

A linear sampling method for inverse problems of diffraction gratings of mixed type

Guanghui Hu^a, Fenglong Qu^b and Bo Zhang^{c,*†}

Communicated by Andreas Kirsch

This paper is concerned with the direct and inverse problem of scattering of a time-harmonic wave by a Lipschitz diffraction grating of mixed type. The scattering problem is modeled by the mixed boundary value problem for the Helmholtz equation in the unbounded half-plane domain above a periodic Lipschitz surface on which a mixed Dirichlet and impedance boundary condition is imposed. We first establish the well-posedness of the direct problem, employing the variational method, and then extend Isakov's method to prove uniqueness in determining the Lipschitz diffraction grating profile by using point sources lying above the structure. Finally, we develop a periodic version of the linear sampling method to reconstruct the diffraction grating. In this case, the far field equation defined on the unit circle is replaced by a near field equation defined on a line above the surface, which is a linear integral equation of the first kind. Numerical results are also presented to illustrate the efficiency of the method in the case when the height of the unknown grating profile is not very large and the noise level of the near field measurements is not very high. Copyright © 2012 John Wiley & Sons, Ltd.

Keywords: inverse problem; diffraction gratings; linear sampling method; mixed boundary condition; Lipschitz surface

1. Introduction

Diffraction gratings are widely used in many areas of science and technology and have a long history (see [1, 2] for the physical and mathematical background). This paper is concerned with the problem of scattering of a time-harmonic (with the time variation $e^{-i\omega t}$, $\omega > 0$) electromagnetic wave by a partially coated perfectly reflecting grating in an isotropic lossless medium, which is modeled by the time-harmonic Maxwell equations together with a mixed boundary condition of perfectly conducting and conductive conditions. In this paper, we assume the grating to be periodic in the x_1 -direction and constant in the other directions and consider the transverse electric polarization case. In this case, the scattering problem is reduced to a mixed problem of Dirichlet and impedance boundary condition for the two-dimensional Helmholtz equation, $(\Delta + k^2)u = 0$, where u is the third coordinate component of the electric field $E = (0, 0, u(x_1, x_2))$ and $k > 0$ is the wave number depending on the index of refraction of the medium. Assume that the diffraction grating is described by a surface profile $\tilde{\Gamma} := \{(x_1, x_2) \in \mathbb{R}^2 : x_2 = f(x_1)\}$ with a 2π -periodic Lipschitz function $f(x_1) > 0$ for $x_1 \in \mathbb{R}$ and the isotropic lossless medium is denoted by $\tilde{\Omega} = \{(x_1, x_2) \in \mathbb{R}^2 : x_2 > f(x_1)\}$.

The direct problem is to compute the scattered field u^s in $\tilde{\Omega}$ when the incident wave u^i and the grating profile $\tilde{\Gamma}$ with the corresponding boundary conditions are given. There always exists a unique solution to the Dirichlet problem (see [3] for the case when the grating surface $\tilde{\Gamma}$ belongs to C^2 and [4] for the case when the grating surface $\tilde{\Gamma}$ is Lipschitz). It is known that the Neumann problem is not necessarily uniquely solvable in general. In this paper, we consider the mixed problem, that is, the problem with a mixed Dirichlet and impedance boundary condition being imposed on $\tilde{\Gamma}$.

We are more interested in the inverse problem of determining the grating profile $\tilde{\Gamma}$ from the knowledge of the scattered field measured on a straight line lying above the grating for a given wavenumber k and given incident waves u^i . Note that the propagating modes (or the 'far field data' in periodic case) for all incident directions are not enough to determine the grating profile uniquely; see [5]. Uniqueness results have been obtained for the cases of Dirichlet and Neumann problems [6–12]. In the case of a lossy medium (i.e., $\text{Im}(k) > 0$), it was shown in [6] that a C^2 -smooth perfectly reflecting grating profile f can be uniquely determined from the scattered

^aWeierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany

^bSchool of Mathematics and Informational Science, Yantai University, Yantai, Shandong, 264005, China

^cLSEC and Institute of Applied Mathematics, AMSS, Chinese Academy of Sciences, Beijing, 100190, China

*Correspondence to: Professor Bo Zhang, Institute of Applied Mathematics, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, 100190, China.

†E-mail: b.zhang@amt.ac.cn

fields for one incident plane wave. In the case of a lossless medium (i.e., $\text{Im}(k) = 0$), in general, global uniqueness with one incident wave is not true for the inverse problem. It has been shown in [11] that a finite number of incident plane waves are sufficient to identify a C^2 perfectly reflecting grating profile from the total field above the structure provided *a priori* information on the height of the grating surface is available. In particular, global uniqueness with one incident direction can be obtained if the wave number or the amplitude is sufficiently small; this, however, is not true for the general case. The uniqueness results of [11] have been extended to the inverse transmission problem in [13] with continuous total field and its normal derivative across the grating profile. Note that a uniqueness result was established in [14] for the inverse transmission problem with general transmission conditions on the grating profile. Global uniqueness results have been established for the inverse Dirichlet and Neumann problems with a minimal number of incident waves for the class of grating profiles given by the graph of a piecewise linear function or a step function in [8, 9]. These results have been extended to the case of general polygonal grating profiles in [7, 10]. It was shown in [7, 10] that without excluding the Rayleigh frequencies, two different directions are sufficient to recover the Dirichlet surface, whereas four are sufficient for the case of Neumann problems. If one excludes the Rayleigh frequencies, one incident wave is sufficient to determine the Dirichlet surface, whereas three are sufficient for the case of Neumann surfaces. It should be remarked that local stability estimates have been obtained in [15] for an inverse periodic medium and in [16] for an inverse transmission problem with a polygonal grating interface. A conditional (global) stability result was established in [17] for the inverse Dirichlet problem. For an overview of inverse diffraction grating problems, see [18].

Efficient numerical methods for the inverse problem studied in this paper are of great importance because of their wide and important applications in many areas. However, it is challenging to design efficient numerical algorithms for such inverse problems because they are both nonlinear and severely ill-posed. For the inverse problem of reconstructing perfectly reflecting grating profiles (i.e., the inverse Dirichlet problem), several numerical reconstruction algorithms have been proposed, such as the conjugate gradient algorithm based on analytic continuation [19], the iterative regularization method [20], the Kirsch–Kress two-step optimization algorithm [4, 21], and the factorization method of Kirsch [22, 23]. Note that the latter two approaches were originally developed for bounded obstacle scattering problems and do not need the solution of the direct scattering problems (see, e.g., [24, 25] and the references quoted there). The factorization method was also applied to the case of impedance boundary conditions [22]. The Kirsch–Kress method proposed in [4, 21] has been extended to an inverse periodic transmission problem in [26] with continuous total field and its normal derivative across the grating profile. A different reconstruction algorithm-based finite element and optimization techniques was proposed in [27] for the inverse periodic transmission problem.

In this paper, we apply the linear sampling method to our inverse problem of diffraction gratings with a mixed Dirichlet and impedance boundary condition on the grating profile. The linear sampling method was originally proposed in [28] for bounded obstacle acoustic scattering and does not need the solution of the direct scattering problem as well as the physical property of the scatterer (see also [29–31] for more details on its mathematical foundation, implementation, and other applications). In the current periodic case, instead of plane waves, we shall use point sources lying on Γ_b as incident waves. This is because uniqueness for the inverse problem using these incident point sources can be guaranteed (see Theorem 3.1) and also these incident point sources have a dense range on the grating surface Γ (see Lemmas 3.2 and 5.1). Furthermore, the far field equation defined on the unit circle for bounded obstacle scattering problems is replaced by a near field equation defined on a line Γ_b above the grating surface. This means that the evanescent waves are always included in our computation so that the quality of the reconstruction can be improved. We also refer to [22] for exploring the number of evanescent modes in order to obtain satisfactory reconstructions based on the factorization method and to [19, 21] using the scattered far field for several incident plane waves based on the optimization method. Another reason for considering near fields in scattering by diffraction gratings is the uniqueness issue that we will address in Section 3 (see Theorem 3.1).

This paper is organized as follows. In Section 2, the well-posedness of the direct scattering problem is established using the variational method. The uniqueness for the inverse problem is proved in Section 3 by Isakov’s method. The linear sampling method is proposed for the inverse Dirichlet problems in Section 4 first and then for the inverse mixed problem in Section 5. Numerical results are presented in Section 6 to illustrate the efficiency of the method.

2. The direct problem

In this section, we establish the well-posedness of the direct scattering problem by employing the variational method. Because of the periodicity of the problem, it can be reduced to a problem in a single period of the grating profile. To this end, we need the following notations:

$$\begin{aligned}\Gamma &= \{x \in \mathbb{R}^2 \mid x_2 = f(x_1), 0 < x_1 < 2\pi\}, \\ \Omega &= \{x \in \mathbb{R}^2 \mid x_2 > f(x_1), 0 < x_1 < 2\pi\}, \\ \Gamma_b &= \{(x_1, b) \mid 0 < x_1 < 2\pi\}, \\ \Omega_b &= \{x \in \Omega \mid x_2 < b\}\end{aligned}$$

for any $b > \max\{f(x_1) \mid x_1 \in \mathbb{R}\}$. Suppose a plane wave given by $u^i = e^{i(\alpha x_1 - \beta x_2)}$ with $(\alpha, \beta) = k(\sin \theta, \cos \theta)$ the incident on Γ from the top, where the wave number k is a positive constant and $\theta \in (-\pi/2, \pi/2)$ is the incident angle. We assume that Γ has a Lipschitz dissection $\Gamma = \Gamma_D \cup \Pi \cup \Gamma_I$, where Γ_D and Γ_I are disjoint and relatively open subsets of Γ having Π as their common boundary

(see [32, p. 99]). Then, in the case of transverse electric polarization for the scattering of u^i by the perfectly conducting diffraction gratings with a partially coated dielectric, the total field $u = u(x_1, x_2)$, which is the sum of u^i and the scattered field u^s , satisfies

$$\Delta u + k^2 u = 0 \quad \text{in } \Omega, \tag{2.1}$$

$$u = 0 \quad \text{on } \Gamma_D, \tag{2.2}$$

$$\frac{\partial u}{\partial \nu} + i\lambda u = 0 \quad \text{on } \Gamma_I, \tag{2.3}$$

where ν is the unit normal of Γ directed into Ω . In the case when $\Gamma_I = \emptyset$, the problem becomes the Dirichlet problem (the periodic structure is a perfectly conducting surface in the electromagnetic case or a sound-soft surface in the acoustic case). In the case when $\Gamma_I \neq \emptyset$, the structure is coated by a thin layer of material on Γ_I and is called a partially coated surface with the surface impedance $\lambda(x)$. In this paper, we assume that λ is a positive constant. We also require the total field u to be α -quasiperiodic in x_1 , which means that

$$u(x_1 + 2\pi, x_2) = e^{2i\alpha\pi} u(x_1, x_2), \tag{2.4}$$

or equivalently $u(x) \exp(-i\alpha x_1)$ is 2π -periodic with respect to x_1 . Note that the incident field u^i is α -quasiperiodic. Under the assumption (2.4), the function $u^s(x) \exp(-i\alpha x_1)$ is 2π -periodic with respect to x_1 and thus can be expanded as a Fourier series:

$$u^s(x_1, x_2) \exp(-i\alpha x_1) = \sum_{n \in \mathbb{Z}} u_n(x_2) e^{inx_1}.$$

Because u^s satisfies the Helmholtz equation (2.1) in Ω , then applying the method of separation of variables allows us to express u^s as a sum of plane waves:

$$u^s = \sum_{n \in \mathbb{Z}} \left[A_n e^{i\alpha_n x_1 + i\beta_n x_2} + B_n e^{i\alpha_n x_1 - i\beta_n x_2} \right], \quad A_n, B_n \in \mathbb{C},$$

where

$$\alpha_n = n + \alpha, \quad \beta_n = \begin{cases} (k^2 - \alpha_n^2)^{1/2} & \text{if } |\alpha_n| \leq k, \\ i(\alpha_n^2 - k^2)^{1/2} & \text{if } |\alpha_n| > k, \end{cases}$$

with $i = \sqrt{-1}$. Physically, the scattered field remains bounded as $x_2 \rightarrow +\infty$, so u^s is only composed of bounded outgoing waves in Ω , leading to the well-known Rayleigh expansion condition:

$$u^s = \sum_{n \in \mathbb{Z}} A_n e^{i\alpha_n x_1 + i\beta_n x_2} \quad \text{for } x_2 > f_+ = \max_{0 < x_1 < 2\pi} \{f(x_1)\} \tag{2.5}$$

with the Rayleigh coefficient $A_n \in \mathbb{C}$. It is clear that u^s in (2.5) can be split into the finite sum $\sum_{|\alpha_n| \leq k}$ of outgoing plane waves and the infinite sum $\sum_{|\alpha_n| > k}$ of exponentially decaying waves, which are called surface or evanescent waves.

