Mathematical Models and Methods in Applied Sciences
Vol. 22, No. 4 (2012) 1150019 (34 pages)

DOI: 10.1142/S0218202511500199

SCATTERING OF PLANE ELASTIC WAVES BY THREE-DIMENSIONAL DIFFRACTION GRATINGS

JOHANNES ELSCHNER* and GUANGHUI HU†

Weierstrass Institute, Mohrenstr. 39,
Berlin 10117, Germany
**johannes.elschner@wias-berlin.de*
†*guanghui.hu@wias-berlin.de*

Received 9 November 2010
Revised 15 March 2011
Communicated by E. Zuazua

The reflection and transmission of a time-harmonic plane wave in an isotropic elastic medium by a three-dimensional diffraction grating is investigated. If the diffractive structure involves an impenetrable surface, we study the first, second, third and fourth kind boundary value problems for the Navier equation in an unbounded domain by the variational approach. A radiation condition based on the Rayleigh expansion of the quasi-periodic solutions is presented. Existence of solutions in Sobolev spaces is established if the grating profile is a two-dimensional Lipschitz surface, while uniqueness is proved only for small frequencies or for all frequencies excluding a discrete set. Similar solvability results are obtained for multilayered transmission gratings in the case of an incident pressure wave. Moreover, by a periodic Rellich identity, uniqueness of the solution to the first kind (Dirichlet) boundary value problem is established for all frequencies under the assumption that the impenetrable surface is given by the graph of a Lipschitz function.

Keywords: Elastic waves; diffraction gratings; Navier equation; variational formulation.

AMS Subject Classification: 74J20, 74B05, 35J55, 35B27

1. Introduction

Since Lord Rayleigh's original work, Ref. 28, grating diffraction problems have received much attention in both the physical and mathematical communities. In recent years, the interest in them has grown immensely because of many industrial applications, e.g. in radar imaging, non-destructive testing, micro-optics or solar energy absorption. We refer to Ref. 9 for historical remarks and details of these applications. Consequently, the scattering of acoustic and electromagnetic waves has been studied extensively concerning theoretical analysis and numerical approximation, using integral equation methods (e.g. Refs. 32, 17, 30 and 34) or variational

†Corresponding author

methods (e.g. Refs. 26, 16, 10, 7, 19, 20, 35 and 8). In particular, the variational approach appeared to be well adapted to the analytical and numerical treatment of rather general two-dimensional and three-dimensional periodic diffractive structures involving complex materials and non-smooth interfaces.

In contrast to the significant progress made for acoustic and electromagnetic waves, there have only been a few papers studying the scattering of elastic waves by unbounded surfaces. However, the relevant phenomena for elastic waves have a wide field of application. For instance, in the fields of geophysics and seismology, the problem of elastic pulse transmission and reflection through the earth is fundamental to the investigation of earthquakes and the utility of controlled explosions in search for oil and ore bodies (see, e.g. Refs. 1, 23, 24, 36 and references therein). Compared to acoustic and electromagnetic scattering, the elasticity problem is more complicated because of the coexistence of compressional and shear waves that propagate at different speeds. The first rigorous attempt to close this gap is due to Arens using the boundary integral equation method; see Refs. 3 and 4 for the scattering by two-dimensional diffraction gratings and Refs. 5 and 6 by general one-dimensional rough surfaces. In particular, existence and uniqueness for the Dirichlet boundary value problem are established in the case that the grating profile Λ is given by the graph of a smooth (C^2) periodic function in Ref. 3. The same Dirichlet problem in general Lipschitz domains is investigated by Elschner and Hu in Ref. 21 via the variational method. It is shown in Ref. 21 that, for either an incident pressure or shear wave, there always exists a quasi-periodic solution to the equivalent variational formulation and hence to the original scattering problem. Moreover, uniqueness can be guaranteed if the grating profile is given by a Lipschitz graph in $\mathbb{R}^2$. Note that the variational approach can be applied to non-smooth domains, without excluding the Rayleigh frequencies.

The aim of this paper is to provide solvability results for both impenetrable and penetrable gratings in three dimensions. Assume a time-harmonic (with time variation of the form $\exp(-i\omega t), \omega > 0$) incident plane wave is scattered by a three-dimensional diffraction grating in an isotropic elastic medium, where the grating profile is represented by a surface Λ which is 2π-periodic in x_1 and x_2. We will consider a broad class of incident plane waves (see (2.15) and (2.16)) under general boundary conditions. If the diffraction grating is impenetrable, the first, second, third and fourth kind boundary value problems for the Navier system are investigated in the unbounded domain above Λ, while the scattering by a multilayered transmission grating is modeled by a corresponding transmission problem on the whole space. We refer to Ref. 27 for an introduction of the boundary value problems of elasticity, including the boundary conditions of the third and fourth kind. The paper is organized as follows.

In Sec. 2, we present mathematical formulations of the scattering problems in the case of an impenetrable grating. Following Refs. 3 and 21, we give an expression of the radiation condition based on the Rayleigh expansion of quasiperiodic solutions to the Helmholtz equation; see Sec. 2.2. Note that the radiation condition of this paper is very similar to that imposed on acoustic waves for two-dimensional diffraction gratings; cf. Ref. 26.

In Sec. 3, we reduce the boundary value problem for the Navier system in the unbounded domain to an equivalent strongly elliptic variational problem in a bounded periodic cell with a nonlocal boundary condition; see Sec. 3.1 for the equivalent variational problem, Sec. 3.2 for properties of the Dirichlet-to-Neumann map, and Sec. 3.3 for the proof of the strong ellipticity of the sesquilinear form generated by the variational formulation. In three dimensions, establishing the strong ellipticity is not trivial and requires a more intricate and careful analysis than for plane elasticity; cf. Ref. 21.

Afterwards, in Sec. 4, we investigate the existence and uniqueness of quasi-periodic solutions for a broad class of incident elastic waves when one of the first, second, third and fourth kind boundary conditions is imposed on the impenetrable surface Λ. For a general Lipschitz profile, existence is established in Sec. 4.2.1 by using Korn's inequality and applying the Fredholm alternative, while uniqueness is proved in Sec. 4.2.2 but only for small frequencies. Using analytic Fredholm theory, the uniqueness result can be extended to all frequencies excluding a discrete set; see Theorem 3(ii). In addition, by a periodic Rellich identity, uniqueness of the solution to the first kind (Dirichlet) boundary value problem is established for all frequencies under the assumption that Λ is given by a Lipschitz graph; see Sec. 4.3. Non-uniqueness examples under the boundary conditions of the second, third and fourth kind are presented in Sec. 4.4.

Finally, in Sec. 5, we extend the solvability results from Sec. 4.2 for impenetrable gratings to the case of scattering by multilayered transmission gratings with several elastic materials.

2. Mathematical Formulations for an Impenetrable Grating

In this section and the following Secs. 3 and 4, we assume the diffraction grating has an impenetrable scattering surface Λ which is 2π-periodic with respect to x_1 and x_2. Let $\Omega := \Omega_\Lambda$ denote the region above Λ filled with an isotropic homogeneous elastic medium characterized by the Lamé constants λ, μ satisfying $\mu > 0,\ \lambda + 2\mu/3 > 0$. Suppose a time-harmonic plane elastic wave u^{in} (with time variation of the form $\exp(-i\omega t), \omega > 0$) is incident on the grating from above. We next formulate the scattering problem for the Navier equation and propose a new radiation condition.

2.1. *Boundary conditions for the Navier equation*

The propagation of time-harmonic elastic waves in Ω is governed by the Navier equation (or system)

$$(\Delta^* + \omega^2)u = 0 \quad \text{in } \Omega, \quad \Delta^* := \mu\Delta + (\lambda+\mu)\text{grad div}, \tag{2.1}$$

$$u = u^{\mathrm{in}} + u^{\mathrm{sc}} \quad \text{in } \Omega, \tag{2.2}$$

where u denotes the total displacement and $u^{\rm sc}$ stands for the scattered field. Let $S^2 := \{x \in \mathbb{R}^3 : \|x\| = 1\}$. The incident plane wave $u^{\rm in}$ is assumed to be either a plane pressure wave of the form

$$u^{\rm in} = u_p^{\rm in}(x) = \hat{\theta} \exp(ik_p\hat{\theta} \cdot x) \quad \text{with } \hat{\theta} = (\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2, -\cos\theta_1) \in S^2, \tag{2.3}$$

or a plane shear wave of the form

$$u^{\rm in} = u_s^{\rm in}(x) = \hat{\theta}^\perp \exp(ik_s\hat{\theta} \cdot x) \quad \text{with } \hat{\theta}^\perp \in S^2, \quad \hat{\theta}^\perp \cdot \hat{\theta} = 0, \tag{2.4}$$

where

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

are the compressional and shear wave numbers respectively, and $\hat{\theta} \in S^2$ denotes the incident direction with the incident angles $\theta_1 \in [0, \pi/2), \theta_2 \in [0, 2\pi)$. Here we have assumed for simplicity that the mass density of the elastic medium is equal to one. Throughout the paper, we write $x' := (x_1, x_2)$ and $\alpha = (\alpha_1, \alpha_2) := k(\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2)$, where $k = k_p$ for the incident pressure wave and $k = k_s$ for the incident shear wave. Note that the incident field $u^{\rm in}$ is α-quasiperiodic in the sense that $u^{\rm in}(x) \exp(-i\alpha \cdot x')$ is 2π periodic with respect to x_1 and x_2. The periodicity of the structure and the form of the incident waves imply that the solution u must also be α-quasiperiodic, i.e.

$$u(x_1 + 2n_1\pi, x_2 + 2n_2\pi, x_3) = \exp(2i(\alpha_1 n_1 + \alpha_2 n_2)\pi) u(x_1, x_2, x_3), \quad x \in \Omega \tag{2.5}$$

for all $n_1, n_2 \in \mathbb{Z}$. On the grating surface Λ, the total displacement u is assumed to fulfill one of the following boundary conditions:

$$\left.\begin{array}{ll} \text{The first kind (Dirichlet) boundary condition:} & u = 0; \\ \text{The second kind (Neumann) boundary condition:} & Tu = 0; \\ \text{The third kind boundary conditions:} & \nu \cdot u = 0,\ \nu \times Tu = 0; \\ \text{The fourth kind boundary conditions:} & \nu \times u = 0,\ \nu \cdot Tu = 0; \end{array}\right\} \tag{2.6}$$

where $\nu := (\nu_1, \nu_2, \nu_3)$ denotes the unit normal vector on Λ pointing into Ω and Tu stands for the *stress vector* or *traction* having the form:

$$Tu = T(\lambda, \mu)u := 2\mu\partial_\nu u + \lambda(\operatorname{div} u)\nu + \mu\nu \times \operatorname{curl} u. \tag{2.7}$$

Here and in the following, the notation $\partial_\nu u = \nu \cdot \nabla u$ is used, and the symbol $\partial_j u$ denotes $\partial u/\partial x_j$. By the Betti formula, the above stress operator plays the role of the normal derivative in the scalar Helmholtz equation; see Ref. 27 for a generalized Betti formula in the three-dimensional case.

2.2. *Radiation condition*

Since the domain Ω is unbounded in the x_3-direction, a radiation condition must be imposed at infinity to ensure well-posedness of the boundary value problem (2.1)–(2.6). Following Refs. 3 and 21 in the two-dimensional case, we put forward a radiation condition based on Rayleigh expansions for solutions to the scalar Helmholtz equation. Noting that the scattered field u^{sc} satisfies the Navier equation (2.1) in Ω, we begin with the decomposition of u^{sc} into a sum of its compressional and shear parts (see Ref. 27)

$$u^{\mathrm{sc}} = \frac{1}{i}(\mathrm{grad}\,\varphi + \mathrm{curl}\,\psi) \quad \text{with } \varphi := -\frac{i}{k_p^2}\,\mathrm{div}\,u^{\mathrm{sc}}, \quad \psi := \frac{i}{k_s^2}\mathrm{curl}\,u^{\mathrm{sc}}, \tag{2.8}$$

where the scalar function φ and the vector function ψ satisfy the homogeneous Helmholtz equations

$$(\Delta + k_p^2)\varphi = 0 \quad \text{and} \quad (\Delta + k_s^2)\psi = 0 \quad \text{in } \Omega. \tag{2.9}$$

Now, we apply the usual outgoing wave condition (Rayleigh expansion) to φ and ψ by assuming (see, e.g. Ref. 26)

$$\varphi(x) = \sum_{n\in\mathbb{Z}^2} A_{p,n}\exp(i\alpha_n\cdot x' + i\beta_n x_3), \quad \psi(x) = \sum_{n\in\mathbb{Z}^2} \tilde{\mathbf{A}}_{s,n}\exp(i\alpha_n\cdot x' + i\gamma_n x_3), \tag{2.10}$$

for $x_3 > \Lambda^+ := \max_{x\in\Lambda}\{x_3\}$, where $A_{p,n} \in \mathbb{C}$ are constants and $\tilde{\mathbf{A}}_{s,n} \in \mathbb{C}^3$ are constant vectors. The parameters β_n and γ_n in (2.10) are defined by

$$\beta_n = \begin{cases} (k_p^2 - |\alpha_n|^2)^{\frac{1}{2}} & \text{if } |\alpha_n| \le k_p, \\ i(|\alpha_n|^2 - k_p^2)^{\frac{1}{2}} & \text{if } |\alpha_n| > k_p, \end{cases} \qquad \gamma_n = \begin{cases} (k_s^2 - |\alpha_n|^2)^{\frac{1}{2}} & \text{if } |\alpha_n| \le k_s, \\ i(|\alpha_n|^2 - k_s^2)^{\frac{1}{2}} & \text{if } |\alpha_n| > k_s, \end{cases} \tag{2.11}$$

respectively, with $\alpha_n = (\alpha_n^{(1)}, \alpha_n^{(2)}) := (\alpha_1 + n_1, \alpha_2 + n_2)$ for $n = (n_1, n_2) \in \mathbb{Z}^2$. Inserting (2.10) into (2.8), we finally obtain a corresponding expansion of u^{sc} into outgoing plane elastic waves:

$$\begin{aligned} u^{\mathrm{sc}}(x) = \sum_{n\in\mathbb{Z}^2} \big\{ & A_{p,n}(\alpha_n, \beta_n)^\top \exp(i\alpha_n\cdot x' + i\beta_n x_3) \\ & + (\alpha_n, \gamma_n) \times \tilde{\mathbf{A}}_{s,n}\exp(i\alpha_n\cdot x' + i\gamma_n x_3)\big\}, \end{aligned} \tag{2.12}$$

or equivalently,

$$\begin{aligned} u^{\mathrm{sc}}(x) = \sum_{n\in\mathbb{Z}^2} \big\{ & A_{p,n}(\alpha_n, \beta_n)^\top \exp(i\alpha_n\cdot x' + i\beta_n x_3) \\ & + \mathbf{A}_{s,n}\exp(i\alpha_n\cdot x' + i\gamma_n x_3)\big\}, \end{aligned} \tag{2.13}$$

with $\mathbf{A}_{s,n} = (A_{s,n}^{(1)}, A_{s,n}^{(2)}, A_{s,n}^{(3)}) := (\alpha_n, \gamma_n) \times \tilde{\mathbf{A}}_{s,n} \in \mathbb{C}^3$ satisfying the orthogonality

$$\mathbf{A}_{s,n} \cdot (\alpha_n, \gamma_n) = 0, \quad \text{for all } n \in \mathbb{Z}^2. \tag{2.14}$$

Throughout the paper, the symbol $(\cdot)^\top$ denotes the transpose of a vector in $\mathbb{C}^2$ or $\mathbb{C}^3$. The series in (2.13), which is referred to as the Rayleigh expansion for elastic waves, is the radiation condition we are going to use in the following sections. The constants $A_{p,n} \in \mathbb{C}, \mathbf{A}_{s,n} \in \mathbb{C}^3$ are also called the Rayleigh coefficients. Since β_n and γ_n are real for at most finitely many indices, we observe that only a finite number of plane waves in (2.12) propagate into the far field, while the remaining part consists of evanescent (or surface) waves decaying exponentially as $x_3 \to +\infty$. Thus, the above expansion converges uniformly with all derivatives in the half-space $\{x \in \mathbb{R}^3 : x_3 \geq a\}$, for any $a > \Lambda^+$. Note that the radiation condition (2.13) is very similar to that imposed on solutions to the scalar Helmholtz equation for two-dimensional diffraction gratings, cf. Ref. 26. Now, we can formulate our diffraction problem as the following boundary value problem.

