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Direct and Inverse Elastic Scattering Problems for Diffraction Gratings

Abstract: This chapter is concerned with the direct and inverse scattering of time-harmonic plane elastic waves by unbounded periodic structures (diffraction gratings). We present a variational approach to forward scattering problems with Lipschitz grating profiles and give a survey of recent uniqueness and existence results. We also report on recent global uniqueness results within the class of piecewise linear grating profiles for the corresponding inverse elastic scattering problems. Moreover, a discrete Galerkin method is presented to efficiently approximate solutions of direct scattering problems via an integral equation approach. Finally, an optimization method for solving the inverse problem of recovering a 2D periodic structure from scattered elastic waves measured above the structure is discussed.

Keywords: diffraction gratings, elastic waves, variational formulation, inverse elastic scattering, uniqueness, reconstruction method

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1 Introduction

Diffraction gratings are widely used in many areas of science and technology and have been investigated since more than 100 years [62]. In recent years, the interest in these areas has grown immensely because of many industrial applications, for example, in radar imaging, nondestructive testing, micro-optics, or solar energy absorption. In particular, the scattering of acoustic and electromagnetic waves in periodic structures has been studied extensively concerning theoretical analysis and numerical approximation, using integral equation methods [32, 64, 67, 68] or variational methods [19–21, 30, 33, 42, 54, 70]. We refer to the monographs [72] for a comprehensive mathematical study and to [15] for the details of the applications of electromagnetic diffraction gratings. However, there have been only a few papers studying the

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scattering of elastic waves by unbounded surfaces. The aim of this survey chapter is to report on recent progress in the analysis and numerics of direct and inverse elastic scattering problems for diffraction gratings.

The relevant phenomena for elastic waves have a wide field of application, particularly in geophysics, seismology and nondestructive testing. For instance, the problem of elastic pulse transmission and reflection through the earth is fundamental to the investigation of earthquakes and the utility of seismic waves in search for oil and ore bodies [2, 48, 49, 71]. Moreover, identifying parallel vertical fractures (which can be modeled as periodic structures) in sedimentary rocks can have significant impact on the production of underground gas and liquids by employing controlled explosions [65]. Inverse elastic scattering problems also arise from detecting cracks and flaws in concrete structures, such as bridges, buildings, dams, highways and so on; see [69, 73] for applications in nondestructive testing.

Compared to acoustic and electromagnetic scattering, the elasticity problem is more complicated due to the coexistence of compressional and shear waves that propagate at different speeds. These two waves are coupled at interfaces where boundary conditions depending on the elastic medium are imposed. The first attempt to rigorously prove solvability of direct elastic scattering problems for unbounded surfaces is due to Arens; see [7, 8] for two-dimensional diffraction gratings and [9, 10] for the more general case of rough surfaces. In [7], existence and uniqueness of quasiperiodic solutions to the Dirichlet problem was established in the case that the grating profile is given by the graph of a smooth periodic function. The existence proof is based on the boundary integral equation method where the solution is sought as the superposition of single and double layer potentials. We also refer to [29] for earlier studies on the scattering of elastic waves in a locally perturbed isotropic half-space with a free boundary using the limiting absorption principle.

In this chapter, we focus on the variational approach, which reduces the forward scattering problem to an equivalent variational formulation in a truncated periodic cell involving a nonlocal boundary (Dirichlet-to-Neumann) operator; see Section 3. We refer to [1, 21, 54] for the variational approach applied to electromagnetic diffraction gratings. This approach appears to be well adapted to the analytical and numerical treatment of rather general two-dimensional and three-dimensional periodic structures involving nonsmooth interfaces and transmission conditions. The variational method can also be applied to elastic scattering by rough surfaces; see [40] for recent existence and uniqueness results in the case of the Dirichlet problem.

The inverse problem of recovering a grating profile from scattered elastic fields is of great practical importance. In contrast to the widespread belief of the uniqueness in bounded obstacle scattering problems with only one incident plane wave, we cannot expect the same global uniqueness in wave diffraction by periodic structures (see, e.g. [41] and [45]). This is mainly due to the Rayleigh expansion radiation condition (RERC) imposed on the scattered field, which involves several propagating modes

without decay as $x_2 \rightarrow \infty$. In general it is difficult to characterize the exceptional grating profiles that cannot be identified by one incident plane wave. However, if the grating profiles are piecewise linear, by the reflection principles for the Helmholtz and Maxwell equations, global uniqueness by finitely many incident waves can be proved for the inverse scattering of time-harmonic electromagnetic waves, including TE and TM polarization [16, 17, 35]. In particular, one can classify and characterize all unidentifiable sets of grating profiles corresponding to one incident plane wave. In Section 4 we review corresponding global uniqueness results in elasticity within the class of polygonal grating profiles under the boundary conditions of the third or fourth kind, which are based on the reflection principle for the Navier system developed in [47]. It is a challenging open problem to extend these results to the case of the boundary conditions of the first or second kind.

The numerical solution of the direct elastic scattering problem under the Dirichlet boundary condition is addressed in Section 5.1 where we present a discrete Galerkin method for solving an equivalent first-kind integral equation. From the numerical view point, the implementation of this method is easier than the integral equation method with a second-kind integral equation that involves the computation of the stress operator on the profile.

The numerical treatment of the corresponding inverse problem is challenging since it is nonlinear and severely ill-posed. There is already a vast literature on the reconstruction of a perfectly conducting profile for the two-dimensional Helmholtz equation. Here we mention a conjugate gradient algorithm based on analytic continuation [53], an iterative regularization method [51], a factorization method [11, 12], and an optimization method [22–24] that follows an approach first developed by Kirsch and Kress for acoustic obstacle scattering (see [27, Chapter 5] and the references therein). In Section 5.2, the two-step algorithm of [22] for the reconstruction of one-dimensional electromagnetic grating profiles is extended to the more complicated case of elastic scattering. The first step of this method is to reconstruct the scattered field from near-field measurements by solving a first-kind integral equation. This step is the linear severely ill-posed part and requires Tikhonov regularization involving the singular value decomposition of the integral operator. The second step is to approximate the grating profile by solving a finite-dimensional least squares problem, which is nonlinear but well-posed.

2 Mathematical formulation of direct and inverse scattering problems

We assume that a periodic surface divides the three-dimensional space into two non-locally perturbed half-spaces filled with homogeneous and isotropic elastic media. Unless otherwise stated, this surface is always assumed to be invariant in the x_3 -

direction, and its cross-section in the (x_1, x_2) -plane is to be represented by a curve Λ which is 2π -periodic in x_1 . We suppose further that all elastic waves propagate perpendicular to the x_3 -axis, so that the problem can be treated as a problem of plane elasticity.

Denote by Ω_Λ the region above the grating in \mathbb{R}^2 . Suppose that a time-harmonic plane elastic wave with the incident angle $\theta \in (-\pi/2, \pi/2)$ is incident on Λ from Ω_Λ . The incident wave is allowed to be either an incident pressure wave taking the form

$$u^{in} = u_p^{in}(x) = \hat{\theta} \exp\left(ik_p x \cdot \hat{\theta}\right) \quad \text{with} \quad \hat{\theta} := (\sin \theta, -\cos \theta)^\top, \quad (3.1)$$

or an incident shear wave taking the form

$$u^{in} = u_s^{in}(x) = \hat{\theta}^\perp \exp\left(ik_s x \cdot \hat{\theta}\right) \quad \text{with} \quad \hat{\theta}^\perp := (\cos \theta, \sin \theta)^\top, \quad (3.2)$$

where

$$k_p := \omega/\sqrt{2\mu + \lambda}, \quad k_s := \omega/\sqrt{\mu}$$

are the compressional and shear wave numbers, respectively, λ and μ are the Lamé constants satisfying $\mu > 0$ and $\lambda + \mu > 0$, $\omega > 0$ denotes the angular frequency of the harmonic motion and the symbol $(\cdot)^\top$ indicates the transpose of a vector in \mathbb{R}^2 . For simplicity we assume the mass density of the elastic medium is equal to one, so that the total displacement $u(x_1, x_2)$, which can be decomposed as the sum of the incident field u^{in} and the scattered field u^{sc} , satisfies the Navier equation (or system):

$$(\Delta^* + \omega^2)u = 0 \quad \text{in} \quad \Omega_\Lambda, \quad \Delta^* := \mu\Delta + (\lambda + \mu) \operatorname{grad} \operatorname{div}. \quad (3.3)$$

We first assume that the grating is impenetrable, and that one of the following boundary conditions is imposed on Λ .

$$\text{First-kind boundary condition:} \quad u = 0, \quad (3.4)$$

$$\text{Second-kind boundary condition:} \quad Tu = 0, \quad (3.5)$$

$$\text{Third-kind boundary conditions:} \quad \mathbf{n} \cdot u = 0, \tau \cdot Tu = 0, \quad (3.6)$$

$$\text{Fourth-kind boundary conditions:} \quad \tau \cdot u = 0, \mathbf{n} \cdot Tu = 0, \quad (3.7)$$

where Tu stands for the *stress vector* or *traction* having the form

$$Tu = 2\mu \partial_{\mathbf{n}} u + \lambda \mathbf{n} \operatorname{div} u + \mu\tau(\partial_2 u_1 - \partial_1 u_2), \quad (3.8)$$

with the exterior unit normal $\mathbf{n} = (n_1, n_2)^\top$ and the unit tangential vector $\tau = (-n_2, n_1)^\top$ on Λ . Here and in the following the notation $\partial_j v = \frac{\partial v}{\partial x_j}$ is used. Note that the boundary condition of the first (second) kind is also referred to as the Dirichlet (Neumann) boundary condition, and that vanishing normal displacement and tangential stress (normal stress and tangential displacement) correspond to the third

(fourth)-kind boundary conditions. We refer to the monograph [57] for a comprehensive treatment of the boundary value problems of elasticity (including the boundary conditions of the third and fourth kind).

The periodicity of the structure together with the form of the incident waves implies that the solution u must be α -quasiperiodic, i.e.

$$u(x_1 + 2\pi, x_2) = \exp(2i\alpha\pi) u(x_1, x_2), \quad (x_1, x_2) \in \Omega_\Lambda, \quad (3.9)$$

where $\alpha := k_p \sin \theta$ is the incident pressure wave (3.1), and $\alpha := k_s \sin \theta$ the incident shear wave (3.2). To ensure well-posedness of the boundary value problem (3.3)–(3.9), a radiation condition must be imposed as $x_2 \rightarrow +\infty$. Observing that the scattered field u^{sc} also satisfies the Navier equation (3.3), we can decompose it into the compressional and shear parts

$$u^{sc} = \frac{1}{i} (\text{grad } \varphi + \overrightarrow{\text{curl}} \psi) \quad \text{with} \quad \varphi := -\frac{i}{k_p^2} \text{div } u^{sc}, \quad \psi := \frac{i}{k_s^2} \text{curl } u^{sc},$$

where the two curl operators in \mathbb{R}^2 are defined by

$$\text{curl } u := \partial_1 u_2 - \partial_2 u_1, \quad u = (u_1, u_2)^\top \quad \text{and} \quad \overrightarrow{\text{curl}} v := (\partial_2 v, -\partial_1 v)^\top,$$

and the scalar functions φ, ψ satisfy the homogeneous Helmholtz equations

$$(\Delta + k_p^2) \varphi = 0 \quad \text{and} \quad (\Delta + k_s^2) \psi = 0 \quad \text{in } \Omega_\Lambda.$$

Applying the Rayleigh expansion for the scalar Helmholtz equation (see e.g. [54]) to φ and ψ , respectively, we finally obtain a corresponding expansion of u^{sc} into outgoing plane elastic waves,

$$u^{sc}(x) = \sum_{n \in \mathbb{Z}} A_{p,n}(\alpha_n, \beta_n)^\top \exp(i\alpha_n x_1 + i\beta_n x_2) + \sum_{n \in \mathbb{Z}} A_{s,n}(\gamma_n, -\alpha_n)^\top \exp(i\alpha_n x_1 + i\gamma_n x_2), \quad (3.10)$$

for $x_2 > \Lambda^+ := \max_{(x_1, x_2) \in \Lambda} x_2$, where the constants $A_{p,n}, A_{s,n} \in \mathbb{C}$ are called the Rayleigh coefficients and

$$\alpha_n := \alpha + n, \quad \beta_n = \beta_n(\theta) := \begin{cases} \sqrt{k_p^2 - \alpha_n^2} & \text{if } |\alpha_n| \leq k_p, \\ i\sqrt{\alpha_n^2 - k_p^2} & \text{if } |\alpha_n| > k_p. \end{cases} \quad (3.11)$$

The parameter $\gamma_n := \gamma_n(\theta)$ is defined analogously as β_n with k_p replaced by k_s . The expansion (3.10) is also called the RERC (see, e.g. [6–8]). We refer to [54] for the RERC of the scalar Helmholtz equation and to [1, 15, 25] in the case of Maxwell’s equations in periodic structures.