We now introduce some periodic and quasiperiodic spaces that are needed in this paper. For $s \in \mathbb{R}$, $s \geq 0$, the Sobolev space $H^s(0, 2\pi)$ of periodic functions is defined as the completion of $\{u|_{[0, 2\pi]} : u \text{ is a trigonometric polynomial}\}$ with respect to the inner product

$$\langle u, v \rangle := \sum_{n \in \mathbb{Z}} (1 + n^2)^s u_n \bar{v}_n,$$

where u_n and v_n are the Fourier coefficients of u and v , respectively. Then the periodic Sobolev space $H_p^s(\Gamma)$ and the α -quasiperiodic Sobolev space $H^s(\Gamma)$ can be defined, respectively, by

$$H_p^s(\Gamma) = \{u : \Gamma \rightarrow \mathbb{C}, u(x_1, f(x_1)) \in H^s(0, 2\pi)\},$$

$$H^s(\Gamma) = \{u : \Gamma \rightarrow \mathbb{C}, u(x_1, f(x_1)) \exp(-i\alpha x_1) \in H^s(0, 2\pi)\}.$$

For $\Gamma_0 \subset \Gamma$, define

$$H^s(\Gamma_0) := \{u|_{\Gamma_0} : u \in H^s(\Gamma)\}, \quad \tilde{H}^s(\Gamma_0) := \{u \in H^s(\Gamma) : \text{supp}(u) \subseteq \bar{\Gamma}_0\}.$$

Then,

$$H^{-1/2}(\Gamma_0) := (\tilde{H}^{1/2}(\Gamma_0))', \quad \tilde{H}^{-1/2}(\Gamma_0) := (H^{1/2}(\Gamma_0))'.$$

Denote by $\langle H^{1/2}(\Gamma_0), \tilde{H}^{-1/2}(\Gamma_0) \rangle$ or $\langle \tilde{H}^{1/2}(\Gamma_0), H^{-1/2}(\Gamma_0) \rangle$, the dual form, which, in our setting, is the extension of the inner product of $L^2(\Gamma_0)$. Recall that $H^{1/2}(\Gamma)$ is the trace space of $H^1(\Omega_b)$ defined by

$$H^1(\Omega_b) = \{v \in H^1(\Omega_b) : v(x_1, x_2) \exp(-i\alpha x_1) \text{ is } 2\pi\text{-periodic with respect to } x_1\}.$$

$H_p^1(\Omega_b)$, $H_p^s(\Gamma_0)$, and $\tilde{H}_p^s(\Gamma_0)$ can be defined similarly as $H^1(\Omega_b)$, $H^s(\Gamma_0)$, and $\tilde{H}^s(\Gamma_0)$, respectively, by replacing α -quasiperiodic functions v with 2π -periodic functions v .

The basic space we use for the direct problem is

$$X = \{v \in H_p^1(\Omega_b) : v = 0 \text{ on } \Gamma_D\}$$

equipped with the Sobolev norm $\|\cdot\|_X$. If $\Gamma_D \neq \emptyset$, then, by Friedrich's inequality, the Sobolev norm $\|\cdot\|_X$ is equivalent to the norm $\|v\|_X$ defined by

$$\|v\|_X = \int_{\Omega_b} |\nabla_\alpha v|^2 dx$$

where $\nabla_\alpha := \nabla + i(\alpha, 0)$. For convenience, we write

$$\Delta_\alpha := \nabla_\alpha \cdot \nabla_\alpha = \Delta + 2i\alpha \partial_1 - \alpha^2, \quad \partial_{v,\alpha} = \frac{\partial}{\partial v} + i\alpha v_1.$$

In this paper, C may denote different positive constants in different places.

Given an incident plane wave $u^i = e^{i(\alpha x_1 - \beta x_2)}$, our goal is to prove that the direct problem (2.1)–(2.5) is well-posed, employing the variational method. To this end, we define the Dirichlet-to-Neumann map $T : H^{1/2}(\Gamma_b) \rightarrow H^{-1/2}(\Gamma_b)$ on an artificial boundary Γ_b by

$$Tv := \sum_{n \in \mathbb{Z}} i\beta_n v_n e^{i\alpha_n x_1} \quad \text{for } v(x_1) = \sum_{n \in \mathbb{Z}} v_n e^{i\alpha_n x_1} \in H^{1/2}(\Gamma_b).$$

The operator T is well defined and bounded because $\beta_n = i|\alpha_n| + O(1/|n|)$ as $|n| \rightarrow +\infty$. Clearly,

$$T(u^s|_{x_2=b}) = \frac{\partial u^s}{\partial x_2} \Big|_{\Gamma_b}, \quad T(u^i|_{x_2=b}) = i\beta e^{-i\beta b} e^{i\alpha x_1} = -\frac{\partial u^i}{\partial x_2} \Big|_{\Gamma_b}.$$

This implies that

$$T(u|_{\Gamma_b}) - \frac{\partial u}{\partial v} \Big|_{\Gamma_b} = 2i\beta e^{-i\beta b} e^{i\alpha x_1}, \tag{2.6}$$

which is equivalent to the Rayleigh expansion (2.5). Let $v(x) = u(x)e^{-i\alpha x_1}$. Then $v \in H_p^1(\Omega_b)$ satisfies $\Delta_\alpha v + k^2 v = 0$ in Ω_b with the boundary conditions

$$v = 0 \text{ on } \Gamma_D, \quad \partial_{v,\alpha} v + i\lambda v = 0 \text{ on } \Gamma_I, \quad Tv - \frac{\partial v}{\partial v} \Big|_{\Gamma_b} = 2i\beta e^{-i\beta b} \text{ on } \Gamma_b.$$

Let $w(x) = v(x) - e^{-i\beta x_2}$. Then the problem (2.1)–(2.3) can be reformulated as follows. Find $w \in H_p^1(\Omega_b)$ such that

$$\Delta_\alpha w + k^2 w = 0 \quad \text{in } \Omega, \tag{2.7}$$

$$w = g \quad \text{on } \Gamma_D, \tag{2.8}$$

$$\partial_{v,\alpha} w + i\lambda w = h \quad \text{on } \Gamma_I, \tag{2.9}$$

$$Tw - \frac{\partial w}{\partial v} = 0 \quad \text{on } \Gamma_b, \tag{2.10}$$

where $g = -e^{-i\alpha x_1} u^i \in H_p^{1/2}(\Gamma_D)$ and $h = -e^{-i\alpha x_1} (\frac{\partial u^i}{\partial v} + i\lambda u^i) \in H_p^{-1/2}(\Gamma_I)$.

Theorem 2.1

For $g \in H_p^{1/2}(\Gamma_D)$ and $h \in H_p^{-1/2}(\Gamma_I)$, if $\Gamma_I \neq \emptyset$, then the problem (2.7)–(2.10) is uniquely solvable in $H_p^1(\Omega_b)$ with the estimate

$$\|w\|_{H_p^1(\Omega_b)} \leq C \left(\|g\|_{H_p^{-1/2}(\Gamma_D)} + \|h\|_{H_p^{-1/2}(\Gamma_I)} \right), \tag{2.11}$$

where C is a positive constant independent of g and h .

Proof

We first prove the uniqueness of the solution. To do this, it is enough to prove that $w = 0$ in Ω_b if $g = 0$ and $h = 0$. Let $g = 0$ and $h = 0$. Then it follows from the weak formulation of the problem (2.7)–(2.10) with the test function replaced by w that

$$\int_{\Omega_b} |\nabla_\alpha w|^2 - k^2 |w|^2 dx - i \int_{\Gamma_I} \lambda |w|^2 ds - \int_{\Gamma_b} \bar{w} Tw ds = 0.$$

Taking the imaginary part of the previous equation gives

$$\int_{\Gamma_l} \lambda |w|^2 ds = -\text{Im} \int_{\Gamma_b} \overline{w} T w ds = -2\pi \sum_{|\alpha_n| \leq k} \beta_n |c_n|^2 \leq 0, \quad c_n = \frac{1}{2\pi} \int_0^{2\pi} w(x_1, b) e^{-inx_1} dx_1.$$

Because $\lambda > 0$, it follows that $w = 0$ on Γ_l , which, together with (2.9), implies that $\partial_{v,\alpha} w = 0$ on Γ_l . By Holmgren's uniqueness theorem and the analyticity of w , we obtain that $w = 0$ in Ω_b .

We now prove the existence of the solution. From [32], it is seen that there exists a $\tilde{g} \in H_p^{1/2}(\Gamma)$ such that \tilde{g} is the extension of g to Γ satisfying that $\|\tilde{g}\|_{H_p^{1/2}(\Gamma)} \leq C \|g\|_{H_p^{1/2}(\Gamma_D)}$, where C is independent of g . Consider the following Dirichlet problem:

$$\Delta_\alpha v_0 + k^2 v_0 = 0 \quad \text{in } \Omega, \quad v_0 = \tilde{g} \quad \text{on } \Gamma, \quad T v_0 - \frac{\partial v_0}{\partial \nu} = 0 \quad \text{on } \Gamma_b.$$

Arguing similarly as in [4], it is easy to show that the aforementioned Dirichlet problem has a unique weak solution $v_0 \in H_p^1(\Omega_b)$ satisfying the estimate

$$\|v_0\|_{H_p^1(\Omega_b)} \leq C \|\tilde{g}\|_{H_p^{1/2}(\Gamma)} \leq C \|g\|_{H_p^{1/2}(\Gamma_D)}, \tag{2.12}$$

where C is a constant independent of \tilde{g} . Let $w_0 = w - v_0$. Then, the problem (2.7)–(2.10) is equivalent to the following problem. Find $w_0 \in X$ such that

$$\Delta_\alpha w_0 + k^2 w_0 = 0 \quad \text{in } \Omega_b, \tag{2.13}$$

$$w_0 = 0 \quad \text{on } \Gamma_D, \tag{2.14}$$

$$\partial_{v,\alpha} w_0 + i\lambda w_0 = \tilde{h} \quad \text{on } \Gamma_l, \tag{2.15}$$

$$T w_0 - \frac{\partial w_0}{\partial \nu} = 0 \quad \text{on } \Gamma_b, \tag{2.16}$$

where $\tilde{h} = -\partial_{v,\alpha} v_0 - i\lambda v_0 + h \in H_p^{-1/2}(\Gamma_l)$. Because Γ_l is Lipschitz, then $\partial_{v,\alpha} v_0 \in H_p^{-1/2}(\Gamma_l)$ should be defined as follows:

$$\int_{\Gamma_l} \overline{\varphi} \partial_{v,\alpha} v_0 ds = \int_{\Omega_b} [-\nabla_\alpha v_0 \cdot \overline{\nabla_\alpha \varphi} + k^2 v_0 \overline{\varphi}] dx + \int_{\Gamma_b} \overline{\varphi} T v_0 ds, \quad \forall \varphi \in X. \tag{2.17}$$

Because w_0 vanishes on Γ_D , we can derive the following variational formulation for the problem (2.13)–(2.16):

$$\int_{\Omega_b} [\nabla_\alpha w_0 \cdot \overline{\nabla_\alpha \varphi} - k^2 w_0 \overline{\varphi}] dx - i \int_{\Gamma_l} \lambda \overline{\varphi} w_0 ds - \int_{\Gamma_b} \overline{\varphi} T w_0 ds = \int_{\Gamma_l} \tilde{h} \overline{\varphi} ds \tag{2.18}$$

for any $\varphi \in X$. Let

$$\begin{aligned} a(w_0, \varphi) &= \int_{\Omega_b} \nabla_\alpha w_0 \cdot \overline{\nabla_\alpha \varphi} dx - \int_{\Gamma_b} \overline{\varphi} T w_0 ds - i \int_{\Gamma_l} \lambda \overline{\varphi} w_0 ds, \\ b(w_0, \varphi) &= - \int_{\Omega_b} k^2 w_0 \overline{\varphi} ds, \quad L(\varphi) = \int_{\Gamma_l} \tilde{h} \overline{\varphi} ds. \end{aligned}$$

Then the variational problem (2.18) becomes

$$a(w_0, \varphi) + b(w_0, \varphi) = L(\varphi) \quad \forall \varphi \in X. \tag{2.19}$$

Set

$$w_n = \frac{1}{2\pi} \int_0^{2\pi} w_0(x_1, b) e^{-inx_1} dx_1, \quad \mathcal{U} = \{n \in \mathbb{Z} : \beta_n \text{ is a real number}\}.$$