Boundary value problem (BVP). Given a grating profile $\Lambda \subset \mathbb{R}^3$ (which is 2π-periodic in x_1 and x_2) and an incident field u^{in} of the form (2.3) or (2.4), find a vector function $u = u^{\text{in}} + u^{\text{sc}} \in H^1_{\text{loc}}(\Omega)^3$ that satisfies (2.1), (2.2), the quasi-periodicity condition (2.5), one of the boundary conditions in (2.6) and the radiation condition (2.13).

We will also consider a general incident pressure wave of the form

$$u^{\text{in}}_{(p)}(x) = \frac{1}{k_p} \sum_{|\alpha_n|<k_p} (\alpha_n, -\beta_n)^\top \exp[i(\alpha_n \cdot x' - \beta_n x_3)] \tag{2.15}$$

with $\alpha = k_p(\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2)$, or an incident shear wave taking the form

$$u^{\text{in}}_{(s)}(x) = \frac{1}{k_s} \sum_{|\alpha_n|<k_s} [(\alpha_n, -\gamma_n) \times \mathbf{Q}_n]^\top \exp[i(\alpha_n \cdot x' - \gamma_n x_3)] \tag{2.16}$$

with $\alpha = k_s(\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2)$, $\mathbf{Q}_n = (q_n^{(1)}, q_n^{(2)}, q_n^{(3)}) \in S^2$, $\mathbf{Q}_n \perp (\alpha_n, -\gamma_n)$. Note that the incident pressure wave (2.3) [respectively shear wave (2.4)] is only one term of the finite sums in (2.15) [respectively (2.16)].

3. Variational Formulation of (BVP)

In this section we propose an equivalent variational formulation of (BVP), following the approach of Refs. 26 and 21 for the scattering of acoustic or elastic waves by two-dimensional diffraction gratings. Since the unbounded domain Ω is periodic in x_1 and x_2, we will restrict ourselves to one periodic cell where the compact imbedding of Sobolev spaces can be applied. Then, with the help of Korn's inequality, the strong ellipticity of the sesquilinear form generated by the variational formulation can be established. This considerably simplifies our mathematical argument, compared to the scattering of elastic waves by general rough surfaces (see Ref. 3 for the integral equation method applied to two dimensions). We also refer to Refs. 11–13 for a rigorous mathematical analysis of rough surface scattering problems for the Helmholtz equation via the variational method in two and three dimensions.

Introduce an artificial boundary

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

and the bounded domain

$$\Omega_b = \Omega_{\Lambda,b} := \{x \in \Omega : 0 < x_1, x_2 < 2\pi, x_3 < b\}.$$

For simplicity we still use Λ to denote one period of the grating surface; see Fig. 1. We assume that Λ is a Lipschitz surface, so that Ω_b is a bounded Lipschitz domain in $\mathbb{R}^3$.

3.1. *An equivalent variational formulation*

In this subsection we establish an equivalent variational formulation posed in the bounded periodic cell Ω_b, which is enforcing the radiation condition on Γ_b.

Let $H^1_\alpha(\Omega_b)$ denote the Sobolev space of scalar functions on Ω_b which are α-quasiperiodic with respect to x_1 and x_2. Introduce the energy space

$$\begin{aligned} V_\alpha &= V_\alpha(\Omega_b) \\ &:= \{u \in H^1_\alpha(\Omega_b)^3 : u \text{ satisfies one of the boundary conditions in (2.6)}\}, \end{aligned}$$

equipped with the norm in the usual Sobolev space $H^1(\Omega_b)^3$ of vector functions. By the first Betti formula, it follows that for $u, \varphi \in V_\alpha$

$$-\int_{\Omega_b} (\Delta^* + \omega^2) u \cdot \overline{\varphi} dx = \int_{\Omega_b} [a(u, \overline{\varphi}) - \omega^2 u \cdot \overline{\varphi}] dx - \int_{\Gamma_b} \overline{\varphi} \cdot Tu ds, \tag{3.1}$$

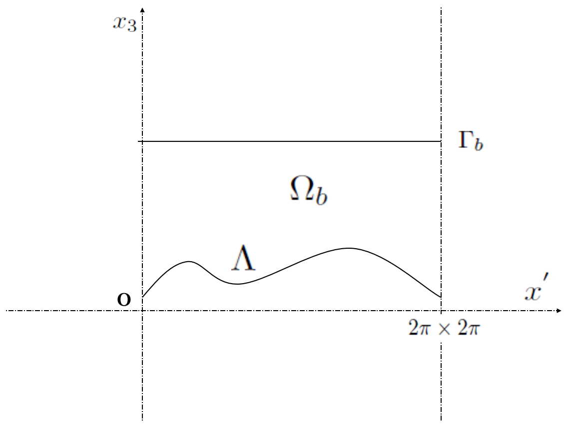

Fig. 1. An impenetrable diffraction grating in $\mathbb{R}^3$.

where the bar indicates the complex conjugate, T is the stress vector defined by (2.7) and

$$a(u,\varphi) = 2\mu \sum_{j,k=1}^{3} \partial_k u_j \partial_k \varphi_j + \lambda(\operatorname{div} u)(\operatorname{div} \varphi) - \mu \operatorname{curl} u \cdot \operatorname{curl} \varphi. \tag{3.2}$$

Moreover, we may rewrite the stress operator Tu in (3.1) as

$$Tu = T(\lambda,\mu)u := 2\mu\partial_3 u + \lambda(\operatorname{div} u)e_3 + \mu e_3 \times \operatorname{curl} u, \quad \text{on } \Gamma_b, \tag{3.3}$$

where $e_3 = (0,0,1)^\top$. Now we introduce the Dirichlet-to-Neumann (DtN) map $\mathcal{T}$ on the artificial boundary Γ_b. For any $u \in H^1_\alpha(\Omega_b)^3$, it is seen from the trace theorem that

$$v := u|_{\Gamma_b} \in H^{1/2}_\alpha(\Gamma_b)^3, \quad \exp(-i\alpha \cdot x')v \in H^{1/2}_{\mathrm{per}}(\Gamma_b)^3$$

where $H^s_\alpha(\Gamma_b)$ and $H^s_{\mathrm{per}}(\Gamma_b)$ denote the Sobolev spaces of order $s \in \mathbb{R}$ of functions on Γ_b that are α-quasiperiodic and periodic respectively. Note that an equivalent norm on $H^s_\alpha(\Gamma_b)^3$ is given by

$$\|v\|_{H^s_\alpha(\Gamma_b)^3} = \left(\sum_{n\in\mathbb{Z}^2} (1+|n|)^{2s}|\hat{v}_n|^2\right)^{1/2},$$

where $\hat{v}_n \in \mathbb{C}^3$ are the Fourier coefficients of $\exp(-i\alpha \cdot x')v(x',b)$.

Definition 1. For any $v \in H^{1/2}_\alpha(\Gamma_b)^3$, the Dirichlet-to-Neumann (DtN) operator $\mathcal{T}v$ is defined as the traction Tu^{sc} on Γ_b, where u^{sc} is the unique α-quasiperiodic solution of the homogeneous Navier equation in $\{x_3 > b\}$ which satisfies the radiation condition at infinity and $u^{\mathrm{sc}} = v$ on Γ_b.

Remark 1. The operator $\mathcal{T}$ is well-defined, since the solution is unique for the scattering by flat surfaces parallel to the (x_1, x_2)-plane under the Dirichlet boundary condition; see Corollary 5 or Theorem 4.

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

$$B(u,\varphi) := \int_{\Omega_b} a(u,\overline{\varphi}) - \omega^2 u \cdot \overline{\varphi}\, dx - \int_{\Gamma_b} \overline{\varphi} \cdot \mathcal{T}u ds, \quad \forall\, u, \phi \in V_\alpha, \tag{3.4}$$

with $\mathcal{T}u := \mathcal{T}(u|_{\Gamma_b})$. Applying Betti's identity (3.1) to a solution $u = u^{\mathrm{sc}} + u^{\mathrm{in}}$ of (BVP) and using the fact that

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

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

$$B(u,\varphi) = \int_{\Gamma_b} f_0 \cdot \overline{\varphi}\, ds, \quad \forall\, \varphi \in V_\alpha. \tag{3.5}$$

Through direct calculations, it can be derived from the definitions of $\mathcal{T}$, T and u^{in} that

$$f_0 = f_{p,0} := Tu_p^{\mathrm{in}} - \mathcal{T}u_p^{\mathrm{in}} = \frac{i}{k_p}\frac{2\omega^2\beta}{\alpha^2+\gamma\beta}\begin{pmatrix}-\alpha^\top\\ \gamma\end{pmatrix}\exp(i\alpha\cdot x' - i\beta b)$$

for an incident pressure wave of the form (2.3), and

$$f_0 = f_{s,0} := Tu_s^{\mathrm{in}} - \mathcal{T}u_s^{\mathrm{in}} = \frac{i}{k_s}\frac{2\omega^2\gamma}{\alpha^2+\gamma\beta}(\hat{\theta}^\perp\times\hat{\theta})^\top\times\begin{pmatrix}\alpha^\top\\ -\beta\end{pmatrix}\exp(i\alpha\cdot x' - i\gamma b)$$

for an incident shear wave of the form (2.4). Here and in the following sections, β and γ denote the values of β_n and γ_n defined by (2.11) with $n=(0,0)$, respectively. Analogously, for the incident shear wave defined by

$$\tilde{u}_s^{\mathrm{in}} := (\hat{\theta}\times\mathbf{Q})^\top\exp(ik_s x\cdot\hat{\theta}),\quad \mathbf{Q}\in S^2,\quad \mathbf{Q}\perp\hat{\theta}, \tag{3.6}$$

one obtains that

$$f_0 = \tilde{f}_{s,0} := T\tilde{u}_s^{\mathrm{in}} - \mathcal{T}\tilde{u}_s^{\mathrm{in}} = \frac{i}{k_s}\frac{2\omega^2\gamma}{\alpha^2+\gamma\beta}\mathbf{Q}^\top\times\begin{pmatrix}\alpha^\top\\ -\beta\end{pmatrix}\exp(i\alpha\cdot x' - i\gamma b).$$

Remark 2. The problems (BVP) and (3.5) are equivalent in the following sense. If $u\in H^1_{\mathrm{loc}}(\Omega)^3$ is a solution of (BVP), then $u|_{\Omega_b}$ satisfies the variational problem (3.5). Conversely, a solution $u\in V_\alpha(\Omega_b)$ of (3.5) can be extended to a solution $u=u^{\mathrm{in}}+u^{\mathrm{sc}}$ of the Navier equation (2.1) for $x_3\geq b$, where u^{sc} is defined as the unique α-quasiperiodic radiating solution of the homogeneous Navier equation in $\{x_3>b\}$ satisfying $u^{\mathrm{sc}}=u-u^{\mathrm{in}}$ on Γ_b.

3.2. *Properties of the Dirichlet-to-Neumann map*

In this subsection, we will show an explicit representation of the DtN map $\mathcal{T}$, and then utilize it to investigate properties of $\mathcal{T}$. In contrast to the case of the scalar Helmholtz equation, the property

$$-\mathrm{Re}\int_{\Gamma_b}\mathcal{T}u\cdot\overline{u}ds\geq 0\quad\text{for all } u\in H_\alpha^{1/2}(\Gamma_b)^3$$

does not hold for the Navier system; cf. Ref. 22, Ref. 12 and the following Lemma 2. Nevertheless, thanks to the periodicity of the structure, the sesquilinear form B appears to be strongly elliptic, since $-\mathrm{Re}\,\mathcal{T}$ can be decomposed into the sum of a positive-definite operator and a finite-dimensional operator over $H_\alpha^{1/2}(\Gamma_b)^3$. However, compared to the two-dimensional case, the arguments are much more involved; cf. Secs. 3.2 and 3.3. In the following, the Fourier coefficients of $\exp(-i\alpha\cdot x')u(x',b)$ and $\exp(-i\alpha\cdot x')(Tu)(x',b)$, denoted by $\hat{u}_n$ and $(\widehat{Tu})_n$ respectively, will be frequently used.

Throughout the paper, we use C to denote a generic constant whose value may change in different inequalities.

