J. Inverse Ill-Posed Probl., Ahead of Print
DOI 10.1515/JIIP.2011.048

Uniqueness in inverse scattering of elastic waves by three-dimensional polyhedral diffraction gratings

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Abstract. We consider the inverse elastic scattering problem of determining a three-dimensional diffraction grating profile from scattered waves measured above the structure. In general, a grating profile cannot be uniquely determined by a single incoming plane wave. We completely characterize and classify the bi-periodic polyhedral structures under the boundary conditions of the third and fourth kinds that cannot be uniquely recovered by only one incident plane wave. Thus we have global uniqueness for a polyhedral grating profile by one incident elastic plane wave if and only if the profile belongs to neither of the unidentifiable classes, which can be explicitly described depending on the incident field and the type of boundary conditions. Our approach is based on the reflection principle for the Navier equation and the reflectional and rotational invariance of the total field.

Keywords. Inverse scattering, uniqueness, three-dimensional diffraction grating, Navier equation, boundary conditions of the third (fourth) kind.

2010 Mathematics Subject Classification. 78A36, 35B27, 35R30, 74B05.

1 Introduction

The problem of recovering a periodic structure from knowledge of the scattered field occurs in many applications, e.g., in diffractive optics and non-destructive testing. We refer to the monograph [7] for the details of these applications. This paper is concerned with uniqueness in inverse scattering of elastic waves by an unbounded bi-periodic structure. The relevant phenomena have a wide field of application. For instance, in geophysics and seismology it is very fundamental to utilize elastic waves to investigate earthquakes and to search for oil and ore bodies (see, e.g., [1], [21], [22], [29] and the references therein).

Assume a time-harmonic incident plane wave is scattered by a three-dimensional diffraction grating in a linear isotropic and homogeneous elastic medium. The diffraction grating is supposed to have an impenetrable bi-periodic surface on which normal displacement and tangential stress (resp. normal stress and tangen-

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

tial displacement) vanish. This gives rise to the so-called third (resp. fourth) kind boundary conditions for the Navier equation. We refer to the monograph [25] for a comprehensive treatment of the boundary value problems of elasticity, including the boundary conditions of the third and fourth kinds. Our goal in this paper is to study the uniqueness of reconstructing a bi-periodic grating profile from near-field data taken on a plane above the grating. The uniqueness issue is always important for finding efficient reconstruction algorithms in practical applications.

There exist several uniqueness results for smooth periodic structures. We refer to [3,6,10,24] for the inverse scattering of acoustic or electromagnetic waves, and to [4] for elastic waves. With a lossy medium above the grating, global uniqueness by one incident plane wave can be easily proved using integration by parts; see [3,6] for the Helmholtz or Maxwell equations. In two dimensions, if some *a priori* information about the height of the grating curve is known, the uniqueness by a finite number of incident plane waves is proved under the Dirichlet boundary condition; see [23] for acoustic waves and [4] for elastic waves, where Schiffer's theorem is established and the spectral properties of the Laplace and Lamé operators in an infinite periodic layer are studied. For bi-periodic structures in $\mathbb{R}^3$, a local uniqueness theorem is proved in [10] by deriving a lower bound of the first Dirichlet eigenvalue of the Maxwell equations in a smooth convex domain. In general, a grating profile can always be uniquely identified by infinitely many quasi-periodic incident plane waves with a fixed phase-shift ([3,24]).

It is known that global uniqueness is impossible with a single incoming plane wave (see e.g. [13, Section 2]). However, if the grating profiles are piecewise linear, one can make use of the reflection principles for the Helmholtz and Maxwell equations to establish global uniqueness with a finite number of incident plane waves; see, e.g., [8, 9, 13, 18, 19] for the inverse scattering of electromagnetic waves, including TE or TM polarization in 2D. Note that the gaps in [18,19] are indicated and fixed in [13]. Relying on the reflection principle for the Navier system developed in [20], we established in [15] the global uniqueness by a minimal number of incident elastic waves within the two-dimensional grating profiles which are given by the graph of a piecewise linear function. Moreover, in [15] all the polygonal grating profiles that cannot be uniquely identified by a single incident plane wave are classified. The purpose of this paper is to find out and characterize all the unidentifiable bi-periodic polyhedral gratings corresponding to one incident pressure or shear wave in $\mathbb{R}^3$. Then, as a consequence, the gratings that do not belong to any of the unidentifiable classes can always be uniquely recovered from the near-field data corresponding to only one incident wave. It remains a challenging open problem to extend our results to the first kind (Dirichlet) or second kind (Neumann) boundary conditions, since there seems to be no reflection principle in these cases.

In this paper we extend our uniqueness result in 2D ([15]) to bi-periodic polyhedral diffractive structures in $\mathbb{R}^3$. Note that our diffraction problem can be reduced to a problem of plane elasticity under the additional assumptions that the three-dimensional grating varies only in x_1 and remain invariant in x_3 and that all elastic waves are propagating perpendicular to the x_3-axis. Thus, it is quite natural to view the unidentifiable grating curves in the (x_1, x_2)-plane as non-uniqueness examples for the inverse scattering by bi-periodic structures in $\mathbb{R}^3$. Nevertheless, we still need to consider the three-dimensional gratings which vary in two directions and the case where the incident wave is not perpendicular to the x_3-axis. Note that the direct diffraction problem has already been investigated in [16]. Using the variational method, we proved the existence of quasi-periodic solutions in Sobolev spaces for an incoming elastic plane wave, while the uniqueness does not hold in general.

Some of our ideas are inspired by recent papers [8, 9] of Bao, Zhang and Zou, where the bi-periodic polyhedral structures that cannot be identified by one incident plane electromagnetic wave are classified and characterized using the dihedral group theory. It is shown in [8] that there exist three classes of unidentifiable polyhedral gratings corresponding to one incident field if Rayleigh frequencies are excluded, and six classes in the resonance case (see [9]), including the flat gratings. It should be remarked that the reflection principle for the Navier equation under the fourth kind boundary conditions takes the same form as that used in [26] for the Maxwell equations. However, the elasticity problem is more complicated because of the coexistence of two different waves, the pressure and shear waves, propagating with different phase velocities and coupled together via the stress operator in the boundary conditions. Moreover, the methods used and the results obtained in paper differ from those in[8, 9] in the following aspects. (1) Our uniqueness results are not restricted to polyhedral grating profiles that are given by the graph of a piecewise linear function. Note that the non-graph grating profiles have many practical applications in diffractive optics and optimal design of complicated grating structures. As one example, we mention the binary grating profiles which are composed of only a finite number of horizontal and vertical planar faces (see [11, 17]). (2) Instead of using the dihedral group theory (first applied to inverse scattering problems in [8, 9]), we derive the unidentifiable classes from the reflectional and rotational invariance of the total field, which is a direct consequence of the reflection principle for the Navier equation. This simplifies our proofs significantly and can be extended to Maxwell equations. (3) Having noticed that the unidentifiable classes defined in [8, 9] may be empty, we enforce explicit conditions on the incident angles and the wave numbers in the definition of the unidentifiable sets to guarantee their existence in the case the elastic scattering. These conditions are derived from the quasi-periodicity of the total field. Each unidentifiable class does exist and is not empty as long as these conditions are fulfilled. Moreover, non-uniqueness examples for bi-periodic structures that vary in both the x_1 and x_2 directions are also presented.

In this paper, we only study uniqueness in the inverse scattering of shear (resp. pressure) waves under the third (resp. fourth) kind boundary conditions. The global uniqueness for general incident plane elastic waves can be established analogously and is omitted here for simplicity. In the case of a plane shear wave incidence, it turns out that there are five classes of unidentifiable grating profiles in the resonance case (see Theorem 2.1), and two classes if Rayleigh frequencies are excluded (see Remark 4.22 (i)), whereas an incident plane pressure wave leads to only one unidentifiable class which only exists in the resonance case. Moreover, it is proved that two incident pressure waves (which is the minimal number) are always enough to uniquely determine a bi-periodic polyhedral surface under the fourth kind boundary conditions; see Remark 5.4.

The outline of the paper is as follows. In Section 2, we rigorously formulate the direct and inverse scattering problems, and present our main results on the inverse problems. A radiation condition based on Rayleigh expansion is used, and an admissible class of bi-periodic grating profiles is defined. In Section 3, the reflection principle for the Navier equation together with the reduction of the total field to a finite number of propagating modes is presented. The aim of Section 4 is to characterize all grating profiles that are unidentifiable by a single incident shear wave under the boundary conditions of the third kind. The non-uniqueness examples for this case are presented in Section 4.5. In the final Section 5, we extend the arguments from Section 4 to the case of inverse scattering of an incident pressure wave under the fourth kind boundary conditions.

We finish this section by introducing some notation that will be used throughout the paper. Denote by $S^2 := \{x \in \mathbb{R}^3 : |x| = 1\}$ the unit sphere in $\mathbb{R}^3$, by $\mathbf{a}^\top$ the transpose of a vector $\mathbf{a} = (a_1, a_2, a_3) \in \mathbb{C}^3$ and by $\mathbf{a}^\perp$ a column vector satisfying $\mathbf{a} \cdot \mathbf{a}^\top = 0$. As usual, $\mathbf{a} \cdot \mathbf{b} := \sum_{j=1}^{3} a_j b_j$ and $\mathbf{a} \times \mathbf{b}$ denotes the vector product of $\mathbf{a} = (a_1, a_2, a_3), \mathbf{b} = (b_1, b_2, b_3) \in \mathbb{C}^3$. The symbol $A^\#$ stands for the number of elements in a set A, while $|A_1 A_2|$ represents the length of a line segment $A_1 A_2$ with end points $A_1, A_2 \in \mathbb{R}^3$. For $C \in \mathbb{C}$, $|C|$ denotes its modulus; if $C \in \mathbb{R}^N$ or $C \in \mathbb{C}^N$ $(N = 2, 3)$, $|C|$ denotes its Euclidean norm. Finally, let $x = (x', x_3)$ with $x' = (x_1, x_2) \in \mathbb{R}^2$.

2 Mathematical formulations and main results

We assume that the diffraction grating involves an impenetrable surface Λ which is 2π-periodic with respect to x_1 and x_2. Let Ω_Λ, the unbounded domain above Λ, be 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 $u^{\rm in}$ (with time variation of the form $\exp(-i\omega t)$, $\omega > 0$) is incident on the grating from above, which is either an incident pressure wave taking the form

$$\begin{aligned} &u^{\rm in} = u_p^{\rm in}(x) = \hat\theta \exp(ik_p\hat\theta\cdot x)\\ &\text{with } \hat\theta = (\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2, -\cos\theta_1) \in S^2, \end{aligned} \tag{2.1}$$

or an incident shear wave of the form

$$u^{\rm in} = u_s^{\rm in}(x) = \hat\theta^\perp \exp(ik_s\hat\theta\cdot x) \quad \text{with} \quad \hat\theta^\perp \in S^2, ; \hat\theta^\perp\cdot\hat\theta = 0, \tag{2.2}$$

where

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

are the compressional and shear wave numbers respectively, and $\hat\theta \in S^2$ denotes the incident direction with the incident angles $\theta_1 \in [0, \pi/2), \theta_2 \in [0, 2\pi)$.

For simplicity we assume the mass density of the elastic medium is equal to one, so that the total displacement $u(x)$, which can be decomposed as the sum of the incident field $u^{\rm in}$ and the scattered field $u^{\rm sc}$, satisfies the Navier equation (or system):

$$(\Delta^* + \omega^2)u = 0 \quad \text{in } \Omega_\Lambda, \quad \Delta^* := \mu\Delta + (\lambda+\mu)\,\mathrm{grad}\,\mathrm{div}\,. \tag{2.3}$$

On the impenetrable surface Λ, the vanishing normal displacement and tangential stress (or normal stress and tangential displacement) lead to the following boundary conditions:

boundary conditions of the third kind: $\nu\cdot u = 0, \quad \nu\times Tu = 0,$ (2.4)

or boundary conditions of the fourth kind: $\nu\times u = 0, \quad \nu\cdot Tu = 0,$ (2.5)

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

$$Tu = T(\lambda,\mu)u := 2\mu\,\partial_\nu u + \lambda(\mathrm{div}\,u)\,\nu + \mu\,\nu\times\mathrm{curl}\,u. \tag{2.6}$$

Here and in the following, $\partial_\nu u = \nu\cdot\nabla u$ is used, and the symbol $\partial_j u$ denotes $\partial u/\partial x_j$.