Then, we have that, for $\varphi \in X$,

$$a(w_0, w_0) = \int_{\Omega_b} |\nabla_\alpha w_0|^2 dx + 2\pi \sum_{n \in \mathbb{Z} \setminus \mathcal{U}} |\beta_n| |w_n|^2 - i2\pi \sum_{n \in \mathcal{U}} \beta_n |w_n|^2 - i \int_{\Gamma_l} \lambda |w_0|^2 ds$$

and

$$|a(w_0, w_0)| \geq \int_{\Omega_b} |\nabla_\alpha w_0|^2 dx + \lambda \int_{\Gamma_l} |w_0|^2 ds \geq C \|w_0\|_{H_p^1(\Omega_b)}^2,$$

where the last inequality is derived by using Friedrich's inequality. From the boundedness of T and the trace theorem, it is seen that

$$|a(w_0, \varphi)| \leq C \|w_0\|_{H_p^1(\Omega_b)} \|\varphi\|_{H_p^1(\Omega_b)} \quad \forall \varphi \in X.$$

Hence, by the Lax–Milgram theorem, the first term $a(\cdot, \cdot)$ of (2.19) gives rise to a bijective operator on X , whereas, because the embedding $X \subset L^2(\Omega_b)$ is compact, the second term $b(\cdot, \cdot)$ defines a compact operator on X . From (2.12) and (2.17) together with the aid of the trace theorem and the boundedness of T , it follows that

$$\begin{aligned} |L(\varphi)| &\leq \int_{\Gamma_l} |\bar{\varphi} \partial_{\nu, \alpha} v_0| ds + \int_{\Gamma_l} |\lambda v_0 \bar{\varphi}| ds + \int_{\Gamma_l} |h \bar{\varphi}| ds \\ &\leq C \left[\|g\|_{H_p^{1/2}(\Gamma_D)} + \|h\|_{H_p^{-1/2}(\Gamma_l)} \right] \|\varphi\|_{H_p^1(\Omega_b)}, \end{aligned}$$

where C is a positive constant independent of g and h . The Riesz representation theorem implies that $L(\cdot)$ defines a linear bounded operator l on X with the estimate

$$\|l\|_1 = \|L\|_{X \rightarrow R} \leq C (\|g\|_{H_p^{1/2}(\Gamma_D)} + \|h\|_{H_p^{-1/2}(\Gamma_l)}).$$

Then a standard argument implies that the Fredholm alternative is applicable, which, together with the uniqueness part of the theorem, implies that the problem (2.19) has a unique solution $w_0 \in X$ satisfying the estimate

$$\|w_0\|_{H_p^1(\Omega_b)} \leq C \|l\|_1 \leq C (\|g\|_{H_p^{1/2}(\Gamma_D)} + \|h\|_{H_p^{-1/2}(\Gamma_l)}).$$

This yields the estimate

$$\begin{aligned} \|w\|_{H_p^1(\Omega_b)} &\leq \|w_0\|_{H_p^1(\Omega_b)} + \|v_0\|_{H_p^1(\Omega_b)} \\ &\leq C (\|g\|_{H_p^{1/2}(\Gamma_D)} + \|h\|_{H_p^{-1/2}(\Gamma_l)}), \end{aligned}$$

where C is a constant independent of g and h . The proof of the theorem is thus completed. \square

For the original scattering problem (2.1)–(2.5), we have the following well-posedness result (Theorem 2.2), which is a corollary of Theorem 2.1. To state this result, we need the free-space quasiperiodic Green function defined by

$$G(x, y) = \sum_{n \in \mathbb{Z}} \frac{i}{4\pi\beta_n} e^{i[\alpha_n(x_1 - y_1) + \beta_n|x_2 - y_2|]} \quad (2.20)$$

where $x, y \in \mathbb{R}^2$ with $x - y \neq n(2\pi, 0)$, $n \in \mathbb{Z}$, and the Rayleigh frequencies $\{k : \beta_n(k) = 0\}$ are excluded. It is known from [3] that $G(x, y)$ is weakly singular at $x = y$ and satisfies the Helmholtz equation in \mathbb{R}_+^2 when $x - y \neq n(2\pi, 0)$, $n \in \mathbb{Z}$.

Theorem 2.2

Let the incident field $u^i(x) = e^{ikx \cdot d}$ or $u^i(x) = G(x, y)$ for $y \in \Omega$. If the impedance coefficient $\lambda > 0$ on Γ_l , then the problem (2.1)–(2.5) is uniquely solvable in $H^1(\Omega_b)$ with the scattered field u^s satisfying that

$$\|u^s\|_{H^1(\Omega_b)} \leq C (\|\tilde{g}\|_{H^{1/2}(\Gamma_D)} + \|\tilde{h}\|_{H^{-1/2}(\Gamma_l)}),$$

where $\tilde{g} = -u^i|_{\Gamma_D} \in H^{1/2}(\Gamma_D)$, $\tilde{h} = -(\frac{\partial u^i}{\partial \nu} + i\lambda u^i)|_{\Gamma_l} \in H^{-1/2}(\Gamma_l)$, and C is a positive constant independent of \tilde{g} and \tilde{h} .

3. The inverse problem

In this section, we consider the inverse problem of determining the diffraction grating profile from a knowledge of the scattered field measured above the diffraction grating by using point sources lying above the grating as incident waves.

For $f_j \in C^{0,1}(0, 2\pi)$ and $\lambda_j > 0$, $j = 1, 2$, and for the incident wave $u^i = G(x, z)$, let $u_j^s(x; z)$ be the scattered field corresponding to $\Gamma_j = \{x \in \mathbb{R}^2 : x_2 = f_j(x_1), 0 < x_1 < 2\pi\}$ and the parameter λ_j , $j = 1, 2$. The purpose of this section is to prove the following uniqueness result on recovering the grating profile f and the parameter λ from the knowledge of the scattered field corresponding to incident point sources.

Theorem 3.1

Assume that $f_j \in C^{0,1}(0, 2\pi)$ is a partially coated diffraction grating profile with mixed sound-soft and impedance boundary conditions on Γ_j and $\lambda_j > 0$, $j = 1, 2$. For a fixed wave number $k > 0$, if the total fields u_1 and u_2 satisfy

$$u_1(x; z_n) = u_2(x; z_n) \quad \forall x \in \Gamma_a$$

for an infinite number of point sources $u^i(x) = G(x, z_n)$, $z_n \in \Gamma_a$, $n = 1, 2, \dots$, then $f_1 = f_2$ and $\lambda_1 = \lambda_2$, where $u_j(x; z_n) = u^i(x) + u_j^s(x; z_n)$, $j = 1, 2$.

To prove this theorem, we need the following denseness result for incident point sources.

Lemma 3.2

Let Λ be the restriction to one period $(0, 2\pi)$ of a 2π -periodic Lipschitz surface below Γ_a . Then the set $\{G(\cdot, z_n)|_\Lambda : z_n \in \Gamma_a, n = 1, 2, \dots\}$ is complete in $H^{1/2}(\Lambda)$.

Proof

Let $\varphi \in \widetilde{H}^{-1/2}(\Lambda)$ be such that

$$\int_\Lambda \overline{\varphi(x)} G(x, z_n) ds(x) = 0, \quad n = 1, 2, \dots$$

Then, to prove the lemma, it is enough to show that $\varphi = 0$ on Λ . Define

$$u(x) = \int_\Lambda G(y, x) \overline{\varphi(y)} ds(y) \quad \text{for } x \in \mathbb{R}_\pi^2 \setminus \Lambda,$$

where $\mathbb{R}_\pi^2 = \{x \in \mathbb{R}^2 : 0 < x_1 < 2\pi\}$. Then

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}_\pi^2 \setminus \Lambda, \quad u(z_n) = 0, \quad n = 1, 2, \dots$$

and $u(x)$ is an $-\alpha$ -quasiperiodic function satisfying the Rayleigh expansion condition above and below the grating Λ . By the unique continuation result for the Helmholtz equation on a line (see [33, Lemma 3.2]), we have $u = 0$ on Γ_a . Consequently, from the uniqueness result of the exterior Dirichlet problem and the analytic continuation of solutions to the Helmholtz equation, it follows that $u \equiv 0$ in $\Omega_\Lambda = \{x \in \mathbb{R}_\pi^2 : x \text{ lies above } \Lambda\}$, which, together with the trace theorem, implies that $u^+ = 0$ in $H^{1/2}(\Lambda)$. Here, the superscripts $+$ and $-$ indicate the limit obtained from Ω_Λ and $\mathbb{R}_\pi^2 \setminus \overline{\Omega_\Lambda}$, respectively. By the continuity of the single layer potential across Λ , it is found that $u^-(z) = 0$ on Λ . Thus, an application of the uniqueness result to the region below Λ gives that $u(x) \equiv 0$ in $\mathbb{R}_\pi^2 \setminus \overline{\Omega_\Lambda}$. Note that the classical layer potential theories on closed surfaces (see [24], [32, Theorem 6.10]) can be carried over to the present periodic case (see, e.g., [34]). Thus, from the jump relation of the normal derivative of the single layer potential u with $H^{-1/2}$ density, it is obtained that $\varphi = 0$ on Λ . The proof is complete. \square

Proof of Theorem 3.1

We first show that $u_1^s(\cdot; z) = u_2^s(\cdot; z)$ in G for any $z \in G_a$, where $G = \Omega_1 \cap \Omega_2$, $\Omega_j = \{x \in \mathbb{R}^2 : x_2 > f_j(x_1), 0 < x_1 < 2\pi\}$, $j = 1, 2$, and $G_a = \{x \in G : x_2 < a\}$. In fact, for each $z \in G_a$, we can always choose a smooth surface Λ lying above ∂G but below z . By Lemma 3.2, $\{G(\cdot, z_n)|_\Lambda : z_n \in \Gamma_a, n = 1, 2, \dots\}$ is dense in $H^{1/2}(\Lambda)$. Thus, for an arbitrarily small $\varepsilon > 0$, there exists a finite sequence $a_n \in \mathbb{C}$ such that

$$\|G(\cdot, z) - \sum_n a_n G(\cdot, z_n)\|_{H^{1/2}(\Lambda)} < \varepsilon.$$

Because both $G(\cdot, z)$ and $\sum_n a_n G(\cdot, z_n)$ satisfy the Helmholtz equation and the Rayleigh expansion condition below Λ , it follows from the well-posedness of the exterior Dirichlet boundary problem that

$$\|G(\cdot, z) - \sum_n a_n G(\cdot, z_n)\|_{H^1(K)} < \varepsilon$$

for a compact subset K lying below Λ such that $\Gamma_1 \cup \Gamma_2 \subset K$. By Theorem 2.2, we obtain that

$$\|u_j^s(x; z) - \sum_n a_n u_j^s(x, z_n)\|_{H^1(G_a)} < C\varepsilon, \quad j = 1, 2.$$

This, together with the fact that $u_1^s(x; z_n) = u_2^s(x; z_n)$ for $x \in G_a$, yields that

$$u_1^s(x; z) = u_2^s(x; z), \quad \forall x \in G, z \in G_a. \tag{3.1}$$

We now prove, by contradiction, that $f_1 = f_2$, similarly as in the proof of Theorem 3.1 in [12]. In fact, if $f_1 \neq f_2$, then we may assume without loss of generality that there is a point $x^* \in \Gamma_1 = \partial\Omega_1$ such that $x_\varepsilon := x^* + \nu(x^*)\varepsilon \in \Omega_1 \cap \Omega_2$ and $B_\varepsilon(x^*) \cap \Gamma_2 = \emptyset$ for some small disk $B_\varepsilon(x^*)$ centered at x^* with radius ε . Consider the following problems:

$$\begin{aligned} \Delta u_j^s(x; x_\varepsilon) + k^2 u_j^s(x; x_\varepsilon) &= 0 && \text{in } \Omega_j, \\ u_j^s(x; x_\varepsilon) &= -G(x, x_\varepsilon) && \text{on } \Gamma_{jD}, \\ \frac{\partial u_j^s(x; x_\varepsilon)}{\partial \nu} + i\lambda_j u_j^s(x; x_\varepsilon) &= -\frac{\partial G(x, x_\varepsilon)}{\partial \nu} - i\lambda_j G(x, x_\varepsilon) && \text{on } \Gamma_{jI}, \end{aligned}$$

where $j = 1, 2$. In the case when $x^* \in \Gamma_{1D}$, $u_1^\varepsilon(x_\varepsilon; x_\varepsilon) \sim O(\ln \varepsilon)$, but $u_2^\varepsilon(x_\varepsilon; x_\varepsilon)$ remains bounded as $\varepsilon \rightarrow 0^+$, whereas in the case when $x^* \in \Gamma_{1I}$, $v(x^*) \cdot \nabla u_1^\varepsilon(x_\varepsilon; x_\varepsilon) \sim O(1/\varepsilon)$, but $v(x^*) \cdot \nabla u_2^\varepsilon(x_\varepsilon; x_\varepsilon)$ remains bounded as $\varepsilon \rightarrow 0^+$. This is a contradiction because, by (3.1), $u_1^\varepsilon(x; x_\varepsilon) = u_2^\varepsilon(x; x_\varepsilon)$ for $x \in \Omega_1 \cap \Omega_2$. Thus we have $f_1 = f_2$.