Since β_n and γ_n in (3.10) are real for at most a finite number of indices n , only a finite number of plane waves in (3.10) propagate into the far field, with the remaining

evanescent waves (or surface waves) decaying exponentially as $x_2 \rightarrow +\infty$. The above expansion converges uniformly with all derivatives in the half-plane $\{x \in \mathbb{R}^2 : x_2 \geq b\}$ for any $b > \Lambda^+$. Now, our direct diffraction problem can be formulated as the following boundary value problem.

(DP): Given a grating profile curve $\Lambda \subset \mathbb{R}^2$ (which is 2π -periodic in x_1) and an incident field u^{in} of the form (3.1) or (3.2), find a vector function $u = u(x; \theta) = u^{in} + u^{sc} \in H_{loc}^1(\Omega_\Lambda)^2$ that satisfies the Navier equation (3.3), one of the boundary conditions in (3.4)–(3.7), the quasiperiodicity (3.9) and the RERC (3.10).

Let $u(x; \theta_j)$ denote solutions of (DP) corresponding to N incident pressure or shear waves u^{in} of the form (3.1) or (3.2) with distinct incident angles $\theta_j \in (-\frac{\pi}{2}, \frac{\pi}{2})$ ($j = 1, 2, \dots, N$). The inverse problem which involves near-field measurements $u(x_1, b)$ for some fixed $b > \Lambda^+$ can be formulated as follows.

(IP): Given N incident angles θ_j , determine the grating profile Λ from the knowledge of the near-field data $u(x_1, b; \theta_j)$ for all $x_1 \in (0, 2\pi)$, $j = 1, 2, \dots, N$.

As mentioned earlier, only a finite number of propagating modes of the compressional and shear parts can be measured far away from the grating surface. From the practical point of view, it is quite natural to reconstruct the unknown grating profile from the far-field data $u_b^\infty(x_1)$ of $u^{sc}(x)$ defined by

$$u_b^\infty(x_1) = \sum_{n \in \mathcal{U}_p} A_{p,n}(\alpha_n, \beta_n)^\top \exp(i\alpha_n x_1 + i\beta_n b) + \sum_{n \in \mathcal{U}_s} A_{s,n}(\gamma_n, -\alpha_n)^\top \exp(i\alpha_n x_1 + i\gamma_n b),$$

where the sets \mathcal{U}_p and \mathcal{U}_s are defined by

$$\mathcal{U}_p = \{n \in \mathbb{Z} : |\alpha_n| \leq k_p\}, \quad \mathcal{U}_s = \{n \in \mathbb{Z} : |\alpha_n| \leq k_s\}.$$

Therefore we also consider the following inverse problem:

(IP*): Determine the grating profile from the far-field data $u_b^\infty(x_1; \theta_j)$, $x_1 \in (0, 2\pi)$, for N incident pressure or shear waves u^{in} with distinct incident angles θ_j , $j = 1, 2, \dots, N$.

Of course, from these data one can only hope to reconstruct a finite number of parameters of the profile (see Section 5.2).

3 Solvability results for direct scattering problems: variational method

3.1 An equivalent variational formulation and its Fredholm property

Following the approach of [54] in the case of the scalar Helmholtz equation, we propose an equivalent variational formulation of the boundary value problem (DP), which is posed in a bounded periodic cell in \mathbb{R}^2 and is enforcing the radiation condition. Introduce an artificial boundary

$$\Gamma_b := \{(x_1, b) : 0 \leq x_1 \leq 2\pi\}, \quad b > \Lambda^+ = \max_{x \in \Lambda} x_2,$$

and the bounded domain

$$\Omega_b := \{(x_1, x_2) \in \Omega_\Lambda : 0 < x_1 < 2\pi, x_2 < b\},$$

lying between the segment Γ_b and one period of the grating profile curve which is denoted by Λ again. We assume that Λ is a Lipschitz curve, so that Ω_b is a bounded Lipschitz domain.

Let $H_\alpha^1(\Omega_b)$ denote the subspace of the Sobolev space $H^1(\Omega_b)$ of scalar functions on Ω_b which are α -quasiperiodic with respect to x_1 . Introduce the variational space

$$V_\alpha = \{u \in H_\alpha^1(\Omega_b)^2 : u \text{ satisfies the corresponding essential boundary condition of (3.4)–(3.7) on } \Lambda\}$$

equipped with the norm in the usual Sobolev space $H^1(\Omega_b)^2$ of vector functions. Note that for the Neumann condition $V_\alpha = H_\alpha^1(\Omega_b)^2$, whereas for the third- and fourth-kind boundary conditions only the first condition of (3.6) and (3.7), respectively, is involved. By the first Betti formula, it follows that for $u, \varphi \in V_\alpha$,

$$-\int_{\Omega_b} (\Delta^* + \omega^2) u \cdot \overline{\varphi} \, dx = \int_{\Omega_b} (a(u, \overline{\varphi}) - \omega^2 u \cdot \overline{\varphi}) \, dx - \int_{\Gamma_b} \overline{\varphi} \cdot T u \, ds, \quad (3.12)$$

where the bar indicates the complex conjugate, and $a(\cdot, \cdot)$ is the symmetric bilinear form defined by

$$\begin{aligned} a(u, \varphi) := & (2\mu + \lambda) (\partial_1 u_1 \partial_1 \varphi_1 + \partial_2 u_2 \partial_2 \varphi_2) + \mu (\partial_2 u_1 \partial_2 \varphi_1 + \partial_1 u_2 \partial_1 \varphi_2) \\ & + \lambda (\partial_1 u_1 \partial_2 \varphi_2 + \partial_2 u_2 \partial_1 \varphi_1) + \mu (\partial_2 u_1 \partial_1 \varphi_2 + \partial_1 u_2 \partial_2 \varphi_1). \end{aligned} \quad (3.13)$$

Let $H_\alpha^s(\Gamma_b)$ denote the Sobolev space of order $s \in \mathbb{R}$ of functions on Γ_b that are α -quasiperiodic. Now we introduce the DtN map \mathcal{T} on the artificial boundary Γ_b .

Definition 3.1. For any $v \in H_\alpha^{1/2}(\Gamma_b)^2$, we define $\mathcal{T}v$ as the traction Tu^{sc} on Γ_b where u^{sc} is the unique α -quasiperiodic solution of the homogeneous Navier equation in $\{x_2 > b\}$ which satisfies (3.10) and $u^{sc} = v$ on Γ_b .

The next lemma is devoted to an explicit representation of \mathcal{T} and its properties.

Lemma 3.2 ([34]).

(i) For $v = \sum_{n \in \mathbb{Z}} \hat{v}_n \exp(i\alpha_n x_1) \in H_\alpha^{1/2}(\Gamma_b)^2$, we have

$$\mathcal{T}v = \mathcal{T}(\omega, \alpha)v = - \sum_{n \in \mathbb{Z}} W_n \hat{v}_n \exp(i\alpha_n x_1), \tag{3.14}$$

where W_n is the 2×2 matrix defined by

$$W_n = W_n(\omega, \alpha) := \frac{1}{i} \begin{pmatrix} \omega^2 \beta_n / d_n & 2\mu\alpha_n - \omega^2 \alpha_n / d_n \\ -2\mu\alpha_n + \omega^2 \alpha_n / d_n & \omega^2 \gamma_n / d_n \end{pmatrix} \tag{3.15}$$

with $d_n := \alpha_n^2 + \beta_n \gamma_n$.

(ii) \mathcal{T} is a bounded linear map from $H_\alpha^{1/2}(\Gamma_b)^2$ to $H_\alpha^{-1/2}(\Gamma_b)^2$.

(iii) For $M_0 > 0$ sufficiently large, we have the decomposition $\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2$, with

$$\mathcal{T}_1 v := - \sum_{|n| > M_0} W_n \hat{v}_n \exp(i\alpha_n x_1) \quad \text{satisfying} \quad \operatorname{Re} \left\{ - \int_{\Gamma_b} \mathcal{T}_1 v \cdot \bar{v} ds \right\} \geq 0,$$

and $\mathcal{T}_2 v := - \sum_{|n| \leq M_0} W_n \hat{v}_n \exp(i\alpha_n x_1)$ for all $v \in H_\alpha^{1/2}(\Gamma_b)^2$.

The first assertion of Lemma 3.2 can be deduced directly from the definition of \mathcal{T} , whereas the second and third assertions follow from the explicit representation of \mathcal{T} .

Next we introduce the sesquilinear form $B(u, \varphi)$ defined by

$$B(u, \varphi) := \int_{\Omega_b} (a(u, \bar{\varphi}) - \omega^2 u \cdot \bar{\varphi}) dx - \int_{\Gamma_b} \bar{\varphi} \cdot \mathcal{T}u ds, \quad \forall u, \varphi \in V_\alpha, \tag{3.16}$$

with $\mathcal{T}u := \mathcal{T}(u|_{\Gamma_b})$. Applying Betti's identity (3.12) to a solution $u = u^{sc} + u^{in}$ of (DP) and using the fact that

$$Tu = T(u^{sc} + u^{in}) = \mathcal{T}u^{sc} + Tu^{in} = \mathcal{T}u + f_0, \quad \text{with} \quad f_0 := Tu^{in} - \mathcal{T}u^{in},$$

we obtain the following variational formulation of (DP): Find $u \in V_\alpha$ such that

$$B(u, \varphi) = \int_{\Gamma_b} f_0 \cdot \bar{\varphi} ds, \quad \forall \varphi \in V_\alpha, \tag{3.17}$$

where

$$f_0 = \begin{cases} 2i\beta_0 k_p (\lambda + 2\mu) d_0^{-1} \exp(i\alpha x_1 - i\beta_0 b) (-\alpha, \gamma_0)^\top & \text{if } u^{in} = u_p^{in}, \\ -2i\gamma_0 k_s \mu d_0^{-1} \exp(i\alpha x_1 - i\gamma_0 b) (\beta_0, \alpha)^\top & \text{if } u^{in} = u_s^{in}. \end{cases} \tag{3.18}$$

The problems (DP) and (3.17) are equivalent in the following sense. If $u \in H_{loc}^1(\Omega_\Lambda)^2$ is a solution of the boundary value problem (DP), then $u|_{\Omega_b}$ satisfies the variational

problem (3.17). Conversely, a solution $u \in V_\alpha$ of (3.17) can be extended to a solution $u = u^{in} + u^{sc}$ of the Navier equation (3.3) for $x_2 \geq b$, where the Rayleigh coefficients $A_{p,n}$ and $A_{s,n}$ of u^{sc} are uniquely determined by the Fourier coefficients \hat{u}_n of $\exp(-i\alpha x_1)(u - u^{in})(x_1, b)$ via the relation

$$\hat{u}_n = \begin{pmatrix} \alpha_n & \gamma_n \\ \beta_n & -\alpha_n \end{pmatrix} \begin{pmatrix} A_{p,n} \exp(i\beta_n b) \\ A_{s,n} \exp(i\gamma_n b) \end{pmatrix}. \tag{3.19}$$

The sesquilinear form B obviously generates a continuous linear operator $\mathcal{B} : V_\alpha \rightarrow V'_\alpha$ such that

$$B(u, \varphi) = (\mathcal{B}u, \varphi)_{\Omega_b} \quad \forall u, \varphi \in V_\alpha. \tag{3.20}$$

Here V'_α denotes the dual of the space V_α with respect to the duality $(\cdot, \cdot)_{\Omega_b}$ extending the scalar product in $L^2(\Omega_b)^2$.