The periodicity of the structure and the form of the incident waves imply that the solution u is α-quasi-periodic, i.e.,

$$u(x_1+2\pi, x_2+2\pi, x_3) = \exp(i2\pi(\alpha_1+\alpha_2))u(x_1,x_2,x_3), \quad x\in\Omega_\Lambda, \tag{2.7}$$

or equivalently, the function $u(x)\exp(-i\alpha\cdot x')$ is 2π-periodic with respect to x_1 and x_2, where $\alpha = (\alpha_1,\alpha_2) = k(\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2)$ with $k = k_p$ for the incident pressure wave (2.1), or $k = k_s$ for the incident shear wave (2.2). To ensure well-posedness of the boundary value problem (2.3)–(2.7), a radiation condition must be imposed as $x_3 \to +\infty$. We note that the scattered field $u^{\rm sc}$, which also satisfies the Navier equation (2.3), can be decomposed into its compressional and shear parts,

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

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

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

Applying the usual Rayleigh expansion to φ and ψ respectively, we finally obtain a corresponding expansion of $u^{\rm sc}$ into outgoing plane elastic waves (see [16]):

$$u^{\rm sc}(x) = \sum_{n\in\mathbb{Z}^2}\Big\{A_{p,n}\,\mathbf{P}_n^\top \exp(i\mathbf{P}_n\cdot x) + A_{s,n}\mathbf{S}_n^\perp \exp(i\mathbf{S}_n\cdot x)\Big\}, \tag{2.10}$$

for $x_3 > \Lambda^+ := \max_{x_3\in\Lambda}\{x_3\}$, where the constants $A_{p,n}, A_{s,n} \in \mathbb{C}$ are called the Rayleigh coefficients, and

$$\mathbf{P}_n = (\alpha_n,\beta_n),\ \ \mathbf{S}_n = (\alpha_n,\gamma_n) \in \mathbb{C}^3,\ \ \mathbf{S}_n^\perp \in \mathbb{C}^3,\ \ |\mathbf{S}_n^\perp| = 1,\ \ \mathbf{S}_n^\perp\cdot\mathbf{S}_n = 0, \tag{2.11}$$

with $\alpha_n = (\alpha_n^{(1)},\alpha_n^{(2)}) := (\alpha_1 + n_1, \alpha_2 + n_2)$ for $n = (n_1,n_2) \in \mathbb{Z}^2$ and the parameters β_n and γ_n given by

$$\begin{aligned}
\beta_n &= \begin{cases} (k_p^2 - |\alpha_n|^2)^{\frac12} & \text{if } |\alpha_n| \le k_p,\\ i\,(|\alpha_n|^2 - k_p^2)^{\frac12} & \text{if } |\alpha_n| > k_p,\end{cases}\\
\gamma_n &= \begin{cases} (k_s^2 - |\alpha_n|^2)^{\frac12} & \text{if } |\alpha_n| \le k_s,\\ i\,(|\alpha_n|^2 - k_s^2)^{\frac12} & \text{if } |\alpha_n| > k_s,\end{cases}
\end{aligned} \tag{2.12}$$

respectively. The expansion in (2.10) is the radiation condition we are going to use in the following; see also [5] and [14] for the radiation condition for plane elasticity. Since β_n and γ_n are real for at most a finite number of indices $n \in \mathbb{Z}^2$, only a finite number of plane waves in (2.10) propagates into the far field, with the remaining evanescent waves (or surface waves) decaying exponentially as $x_3 \to +\infty$.

The above expansion (2.10) converges uniformly with all derivatives in the half-space $\{x \in \mathbb{R}^3 : x_3 \geq b\}$ for any $b > \Lambda^+$. For fixed incident angles $\theta_1 \in [0, \pi/2)$, $\theta_2 \in [0, 2\pi)$, define

$$\pi_p := \{n \in \mathbb{Z}^2 : \beta_n(\alpha, k_p) = 0\}, \quad \pi_s := \{n \in \mathbb{Z} : \gamma_n(\alpha, k_s) = 0\}. \quad (2.13)$$

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 resp. shear part are excluded if $\pi_p = \emptyset$ resp. $\pi_s = \emptyset$.

Now, our direct diffraction problem can be formulated as the following boundary value problem.

Direct problem (DP). Given a grating profile surface $\Lambda \subset \mathbb{R}^3$ (which is 2π-periodic in x_1 and x_2) and an incident field u^{in} of the form (2.1) or (2.2), find a vector function $u = u(x; \theta_1, \theta_2) = u^{\text{in}} + u^{\text{sc}} \in H^1_{\text{loc}}(\Omega_\Lambda)^3$ that satisfies the Navier equation (2.3), one of the boundary conditions in (2.4) and (2.5), the α-quasi-periodicity (2.7) and the radiation condition (2.10).

If Λ is a Lipschitz surface in $\mathbb{R}^3$, there always exists a solution u to (DP), while the uniqueness can be guaranteed only for small frequencies ω or for all frequencies excluding a discrete set; see Elschner & Hu [16] for a proof using the variational method. Since the surface waves are exponentially decaying and thus can hardly be measured far away from the grating, our inverse problem involves near-field measurements $u(x', b)$ for some fixed $b > \Lambda^+$.

Inverse problem (IP). Given an incident pressure wave of the form (2.1) or an incident shear wave of the form (2.2), determine the grating profile Λ from the knowledge of the near-field data $u(x_1, x_2, b)$ for all $x_1, x_2 \in (0, 2\pi)$ and some $b > \Lambda^+$, where $u(x)$ is a (not necessarily unique) solution of (DP) corresponding to the incident field.

Note that the formulation of (IP) makes sense if there only exists a solution u of (DP). In this paper we are mainly interested in the following uniqueness questions about (IP):

Let the incident angles θ_1, θ_2 be fixed, and let $\mathcal{A}$ be an admissible class of grating profiles. Suppose that the two gratings $\Lambda_1, \Lambda_2 \in \mathcal{A}$ produce the total fields u_j $(j = 1, 2)$ for an incident pressure resp. shear wave of the form (2.1) resp. (2.2). Does the relation

$$u_1(x', b) = u_2(x', b), \ \ \forall\, x_1, x_2 \in (0, 2\pi), \ \text{for some } b > \max\{\Lambda_1^+, \Lambda_2^+\} \quad (2.14)$$

imply $\Lambda_1 = \Lambda_2$? If not, what kind of geometric characteristics do Λ_1 and Λ_2 share in order to generate the same total field on $x_3 = b$?

In this paper, a grating profile $\Lambda \in \mathcal{A}$ is required to be a bi-periodic polyhedral Lipschitz surface, consisting of a finite number of planar faces in one periodic cell $(0, 2\pi) \times (0, 2\pi)$. Without loss of generality, we always assume that Λ is not constant in x_1 and is allowed to be invariant in x_2. Thus, we define the admissible class $\mathcal{A}$ by

$$\mathcal{A} = \big\{\Lambda : \Lambda \text{ is a polyhedral surface in } \mathbb{R}^3 \text{ which is } 2\pi\text{-periodic in } x_1 \text{ and } x_2, \text{ and } \Lambda \text{ is not constant in } x_1\text{-direction}\big\}. \tag{2.15}$$

Note that a flat grating of the form $\{x_3 = c\}$ for some $c \in \mathbb{R}$, which is constant in both x_1 and x_2, is excluded from the admissible class $\mathcal{A}$. We do not consider such flat gratings because they cannot be uniquely identified from the near-field data corresponding to a finite number of incident plane waves. This can be readily deduced from the explicit solutions of (DP) for flat gratings under the third or fourth kind boundary conditions; see [15] for the non-uniqueness examples in 2D and [16] for the explicit direct solutions to the homogeneous problem (DP) (with $u^{\mathrm{in}} = 0$) in 3D. By [16, Section 4.3], we know that there always exists a solution to (DP) for any $\Lambda \in \mathcal{A}$.

Concerning the admissible class $\mathcal{A}$, we distinguish its two subclasses $\mathcal{A}_1$ and $\mathcal{A}_2$ by defining

$$\mathcal{A}_1 := \{\Lambda \in \mathcal{A} : \ \Lambda \text{ is constant in } x_2\},$$
$$\mathcal{A}_2 := \{\Lambda \in \mathcal{A} : \Lambda \text{ is not constant in } x_2\}.$$

The grating profiles from $\mathcal{A}_1$ vary only in x_1 and remain invariant in x_2, whereas those from $\mathcal{A}_2$ vary in both x_1 and x_2. By the definition of $\mathcal{A}$, we have

$$\mathcal{A} = \mathcal{A}_1 \cup \mathcal{A}_2.$$

In this paper, it is supposed for simplicity that

$$\text{either} \quad \Lambda_1, \Lambda_2 \in \mathcal{A}_1, \quad \text{or} \quad \Lambda_1, \Lambda_2 \in \mathcal{A}_2. \tag{2.16}$$

Throughout the paper we assume without loss of generality that one of the two grating profiles, say Λ_1, contains the origin O of the coordinate system in the following way. If $\Lambda_1 \in \mathcal{A}_1$, the origin O is supposed to be located at the intersection line l of two neighboring faces of Λ_1, so that l coincides with the x_2-axis. If $\Lambda_1 \in \mathcal{A}_2$, the origin is supposed to coincide with one corner point of Λ_1, where at least three faces of Λ_1 meet together.

Now we present the main uniqueness theorems of this paper as follows.

Theorem 2.1. *Assume the incident wave is an incident shear wave of the form* (2.2). *Let the total fields $u_j(x)$ $(j = 1, 2)$ satisfy the direct problem* (DP) *corresponding to the grating profiles $\Lambda_j \in \mathcal{A}$ under the boundary conditions of the third* *kind. Then, under the assumption* (2.16)*, the relation* (2.14) *implies that*

$$\text{either } \Lambda_1 = \Lambda_2, \quad \text{or } \Lambda_1, \Lambda_2 \in U_j \quad \text{for some } j \in \{1,2,3,4,5\}, \qquad (2.17)$$

where $U_j \subset \mathcal{A}_1$ *for* $j = 1,2,3,4$ *and* $U_5 \subset \mathcal{A}_2$*, which are defined respectively in Sections* 4.3 *and* 4.4*, are five classes of unidentifiable grating profiles corresponding to the incident shear wave of the form* (2.2)*. Moreover, for each index* $j \in \{1,2,3,4,5\}$*, the different grating profiles from* U_j *generate the same total field of the specific form presented in Lemmas* 4.10*,* 4.12*,* 4.14*,* 4.16 *and* 4.21 *respectively.*

Theorem 2.2. *Assume the incident wave is an incident pressure wave of the form* (2.1)*. Let the total fields* $u_j(x)$ $(j = 1,2)$ *satisfy the direct problem* (DP) *corresponding to the grating profiles* $\Lambda_j \in \mathcal{A}$ *under the boundary conditions of the fourth kind. Then, under the assumption* (2.16)*, the relation* (2.14) *implies that*

$$\text{either } \Lambda_1 = \Lambda_2, \quad \text{or } \Lambda_1, \Lambda_2 \in U_2(\theta_1, \theta_2, k_p).$$

Furthermore, if we have $\Lambda_1, \Lambda_2 \in U_2(\theta_1, \theta_2, k_p)$ *and* $\Lambda_1 \neq \Lambda_2$*, then the total field* $u = u_1 = u_2$ *takes the form*

$$u = \hat{\theta} \exp(i k_p x \cdot \hat{\theta}) + \mathrm{Rot}_\pi(\hat{\theta}) \exp(i k_p x \cdot \mathrm{Rot}_\pi(\hat{\theta})) \\ - (1/k_p)\mathbf{P} \exp(i x \cdot \mathbf{P}) - (1/k_p)\,\mathrm{Rot}_\pi(\mathbf{P}) \exp(i x \cdot \mathrm{Rot}_\pi(\mathbf{P})),$$

where $\mathrm{Rot}_\pi(\cdot)$ *denotes the rotation around the* x_2*-axis by the angle* π*,* $\mathbf{P}$ *and* $\mathrm{Rot}_\pi(\mathbf{P})$ *are defined in Lemma* 5.3 (1)*.*

3 Auxiliary lemmas

In this section we present some auxiliary lemmas which play an import role in the proof of our uniqueness results. The following one is elementary (see [8] for a proof).

Lemma 3.1. *Let* $a_j \in \mathbb{C}^3$*, and let* $\lambda_j \in \mathbb{R}$ *be distinct numbers* $(j = 1,2,\ldots,m)$*. If*

$$\sum_{j=1}^{m} a_j \exp(i\lambda_j t) = 0, \quad \forall\, t \in \mathbb{R},$$

then $a_j = (0,0,0)^\top$*,* $j = 1,2,\ldots,m$*.*

Definition 3.2. Let Π be a two-dimensional plane in $\mathbb{R}^3$ and let u be a solution to (2.3). A non-void open connected component Θ of $\Pi \cap \overline{\Omega}_\Lambda$ will be called *a perfect set of* u if u satisfies the third resp. fourth kind boundary conditions on Θ.