We next prove that $\lambda_1 = \lambda_2$. Let $\Gamma_1 = \Gamma_2 = \Gamma$. Then $u_1 = u_2$ and $\partial u_1 / \partial \nu = \partial u_2 / \partial \nu$ on Γ . The boundary conditions

$$u_j = 0 \text{ on } \Gamma_{jD}, \quad \frac{\partial u_j}{\partial \nu} + i\lambda_j u_j = 0 \text{ on } \Gamma_{jI}$$

imply that $\Gamma_{1D} \cap \Gamma_{2I} = \emptyset$, because, otherwise, $u_1 = \partial u_1 / \partial \nu = 0$ on an open arc of Γ ; therefore, by Holmgren's uniqueness theorem, $u = 0$ in Ω , which is impossible. Thus, $\Gamma_{1I} = \Gamma_{2I} := \Gamma_I$, which yields that $(\lambda_1 - \lambda_2)u_1 = 0$ on Γ_I . Because $u_1 \neq 0$ in Ω , we have $\lambda_1 = \lambda_2$. The theorem is proved. \square

Remark 3.3

Our proof can be easily extended to the nonconstant impedance case, so Theorem 3.1 remains true if the impedance coefficient λ is a continuous function on Γ_I .

4. The linear sampling method for the Dirichlet problem

In this section, we consider the linear sampling method for the case when $\Gamma_I = \emptyset$, that is, the Dirichlet problem. To this end, we introduce the following operators. For $g \in L^2(\Gamma_a) := H^0(\Gamma_a)$ and $h \in H^{-1/2}(\Gamma)$, define

$$\begin{aligned} (Hg)(x) &= \int_{\Gamma_a} G(x, y)g(y)ds(y) \quad x \in \Gamma, \\ (S_1 h)(x) &= \int_{\Gamma} G(x, y)h(y)ds(y) \quad x \in \Gamma_a, \\ (S_2 h)(x) &= \int_{\Gamma} G(x, y)h(y)ds(y) \quad x \in \Gamma. \end{aligned}$$

Properties of these operators are summarized in the following lemma.

Lemma 4.1

- (i) $H : L^2(\Gamma_a) \rightarrow H^{1/2}(\Gamma)$ is an injective, bounded operator with dense range in $H^{1/2}(\Gamma)$.
- (ii) $S_1 : H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma_a)$ is an injective, compact operator with dense range in $H^{1/2}(\Gamma_a)$.
- (iii) The operator $S_2 : H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma)$ is a norm isomorphism.

Proof

- (i) For $x \in \Gamma$ and $y \in \Gamma_a$, the kernel $G(x, y)$ is continuous, which, together with a simple calculation of $\|H\varphi\|_{H^{1/2}(\Gamma)}$, implies the boundedness of H . From the proof of Lemma 3.2, it is seen that the dual operator $H^* : H^{-1/2}(\Gamma) \rightarrow L^2(\Gamma_a)$ of H defined by

$$(H^* \varphi)(y) = \int_{\Gamma} \overline{G(x, y)} \varphi(x) ds(x) = 0, \quad \varphi \in H^{-1/2}(\Gamma),$$

is injective. Thus, the range of H is dense in $H^{1/2}(\Gamma)$. The proof of Lemma 3.2 also yields that H is injective.

- (ii) The compactness of S_1 follows from the continuity of the kernel $G(x, y)$ for $x \in \Gamma_a$ and $y \in \Gamma$, whereas the injectivity and denseness property of S_1 follow from the proof of Lemma 3.2.
- (iii) From [23, Lemma 2.3], it is known that S_2 is a norm isomorphism. \square

We now take point sources $G(x, y)$ with $y \in \Gamma_a$ defined by (2.20) as incident waves $u_y^i(x)$ and write $u_y^s(x)$ for the scattered solution of the problem (2.1)–(2.3) corresponding to $u_y^i(x)$. To derive a periodic version of the linear sampling method, we consider the following near field equation:

$$\int_{\Gamma_a} u_y^s(x)g(y)ds(y) = G(x, z), \quad x \in \Gamma_a \tag{4.1}$$

for $z \in \mathbb{R}_x^2$. The near field operator $N : H^{1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma_a)$ is defined by

$$Nw = V|_{\Gamma_a}, \tag{4.2}$$

where V is the α -quasiperiodic solution to the exterior boundary value problem for the Helmholtz equation $\Delta V + k^2 V = 0$ with the Dirichlet boundary value w on Γ and satisfying the Rayleigh expansion condition (2.5). Note that the definition of the near

field operator N here differs from that in [22, Formula (9)], which corresponds to the input–output operator. For $h \in H^{-1/2}(\Gamma)$ and $g \in L^2(\Gamma_a)$, define

$$\begin{aligned}(\tilde{S}h)(x) &= \int_{\Gamma} G(x, y)h(y)ds(y), \quad x \in \mathbb{R}^2_{\pi} \setminus \Gamma, \\(Fg)(x) &= \int_{\Gamma_a} u_y^s(x)g(y)ds(y), \quad x \in \Gamma_a.\end{aligned}$$

Obviously,

$$\begin{aligned}(\tilde{S}h)(x)|_{\Gamma} &= (S_2h)(x), & (\tilde{S}h)(x)|_{\Gamma_a} &= (S_1h)(x), \\(Fg)(x) &= -(NHg)(x), & (S_1h)(x) &= (NS_2h)(x),\end{aligned}$$

which implies that

$$F(g) = -S_1S_2^{-1}H(g), \quad \text{Range}(S_1) = \text{Range}(N). \tag{4.3}$$

Clearly, the near field equation (4.1) is equivalent to

$$(Fg)(x) = G(x, z), \quad x \in \Gamma_a \tag{4.4}$$

for $z \in \mathbb{R}^2_{\pi}$.

The region Ω can be characterized by the following lemma, which is a corollary of Theorems 3.3 and 3.4 in [23].

Lemma 4.2

$G(\cdot, z)|_{\Gamma_a}$ is in the range of N if and only if $z \in \mathbb{R}^2_{\pi} \setminus \overline{\Omega}$.

Now, we present the main theorem for the Dirichlet problem.

Theorem 4.3

Assume that the incident field $u_y^i(x) = G(x, y)$ and Γ is Lipschitz with $\Gamma_l = \emptyset$.

(i) If $z \in \mathbb{R}^2_{\pi} \setminus \overline{\Omega}$, then for any $\varepsilon > 0$, there exists $g_z^{\varepsilon} \in L^2(\Gamma_a)$ such that

$$\|Fg_z^{\varepsilon} - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < \varepsilon \quad \text{and} \quad \|g_z^{\varepsilon}\|_{L^2(\Gamma_a)} \rightarrow \infty \quad \text{as } z \rightarrow \Gamma^-.$$

(ii) If $z \in \Omega$, then for any $\varepsilon > 0$ and $\delta > 0$, there exists $g_z^{\varepsilon, \delta} \in L^2(\Gamma_a)$ such that

$$\|Fg_z^{\varepsilon, \delta} - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < \varepsilon + \delta \quad \text{and} \quad \|g_z^{\varepsilon, \delta}\|_{L^2(\Gamma_a)} \rightarrow \infty \quad \text{as } \delta \rightarrow 0.$$

Proof

(i) If $z \in \mathbb{R}^2_{\pi} \setminus \overline{\Omega}$, then $-G(\cdot, z)|_{\Gamma_a} = N(-G(\cdot, z)|_{\Gamma})$ is in the range of S_1 . Thus, there exists $h_z \in H^{-1/2}(\Gamma)$ such that $(S_1h_z)(x) = -G(x, z)$ for $x \in \Gamma_a$. Because $S_2h_z \in H^{1/2}(\Gamma)$, then, by Lemma 4.1, for any $\varepsilon > 0$, there is $g_z^{\varepsilon} \in L^2(\Gamma_a)$ such that

$$\|Hg_z^{\varepsilon} - S_2h_z\|_{H^{1/2}(\Gamma)} < \varepsilon, \tag{4.5}$$

$$\|S_2^{-1}Hg_z^{\varepsilon} - h_z\|_{H^{-1/2}(\Gamma)} < C\varepsilon \tag{4.6}$$

for some constant $C > 0$. From the boundedness of S_1 and (4.3), it follows that

$$\|S_1S_2^{-1}Hg_z^{\varepsilon} - S_1h_z\|_{H^{1/2}(\Gamma_a)} < C\varepsilon,$$

$$\|Fg_z^{\varepsilon} - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < C\varepsilon.$$

Because $-G(x, z) = (S_1h_z)(x) = (NS_2h_z)(x)$ for $x \in \Gamma_a$ and $-G(\cdot, z)|_{\Gamma_a} = N(-G(\cdot, z)|_{\Gamma})$, we have $-G(\cdot, z)|_{\Gamma} = S_2h_z$. By (4.5), we get

$$\begin{aligned}\lim_{z \rightarrow \Gamma^-} \|Hg_z^{\varepsilon}\|_{H^{1/2}(\Gamma)} &\geq \lim_{z \rightarrow \Gamma^-} \|S_2h_z\|_{H^{1/2}(\Gamma)} - \varepsilon \\&\geq \lim_{z \rightarrow \Gamma^-} \|G(\cdot, z)\|_{H^{1/2}(\Gamma)} - \varepsilon \\&= \infty,\end{aligned}$$

which, together with the boundedness of H (Lemma 4.1 (i)), implies that

$$\|g_z^{\varepsilon}\|_{L^2(\Gamma_a)} \rightarrow \infty \quad \text{as } z \rightarrow \Gamma^-.$$

(ii) If $z \in \Omega$, then, by Lemma 4.2, $G(\cdot, z)$ is not in the range of N and is therefore not in the range of S_1 either. This means that the equation

$$S_1 h_z = G(\cdot, z)|_{\Gamma_a} \tag{4.7}$$

has no solution in $H^{-1/2}(\Gamma)$. However, because $S_1 : H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma_a)$ is compact and has a dense range in $H^{1/2}(\Gamma_a)$, then for each $\delta > 0$, we may obtain an approximate solution to the equation (4.7) by using the Tikhonov regularization:

$$h_z^{\gamma(\delta)} = \sum_{n \in \mathbb{N}} \frac{\mu_n}{\gamma(\delta) + \mu_n^2} (G(\cdot, z), g_n) \varphi_n.$$

Here, (μ_n, φ_n, g_n) is a singular system of S_1 and $\gamma(\delta)$ is the regularization parameter chosen by the following Morozov discrepancy principle (see [24]):

$$\|S_1 h_z^{\gamma(\delta)} - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} = \delta,$$

or equivalently,

$$\sum_{n \in \mathbb{N}} \frac{\Lambda^2}{(\Lambda + \mu_n^2)^2} |(G(\cdot, z), g_n)|^2 = \delta^2. \tag{4.8}$$

From Picard's Theorem (see [24]) and (4.8), it follows that

$$\|h_z^{\gamma(\delta)}\|_{H^{-1/2}(\Gamma)} \rightarrow \infty, \quad \gamma(\delta) \rightarrow 0, \quad \text{as } \delta \rightarrow 0. \tag{4.9}$$

By Lemma 4.1, it is seen that, for any $\varepsilon > 0$, there exists $g_z^{\varepsilon, \delta} \in L^2(\Gamma_a)$ such that

$$\|S_2^{-1} H g_z^{\varepsilon, \delta} - h_z^{\gamma(\delta)}\|_{H^{1/2}(\Gamma_a)} < \varepsilon. \tag{4.10}$$

From this, it follows that

$$\|S_1 S_2^{-1} H g_z^{\varepsilon, \delta} - S_1 h_z^{\gamma(\delta)}\|_{H^{1/2}(\Gamma_a)} = \|F g_z^{\varepsilon, \delta} + S_1 h_z^{\gamma(\delta)}\|_{H^{1/2}(\Gamma_a)} < C\varepsilon.$$

This, together with (4.9), implies that

$$\|F g_z^{\varepsilon, \delta} - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < C\varepsilon + \delta.$$

Combining (4) and (4.10) gives

$$\|g_z^{\varepsilon, \delta}\|_{L^2(\Gamma)} \rightarrow \infty, \quad \|H g_z^{\varepsilon, \delta}\|_{H^{1/2}(\Gamma)} \rightarrow \infty \quad \text{as } \delta \rightarrow 0.$$

The proof is thus complete. □

5. The linear sampling method for the mixed problem

In this section, we extend the linear sampling method for the Dirichlet problem to the mixed problem, that is, the case when $\Gamma_I \neq \emptyset$. In this case, the near field operator $N : H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma_I) \rightarrow H^{1/2}(\Gamma_a)$ is defined by

$$N(\varphi, \psi) = u^s|_{\Gamma_a}, \quad h_1 \in H^{1/2}(\Gamma_D), h_2 \in H^{-1/2}(\Gamma_I),$$

where u^s satisfying the Rayleigh expansion (2.5) is the unique solution to

$$\Delta u^s + k^2 u^s = 0 \text{ in } \Omega, \quad u^s = \varphi \text{ on } \Gamma_D, \quad \partial_\nu u^s + i\lambda u^s = \psi \text{ on } \Gamma_I. \tag{5.1}$$

It should be pointed out that, in this section, the incident wave $u_y^i(x)$ is taken as

$$u_y^i(x) := u^i(x, y) = \overline{G(y, x)},$$

which is different from the previous section. By the definition of $G(x, y)$ it is seen that such $u_y^i(x)$ satisfies the Rayleigh expansion condition (2.5) and therefore propagates upward and does not appear to be meaningful as incident waves. However, in the next section, we will present the method of Arens and Kirsch [23] for generating the scattered field using the aforementioned incident waves.