Lemma 1. *For* $v = \sum_{n\in\mathbb{Z}^2} \hat{v}_n \exp(i\alpha_n \cdot x') \in H_\alpha^{1/2}(\Gamma_b)^3$, *we have*

$$\mathcal{T}v = \mathcal{T}(\omega,\alpha)v = \sum_{n\in\mathbb{Z}^2} iW_n \hat{v}_n \exp(i\alpha_n \cdot x'),$$

where W_n *is the* 3×3 *matrix defined by*

$$W_n = W_n(\omega,\alpha) := \frac{1}{|\alpha_n|^2 + \beta_n\gamma_n} \begin{pmatrix} a_n & b_n & c_n \\ b_n & d_n & e_n \\ -c_n & -e_n & f_n \end{pmatrix}, \tag{3.7}$$

with

$$\begin{aligned} a_n &:= \mu[(\gamma_n - \beta_n)(\alpha_n^{(2)})^2 + k_s^2\beta_n], \quad b_n := -\mu\alpha_n^{(1)}\alpha_n^{(2)}(\gamma_n - \beta_n), \\ c_n &:= (2\mu\alpha_n^2 - \omega^2 + 2\mu\gamma_n\beta_n)\alpha_n^{(1)}, \quad e_n := (2\mu\alpha_n^2 - \omega^2 + 2\mu\gamma_n\beta_n)\alpha_n^{(2)}, \\ d_n &:= \mu[(\gamma_n - \beta_n)(\alpha_n^{(1)})^2 + k_s^2\beta_n], \quad f_n := \gamma_n\omega^2. \end{aligned}$$

Proof. Assume u is a radiating solution of the form (2.13). Then the Fourier coefficients of $\exp(-i\alpha\cdot x')u(x)|_{\Gamma_b}$ can be written as

$$\hat{u}_n := \begin{pmatrix} \alpha_n^{(1)} & 1 & 0 & 0 \\ \alpha_n^{(2)} & 0 & 1 & 0 \\ \beta_n & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} A_{p,n}e^{i\beta_n b} \\ \mathbf{A}_{s,n}^\top e^{i\gamma_n b} \end{pmatrix} =: D_n A_n, \tag{3.8}$$

or equivalently, by recalling the orthogonality relation (2.14),

$$\begin{pmatrix} \hat{u}_n \\ 0 \end{pmatrix} = \begin{pmatrix} \alpha_n^{(1)} & 1 & 0 & 0 \\ \alpha_n^{(2)} & 0 & 1 & 0 \\ \beta_n & 0 & 0 & 1 \\ 0 & \alpha_n^{(1)} & \alpha_n^{(2)} & \gamma_n \end{pmatrix} \begin{pmatrix} A_{p,n}e^{i\beta_n b} \\ A_{s,n}^{(1)}e^{i\gamma_n b} \\ A_{s,n}^{(2)}e^{i\gamma_n b} \\ A_{s,n}^{(3)}e^{i\gamma_n b} \end{pmatrix} =: \tilde{D}_n A_n. \tag{3.9}$$

Through direct calculations, it follows from (3.9) that

$$A_n = \tilde{D}_n^{-1} \begin{pmatrix} \hat{u}_n \\ 0 \end{pmatrix} = D_n^{-1}\hat{u}_n, \tag{3.10}$$

where $\tilde{D}_n^{-1}$ denotes the inverse matrix of $\tilde{D}_n$, and D_n^{-1} is the 4×3 matrix defined by

$$D_n^{-1} := \frac{1}{\gamma_n\beta_n + |\alpha_n|^2} \begin{pmatrix} \alpha_n^{(1)} & \alpha_n^{(2)} & \gamma_n \\ \gamma_n\beta_n + (\alpha_n^2)^2 & -\alpha_n^{(1)}\alpha_n^{(2)} & -\gamma_n\alpha_n^{(1)} \\ -\alpha_n^{(1)}\alpha_n^{(2)} & \gamma_n\beta_n + (\alpha_n^{(1)})^2 & -\gamma_n\alpha_n^{(2)} \\ -\alpha_n^{(1)}\beta_n & -\alpha_n^{(2)}\beta_n & |\alpha_n|^2 \end{pmatrix}.$$

On the other hand, applying the stress operator T (see (3.3)) to the radiating solution $u|_{\Gamma_b}$ yields

$$Tu = i\left\{\begin{pmatrix} 2\mu\beta_n\alpha_n^{(1)} \\ 2\mu\beta_n\alpha_n^{(2)} \\ 2\mu\beta_n^2 + \lambda k_p^2 \end{pmatrix} A_{p,n}e^{i\beta_n b} + \begin{pmatrix} \mu\gamma_n & 0 & \mu\alpha_n^{(1)} \\ 0 & \mu\gamma_n & \mu\alpha_n^{(2)} \\ 0 & 0 & 2\mu\gamma_n \end{pmatrix} \mathbf{A}_{s,n}^\top e^{i\gamma_n b}\right\} e^{i\alpha_n\cdot x'}.$$

This together with (3.10) allows us to write the Fourier coefficients of $\exp(-i\alpha \cdot x')(Tu)(x)|_{\Gamma_b}$ as

$$\begin{aligned} \widehat{(Tu)}_n &= i\begin{pmatrix} 2\mu\beta_n\alpha_n^{(1)} & \mu\gamma_n & 0 & \mu\alpha_n^{(1)} \\ 2\mu\beta_n\alpha_n^{(2)} & 0 & \mu\gamma_n & \mu\alpha_n^{(2)} \\ 2\mu\beta_n^2 + \lambda k_p^2 & 0 & 0 & 2\mu\gamma_n \end{pmatrix} \begin{pmatrix} A_{p,n}e^{i\beta_n b} \\ \mathbf{A}_{s,n}e^{i\gamma_n b} \end{pmatrix} \qquad (3.11) \\ &=: iG_nA_n \\ &= iG_nD_n^{-1}\hat{u}_n \qquad (3.12) \\ &= iW_n\hat{u}_n, \end{aligned}$$

where $W_n := G_nD_n^{-1}$ coincides with the matrix defined in (3.7). The proof is thus complete. □

For a matrix $M \in \mathbb{C}^{3\times 3}$, we define its real part by $\operatorname{Re} M := (M + M^*)/2$, and write $\operatorname{Re} M > 0$ if $\operatorname{Re} M$ is positive-definite. Here M^* is the adjoint matrix of M with respect to the scalar product $(\cdot,\cdot)_{\mathbb{C}^3}$ in $\mathbb{C}^3$.

Lemma 2. *Let W_n be defined as in* (3.7).

(i) *Given a fixed frequency $\omega > 0$, we have $\operatorname{Re}(-iW_n) > 0$ for all sufficiently large $|n|$.*

(ii) *There exists a sufficiently small frequency $\omega_0 > 0$ such that*

$$\operatorname{Re}(-iW_nz, z)_{\mathbb{C}^3} \geq C|n||z|^2, \quad \forall\, z \in \mathbb{C}^3, \quad \omega \in (0,\omega_0], \quad n \neq (0,0)$$

with some constant $C > 0$ independent of ω and n.

(iii) *The DtN map $\mathcal{T}$ is a bounded operator from $H_\alpha^{1/2}(\Gamma_b)^3$ to $H_\alpha^{-1/2}(\Gamma_b)^3$.*

Proof. (i) For sufficiently large $|n|$, we first observe that $\beta_n = i|\beta_n|, \gamma_n = i|\gamma_n|$, and thus

$$iW_n = \frac{-1}{|\alpha_n|^2 - |\beta_n||\gamma_n|}\begin{pmatrix} a_n' & b_n' & -i\alpha_n^{(1)}c_n' \\ b_n' & d_n' & -i\alpha_n^{(2)}c_n' \\ i\alpha_n^{(1)}c_n' & i\alpha_n^{(2)}c_n' & f_n' \end{pmatrix} =: \frac{-W_n'}{|\alpha_n|^2 - |\beta_n||\gamma_n|}, \qquad (3.13)$$

where

$$a_n' := \mu[(|\gamma_n| - |\beta_n|)(\alpha_n^{(2)})^2 + k_s^2|\beta_n|] \in \mathbb{R}, \quad b_n' := -\mu\alpha_n^{(1)}\alpha_n^{(2)}(|\gamma_n| - |\beta_n|) \in \mathbb{R},$$
$$c_n' := (2\mu|\alpha_n|^2 - \omega^2 - 2\mu|\gamma_n||\beta_n|) \in \mathbb{R}, \; d_n' := \mu[(|\gamma_n| - |\beta_n|)(\alpha_n^{(1)})^2 + k_s^2|\beta_n|] \in \mathbb{R},$$
$$f_n' := |\gamma_n|\omega^2 \in \mathbb{R}.$$

Using Taylor expansions, one may check that, for fixed $\omega > 0$,

$$|\alpha_n|^2 - |\beta_n||\gamma_n| \to \frac{k_p^2 + k_s^2}{2} \quad \text{as } |n| \to +\infty. \tag{3.14}$$

From the definition of W_n' in (3.13), we observe that $\operatorname{Re} W_n' = W_n'$, that is, W_n' coincides with its real part. Hence it remains to prove that W_n' is positive-definite for all sufficiently large $|n|$. To this end, we only need to verify that

$$\text{(I)}\, a_n' > 0, \quad \text{(II)} \begin{vmatrix} a_n' & b_n' \\ b_n' & d_n' \end{vmatrix} > 0, \quad \text{(III)}\det(W_n') > 0, \;\text{ for all sufficiently large } |n|.$$

Noting that $|\gamma_n|^2 = |\alpha_n|^2 - k_s^2$, $|\beta_n|^2 = |\alpha_n|^2 - k_p^2$ for large $|n|$, we shall prove (I), (II) and (III) as follows.

(I) For sufficiently large $|n|$, it is obvious that

$$\begin{aligned} a_n' &= \mu[(|\gamma_n| - |\beta_n|)(\alpha_n^{(2)})^2 + k_s^2|\beta_n|] \\ &= \mu\left[\frac{(k_p^2 - k_s^2)(\alpha_n^{(2)})^2}{|\gamma_n| + |\beta_n|} + \frac{k_s^2|\gamma_n|^2 + k_s^2|\gamma_n||\beta_n|}{|\gamma_n| + |\beta_n|}\right] \\ &= \frac{\mu}{|\gamma_n| + |\beta_n|}[k_p^2(\alpha_n^{(2)})^2 + k_s^2(\alpha_n^{(1)})^2 + k_s^2|\gamma_n||\beta_n| - k_s^2k_p^2] \\ &> 0. \end{aligned} \tag{3.15}$$

(II) By arguing as in (3.15), one arrives at

$$g_n := (|\gamma_n| - |\beta_n|)|\alpha_n|^2 + k_s^2|\beta_n| > 0, \quad \text{if } |n| \text{ is sufficiently large.} \tag{3.16}$$

Thus,

$$\begin{aligned} \begin{vmatrix} a_n' & b_n' \\ b_n' & d_n' \end{vmatrix} &= a_n'd_n' - (b_n')^2 \\ &= \mu^2[(|\gamma_n| - |\beta_n|)(\alpha_n^{(2)})^2 + k_s^2|\beta_n|]\,[(|\gamma_n| - |\beta_n|)(\alpha_n^{(1)})^2 + k_s^2|\beta_n|] \\ &\quad - \mu^2(\alpha_n^{(1)}\alpha_n^{(2)})^2(|\gamma_n| - |\beta_n|)^2 \\ &= \mu^2k_s^2|\beta_n|\,[(|\gamma_n| - |\beta_n|)|\alpha_n|^2 + k_s^2|\beta_n|] \\ &= \mu^2k_s^2|\beta_n|\,g_n \\ &> 0. \end{aligned} \tag{3.17}$$

(III) It can be verified that

$$\begin{vmatrix} a_n & b_n & -c_n \\ b_n & d_n & -e_n \\ c_n & e_n & f_n \end{vmatrix} = \begin{vmatrix} a_n & b_n \\ b_n & d_n \end{vmatrix} f_n + (a_n e_n^2 - 2b_n e_n c_n + d_n c_n^2).$$

Hence, from (3.17) and the definition of W_n' it follows that

$$\begin{aligned} &\det(W_n') \\ &\quad= \begin{vmatrix} a_n' & b_n' \\ b_n' & d_n' \end{vmatrix} f_n' + \left[a_n'(i\alpha_n^{(2)} c_n')^2 - 2b_n'(i\alpha_n^{(2)} c_n')\,(i\alpha_n^{(1)} c_n') + d_n'(i\alpha_n^{(1)} c_n')^2\right] \\ &\quad= (\mu^2 k_s^2\,|\beta_n|\,g_n)\,(|\gamma_n|\omega^2) + (c_n')^2\,\underbrace{\left[2b_n'\alpha_n^{(1)}\alpha_n^{(2)} - a_n'(\alpha_n^{(2)})^2 - d_n'(\alpha_n^{(1)})^2\right]}_{h_n}. \end{aligned} \tag{3.18}$$

In view of the definitions of a_n', b_n', d_n' at the beginning of the proof and that of g_n in (3.16), there holds

$$\begin{aligned} h_n &:= 2b_n'\alpha_n^{(1)}\alpha_n^{(2)} - a_n'(\alpha_n^{(2)})^2 - d_n'(\alpha_n^{(1)})^2 \\ &= 2\mu(\alpha_n^{(1)}\alpha_n^{(2)})^2(|\beta_n| - |\gamma_n|) - \mu(\alpha_n^{(2)})^2[(\alpha_n^{(2)})^2(|\gamma_n| - |\beta_n|) + k_s^2|\beta_n|)] \\ &\quad - \mu(\alpha_n^{(1)})^2[(\alpha_n^{(1)})^2(|\gamma_n| - |\beta_n|) + k_s^2|\beta_n|)] \\ &= \mu(|\beta_n| - |\gamma_n|)|\alpha_n|^4 - \mu k_s^2\,|\beta_n|\,|\alpha_n|^2 \\ &= -\mu|\alpha_n|^2[(|\gamma_n| - |\beta_n|)|\alpha_n|^2 + k_s^2|\beta_n|] \\ &= -\mu|\alpha_n|^2 g_n. \end{aligned} \tag{3.19}$$

Inserting (3.19) into (3.18) and recalling the definition of c_n', we obtain

$$\begin{aligned} \det(W_n') &= \mu^3 k_s^4\,|\beta_n|\,|\gamma_n|\,g_n - \mu^3[2|\gamma_n|\,|\beta_n| - |\gamma_n|^2 - |\alpha_n|^2]^2\,|\alpha_n|^2\,g_n \\ &= \mu^3 g_n\left\{|\beta_n|\,|\gamma_n| k_s^4 - |\alpha_n|^2[2|\gamma_n|(|\gamma_n| - |\beta_n|) + k_s^2]^2\right\} \\ &= \mu^3 g_n|\alpha_n|^2\left\{\frac{|\beta_n|}{|\alpha_n|}\frac{|\gamma_n|}{|\alpha_n|}k_s^4 - \left[\frac{2|\gamma_n|(k_p^2 - k_s^2)}{|\gamma_n| + |\beta_n|} + k_s^2\right]^2\right\}. \end{aligned} \tag{3.20}$$

Since

$$\frac{|\beta_n|}{|\alpha_n|} \to 1, \quad \frac{|\gamma_n|}{|\alpha_n|} \to 1, \quad \frac{2|\gamma_n|(k_p^2 - k_s^2)}{|\gamma_n| + |\beta_n|} \to k_p^2 - k_s^2, \quad g_n > 0 \quad \text{as } |n| \to +\infty,$$

we finally conclude from (3.20) and the fact $0 < k_p < k_s$ that

$$\det(W_n') > 0 \quad \text{for all sufficiently large } |n|.$$

This finishes the proof of assertion (i).