Denote by $\mathrm{Ref}_\Pi(\cdot)$ the reflection with respect to a plane Π in $\mathbb{R}^3$, and by $\mathrm{Ref}'_\Pi(\cdot)$ the reflection with respect to the plane Π' that passes through the origin O and is parallel to Π. In this paper a reflection or rotation operator is also applied to a complex-valued function or vector by acting on its real and imaginary parts respectively. Analogously, we say that a plane Π passes through a complex vector $\mathbf{a} = \mathbf{b} + i\mathbf{c} \in \mathbb{C}^3$ (i.e., $\mathbf{a} \in \Pi$) for $\mathbf{b}, \mathbf{c} \in \mathbb{R}^3$ if Π passes through both of the points $\mathbf{b}, \mathbf{c} \in \mathbb{R}^3$.

The following reflection principle for the Navier equation is the main tool for proving uniqueness in our inverse diffraction problems.

Lemma 3.3 (Reflection principle for the Navier equation). *Assume that $\Omega \subset \mathbb{R}^3$ is a symmetric domain with respect to a perfect set $\Theta \subset \Pi$ of u, and that the function u satisfies the Navier equation $(\triangle^* + \omega^2)u = 0$ in Ω.*

(1) *If $\tilde{\Theta}$ is another perfect set of u in $\overline{\Omega}$, then $\mathrm{Ref}_\Pi(\tilde{\Theta}) \subset \overline{\Omega}$ is also a perfect set of u.*

(2) *There holds*

$$u(x) \pm \mathrm{Ref}'_\Pi(u(\mathrm{Ref}_\Pi(x))) = 0 \quad \text{in } \Omega, \tag{3.1}$$

where $+$ resp. $-$ is taken corresponding to the fourth resp. third kind boundary conditions on Θ.

The first assertion of Lemma 3.3 is proved by Elschner & Yamamoto in [20], where the identities (3.1) are implicitly contained. Note that the reflection principle under the fourth kind boundary conditions takes the same form as that for Maxwell's equations proved in [26]; see also [8] and [27]. If Π passes through the origin O, then the identities in (3.1) take the form

$$\mathrm{Ref}_\Pi(u(x)) \pm u(\mathrm{Ref}_\Pi(x)) = 0 \quad \text{in } \Omega, \tag{3.2}$$

which will be frequently used in the subsequent analysis; see Figure 1.

In the following, we denote by $u_j := u_j(x; \theta_1, \theta_2)$ the corresponding total fields produced by the grating profiles $\Lambda_j \in \mathcal{A}$ $(j = 1, 2)$. Assume

$$u_1(x', b) = u_2(x', b), \quad x' = (x_1, x_2) \in (0, 2\pi) \times (0, 2\pi) \tag{3.3}$$

for some $b > \max\{\Lambda_1^+, \Lambda_2^+\}$. Denote $\Omega_b := \{x \in \mathbb{R}^3 : x_3 > b\}$, $\Gamma_b := \{x_3 = b\}$.

Next, based on the reflection principle for the Navier equation, we prove that, under the condition (3.3), the total fields u_j $(j = 1, 2)$ can be reduced to a finite number of propagating modes. To do this, we employ the arguments used in [2,20] to find an unbounded perfect set which extends to Ω_b. We first recall a fundamental property for a connected set (see [12, Theorem 3.19.9]) which will be used in our subsequent analysis.

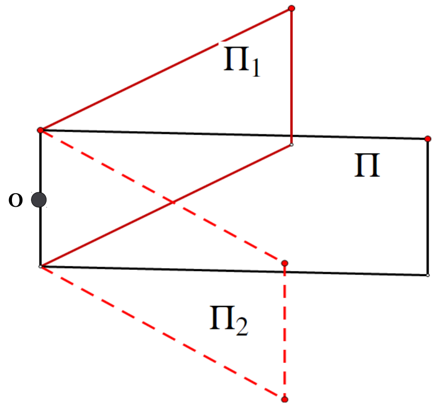

Figure 1. If $(\Delta^* + \omega^2)u = 0$ in $\mathbb{R}^3$ and u satisfies the third resp. fourth kind boundary conditions on the plane Π, then the relation (3.2) holds in $\mathbb{R}^3$. In particular, if u satisfies the third resp. fourth kind boundary conditions on both Π and Π_1, then the same boundary conditions hold on $\Pi_2 := \mathrm{Ref}_\Pi(\Pi_1)$.

Lemma 3.4. *Let A, B be two subsets of $\mathbb{R}^3$, and assume that B is connected such that $B \cap A \neq \emptyset$ and $B \cap (\mathbb{R}^3 \backslash A) \neq \emptyset$. Then $\partial A \cap B \neq \emptyset$.*

Lemma 3.5. *If relation* (3.3) *holds for two different grating profiles $\Lambda_1, \Lambda_2 \in \mathcal{A}$, then*

(1) *Under the boundary conditions of the third (fourth) kind, there always exists a perfect set Θ of both u_1 and u_2 such that $\Theta \cap \Omega_b \neq \emptyset$.*

(2) *Both of the total fields $u_j = u^{\mathrm{in}} + u_j^{\mathrm{sc}}$, $j = 1, 2$, can be reduced to a finite sum of propagating waves,*

$$u_1 = u_2 = u^{\mathrm{in}} + \sum_{|\alpha_n| \leq k_p} A_{p,n} \mathbf{P}_n^\top e^{ix\cdot \mathbf{P}_n} + \sum_{|\alpha_n| \leq k_s} A_{s,n} \mathbf{S}_n^\perp e^{ix\cdot \mathbf{S}_n} \tag{3.4}$$

in $x_3 > \max\{\Lambda_1^+, \Lambda_2^+\}$, where $\mathbf{P}_n$ and $\mathbf{S}_n$ are defined in (2.11).

Proof. (1) It follows from the standard elliptic regularity theory that the solution $u_j \in H^1_{\mathrm{loc}}(\Omega_{\Lambda_j})^3$ to the corresponding problem (DP) is infinitely smooth up to Λ_j except for vertices and edges, and u_j is real-analytic in Ω_{Λ_j}. By assumption (3.3) and the uniqueness of the Dirichlet problem in Ω_b [16], we see that $u_1 = u_2$ for $x_3 > b$. Then, applying the unique continuation of solutions to the Navier equation gives $u_1 = u_2$ in Ω, where Ω denotes the unbounded connected component of

$\Omega_{\Lambda_1} \cap \Omega_{\Lambda_2}$ which contains the plane Γ_b. It follows from $\Lambda_1 \neq \Lambda_2$, the connectedness of Ω_{Λ_1} and Ω_{Λ_2} and Lemma 3.4 that $\partial\Omega \not\subseteq \Lambda_1 \cap \Lambda_2$ (see [26, Theorem 1]). Thus, by periodicity we may assume without loss of generality that

$$S := \tilde{\Omega}_{\Lambda_1} \cap \partial\Omega \neq \emptyset \quad \text{with } \tilde{\Omega}_{\Lambda_1} := \{x \in \Omega_{\Lambda_1} : x_1, x_2 \in (0, 2\pi)\}.$$

Then there is an open connected subset $F \subset S$ of a plane Π satisfying $F \subset \Omega_{\Lambda_1}$, and thus a perfect set Θ of u_1 in Ω_{Λ_1} such that $F \subset \Theta \subset \Pi$. If Θ can be extended to $\{x_3 > b\}$, we already have the desired perfect set; otherwise, the set Ξ defined by

$$\Xi := \left\{\Theta : \Theta \text{ is a perfect set of } u_1 \text{ in } \Omega_{\Lambda_1} \text{ with } \Theta \cap \tilde{\Omega}_{\Lambda_1} \neq \emptyset \text{ and } \Theta \cap \Omega_b = \emptyset\right\}$$

is not empty. Proceeding similarly to the case of scattering by polygonal and polyhedral bounded obstacles (see, e.g., [2,20,26,28]), we now combine the reflection principle for the Navier equation with a path argument to obtain the desired perfect set which can be extended to Ω_b.

Choose a point $P \in F \subset \partial\Omega \cap \tilde{\Omega}_{\Lambda_1}$ and a continuous and injective path $\gamma(t)$, $t \geq 0$, starting at $P = \gamma(0)$ and leading to infinity in the unbounded connected component $\tilde{\Omega}$ of $\Omega \cap \{x \in \mathbb{R}^3 : -2\pi < x_1, x_2 < 4\pi\}$, for $t > 0$. Let $\mathcal{M}$ be the set of intersection points of γ with all perfect set of u_1 from the class Ξ. Then $\mathcal{M} \neq \emptyset$, and $\mathcal{M}$ is obviously bounded. Furthermore, the set Ξ is closed, and hence compact. In fact, let $\{x_n\}$ be a sequence of intersection points of perfect sets $\Theta_n \in \Xi$, $x_n \in \Theta_n$, with the path γ, such that x_n converges to a point $\tilde{x} \in \gamma$. Choosing a unit normal ν_n to Θ_n and passing to a convergent subsequence $\nu_n \to \tilde{\nu}$, we can prove (see the proof of [28, Lemma 2]) that the plane $\tilde{\Pi}$ through $\tilde{x}$ with unit normal $\tilde{\nu}$ contains a perfect set $\tilde{\Theta}$ of u_1 such that $\tilde{x} \in \tilde{\Theta}$. We can assume that $\Theta \in \Xi$ since, otherwise, we already have a perfect set that extends to Ω_b. Thus there exists $t_0 \geq 0$ such that $\gamma(t_0) \in \mathcal{M}$ and no perfect set of Ξ can intersect $\gamma(t)$ for $t > t_0$. Let $\Theta_0 \subset \Pi_0$ be a perfect set of Ξ passing $\gamma(t_0)$ and lying on a plane Π_0. We now apply the reflection principle of Lemma 3.3 to prove the existence of a perfect set Θ^* of u_1 intersecting $\gamma(t)$ at some $t^* > t_0$, which gives the desired unbounded perfect set or a contradiction to the assumption that $\Lambda_1 \neq \Lambda_2$.

Let $x^+ = \gamma(t_0 + \epsilon)$ for some sufficiently small $\epsilon > 0$, and let $x^- = \mathrm{Ref}_{\Pi_0}(x^+)$. Denote by $G^\pm$ the connected component of $\Omega_{\Lambda_1} \backslash \Theta_0$ containing $x^\pm$, and let $E^\mp$ be the connected component of $\mathrm{Ref}_{\Pi_0}(G^\mp) \cap G^\pm$ containing $x^\pm$. Defining E by $E = E^+ \cup \Theta_0 \cup E^-$, we see that E is a connected open set whose boundary consists of faces of Λ_1 and $\mathrm{Ref}_{\Pi_0}(\Lambda_1)$. By Lemma 3.3, u_1 satisfies the boundary condition (2.4) resp. (2.5) on ∂E and $E \cap \Pi_0$.

Next we claim that the projection of the set E on the x_3 axis, $\mathrm{pr}(E)$, is bounded. In fact, if Π_0 is parallel to the (x_1, x_2)-plane, then $\mathrm{pr}(E)$ is obviously bounded since E is symmetric with respect to Π_0. It remains to consider the case when Π_0 is not parallel to the (x_1, x_2)-plane. Then we may assume that $\mathrm{pr}(E \cap \Pi_0)$ and $\mathrm{pr}(\partial E)$ are both bounded; otherwise Π_0 already contains a perfect set extending to Ω_b, or a face of ∂E can be extended to such a perfect set. Therefore, if $\mathrm{pr}(E)$ were unbounded, then E would contain a half-space $\{x_3 > a\}$ for some $a > 0$ sufficiently large, which contradicts the boundedness of $\mathrm{pr}(E \cap \Pi_0)$.

Since $\mathrm{pr}(E)$ is bounded and the connected set $\Gamma := \{\gamma(t) : t \geq t_0\}$ extends to infinity in $\tilde{\Omega}$, it follows from Lemma 3.4 with $A = E$ and $B = \Gamma$ that there exists $t^* > t_0$ such that $\gamma(t^*) \in \partial E$. Consequently, there is a perfect set $\Theta^* \notin \Xi$ of u_1 passing $\gamma(t^*)$, so that $\Theta^* \cap \Omega_b \neq \emptyset$. Finally, it is seen from $u_1 = u_2$ in Ω that Θ^* is also a perfect set of u_2. This completes the proof of the first assertion.

(2) We will prove the second assertion under the fourth kind boundary conditions. The proof under the third kind boundary conditions is analogous. Let Θ be the perfect set involved in assertion (1) lying on a plane Π. We consider the following two cases.

Case (i): Π is parallel to $\{x_3 = 0\}$.