We write the near field equation (4.1) as

$$(Fg) = -(NHg), \tag{5.2}$$

where $H: L^2(\Gamma_a) \rightarrow H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma_I)$ is now defined by

$$(Hg)(x) = \begin{cases} \int_{\Gamma_a} u_y^j(x)g(y)ds(y), & x \in \Gamma_D, \\ \left(\frac{\partial}{\partial \nu(x)} + i\lambda\right) \int_{\Gamma_a} u_y^j(x)g(y)ds(y), & x \in \Gamma_I. \end{cases}$$

Lemma 5.1

The range of H is dense in $H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma_I)$.

Proof

Let $\varphi \times \psi \in \widetilde{H}^{-1/2}(\Gamma_D) \times \widetilde{H}^{1/2}(\Gamma_I)$. To prove the lemma, it is enough to show that $\varphi = 0$ and $\psi = 0$ under the assumption that

$$\langle Hg, \varphi \times \psi \rangle := \langle Hg, \varphi \rangle_{H^{1/2}(\Gamma_D) \times \widetilde{H}^{-1/2}(\Gamma_D)} + \langle Hg, \psi \rangle_{H^{-1/2}(\Gamma_I) \times \widetilde{H}^{1/2}(\Gamma_I)} = 0 \tag{5.3}$$

for any $g \in L^2(\Gamma_a)$. By (5.3), we obtain that

$$\int_{\Gamma_D} \int_{\Gamma_a} u^i(x,y)g(y)ds(y)\overline{\varphi}(x)ds(x) + \int_{\Gamma_I} \left(\frac{\partial}{\partial \nu(x)} + i\lambda\right) \int_{\Gamma_a} u_y^i(x)g(y)ds(y)\overline{\psi}(x)ds(x) = 0,$$

which gives on exchanging the order of integration that

$$\int_{\Gamma_D} u_y^i(x)\overline{\varphi}(x)ds(x) + \int_{\Gamma_I} \left(\frac{\partial}{\partial \nu(x)} + i\lambda\right)u_y^i(x)\overline{\psi}(x)ds(x) = 0, \quad \text{for almost all } y \in \Gamma_a.$$

Let

$$u(y) = \int_{\Gamma_D} G(y,x)\varphi(x)ds(x) + \int_{\Gamma_I} \left(\frac{\partial}{\partial \nu(x)} - i\lambda\right)G(y,x)\psi(x)ds(x).$$

Then $u(y)$ is a α -quasiperiodic solution of the Helmholtz equation in $\mathbb{R}^2_\pi \setminus \Gamma$ with the Dirichlet condition on Γ_a . Furthermore, $u(y)$ propagates upward above Γ satisfying the Rayleigh expansion condition (2.5) and downward below Γ satisfying the Rayleigh expansion condition (2.5) with α replaced by $-\alpha$. From the uniqueness of the exterior Dirichlet problem and the analyticity of $u(y)$, it is found that $u(y) \equiv 0$ in Ω . By the jump relations of the single and double layer potentials, we get

$$u^+|_{\Gamma_D} - u^-|_{\Gamma_D} = 0, \quad \left(\frac{\partial u^+}{\partial \nu} - i\lambda u^+\right)\Big|_{\Gamma_I} - \left(\frac{\partial u^-}{\partial \nu} - i\lambda u^-\right)\Big|_{\Gamma_I} = 0,$$

where the superscripts $+$ and $-$ indicate the limit obtained from Ω and $\mathbb{R}^2_\pi \setminus \overline{\Omega}$, respectively. Thus,

$$\begin{aligned} \Delta u + k^2 u &= 0 & \text{in } \mathbb{R}^2_\pi \setminus \overline{\Omega}, \\ u^- &= 0 & \text{on } \Gamma_D, \\ \frac{\partial u^-}{\partial \nu} - i\lambda u^- &= 0 & \text{on } \Gamma_I. \end{aligned}$$

A similar argument as in Section 2 can be used to show the existence of a unique solution to the aforementioned scattering problem satisfying the Rayleigh expansion condition (2.5) with α replaced by $-\alpha$. In particular, we have $u \equiv 0$ in $\mathbb{R}^2_\pi \setminus \overline{\Omega}$. By the jump relation across Γ of the potential u again, we get

$$0 = \frac{\partial u^+}{\partial \nu}\Big|_{\Gamma_D} - \frac{\partial u^-}{\partial \nu}\Big|_{\Gamma_D} = -\varphi, \quad 0 = u^+|_{\Gamma_I} - u^-|_{\Gamma_I} = \psi.$$

This completes the proof of the lemma. □

We now derive a periodic Green representation formula.

Lemma 5.2

If $u \in H^1(\Omega_b)$ for any $b > \max_{t \in \mathbb{R}} f(t)$ and satisfies the Rayleigh expansion condition (2.5), then for every $x \in \Omega$, we have

$$u(x) = \int_{\Gamma} \left[u(y) \frac{\partial G(x,y)}{\partial \nu(y)} - \frac{\partial u(y)}{\partial \nu(y)} G(x,y) \right] ds(y),$$

where $G(x,y)$ is the quasiperiodic Green function defined by (2.20).

Proof

Fix $x = (x_1, x_2) \in \Omega$ and choose $b > x_2$. Denote by $B(x, \delta)$ the small ball centered at x with radius δ such that $B(x, \delta) \subset \Omega_b$. The application of the second Green formula to the region $\Omega_b \setminus B(x, \delta)$ gives

$$\begin{aligned} 0 &= \int_{\partial(\Omega_b \setminus B(x, \delta))} \left[\frac{\partial u(y)}{\partial v(y)} G(x, y) - u(y) \frac{\partial G(x, y)}{\partial v(y)} \right] ds(y) \\ &= \left(- \int_{\Gamma} + \int_{\Gamma_b} + \int_{\partial B(x, \delta)} + \int_{\Gamma'} \right) \left[\frac{\partial u(y)}{\partial v(y)} G(x, y) - u(y) \frac{\partial G(x, y)}{\partial v(y)} \right] ds(y) \\ &:= I_1 + I_2 + I_3 + I_4, \end{aligned} \tag{5.4}$$

where $\Gamma' = \{(0, y_2) \cup (2\pi, y_2) : f(0) < y_2 < b\}$. From the Rayleigh expansion condition (2.5) of u and the definition of $G(x, y)$, it is seen that

$$\begin{aligned} I_2 &= \int_{\Gamma_b} \left[\frac{\partial u(y)}{\partial v(y)} G(x, y) - u(y) \frac{\partial G(x, y)}{\partial v(y)} \right] ds(y) \\ &= \int_0^{2\pi} \left[\frac{\partial u(y)}{\partial y_2} G(x, y) - u(y) \frac{\partial G(x, y)}{\partial y_2} \right] dy_1 = 0. \end{aligned} \tag{5.5}$$

From the periodicity of $f(x_1)$ with period 2π , it follows that

$$I_4 = \int_{\Gamma'} \left[\frac{\partial u(y)}{\partial v(y)} G(x, y) - u(y) \frac{\partial G(x, y)}{\partial v(y)} \right] ds(y) = 0. \tag{5.6}$$

Denote by $H_0^{(1)}(t)$ the Hankel function of the first kind of order zero. Then $\Phi(x, y) := (i/4)H_0^{(1)}(k|x - y|)$ is the fundamental solution of the Helmholtz equation in \mathbb{R}^2 . It has been shown in [3] that $G(x, y)$ has the same singularity as $\Phi(x, y)$ and that $\Phi(x, y) - G(x, y)$ is analytic in $[(0, 2\pi) \times \mathbb{R}] \times [(0, 2\pi) \times \mathbb{R}]$. Thus,

$$\begin{aligned} I_3 &= \int_{\partial B(x, \delta)} \left[\frac{\partial u(y)}{\partial v(y)} G(x, y) - u(y) \frac{\partial G(x, y)}{\partial v(y)} \right] ds(y) \\ &= \int_{\partial B(x, \delta)} \left[\frac{\partial u(y)}{\partial v(y)} [G(x, y) - \Phi(x, y)] - u(y) \frac{\partial [G(x, y) - \Phi(x, y)]}{\partial v(y)} \right] ds(y) \\ &\quad + \int_{\partial B(x, \delta)} \left[\frac{\partial u(y)}{\partial v(y)} \Phi(x, y) - u(y) \frac{\partial \Phi(x, y)}{\partial v(y)} \right] ds(y) \rightarrow -u(x), \end{aligned} \tag{5.7}$$

as $\delta \rightarrow 0$. Combining (5.4)–(5.7) and letting $\delta \rightarrow 0$ give the required result. The proof is thus complete. □

Lemma 5.3

The near field operator N is injective and compact with dense range in $H^{1/2}(\Gamma_a)$.

Proof

By the well-posedness of the exterior mixed boundary problem (2.7)–(2.10), it is easy to see that N is injective and bounded. By the definition of N , there exists a function u satisfying the Rayleigh expansion condition (2.5) such that $N(\varphi, \psi) = u(\cdot)|_{\Gamma_a}$. The near field operator N can be decomposed into $N = N_1 N_2$, where

$$N_1 : H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma), \quad N_2 : H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma_a)$$

are defined by

$$N_1(\varphi, \psi) = (u|_{\Gamma}, \partial_\nu u|_{\Gamma}), \quad N_2(u|_{\Gamma}, \partial_\nu u|_{\Gamma}) := u|_{\Gamma_a},$$

respectively. From the well-posedness of the exterior mixed boundary problem, it is seen that N_1 is bounded, and from Lemma 5.2, it follows that N_2 is compact. Thus, N is a compact operator.