(ii) To prove the second assertion for small frequencies, we need to analyze the asymptotic behavior of $\mathrm{Re}(iW_n)$ as $\omega \to 0^+$. In the following, for a sequence $\{a_j\}$, we write $a_j \sim a_0$ as $j \to +\infty$ if $a_j/a_0 \to 1$ as $j \to +\infty$. Since

$$\beta_n = i\sqrt{|\alpha_n|^2 - k_p^2} \sim i|n|, \quad \gamma_n = i\sqrt{|\alpha_n|^2 - k_s^2} \sim i|n| \quad \text{as } \omega \to 0^+, \tag{3.21}$$

uniformly in $n \neq (0,0)$, the matrix iW_n with $n \neq (0,0)$ takes the same form as in (3.13) for small frequencies. Furthermore, it follows from the behavior of β_n and γ_n in (3.21) in combination with the identities in (3.15)–(3.17) and (3.20) that

$$a_n' \sim \omega^2|n|C_1(\lambda,\mu), \quad g_n \sim \omega^2|n|C_2(\lambda,\mu), \tag{3.22}$$

$$\begin{vmatrix} a_n' & b_n' \\ b_n' & d_n' \end{vmatrix} \sim \omega^4|n|^2C_3(\lambda,\mu), \quad \det(W_n') \sim \omega^6|n|^3C_4(\lambda,\mu), \tag{3.23}$$

as $\omega \to 0^+$ uniformly in $n \neq (0,0)$, where $C_j(\lambda,\mu)$ $(j = 1,2,3,4)$ are positive constants only depending on λ and μ; note that $\omega^2 = \mu k_s^2 = (\lambda+2\mu)k_p^2$. In addition, we get

$$\delta_n := |\alpha_n|^2 - |\beta_n|\,|\gamma_n| = \omega^2\frac{3\mu+\lambda}{2\mu(2\mu+\lambda)} + \mathcal{O}(\omega^4) \quad \text{as } \omega \to 0. \tag{3.24}$$

From (3.22)–(3.24), we then obtain the inequalities

$$\frac{a_n'}{|n|\delta_n} \geq C, \quad \frac{1}{|n|^2(\delta_n)^2}\begin{vmatrix} a_n' & b_n' \\ b_n' & d_n' \end{vmatrix} \geq C, \quad \frac{\det(W_n')}{|n|^3(\delta_n)^3} \geq C, \tag{3.25}$$

uniformly in $n \neq (0,0)$, for all sufficiently small ω and some constant $C > 0$. Combining (3.24), (3.25) and (3.13) yields the second assertion.

(iii) Since the asymptotic behavior in (3.21) remains valid as $|n| \to +\infty$, there holds

$$|\beta_n - \gamma_n| \sim \frac{1}{|n|^2}\frac{k_s^2 - k_p^2}{2} \quad \text{as } |n| \to +\infty.$$

It follows from (3.7) and (3.14) that

$$|a_n|,\ |b_n|,\ |c_n|,\ |d_n|,\ |e_n|,\ |f_n| \leq |n|C(\lambda,\mu), \quad \text{for sufficiently large } |n|,$$

with some constant $C(\lambda,\mu) > 0$, implying the inequality $|(W_n\hat{v}_n, \hat{v}_n)_{\mathbb{C}^3}| \leq C|n||\hat{v}_n|^2$ for some constant $C > 0$ uniformly in $n \in \mathbb{Z}^2$. By the definition of $\|\cdot\|_{H_\alpha^s(\Gamma_b)^3}$, the boundedness of $\mathcal{T}$ mapping $H_\alpha^{1/2}(\Gamma_b)^3$ into $H_\alpha^{-1/2}(\Gamma_b)^3$ follows in a standard way. $\square$

3.3. *Strong ellipticity*

Let V'_α denote the dual of V_α with respect to the L^2 scalar product. By Lemma 2(iii), there exists a continuous linear operator $\mathcal{B} : V_\alpha \to V'_\alpha$ associated with the sesquilinear form B such that

$$B(u, \varphi) = (\mathcal{B}u, \varphi) \quad \text{for all } \varphi \in V_\alpha. \tag{3.26}$$

Definition 2. A bounded sesquilinear form $B(\cdot, \cdot)$ given on some Hilbert space X is called strongly elliptic if there exists a compact form $q(\cdot, \cdot)$ such that

$$|\mathrm{Re}\, B(u, u)| \geq C\, \|u\|_X^2 - q(u, u) \quad \forall\, u \in X.$$

The following theorem establishes the strong ellipticity of the sesquilinear form B defined in (3.4).

Theorem 1. *Assume* Λ *is a Lipschitz surface. Then the sesquilinear form* B *is strongly elliptic over* V_α *under each of the boundary conditions in* (2.6). *Moreover, the operator* $\mathcal{B}$ *defined by* (3.26) *is always a Fredholm operator with index zero.*

Proof. The bilinear form $a(\cdot, \cdot)$ defined by (3.2) can be written as

$$a(u, v) = \lambda\, \mathrm{div}\, u\, \mathrm{div}\, v + 2\mu \sum_{i,j=1}^{3} \varepsilon_{ij}(u)\varepsilon_{ij}(v), \quad \varepsilon_{ij}(u) := (\partial_j u_i + \partial_i u_j)/2.$$

Under our assumptions on the Lamé constants, $\mu > 0, \lambda + 2\mu/3 > 0$, we have the estimate (see Ref. 25)

$$\int_{\Omega_b} a(u, \overline{u})dx \geq C(\Omega_b) \sum_{i,j=1}^{3} \|\varepsilon_{ij}(u)\|^2_{L^2(\Omega_b)}, \quad \forall\, u \in H^1(\Omega_b)^3. \tag{3.27}$$

By the well-known Korn's inequality (see e.g. Refs. 29 and 18), there holds

$$\sum_{i.j=1}^{3} \|\varepsilon_{ij}(u)\|^2_{L^2(\Omega_b)} + \sum_{i=1}^{3} \|u_i\|^2_{L^2(\Omega_b)} \geq C(\Omega_b)\|u\|^2_{H^1(\Omega_b)^3}, \quad \forall\, u \in H^1(\Omega_b)^3. \tag{3.28}$$

Hence,

$$\int_{\Omega_b} (a(u, \overline{u}) - \omega^2|u|^2)dx \geq C(\Omega_b)\|u\|^2_{H^1(\Omega_b)^3} - (C(\Omega_b) + \omega^2)\|u\|^2_{L^2(\Omega_b)}.$$

The compactness of the imbedding $H^1(\Omega_b) \hookrightarrow L^2(\Omega_b)$ implies that the operator $\mathcal{K} : V_\alpha \to V'_\alpha$ defined by

$$(\mathcal{K}u, \varphi)_{\Omega_b} = \int_{\Omega_b} u \cdot \bar{\varphi} dx, \quad \forall\, u, \varphi \in V_\alpha \tag{3.29}$$

is compact. Thus, to prove the strong ellipticity of the form B defined in (3.4), it is now sufficient to verify that $\mathcal{T}$ is the sum of a finite-dimensional operator and an operator $\mathcal{T}_1$ satisfying

$$\mathrm{Re}\left\{ - \int_{\Gamma_b} \overline{u} \cdot \mathcal{T}_1 u ds \right\} \geq 0, \quad \forall\, u \in H^1_\alpha(\Omega_b)^3. \tag{3.30}$$

To do so, we set

$$\mathcal{T}_1 u := \sum_{|n|\geq n_0} iW_n \hat{u}_n, \quad \mathcal{T}_0 u := \mathcal{T} u - \mathcal{T}_1 u = \sum_{|n|<n_0} iW_n \hat{u}_n,$$

where the matrices W_n are defined as in (3.7), and $n_0 \in \mathbb{N}$ is sufficiently large so that by Lemma 2(i)

$$\mathrm{Re}(-iW_n z, z)_{\mathbb{C}^2} \geq 0, \quad \forall\, z \in \mathbb{C}^2, \quad \forall\, |n| \geq n_0. \tag{3.31}$$

Then we have the decomposition $\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_0$, where $\mathcal{T}_1$ satisfies (3.30) and $\mathcal{T}_0$ is a finite-dimensional operator. This finishes the proof of the strong ellipticity of B over V_α, from which the Fredholm property of $\mathcal{B}$ follows. □

4. Solvability Results for Impenetrable Gratings

Relying on the strong ellipticity of the sesquilinear form B established in Theorem 1, we next show existence and uniqueness results for impenetrable gratings under the first, second, third and fourth kind of boundary conditions. According to the Fredholm alternative, existence of solutions can always be guaranteed as long as uniqueness holds. However, as we will see in Sec. 4.4, uniqueness for all frequencies cannot be expected under the second, third and fourth kind of boundary conditions, because this even does not hold for a flat grating. Using properties of the DtN map and Korn's inequality, we can prove the uniqueness for small frequencies, and thus for all frequencies excluding a discrete set by employing analytic Fredholm theory. Note that the non-uniqueness examples shown in Sec. 4.4 for flat gratings cannot occur if ω is sufficiently small. Moreover, existence for special incident waves can be established even if there is no uniqueness; see Sec. 4.2.1. In the case of the Dirichlet boundary condition, we shall prove uniqueness for all frequencies if the grating profile Λ is given by the graph of a Lipschitz function; see Sec. 4.3.

We begin with the following auxiliary lemma which plays an important role in the subsequent analysis.

4.1. *An auxiliary lemma*

Lemma 3. *Assume $u \in V_\alpha$ is a radiating solution of the form* (2.13). *If $\mathcal{B}u = 0$, then*

$$A_{p,n} = 0 \quad \textit{for } |\alpha_n| < k_p \quad \textit{and} \quad \mathbf{A}_{s,n} = 0 \quad \textit{for } |\alpha_n| < k_s. \tag{4.1}$$

Proof. Taking imaginary parts in the variational equation (3.5) with $\varphi = u$ and $f_0 = 0$ yields

$$0 = \mathrm{Im}(\mathcal{B}u, u) = \mathrm{Im}\, B(u, u) = -\mathrm{Im} \int_{\Gamma_b} \overline{u} \cdot \mathcal{T} u ds. \tag{4.2}$$

In the sequel, we are going to prove that

$$\operatorname{Im}\int_{\Gamma_b}\overline{u}\cdot\mathcal{T}u ds = 4\pi^2\left(\sum_{|\alpha_n|<k_p}\beta_n|A_{p,n}|^2\,\omega^2+\sum_{|\alpha_n|<k_s}\gamma_n|\mathbf{A}_{s,n}|^2\mu\right), \tag{4.3}$$

which together with (4.2) implies the lemma.

Recalling the Fourier coefficients of $\exp(-i\alpha\cdot x')u(x)|_{\Gamma_b}$, $\hat{u}_n := D_nA_n$, defined as in (3.8), and those of $\exp(-i\alpha\cdot x')Tu(x)|_{\Gamma_b}$, $(\widehat{Tu})_n := iG_nA_n$, defined as in (3.11) and (3.12), we have

$$\operatorname{Im}\int_{\Gamma_b}\overline{u}\cdot\mathcal{T}u ds = \operatorname{Im}\int_{\Gamma_b}\overline{u}\cdot Tu ds = 4\pi^2\operatorname{Im}\sum_{n\in\mathbb{Z}^2}(iG_nA_n, D_nA_n)_{\mathbb{C}^3} \tag{4.4}$$

$$= 4\pi^2\sum_{n\in\mathbb{Z}^2}(\operatorname{Re}(D_n^*G_n)A_n, A_n)_{\mathbb{C}^3}, \tag{4.5}$$

where D_n^* denotes the adjoint matrix of D_n. By direct calculations, we see that

$$D_n^*G_n = \begin{pmatrix} 2\mu\beta_n(|\alpha_n|^2+|\beta_n|^2)+\lambda\overline{\beta}_nk_p^2 & \mu\gamma_n\alpha_n^{(1)} & \mu\gamma_n\alpha_n^{(2)} & \mu(|\alpha_n|^2+2\overline{\beta}_n\gamma_n) \\ 2\mu\beta_n\alpha_n^{(1)} & \mu\gamma_n & 0 & \mu\alpha_n^{(1)} \\ 2\mu\beta_n\alpha_n^{(2)} & 0 & \mu\gamma_n & \mu\alpha_n^{(2)} \\ 2\mu\beta_n^2+\lambda k_p^2 & 0 & 0 & 2\mu\gamma_n \end{pmatrix}.$$

To obtain the real part of $D_n^*G_n$, we decompose the above 4×4 matrix into the sum $J_1+J_2+J_3$, where

$$J_1 := \begin{pmatrix} 2\mu\beta_n(|\alpha_n|^2+|\beta_n|^2)+\lambda\overline{\beta}_nk_p^2 & 0 & 0 & 0 \\ 0 & \mu\gamma_n & 0 & 0 \\ 0 & 0 & \mu\gamma_n & 0 \\ 0 & 0 & 0 & \mu\gamma_n \end{pmatrix},$$

$$J_2 := \begin{pmatrix} 0 & \mu\gamma_n\alpha_n^{(1)} & \mu\gamma_n\alpha_n^{(2)} & \mu(|\alpha_n|^2+2\overline{\beta}_n\gamma_n) \\ 2\mu\beta_n\alpha_n^{(1)} & 0 & 0 & 0 \\ 2\mu\beta_n\alpha_n^{(2)} & 0 & 0 & 0 \\ 2\mu\beta_n^2+\lambda k_p^2 & 0 & 0 & 0 \end{pmatrix},$$

$$J_3 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu\alpha_n^{(1)} \\ 0 & 0 & 0 & \mu\alpha_n^{(2)} \\ 0 & 0 & 0 & \mu\gamma_n \end{pmatrix}.$$