Theorem 3.3 ([34]). *Assume that the grating profile Λ is a Lipschitz curve. Then the sesquilinear form B defined in (3.16) is strongly elliptic over V_α . Moreover, the operator \mathcal{B} defined by (3.20) is always a Fredholm operator with index zero.*

Proof. Using the well-known Korn’s inequality (see [31, Chapter 3], [63, Chapter 10]), we obtain

$$\int_{\Omega_b} a(u, \bar{u}) dx \geq C_1 \|u\|_{H^1(\Omega_b)^2}^2 - C_2 \|u\|_{L^2(\Omega_b)^2}^2, \quad \forall u \in H^1(\Omega_b)^2,$$

for some constants $C_1, C_2 > 0$ independent of u . On the other hand, it follows from Lemma 3.2 (iii) that $-\mathcal{T}$ can be decomposed into the sum of the positive definite operator $-\mathcal{T}_1$ and the finite rank operator $-\mathcal{T}_2$. Therefore, the sesquilinear form B is strongly elliptic and the operator \mathcal{B} is a Fredholm operator with index zero. \square

In contrast to properties of the DtN map for the periodic scalar Helmholtz equation, the operator $-\mathcal{T}$ for the Navier equation is no longer positive definite (cf. Lemma 3.2 (iii) and [44]). Thanks to the periodicity of the domain, we can still justify the Fredholm property of \mathcal{B} . Concerning the DtN map for the biperiodic Maxwell equations, we refer to [1, 19, 70].

3.2 Uniqueness and existence for direct scattering problems

We rewrite problem (3.17) in the form

$$\mathcal{B}u = \mathcal{F}_0, \quad \mathcal{F}_0 \in V'_\alpha, \tag{3.21}$$

where \mathcal{F}_0 is given by the right-hand side of (3.17). We have the following solvability results for (DP).

Theorem 3.4 ([34]).

- (i) *If the grating profile Λ is a Lipschitz curve, then there always exists a solution of (DP) under the boundary conditions of the first, second, third or fourth kind. Moreover, uniqueness holds for small frequencies, and for all frequencies excluding a discrete set with the only accumulation point at infinity.*
- (ii) *If Λ is the graph of a Lipschitz function, then for any frequency $\omega > 0$ there exists a unique solution of (DP) under the Dirichlet boundary condition.*

Proof. (i) By the Fredholm alternative and Theorem 3.3, equation (3.21) is solvable if the right-hand side \mathcal{F}_0 is orthogonal to all solutions v of the homogeneous adjoint equation $\mathcal{B}^*v = 0$. Note that such v can always be extended to a solution of (3.3) in the unbounded domain Ω_Λ by setting

$$v(x) = \sum_{n \in \mathbb{Z}} A_{p,n} (\alpha_n, -\bar{\beta}_n)^\top \exp(i \alpha_n x_1 - i \bar{\beta}_n x_2) + \sum_{n \in \mathbb{Z}} A_{s,n} (-\bar{\gamma}_n, -\alpha_n)^\top \exp(i \alpha_n x_1 - i \bar{\gamma}_n x_2),$$

for $x_2 \geq b$, where the Rayleigh coefficients $A_{p,n}, A_{s,n}$ are determined by the n th Fourier coefficient \hat{v}_n of $e^{-i\alpha x_1} v|_{\Gamma_b}$ via an analogous relation to (3.19) with β_n, γ_n replaced by $\bar{\beta}_n, \bar{\gamma}_n$, respectively. On the other hand, it can be derived from

$$0 = (\mathcal{B}^*v, \psi)_{\Omega_b} = (v, \mathcal{B}\psi)_{\Omega_b} = \overline{B(\psi, v)}, \quad \forall \psi \in V_\alpha$$

that v has vanishing Rayleigh coefficients of the incoming modes (see [34]):

$$A_{p,n} = 0 \quad \text{for } |\alpha_n| < k_p \quad \text{and} \quad A_{s,n} = 0 \quad \text{for } |\alpha_n| < k_s. \quad (3.22)$$

Using (3.22), we arrive at

$$(F_0, v)_{\Omega_b} = \int_{\Gamma_b} f_0 \cdot \bar{v} ds = 0,$$

with f_0 given in (3.18). Applying the Fredholm alternative yields the existence of a solution to (DP).

We next prove uniqueness for small frequencies. If $B(u, u) = 0$ for some $u \in V_\alpha$, then it follows from [34, Lemma 4] that the Rayleigh coefficient of order zero of u vanishes. This together with the asymptotic behavior of the matrix W_n (see [34, Lemma 2]) as $\omega \rightarrow 0^+$ leads to the estimate

$$\operatorname{Re} \left\{ - \int_{\Gamma_b} \bar{u} \cdot \mathcal{T} u ds \right\} \geq C \|u\|_{H_\alpha^{1/2}(\Gamma_b)^2}^2,$$

for some constant $C > 0$ independent of u and ω . Then, one can prove the coercivity of the sesquilinear form B via the estimate (cf. [34, Remark 2])

$$B(u, u) \geq \int_{\Omega_b} a(u, \bar{u}) dx + C \|u\|_{H_\alpha^{1/2}(\Gamma_b)^2}^2 - \omega^2 \|u\|_{L^2(\Omega_b)^2}^2 \geq C_1 \|u\|_{H_\alpha^1(\Omega_b)^2}^2,$$

which implies that $u = 0$ if ω is sufficiently small. In view of the analytic Fredholm theory (see e.g. [27, Theorem 8.26] or [50, Theorem I. 5. 1]), we obtain uniqueness and existence for all frequencies $\omega \in \mathbb{R}^+ \setminus \mathcal{D}$, where \mathcal{D} is a discrete set including the Rayleigh frequencies. Moreover, we conclude from the arguments in [34, Theorem 6] or [42, Theorem 3.3] that \mathcal{D} cannot have a finite accumulation point.

(ii) If Λ is the graph of a smooth function f and $u = 0$ on Λ , by a periodic Rellich identity we have (see [34])

$$\begin{aligned}
 0 &= -2\text{Re} \int_{\Omega_b} (\Delta^* + \omega)u \cdot \partial_2 \bar{u} \, dx \\
 &= \left(\int_{\Lambda} + \int_{\Gamma_b} \right) \left(2\text{Re}(Tu \cdot \partial_2 \bar{u}) - a(u, \bar{u})n_2 + \omega^2 |u|^2 n_2 \right) ds \quad (3.23) \\
 &= \int_{\Lambda} (\mu |\partial_n u|^2 + (\lambda + \mu) |\text{div} u|^2) n_2 \, ds.
 \end{aligned}$$

Since $n_2 = -1/\sqrt{1 + |f'|^2} < 0$, there holds $\partial_n u = u = 0$ on Λ . Applying Holmgren’s theorem leads to uniqueness at arbitrary frequency. By Theorem 3.3, existence follows directly from uniqueness via the Fredholm alternative. Note that the integral in (3.23) over Λ does not make sense for Lipschitz graphs. To deal with the Lipschitz boundary, one can adapt Nečas’ method [66, Chap. 5] of approximating the grating profile by smooth graphs. For the details we refer to [44] and [34]. □

Theorem 3.4 (ii) generalizes the results of [44, 54] for the scalar quasiperiodic Helmholtz equation to the case of the Navier equation. More general Rellich identities for the Navier equation (on bounded domains) can be found in [28]. The well-posedness for the boundary value problem with mixed Dirichlet and impedance boundary conditions can also be established for all frequencies, provided Λ is a Lipschitz curve [34]. The uniqueness to (DP) under the second, third, and fourth-kind boundary conditions is not true in general. Nonuniqueness examples can be constructed for a flat grating in the resonance case (see [39]).

3.3 Uniqueness and existence for transmission gratings

Suppose the whole (x_1, x_2) -plane is filled with elastic materials that are homogeneous above and below a certain interface Λ of period 2π . Let Ω^\pm be the unbounded domains above and below Λ , respectively. We assume that the Lamé coefficients μ^\pm, λ^\pm in Ω^\pm are constants satisfying $\mu^\pm > 0, \lambda^\pm + \mu^\pm > 0$, and that the mass densities ρ^\pm are positive constants in these subdomains. Let $k_p^\pm := \omega \sqrt{\rho^\pm / (2\mu^\pm + \lambda^\pm)}$, $k_s^\pm := \omega \sqrt{\rho^\pm / \mu^\pm}$ be the corresponding compressional and shear wave numbers, respectively. In Section 3, we assume that a time-harmonic plane elastic wave u^{in} with

incident angle θ is incident on Λ from Ω^+ , which is either an incident pressure wave of the form (3.1), or an incident shear wave of the form (3.2), with k_p, k_s replaced by k_p^+, k_s^+ . We then look for the total displacement field u

$$u = u^{in} + u^+ \text{ in } \Omega^+, \quad u = u^- \text{ in } \Omega^-, \tag{3.24}$$

where the scattered fields u^\pm satisfy the corresponding Navier equations

$$(\Delta^* + \omega^2 \rho^\pm) u^\pm = 0 \text{ in } \Omega^\pm, \tag{3.25}$$

with the α -quasiperiodicity condition

$$u^\pm(x_1 + 2\pi, x_2) = \exp(2i\alpha\pi) u^\pm(x_1, x_2). \tag{3.26}$$

On the interface the continuity of the displacement and the stress lead to the transmission conditions

$$u^{in} + u^+ = u^-, \quad T^+(u^{in} + u^+) = T^- u^- \text{ on } \Lambda, \tag{3.27}$$

where the corresponding stress operators are defined as in (3.8), with μ, λ replaced by μ^\pm, λ^\pm . Finally, we need to impose appropriate radiation conditions on the scattered fields u^\pm as $x_2 \rightarrow \pm\infty$. Introduce the notation

$$\Lambda^+ := \max_{(x_1, x_2) \in \Lambda} x_2, \quad \Lambda^- := \min_{(x_1, x_2) \in \Lambda} x_2,$$

and define β_n^\pm and γ_n^\pm as in (3.11) with k_p, k_s replaced by k_p^\pm, k_s^\pm . Then we insist that the scattered fields u^\pm admit the following Rayleigh expansions (cf. (3.10)), for $x_2 \gtrless \Lambda^\pm$:

$$u^\pm(x) = \sum_{n \in \mathbb{Z}} \left\{ A_{p,n}^\pm (\alpha_n, \pm\beta_n^\pm)^\top \exp(i\alpha_n x_1 \pm i\beta_n^\pm x_2) + A_{s,n}^\pm (\pm\gamma_n^\pm, -\alpha_n)^\top \exp(i\alpha_n x_1 \pm i\gamma_n^\pm x_2) \right\}. \tag{3.28}$$

Transmission problem (TP): Given a grating profile curve $\Lambda \subset \mathbb{R}^2$ (which is 2π -periodic in x_1) and an incident plane pressure or shear wave u^{in} , find a vector function $u \in H_{loc}^1(\mathbb{R}^2)^2$ that satisfies (3.24)–(3.28).