We can assume $\Pi = \{x_3 = d\} \subset \overline{\Omega}$ for some $d > b$ and that the fourth kind boundary conditions are fulfilled on Π. In this case of a flat grating, the non-trivial solutions to the homogeneous scattering problem (DP) (with $u^{\mathrm{in}} = 0$) are known explicitly [16]. Therefore we obtain that

$$u(x) = \frac{1}{k_p}\begin{pmatrix}\alpha^\top \\ -\beta\end{pmatrix} e^{i(\alpha\cdot x' - \beta x_3)} - \frac{1}{k_p}\begin{pmatrix}\alpha^\top \\ \beta\end{pmatrix} e^{i(\alpha\cdot x' + \beta(x_3 - 2d))} + e_3^\top \sum_{\gamma_n = 0} C_n e^{i\alpha_n\cdot x'}$$

for the incident pressure wave of the form (2.1), and

$$u(x) = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} e^{i(\alpha\cdot x' - \gamma x_3)} - \begin{pmatrix} q_1 \\ q_2 \\ -q_3 \end{pmatrix} e^{i(\alpha\cdot x' + \gamma(x_3 - 2d))} + e_3^\top \sum_{\gamma_n = 0} C_n e^{i\alpha_n\cdot x'}$$

for the incident shear wave of the form (2.2) with $\hat{\theta}^\perp = (q_1, q_2, q_3)^\top \in S^2$, where $C_n \in \mathbb{C}$ are arbitrary constants and $e_3 = (0, 0, 1)$. Thus, the total field indeed takes the form (3.4).

Case (ii): Π is not parallel to $\{x_3 = 0\}$.

Following [15, 18] in spirit, we shall study this case using properties of almost-periodic functions. From the beginning part of the proof of assertion (1) and by (2.10) and (3.3), we can write

$$u(x) = u_1(x) = u_2(x) = I(x) + \sum_{|\alpha_n| > k_p} I_{p,n}(x) + \sum_{|\alpha_n| > k_s} I_{s,n}(x)$$

in $x_3 > \max\{\Lambda_1^+, \Lambda_2^+\}$, where

$$\begin{aligned} I_{p,n}(x) &:= A_{p,n}\mathbf{P}_n^\top e^{ix\cdot\mathbf{P}_n}, \\ I_{s,n}(x) &:= A_{s,n}\mathbf{S}_n^\perp e^{ix\cdot\mathbf{S}_n}, \\ I(x) &:= u^{\rm in}(x) + \sum_{|\alpha_n|\le k_p} I_{p,n}(x) + \sum_{|\alpha_n|\le k_s} I_{s,n}(x). \end{aligned}$$

Thus $I(x)$ consists of a finite number of propagating waves of the compressional and shear parts, including the incident wave $u^{\rm in}$, whereas $u(x) - I(x)$ consists of infinitely many surface waves decaying exponentially as $x_3 \to +\infty$. It suffices to prove that $A_{p,n} = 0$ for all $|\alpha_n| > k_p$ and $A_{s,n} = 0$ for all $|\alpha_n| > k_s$.

Defining

$$A^* = \min\Big\{\inf_{|\alpha_n|>k_p}\{|\beta_n|\}, \inf_{|\alpha_n|>k_s}\{|\gamma_n|\}\Big\}$$

and

$$\Upsilon := \{n \in \mathbb{Z}^2 : \gamma_n = iA^* \text{ or } \beta_n = iA^*\},$$

we first prove that $A_{p,n} = A_{s,m} = 0$ if $\beta_n = iA^*$ or $\gamma_m = iA^*$.

It follows from the existence of the perfect set Θ in the first assertion that there always exists a ray $l \subset \Theta$ starting from some point $z = (z_1, z_2, z_3) \in \Omega_b$ such that the third Cartesian components of the points of l tend to $+\infty$. Without loss of generality the ray l takes the form

$$l = \Big\{x(t) : \frac{x_1 - z_1}{a} = \frac{x_2 - z_2}{b} = \frac{x_3 - z_3}{c} = t,\ t \ge 0\Big\},$$

for some $a, b \in \mathbb{R}, c > 0$ such that $\overrightarrow{l} = (a, b, c) \in S^2$ is orthogonal to the normal direction ν of the perfect plane Θ. Since the set Υ consists of a finite number of indices, we may assume further that $\alpha_n \cdot (a, b)^\top \ne \alpha_m \cdot (a, b)^\top$ for any $n \ne m$, $n, m \in \Upsilon$; otherwise we may replace the ray $l \subset \Theta$ by another ray $l' \subset \Theta$ with the unit direction

$$\overrightarrow{l}' = (a', b', c') \in S^2, \quad c' > 0,$$

such that the third components of l' also tend to $+\infty$ and the norm $\|\overrightarrow{l} - \overrightarrow{l}'\|$ is as small as we like. We then have

$$0 = \nu\times u|_l = \Big[\nu\times I(x) + \sum_{|\alpha_n|>k_p} \nu\times I_{p,n}(x) + \sum_{|\alpha_n|>k_s} \nu\times I_{s,n}(x)\Big]\Big|_{x=x(t)} \quad (3.5)$$

for all $t \ge 0$. Noting that $\nu \times I(x)|_{x=x(t)}$ is an almost periodic function in t, and that $\nu\times I_{p,n}(x)|_{x=x(t)}$ for $|\alpha_n| > k_p$, $\nu\times I_{s,n}(x)|_{x=x(t)}$ for $|\alpha_n| > k_s$ are exponentially decaying functions as $t \to +\infty$, we obtain from (3.5) that (see [18, p. 784] for the 2D case)

$$\begin{aligned}
&\max_{x\in l}|\nu \times I(x)| \\
&\qquad = \limsup_{t\to+\infty} |\nu \times I(x)|_{x=x(t)}| \\
&\qquad = \limsup_{t\to+\infty}\left\{\left|\sum_{|\alpha_n|>k_p} \nu \times I_{p,n}(x)|_{x=x(t)} + \sum_{|\alpha_n|>k_s} \nu \times I_{s,n}(x)|_{x=x(t)}\right|\right\} \\
&\qquad = 0,
\end{aligned}$$

which implies that $\nu \times I(x) \equiv 0$ for all $x \in l$. Using (3.5) again, we arrive at

$$\sum_{|\alpha_n|>k_p} A_{p,n}\nu \times \mathbf{P}_n^\top e^{ix\cdot\mathbf{P}_n} + \sum_{|\alpha_n|>k_s} A_{s,n}\nu \times \mathbf{S}_n^\perp e^{ix\cdot\mathbf{S}_n} = 0, \quad x \in l. \tag{3.6}$$

Multiplying (3.6) by $\exp(A^*(ct + z_3))$ and letting $x \in l$, $|x| \to +\infty$, we obtain by recalling the definitions of $\mathbf{P}_n$ and $\mathbf{S}_n$ in (2.11) that

$$\begin{aligned}
0 = &\sum_{\beta_n=iA^*} A_{p,n}\nu \times (\alpha_n, i|\beta_n|)\exp(i\alpha_n \cdot \tilde{x}(t)) \\
&\qquad + \sum_{\gamma_n=iA^*} A_{s,n}\nu \times \mathbf{S}_n^\perp \exp(i\alpha_n \cdot \tilde{x}(t)), \quad t > 0,
\end{aligned}$$

where $\tilde{x}(t) := (at + z_1, bt + z_2)^\top \in \mathbb{R}^2$. Then, it follows from Lemma 3.1 that

$$\begin{aligned}
A_{p,n}\, \nu \times (\alpha_n, i|\beta_n|) = 0 &\qquad \text{for} \quad \beta_n = iA^*, \\
A_{s,m}\, \nu \times \mathbf{S}_m^\perp = 0 &\qquad \text{for} \quad \gamma_m = iA^*.
\end{aligned}$$

Since the normal ν to the plane Π is not parallel to e_3 and the third components of $\mathbf{P}_n = (\alpha_n, i|\beta_n|)$ for $|\alpha_n| > k_p$ and $\mathbf{S}_n = (\alpha_n, i|\gamma_n|)$ for $|\alpha_n| > k_s$ are purely imaginary, by simple calculations one may check that

$$\nu \times (\alpha_n, i|\beta_n|) \neq O, \quad \nu \times \mathbf{S}_n^\perp \neq O, \quad \text{with } O = (0,0,0),$$

which leads to $A_{p,n} = A_{s,m} = 0$ for $\beta_n = \gamma_m = iA^*$.

Setting

$$A^{**} = \min\left\{\inf_{|\alpha_n|>k_p}\{|\beta_n| : |\beta_n| > A^*\}, \inf_{|\alpha_n|>k_s}\{|\gamma_n| : |\gamma_n| > A^*\}\right\}$$

and repeating the argument above, we finally conclude that

$$A_{p,n} = 0 \text{ for all } |\alpha_n| > k_p \quad \text{and} \quad A_{s,n} = 0 \text{ for all } |\alpha_n| > k_s.$$

This implies that the total fields u_j $(j = 1, 2)$ take the form (3.4) and completes the proof of the second assertion. □

4 Inverse scattering of an incident shear wave under the boundary conditions of the third kind

We make the following assumptions throughout this section.

(A1) The incident wave is the incident shear wave defined in (2.2), i.e.,

$$u^{\mathrm{in}} := \hat{\theta}^{\perp} \exp(ik_s x \cdot \hat{\theta})$$

with the incident direction $\hat{\theta} = (\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2, -\cos\theta_1)$ and the incident angles $\theta_1 \in [0, \frac{\pi}{2})$, $\theta_2 \in [0, 2\pi)$.

(A2) The total fields $u_j(x)$ $(j = 1,2)$ satisfy problem (DP) corresponding to the different grating profiles Λ_j under the boundary conditions of the third kind and fulfill the relation (3.3).

Under the above assumptions **(A1)** and **(A2)**, it follows from Lemma 3.5 (2) that $u = u_1 = u_2$ can be reduced to a finite sum of propagating modes in Ω. Thus, each u_j $(j = 1,2)$ can be extended to an analytic function in the whole space by (3.4) and $u = u_1 = u_2$ in $\mathbb{R}^3$. Let Λ denote one of the profiles Λ_j $(j = 1,2)$, and define $(\alpha, \gamma) := (\alpha_0, \gamma_0) = k_s(\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2, \cos\theta_1)$.

The remaining part of this section is organized as follows. In Sections 4.1–4.2, we derive the reflectional and rotational invariance of the total field using the reflection principle for the Navier equation. The unidentifiable grating profiles from $\mathcal{A}_1$ and $\mathcal{A}_2$ are characterized and classified in Sections 4.3 and 4.4, respectively, which would lead to Theorem 2.1 directly. The corresponding non-uniqueness examples will be presented in Section 4.5.

4.1 Reflectional invariance

By (3.4), we can write the total field $u = u_1 = u_2$ as

$$u = \sum_{n \in P} A_{p,n} \mathbf{P}_n^{\top} \exp(ix \cdot \mathbf{P}_n) + \sum_{n \in S} A_{s,n} \mathbf{S}_n^{\perp} \exp(ix \cdot \mathbf{S}_n) \quad \text{in } \mathbb{R}^3, \tag{4.1}$$

where

$$P := \{n \in \mathbb{Z}^2 : |\alpha_n| \le k_p, A_{p,n} \ne 0\},$$
$$S := \{n \in \mathbb{Z}^2 : |\alpha_n| \le k_s, A_{s,n} \ne 0\} \cup \{\kappa\},$$

and $\mathbf{S}_\kappa := (\alpha, -\gamma)^{\top}$, $A_{s,\kappa} = 1$, the vectors $\mathbf{S}_n$ for $n \ne \kappa$ and $\mathbf{P}_n$ for all $n \in \mathbb{Z}^2$ are defined in (2.11).

Define

$$\mathcal{P} = \{\mathbf{P}_n : n \in P\}, \quad \mathcal{S} = \{\mathbf{S}_n : n \in S\}.$$

We observe that $\mathscr{P}$ consists of a finite number of upward propagating directions of the compressional part, whereas $\mathscr{S}\backslash\mathbf{S}_\kappa$ consists of finitely many upward propagating directions of the shear part and $\mathbf{S}_\kappa$ denotes the downward incident direction. By the definitions of α_n, β_n and γ_n (see (2.12)), we have $\mathscr{P} \subset B_{k_p}(O)$ and $\mathscr{S} \subset B_{k_s}(O)$, where $B_r(O) := \{x \in \mathbb{R}^3 : |x| = r\}$ denotes the sphere centered at the origin O with radius r.

Remark 4.1. Since a plane shear wave of the form $u^{\mathrm{in}} = A_{s,\kappa}\mathbf{S}_\kappa^\perp \exp(ix \cdot \mathbf{S}_\kappa)$ is taken as the incident wave, the incident direction $\mathbf{S}_\kappa$ is the only element in $\mathscr{S}$ whose x_3-component is negative, while the third components of the elements in $\mathscr{P}$ and $\mathscr{S}\backslash\mathbf{S}_\kappa$ are all non-negative. Furthermore, if $\pi_p = \emptyset$, then each element of $\mathscr{P}$ has a positive x_3-component, and if $\pi_s = \emptyset$, the x_3-components of the elements in $\mathscr{S}\backslash\mathbf{S}_\kappa$ are all positive; see Figure 2. Recall that π_p and π_s are defined in (2.13).