Then, using the relations

$$\alpha_n^{(1)}A_{s,n}^{(1)}+\alpha_n^{(2)}A_{s,n}^{(2)}+\gamma_nA_{s,n}^{(3)}=0,\quad |\alpha_n|^2+\beta_n^2=k_p^2,\quad |\alpha_n|^2+\gamma_n^2=k_s^2$$

for all $n \in \mathbb{Z}^2$, we obtain

$$(J_2 A_n, A_n) = (\tilde{J}_2 A_n, A_n), \quad (J_3 A_n, A_n) = 0 \quad \text{for all } n \in \mathbb{Z}^2, \tag{4.6}$$

where $\tilde{J}_2$ is the 4×4 matrix whose $(1,4)$th entry is $2\mu|\alpha_n|^2+2\mu\overline{\beta}_n\gamma_n-\omega^2$, its $(4,1)$th entry is $-2\mu|\alpha_n|^2 - 2\mu\beta_n\overline{\gamma}_n + \omega^2$, and the other entries are zeros. Furthermore, we arrive at

$$((\operatorname{Re} J_1)A_n, A_n) = \begin{cases} \omega^2\beta_n|A_{p,n}|^2 + \mu\gamma_n|\mathbf{A}_{s,n}|^2 & \text{if } |\alpha_n| < k_p, \\ \mu\gamma_n|\mathbf{A}_{s,n}|^2 & \text{if } k_p \le |\alpha_n| < k_s, \\ 0 & \text{if } k_s \le |\alpha_n|. \end{cases} \tag{4.7}$$

Noting that $\operatorname{Re}\tilde{J}_2 = 0$, we conclude from (4.4)–(4.7) that the identity (4.3) holds. The proof is thus complete. □

Remark 3. If $u \in V_\alpha$ is a radiating solution of the form (2.12) and satisfies $\mathcal{B}u = 0$, then the identity (4.3) takes the form

$$\operatorname{Im}\int_{\Gamma_b} \overline{u}\cdot\mathcal{T}u ds = 4\pi^2\omega^2\left(\sum_{|\alpha_n|<k_p}\beta_n\,|A_{p,n}|^2 + \sum_{|\alpha_n|<k_s}\gamma_n|\tilde{\mathbf{A}}_{s,n}|^2\right) \tag{4.8}$$

which also implies (4.1). Note that the quantity in (4.8) denotes the energy flux through Γ_b, and that an analogous identity to (4.8) has been proved in Refs. 21 and 3 for two-dimensional gratings.

4.2. *Solvability for general Lipschitz grating profiles*

We assume the impenetrable grating profile Λ is a Lipschitz surface on which one of the boundary conditions in (2.6) is imposed. By (3.26), we rewrite the variational formulation (3.5) as

$$\mathcal{B}u = \mathcal{F}_0, \tag{4.9}$$

where $\mathcal{F}_0 \in V'_\alpha$ is defined by the right-hand side of (3.5). Equation (4.9) is equivalent to the boundary value problem (BVP) in the sense of Remark 2. Lemma 3 only tells us that a radiating solution to the homogeneous equation $(\mathcal{B}u, u) = 0$ has vanishing propagating modes. Obviously this does not imply the uniqueness. Next, we establish an existence result for the incident pressure waves (2.15) or the incident shear waves (2.16) for any $\omega > 0$, and then present a uniqueness result for small frequencies.

4.2.1. *Existence*

Theorem 2. *Let the grating profile Λ be given by a Lipschitz surface in $\mathbb{R}^3$. Then, for all incident plane waves of the form* (2.15) *or* (2.16), *there always exists a* *solution* $u \in V_\alpha$ *to the variational problem* (3.5) *and hence to* (BVP) *under each of the boundary conditions in* (2.6).

Proof. By Theorem 1, Eq. (4.9) is solvable if its right-hand side $\mathcal{F}_0$ is orthogonal (with respect to the duality $(\cdot,\cdot)_{\Omega_b}$ extending the scalar product in $L^2(\Omega_b)^3$) 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 (2.1) in the unbounded domain Ω by setting

$$v(x) = \sum_{n\in\mathbb{Z}^2} \big\{ A_{p,n}(\alpha_n, -\overline{\beta}_n)^\top \exp(i\alpha_n\cdot x' - i\overline{\beta}_n x_3) + \mathbf{A}_{s,n}\exp(i\alpha_n\cdot x' - i\overline{\gamma}_n x_s)\big\}, \tag{4.10}$$

for $x_3 \geq b$, where the Rayleigh coefficients $\mathbf{A}_{s,n} \in \mathbb{C}^3$ fulfill the orthogonality relation $\mathbf{A}_{s,n}\cdot(\alpha_n^{(1)}, \alpha_n^{(2)}, -\overline{\gamma}_n) = 0$, and $A_{p,n}, \mathbf{A}_{s,n}$ are determined by the nth Fourier coefficient $\hat{v}_n$ of $e^{-i\alpha\cdot x'}v|_{\Gamma_b}$ via the following relation:

$$\begin{pmatrix}\hat{v}_n\\ 0\end{pmatrix} = \begin{pmatrix} \alpha_n^{(1)} & 1 & 0 & 0\\ \alpha_n^{(2)} & 0 & 1 & 0\\ -\overline{\beta}_n & 0 & 0 & 1\\ 0 & \alpha_n^{(1)} & \alpha_n^{(2)} & -\overline{\gamma}_n\end{pmatrix}\begin{pmatrix} A_{p,n}e^{-i\overline{\beta}_n b}\\ \mathbf{A}_{s,n}^\top e^{-i\overline{\gamma}_n b}\end{pmatrix}.$$

Analogously to Lemma 3, it can be derived from

$$(\mathcal{B}^* v, \psi)_{\Omega_b} = (v, \mathcal{B}\psi)_{\Omega_b} = \overline{B(\psi, v)} = 0, \quad \forall\,\psi\in V_\alpha \tag{4.11}$$

that

$$A_{p,n} = 0 \quad \text{for } |\alpha_n| < k_p \quad \text{and} \quad \mathbf{A}_{s,n} = 0 \quad \text{for } |\alpha_n| < k_s. \tag{4.12}$$

This means that v has vanishing Rayleigh coefficients of the incoming modes, giving that

$$\hat{v}_n = \begin{cases} (0,0,0)^\top & \text{if } |\alpha_n| < k_p < k_s,\\ (\alpha_n^{(1)}, \alpha_n^{(2)}, -\overline{\beta}_n)^\top A_{p,n}\exp(-i\overline{\beta}_n b) & \text{if } k_p \leq |\alpha_n| < k_s.\end{cases}$$

On the other hand, through direct calculations we deduce that $f_0 := Tu^{\mathrm{in}} - \mathcal{T}u^{\mathrm{in}}$ takes the form

$$f_0 = \sum_{|\alpha_n|<k_p} \frac{i}{k_p}\frac{2\omega^2\beta_n}{|\alpha_n|^2 + \gamma_n\beta_n}\begin{pmatrix}-\alpha_n^\top\\ \gamma_n\end{pmatrix} e^{-i\beta_n b}e^{i\alpha_n\cdot x'} =: \sum_{|\alpha_n|<k_p} h_n e^{i\alpha_n\cdot x'} \tag{4.13}$$

for the incident pressure wave $u^{\mathrm{in}}_{(p)}$ defined in (2.15), which leads to

$$\mathcal{F}_0(v) = \int_{\Gamma_b} f_0\cdot\overline{v}\,ds = 4\pi^2\sum_{|\alpha_n|<k_p} h_n\cdot\overline{\hat{v}_n} = 0.$$

For the incident shear wave $u^{\rm in}_{(s)}$ defined in (2.16), we obtain

$$\begin{aligned} f_0 &= \sum_{|\alpha_n|<k_s} \frac{i}{k_s} \frac{2\omega^2\gamma_n}{|\alpha_n|^2+\beta_n\gamma_n} \mathbf{Q}_n^\top \times \begin{pmatrix} \alpha_n^\top \\ -\beta_n \end{pmatrix} e^{-i\gamma_n b} e^{i\alpha_n\cdot x'} \\ &=: \sum_{|\alpha_n|<k_s} g_n e^{i\alpha_n\cdot x'} \end{aligned} \tag{4.14}$$

so that

$$\begin{aligned} \mathcal{F}_0(v) &= \int_{\Gamma_b} f_0\cdot \overline{v} ds \\ &= 4\pi^2 \sum_{|\alpha_n|<k_s} g_n\cdot \overline{\hat{v}_n} \\ &= 4\pi^2 \sum_{|\alpha_n|<k_s} \frac{i}{k_s} \frac{2\omega^2\gamma_n}{|\alpha_n|^2+\beta_n\gamma_n} e^{-i\gamma_n b} \left\{ \mathbf{Q}_n^\top \times \begin{pmatrix} \alpha_n^\top \\ -\beta_n \end{pmatrix} \right\} \cdot \begin{pmatrix} \alpha_n^\top \\ -\beta_n \end{pmatrix} \overline{A}_{p,n} e^{i\beta_n b} \\ &= 0. \end{aligned}$$

Therefore, the right-hand side of Eq. (4.9) is always orthogonal to each solution of (4.11). Applying the Fredholm alternative, we finish the proof. □

4.2.2. *Uniqueness*

Theorem 3. *Assume the grating profile Λ is given by a Lipschitz surface and $u^{\rm in}$ is an incident pressure wave (where $\alpha = k_p(\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2)$). Then, under each of the boundary conditions in* (2.6), *we have*

(i) *There exists a small frequency $\omega_0 > 0$ such that the variational problem* (3.5) *admits a unique solution $u \in V_\alpha(\Omega_b)$ for all incident angles and for all frequencies $\omega \in (0, \omega_0]$.*
(ii) *For all but a sequence of countable frequencies $\omega_j, \omega_j \to \infty$, the variational problem* (3.5) (*with fixed incidence angles θ_1 and θ_2*) *admits a unique solution $u \in V_\alpha(\Omega_b)$.*

Proof. (i) Assuming $u \in V_\alpha(\Omega_b)$ is a solution to the homogeneous problem (3.5) so that $(\mathcal{B}u, u) = B(u,u) = 0$, we shall prove that $u = 0$ in Ω_b if ω is sufficiently small. We decompose the operator $\mathcal{B}$ into the sum of $\mathcal{A}+\mathcal{K}$, where $\mathcal{K}$ and $\mathcal{A}$ are defined by

$$(\mathcal{K}v,\varphi)_{\Omega_b} = -\omega^2\int_{\Omega_b} v\cdot\overline{\varphi} ds, \quad (\mathcal{A}v,\varphi)_{\Omega_b} = \int_{\Omega_b} a(v,\overline{\varphi})dx - \int_{\Gamma_b} \overline{\varphi}\cdot \mathcal{T}v ds \tag{4.15}$$

for any $v, \varphi \in V_\alpha$. Since $\alpha = k_p(\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2)$ for an incident pressure wave, we have $|\alpha| = |k_p\sin\theta_1| < k_p$ for all $\theta_1 \in [0, \pi/2)$. Thus it follows from Lemma 3 that the $(0,0)$th Fourier coefficient of $\exp(-i\alpha\cdot x')u(x)|_{\Gamma_b}$ is $\hat{u}_0 = (0,0,0)$.

By Lemma 2(ii), there exists a sufficiently small frequency $\omega_0 > 0$ and a constant $C > 0$ such that, for any $\omega \in (0, \omega_0]$,

$$
\begin{aligned}
\operatorname{Re}\left\{-\int_{\Gamma_b} \overline{u} \cdot \mathcal{T} u ds\right\} &= 4\pi^2 \sum_{n\neq 0} \operatorname{Re}(-iW_n \hat{u}_n, \hat{u}_n)_{\mathbb{C}^3} + 4\pi^2 \operatorname{Re}(-iW_0 \hat{v}_0, \hat{u}_0)_{\mathbb{C}^3} \\
&= 4\pi^2 \sum_{n\neq 0} \operatorname{Re}(-iW_n \hat{u}_n, \hat{u}_n)_{\mathbb{C}^3} \\
&\geq C\|u\|^2_{H^{1/2}_\alpha(\Gamma_b)^3},
\end{aligned}
\tag{4.16}
$$

where $\hat{u}_n$ are the Fourier coefficients of $\exp(-i\alpha \cdot x')u(x', b)$ and C does not depend on ω and n. Using (3.28) and the arguments in the proof of Ref. 18, one can prove that

$$
\|v\|^2_{H^1(\Omega_b)^3} \leq C(\Omega_b) \left(\|v\|^2_{L^2(\Gamma_b)^3} + \sum_{i,j=1}^{3} \|\varepsilon_{ij}(v)\|^2_{L^2(\Omega_b)} \right), \quad \forall\, v \in H^1(\Omega_b)^3.
$$

Together with (3.27), this implies that

$$
|v| := \left(\int_{\Omega_b} a(v, \overline{v}) dx + \|v\|_{H^{1/2}_\alpha(\Gamma_b)^3} \right)^{1/2}
$$

is an equivalent norm of v in $V_\alpha(\Omega_b)$. Thus, combining (4.15) and (4.16) gives

$$
0 = \operatorname{Re}(\mathcal{B}u, u) \geq C\|u\|^2_{V_\alpha(\Omega_b)} - \omega^2 \|u\|^2_{L^2(\Omega_b)^3},
$$

where $C > 0$ does not depend on ω, whence $u = 0$ follows if ω is sufficiently small.

(ii) Relying on the above uniqueness result for small frequencies and employing analytic Fredholm theory, one can prove the invertibility of the operator $\mathcal{B}$ for all frequencies $\omega > 0$ with the possible exception of a discrete set in $(0, \infty)$. The proof is omitted since it can be carried out with minor modifications of that in Elschner and Hu[21] for two-dimensional transmission gratings. □

Remark 4. (i) For an incident shear wave (where $\alpha = k_s(\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2)$), Theorem 3 holds under the additional assumption that $k_s \sin\theta_1 < k_p$. This assumption ensures $\hat{u}_0 = (0, 0, 0)$ in the proof of assertion (i) so that the estimate (4.16) remains true.

(ii) Under the second, third and fourth kind boundary conditions, Theorem 3 does not hold for all frequencies. Non-uniqueness examples will be presented in Sec. 4.4 for flat gratings.

4.3. *Uniqueness for the first kind (Dirichlet) boundary value problem*

In this subsection, we assume the grating profile Λ is given by a Lipschitz graph, $x_3 = f(x_1, x_2)$, where f is 2π-periodic with respect to x_1 and x_2, and suppose the

Dirichlet boundary condition $u = 0$ is imposed on Λ. Our main task is to prove the following uniqueness result for all frequencies.