We now prove that the range of N is dense in $H^{1/2}(\Gamma_a)$. To this end, let $h \in \widetilde{H}^{-1/2}(\Gamma_a)$ be such that

$$\langle N(\varphi, \psi), h \rangle_{H^{1/2}(\Gamma_a) \times \widetilde{H}^{-1/2}(\Gamma_a)} = 0, \quad \forall \varphi \in H^{1/2}(\Gamma_D), \psi \in H^{-1/2}(\Gamma). \tag{5.8}$$

Then, it is sufficient to prove that $h = 0$. By Lemma 5.2, we have

$$\begin{aligned} &\langle N(\varphi, \psi), h \rangle_{H^{1/2}(\Gamma_a) \times \widetilde{H}^{-1/2}(\Gamma_a)} \\ &= \int_{\Gamma_a} u(x) \bar{h}(x) ds(x) \\ &= \int_{\Gamma_a} \left(\int_{\Gamma} \left[u(y) \frac{\partial G(x, y)}{\partial v(y)} - \frac{\partial u(y)}{\partial v(y)} G(x, y) \right] ds(y) \right) \bar{h}(x) ds(x) \\ &= \int_{\Gamma} \left[u(y) \frac{\partial V_h(y)}{\partial v(y)} - \frac{\partial u(y)}{\partial v(y)} V_h(y) \right] ds, \end{aligned} \tag{5.9}$$

where $V_h(y) = \int_{\Gamma_a} G(x, y) \bar{h}(x) ds(x)$, $y \in \mathbb{R}^2_\pi \setminus \Gamma_a$. Let \tilde{u}_h be the $(-\alpha)$ -quasiperiodic radiating solution to the problem:

$$\Delta \tilde{u}_h + k^2 \tilde{u}_h = 0 \quad \text{in } \Omega, \tag{5.10}$$

$$\tilde{u}_h = V_h \quad \text{on } \Gamma_D, \tag{5.11}$$

$$\frac{\partial \tilde{u}_h}{\partial \nu} + i\lambda \tilde{u}_h = \frac{\partial V_h}{\partial \nu} + i\lambda V_h \quad \text{on } \Gamma_I. \tag{5.12}$$

From the second Green formula and the Rayleigh expansion of \tilde{u}_h and u , it follows that

$$\int_{\Gamma} \left[u \frac{\partial \tilde{u}_h}{\partial \nu} - \frac{\partial u}{\partial \nu} \tilde{u}_h \right] ds = \int_{\Gamma_a} \left[u \frac{\partial \tilde{u}_h}{\partial \nu} - \frac{\partial u}{\partial \nu} \tilde{u}_h \right] ds = 0,$$

which, together with (5.11) and (5.12), implies that

$$-\int_{\Gamma_D} V_h \frac{\partial u}{\partial \nu} ds + \int_{\Gamma_I} \left[u \frac{\partial V_h}{\partial \nu} + i\lambda u V_h \right] ds = -\int_{\Gamma_D} \varphi \frac{\partial \tilde{u}_h}{\partial \nu} ds + \int_{\Gamma_I} \tilde{u}_h \psi ds.$$

This, together with (5.9), yields

$$\begin{aligned} & \langle N(\varphi \times \psi), h \rangle_{H^{1/2}(\Gamma_a) \times H^{-1/2}(\Gamma_a)} \\ &= \int_{\Gamma_D} \left[\varphi \frac{\partial V_h}{\partial \nu} - \frac{\partial u}{\partial \nu} V_h \right] ds + \int_{\Gamma_I} \left[u \frac{\partial V_h}{\partial \nu} + i\lambda u V_h \right] ds - \int_{\Gamma_I} \psi V_h ds \\ &= \int_{\Gamma_D} \varphi \left(\frac{V_h}{\partial \nu} - \frac{\partial \tilde{u}_h}{\partial \nu} \right) ds + \int_{\Gamma_I} \psi (\tilde{u}_h - V_h) ds. \end{aligned}$$

From this equation, it can be seen that the dual operator of N is given by

$$N^*h = \left(\frac{\partial \bar{V}_h}{\partial \nu} - \frac{\partial \bar{\tilde{u}}_h}{\partial \nu}, \bar{\tilde{u}}_h - \bar{V}_h \right) \in \tilde{H}^{-1/2}(\Gamma_D) \times \tilde{H}^{1/2}(\Gamma_I).$$

From (5.8), we see that $N^*h = 0$, so

$$\frac{\partial V_h}{\partial \nu} = \frac{\partial \tilde{u}_h}{\partial \nu} \quad \text{on } \Gamma_D, \quad \tilde{u}_h = V_h \quad \text{on } \Gamma_I. \tag{5.13}$$

Combining (5.11), (5.12), and (5.13) gives that $\partial V_h / \partial \nu = \partial \tilde{u}_h / \partial \nu$ and $\tilde{u}_h = V_h$ on Γ . Thus, by Holmgren's uniqueness theorem, $\tilde{u}_h = V_h$ in Ω_a . Because $\tilde{u}_h = V_h$ on Γ_a and both $\tilde{u}_h(x)$ and $V_h(x)$ satisfy the $(-\alpha)$ -quasiperiodic Rayleigh expansion condition for $x_2 > a$, it follows from the uniqueness result of the exterior Dirichlet problem that $\tilde{u}_h = V_h$ for $x_2 > a$. Now, in view of the fact that \tilde{u}_h is analytic in Ω , we have by the jump relation of $\partial V_h(y) / \partial \nu(y)$ as $y \rightarrow \Gamma_a^-$ that

$$\bar{h} = \frac{\partial V_h^+}{\partial \nu} \Big|_{\Gamma_a} - \frac{\partial V_h^-}{\partial \nu} \Big|_{\Gamma_a} = \frac{\partial \tilde{u}_h^+}{\partial \nu} \Big|_{\Gamma_a} - \frac{\partial \tilde{u}_h^-}{\partial \nu} \Big|_{\Gamma_a} = 0,$$

which completes the proof of the lemma. □

We are now ready to analyze the near field equation (5.2). Combining Lemmas 5.1 and 5.3, the linear sampling method for the mixed problem can be proved, similarly as in the case of Dirichlet problems.

Theorem 5.4

Assume that $\Gamma_I \neq \emptyset$ and assume that $u_y^\varepsilon(x)$ is the unique scattered solution corresponding to the incident wave $u_y^i(x) = \overline{G(y, x)}$, $y \in \Gamma_a$.

(i) If $z \in \mathbb{R}^2_\pi \setminus \overline{\Omega}$, then for any $\varepsilon > 0$, there exists $g_z^\varepsilon \in L^2(\Gamma_a)$ such that

$$\|Fg_z^\varepsilon - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < \varepsilon, \quad \|g_z^\varepsilon\|_{L^2(\Gamma_a)} \rightarrow \infty \quad \text{as } z \rightarrow \Gamma^-.$$

(ii) If $z \in \Omega$, then for any $\varepsilon > 0$ and $\delta > 0$, there exists $g_z^{\varepsilon, \delta} \in L^2(\Gamma_a)$ such that

$$\|Fg_z^{\varepsilon, \delta} - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < \varepsilon + \delta, \quad \|g_z^{\varepsilon, \delta}\|_{L^2(\Gamma_a)} \rightarrow \infty \quad \text{as } \delta \rightarrow 0.$$

Proof

- (i) Let $z \in \mathbb{R}^2_\pi \setminus \bar{\Omega}$. In this case, $-G(\cdot, z)|_{\Gamma_a} = N(h_1, h_2)$ with $h_1 = -G(\cdot, z)|_{\Gamma_D}$ and $h_2 = -\left(\frac{\partial}{\partial \nu} + i\lambda\right)G(\cdot, z)|_{\Gamma_1}$. By Lemma 5.1, there is $g_z^\varepsilon \in L^2(\Gamma_a)$ satisfying that

$$\|Hg_z^\varepsilon - (h_1, h_2)\|_{H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma_1)} < \varepsilon.$$

By the boundedness of N , we have

$$\|NHg_z^\varepsilon - N(h_1, h_2)\|_{H^{1/2}(\Gamma_a)} < C\varepsilon,$$

that is,

$$\|Fg_z^\varepsilon - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < C\varepsilon.$$

Further, when $z \rightarrow \Gamma^-$, we get

$$\lim_{z \rightarrow \Gamma^-} \|Hg_z^\varepsilon\|_{H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)} \geq \lim_{z \rightarrow \Gamma^-} \|(h_1, h_2)\|_{H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)} - \varepsilon = \infty,$$

which implies that $\|g_z^\varepsilon\|_{L^2(\Gamma_a)} \rightarrow \infty$ as $z \rightarrow \Gamma^-$.

- (ii) If $z \in \Omega$ then, by Lemma 4.2, $G(\cdot, z)$ is not in the range of N , so $N(h_1, h_2) = G(\cdot, z)|_{\Gamma_a}$ has no solution in $H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma_1)$. However, because $N: H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma_1) \rightarrow H^{1/2}(\Gamma_a)$ is compact and has a dense range in $H^{1/2}(\Gamma_a)$, then for every $\delta > 0$, we may solve $N(h_1^{\gamma(\delta)}, h_2^{\gamma(\delta)}) = G(\cdot, z)|_{\Gamma_a}$ by the Tikhonov regularization with the parameter $\gamma = \gamma(\delta)$ determined by the Morozov discrepancy principle such that

$$\|N(h_1^{\gamma(\delta)}, h_2^{\gamma(\delta)}) - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < \delta, \tag{5.14}$$

$$\|(h_1^{\gamma(\delta)}, h_2^{\gamma(\delta)})\|_{H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma_1)} \rightarrow \infty, \quad \gamma(\delta) \rightarrow 0, \quad \text{as } \delta \rightarrow 0. \tag{5.15}$$

It follows from Lemma 5.3 that for any $\varepsilon > 0$, there exists $g_z^{\varepsilon, \delta} \in L^2(\Gamma_a)$ such that

$$\|Hg_z^{\varepsilon, \delta} - (h_1^{\gamma(\delta)}, h_2^{\gamma(\delta)})\|_{H^{1/2}(\Gamma_D) \times H^{-1/2}(\Gamma_1)} < \varepsilon, \tag{5.16}$$

which implies that

$$\|NHg_z^{\varepsilon, \delta} - N(h_1^{\gamma(\delta)}, h_2^{\gamma(\delta)})\|_{H^{1/2}(\Gamma_a)} = \|Fg_z^{\varepsilon, \delta} + N(h_1^{\gamma(\delta)}, h_2^{\gamma(\delta)})\|_{H^{1/2}(\Gamma_a)} < C\varepsilon.$$

This, together with (5.14) and (5.16), gives

$$\|Fg_z^{\varepsilon, \delta} - G(\cdot, z)\|_{H^{1/2}(\Gamma_a)} < C\varepsilon + \delta.$$

Combining (5.16) and (5.15), we obtain that

$$\|g_z^{\varepsilon, \delta}\|_{L^2(\Gamma)} \rightarrow \infty, \quad \text{as } \delta \rightarrow 0.$$

The theorem is thus proved. □

6. Numerical experiments

As mentioned in Section 4, the incident waves $u_y^i(x) = \overline{G(y, x)}$ are not of physical relevance because they propagate away from the surface. Thus, the scattered field $u_y^s(x)$ corresponding to $u_y^i(x)$ cannot be generated directly. We now use the method of Arens and Kirsch [23] to generate $u_y^s(x)$. Note first that for $y \in \Gamma_a$ and $x \in \Omega_a$,

$$\begin{aligned} G(x, y) - \overline{G(y, x)} &= \frac{i}{4\pi k} \left\{ \sum_{\alpha_n \leq k} \frac{1}{\beta_n} e^{i(\alpha_n(x_1 - y_1) - \beta_n|x_2 - y_2|)} + \sum_{\alpha_n \leq k} \frac{1}{\beta_n} e^{i(\alpha_n(x_1 - y_1) + \beta_n|x_2 - y_2|)} \right\} \\ &:= \Delta^{(U)}(x, y) + \Delta^{(D)}(x, y). \end{aligned} \tag{6.1}$$

It is clear that $\Delta^{(U)}(x, y)$ and $\Delta^{(D)}(x, y)$ are upwards and downwards propagating modes, respectively. Set $\tilde{u}_y^l(x) = G(x, y) - \Delta^{(D)}(x, y)$. Then $\tilde{u}_y^l(x)$ is propagating downwards towards the scattering surface. Denote by $\tilde{u}^s(x, y)$ the corresponding scattered field with respect to the boundary value problem (2.7)–(2.10). Then, it is seen from (6.1) and the boundary value of $\tilde{u}^s(x, y)$ that

$$\begin{aligned} (\tilde{u}^s(\cdot, y) + \Delta^{(U)}(\cdot, y))|_{\Gamma_D} &= \tilde{u}^s(\cdot, y)|_{\Gamma_D} + G(\cdot, y)|_{\Gamma_D} - \overline{G(y, \cdot)}|_{\Gamma_D} - \Delta^{(U)}(\cdot, y)|_{\Gamma_D} \\ &= -\overline{G(y, \cdot)}|_{\Gamma_D}. \end{aligned}$$

Similarly, we have

$$\begin{aligned} \left(\frac{\partial}{\partial \nu} + i\lambda\right) (\tilde{u}^s(\cdot, y) + \Delta^{(U)}(\cdot, y))|_{\Gamma_I} &= \left(\frac{\partial}{\partial \nu} + i\lambda\right) (\tilde{u}^s(\cdot, y) + G(\cdot, y) - \Delta^{(U)}(\cdot, y))|_{\Gamma_I} - \left(\frac{\partial}{\partial \nu} + i\lambda\right) (\overline{G(y, \cdot)})|_{\Gamma_I} \\ &= -\left(\frac{\partial}{\partial \nu} + i\lambda\right) (\overline{G(y, \cdot)})|_{\Gamma_I}. \end{aligned}$$