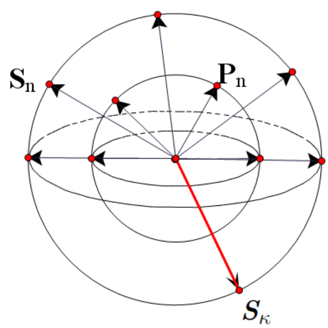

Figure 2. $\mathbf{P}_n \in \mathscr{P} \subset B_{k_p}(O)$, $\mathbf{S}_n \in \mathscr{S} \subset B_{k_s}(O)$. The incident direction $\mathbf{S}_\kappa$ is the only direction propagating downward.

A two-dimensional plane will be called a perfect plane of u if u satisfies the third kind boundary conditions on the whole plane. Since both the normal and tangential vectors of a plane are constant vectors and u is analytic in $\mathbb{R}^3$, each face of Λ can be extended to a perfect plane in $\mathbb{R}^3$. By our assumption on the choice of the origin, we may always assume $O \in l = \Pi_1 \cap \Pi_2$, where Π_1 and Π_2 are two perfect planes of u extending two faces of Λ_1. Define

$$D_l := \{\Pi : \Pi \text{ is a perfect plane of } u \text{ that passes through the straight line } l\}. \quad (4.2)$$

Then we know that $\Pi_1, \Pi_2 \in D_l$, or equivalently, $D_l^\# \geq 2$. Moreover, using the reflection principle one can verify that

Lemma 4.2. *D_l consists of a finite number of perfect planes which form an equiangular system of planes in $\mathbb{R}^3$.*

For the proof of Lemma 4.2, we refer to [8] in the case of Maxwell's equations and to [13] in the case of the Helmholtz equation. Note that this result is already implicitly contained in [18] and [19] in the 2D case. By Lemma 4.2, we know that $D_l^{\#} < \infty$ and each dihedral angle formed by two neighboring planes in the set D_l is $\pi/D_l^{\#}$.

Since $O \in \Pi$, for any $\Pi \in D_l$, we may write the relation (3.2) as

$$0 = \sum_{n\in P} A_{p,n}\Big[\mathbf{P}_n^{\top} \exp(ix\cdot\mathbf{P}_n) - \mathrm{Ref}_{\Pi}(\mathbf{P}_n^{\top}) \exp(ix\cdot \mathrm{Ref}_{\Pi}(\mathbf{P}_n))\Big]$$
$$+ \sum_{n\in S} A_{s,n}\Big[\mathbf{S}_n^{\perp} \exp(ix\cdot\mathbf{S}_n) - \mathrm{Ref}_{\Pi}(\mathbf{S}_n^{\perp}) \exp(ix\cdot \mathrm{Ref}_{\Pi}(\mathbf{S}_n))\Big],$$

under the boundary conditions of the third kind. Applying Lemma 3.1 to the above identity, we obtain the reflectional invariance of the propagating directions in $\mathcal{P}$ and $\mathcal{S}$, which is stated in the following lemma.

Lemma 4.3 (Reflectional invariance). *Assume Π is a perfect plane from D_l. We have*

(1) $\mathrm{Ref}_{\Pi}(\mathcal{P}) = \mathcal{P}$, $\mathrm{Ref}_{\Pi}(\mathcal{S}) = \mathcal{S}$.

(2) *If* $\mathrm{Ref}_{\Pi}(\mathbf{P}_n) = \boldsymbol{P}_m$ *for some $n, m \in P$, then $A_{p,n} = A_{p,m}$.*

(3) *If* $\mathrm{Ref}_{\Pi}(\mathbf{S}_n) = \mathbf{S}_m$ *for some $n, m \in S$, then $A_{s,n}\ \mathrm{Ref}_{\Pi}(\mathbf{S}_n^{\perp}) = A_{s,m}\, \mathbf{S}_m^{\perp}$.*

Define $U_n(x) := \mathbf{P}_n^{\top} \exp(ix\cdot\mathbf{P}_n)$, $V_n(x) := \mathbf{S}_n^{\perp} \exp(ix\cdot\mathbf{S}_n)$. As a consequence of Lemma 4.3, we obtain

Corollary 4.4. (1) *If* $\mathrm{Ref}_{\Pi}(\mathbf{S}_n) = \mathbf{S}_n$ *for some plane $\Pi \in D_l$, then it holds that* $\mathbf{S}_n^{\perp} = \mathrm{Ref}_{\Pi}(\mathbf{S}_n^{\perp})$*, i.e.,* $\mathbf{S}_n \in \Pi$ *implies that* $\mathbf{S}_n^{\perp} \in \Pi$.

(2) *Two different perfect planes from the set D_l cannot pass through the same point* $\mathbf{S}_n \in \mathcal{S}$.

(3) *The function $U_n(x)$ for $|\alpha_n| \le k_p$ satisfies the third kind boundary conditions on $\Pi \in D_l$ if and only if $\boldsymbol{P}_n \in \Pi$, i.e., the perfect plane passes through $\boldsymbol{P}$. The function $V_n(x)$ for $|\alpha_n| \le k_s$ satisfies the third kind boundary conditions on $\Pi \in D_l$ if and only if* $\mathbf{S}_n$, $\mathbf{S}_n^{\perp} \in \Pi$*, i.e., the perfect plane Π passes through both* $\mathbf{S}_n$ *and* $\mathbf{S}_n^{\perp}$.

Proof. Since $A_{s,n} \neq 0$ for any $n \in S$, the first assertion follows directly from Lemma 4.3 (3), and the second assertion follows from the first one. Using Lemma 4.3 in combination with the definition of the stress operator T in (2.6), one can easily prove the third assertion. □

4.2 Rotational invariance

Let the straight line l and the perfect planes $\Pi_1, \Pi_2 \in D_l$ be given as in Section 4.1. We need the following notation to prove the rotational invariance of $\mathcal{P}$ and $\mathcal{S}$.

(1) $\mathrm{Rot}_\varphi(\cdot)$: The rotation around the x_2-axis by the angle $\varphi \in [0, 2\pi)$. We assume that $\mathrm{Rot}_{\pi/2}$ rotates the positive x_1-axis towards the positive x_3-axis so that the rotation direction of $\mathrm{Rot}_\varphi(\cdot)$ is determined. $\mathrm{Rot}_{l,\varphi}(\cdot)$: The rotation around the straight line l by the angle $\varphi \in [0, 2\pi)$ with some specified direction.

(2) ν_l: The unit vector parallel to l. The third component of ν_l is supposed to be non-negative.

(3) Π^*: The plane perpendicular to l and passing through the origin.

(4) $\mathrm{Rot}^*_\varphi(\cdot)$: The rotation around O by the angle φ defined on the plane Π^*. The rotation direction of Rot^*_φ coincides with that of $\mathrm{Rot}_{l,\varphi}$. $\mathrm{Ref}^*_{l_1}(\cdot)$: The reflection with respect to the straight line $l_1 \subset \Pi^*$ defined on Π^*.

(5) $H(\cdot)$: The projection operator from $\mathbb{R}^3$ to Π^*.

Lemma 4.5. *The rotation* $\mathrm{Rot}_{l,2\pi/D_l^\#}$ *can be written as*

$$\mathrm{Rot}_{l,2\pi/D_l^\#}(x) = \mathrm{Ref}_{\tilde{\Pi}_1}\,\mathrm{Ref}_{\tilde{\Pi}_2}(x), \quad x \in \mathbb{R}^3,$$

where $\tilde{\Pi}_1, \tilde{\Pi}_2$ *are two neighboring planes from* D_l.

Proof. For $x \in \mathbb{R}^3$, there holds the decomposition $x = (x \cdot \nu_l)\nu_l + H(x)$. Thus

$$\begin{aligned}\mathrm{Rot}_{l,2\pi/D_l^\#}(x) &= (x \cdot \nu_l)\nu_l + \mathrm{Rot}_{l,2\pi/D_l^\#}(H(x))\\ &= (x \cdot \nu_l)\nu_l + \mathrm{Rot}^*_{2\pi/D_l^\#}(H(x)),\end{aligned}$$

and for any two neighboring planes $\tilde{\Pi}_1, \tilde{\Pi}_2 \in D_l$,

$$\begin{aligned}\mathrm{Ref}_{\tilde{\Pi}_1}\,\mathrm{Ref}_{\tilde{\Pi}_2}(x) &= (x \cdot \nu_l)\nu_l + \mathrm{Ref}_{\tilde{\Pi}_1}\,\mathrm{Ref}_{\tilde{\Pi}_2}(H(x))\\ &= (x \cdot \nu_l)\nu_l + \mathrm{Ref}^*_{l_1}\,\mathrm{Ref}^*_{l_2}(H(x)),\end{aligned}$$

where $l_j = \tilde{\Pi}_j \cap \Pi^*$ for $j = 1, 2$. It is seen from Lemma 4.2 that the angle formed by l_1 and l_2 is $2\pi/D_l^\#$. This implies that either

$$\mathrm{Rot}^*_{2\pi/D_l^\#}(H(x)) = \mathrm{Ref}^*_{l_1}\,\mathrm{Ref}^*_{l_2}(H(x))$$

or

$$\mathrm{Rot}^*_{2\pi/D_l^\#}(H(x)) = \mathrm{Ref}^*_{l_2}\,\mathrm{Ref}^*_{l_1}(H(x)),$$

which completes the proof. □

Lemma 4.6 (Rotational invariance). *We have that*

$$\mathrm{Rot}_{l,2\pi/D_l^\#}(u(x)) = u(\mathrm{Rot}_{l,2\pi/D_l^\#}(x)),$$
$$\mathrm{Rot}_{l,2\pi/D_l^\#}(\mathcal{P}) = \mathcal{P},$$
$$\mathrm{Rot}_{l,2\pi/D_l^\#}(\mathcal{S}) = \mathcal{S}.$$

Proof. Combining (3.2) and the above Lemma 4.5 gives

$$\begin{aligned}\mathrm{Rot}_{l,2\pi/D_l^\#}(u(x)) &= \mathrm{Ref}_{\tilde{\Pi}_1}\,\mathrm{Ref}_{\tilde{\Pi}_2}(u(x)) = \mathrm{Ref}_{\tilde{\Pi}_1}\big(u(\mathrm{Ref}_{\tilde{\Pi}_2}(x))\big)\\ &= u\big(\mathrm{Ref}_{\tilde{\Pi}_1}\,\mathrm{Ref}_{\tilde{\Pi}_2}(x)\big) = u\big(\mathrm{Rot}_{l,2\pi/D_l^\#}(x)\big),\end{aligned}$$

where $\tilde{\Pi}_1$ and $\tilde{\Pi}_2$ are two neighboring perfect planes from D_l. This together with Lemma 3.1 implies the other two equalities in Lemma 4.6 for $\mathcal{P}$ and $\mathcal{S}$. □

From Lemma 4.6, we see that the multiple action of the rotation $\mathrm{Rot}_{l,2\pi/D_l^\#}$ on a propagating direction of the compressional (resp. shear) part produces a propagating direction that still belongs to the compressional (resp. shear) part. Therefore, we obtain

Corollary 4.7. *We have*

$$\begin{aligned}G_{l,\mathbf{P}} &:= \{\mathrm{Rot}_{l,2j\pi/D_l^\#}(\mathbf{P}) : j = 1,2,\ldots,D_l^\#\} \subset \mathcal{P}, \quad \forall\,\mathbf{P} \in \mathcal{P},\\ G_{l,\mathbf{S}} &:= \{\mathrm{Rot}_{l,2j\pi/D_l^\#}(\mathbf{S}) : j = 1,2,\ldots,D_l^\#\} \subset \mathcal{S}, \quad \forall\,\boldsymbol{S} \in \mathcal{S}.\end{aligned} \tag{4.3}$$

Note that the set $G_{l,\mathbf{P}}$ (resp. $G_{l,\mathbf{S}}$) consists of the vertices of some $D_l^\#$-sided regular polygon centered at a point $O' \in l$, where the line segment $O'\mathbf{P}$ (resp. $O'\mathbf{S}$) is perpendicular to the straight line l in $\mathbb{R}^3$. In addition, using Lemma 4.3 one can prove that, for $1 \le j \le D^\#$,

$$\begin{aligned}A_{p,m}\,\mathbf{P}_m &= A_{p,n}\ \mathrm{Rot}_{l,2j\pi/D_l^\#}(\mathbf{P}_n) \qquad \text{if} \quad \mathrm{Rot}_{l,2j\pi/D_l^\#}(\mathbf{P}_n) = \mathbf{P}_m,\\ A_{s,m}\,\mathbf{S}_m^\perp &= A_{s,n}\ \mathrm{Rot}_{l,2j\pi/D_l^\#}(\mathbf{S}_n^\perp) \qquad \text{if} \quad \mathrm{Rot}_{l,2j\pi/D_l^\#}(\mathbf{S}_n) = \mathbf{S}_m.\end{aligned}$$

4.3 Unidentifiable grating profiles which remain invariant in x_2-direction

The main task of this subsection is to find all the grating profiles in $\mathcal{A}_1$ that cannot be uniquely identified by one incident shear wave under the boundary conditions of the third kind. We make the additional assumption that

(A3) $\Lambda_1, \Lambda_2 \in \mathcal{A}_1$, so that both Λ_1 and Λ_2 remain invariant in the x_2-direction. We may suppose that the x_2-axis coincides with the intersection line of the perfect planes Π_1, Π_2 extending two neighboring faces of Λ_1. For simplicity, we use the symbols Rot_φ, D, $G_{\mathbf{P}}$, $G_{\mathbf{S}}$ to denote $\mathrm{Rot}_{l,\varphi}$, D_l, $G_{l,\mathbf{P}}$, $G_{l,\mathbf{S}}$, respectively, with the straight line l replaced by the x_2-axis. Then $\Pi_1, \Pi_2 \in D$, and by Lemma 4.2, $2 \le D^\# < \infty$. Recalling the incident direction $\mathbf{S}_\kappa = k_s\hat{\theta}$, with the incident angle $\hat{\theta}$ defined in (2.1), by (4.3) we have that $G_{\mathbf{S}_\kappa} \subset \Pi := \{x_2 = k_s \sin\theta_1 \sin\theta_2\}$.