Theorem 4. *If Λ is a Lipschitz graph, then the operator $\mathcal{B} : V_\alpha \to V'_\alpha$ is invertible for the Dirichlet boundary value problem. In particular, the variational problem* (3.5) *and hence problem* (*BVP*) *have a unique solution for all incident waves under the Dirichlet boundary condition on Λ.*

By Theorem 1, we only need to prove uniqueness. To this end, we first investigate the uniqueness for smooth graphs when $f(x_1, x_2)$ is a C^2 function over $\mathbb{R}^2$. In this case, the third component of the unit normal $\nu := (\nu_1, \nu_2, \nu_3)$ on Λ can be written as

$$\nu_3 = \frac{1}{\sqrt{1 + |\nabla_{x'} f(x')|^2}} \geq C_f > 0$$

for some constant $C_f > 0$ depending only on the Lipschitz constant of f, and by the standard elliptic regularity we have $u \in H^2(\Omega_b) \cap V_\alpha(\Omega_b)$. It is always assumed that the normal on Γ_b points into the region $x_3 > b$. We next establish a periodic Rellich identity for the Navier system in $\mathbb{R}^3$.

Lemma 4. (Periodic Rellich identity for the Navier equation) *If $u \in H^2_\alpha(\Omega_b)$, then*

$$\begin{aligned} &2\,\mathrm{Re} \int_{\Omega_b} (\Delta^* + \omega^2) u \cdot \partial_3 \overline{u} dx \\ &\quad = \left(-\int_\Lambda + \int_{\Gamma_b} \right) \left\{ 2\,\mathrm{Re}\,(Tu \cdot \partial_3 \overline{u}) - \nu_3 a(u, \overline{u}) + \omega^2 |u|^2 \right\} ds. \end{aligned}$$

Proof. Using integration by parts and the first Betti formula, we have

$$\omega^2 \int_{\Omega_b} u \cdot \partial_3 \overline{u} dx = \omega^2 \left(-\int_\Lambda \nu_3 |u|^2 ds + \int_{\Gamma_b} \nu_3 |u|^2 ds - \int_{\Omega_b} \partial_3 u \cdot \overline{u} dx \right)$$

and

$$\begin{aligned} &\int_{\Omega_b} \Delta^* u \cdot \partial_3 \overline{u} dx \\ &\quad = \left(-\int_\Lambda + \int_{\Gamma_b} \right) Tu \cdot \partial_3 \overline{u} ds - \int_{\Omega_b} a(u, \partial_3 \overline{u}) dx \\ &\quad = \left(-\int_\Lambda + \int_{\Gamma_b} \right) Tu \cdot \partial_3 \overline{u} ds + \int_{\Omega_b} a(\partial_3 u, \overline{u}) dx + \left(\int_\Lambda - \int_{\Gamma_b} \right) \nu_3 a(u, \overline{u}) ds \\ &\quad = \left(-\int_\Lambda + \int_{\Gamma_b} \right) 2\,\mathrm{Re}(Tu \cdot \partial_3 \overline{u}) ds - \int_{\Omega_b} \Delta^* \overline{u} \cdot \partial_3 u dx + \left(\int_\Lambda - \int_{\Gamma_b} \right) \nu_3 a(u, \overline{u}) ds. \end{aligned}$$

Note that the contributions of the integrals over vertical surfaces cancel because of the α-quasi-periodicity of u over Ω_b. The periodic Rellich identity for the Navier equation in Lemma 4 follows directly from the previous two identities. $\square$

We refer to Refs. 10 and 22 for the periodic Rellich identity for the scalar Helmholtz equation and to Ref. 21 for the two-dimensional Navier system. Here we have presented a more direct proof. See also Ref. 15 for a general form of the Rellich identity in bounded domains.

Lemma 5. *If $u \in H^{3/2+\epsilon}(\Omega_b)$ for some $\epsilon > 0$ and $u = 0$ on Λ, then*

(i) $\nu \cdot \partial_3 \overline{u}\, \operatorname{div} u = \nu_3 |\operatorname{div} u|^2$, $\partial_3 u = \nu_3 \partial_\nu u$ *on* Λ,
(ii) $\partial_\nu u + \nu \times \operatorname{curl} u - \nu \operatorname{div} u = 0$ *on* Λ,
(iii) $Tu \cdot \partial_3 \overline{u} = \mu |\partial_\nu u|^2 \nu_3 + (\lambda + \mu)|\operatorname{div} u|^2 \nu_3$ *on* Λ,
(iv) $a(u, \overline{u})\nu_3 = \mu |\partial_\nu u|^2 \nu_3 + (\lambda + \mu)|\operatorname{div} u|^2 \nu_3$ *on* Λ.

Proof. Since $u \in H^{3/2+\epsilon}(\Omega_b)$ for some $\epsilon > 0$, ∇u exists almost everywhere on Λ. By the assumption that $u = (u_1, u_2, u_3) = 0$ on Λ, there holds $\nu \times \nabla u_j = 0$ for $j = 1, 2, 3$, i.e.

$$\nu_2 \partial_3 u_j - \nu_3 \partial_2 u_j = 0, \quad \nu_3 \partial_1 u_j - \nu_1 \partial_3 u_j = 0, \quad \nu_1 \partial_2 u_j - \nu_2 \partial_1 u_j = 0 \quad \text{on } \Lambda. \tag{4.17}$$

The assertions (i), (ii) and (iv) can be proved directly by using (4.17), while the third one follows from (ii) and the definition of T in (2.7). □

Corollary 5. *Suppose that the grating profile Λ is given by a C^2 graph and that a radiating solution $u \in V_\alpha(\Omega_b)$ satisfies $\mathcal{B}u = 0$ under the Dirichlet boundary condition. Then $u = 0$ in $V_\alpha(\Omega_b)$.*

The uniqueness result of Corollary 5 was proved in Ref. 26 for the scalar Helmholtz equation and in Refs. 3 and 21 for the two-dimensional Navier system. See also Arens[5] for the uniqueness of scattering of elastic waves by a rough surface in $\mathbb{R}^2$.

Proof of Corollary 5. Combining the Dirichlet boundary condition on Λ, Lemmas 4 and 5(iii), (iv), we find

$$\begin{aligned} &\int_\Lambda \big(\mu |\partial_\nu u|^2 \nu_3 + (\lambda + \mu)|\operatorname{div} u|^3 \nu_3\big) ds \\ &\quad = \int_{\Gamma_b} (2 \operatorname{Re}(Tu \cdot \partial_3 \overline{u}) - \nu_3 a(u, \overline{u}) + \omega^2 |u|^2) ds. \end{aligned} \tag{4.18}$$

Next we prove that the right-hand side of (4.18) vanishes. Let $u \in V_\alpha$ be a radiating solution of the form (2.13) satisfying $\mathcal{B}u = 0$. By Lemma 3, we know that u takes the form

$$\begin{aligned} u = v &+ \sum_{|\alpha_n| > k_p} A_{p,n} (\alpha_n, \beta_n)^\top \exp(i\alpha_n \cdot x' + i\beta_n x_3) \\ &+ \sum_{|\alpha_n| > k_s} \mathbf{A}_{s,n} \exp(i\alpha_n \cdot x' + i\gamma_n x_3), \end{aligned}$$

where

$$v(x) = \sum_{|\alpha_n|=k_p} A_{p,n} \begin{pmatrix} \alpha_n^\top \\ 0 \end{pmatrix} \exp(i\alpha_n \cdot x') + \sum_{|\alpha_n|=k_s} \mathbf{A}_{s,n} \exp(i\alpha_n \cdot x').$$

One can see from the periodic Rellich identity that the right-hand side of (4.18) does not depend on the choice of b. Thus, for any $\epsilon > 0$, there exist $c > 0$ sufficiently large so that

$$\begin{aligned}
&\int_{\Gamma_b} 2\,\mathrm{Re}(Tu \cdot \partial_3 \overline{u}) - \nu_3 a(u, \overline{u}) + \omega^2 |u|^2 ds \\
&\qquad - \int_{\Gamma_b} 2\,\mathrm{Re}(Tv \cdot \partial_3 \overline{v}) - \nu_3 a(v, \overline{v}) + \omega^2 |v|^2 ds \\
&\quad = \int_{\Gamma_c} \{(2\,\mathrm{Re}(Tu \cdot \partial_3 \overline{u}) - \nu_3 a(u, \overline{u}) + \omega^2 |u|^2)\} ds \\
&\qquad - \int_{\Gamma_c} \{(2\,\mathrm{Re}(Tv \cdot \partial_3 \overline{v}) - \nu_3 a(v, \overline{v}) + \omega^2 |v|^2)\} ds \\
&\quad < \epsilon,
\end{aligned}$$

since the integrands on Γ_c only consist of exponentially decaying functions as $c \to +\infty$. This gives rise to the equality

$$\begin{aligned}
&\int_{\Gamma_b} 2\,\mathrm{Re}(Tu \cdot \partial_3 \overline{u}) - \nu_3 a(u, \overline{u}) + \omega^2 |u|^2 ds \\
&\qquad = \int_{\Gamma_b} 2\,\mathrm{Re}(Tv \cdot \partial_3 \overline{v}) - \nu_3 a(v, \overline{v}) + \omega^2 |v|^2 ds.
\end{aligned}$$

Noting that $\partial_3 v = 0$ in $\mathbb{R}^3$, by direct calculations one may readily check that

$$\int_{\Gamma_b} (-a(v, \overline{v}) + \omega^2 |v|^2) ds = 0.$$

Together with (4.18), this gives the identity

$$\int_{\Lambda} (\mu |\partial_\nu u|^2 \nu_3 + (\lambda + \mu) |\mathrm{div}\, u|^2 \nu_3) ds = 0,$$

from which $\partial_\nu u = 0$ on Λ follows. Finally, as a consequence of Holmgren's uniqueness theorem, it holds that $u = 0$ in $V_\alpha(\Omega_b)$ for any $b > \Lambda^+$. □

Relying on the above uniqueness result for C^2 graphs, we adapt Nečas' approach in Ref. 31 of approximating a Lipschitz graph by smooth surfaces to prove Theorem 4. In the following, we sketch the proof of Theorem 4, referring to Elschner and Hu[21] for the details in the case of plane elasticity, which can be carried over to the 3D case.

Proof of Theorem 4. Step 1. Choose C^∞ graphs $\Lambda_j = \Lambda_{f_j} := \{x_3 = f_j(x') : x' \in (0, 2\pi) \times (0, 2\pi)\}$ such that the Lipschitz constants of f_j are uniformly bounded in j, and

$$\Omega_b^j = \Omega_{\Lambda_j, b} \subset \Omega_b, \quad \max\{|f_j(x') - f(x')| : x' \in [0, 2\pi] \times [0, 2\pi]\} \to 0, \quad \text{as } j \to \infty.$$

Consider the inhomogeneous boundary value problem

$$\begin{aligned} (\Delta^* + \omega^2 + i)u^j = iu \quad \text{in } \Omega_b^j, \\ u^j|_{\Lambda_j} = 0, \quad Tu^j - \mathcal{T}(\omega, \alpha)u^j = 0 \quad \text{on } \Gamma_b, \end{aligned} \tag{4.19}$$

and its equivalent variational formulation

$$\int_{\Omega_b^j} [a(u^j, \overline{\varphi}) - (\omega^2 + i)u^j \cdot \overline{\varphi}]dx - \int_{\Gamma_b} \overline{\varphi} \cdot \mathcal{T}(\omega, \alpha)u^j ds = -\int_{\Omega_b} iu \cdot \overline{\varphi} dx \tag{4.20}$$

for $\varphi \in V_\alpha(\Omega_b^j)$. Analogously to Corollary 4, one can prove that there exists a unique solution $u^j \in V_\alpha(\Omega_b^j)$ to the above variational formulation and hence to (4.19). Extending u^j by zero to $\Omega_b \backslash \Omega_b^j$, we have $u^j \to u$ in $V_\alpha(\Omega_b)$ as $j \to \infty$.

Step 2. Rewrite the boundary value problem (4.19) as

$$\begin{aligned} (\Delta^* + \omega^2)u^j = h_j := i(u - u_j) \quad \text{in } \Omega_b^j, \\ u|_{\Lambda_j} = 0, \quad Tu^j - \mathcal{T}(\omega, \alpha)u^j = 0 \quad \text{on } \Gamma_b. \end{aligned} \tag{4.21}$$

The unique solution u^j to the above problem satisfies the identity

$$\int_{\Omega_b^j} \left[a(u^j, \overline{u}_j) - \omega^2 |u^j|^2\right] dx - \int_{\Gamma_b} \overline{u^j} \cdot \mathcal{T}(\omega, \alpha)u^j ds = -\int_{\Omega_b} h^j \cdot \overline{u^j} dx. \tag{4.22}$$

Then, taking imaginary part of (4.22) and using the identity (4.3), we get

$$I_j := 4\pi^2 \left(\sum_{|\alpha_n| < k_p} \omega^2 \beta_n \, |A_{p,n}^j|^2 + \sum_{|\alpha_n| < k_s} \mu \gamma_n \, |\mathbf{A}_{s,n}^j|^2 \right) = \operatorname{Im} \int_{\Omega_b} h^j \cdot \overline{u^j} dx,$$

where $A_{p,n}^j$ and $\mathbf{A}_{s,n}^j$ are the Rayleigh coefficients of u^j of the form (2.13). Noting that $u^j \to u$ in $V_\alpha(\Omega_b)$ from Step 1, we have $I_j \to 0$ and thus $|A_{p,n}^j|$, $|\mathbf{A}_{s,n}^j| \to 0$ as $j \to \infty$.