Introduce artificial boundaries

$$\Gamma^\pm := \{(x_1, b^\pm) : 0 \leq x_1 \leq 2\pi\}, \quad b^+ > \Lambda^+, \quad b^- < \Lambda^-$$

and the bounded domains

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

The DtN maps \mathcal{T}^\pm on the artificial boundaries Γ^\pm have the Fourier series representations (cf. Lemma 3.2 (i))

$$\mathcal{T}^\pm u^\pm := - \sum_{n \in \mathbb{Z}} W_n^\pm \hat{u}_n^\pm \exp(i\alpha_n x_1), \quad u^\pm = \sum_{n \in \mathbb{Z}} \hat{u}_n^\pm \exp(i\alpha_n x_1) \in H_\alpha^{1/2}(\Gamma^\pm)^2,$$

where the matrices $W_n^\pm = W_n^\pm(\omega, \alpha)$ take the form (cf. (3.15))

$$W_n^\pm := \frac{1}{i} \begin{pmatrix} \omega^2 \rho^\pm \beta_n^\pm / d_n^\pm & 2\mu^\pm \alpha_n - \omega^2 \rho^\pm \alpha_n / d_n^\pm \\ -2\mu^\pm \alpha_n + \omega^2 \rho^\pm \alpha_n / d_n^\pm & \omega^2 \rho^\pm \gamma_n^\pm / d_n^\pm \end{pmatrix},$$

with $d_n^\pm := \alpha_n^2 + \beta_n^\pm \gamma_n^\pm$. Applying the first Betti formula on each subdomain Ω^\pm to a solution of (TP), and using the transmission conditions (3.27), we obtain the following variational formulation of (TP) on the bounded domain Ω : Find $u \in H_\alpha^1(\Omega)^2$ such that

$$\begin{aligned} B(u, \varphi) &:= \int_{\Omega_b} (a(u, \overline{\varphi}) - \omega^2 \rho u \cdot \overline{\varphi}) dx - \int_{\Gamma^+} \overline{\varphi} \cdot \mathcal{T}^+ u ds - \int_{\Gamma^-} \overline{\varphi} \cdot \mathcal{T}^- u ds \\ &= \int_{\Gamma^+} f_0 \cdot \overline{\varphi} ds, \quad \forall \varphi \in H_\alpha^1(\Omega)^2. \end{aligned} \tag{3.29}$$

Here the domain integral is understood as the sum of the integrals

$$\int_{\Omega_b^\pm} (a^\pm(u, \overline{\varphi}) - \omega^2 \rho^\pm u \cdot \overline{\varphi}) dx,$$

where the bilinear forms a^\pm are defined as in (3.13), with μ, λ replaced by μ^\pm, λ^\pm , and the function f_0 on the right-hand side is defined analogously as in (3.18), with $\beta_0, \gamma_0, k_p, k_s, \lambda, \mu$ replaced by $\beta_0^+, \gamma_0^+, k_p^+, k_s^+, \lambda^+, \mu^+$, respectively. As in (3.20), the sesquilinear form B defined in (3.29) generates a continuous linear operator \mathcal{B} from $H_\alpha^1(\Omega_b)^2$ into its dual $(H_\alpha^1(\Omega_b)^2)'$, with respect to the pairing $(u, \varphi)_{\Omega_b} = \int_{\Omega_b} u \cdot \overline{\varphi}$, via

$$B(u, \varphi) = (\mathcal{B}u, \varphi)_{\Omega_b}, \quad \forall u, \varphi \in H_\alpha^1(\Omega_b)^2. \tag{3.30}$$

The following result extends Theorems 3.3 and 3.4 (i) to problem (TP).

Theorem 3.5 ([34]).

- (i) *The sesquilinear form B defined by (3.29) is strongly elliptic over $H_\alpha^1(\Omega)^2$, and the operator \mathcal{B} defined in (3.30) is Fredholm with index zero.*
- (ii) *For an incident plane pressure or shear wave, there always exists a solution to the variational problem (3.29) and hence to problem (TP).*
- (iii) *Assume that u^{in} is an incident pressure wave of the form (3.1) (with $k_p = k_p^+$). Then, there exists a sufficiently small frequency $\omega_0 > 0$ such that the variational problem (3.29) admits a unique solution $u \in H_\alpha^1(\Omega_b)^2$ for all incident angles and for all frequencies $\omega \in (0, \omega_0]$. Moreover, for all but a sequence of countable frequencies $\omega_j \rightarrow \infty$, the variational problem (3.29) admits a unique solution.*

(iv) For an incident shear wave of the form (3.2), the results of the third assertion remain valid under one of the following additional assumptions:

- (1) $k_p^+ > k_s^+ \sin \theta$, or equivalently, $\mu^+ / (2\mu^+ + \lambda^+) > \sin^2 \theta$,
- (2) $k_p^- > k_s^+$, or equivalently, $\rho^- / (2\mu^- + \lambda^-) > \rho^+ / \mu^+$.

Remark 3.6. Assume that the elastic material is homogeneous above some periodic Lipschitz interface and below another periodic Lipschitz interface, whereas the elastic medium between the two interfaces may be inhomogeneous with piecewise constant Lamé parameters λ , μ and density ρ having jumps at certain (finitely many) disjoint periodic Lipschitz interfaces. Then Theorem 3.5 can be easily extended to these more general periodic diffractive structures.

In general, the uniqueness result of Theorem 3.4 (ii) does not hold for the transmission problem (TP). Even in the special case of two half-planes with certain elastic parameters λ^\pm , μ^\pm , ρ^\pm and the transmission conditions (3.27) on the line $\{x_2 = 0\}$, there may exist nontrivial solutions of the homogeneous problem (Rayleigh surface waves) that decay exponentially as $x_2 \rightarrow \pm\infty$ [3]. Hence additional conditions must be imposed on the elastic parameters to guarantee the uniqueness. As an example, we present a new uniqueness result for (TP) at any frequency of the incident wave.

Theorem 3.7. Assume that the interface Λ is given by the graph of a 2π -periodic Lipschitz function $x_2 = f(x_1)$. Suppose further that $\rho^+ \neq \rho^-$ and that the Lamé constants λ^\pm, μ^\pm in Ω_b^\pm satisfy $\lambda^+ = \lambda^-, \mu^+ = \mu^-$. Then there exists a unique solution u to problem (TP).

Proof. By Theorem 3.5 (i), we only need to prove $u = 0$ provided that $u^{in} = 0$. Suppose first that the grating profile is given by a C^∞ -smooth function f . Applying the Rellich identity (3.23) to u^\pm in Ω_b^\pm yields (cf. (3.23))

$$\begin{aligned} 0 &= -2\operatorname{Re} \int_{\Omega_b^\pm} (\Delta^* + \omega) u^\pm \cdot \partial_2 \bar{u}^\pm dx \\ &= \left(\pm \int_\Lambda + \int_{\Gamma^\pm} \right) 2\operatorname{Re}(T^\pm u^\pm \cdot \partial_2 \bar{u}^\pm) - a^\pm(u^\pm, \bar{u}^\pm) n_2 + \omega^2 \rho^\pm |u^\pm|^2 n_2 ds, \quad (3.31) \\ &= \pm \int_\Lambda 2\operatorname{Re}(T^\pm u^\pm \cdot \partial_2 \bar{u}^\pm) - a^\pm(u^\pm, \bar{u}^\pm) n_2 + \omega^2 \rho^\pm |u^\pm|^2 n_2 ds. \end{aligned}$$

Note that the normal to Λ is directed into Ω^- . Making use of the transmission conditions (3.27) with $u^{in} = 0, \lambda^+ = \lambda^-, \mu^+ = \mu^-$, we deduce that $\nabla u^+ = \nabla u^-$ on Λ , leading to

$$T^+ u^+ \cdot \partial_2 \bar{u}^+ = T^- u^- \cdot \partial_2 \bar{u}^-, \quad a^+(u^+, \bar{u}^+) = a^-(u^-, \bar{u}^-) \quad \text{on } \Lambda.$$

Thus, from (3.31) we see that

$$0 = \omega^2(\rho^+ - \rho^-) \int_{\Lambda} |u^+|^2 n_2 ds.$$

This relation combined with $n_2 = -1/\sqrt{1 + |f'|^2} < 0$ and the transmission condition (3.27) gives $u^+ = u^- = 0$ on Λ . By the uniqueness to the forward scattering problem with the Dirichlet boundary condition (see Theorem 3.4 (ii)), we conclude that $u^\pm = 0$ in Ω_b^\pm . Thus $u = 0$ in Ω_b . In the general case we proceed analogously to Theorem 3.4 (ii) by using Nečas' method [66, Chap. 5] of approximating the Lipschitz grating profile by smooth graphs. \square

Remark 3.8. The solvability results in Theorems 3.4, 3.5 and 3.7 can be generalized to biperiodic diffraction gratings in \mathbb{R}^3 . However, to prove an analog of Lemma 3.2 for the DtN map, a more sophisticated analysis than for plane elasticity is needed. Note that the 2×2 matrix W_n in (3.14) must be replaced by a 3×3 matrix in the biperiodic case. For further details we refer to [39].

4 Uniqueness for inverse scattering problems

In this section, we will review recent uniqueness results for inverse elastic scattering by periodic structures. Suppose that the two gratings Λ_1, Λ_2 generate the total fields $u_j(x; \theta_m)$ ($j = 1, 2$) for the incident plane wave of the form (3.1) or (3.2) with the incident angle $\theta = \theta_m$. We are interested in the following uniqueness questions about the inverse problem (IP). Does the relation

$$u_1(x_1, b; \theta_m) = u_2(x_1, b; \theta_m), \quad \forall x_1 \in (0, 2\pi), \text{ for } m = 1, 2, \dots, M,$$

with some sufficiently large b imply $\Lambda_1 = \Lambda_2$? If yes, what is the minimal number of incident elastic waves needed to assure uniqueness? Moreover, can we describe the exceptional classes of grating profiles that generate the same near field data on $x_2 = b$? A first answer related to these questions is given in [6] for the Dirichlet boundary condition with several incident frequencies.

Investigating the eigenvalues and quasiperiodic eigenfunctions of Lamé operator in a periodic layer, it is proved in [6] that a Dirichlet C^2 -smooth surface can be uniquely determined from the scattered fields corresponding to incident pressure waves for one incident angle and an interval of wave numbers. Moreover, a finite number of wave numbers is enough if some a priori information about the height of the grating is available. In particular, uniqueness with one incident pressure wave holds if the height is sufficiently small. This extends the paper by Hettlich and Kirsch on the periodic analog of Schiffer's theorem (see [52]) to the case of elastic scattering. We further refer to [6, Theorem 5] for the minimal number of compressional wave numbers need-

ed to guarantee uniqueness. See also [5, 14, 18, 55] for other uniqueness results within smooth periodic profiles in inverse scattering of acoustic and electromagnetic waves.

As already mentioned in the introduction, there are recent uniqueness results on inverse acoustic and electromagnetic scattering by polygonal and polyhedral obstacles and diffraction gratings [4, 16, 17, 26, 35, 41, 45, 46, 59, 61]. These results are essentially based on reflection principles for the Helmholtz and Maxwell equations. In this section, we present corresponding uniqueness theorems for polygonal elastic diffraction gratings under the third or fourth-kind boundary conditions, where a reflection principle is available. There seems to be no reflection principle for the Navier equation under the physically more relevant boundary conditions of the first (Dirichlet) or second (Neumann) kind. Thus it is still a challenging problem to study uniqueness in the inverse problem under these boundary conditions.

Let \mathcal{A} be our admissible class of periodic structures defined by

$$\mathcal{A} := \{\Lambda : \Lambda = (x_1, f(x_1)), \text{ where } f \text{ is a continuous piecewise linear function of period } 2\pi \text{ satisfying } \max_{x_1 \in \mathbb{R}} \{f(x_1)\} < b, \text{ and the graph of } f \text{ restricted to } [0, 2\pi] \text{ consists of finitely many line segments and is not a straight line parallel to the } x_1\text{-axis}\}.$$

Note that flat gratings are excluded from our admissible class \mathcal{A} , because such gratings cannot be uniquely determined by a fixed number of incident pressure or shear waves [36, Section 4].

4.1 Inverse scattering of incident pressure waves

In this section, we make the following assumptions.