Lemma 4.8. *Under the assumptions* **(A1)–(A3)**, *we have*

(1) $2 \le D^\# \le 4$.

(2) *If* $D^\# = 2$, *then setting* $Q_s := \{(\pm\alpha_n^{(1)}, \alpha_n^{(2)}, 0) : |\alpha_n|^2 = k_s^2\}$ *we have*

$$\{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa)\} \subseteq \mathcal{S} \subseteq \{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa)\} \cup Q_s, \quad \mathcal{P} \subseteq Q_p. \tag{4.4}$$

Moreover, if there exists some $\mathbf{P}_n \in \mathcal{P}\backslash\{\pm k_p e_2\}$ *or* $\mathbf{S}_n \in Q_s \cap \mathcal{S}$, *then we have* $\alpha_1 = k_s \sin\theta_1 \cos\theta_2 = 0$ *and* $D = \Pi_1 \cup \Pi_2$ *with* $\Pi_1 = \{x_1 = 0\}$, $\Pi_2 = \{x_3 = 0\}$.

(3) *If* $D^\# = 3$, *then*

$$\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_{2\pi/3}(\mathbf{S}_\kappa), \mathrm{Rot}_{4\pi/3}(\mathbf{S}_\kappa)\}, \quad \mathcal{P} \subseteq \{\pm k_p e_2\}.$$

(4) *If* $D^\# = 4$, *then*

$$\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_{\pi/2}(\mathbf{S}_\kappa), \mathrm{Rot}_\pi(\mathbf{S}_\kappa), \mathrm{Rot}_{3\pi/2}(\mathbf{S}_\kappa)\}, \quad \mathcal{P} \subseteq \{\pm k_p e_2\}.$$

Proof. (1) By Corollary 4.7, we observe that $G_{\mathbf{S}_\kappa} \subset \mathcal{S}$ consists of the $D^\#$ vertices of some regular polygon centered at $(0, k_s \sin\theta_1 \sin\theta_2, 0) \in \Pi$ and that the x_2-axis is perpendicular to the plane Π. If $D^\# \ge 5$, then there are at least two elements in $G_{\mathbf{S}_\kappa}$, each of them has a negative x_3-component. However, this is impossible by Remark 4.1. Since $\Pi_1, \Pi_2 \in D$, we arrive at $2 \le D^\# \le 4$.

(2) Assume $D^\# = 2$ with $D = \{\Pi_1, \Pi_2\}$. From Lemma 4.2 above, we see that $\Pi_1 \perp \Pi_2$, i.e., the dihedral angle between Π_1 and Π_2 is the right angle. Applying the rotational invariance gives the relation $\mathrm{Rot}_\pi(\mathbf{S}_n) \in \mathcal{S}$ for all $\mathbf{S}_n \in \mathcal{S}$, and in particular $\mathrm{Rot}_\pi(\mathbf{S}_\kappa) \in \mathcal{S}$. Thus

$$\{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa)\} \subseteq \mathcal{S}.$$

Since $\mathrm{Rot}_\pi(x) = (-x_1, x_2, -x_3)$ for $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, all the points in $\mathcal{S}\backslash\{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa)\}$ are located on the circle $B_{k_s}(O) \cap \{x_3 = 0\}$ and are symmetric with respect to the x_2-axis. This implies that the elements of $\mathcal{S}$ satisfy the relation (4.4). The relation (4.4) for the elements of $\mathcal{P}$ can be proved similarly.

If there exists some $n \in \mathbb{Z}^2$ such that $\mathbf{P}_n = (\alpha_n^{(1)}, \alpha_n^{(2)}, 0) \in \mathcal{P}\backslash\{\pm k_p e_2\}$, then by the rotational invariance,

$$\mathrm{Rot}_\pi(\mathbf{P}_n) = (-\alpha_n^{(1)}, \alpha_n^{(2)}, 0) \in \mathcal{P}\backslash\{\pm k_p e_2\}.$$

Note that $\{\pm k_p e_2\}$ is a subset of Q_p. As Π_j $(j = 1, 2)$ passes through the x_2-axis, the reflectional invariance applied to $\mathcal{P}$ yields that one plane in D, say Π_1, coincides with $\{x_1 = 0\}$, while the other plane can be written as $\Pi_2 = \{x_3 = 0\}$. Since

$$\mathrm{Rot}_\pi(\mathbf{S}_\kappa) = k_s(-\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2, \cos\theta_1) \in \mathcal{S},$$

by the reflectional invariance it holds that

$$\mathrm{Ref}_{\Pi_2}(\mathrm{Rot}_\pi(\mathbf{S}_\kappa)) = k_s(-\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2, -\cos\theta_1) \in \mathcal{S}$$

with a negative x_3-component, $-\cos\theta_1$. However, recalling that $\mathbf{S}_\kappa$ is the only element in $\mathcal{S}$ whose x_3-component is negative, we obtain

$$\mathrm{Ref}_{\Pi_2}(\mathrm{Rot}_\pi(\mathbf{S}_\kappa)) = \mathbf{S}_\kappa = k_s(\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2, -\cos\theta_1),$$

which implies that $\alpha_1 = k_s\sin\theta_1\cos\theta_2 = 0$. The case of $\mathbf{S}_n \in Q_s \cap \mathcal{S} \neq \emptyset$ for some $n \in S$ can be proved similarly.

(3) If $D^\# = 3$, it is seen from (4.3) that

$$G_{\mathbf{S}_\kappa} = \{\mathbf{S}_\kappa, \mathrm{Rot}_{2\pi/3}(\mathbf{S}_\kappa), \mathrm{Rot}_{4\pi/3}(\mathbf{S}_\kappa)\} \subseteq \mathcal{S}.$$

If $\mathbf{S}_n \in \mathcal{S}\backslash G_{\mathbf{S}_\kappa}$ for some $n \in S$, then one element in $G_{\mathbf{S}_n} \subseteq \mathcal{S}$ must have a negative x_3-component, contradicting Remark 4.1. Thus $G_{\mathbf{S}_\kappa} = \mathcal{S}$. In addition, one further obtains that $\mathbf{S}_\kappa$ must lie on one perfect plane from D, say Π_1, while $\mathrm{Rot}_{2\pi/3}(\mathbf{S}_\kappa)$ and $\mathrm{Rot}_{4\pi/3}(\mathbf{S}_\kappa)$ belong to the other two perfect planes $\Pi_3 \in D$ and $\Pi_2 \in D$, respectively; see Figure 3. In fact, if $\mathbf{S}_\kappa$ does not belong to any perfect plane in D, a contradiction to Remark 4.1 can be derived by employing the reflectional invariance.

If $\mathbf{P} \in \mathcal{P}$, then by equation (4.3) we get $G_\mathbf{P} \subseteq \mathcal{P}$. However, this is possible only if $\mathbf{P} \in \{\pm k_p e_2\}$, because the x_3-components of the elements in $\mathcal{P}$ are all non-negative and the perfect planes in D all pass through the x_2-axis. Thus $\mathcal{P} \subseteq \{\pm k_p e_2\}$.

(4) The case of $D^\# = 4$ can be proved analogously to that of $D^\# = 3$. □

We remark that all the possible propagating directions of the total field, indicated in Lemma 4.8, are determined by the form of the incident shear wave. Employing the reflectional and rotational invariance of these directions and the perfect planes that pass through the origin, we can determine each perfect plane in D, while the perfect planes that do not pass through the origin can be determined via a coordinate translation. This will be carried out in the following sections. Since

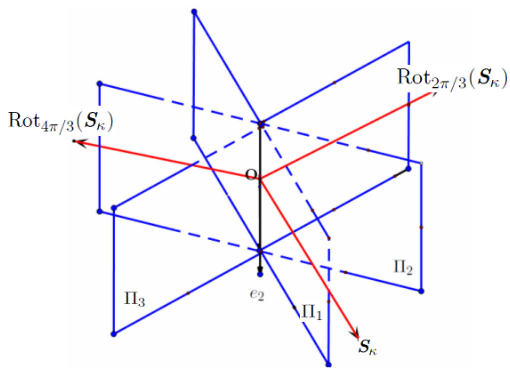

Figure 3. $\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_{\pi/3}(\mathbf{S}_\kappa), \mathbf{S}, \mathrm{Rot}_{2\pi/3}(\mathbf{S})\}$ if $D^\# = 3$.

each face of $\Lambda_1 \cup \Lambda_2$ can be extended to a perfect plane, all the unidentifiable grating profiles can be characterized. We next proceed by considering the possible number of elements in D separately.

Unidentifiable grating profiles in the case $D^\# = 2$

Lemma 4.9. *Suppose that* **(A1)–(A3)** *hold,* $D^\# = 2$ *and that one plane from* D*, say* Π_1*, passes through* $\mathbf{S}_\kappa$*. Then* $D = \{\Pi_1, \Pi_2\}$ *with* $\Pi_1 \perp \Pi_2$*, and the normal directions* ν_{Π_j} *corresponding to* Π_j $(j = 1, 2)$ *are given by*

$$\begin{aligned} \nu_{\Pi_1} &= \hat{\theta} \times e_2 = (\cos\theta_1, 0, -\sin\theta_1\cos\theta_2), \\ \nu_{\Pi_2} &= e_2 \times \nu_{\Pi_1} = (\sin\theta_1\cos\theta_2, 0, -\cos\theta_1), \end{aligned} \tag{4.5}$$

so that the plane Π_j *is defined by* $\nu_{\Pi_j} \cdot x = 0$ *for* $j = 1, 2$*. In addition,* $\nu_{\Pi_1} \perp \hat{\theta}^\perp$*.*

Proof. That $D = \{\Pi_1, \Pi_2\}$ with $\Pi_1 \perp \Pi_2$ follows from Lemma 4.2 applied to the case $D^\# = 2$. Since $\mathrm{Ref}_{\Pi_1}(\mathbf{S}_\kappa) = \mathbf{S}_\kappa$ and $\nu_{\Pi_1} \perp \nu_{\Pi_2}$, we may write $\nu_{\Pi_1} = \hat{\theta} \times e_2$ and $\nu_{\Pi_2} = e_2 \times \nu_{\Pi_1}$, noting that $\mathbf{S}_\kappa = k_s \hat{\theta}$ and that both Π_1 and Π_2 pass through the x_2-axis. It is seen from Corollary 4.4 (1) that $\hat{\theta}^\perp \in \Pi_1$ and thus $\nu_{\Pi_1} \perp \hat{\theta}^\perp$. □

Since $D^\# = 2$, using $\mathrm{Rot}_\pi(\cdot) = \mathrm{Ref}_{\Pi_1}\mathrm{Ref}_{\Pi_2}(\cdot) = \mathrm{Ref}_{\Pi_2}\mathrm{Ref}_{\Pi_1}(\cdot)$ we obtain that (see Figure 4, left)

$$\begin{aligned} \mathrm{Ref}_{\Pi_2}(\mathbf{S}_\kappa) &= \mathrm{Rot}_\pi(\mathbf{S}_\kappa), \\ \mathrm{Ref}_{\Pi_1}(\mathbf{S}_\kappa) &= \mathbf{S}_\kappa, \\ \mathrm{Ref}_{\Pi_1}(\mathrm{Rot}_\pi(\mathbf{S}_\kappa)) &= \mathrm{Rot}_\pi(\mathbf{S}_\kappa). \end{aligned} \tag{4.6}$$

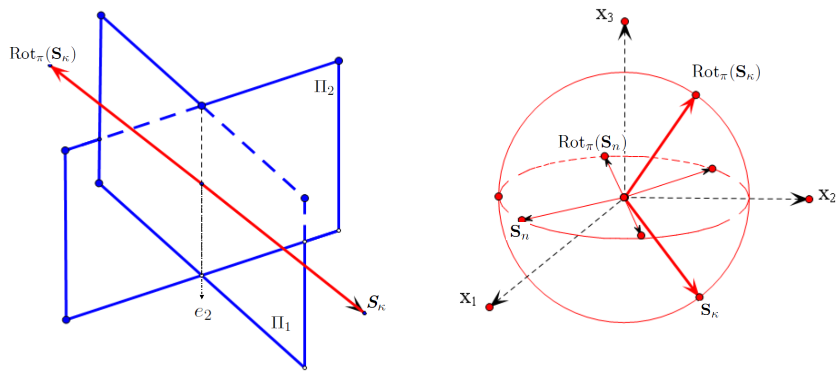

Figure 4. The elements of $\mathcal{S}$ in the case of $D = \{\Pi_1, \Pi_2\}$ with $\mathbf{S}_\kappa = k_s\hat{\theta} \in \Pi_1$. Left figure: $\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa)\}$ if $\alpha_1 = k_s \sin\theta_1 \cos\theta_2 \neq 0$; Right figure: $\mathcal{S} \subseteq \{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa)\} \cup Q_s$, with $\mathbf{S}_n \in Q_s$ for some $n \in \pi_s$, if $\alpha_1 = k_s \sin\theta_1 \cos\theta_2 = 0$.