Step 3. Applying the periodic Rellich identity (Lemma 4) to problem (4.21), we obtain

$$\begin{aligned} 2 \operatorname{Re} \int_{\Omega_b} h^j \cdot \partial_3 \overline{u^j} dx = \int_{\Lambda_j} (\mu \, |\partial_\nu u^j|^2 + (\lambda + \mu) \, |\operatorname{div} u^j|^2) \nu_3 ds \\ + 4\pi^2 \left(\sum_{|\alpha_n| < k_p} \omega^2 \beta_n^2 \, |A_{p,n}^j|^2 + \sum_{|\alpha_n| < k_s} \mu^2 \gamma_n^2 \, |\mathbf{A}_{s,n}^j|^2 \right), \end{aligned}$$

leading to

$$\int_{\Lambda_j} |\partial_\nu u^j|^2 ds \to 0, \quad j \to \infty.$$

This together with the Dirichlet boundary condition $u^j|_{\Lambda_j} = 0, j \in \mathbb{N}$, yields that $Tu^j|_{\Lambda_j} \to 0$ in $L^2(0, 2\pi)^3$. Finally, by passing to the limit in Betti's identity

$$\int_{\Lambda_j} \overline{\varphi} \cdot Tu^j ds = B(u^j, \varphi) + \int_{\Omega_b} h^j \cdot \overline{u^j} dx, \quad \forall \varphi \in H^1_\alpha(\Omega_b)^3,$$

we obtain $B(u, \varphi) = 0$ for all $\varphi \in H^1_\alpha(\Omega_b)^3$ and thus $Tu|_\Lambda = 0$. Applying the unique continuation principle completes the proof. □

Remark 5. Assume Λ has a Lipschitz dissection $\Lambda = \Lambda_D \cup \Sigma \cup \Lambda_I$, where Λ_D and Λ_I are two disjoint and relative open subsets of Λ having Σ as their common boundary (see Ref. 29). Consider the mixed Dirichlet and Robin boundary conditions

$$u = 0 \quad \text{on } \Lambda_D, \quad Tu - i\eta u = 0 \quad \text{on } \Lambda_I, \tag{4.23}$$

with a constant $\eta \in \mathbb{C}$ satisfying $\mathrm{Re}\, \eta > 0$. If $\Lambda_I \neq \emptyset$ and Λ is given by a Lipschitz surface, then, there always exists a unique solution $u \in E_\alpha := \{u \in H^1_\alpha(\Omega_b)^3 : u = 0 \text{ on } \Lambda_D\}$ to (BVP) under the above mixed boundary conditions (4.23). Note that in this case, uniqueness follows easily from the Robin boundary conditions on Λ_I. See Refs. 21 and 3 for the proof in the 2D case.

All the existence and uniqueness results in Sec. 4 remain true, if Λ is given by a polyhedral surface (in Lemma 3, Theorems 2 and 3) or by the graph of a piecewise linear function (in Theorem 4). Note that the Betti formula can always be applied to a polyhedral domain which is not necessarily a Lipschitz domain in $\mathbb{R}^3$. To prove Theorem 4 for polyhedral gratings, one may directly obtain the uniqueness from Corollary 5, since in this case each solution belongs to $H^{3/2+\epsilon}(\Omega_b)$ for any $\epsilon > 0$ so that Lemmas 4 and 5 are still valid. Moreover, Theorem 4 can be extended to a polyhedral profile on which the third component of the normal vanishes on a subset and has a positive lower bound on the other parts. Such a polyhedral surface may not be a graph, e.g. the cubic grating where the profile consists of a finite number of horizontal and vertical planes only.

4.4. *Non-uniqueness examples under the second, third and fourth kind boundary conditions*

Assume that Λ is a flat grating given by $\Gamma_0 := \{(x_1, x_2, 0) : 0 < x_1, x_2 < 2\pi\}$. We shall present non-uniqueness examples for this flat grating Λ under the second, third and fourth kind boundary conditions. To do this, we construct nontrivial solutions to the homogeneous problem (BVP) (for $u^{\rm in} = 0$), provided that Rayleigh frequencies occur in the expansion (2.13).

Suppose that u is a radiating solution of the form (2.13) in $x_3 > 0$, and that the Neumann boundary condition is imposed on $\{x_3 = 0\}$. Since the unit normal ν on Λ coincides with e_3, the boundary condition $Tu = 0$ on Λ can be written as

$$e_3 \cdot Tu = 2\mu\partial_3 u_3 + \lambda \operatorname{div} u = \lambda(\partial_1 u_1 + \partial_2 u_2) + (\lambda + 2\mu)\partial_3 u_3 = 0,$$

$$e_3 \times Tu = 2\mu e_3 \times \partial_3 u + \mu e_3 \times (e_3 \times \operatorname{curl} u) = \mu(-\partial_3 u_2 - \partial_2 u_3, \partial_3 u_1 + \partial_1 u_3, 0) = 0.$$

Applying the above two identities to the radiating solution u of the form (2.13) and using the orthogonality relation (2.14), we obtain

$$0 = i \begin{pmatrix} \lambda k_p^2 + 2\mu\beta_n^2 & 0 & 0 & 2\mu\gamma_n \\ 2\alpha_n^{(2)}\beta_n & 0 & \gamma_n & \alpha_n^{(2)} \\ 2\alpha_n^{(1)}\beta_n & \gamma_n & 0 & \alpha_n^{(1)} \\ 0 & \alpha_n^{(1)} & \alpha_n^{(2)} & \gamma_n \end{pmatrix} \begin{pmatrix} A_{p,n} \\ \mathbf{A}_{s,n}^\top \end{pmatrix} := iE_n A_n. \tag{4.24}$$

It is not difficulty to check that

$$\det(E_n) = \gamma_n[(\lambda k_p^2 + 2\mu\beta_n^2)(|\alpha_n|^2 - \gamma_n^2) - 4\mu\beta_n\gamma_n|\alpha_n|^2]. \tag{4.25}$$

Thus $\det(E_n) = 0$ if $\gamma_n = 0$, or $\beta_n = 0$ and $\gamma_n^2 = k_p^2$. If $\gamma_n = 0$, it follows from (4.24) that

$$A_{p,n} = 0, \quad A_{s,n}^{(3)} = 0, \quad \alpha_n^{(1)} A_{s,n}^{(1)} + \alpha_n^{(2)} A_{s,n}^{(2)} = 0,$$

leading to

$$u = \sum_{\gamma_n = 0} C_n(-\alpha_n^{(2)}, \alpha_n^{(1)}, 0)^\top \exp(i\alpha_n \cdot x'), \tag{4.26}$$

where $C_n \in \mathbb{C}$ are arbitrary constants. If $\beta_n = 0$ and $\gamma_n^2 = k_p^2$ for some $n \in \mathbb{Z}^2$, we deduce from (4.24) that

$$A_{s,n}^{(3)} = \frac{\lambda k_p^2}{2\mu\gamma_n} A_{p,n}, \quad A_{s,n}^{(1)} = -\frac{\lambda}{2\mu}\alpha_n^{(1)} A_{p,n}, \quad A_{s,n}^{(2)} = -\frac{\lambda}{2\mu}\alpha_n^{(2)} A_{p,n}.$$

In this case, we have

$$u = \sum_{\beta_n = 0, \gamma_n^2 = k_p^2} A_{p,n} \left\{ \begin{pmatrix} \alpha_n^\top \\ 0 \end{pmatrix} + \frac{\lambda}{2\mu} \begin{pmatrix} -\alpha_n^\top \\ -k_p^2/\gamma_n \end{pmatrix} \exp(i\gamma_n x_3) \right\} \exp(i\alpha_n \cdot x'), \tag{4.27}$$

with $A_{p,n} \in \mathbb{C}$. Thus the non-uniqueness examples for the second boundary value problem can be constructed from (4.26) and (4.27).

We next consider the third (respectively fourth) kind boundary conditions, which take the form

$$u_3 = \partial_3 u_1 = \partial_3 u_2 = 0 \quad \text{respectively } \partial_3 u_3 = u_1 = u_2 = 0 \quad \text{on } \{x_3 = 0\}.$$

Inserting the Rayleigh expansion (2.13) into the above boundary conditions and using the fact that $\{\exp(i\alpha_n \cdot x') : n \in \mathbb{Z}^2\}$ is an orthogonal basis of $L^2((0, 2\pi) \times (0, 2\pi))^3$, one can prove that

Proposition 6. (1) *Under the third kind boundary conditions, $\nu \times Tu = \nu \cdot u = 0$, on $\{x_3 = 0\}$, the nontrivial solution to the homogeneous problem (BVP) takes the form*

$$u = \sum_{\beta_n=0} A_{p,n}(\alpha_n^{(1)}, \alpha_n^{(2)}, 0)^\top \exp(i\alpha_n \cdot x') \quad \text{with } A_{p,n} \in \mathbb{C}, \ \text{ in } x_3 > 0,$$

provided that a Rayleigh frequency of the compressional part occurs, i.e. the set $\{n \in \mathbb{Z}^2 : \beta_n = 0\} \neq \emptyset$.

(2) *Under the fourth kind of boundary conditions, $\nu \cdot Tu = \nu \times u = 0$, on $\{x_3 = 0\}$, the nontrivial solution to the homogeneous problem (BVP) takes the form*

$$u = e_3 \sum_{\gamma_n=0} A_{s,n}^{(3)} \exp(i\alpha_n \cdot x') \quad \text{with } A_{s,n}^{(3)} \in \mathbb{C}, \ \text{in } x_3 > 0,$$

provided that a Rayleigh frequency of the shear part occurs, i.e. the set $\{n \in \mathbb{Z}^2 : \gamma_n = 0\} \neq \emptyset$.

We omit the proofs of these results for the sake of brevity. Note that the solutions to the problem (BVP) for a flat grating under the boundary conditions of the third (respectively fourth) kind must be unique if Rayleigh frequencies of the compressional (respectively shear) part are excluded.

5. Solvability Results for Multilayered Diffraction Gratings

The aim of this section is to provide a solvability theory of multilayered diffraction problems for several elastic materials, extending the results for impenetrable gratings to transmission gratings. Suppose the whole space $\mathbb{R}^3$ is divided by several disjoint interfaces Λ_j $(j = 1, 2, \ldots, N)$ into $N + 1$ sections Ω_j $(j = 0, 1, \ldots, N)$ which are filled with different homogeneous elastic materials. For simplicity we assume throughout this section that $N = 2$ and Λ_j are Lipschitz surfaces which are periodic with respect to x_1 and x_2; see Fig. 2. We assume further that a time-harmonic plane elastic wave U^{in} with the incident angles $\theta_1 \in [0, \pi/2), \theta_2 \in [0, 2\pi)$ is incident on the grating from the upper half-space Ω_0, and that both the displacement and stress are continuous across each interface Λ_j.

We introduce the following notations for several elastic materials. Let μ_j, λ_j denote the Lamé coefficients in Ω_j satisfying $\mu_j > 0, \lambda_j + 2\mu_j/3 > 0$; $\rho_j > 0$ denotes the mass densities in Ω_j, which are positive constants; let $k_{p,j} := \omega\sqrt{\rho_j/(2\mu_j + \lambda_j)}, k_{s,j} := \omega\sqrt{\rho_j/\mu_j}$ denote the corresponding compressional and shear wave numbers in Ω_j; T_j stands for the stress operators defined as in (2.7),

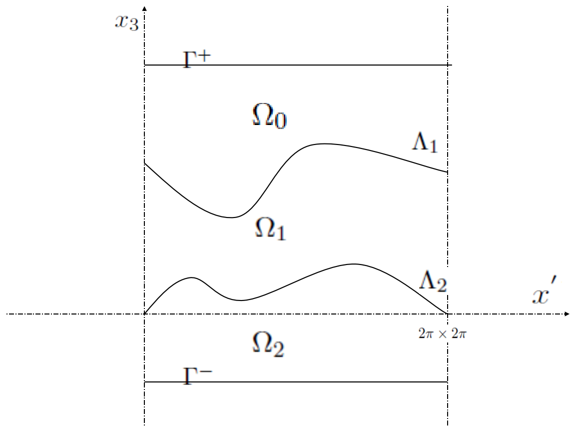

Fig. 2. A multilayered diffraction grating.

with μ, λ replaced by μ_j, λ_j; and $\beta_{n,j}, \gamma_{n,j}$ $(j = 0, 2)$ are the parameters defined as in (2.11) with k_p, k_s replaced by $k_{p,j}, k_{s,j}$. Throughout this section, we assume U^{in} is either an incident pressure wave of the form (2.15) with k_p replaced by $k_{p,0}$, or an incident shear wave of the form (2.16) with k_s replaced by $k_{s,0}$.

Then we are looking for the total displacement field u,

$$u = U^{\mathrm{in}} + U_0 \quad \text{in } \Omega_0, \quad u = U_j \quad \text{in } \Omega_j, \quad j = 1, 2 \tag{5.1}$$

satisfying the Navier equations

$$(\Delta^* + \omega^2 \rho_j) U_j = 0 \quad \text{in } \Omega_j, \quad j = 0, 1, 2, \tag{5.2}$$

with the α-quasi-periodicity condition

$$u(x' + 2n\pi, x_3) = \exp(i 2\pi \alpha \cdot n) u(x_1, x_2, x_3), \quad \forall n \in \mathbb{Z}^2. \tag{5.3}$$

Here $\alpha := k(\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2)$ with $k = k_{p,0}$ for the incident pressure wave, or $k = k_s$ for the incident shear wave. On the interfaces the continuity of the displacement and the stress lead to the transmission conditions

$$U^{\mathrm{in}} + U_0 = U_1, \quad T_0(U^{\mathrm{in}} + U_0) = T_1(U_1) \quad \text{on } \Lambda_1, \tag{5.4}$$

$$U_1 = U_2, \quad T_1(U_1) = T_2(U_2) \quad \text{on } \Lambda_2. \tag{5.5}$$

Finally, we impose the following radiation conditions on the scattered fields U_j $(j = 0, 2)$ (cf. (2.13)):

$$\begin{aligned} U_0(x) = \sum_{n \in \mathbb{Z}^2} \big\{ & A_{p,n}^{+} (\alpha_n, \beta_{n,0})^\top \exp(i\alpha_n \cdot x' + i\beta_{n,0} x_3) \\ & + \mathbf{A}_{s,n}^{+} \exp(i\alpha_n \cdot x' + i\gamma_{n,0} x_3) \big\} \end{aligned} \tag{5.6}$$

for $x_3 > \Lambda_1^+ := \max_{x\in\Lambda_1} x_3$, and

$$U_2(x) = \sum_{n\in\mathbb{Z}^2} \big\{A_{p,n}^-(\alpha_n, -\beta_{n,2})^\top \exp(i\alpha_n\cdot x' - i\beta_{n,2}x_3) + \mathbf{A}_{s,n}^- \exp(i\alpha_n\cdot x' - i\gamma_{n,2}x_3)\big\} \tag{5.7}$$

for $x_3 < \Lambda_2^- := \min_{x\in\Lambda_2} x_3$, where $\mathbf{A}_{s,n}^\pm \in \mathbb{C}^3$ fulfill the orthogonality relations

$$\mathbf{A}_{s,n}^+\cdot(\alpha_n, \gamma_{n,0}) = 0, \quad \mathbf{A}_{s,n}^-\cdot(\alpha_n, -\gamma_{n,2}) = 0 \quad \text{for all } n = (n_1, n_2)\in\mathbb{Z}^2.$$

The diffraction problem for transmission gratings can now be formulated as the following boundary value problem.