- (A1) $u^{in} = u_p^{in} := \hat{\theta} \exp(ik_p x \cdot \hat{\theta})$ with some fixed incident angle $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$.
- (A2) Without loss of generality, one of the profiles $\Lambda_1, \Lambda_2 \in \mathcal{A}$ has a corner point at the origin $O = (0, 0)$.
- (A3) The corresponding total fields u_1 and u_2 both satisfy the third (or fourth) kind boundary conditions on Λ_1 and Λ_2 , and they coincide on Γ_b :

$$u_1(x_1, b; \theta) = u_2(x_1, b; \theta), \quad x_1 \in (0, 2\pi). \tag{3.32}$$

Introduce the (exceptional) class of polygonal grating profiles $\mathcal{D}_2(\theta, k_p)$ by

$$\mathcal{D}_2(\theta, k_p) := \{\Lambda \in \mathcal{A} : \text{each line segment of } \Lambda \text{ lies on a straight line defined by } x_2 = x_1 \tan \varphi + \frac{2\pi}{k_p \cos \theta} n \text{ for some } n \in \mathbb{Z} \text{ with } \varphi \in \{\frac{\theta}{2} + \frac{\pi}{4}, \frac{\theta}{2} - \frac{\pi}{4}\}\}$$

if $k_p(1 \pm \sin \theta) \in \mathbb{Z}$, and by $\mathcal{D}_2(\theta, k_p) := \emptyset$ otherwise. See Figure 3.1 for two different grating profiles from the class $\mathcal{D}_2(\theta, k_p)$ with $\theta = -\frac{\pi}{6}, k_p = 2$. In fact, the set $\mathcal{D}_2(\theta, k_p)$ contains grating profiles which only depend on the incident pressure

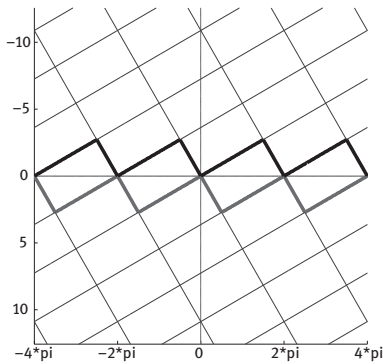


Figure 3.1: (See Color Plates for a color version.) $\mathcal{D}_2(\theta, k_p)$ with $\theta = -\frac{\pi}{6}$, $k_p = 2$.

wave. One can prove that $\mathcal{D}_2(\theta, k_p) \neq \emptyset$ for all k_p and θ satisfying $k_p(1 \pm \sin \theta) \in \mathbb{Z}$ [36, Lemma 11].

Given a fixed incident angle θ , define

$$\pi_p := \{n \in \mathbb{Z} : \beta_n(\theta) = 0\}, \quad \pi_s := \{n \in \mathbb{Z} : \gamma_n(\theta) = 0\}.$$

We say that a Rayleigh frequency occurs if either $\pi_p \neq \emptyset$ or $\pi_s \neq \emptyset$, and that Rayleigh frequencies of the compressional (shear) part are excluded if $\pi_p = \emptyset$ ($\pi_s = \emptyset$). Let us now give the main theorem for the fourth-kind boundary conditions.

Theorem 3.9 ([36]). *Assume the boundary conditions of the fourth kind (3.7) are imposed on Λ_1 and Λ_2 . Then the relation (3.32) implies that one of the following cases must occur:*

- (i) $\Lambda_1 = \Lambda_2$.
- (ii) $\Lambda_1, \Lambda_2 \in \mathcal{D}_2(\theta, k_p)$, $\pi_p = \emptyset$, and the total field takes the form

$$u = \hat{\theta} \exp(ik_p x \cdot \hat{\theta}) - \hat{\theta} \exp(-ik_p x \cdot \hat{\theta}) - e_1 \exp(ik_p x_1) + e_1 \exp(-ik_p x_1)$$

with $u = u_j$ ($j = 1, 2$), $e_1 = (1, 0)^\top$.

It follows from Theorem 3.9 (ii) that the class $\mathcal{D}_2(\theta, k_p)$ contains the exceptional grating profiles which generate the same total field, with a finite number of propagating modes only involved in the compressional part of the scattered field. Nonuniqueness examples to (IP) with one incident pressure wave can be easily constructed from the set $\mathcal{D}_2(\theta, k_p)$ (see e.g. [36, Section 6.2]).

The following reflection principle for the Navier equation is the main tool for proving Theorem 3.9 and the other theorems below. We denote by R_l the reflection with respect to a line l in \mathbb{R}^2 , and by R'_l the reflection with respect to the line l' that passes through the origin O and is parallel to l .

Lemma 3.10 ([36]). (*Reflection principle for the Navier equation*) Let Ω be a symmetric domain with respect to a line l , and let $\tilde{l} \subset \Omega$ be a subset of another line such that $R_l(\tilde{l}) \subset \Omega$. Assume $u \in H^1(\Omega)^2$ satisfies the Navier equation $\Delta^* u + \omega^2 u = 0$ in Ω .

(i) If u satisfies the boundary conditions of the fourth kind (3.7) on $l \cap \Omega$, then

$$u(x) + R'_l(u(R_l(x))) = 0 \quad \text{in } \Omega. \tag{3.33}$$

(ii) If u satisfies the boundary conditions of the third kind (3.6) on $l \cap \Omega$, then

$$u(x) - R'_l(u(R_l(x))) = 0 \quad \text{in } \Omega. \tag{3.34}$$

(iii) In particular, if u satisfies the fourth respectively third-kind boundary conditions on both l and \tilde{l} in Ω , then the same boundary conditions hold on $R_l(\tilde{l})$.

The original version of the reflection principle for the Navier equation can be found in [47], where it was proved in the three-dimensional case when the domain Ω is symmetric with respect to the (x_1, x_2) -plane. The proof readily carries over to a two-dimensional domain Ω in the above lemma. Note that the relations (3.33) and (3.34) are similar to those given in [60, 61] for the Maxwell equations.

Proof of Theorem 3.9. From the assumption (3.32) and the unique continuation of solutions to the Navier equation, it follows that $u_1(x) = u_2(x)$ for all x lying above the profiles Λ_1 and Λ_2 . Relying on the analyticity of u_j and the reflection principle in Lemma 3.10, one can always find an “exit” ray l extending to infinity in $x_2 > b$ such that u_j ($j = 1, 2$) satisfies the fourth-kind boundary conditions on l . Applying properties of almost periodic functions to $u_j|_l$ gives the vanishing Rayleigh coefficients $A_{p,n} = 0$ for $|\alpha_n| > k_p$ and $A_{s,n} = 0$ for $|\alpha_n| > k_s$. Therefore, both of the total fields $u_j = u^{in} + u_j^{sc}$, $j = 1, 2$, can be reduced to a finite sum of propagating waves, i.e.

$$\begin{aligned} u_1 = u_2 = u^{in} &+ \sum_{|\alpha_n| \leq k_p} A_{p,n}(\alpha_n, \beta_n)^\top e^{i(\alpha_n x_1 + \beta_n x_2)} \\ &+ \sum_{|\alpha_n| \leq k_s} A_{s,n}(\gamma_n, -\alpha_n)^\top e^{i(\alpha_n x_1 + \gamma_n x_2)} \end{aligned}$$

for $x_2 > b$, which can be analytically extended to the whole plane. Further, it can be derived from the reflection relation (3.33) that the solution u and its finite number of propagating directions exhibit some rotational and reflection invariance (see [36, Lemmas 6 and 7]) around the origin. This symmetry implies further that $A_{s,n} = 0$ for all $|\alpha_n| \leq k_s$, due to the incident pressure wave u_p^{in} and the assumption that Λ_j ($j = 1, 2$) is the graph of a function [36, Lemma 8]. Therefore, the total field only consists of the compressional part with a finite number of propagating directions lying on the circle $|x| = k_p$. Among these directions, only the incident wave of direction $(\alpha, -\beta)^\top$ is propagating downward, whereas the other waves of directions $(\alpha_n, \beta_n)^\top$ are propagating upward when $\beta_n > 0$ or along the x_1 -axis when $\beta_n = 0$.

From the reflectional and rotational invariance of these directions, one can describe each propagating direction of the compressional part and its corresponding Rayleigh coefficient in terms of the incident compressional wave number k_p and the incident angle θ . This implies the representation of the total field in Theorem 3.9 (ii) and leads to the definition of the unidentifiable set $\mathcal{D}_2(\theta, k_p)$ (see [36]). \square

The following results can be obtained directly from Theorem 3.9.

Remark 3.11.

- (i) Let $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$. If $\mathcal{D}_2(\theta, k_p) = \emptyset$ or $\Lambda \notin \mathcal{D}_2(\theta, k_p)$, then one incident pressure wave with the incident angle θ uniquely determines $\Lambda \in \mathcal{A}$. Since $\mathcal{D}_2(\theta, k_p) = \emptyset$ if $\pi_p = \emptyset$, we have uniqueness with one incident pressure wave provided the Rayleigh frequencies of the compressional part are excluded.
- (ii) Two incident pressure waves are always sufficient to uniquely determine $\Lambda \in \mathcal{A}$ since

$$\mathcal{D}_2(\theta_1, k_p) \cap \mathcal{D}_2(\theta_2, k_p) = \emptyset, \quad \theta_1 \neq \theta_2.$$

Before stating the main theorem for the third-kind boundary conditions, we introduce the following three (exceptional) classes of polygonal periodic structures.

For $2k_p \sin \theta \in \mathbb{Z}$, let

$$\begin{aligned} \mathcal{N}_2(\theta, k_p) := \{ \Lambda \in \mathcal{A} : \text{each line segment of } \Lambda \text{ lies on a straight line defined} \\ \text{by } x_2 = x_1 \tan \theta + \frac{\pi}{k_p \cos \theta} n \text{ for some } n \in \mathbb{Z}, \text{ or} \\ x_2 = x_1 \tan(\theta + \frac{\pi}{2}) + c \text{ for some } c \in \mathbb{R} \}, \end{aligned}$$

and if $2k_p \sin \theta \notin \mathbb{Z}$, set $\mathcal{N}_2(\theta, k_p) := \emptyset$. Moreover,

$$\begin{aligned} \mathcal{N}_3(\theta, k_p) := \{ \Lambda \in \mathcal{A} : \text{each line segment of } \Lambda \text{ lies on a straight line defined} \\ \text{by } x_2 = x_1 \tan \varphi + \frac{2\pi}{k_p \sqrt{3} \cos \varphi} n \text{ for some } n \in \mathbb{Z}, \text{ with} \\ \varphi \in \{ \theta + \frac{5\pi}{6}, \theta + \frac{\pi}{6}, \theta - \frac{\pi}{2} \} \} \end{aligned}$$

if $\theta \in [-\frac{\pi}{6}, \frac{\pi}{6}]$ and $k_p \sqrt{3} \sin(\frac{\pi}{6} \pm \theta) \in \mathbb{Z}$, and $\mathcal{N}_3(\theta, k_p) := \emptyset$ otherwise. Finally,

$$\begin{aligned} \mathcal{N}_4(0, k_p) := \{ \Lambda \in \mathcal{A} : \text{each line segment of } \Lambda \text{ lies on a straight line defined} \\ \text{by } x_2 = \pm x_1 + \frac{2\pi}{k_p} n \text{ for some } n \in \mathbb{Z}, \text{ or} \\ x_2 = \frac{\pi}{k_p} m \text{ for some } m \in \mathbb{Z} \} \end{aligned}$$

if $\theta = 0$ and $k_p \in \mathbb{Z}$, and $\mathcal{N}_4(0, k_p) := \emptyset$ otherwise. See Figure 3.2 for examples of the triangular grids on which the profiles of $\mathcal{N}_3(\theta, k_p)$ and $\mathcal{N}_4(0, k_p)$ are located.

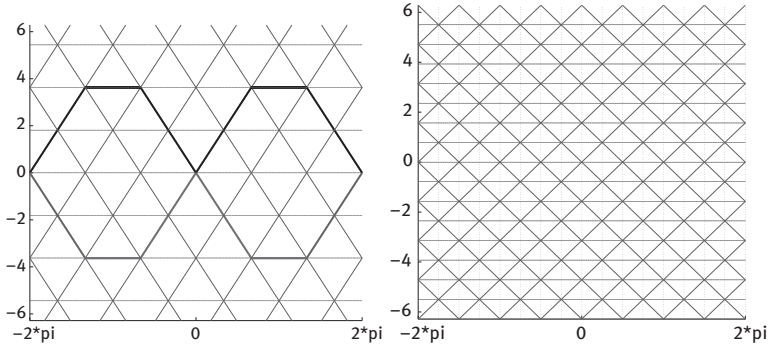


Figure 3.2: (See Color Plates for a color version.) Left: $\mathcal{N}_3(\theta, k_p)$ with $\theta = -\frac{\pi}{6}, k_p = 2$. Right: $\mathcal{N}_4(0, k_p)$ with $k_p = 4$.