We next introduce the first class $U_1 := U_1(\theta_1, \theta_2, k_s, \hat{\theta}^\perp)$ of unidentifiable grating profiles. Let $\nu_{\Pi_j} \in \mathbb{R}^3$ $(j = 1, 2)$ be defined by (4.5). If $\nu_{\Pi_1} \cdot \hat{\theta}^\perp = 0$ and $2k_s \sin\theta_1 \cos\theta_2 \in \mathbb{Z}$, U_1 is defined as

$$\begin{aligned} U_1 = \Big\{\Lambda \in \mathcal{A}_1 :\ & \text{each face of } \Lambda \text{ lies on a plane defined by } \nu_{\Pi_1} \cdot x + C = 0 \\ & \text{for some } C \in \mathbb{R}, \text{ or on a plane given by } \nu_{\Pi_2} \cdot x + m\pi/k_s = 0 \\ & \text{for some } m \in \mathbb{Z}, \text{ where } \nu_{\Pi_j} \text{ are defined in (4.5)}\Big\}. \end{aligned}$$

If $\nu_{\Pi_1} \cdot \hat{\theta}^\perp \neq 0$ or $2k_s \sin\theta_1 \cos\theta_2 \notin \mathbb{Z}$, the set U_1 is defined as the empty set.

Lemma 4.10. *Under the assumptions of Lemma* 4.9, *we have* $\Lambda_1, \Lambda_2 \in U_1$, *and the total field* $u = u_1 = u_2$ *takes the form*

$$\begin{aligned} u = \ & \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta}) + \mathrm{Rot}_\pi(\hat{\theta}^\perp) \exp(ik_s x \cdot \mathrm{Rot}_\pi(\hat{\theta})) \\ & + [C^+ \exp(ik_p x_2) - C^- \exp(-ik_p x_2)] e_2 \\ & + \sum_{n \in \tilde{\pi}_p} \Big[(n_1, \alpha_n^{(2)}, 0)^\top \exp(in_1 x_1 + i\alpha_n^{(2)} x_2) \\ & \qquad + (-n_1, \alpha_n^{(2)}, 0)^\top \exp(-in_1 x_1 + i\alpha_n^{(2)} x_2) \Big] A_{p,n} \\ & + \sum_{n \in \pi_s} \Big[(-\alpha_n^{(2)}, n_1, 0)^\top \exp(in_1 x_1 + i\alpha_n^{(2)} x_2) \\ & \qquad + (\alpha_n^{(2)}, n_1, 0)^\top \exp(-in_1 x_1 + i\alpha_n^{(2)} x_2) \Big] A_{s,n}, \end{aligned}$$

where $\tilde{\pi}_p = \{n \in \pi_p : (\alpha_n, 0) \notin \{\pm k_p e_2\}\}$, *and* $C^\pm, A_{p,n}, A_{s,n} \in \mathbb{C}$ *are determined as follows. If* $\pm k_p - k_s \sin\theta_1 \sin\theta_2 \in \mathbb{Z}$ *and* $k_s \sin\theta_1 \cos\theta_2 \in \mathbb{Z}$, *then* $C^\pm$

is an arbitrary constant; otherwise $C^{\pm} = 0$*. For* $n = (n_1, n_2) \in \tilde{\pi}_p$ *(resp.* π_s*), the Rayleigh coefficient* $A_{p,n}$ *(resp.* $A_{s,n}$*) is an arbitrary constant if* $\sin\theta_1 \cos\theta_2 = 0$ *and* $\frac{C}{\pi \cos\theta_1} n_1 \in \mathbb{Z}$ *for each* C *involved in the definition of* U_1*; otherwise, we have* $A_{p,n} = 0$ *(resp.* $A_{s,n} = 0$*).*

Proof. We first check that the total field u indeed takes the form as indicated above. Noting that $\{\pm k_p e_2\} \subseteq Q_p$, by Lemma 4.8 (2), we may write the compressional part of u as

$$\begin{aligned} u_p = {} & [C^+ \exp(i k_p x_2) - C^- \exp(-i k_p x_2)] e_2 \\ & + \sum_{n \in \tilde{\pi}_p} \Big[A^+_{p,n} (\alpha_n^{(1)}, \alpha_n^{(2)}, 0)^\top \exp(i\alpha_n^{(1)} x_1 + i\alpha_n^{(2)} x_2) \\ & \qquad + A^-_{p,n} (-\alpha_n^{(1)}, \alpha_n^{(2)}, 0)^\top \exp(-i\alpha_n^{(1)} x_1 + i\alpha_n^{(2)} x_2) \Big], \end{aligned}$$

where $\tilde{\pi}_p = \{n \in \pi_p : (\alpha_n, 0) \notin \{\pm k_p e_2\}\}$, and $C^{\pm}, A^{\pm}_{p,n} \in \mathbb{C}$. If $A^+_{p,n} \neq 0$, then

$$(\alpha_n^{(1)}, \alpha_n^{(2)}, 0) \in \mathcal{P} \backslash \{\pm k_p e_2\};$$

if $A^-_{p,n} \neq 0$, then

$$(-\alpha_n^{(1)}, \alpha_n^{(2)}, 0) \in \mathcal{P} \backslash \{\pm k_p e_2\}.$$

Using Lemma 4.8 (2) and Lemma 4.3 (2), we see that $A^-_{p,n} = A^+_{p,n} =: A_{p,n} \neq 0$ and $\alpha_1 = k_s \sin\theta_1 \cos\theta_2 = 0$ if either $A^+_{p,n} \neq 0$ or $A^-_{p,n} \neq 0$. On the other hand, if $C^{\pm} \neq 0$, the α-quasi-periodicity (2.7) of u_p gives the relations

$$\pm k_p - k_s \sin\theta_1 \sin\theta_2 \in \mathbb{Z} \quad \text{and} \quad k_s \sin\theta_1 \cos\theta_2 \in \mathbb{Z}.$$

Analogously, using the relations in (4.6) and Lemma 4.3 (3), we obtain that the shear part u_s takes the form

$$\begin{aligned} u_s = {} & \hat{\theta}^{\perp} \exp(i k_s x \cdot \hat{\theta}) + \mathrm{Rot}_\pi(\hat{\theta}^{\perp}) \exp(i k_s x \cdot \mathrm{Rot}_\pi(\hat{\theta})) \\ & + \sum_{n \in \pi_s} \Big[(-\alpha_n^{(2)}, n_1, 0)^\top \exp(i n_1 x_1 + i\alpha_n^{(2)} x_2) \\ & \qquad + (\alpha_n^{(2)}, n_1, 0)^\top \exp(-i n_1 x_1 + i\alpha_n^{(2)} x_2) \Big] A_{s,n} \end{aligned}$$

and that $\alpha_1 = k_s \sin\theta_1 \cos\theta_2 = 0$ if $A_{s,n} \neq 0$ for some $n \in \pi_s$. In addition, it is seen from

$$\mathrm{Rot}_\pi(\hat{\theta}) = (-\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2, \cos\theta_1)$$

and the α-quasi-periodicity of u_s that it holds $2k_s \sin\theta_1 \cos\theta_2 \in \mathbb{Z}$, and from Corollary 4.4 (1) that $\nu_{\Pi_1} \cdot \hat{\theta}^{\perp} = 0$.

In summary, the total field $u = u_p + u_s$ indeed takes the form given in Lemma 4.10, and

- $\nu_{\Pi_1} \cdot \hat{\theta}^{\perp} = 0$, $2k_s \sin\theta_1 \cos\theta_2 \in \mathbb{Z}$,
- $A^+_{p,n} \neq 0$ or $A^-_{s,n} \neq 0$ implies $\sin\theta_1 \cos\theta_2 = 0$,
- $C^{\pm} \neq 0$ implies $\pm k_p - k_s \sin\theta_1 \sin\theta_2 \in \mathbb{Z}$, $k_s \sin\theta_1 \cos\theta_2 \in \mathbb{Z}$.

Next we shall prove that $\Lambda_1, \Lambda_2 \in U_1$. To this end, we need to determine the planes containing a face of $\Lambda_1 \cup \Lambda_2$ that do not pass through the origin.

Let

$$\Pi_0 : \nu_0 \cdot x + \nu_0 \cdot y = 0 \quad \text{with some fixed } y \in \mathbb{R}^3,\ \nu_0 \in \mathbb{R}^3$$

be another perfect plane of u, extending some face of $\Lambda_1 \cup \Lambda_2$ on which the total field u defined in Lemma 4.10 satisfies the boundary conditions of the third kind. Define $v(x) := u(x-y)$. Then, the shear part of v, $v_s(x) = u_s(x-y)$, can be decomposed into the sum $V_s + \sum_{n\in\pi_s} A_{s,n} V_{s,n}$, where

$$\begin{aligned} V_s(x) = {} & \hat{\theta}^{\perp} \exp(ik_s x\cdot\hat{\theta}) \exp(-ik_s y\cdot\hat{\theta}) \\ & + \mathrm{Rot}_\pi(\hat{\theta}^{\perp}) \exp(ik_s x\cdot \mathrm{Rot}_\pi(\hat{\theta})) \exp(-ik_s y\cdot\mathrm{Rot}_\pi(\hat{\theta})), \end{aligned} \tag{4.7}$$

$$\begin{aligned} V_{s,n}(x) = {} & (-\alpha_n^{(2)}, n_1, 0)^\top \exp(in_1x_1 + i\alpha_n^{(2)}x_2) \exp(-in_1y_1 - i\alpha_n^{(2)}y_2) \\ & + (\alpha_n^{(2)}, n_1, 0)^\top \exp(-in_1x_1 + i\alpha_n^{(2)}x_2) \\ & \times \exp(in_1y_1 - i\alpha_n^{(2)}y_2), \end{aligned} \tag{4.8}$$

while the compressional part of v, $v_p(x) = u_p(x-y)$, can be written as

$$v_p = V_p + \sum_{n\in\tilde{\pi}_p} A_{p,n} V_{p,n},$$

where

$$\begin{aligned} V_p(x) = {} & e_2[C^+ \exp(ik_px_2)\exp(-ik_py_2) \\ & - C^- \exp(-ik_px_2)\exp(ik_py_2)], \end{aligned} \tag{4.9}$$

$$\begin{aligned} V_{p,n}(x) = {} & (n_1, \alpha_n^{(2)}, 0)^\top \exp(in_1x_1 + i\alpha_n^{(2)}x_2) \exp(-in_1y_1 - i\alpha_n^{(2)}y_2) \\ & + (-n_1, \alpha_n^{(2)}, 0)^\top \exp(-in_1x_1 + i\alpha_n^{(2)}x_2) \\ & \times \exp(in_1y_1 - i\alpha_n^{(2)}y_2). \end{aligned} \tag{4.10}$$

The function $v(x)$ satisfies the Navier equation in $\mathbb{R}^3$ with the third kind boundary conditions on the plane $\Pi_0' : \nu_0 \cdot x = 0$. One may further observe that v has the same propagating directions as u. Since $\Lambda_j \in \mathcal{A}_1$, $j = 1, 2$, we know that Π_0' passes through the x_2-axis, and that either $\Pi_0' = \Pi_2$ or $\Pi_0' = \Pi_1$ holds.