Transmission problem (TP). Given two surfaces $\Lambda_1, \Lambda_2 \subset \mathbb{R}^3$ (which are 2π-periodic in x_1 and x_2) and an incident plane pressure or shear wave $U^{\rm in}$, find a vector function $u \in H^1_{\rm loc}(\mathbb{R}^3)^3$ that satisfies (5.1)–(5.7).

Following the approach of Sec. 3, we reduce the problem (TP) to a variational problem in a bounded periodic cell in $\mathbb{R}^3$, enforcing the transmission and radiation conditions. In this case, we introduce the artificial boundaries

$$\Gamma^\pm := \{(x', b^\pm) : 0\le x_1, x_2 \le 2\pi\}, \quad \text{for some } b^+ > \Lambda_1^+, b^- < \Lambda_2^-,$$

so that we have the bounded domain

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

The DtN maps $\mathcal{T}^\pm$ on the artificial boundaries $\Gamma^\pm$ have the Fourier series representations (cf. Lemma 1)

$$\begin{aligned} \mathcal{T}^\pm u^\pm &:= \sum_{n\in\mathbb{Z}^2} iW_n^\pm \hat{u}_n^\pm \exp(i\alpha\cdot x'),\\ u^\pm &= \sum_{n\in\mathbb{Z}^2} \hat{u}_n^\pm \exp(i\alpha\cdot x') \in H_\alpha^{1/2}(\Gamma^\pm)^3, \end{aligned} \tag{5.8}$$

where the matrices $W_n^\pm = W_n^\pm(\omega,\alpha)$ are defined as in (3.7) with ω, μ, λ replaced by $\omega\rho_j, \mu_j, \lambda_j$ ($j = 0$ for W_n^+ and $j = 2$ for W_n^-) respectively. Applying the first Betti formula on each sub-domain $\Omega_j \cap \Omega_b$ ($j = 0, 1, 2$) to a solution of (TP), and using the transmission conditions (5.4) and (5.5) at the interfaces and the DtN operators (5.8), we obtain the following variational formulation of (TP) on the bounded domain Ω: Find $u \in H_\alpha^1(\Omega)^3$ such that

$$\begin{aligned} B(u,\varphi) &:= \int_\Omega (a(u,\overline{\varphi}) - \omega^2\rho u\cdot\overline{\varphi})dx - \int_{\Gamma^+} \overline{\varphi}\cdot\mathcal{T}^+ u ds - \int_{\Gamma^-}\overline{\varphi}\cdot\mathcal{T}^- u ds\\ &= \int_{\Gamma^+} f_0\cdot\overline{\varphi} ds, \quad \forall\,\varphi\in H_\alpha^1(\Omega)^3. \end{aligned} \tag{5.9}$$

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

$$\sum_{j=0}^{2} \int_{\Omega_j \cap \Omega_b} (a_j(u, \overline{\varphi}) - \omega^2 \rho_j u \cdot \overline{\varphi}) dx,$$

where the bilinear forms a_j are defined as in (3.2), with μ, λ replaced by μ_j, λ_j. The right-hand side $f_0 := T(U^{\text{in}}) - \mathcal{T}(U^{\text{in}})$ takes the same form as in (4.13) or (4.14), with $k_p, k_s, \beta_n, \gamma_n$ replaced by $k_{p,j}, k_{s,j}, \beta_{n,j}, \gamma_{n,j}$. As in (3.26), the sesquilinear form B defined in (5.9) generates a continuous linear operator $\mathcal{B}$ from $H^1_\alpha(\Omega)^3$ into its dual $(H^1_\alpha(\Omega)^3)'$, with respect to the pairing $(u, \varphi)_\Omega = \int_\Omega u \cdot \bar{\varphi} dx$, via

$$B(u, \varphi) = (\mathcal{B}u, \varphi)_\Omega, \quad \forall\, u,\ \varphi \in H^1_\alpha(\Omega)^3. \tag{5.10}$$

The following lemma extends Lemma 3 to the transmission case.

Lemma 6. *Let $\mathcal{B}$ be the operator defined in* (5.10). *If a radiating solution $u \in H^1_\alpha(\Omega)^2$ satisfies $\mathcal{B}u = 0$, then*

$$A^+_{p,n} = 0 \quad \text{for } |\alpha_n| < k_{p,0} \quad \text{and} \quad \mathbf{A}^+_{s,n} = 0 \quad \text{for } |\alpha_n| < k_{s,0},$$

$$A^-_{p,n} = 0 \quad \text{for } |\alpha_n| < k_{p,2} \quad \text{and} \quad \mathbf{A}^-_{s,n} = 0 \quad \text{for } |\alpha_n| < k_{s,2}.$$

The following results extend Theorems 1 and 2 to the transmission problem. For the proofs of Theorems 7 and 8, we refer to Ref. 21 in the case of plane elasticity which can be carried over to three dimensions.

Theorem 7. (i) *The sesquilinear form B defined by* (5.9) *is strongly elliptic over $H^1_\alpha(\Omega)^3$, and the operator $\mathcal{B}$ defined in* (5.10) *is Fredholm with index zero.*

(ii) *For an incident plane wave U^{in} of the form* (2.15) *or* (2.16), *there always exists a solution to the variational problem* (5.9) *and hence to problem* (TP).

Theorem 8. *Let U^{in} be an incident pressure wave of the form* (2.15), *where $\alpha := k_{p,0}(\sin\theta_1 \cos\theta_2,\ \sin\theta_1 \sin\theta_2)$.*

(i) *There exists $\omega_0 > 0$ such that the variational problem* (5.9) *admits a unique solution $u \in H^1_\alpha(\Omega)^3$ for all incident angles and for all frequencies $\omega \in (0, \omega_0]$.*
(ii) *For all but a sequence of countable frequencies $\omega_j, \omega_j \to \infty$, the variational problem* (5.9) (*with fixed incident angles θ_1 and θ_2*) *admits a unique solution $u \in H^1_\alpha(\Omega)^3$.*

Remark 6. In the case of an incident shear wave U^{in} of the form (2.16) with $\alpha := k_{s,0}(\sin\theta_1 \cos\theta_2,\ \sin\theta_1 \sin\theta_2)$, Theorem 8 holds under one of the following additional assumptions

(a) $k_{s,0} \sin\theta_1 < k_{p,0}$, or equivalently, $\frac{\sin^2\theta_1}{\mu_0} < \frac{1}{\lambda_0 + 2\mu_0}$;
(b) $k_{s,0} \sin\theta_1 < k_{p,2}$, or equivalently, $\frac{\sin^2\theta_1 \rho_0}{\mu_0} < \frac{\rho_2}{\lambda_2 + 2\mu_2}$.

Note that by Lemma 6, the $(0,0)$th Fourier coefficient of $\exp(-i\alpha\cdot x')U_0(x)|_{\Gamma^+}$ vanishes if (a) holds, while that of $\exp(-i\alpha\cdot x')U_2(x)|_{\Gamma^-}$ vanishes if (b) holds. Thus an analogous estimate to (4.16) on Γ^+ or Γ^- can be derived; see the proof of Theorem 3(i) and Remark 4.

The uniqueness of (TP) does not hold for all frequencies, even in the special case of one interface $\Lambda_1 := \{x_3 = 0\}$ dividing $\mathbb{R}^3$ into two half-spaces $\Omega_0 := \{x_3 > 0\}$ and $\Omega_1 := \{x_3 < 0\}$ with certain elastic parameters λ_j, μ_j, ρ_j $(j = 0, 1)$. If all elastic waves are assumed to be propagating perpendicular to the x_3-axis, this problem can be reduced to a problem of plane elasticity over the (x_1, x_2)-plane with the continuity of the displacement and stress on the line $\{x_2 = 0\}$ in $\mathbb{R}^2$. It was shown in Ref. 2 that there may exist nontrivial solutions (Rayleigh surface waves) of the two-dimensional homogeneous problem that decay exponentially as $x_2 \to \pm\infty$. Hence additional conditions must be imposed on the elastic parameters or grating profiles to guarantee uniqueness for (TP). In this direction, we refer to Refs. 10 and 13 for non-trapping conditions on the refractive index in the case of the Helmholtz equation.

Remark 7. We think that our H^1_α-solvability result of Theorem 8 can be extended to periodic interpenetrating (intersecting) interfaces, at least in the case of polyhedral grating profiles. We refer e.g. to Ref. 33 for general elliptic transmission problems on bounded domains.

Acknowledgment

The second author gratefully acknowledges the support by the German Research Foundation (DFG) under Grant No. EL 584/1-2.

References

1. I. Abubakar, Scattering of plane elastic waves at rough surface I, *Proc. Cambridge Philos. Soc.* **58** (1962) 136–157.
2. J. D. Achenbach, Wave propagation in elastic solids, in: North-Holland Series in Applied Mathematics and Mechanics, Vol. 16, eds. H. A. Lauwerier and W. T. Koiter (North-Holland, 1973), pp. 165–201.
3. T. Arens, The scattering of plane elastic waves by a one-dimensional periodic surface, *Math. Methods Appl. Sci.* **22** (1999) 55–72.
4. T. Arens, A new integral equation formulation for the scattering of plane elastic waves by diffraction gratings, *J. Integral Equations Appl.* **11** (1999) 275–297.
5. T. Arens, Uniqueness for elastic wave scattering by rough surfaces, *SIAM J. Math. Anal.* **33** (2001) 461–471.
6. T. Arens, Existence of solution in elastic wave scattering by unbounded rough surfaces, *Math. Methods Appl. Sci.* **25** (2002) 507–528.
7. G. Bao, Finite element approximation of time harmonic waves in periodic structures, *SIAM J. Numer. Anal.* **32** (1995) 1155–1169.
8. G. Bao, Z. Chen and H. Wu, Adaptive finite-element method for diffraction gratings, *J. Opt. Soc. Amer. A* **22** (2005) 1106–1114.

9. G. Bao, L. Cowsar and W. Masters (eds.), *Mathematical Modeling in Optical Science* (SIAM, 2001).
10. A. S. Bonnet-Bendhia and F. Starling, Guided waves by electromagnetic gratings and non-uniqueness examples for the diffraction problem, *Math. Methods Appl. Sci.* **17** (1994) 305–338.
11. S. N. Chandler-Wilde and J. Elschner, Variational approach in weighted Sobolev spaces to scattering by unbounded rough surfaces, *SIAM J. Math. Anal.* **42** (2010) 2554–2580.
12. S. N. Chandler-Wilde and P. Monk, Existence, uniqueness and variational methods for scattering by unbounded rough surfaces, *SIAM J. Math. Anal.* **37** (2005) 598–618.
13. S. N. Chandler-Wilde, P. Monk and M. Thomas, The mathematics of scattering by unbounded, rough, inhomogeneous layers, *J. Comp. Appl. Math.* **204** (2007) 549–559.
14. D. Colton and R. Kress, *Inverse Acoustic and Electromagnetic Scattering*, 2nd edn. (Springer, 1998).
15. P. Cummings and X. Feng, Sharp regularity coefficient estimates for complex-valued acoustic and elastic Helmholtz equations, *Math. Models Methods Appl. Sci.* **16** (2006) 139–160.
16. D. C. Dobson, A variational method for electromagnetic diffraction in biperiodic structures, *Model. Math. Anal. Numer.* **28** (1994) 419–439.
17. D. Dobson and A. Friedman, The time-harmonic Maxwell equations in a doubly periodic structure, *J. Math. Anal. Appl.* **166** (1992) 507–528.
18. G. Duvaut and J. L. Lions, *Inequalities in Mechanics and Physics* (Springer, 1976).
19. J. Elschner and G. Schmidt, Diffraction in periodic structures and optimal design of binary gratings I. Direct problems and gradient formulas, *Math. Methods Appl. Sci.* **21** (1998) 1297–1342.
20. J. Elschner, R. Hinder, F. Penzel and G. Schmidt, Existence, uniqueness and regularity for solutions of the conical diffraction problem, *Math. Models Methods Appl. Sci.* **10** (2000) 317–341.
21. J. Elschner and G. Hu, Variational approach to scattering of plane elastic waves by diffraction gratings, *Math. Methods Appl. Sci.* **33** (2010) 1924–1941.
22. J. Elschner and M. Yamamoto, An inverse problem in periodic diffractive optics: Reconstruction of Lipschitz grating profiles, *Appl. Anal.* **81** (2002) 1307–1328.
23. J. T. Fokkema, Reflection and transmission of elastic waves by the spatially periodic interface between two solids (theory of the integral-equation method), *Wave Motion* **2** (1980) 375–393.
24. J. T. Fokkema and P. M. van den Berg, Elastodynamic diffraction by a periodic rough surface (stress-free boundary), *J. Acoust. Soc. Am.* **62** (1977) 1095–1101.
25. G. C. Hsiao and W. L. Wendland, *Boundary Integral Equations* (Springer, 2008).
26. A. Kirsch, Diffraction by periodic structures, in *Proc. Lapland Conf. Inverse Problems*, eds. Päivärinta *et al.* (Springer, 1993), pp. 87–102.
27. V. D. Kupradze *et al.*, *Three-Dimensional Problems of the Mathematical Theory of Elasticity and Thermoelasticity* (North-Holland, 1979).
28. J. W. S. Lord Rayleigh, On the dynamical theory of gratings, *Proc. Roy. Soc. Lond. A* **79** (1907) 399–416.
29. W. McLean, *Strongly Elliptic Systems and Boundary Integral Equations* (Cambridge Univ. Press, 2000).
30. A. Meier, T. Arens, S. N. Chandler-Wilde and A. Kirsch, A Nyström method for a class of integral equations on the real line with applications to scattering by diffraction gratings and rough surfaces, *J. Integral Equations Appl.* **12** (2000) 281–321.
31. J. Nečas, *Les Méthodes Directes en Théorie des Équations Elliptiques* (Masson, 1967).

32. J. C. Nedelec and F. Starling, Integral equation methods in a quasi-periodic diffraction problem for the time-harmonic Maxwell's equations, *SIAM J. Math. Anal.* **22** (1991) 1679–1701.
33. S. Nicaise and A. M. Sändig, General interface problems I, *Math. Methods Appl. Sci.* **17** (1994) 395–429.
34. A. Rathsfeld, G. Schmidt and B. H. Kleemann, On a fast integral equation method for diffraction gratings, *Commun. Comput. Phys.* **1** (2006) 984–1009.
35. G. Schmidt, On the diffraction by biperiodic anisotropic structures, *Appl. Anal.* **82** (2003) 75–92.
36. J. W. C. Sherwood, Elastic wave propagation in a semi-infinite solid medium, *Proc. Phys. Soc.* **71** (1958) 207–219.