Theorem 3.12 ([36]). *Assume the third-kind boundary conditions (3.6) are imposed on Λ_1 and Λ_2 . Then the relation (3.32) implies one of the following cases:*

- (i) $\Lambda_1 = \Lambda_2$.
- (ii) (a) $\Lambda_1, \Lambda_2 \in \mathcal{N}_2(\theta, k_p), \pi_p = \emptyset$, and the total field takes the form

$$u(x) = \hat{\theta} \exp(ik_p x \cdot \hat{\theta}) - \hat{\theta} \exp(-ik_p x \cdot \hat{\theta}).$$

- (b) $\Lambda_1, \Lambda_2 \in \mathcal{D}_2(\theta, k_p), \pi_p \neq \emptyset$, and the total field can be written as

$$u(x) = \hat{\theta} \exp(ik_p x \cdot \hat{\theta}) - \hat{\theta} \exp(-ik_p x \cdot \hat{\theta}) + e_1 \exp(ik_p x_1) - e_1 \exp(-ik_p x_1).$$

- (iii) $\Lambda_1, \Lambda_2 \in \mathcal{N}_3(\theta, k_p)$ with $\theta \in [-\frac{\pi}{6}, \frac{\pi}{6}]$. In this case, $\pi_p \neq \emptyset$ if $\theta = \frac{\pi}{6}$ or $\theta = -\frac{\pi}{6}$, and the total field takes the form

$$u(x) = \hat{\theta} \exp(ik_p x \cdot \hat{\theta}) + \text{Rot}_{\frac{2\pi}{3}}(\hat{\theta}) \exp(ik_p x \cdot \text{Rot}_{\frac{2\pi}{3}}(\hat{\theta})) + \text{Rot}_{\frac{4\pi}{3}}(\hat{\theta}) \exp(ik_p x \cdot \text{Rot}_{\frac{4\pi}{3}}(\hat{\theta})),$$

where Rot_φ denotes the rotation around the origin O by the angle φ .

- (iv) $\Lambda_1, \Lambda_2 \in \mathcal{N}_4(0, k_p), \theta = 0, \pi_p \neq \emptyset$, and the total field can be written as

$$u(x) = -e_2 \exp(-ik_p x_2) + e_2 \exp(ik_p x_2) + e_1 \exp(ik_p x_1) - e_1 \exp(-ik_p x_1).$$

Here $u = u_j$ ($j = 1, 2$), $e_1 = (1, 0)^\top$ and $e_2 = (0, 1)^\top$.

Corollary 3.13. *Suppose that the assumptions of Theorem 3.12 are satisfied. If (3.32) holds for four incident pressure waves with distinct incident angles, then Λ_1 and Λ_2 must be identical, while three incident waves are always enough to imply $\Lambda_1 = \Lambda_2$ if the Rayleigh frequencies of the compressional part for each incident angle are excluded.*

We refer to [35, Corollary 5] for additional conditions on the incident angles and the compressional wave number k_p guaranteeing that each grating profile $\Lambda \in \mathcal{A}$ can be uniquely determined by three incident pressure waves under the third-kind boundary conditions.

4.2 Inverse scattering of incident shear waves

In this section, we assume that the profiles $\Lambda_1, \Lambda_2 \in \mathcal{A}$ satisfy the conditions (A2) and (A3) again, whereas u^{in} in (A1) has to be replaced by the incident shear wave $u_s^{in}(x) = \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta})$. Then the uniqueness results of [36] for incident plane shear waves may be stated as follows.

Theorem 3.14. *Assume the boundary conditions of the third kind (3.6) are imposed on Λ_1 and Λ_2 . Then the relation (3.32) implies one of the following cases:*

- (i) $\Lambda_1 = \Lambda_2$.
- (ii) $\Lambda_1, \Lambda_2 \in \mathcal{D}_2(\theta, k_s)$, $\pi_s = \emptyset$, and the total field takes the form

$$u(x) = \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta}) - \hat{\theta}^\perp \exp(-ik_s x \cdot \hat{\theta}) + e_2 \exp(ik_s x_1) - e_2 \exp(-ik_s x_1)$$

with $u = u_j$ ($j = 1, 2$), $e_2 = (0, 1)^\top$.

Theorem 3.15. *Let the fourth-kind boundary conditions (3.7) be satisfied on Λ_1 and Λ_2 , and assume that (3.32) holds. Then one of the following cases must occur:*

- (i) $\Lambda_1 = \Lambda_2$.
- (ii) (a) $\Lambda_1, \Lambda_2 \in \mathcal{N}_2(\theta, k_s)$, $\pi_s = \emptyset$, and the total field takes the form

$$u(x) = \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta}) - \hat{\theta}^\perp \exp(-ik_s x \cdot \hat{\theta}).$$

- (b) $\Lambda_1, \Lambda_2 \in \mathcal{D}_2(\theta, k_s)$, $\pi_s \neq \emptyset$, and the total field takes can be written as

$$u = \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta}) - \hat{\theta}^\perp \exp(-ik_s x \cdot \hat{\theta}) - e_2 \exp(ik_s x_1) + e_2 \exp(-ik_s x_1).$$

- (iii) $\Lambda_1, \Lambda_2 \in \mathcal{N}_3(\theta, k_s)$ with $\theta \in [-\frac{\pi}{6}, \frac{\pi}{6}]$. In this case, $\pi_s \neq \emptyset$ if $\theta = \frac{\pi}{6}$ or $\theta = -\frac{\pi}{6}$, and the total field takes the form

$$\begin{aligned} u(x) &= \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta}) + (\text{Rot}_{\frac{2\pi}{3}}(\hat{\theta}))^\perp \exp(ik_s x \cdot \text{Rot}_{\frac{2\pi}{3}}(\hat{\theta})) \\ &\quad + (\text{Rot}_{\frac{4\pi}{3}}(\hat{\theta}))^\perp \exp(ik_s x \cdot \text{Rot}_{\frac{4\pi}{3}}(\hat{\theta})). \end{aligned}$$

- (iv) $\Lambda_1, \Lambda_2 \in \mathcal{N}_4(0, k_s)$, $\theta = 0$, $\pi_s \neq \emptyset$, and the total field can be written as

$$u(x) = e_1 \exp(-ik_s x_2) - e_1 \exp(ik_s x_2) + e_2 \exp(ik_s x_1) - e_2 \exp(-ik_s x_1).$$

As the counterpart of Remark 3.11 and Corollary 3.13, we have the following uniqueness results with the minimal number of incident shear waves.

Corollary 3.16. *Two (four) incident shear waves with distinct incidence angles are sufficient to uniquely determine a grating profile $\Lambda \in \mathcal{A}$ under the boundary conditions of the third (fourth) kind. If the Rayleigh frequencies of the shear part are excluded, then the minimal number is one (three).*

Remark 3.17. The uniqueness results in Section 4 generalize those for acoustic and electromagnetic gratings [35] to the elastic case. As one would expect, the derivation of the unidentifiable classes in 3D is more complicated than in 2D, since we must take into account biperiodic structures which vary in both x_1 and x_2 and where the incident wave is not perpendicular to the x_3 -axis. In general, there exist five (two) classes of unidentifiable polyhedral grating profiles in the case of plane shear (pressure) wave incidence under the boundary conditions of the third (fourth) kind [37].

5 Numerical solution of direct and inverse scattering problems

5.1 A discrete Galerkin method for (DP)

In this section, we discuss the numerical treatment of the direct scattering problem for the Dirichlet boundary condition. The approach is based on the discrete Galerkin method proposed by Atkinson [13] for solving an equivalent integral equation of first kind. A similar method is used in [56] for solving the forward problem of elastic scattering from an open arc in \mathbb{R}^2 . As mentioned in the introduction, the implementation of this method is easier than the integral equation method with a second-kind integral equation. This approach also leads to the unique solvability of the forward scattering problem for the Dirichlet boundary condition (see [38, Lemma 4.1]). In the sequel, we assume that the incident wave is an incident pressure wave, and that Λ is the graph of some C^2 -smooth periodic function f . For piecewise linear gratings where the scattered field may be singular at corner points, one can adopt a mesh grading transformation to parameterize the grating profile (see [38, 43]). In this section, it is supposed that $\pi_p = \pi_s = \emptyset$, that is, the Rayleigh frequencies are excluded.

We first recall the free space fundamental solution $\Phi_k(x, y)$ to the Helmholtz equation $(\Delta + k^2)u = 0$ given by

$$\Phi_k(x, y) = \frac{i}{4} H_0^{(1)}(k|x - y|), \quad x \neq y, \quad x = (x_1, x_2), \quad y = (y_1, y_2) \in \mathbb{R}^2,$$

with $H_0^{(1)}(t)$ being the first-kind Hankel function of order zero, and then recall the α -quasiperiodic fundamental solution to the Helmholtz equation defined by (see

e.g. [58])

$$\begin{aligned} G_k(x, y) &= \sum_{n \in \mathbb{Z}} \exp(-i\alpha 2\pi n) \Phi_k(x + n(2\pi, 0), y) \\ &= \frac{i}{4\pi} \sum_{n \in \mathbb{Z}} \frac{1}{\beta_n} \exp(i\alpha_n(x_1 - y_1) + i\beta_n|x_2 - y_2|), \end{aligned} \quad (3.35)$$

for $x - y \neq n(2\pi, 0)$, $n \in \mathbb{Z}$, where β_n are defined as in (3.11) with k_p replaced by k . The free space fundamental solution to the Navier equation (3.3) is given by (see [56])

$$\Gamma(x, y) = \frac{1}{\mu} \Phi_{k_s}(x, y) I + \frac{1}{\omega^2} \text{grad}_x \text{grad}_x^T [\Phi_{k_s}(x, y) - \Phi_{k_p}(x, y)],$$

where I stands for the 2×2 unit matrix. Then, the α -quasiperiodic fundamental solution (Green’s tensor) to the Navier equation (3.3) takes the form

$$\Pi(x, y) := \sum_{n \in \mathbb{Z}} \exp(-i\alpha 2\pi n) \Gamma(x + n(2\pi, 0), y)$$

for $x - y \neq n(2\pi, 0)$, $n \in \mathbb{Z}$. The convergence of the above series for $\Pi(x, y)$ is discussed in [7, Section 6]. Define

$$\begin{pmatrix} P_{11}^{(n)} & P_{12}^{(n)} \\ P_{21}^{(n)} & P_{22}^{(n)} \end{pmatrix} = \frac{i}{4\pi\omega^2\beta_n} \begin{pmatrix} \alpha_n^2 & \alpha_n\beta_n \\ \alpha_n\beta_n & \beta_n^2 \end{pmatrix} =: P^{(n)}, \quad (3.36)$$

$$\begin{pmatrix} S_{11}^{(n)} & S_{12}^{(n)} \\ S_{21}^{(n)} & S_{22}^{(n)} \end{pmatrix} = \frac{i}{4\pi\mu\gamma_n} I - \frac{i}{4\pi\omega^2\gamma_n} \begin{pmatrix} \alpha_n^2 & \alpha_n\gamma_n \\ \alpha_n\gamma_n & \gamma_n^2 \end{pmatrix} =: S^{(n)}. \quad (3.37)$$

We can derive from (3.35) that $\Pi(x, y)$ takes the form

$$\begin{aligned} \Pi(x, y) &= \sum_{n \in \mathbb{Z}} P^{(n)} \exp(i[\alpha_n(x_1 - y_1) + \beta_n|x_2 - y_2|]) \\ &\quad + \sum_{n \in \mathbb{Z}} S^{(n)} \exp(i[\alpha_n(x_1 - y_1) + \gamma_n|x_2 - y_2|]). \end{aligned} \quad (3.38)$$

Our approach is based on the following decomposition of the α -quasiperiodic fundamental solution $\Pi(x, y)$ and the periodicity of the grating surface.

Lemma 3.18 ([38]). *On the profile Λ , the α -quasiperiodic Green’s tensor $\Pi(x, y)$ has a logarithmic singularity of the form*

$$\Pi(x, y) = -\eta_1 \frac{1}{\pi} \ln(|x - y|) I + \Pi^*(x, y), \quad \eta_1 = \frac{1}{\omega^2} (k_s^2 + k_p^2), \quad (3.39)$$

where $\Pi^*(x, y)$ is a continuously differentiable matrix in the variables $x, y \in \Lambda$.