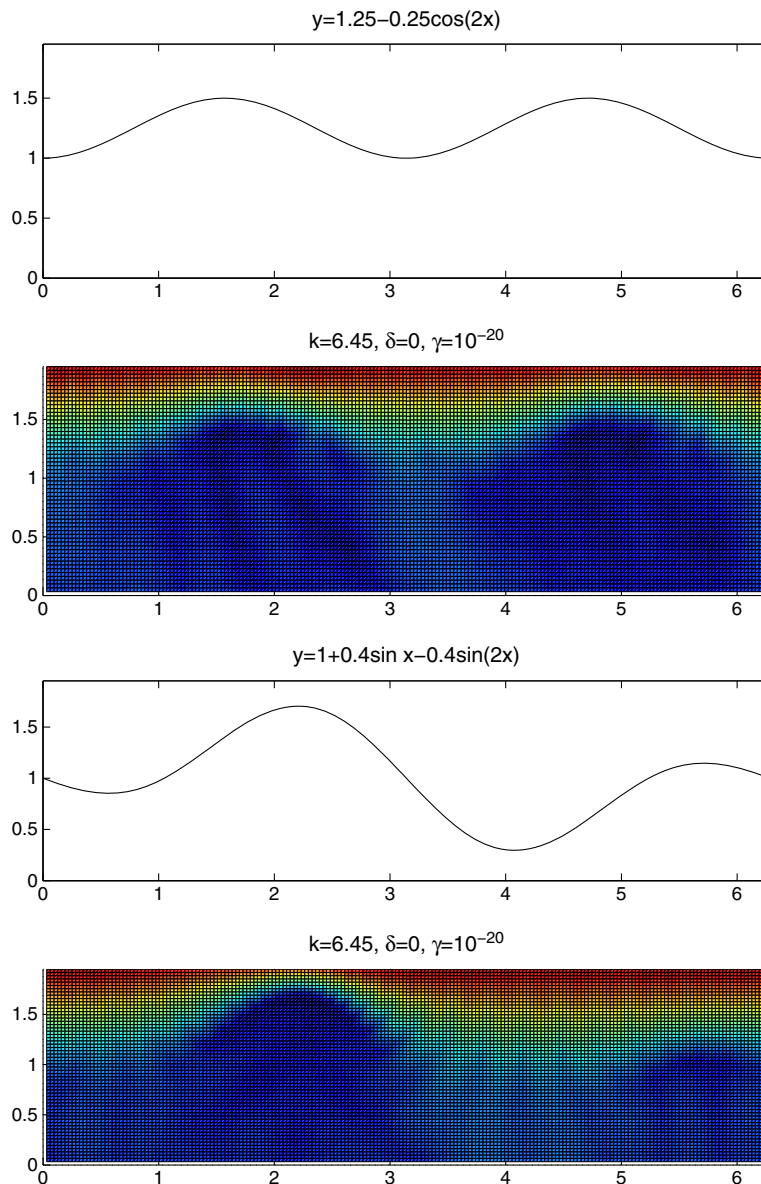


Figure 1. Example 6.1: two Fourier, perfectly reflecting grating profiles to be reconstructed and their numerical reconstructions from exact data (i.e., $\delta = 0$).

Then by the uniqueness of the direct problem, it follows that $u_y^s(x) = \tilde{u}^s(x, y) + \Delta^{(U)}(x, y)$ for $x \in \Omega_a$. Thus, the scattered field $u_y^s(x)$ can be exactly generated using the incident field $\tilde{u}_y^i(x)$.

Our reconstruction algorithm consists of the following steps:

- Step 1. Select a mesh of sampling points in a computing region $\Sigma_a = \{x \in \mathbb{R}^2 : 0 < x_2 < a, 0 < x_1 < 2\pi\}$, which contains the grating surface.
- Step 2. Make use of the Tikhonov regularization and the Morozov discrepancy principle to compute an approximate solution g_z^ε to the near field equation (4.1) or (5.2).
- Step 3. Consider $\|g_z^\varepsilon\|_{L^2(\Gamma_a)}$ as an indicator function of sampling points z and get the contour plot of the function $z \rightarrow \ln(\|g_z^\varepsilon\|_{L^2(\Gamma_a)})$.

To implement Step 2, one needs to calculate the α -quasiperiodic Green function $G(x, z)$ for $x = (x_1, x_2) \in \Gamma_a, z = (z_1, z_2) \in \Sigma_a$. In this paper, we apply Ewald's method (see, e.g. [35, 36]) to accelerate the evaluation of the Green's function $G(x, z)$. In order to illustrate the performance of the aforementioned reconstruction algorithm, we now present some numerical examples.

In the following experiments, we always assume that the unknown profile lies between the lines $x_2 = 0$ and $x_2 = 2$ and that both the incident point sources and the detecting positions are located at $\Gamma_a = \{(x_1, 2) : x_1 \in (0, 2\pi)\}$, that is, $a = 2$. The incident angle is always

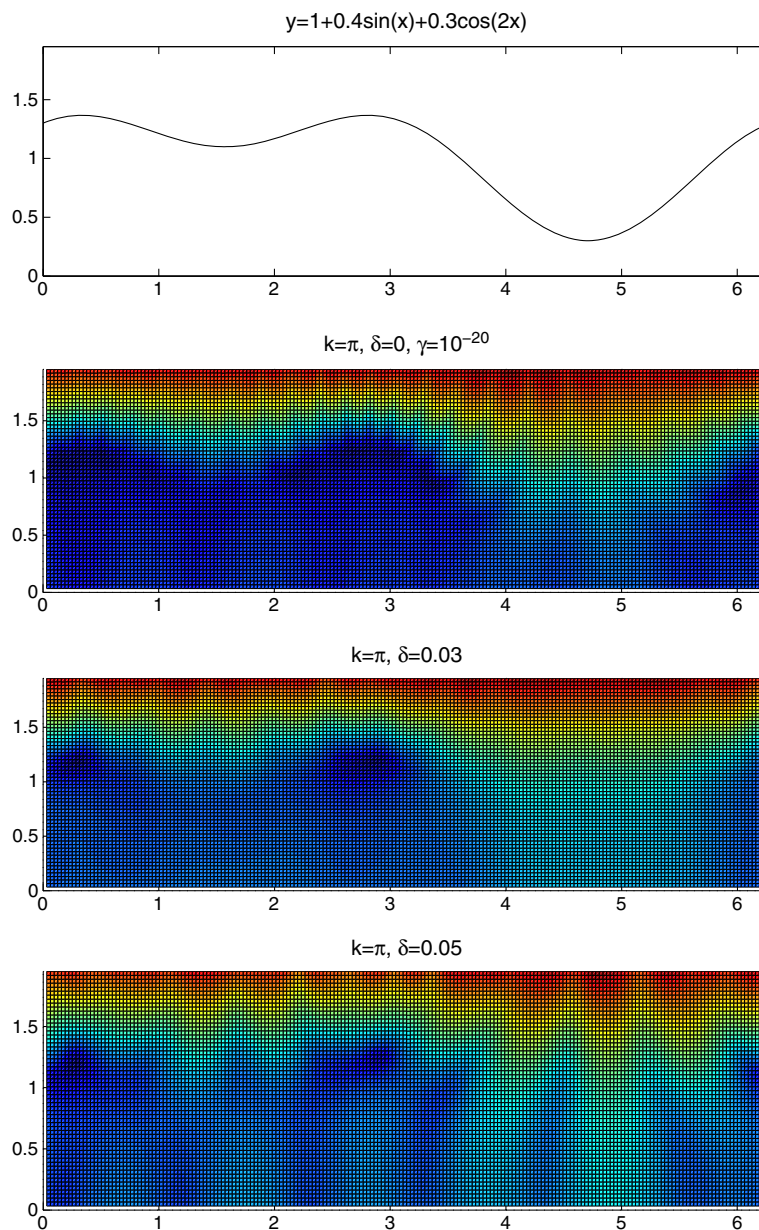


Figure 2. Example 6.2: a Fourier, perfectly reflecting grating profile to be reconstructed (top) and its numerical reconstructions from exact data ($\delta = 0$) and noise data with different noise levels ($\delta = 0.03, 0.05$).

taken as $\theta = 0$. We plot the function $z \rightarrow \ln(\|g_z^\varepsilon\|_{L^2(\Gamma_a)})$ over a 200×60 grid lying on the region $[0, 2\pi] \times [0, 1.95]$. Each of the reconstructions discussed later can be finished within 50 s on one MATLAB work station provided the near field data $u_y^s(x_1, a)$, $0 < x_1 < 2\pi$ for all incident point sources $y \in \Gamma_a$ can be obtained in advance. We use 257 incident point sources $u_y^i(x)$ with the source point y equivalently distributing on Γ_a . It should be noted that the right-hand side of (4.1) is becoming singular as z moves to Γ_a so the values of $\|g_z^\varepsilon\|_{L^2(\Gamma_a)}$ at the sampling points near Γ_a are always larger than those at other sampling points.

In Examples 6.1 and 6.2, we will consider the reconstruction of smooth perfectly reflecting grating profiles by assuming that $\Gamma_l = \emptyset$.

Example 6.1 (Reconstruction of Fourier gratings using exact data)

Suppose the grating profile $\Gamma = \{x : x_2 = f(x_1)\}$ is given by the graph of a trigonometric polynomial (Figure 1):

$$f(x_1) = f_1(x_1) = 1.25 - 0.25 \cos(2x_1), \quad x_1 \in \mathbb{R},$$

$$\text{or } f(x_1) = f_2(x_1) = 1 + 0.4 \sin(x_1) - 0.4 \sin(2x_1), \quad x_1 \in \mathbb{R}.$$

The height of f_1 is 0.5, whereas that of f_2 is greater than 1. The wave number is set as $k = 6.45$, which implies that each incident point source has 13 incoming plane waves and that each scattered field has 13 outgoing modes. The near field measurements for each incident point source are generated by solving the direct problem using the discrete collocation method proposed in [37]. We get an approximate solution to the equation (4.1) using unperturbed near field data on Γ_a with the regularization parameter $\gamma = 10^{-20}$. The results are shown in Figure 1. The reconstruction of f_1 is satisfactory, but the reconstruction on the downward convex part of f_1 is not very good.

Example 6.2 (Reconstruction of Fourier gratings using noisy data)

Here we perform a numerical experiment for the profile function discussed in [22] (see the top picture in Figure 2):

$$f(x_1) = 1 + 0.4 \sin(x_1) + 0.3 \cos(2x_1), \quad x_1 \in \mathbb{R}.$$

The exact near field data are perturbed with the following random errors:

$$u_y^s(t_j, a) + \delta u_y^s(t_j, a) \omega_j,$$

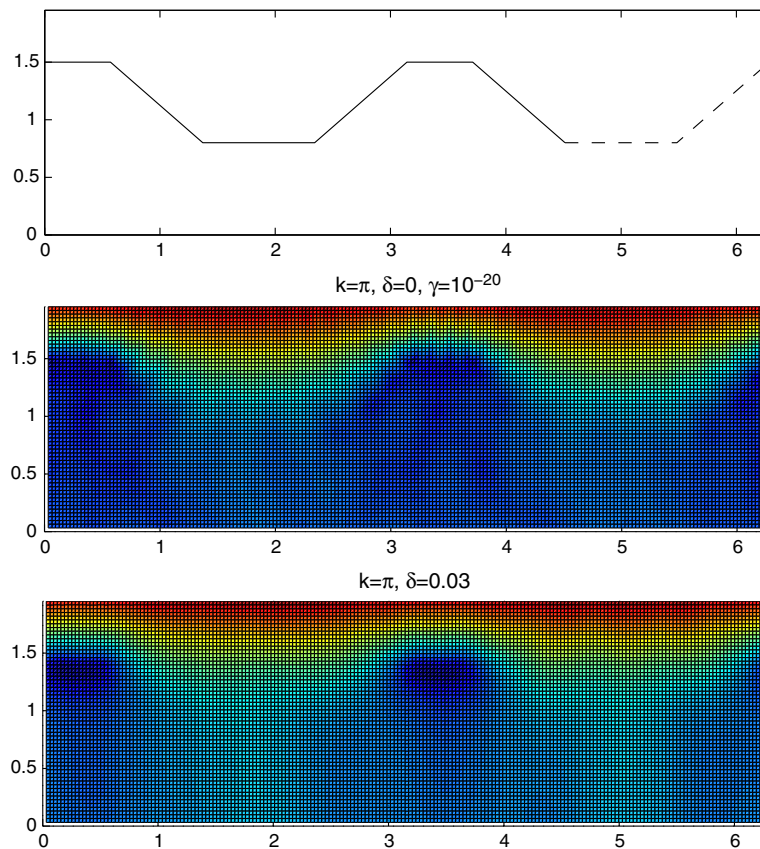


Figure 3. Example 6.3: a piecewise linear two-tower, mixed-type grating profile of fixed height 0.7 to be reconstructed (top) and its reconstructions from exact data ($\delta = 0$) and noise data ($\delta = 0.03$). An impedance condition is imposed on the dashed line part, and a Dirichlet condition is imposed on the remaining part.

where $\delta \geq 0$ is the noise level, t_j is an equidistant partition of $[0, 2\pi]$, and ω_j are random values between -1 and 1 . The wave number is set as $k = \pi$, where the incident point source (respectively the scattered field) involves seven incoming (outgoing) plane waves. We choose the regularization parameter $\gamma = 10^{-20}$ for the unperturbed data (i.e., $\delta = 0$) and determine γ by the Morozov discrepancy principle. Figure 2 shows the contour plot of $\ln(\|g_z\|_{L^2(\Gamma_{\delta})})$ as a function of z for different noise levels $\delta = 0, \delta = 0.03$, and $\delta = 0.05$. Noisy data with a noise level of $\delta = 3\%$ still produces acceptable results except for the downmost part, but the reconstruction with $\delta = 5\%$ turns out to be blurred; see Figure 2.

