enough, taking four or five seconds altogether on a workstation. The results proved to be stable with respect to rather large variations of the used initial guess. So, for obtaining the same results for the target profile, the parameters c_0, c_1 of the starting profile could be varied between 0.5 and 1.0, and between 0.2 and -0.05, respectively.

Some of our computational results are additionally depicted in Figures 1 and 2.

	target	initial	800it	50it	100it
c_0	.633	.6	.679	.637	.653
c_1	.000	.0	.025	.008	.011
c_2	.000	.0	.017	-.002	-.000
c_3	.000	.0	.002	.000	-.001
c_4	.000	.0	.006	.000	-.003
c_5	.000	.0	.006	.000	-.001
c_6	-.027	.0	-.004	-.009	-.017
c_7	.000	.0	.039	.008	.013
c_8	-.040	.0	.024	.002	.003
d_1	.000	.0	.004	-.003	-.000
d_2	.000	.0	.005	-.001	.004
d_3	.113	.0	.121	.050	.079
d_4	.169	.0	.185	.081	.126
d_5	.000	.0	-.005	.003	.001
d_6	.000	.0	-.015	.001	-.002
d_7	.000	.0	-.002	.001	-.001
d_8	.000	.0	.000	.000	-.001

Table 2: Case (6.7)

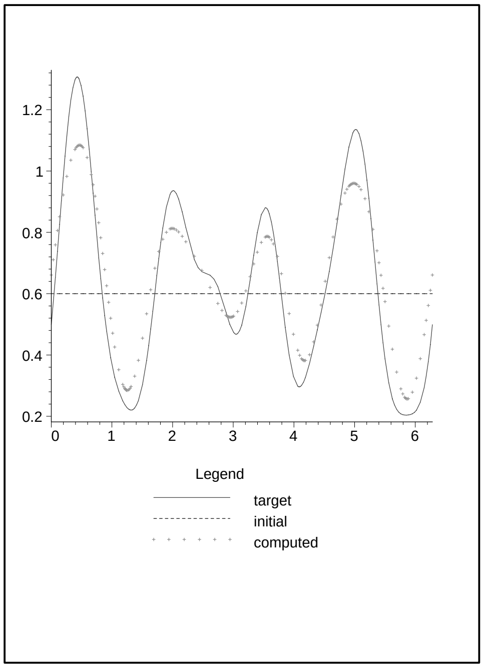

Figure 1: Case (6.7), 100 iterations

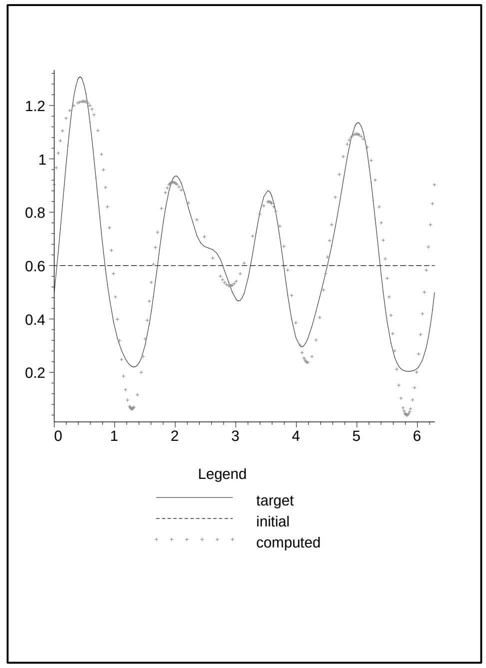

Figure 2: Case (6.7), 800 iterations

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References

[1] T. Arens, A. Kirsch, The factorization method in inverse scattering from periodic structures, Inverse Problems **19** (2003) 1195-1211.

[2] G. Bao, L. Cowsar, W. Masters (eds.), Mathematical Modeling in Optical Science, SIAM, Philadelphia, 2001.

[3] A.-S. Bonnet-Bendhia, F. Starling, Guided waves by electromagnetic gratings and non-uniqueness examples for the diffraction problem, Math. Meth. Appl. Sci. **17** (1994) 305–338.

[4] G. Bruckner, J. Elschner, A two-step algorithm for the reconstruction of perfectly reflecting periodic profiles, Inverse Problems 19 (2003) 315-329.

[5] G. Bruckner, J. Elschner, M. Yamamoto, An optimization method for grating profile reconstruction, in: Progress in Analysis, Proceed. 3rd ISAAC congress, World Scientific, Singapore, 2003, pp. 1391-1404.

[6] X. Chen, A. Friedman, Maxwell's equation in a periodic structure, Trans. Amer. Math. Soc. **323** (1991) 465-507.

[7] D. Colton, R. Kress, Inverse Acoustic and Electromagnetic Scattering Theory, 2nd Edition, Springer, Berlin, 1998.

[8] M. Costabel, Boundary integral operators on Lipschitz domains: Elementary results, SIAM J. Math. Anal. **19** (1988) 613-626.

[9] D.C. Dobson, Optimal design of periodic antireflective structures for the Helmholtz equation, European J. Appl. Math. **4** (1993) 321-340.

[10] J. Elschner, G.C. Hsiao, A. Rathsfeld, Grating profile reconstruction based on finite elements and optimization techniques, SIAM J. Appl. Math., to appear.

[11] J. Elschner, G. Schmidt, Diffraction in periodic structures and optimal design of binary gratings I: Direct problems and gradient formulas, Math. Meth. Appl. Sci. **21** (1998) 1297-1342.

[12] J. Elschner, G. Schmidt, M. Yamamoto, An inverse problem in periodic diffractive optics: global uniqueness with a single wavenumber, Inverse Problems 19 (2003) 779-787.

[13] J. Elschner, M. Yamamoto, An inverse problem in periodic diffractive optics: Reconstruction of Lipschitz grating profiles, Applicable Analysis **81** (2002) 1307-1328.

[14] F. Hettlich, Iterative regularization schemes in inverse scattering by periodic structures, Inverse Problems **18** (2002) 701-714.

[15] K. Ito, F. Reitich, A high-order perturbation approach to profile reconstruction: I.Perfectly conducting gratings. Inverse Problems **15** (1999) 1067-1085.

[16] C.E. Kenig, Harmonic Analysis Techniques for Second Order Elliptic Boundary Value Problems, CBMS Regional Conference Series in Mathematics, No.83, American Mathematical Society, Providence, 1994.

[17] A. Kirsch, R. Kress, An optimization method in inverse acoustic scattering, in: Boundary elements IX, Vol. 3 (eds. Brebbia et al), Springer, Berlin, 1987, pp. 3-18.

[18] M. Mitrea, Boundary value problems and Hardy spaces associated to the Helmholtz equation in Lipschitz domains, J. Math. Anal. Appl. **202** (1996) 819-842.

[19] J. Nečas, Les Méthodes Directes en Théorie des Équations Elliptiques, Masson, Paris, 1967.

[20] J.C. Nedelec, F. Starling, Integral equation methods in a quasi–periodic diffraction problem for the time–harmonic Maxwell equation, SIAM J. Math. Anal. **22** (1991) 1679-1701.

[21] R. Petit (ed.), Electromagnetic Theory of Gratings, Springer, Berlin, 1980.

[22] G. Verchota, Layer potentials and regularity for the Dirichlet problem for Laplace's equation, J. Funct. Anal. **59** (1984) 572-611.

[23] A. Zinn, The numerical solution of an inverse scattering problem for time–harmonic acoustic waves, in: Inverse Problems and Imaging (ed. Roach), Pitman Research Notes in Mathematics Series, Vol. 245, Longman, London, 1991, pp. 242-263.