To solve problem (DP) under the boundary condition (3.4), we make the ansatz for the scattered field u^{sc} in the form

$$u^{sc}(x) = \int_{\Lambda} \Pi(x, y) \phi(y) ds(y), \quad x \in \Omega_{\Lambda}$$

with some unknown α -quasiperiodic function $\phi(\gamma) \in L^2(\Lambda)^2$. Then we only need to solve the linear first-kind integral equation

$$\int_{\Lambda} \Pi(x, \gamma) \phi(\gamma) ds(\gamma) = -u^{in}(x), \quad x \in \Lambda. \tag{3.40}$$

Set

$$\begin{aligned} x &= (t, f(t)), \quad \gamma = (s, f(s)), \\ g(t) &:= -u^{in}(t, f(t)) \exp(-i\alpha t), \\ \rho(s) &:= \phi(s, f(s)) \exp(-i\alpha s) \sqrt{1 + f'(s)^2}, \\ K(t, s) &:= \Pi(t, f(t); s, f(s)) \exp(i\alpha(s - t)). \end{aligned}$$

Multiplying (3.40) by $\exp(-i\alpha t)$ gives the equivalent form

$$\int_0^{2\pi} K(t, s) \rho(s) ds = g(t), \quad 0 \leq t \leq 2\pi. \tag{3.41}$$

Note that $\rho(t), g(t)$ are both 2π -periodic with respect to t . It follows from the decomposition in (3.39) that

$$K(t, s) = -\eta_1 \frac{1}{\pi} \ln \left| 2e^{-1/2} \sin \left(\frac{t-s}{2} \right) \right| I + H(t, s),$$

where $H(t, s)$ is a continuously differentiable function on $\mathbb{R} \times \mathbb{R}$. Define the integral operators

$$\begin{aligned} A\rho(t) &:= -\eta_1 \frac{1}{\pi} \int_0^{2\pi} \ln \left| 2e^{-1/2} \sin \left(\frac{t-s}{2} \right) \right| I \rho(s) ds, \\ B\rho(t) &:= \int_0^{2\pi} H(t, s) \rho(s) ds. \end{aligned}$$

Let $H_p^1(0, 2\pi)$ denote the Sobolev space of 2π -periodic functions on $(0, 2\pi)$. Then, solving the first-kind integral equation (3.41) can be transformed into:

$$\text{Given } g \in H_p^1(0, 2\pi)^2, \text{ find } \rho(t) \in L^2(0, 2\pi)^2 \text{ such that } A\rho + B\rho = g. \tag{3.42}$$

Let further J_n denote the $(2n + 1)$ -dimensional space of trigonometric polynomials of degree not greater than n , with the basis given by $\{\varphi_m(t) := e^{imt}, -n \leq m \leq n\}$. Then the orthogonal projection P_n of $L^2(0, 2\pi)^2$ onto J_n^2 takes the form

$$(P_n \rho)(t) = \frac{1}{\sqrt{2\pi}} \sum_{m=-n}^n \rho_m e^{imt}, \quad \rho_m = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \rho(s) e^{-ims} ds \in \mathbb{C}^2,$$

and the corresponding Galerkin method for (3.42) consists of solving the projection equation

$$(A + P_n B)\rho_n = P_n g, \quad \text{for } \rho_n = \sum_{j=-n}^n c_j \varphi_j(t) \in \mathcal{J}_n^2, \quad c_j \in \mathbb{C}^2. \quad (3.43)$$

Let $C_p[0, 2\pi]$ denote the continuous complex-valued 2π -periodic functions in t . The basic idea of the discrete Galerkin method proposed in [13] is to replace the orthogonal projection P_n by the interpolatory projection $Q_n : C_p[0, 2\pi]^2 \rightarrow \mathcal{J}_n^2$ at the equidistant grid points $t_j = jh, h = 2\pi/(2n + 1)$, and to approximate (3.43) by

$$(A + Q_n B_n)\rho_n = Q_n g, \quad \rho_n \in \mathcal{J}_n^2, \quad (3.44)$$

where the integral operator B is approximated by a finite-dimensional operator using the trapezoidal rule

$$B_n \rho_n(t) = h \sum_{j=0}^{2n} H(t, t_j) \rho_n(t_j). \quad (3.45)$$

To avoid the computation of $H(t, s)$ for $t = s$ (i.e. the diagonal terms), we introduce the collocation points $s_k = kh + h/2, k = 0, 1, \dots, 2n$, which is a shift of the equidistant grid points t_j . Then, problems (3.44) and (3.45) are equivalent to

$$\sum_{j=-n}^n \left[\frac{\eta_1 \varphi_j(s_k)}{\max\{1, |j|\}} I + B_n \varphi_j(s_k) \right] c_j = g(s_k), \quad k = 0, 1, \dots, 2n.$$

Using (3.45) and the orthogonality of φ_m , the previous finite linear system becomes (see also [43, section 3])

$$\sum_{j=0}^{2n} \left[\eta_1 \sigma_{kj} + hH(s_k, t_j) \right] \rho_n(t_j) = g(s_k), \quad k = 0, 1, \dots, 2n, \quad (3.46)$$

in terms of the unknown density ρ , where

$$\sigma_{kj} = \frac{1}{2\pi} h \sum_{m=-n}^n \varphi_m(s_k) \overline{\varphi_j(t_m)} / \max\{1, |m|\}.$$

Note that $s_k \neq t_j$ for all $k, j = 0, 1, \dots, 2n$, and that the σ_{kj} can be readily computed employing the fast Fourier transform. Solving the linear system (3.46) in the unknowns $\rho_n(t_j)$ then gives an approximate solution $\rho_n \in \mathcal{J}_n$ of the integral equation (3.40). We refer to [13] for a convergence analysis of this approximation method.

5.2 A two-step algorithm for (IP)

In this section, we present a numerical method for the profile reconstruction problem (IP) in the case that the Dirichlet condition is imposed on the unknown profile Λ .

We assume that Λ is the graph of a sufficiently smooth 2π -periodic function f , and suppose that we have the a priori information that Λ lies between the horizontal lines $\{x_2 = 0\}$ and $\{x_2 = b\}$ for some $b > 0$. For simplicity we restrict ourselves to the case of one incident wave with incidence angle θ . We can rewrite the corresponding near-field data $u_b^{sc}(x_1) = u^{sc}(x_1, b)$ and far-field data $u_b^\infty(x_1)$ as

$$u_b^{sc}(x_1) = \sum_{n \in \mathbb{Z}} \mathbf{A}_n(\theta) \exp(i\alpha_n x_1), \quad u_b^\infty(x_1) = \sum_{n \in \mathcal{U}_s} \mathbf{A}_n^\infty(\theta) \exp(i\alpha_n x_1), \quad (3.47)$$

where

$$\begin{aligned} \mathbf{A}_n(\theta) &= A_{p,n}(\alpha_n, \beta_n)^T e^{i\beta_n b} + A_{s,n}(-\gamma_n, \alpha_n)^T e^{i\gamma_n b}, \\ \mathbf{A}_n^\infty(\theta) &= \begin{cases} \mathbf{A}_n(\theta), & \text{if } n \in \mathcal{U}_p, \\ A_{p,n}(\alpha_n, \beta_n)^T e^{i\beta_n b}, & \text{if } n \in \mathcal{U}_s \setminus \mathcal{U}_p. \end{cases} \end{aligned}$$

We consider the following inverse problem, which is a slightly more general version of problem (IP*) formulated at the end of Section 2 (in the case of a single incidence angle).

(IP'): Given a finite number of Rayleigh coefficients $\mathbf{A}_n(\theta)$, $|n| < K$, for some $K \in \mathbb{N}$, determine the unknown grating profile Λ .

Note that the far-field data $\mathbf{A}_n^\infty(\theta)$, $n \in \mathcal{U}_s$, are covered if K is sufficiently large. Since (IP') is nonlinear and severely ill-posed, it is quite natural to apply regularization and optimization techniques. Introduce the Hilbert space $X = L^2(0, 2\pi)^2$ with the scalar product

$$(u(t), v(t)) := \frac{1}{2\pi} \int_0^{2\pi} u(t) \cdot \overline{v(t)} dt,$$

and the norm $\|u\| := \sqrt{(u, u)}$. Define the linear operators $J, S_f : X \rightarrow X$ by

$$\begin{aligned} J\varphi(x_1) &:= \frac{1}{2\pi} \int_0^{2\pi} \Pi(x_1, b; t, 0) \varphi(t) dt, \\ S_f\varphi(x_1) &:= \frac{1}{2\pi} \int_0^{2\pi} \Pi(x_1, f(x_1); t, 0) \varphi(t) dt. \end{aligned}$$

The Kirsch–Kress method adapted to our diffraction problem consists of solving the optimization problem

$$\|T\varphi - u_b\|^2 + \gamma \|\varphi\|^2 + \eta \left\| u^{in} \circ f + S_f\varphi \right\|^2 \rightarrow \inf_{f \in \mathcal{M}, \varphi \in X}, \quad (3.48)$$

where $\gamma > 0$ denotes the regularization parameter, $\eta > 0$ is a coupling parameter and \mathcal{M} is an admissible set of profile functions with uniformly bounded $C^{0,1}$ -norm.

The convergence analysis for problem (3.48) is presented in [44] in the case of the quasiperiodic Helmholtz equation, which we think can carry over to the quasiperiodic Navier equation. Since the combined optimization scheme (3.48) requires the determination of two unknown functions f and φ , to reduce the computational effort, we extend the two-step inversion algorithm proposed in [22] for electromagnetic gratings to the inverse elastic scattering problem (IP').

Step 1: Reconstruct the scattered field from the near-field data $u_b^{sc}(x_1)$.

We try to represent the scattered field u^{sc} as the single layer potential

$$u^{sc}(x) = \frac{1}{2\pi} \int_0^{2\pi} \Pi(x_1, x_2; t, 0) \varphi(t) dt, \quad x \in \Omega_\Lambda$$

with some unknown α -quasiperiodic function $\varphi(t) \in X$. Then we only need to solve the first-kind integral equation

$$J\varphi(x_1) = u_b^{sc}(x_1), \quad x_1 \in (0, 2\pi). \tag{3.49}$$

Expand $\varphi(t) \in X$ into the Fourier series

$$\varphi(t) = \sum_{n \in \mathbb{Z}} \varphi_n \exp(i\alpha_n t), \quad \varphi_n := (\varphi_n^{(1)}, \varphi_n^{(2)}) \in \mathbb{C}^2.$$

Then, it follows from (3.36)–(3.38) that the operator J takes the form

$$J\varphi(x_1) = \sum_{n \in \mathbb{Z}} M^{(n)} \varphi_n \exp(i\alpha_n x_1), \quad M^{(n)} := (P^{(n)} \exp(i\beta_n b) + S^{(n)} \exp(i\gamma_n b)).$$

Since the operator J is compact on X , we consider the Tikhonov regularized version $\gamma\varphi + J^*J\varphi = J^*u_b^{sc}$ of equation (3.49) with the regularization parameter $\gamma > 0$, where J^* denotes the adjoint operator of J . Let the singular value decomposition of $M^{(n)}$ be given by $M^{(n)} = U^{(n)} \Sigma^{(n)} (V^{(n)})^*$, where

$$U^{(n)} = (U_1^{(n)}, U_2^{(n)}), \quad V^{(n)} = (V_1^{(n)}, V_2^{(n)}), \quad \Sigma^{(n)} = \text{diag}(\sigma_1^{(n)}, \sigma_2^{(n)}).$$

with $U_j^{(n)}, V_j^{(n)} \in \mathbb{C}^2$ being column vectors and $\sigma_j^{(n)} \in \mathbb{R}^+$ for $n \in \mathbb{Z}, j = 1, 2$. Then, the regularized solution φ_γ is given by (see [27, Chapter 4])

$$\begin{aligned} \varphi_\gamma &= \sum_{n \in \mathbb{Z}} \sum_{j=1}^2 \frac{\sigma_j^{(n)}}{(\sigma_j^{(n)})^2 + \gamma} (u_b^{sc}, U_j^{(n)} \exp(i\alpha_n t)) V_j^{(n)} \exp(i\alpha_n t) \\ &\approx \sum_{|n| \leq K} \sum_{j=1}^2 \frac{\sigma_j^{(n)}}{(\sigma_j^{(n)})^2 + \gamma} (\mathbf{A}_n \cdot \overline{U_j^{(n)}}) V_j^{(n)} \exp(i\alpha_n t) \end{aligned}$$

in the case that near-field data are given, where $\mathbf{A}_n \in \mathbb{C}^2$ are defined in (3.47). Now we can represent φ_γ as

$$\varphi_\gamma = \sum_{|n| \leq K} \varphi_\gamma^{(n)} \exp(i\alpha_n t), \quad \varphi_\gamma^{(n)} := \sum_{j=1}^2 \frac{\sigma_j^{(n)}}{(\sigma_j^{(n)})^2 + \gamma} (\mathbf{A}_n \cdot \overline{U_j^{(n)}}) V_j^{(n)}. \tag{3.50}$$

When far-field data are given, we only need to replace u_b^{sc}, \mathbf{A}_n by $u_\infty^{sc}, \mathbf{A}_n^\infty$, respectively.