Example 6.3 (Reconstruction of piecewise linear gratings)

Consider a piecewise linear two-tower profile of fixed height 0.7 given by the top picture in Figure 3. We impose the Robin boundary condition with the impedance coefficient $\lambda = 0.05$ on the dashed line part and the Dirichlet boundary condition on the remaining part of the grating surface. The scattering data are obtained by the numerical solution of the direct scattering problem using the adaptive finite element method with perfectly matched layers proposed in [38, 39]. In our computation, the perfectly matched layer is chosen to lie between $x_2 = 2$ and $x_2 = 3$. Our computation on the inverse problem is carried out using both unperturbed and noisy data, with the results shown in Figure 3. Reconstruction of the bottom part is still not satisfactory, but the topmost part can always be perfectly identified.

Example 6.4 (Reconstruction of binary gratings)

We finally consider a perfectly conducting binary grating profile, which consists of only a finite number of horizontal and vertical line segments. The periodic profile is shown by the top picture in Figure 4 with a fixed height 0.5. Note that the binary grating profile is not the graph of any 2π -periodic continuous function. However, one can still carry over the linear sampling method for the inverse problem and the well-posedness result for the direct problem to this case. The computational results with exact and noisy data are presented in Figure 4. We find that the reconstruction in this case is rather sensitive to the noise level. Even 1% perturbation of the exact data (i.e., noise data with a noise level of $\delta = 1\%$) can lead to a large deviation of the original profile. We have also tried to select the regularization parameter by trial, but this gives no improvement in the noise case.

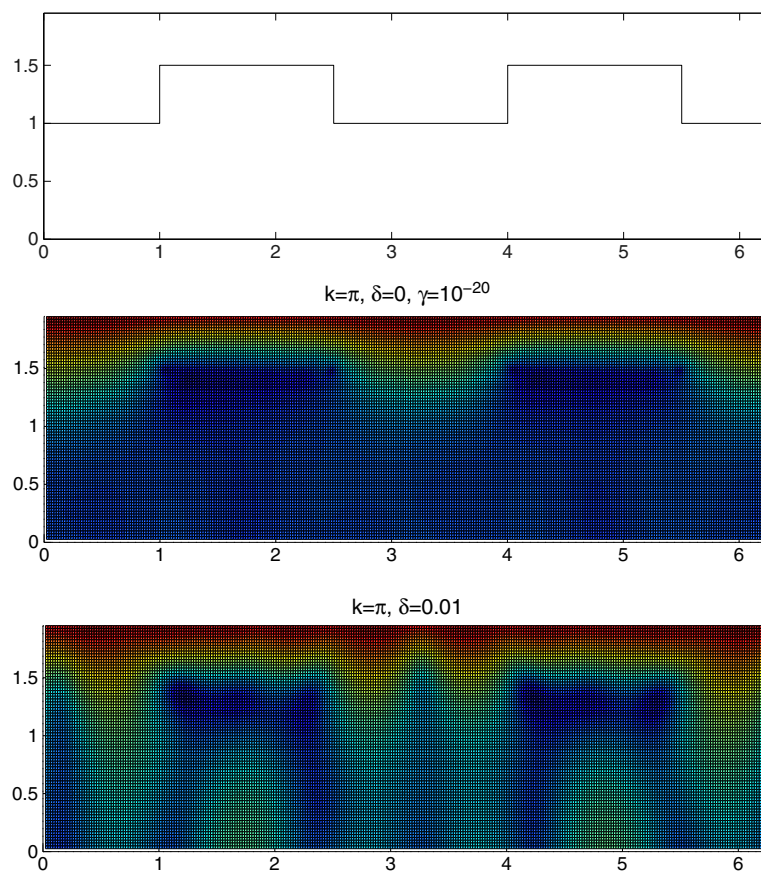


Figure 4. Example 6.4: a step, perfectly reflecting grating profile to be reconstructed (top) and its reconstructions from exact data ($\delta = 0$) and noise data ($\delta = 0.01$).

7. Conclusions

We study the direct and inverse problem of scattering of a time-harmonic incident point source wave by a Lipschitz diffraction grating of mixed type. The linear sampling method proposed for bounded obstacle scattering problems is generalized to the periodic case. We presented numerical examples for reconstructing three kinds of grating profiles: (i) smooth Fourier gratings; (ii) piecewise linear gratings; and (iii) binary gratings. The computational results indicate that acceptable results can be achieved provided the height of the probed diffraction grating profile is not very large and the noise level of the near field measurements is not very high. A numerical example for diffraction gratings of mixed type is also presented. Further work is still required to investigate the performance of the inversion algorithm depending on the wavenumber, the incident angle, the detecting position, and the amplitude of the gratings.

Acknowledgements

The authors would like to thank Haijun Wu of Nanjing University, China, for sending us the adaptive finite element code with a perfectly matched layer technique in MATLAB for solving the direct scattering problem by diffraction gratings. We also greatly acknowledge the anonymous referees for their valuable suggestions and comments that improve the original manuscript significantly.

The work of the first author (G. H.) was supported by the German Research Foundation (DFG) under grant EL 584/1-2, the work of the second author (F. Q.) was supported by the Tianyuan Youth Foundations for Mathematics of NNSF of China grant 11026098 and 11026150, and the work of the third author (B. Z.) was supported by the NNSF of China grant 11071244.

References

- Bao G, Cowsar L. In *Mathematical Modeling in Optical Science*, Masters W (ed.). SIAM: Philadelphia, USA, 2001.
- Petit R (ed.). *Electromagnetic Theory of Gratings*. Springer: Berlin, 1980.
- Kirsch A. Diffraction by periodic structures. In *Proceedings of The Lapland Conference on Inverse Problems*, Päivärinta et al. (ed.). Springer: Berlin, 1993; 87–102.
- Elschner J, Yamamoto M. An inverse problem in periodic diffractive optics: reconstruction of Lipschitz grating profiles. *Applicable Analysis* 2002; **81**:1307–1328.
- Kirsch A. An inverse scattering problem for periodic structures. In *Inverse Scattering and Potential Problems in Mathematical Physics*. Lang, Frankfurt am Main, 1995; 75–93.
- Bao G. A uniqueness theorem for an inverse problem in periodic diffractive optics. *Inverse Problems* 1994; **10**:335–340.
- Elschner J, Hu G. Global uniqueness in determining polygonal periodic structures with a minimal number of incident plane waves. *Inverse Problems* 2010; **26**:115002 (23pp).
- Elschner J, Schmidt G, Yamamoto M. An inverse problem in periodic diffractive optics: global uniqueness with a single wavenumber. *Inverse Problems* 2003; **19**:779–787.
- Elschner J, Schmidt G, Yamamoto M. Global uniqueness in determining rectangular periodic structures by scattering data with a single wavenumber. *Journal of Inverse and Ill-Posed Problems* 2003; **11**:235–244.
- Elschner J, Yamamoto M. Uniqueness in determining polygonal periodic structures. *Zeitschrift für Analysis und ihre Anwendungen* 2007; **26**:165–177.
- Hettlich F, Kirsch A. Schiffer's theorem in inverse scattering theory for periodic structures. *Inverse Problems* 1997; **13**:351–361.
- Kirsch A. Uniqueness theorems in inverse scattering theory for periodic structures. *Inverse Problems* 1994; **10**:145–152.
- Elschner J, Yamamoto M. Uniqueness results for an inverse periodic transmission problem. *Inverse Problems* 2004; **20**:1841–1852.
- Strycharz B. Uniqueness in the inverse transmission scattering problem for periodic media. *Mathematical Methods in the Applied Sciences* 1999; **22**:753–772.
- Bao G, Friedman A. Inverse problem for scattering by periodic structures. *Archive for Rational Mechanics and Analysis* 1995; **132**:49–72.
- Elschner J, Schmidt G. Inverse scattering for periodic structures: stability of polygonal interfaces. *Inverse Problems* 2001; **17**:1817–1829.
- Bruckner G, Cheng J, Yamamoto M. Inverse problems of diffractive optics: condition stability. *Inverse Problems* 2002; **18**:415–434.
- Bao G, Dobson DC, Cox JA. Mathematical studies in rigorous grating theory. *Journal of the Optical Society of America A* 1995; **12**:1029–1042.
- Ito K, Reitich F. A high-order perturbation approach to profile reconstruction: I. Perfectly conducting grating. *Inverse Problems* 1999; **15**:1067–1085.
- Hettlich F. Iterative regularization schemes in inverse scattering by periodic structures. *Inverse Problems* 2002; **18**:701–714.
- Bruckner G, Elschner J. A two-step algorithm for the reconstruction of perfectly reflecting periodic profiles. *Inverse Problems* 2003; **19**:315–329.
- Arens T, Grinberg N. A complete factorization method for scattering by periodic surface. *Computing* 2005; **75**:111–132.
- Arens T, Kirsch A. The factorization method in inverse scattering from periodic structures. *Inverse Problems* 2003; **19**:1195–1211.
- Colton D, Kress R. *Inverse Acoustic and Electromagnetic Scattering Theory*, (2nd Edition). Springer: Berlin, 1998.
- Kirsch A, Grinberg N. *The Factorization Method for Inverse Problems*. Oxford University Press: Oxford, 2008.
- Bruckner G, Elschner J. The numerical solution of an inverse periodic transmission problem. *Mathematical Methods in the Applied Sciences* 2005; **28**:757–778.
- Elschner J, Hsiao GC, Rathsfeld A. Grating profile reconstruction based on finite elements and optimization techniques. *SIAM Journal on Applied Mathematics* 2003; **64**:525–545.
- Colton D, Kirsch A. A simple method for solving inverse scattering problems in the resonance region. *Inverse Problems* 1996; **12**:383–393.
- Cakoni F, Colton D. On the mathematical basis of the linear sampling method. *Georgian Mathematical Journal* 2003; **10**:411–425.
- Cakoni F, Colton D. *Qualitative Methods in Inverse Scattering Theory*. Springer: Berlin, 2005.
- Colton D, Haddar H, Piana M. The linear sampling method in inverse electromagnetic scattering theory. *Inverse Problems* 2003; **19**:S105–S137.
- McLean W. *Strongly Elliptic Systems and Boundary Integral Equations*. Cambridge University Press: Cambridge, 2000.
- Bruckner G, Cheng J, Yamamoto M. Uniqueness of determining a periodic structure from discrete far field observations, 2000. WIAS Preprint No. 605 Available from: <http://www.wias-berlin.de/main/publications/>.
- Schmidt G. Integral equations for conical diffraction by coated gratings. *Journal of Integral Equations and Applications* 2011; **23**:71–112.

35. Linton CM. The Green's function for the two-dimensional Helmholtz equation in periodic domains. *Journal of Engineering Mathematics* 1998; **33**:377–401. DOI: 10.1023/A:1004377501747.
36. Rathsfeld A, Schmidt G, Kleemann BH. On a fast integral equation method for diffraction gratings. *Communications in Computational Physics* 2006; **1**:984–1009.
37. Atkinson KE. A discrete Galerkin method for first kind integral equations with a logarithmic kernel. *Journal of Integral Equations and Applications* 1988; **1**:343–363.
38. Bao G, Chen Z, Wu H. An adaptive finite element method for diffraction gratings. *Journal of the Optical Society of America A* 2005; **22**:1106–1114.
39. Chen Z, Wu H. An adaptive finite element method with perfectly matched absorbing layers for the wave scattering by periodic structures. *SIAM Journal on Numerical Analysis* 2003; **41**:799–826.