Step 2: Determine the grating profile function f by minimizing the defect

$$\|u^{in} \circ f + S_f \varphi\| \rightarrow \inf_{f \in \mathcal{M}} \tag{3.51}$$

over some admissible set \mathcal{M} of profile functions.

Having computed φ_y from the first step, we may consider $S_f(\varphi_y)$ as an approximation of the scattered field on the grating profile. We now turn to investigating the nonlinear least-squares minimization problem (3.51). Using (3.36)–(3.38) and (3.50), we see that the integral operator S_f takes the form

$$S_f \varphi_y(x_1) = \sum_{|n| \leq K} P^{(n)} \varphi_y^{(n)} e^{i\alpha_n x_1 + i\beta_n f(x_1)} + S^{(n)} \varphi_y^{(n)} e^{i\alpha_n x_1 + i\gamma_n f(x_1)}.$$

Hence, problem (3.51) is equivalent to

$$\left\| \hat{\theta} e^{-i\beta f(t)} + \sum_{|n| \leq K} \left(P^{(n)} \varphi_y^{(n)} e^{i\beta_n f(t)} + S^{(n)} \varphi_y^{(n)} e^{i\gamma_n f(t)} \right) e^{int} \right\|^2 \rightarrow \inf_{f \in \mathcal{M}}, \tag{3.52}$$

where, for C^2 -smooth grating profiles, an admissible set \mathcal{M} is given by

$$\mathcal{M} = \left\{ f(t) = a_0 + \sum_{m=1}^M a_m \cos(mt) + a_{M+m} \sin(mt) \right\}, \tag{3.53}$$

with some fixed number $M \in \mathbb{N}$ and bounded Fourier coefficients a_j . We discretize the objective functional in (3.52) by the trapezoidal rule and then solve the resulting minimization problem in a finite-dimensional space.

Here we present two numerical examples using the two-step algorithm. Take $k_s = 4.45$, $\omega = 5$, and probe the unknown grating profile by a single incident pressure wave with $\theta = 0$ and $k_p = 4.2$. With these settings we have $\mathcal{U}_p = \mathcal{U}_s = \{n \in \mathbb{Z} : |n| \leq 4\}$. In the following Examples 3.19 and 3.20, unless otherwise stated we always set $K = 7$ in (3.50) and (3.52). This implies that all propagating modes of the compressional and shear parts corresponding to $|n| \leq 4$ are used, while six additional evanescent modes corresponding to $5 \leq |n| \leq 7$ are also taken into account.

Example 3.19 (Fourier gratings). Suppose that the grating profile function is given by the finite Fourier series

$$f(t) = 2 + \zeta(\cos(t) + \cos(2t) + \cos(3t)), \quad \zeta = 0.05\pi,$$

where ζ characterizes the steepness of the profile. We used exact near-field data to reconstruct this profile function, which has the form (3.53) with $M = 3$. To generate

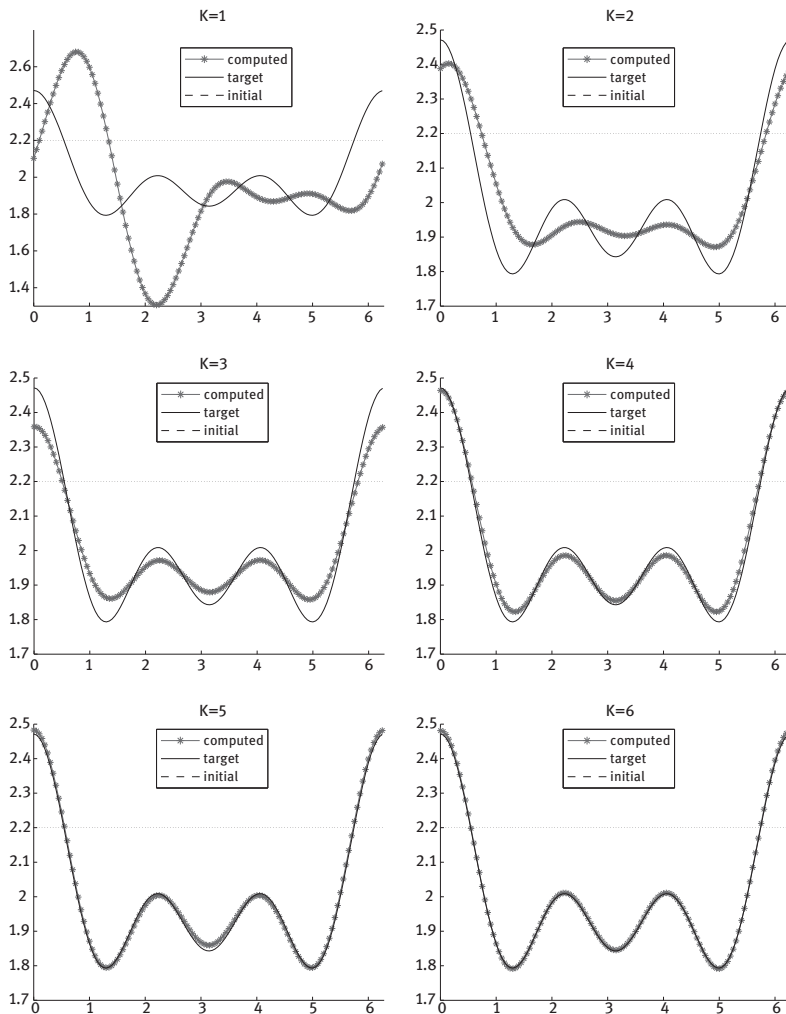


Figure 3.3: (See Color Plates for a color version.) Sensitivity of the method to the parameter K in Example 3.19.

the synthetic data, the discrete trigonometric Galerkin method of Section 5.1 was employed. Figure 3.3 illustrates the sensitivity of the method to the parameter K , from which we see that the propagating modes corresponding to $K = 4$ (i.e., only far-field data are used) lead to satisfactory results. The reconstruction from noisy data even with noise level $\delta = 10\%$ can still produce good results in the case $K = 7$. However, the results are not acceptable if we increase the steepness to 0.1π .

Example 3.20 (General smooth gratings). Suppose that Λ is the graph given by the function

$$f(t) = 1.5 + 0.2 \exp(\sin(3t)) + 0.3 \exp(\sin(3t)),$$

which can be approximated by the truncated Fourier series

$$f^*(t) = 2.133 - 0.0543 \cos(6t) - 0.0814 \cos(8t) + 0.22606 \sin(3t) + 0.339 \sin(4t)$$

with four interior local minima. In this case we chose $M = 8$ in (3.53), with a total of 17 parameters to be determined. The computational results are presented in Figures 3.4 and 3.5. Since the steepness of Λ is relatively large, the downward convex part of the grating surface is not well-reconstructed. One can see from Figure 3.4 that data with 10% noise lead to a larger deviation in contrast to the profile reconstructed from data corresponding to a noise of 5%.

Our experiments have shown that the reconstruction with $K < 7$ also leads to a large deviation and that the one with $K \geq 8$ only slightly improves the computational results in Figure 3.4. Figure 3.5 demonstrates the computational results from different initial guesses using unperturbed propagating modes.

The two-step algorithm is easily implemented, and satisfactory reconstructions can be obtained with a low computational effort for suitable initial values of grating parameters. This is mainly because the singular value decomposition of the derived first-kind integral equation can be readily achieved, and only the unknown grating

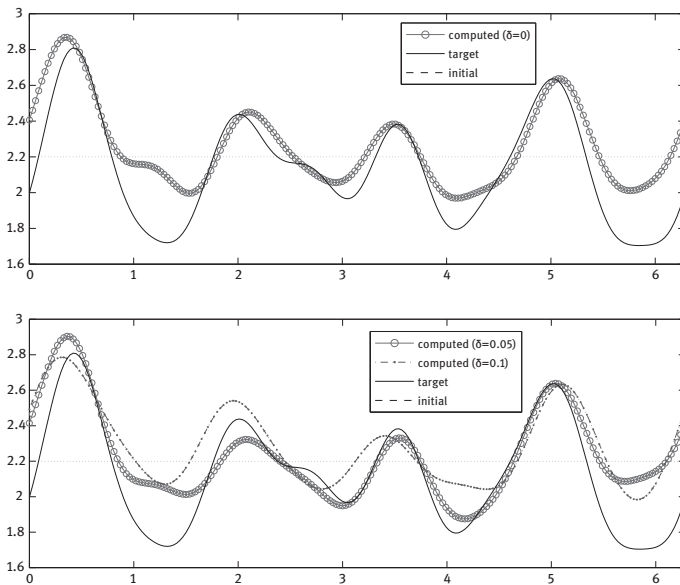


Figure 3.4: (See Color Plates for a color version.) Example 3.20. $K = 7$, $M = 8$.

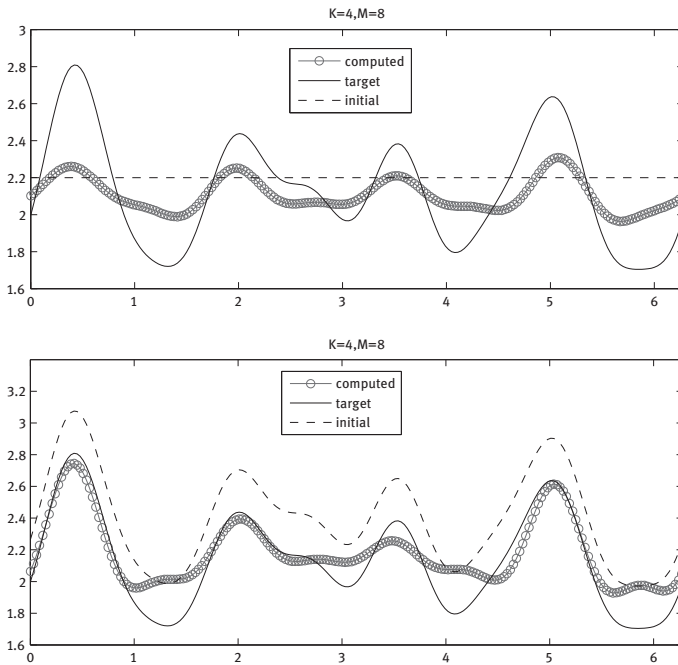


Figure 3.5: (See Color Plates for a color version.) Example 3.20. $K = 4$, $M = 8$, $\delta = 0$.

profile function needs to be determined in the second step. Moreover, no direct scattering problems need to be solved in the process of the inversion algorithm. As our experience has shown in [22–24], the two step algorithm is in general faster and more accurate than the minimization of the combined cost functional. The reconstruction scheme can also be applied to piecewise linear grating profiles with a finite number of corners (see [38]), and it can be readily adapted to the case of several incident angles or a finite number of incident frequencies. However, the convergence of the two-step algorithm is still open.

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