Case (i) $\Pi_0' = \Pi_2$.

In this case, we have $\nu_0 = \nu_{\Pi_2}$, and by (4.6), $\mathrm{Ref}_{\Pi_0'}(\mathbf{S}_\kappa) = \mathrm{Rot}_\pi(\mathbf{S}_\kappa)$. Applying Lemma 4.3 (3) to V_s gives the relation

$$\exp(-ik_s y \cdot \hat{\theta}) = \exp(-ik_s y \cdot \mathrm{Rot}_\pi(\hat{\theta})),$$

which implies that

$$k_s y \cdot (\hat{\theta} - \mathrm{Rot}_\pi(\hat{\theta})) = 2m\pi$$

for some $m \in \mathbb{Z}$. Since $\hat{\theta} - \mathrm{Rot}_\pi(\hat{\theta}) = 2\nu_{\Pi_2}$, we obtain that $y \cdot \nu_{\Pi_2} = m\pi/k_s$ for some $m \in \mathbb{Z}$. If $A_{s,n} \neq 0$ for some $n \in \pi_s$, then by Lemma 4.8 (2), we have $\alpha_1 = 0$, $\Pi_0' = \{x_3 = 0\}$ and $\nu_0 = \nu_{\Pi_2} = (0, 0, -\cos\theta_1)$. Thus $Q_s \subset \Pi_0'$. By Corollary 4.4 (3), this implies that the function $V_{s,n}$ defined in (4.8) always satisfy the Navier equation and the boundary conditions of the third kind on Π_0'. We obtain the same for the function $V_{p,n}$ defined in (4.9) since $Q_p \subset \{x_3 = 0\}$ using similar arguments and Lemma 4.8 (2) above. Therefore, Π_0 can be written as $\{x \in \mathbb{R}^3 : \nu_{\Pi_2} \cdot x + m\pi/k_s = 0\}$ for some $m \in \mathbb{Z}$, and Π_0 coincides with Π_2 if $m = 0$.

Case (ii) $\Pi_0' = \Pi_1$.

In this case, we have $\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa) \in \Pi_0'$ and $\nu_0 = \nu_{\Pi_1}$. Since Π_0' passes through the x_2-axis and both $\mathbf{S}_\kappa$ and $\mathrm{Rot}_\pi(\mathbf{S}_\kappa)$ belong to Π_0', the functions V_p and V_s, defined by (4.9) and (4.7) respectively, both satisfy the boundary conditions of the third kind on the plane $\{\nu_{\Pi_1} \cdot x + C = 0\}$, where $C = \nu_{\Pi_1} \cdot y$ for some $y = (y_1, y_2, y_3) \in \mathbb{R}^3$.

If $A_{p,n} \neq 0$ for some $n \in \tilde{\pi}_p$ (resp. $A_{s,n} \neq 0$ for some $n \in \pi_s$), it is seen from Lemma 4.8 (2) that $\Pi_0' = \Pi_1 = \{x_1 = 0\}$, $\nu_{\Pi_1} = (\cos\theta_1, 0, 0)$, and thus

$$\mathrm{Ref}_{\Pi_0'}\{(n_1, \alpha_n^{(2)}, 0)\} = \{(-n_1, \alpha_n^{(2)}, 0)\}.$$

Together with Lemma 4.3 (2) applied to (4.10) (resp. Lemma 4.3 (3) applied to (4.8)), this gives the identity

$$\exp(-in_1 y_1 - i\alpha_n^{(2)} y_2) = \exp(in_1 y_1 - i\alpha_n^{(2)} y_2),$$

which implies that $n_1 y_1 = m\pi$ for some $m \in \mathbb{Z}$. Therefore,

$$C = y \cdot \nu_{\Pi_1} = y_1 \cos\theta_1 = \frac{m\pi}{n_1}\cos\theta_1, \quad \text{for some } m \in \mathbb{Z}, \quad \forall\, n = (n_1, n_2) \in \tilde{\pi}_p \cup \pi_s.$$

It means that if $A_{p,n} \neq 0$ for some $n = (n_1, n_2) \in \tilde{\pi}_p$ or if $A_{s,n} \neq 0$ for some $n = (n_1, n_2) \in \pi_s$, then

$$\frac{C}{\pi \cos\theta_1} n_1 \in \mathbb{Z}, \quad \text{for each } C \text{ involved in the definition of } U_1.$$

The proof of Lemma 4.10 is thus complete. □

Lemma 4.11. *Suppose that* **(A1)–(A3)** *hold,* $D^{\#} = 2$*, and that each plane from* D *does not pass through* $\boldsymbol{S}_\kappa$*. Then*

(1) $\mathcal{S} = \{\boldsymbol{S}_\kappa, \mathrm{Rot}_\pi(\boldsymbol{S}_\kappa), \boldsymbol{S}, \mathrm{Rot}_\pi(\boldsymbol{S})\}$*, where* $\boldsymbol{S}_\kappa$ *is the incident direction, and* $\boldsymbol{S}$*,* $\mathrm{Rot}_\pi(\boldsymbol{S})$ *are given by*

$$\begin{aligned} \boldsymbol{S} &= k_s\Big(\sqrt{1-\sin^2\theta_1\sin^2\theta_2}, \sin\theta_1\sin\theta_2, 0\Big), \\ \mathrm{Rot}_\pi(\boldsymbol{S}) &= k_s\Big(-\sqrt{1-\sin^2\theta_1\sin^2\theta_2}, \sin\theta_1\sin\theta_2, 0\Big). \end{aligned} \tag{4.11}$$

(2) $D = \{\Pi_1, \Pi_2\}$ *with* $\Pi_1 \perp \Pi_2$*. Moreover, the normal directions* ν_{Π_j} *corresponding to* Π_j $(j = 1, 2)$ *are given by*

$$\begin{aligned} \nu_{\Pi_1} &= \Big(\sqrt{1-\sin^2\theta_1\sin^2\theta_2} - \sin\theta_1\cos\theta_2, 0, \cos\theta_1\Big), \\ \nu_{\Pi_2} &= \Big(-\sqrt{1-\sin^2\theta_1\sin^2\theta_2} - \sin\theta_1\cos\theta_2, 0, \cos\theta_1\Big). \end{aligned} \tag{4.12}$$

(3) *We have*

$$k_s\Big(\sin\theta_1\cos\theta_2 - \sqrt{1-\sin^2\theta_1\sin^2\theta_2}\Big) \in \mathbb{Z},$$

$$k_s\Big(\sin\theta_1\cos\theta_2 + \sqrt{1-\sin^2\theta_1\sin^2\theta_2}\Big) \in \mathbb{Z}.$$

(4) $\mathcal{P} \subseteq \{\pm k_p e_2\}$.

Proof. (1) Since $D^{\#} = 2$, by Lemma 4.2 we have $D = \{\Pi_1, \Pi_2\}$ with $\Pi_1 \perp \Pi_2$. Noting that $\mathbf{S}_\kappa \notin \Pi_j$ $(j = 1, 2)$, without loss of generality we may assume (see Figure 5)

$$\begin{aligned} \mathrm{Ref}_{\Pi_1}(\mathbf{S}_\kappa) &= (\alpha_n^{(1)}, \alpha_n^{(2)}, 0) := \mathbf{S}, \\ \mathrm{Ref}_{\Pi_1}(\mathrm{Rot}_\pi(\mathbf{S}_\kappa)) &= (-\alpha_n^{(1)}, \alpha_n^{(2)}, 0) \end{aligned} \tag{4.13}$$

for some $n \in \pi_s$. We claim that $\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa), (\pm\alpha_n^{(1)}, \alpha_n^{(2)}, 0)\}$. To prove this, we suppose there exists some $m = (m_1, m_2) \in \pi_s$ such that $n \neq m$ and $\{(\pm\alpha_m^{(1)}, \alpha_m^{(2)}, 0)\} \subset \mathcal{S}$. It follows from Corollary 4.4 (3) that $\{(\pm\alpha_m^{(1)}, \alpha_m^{(2)}, 0)\}$ does not coincide with $\{\pm k_s e_2\}$ and from equation (4.13) that $\Pi_1 \neq \{x_3 = 0\}$. Thus the elements in $\mathrm{Ref}_{\Pi_1}\{(\pm\alpha_m^{(1)}, \alpha_m^{(2)}, 0)\} \subset \mathrm{Ref}_{\Pi_1}\{x_3 = 0\}$ do not belong to the set Q_s defined by (4.4). In view of Lemma 4.9 (2), we have

$$\mathrm{Ref}_{\Pi_1}\{(\pm\alpha_m^{(1)}, \alpha_m^{(2)}, 0)\} = \{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa)\}.$$

However, this contradicts (4.13) and the fact that $n \neq m$. Thus

$$\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa), \mathbf{S}, \mathrm{Rot}_\pi(\mathbf{S}\}.$$

We see from $\mathbf{S} \in B_{k_s}(O)$ that $\alpha_n^{(1)}$ and $\alpha_n^{(2)}$ satisfy

$$(\alpha_n^{(1)})^2 + (\alpha_n^{(2)})^2 = k_s^2 \quad \text{and} \quad \alpha_n^{(2)} = k_s \sin\theta_1 \sin\theta_2,$$

which together with (4.13) yields the first assertion.

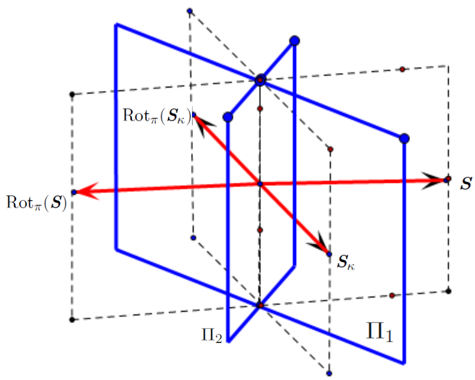

Figure 5. $\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa), \mathbf{S}, \mathrm{Rot}_\pi(\mathbf{S})\}$ if $D^\# = 2$ and $\mathbf{S}_\kappa \notin \Pi_j$ for $j = 1, 2$.

(2) The identities in (4.13) lead to $\mathrm{Ref}_{\Pi_1}(\mathbf{S}_\kappa) = \mathbf{S}$ and $\mathrm{Ref}_{\Pi_2}(\mathbf{S}_\kappa) = \mathrm{Rot}_\pi(\mathbf{S})$, from which we obtain that the normal directions ν_{Π_j} corresponding to Π_j are given by

$$\nu_{\Pi_1} = \frac{1}{k_s}(\mathbf{S} - \mathbf{S}_\kappa) = \Big(\sqrt{1 - \sin^2\theta_1 \sin^2\theta_2} - \sin\theta_1\cos\theta_2,\ 0\ \cos\theta_1\Big),$$

$$\nu_{\Pi_2} = \frac{1}{k_s}(\mathrm{Rot}_\pi(\mathbf{S}) - \mathbf{S}_\kappa) = \Big(-\sqrt{1 - \sin^2\theta_1 \sin^2\theta_2} - \sin\theta_1\cos\theta_2,\ 0\ \cos\theta_1\Big).$$

(3) The relations in the third assertion follow from the α-quasi-periodicity condition (2.7) applied to the four propagating directions of the shear part $\mathcal{S}$ indicated in Lemma 4.11 (1).

(4) If $\mathcal{P} \backslash \{\pm k_p e_2\} \neq \emptyset$, it follows from Lemma 4.9 (2) that $\sin\theta_1 \cos\theta_2 = 0$ and $\Pi_1 = \{x_1 = 0\}$. This implies that $\mathbf{S}_\kappa \in \Pi_1$, contradicting the assumption that no plane from D passes through $\mathbf{S}_\kappa$. Thus $\mathcal{P} \subseteq \{\pm k_p e_2\}$. □

Now we introduce the second class $U_2 = U_2(\theta_1, \theta_2, k_s)$ of unidentifiable grating profiles by setting

$$U_2 := \big\{\Lambda \in \mathcal{A}_1 : \text{each face of } \Lambda \text{ lies on a plane defined by } \nu_{\Pi_j} \cdot x + 2m\pi = 0 \\ \text{for some } m \in \mathbb{Z},\ j = 1, 2, \text{ with } \nu_{\Pi_j} \text{ given by (4.12)}\big\}$$

if $-k_s(\sin\theta_1\cos\theta_2 \pm \sqrt{1 - \sin^2\theta_1 \sin^2\theta_2}) \in \mathbb{Z}$, and by $U_2 := \emptyset$ otherwise.

Lemma 4.12. *Under the assumptions of Lemma* 4.11*, we have* $\Lambda_1, \Lambda_2 \in U_2$*, and the total field* $u = u_1 = u_2$ *takes the form*

$$u = \hat{\theta}^{\perp} \exp(ik_s x \cdot \hat{\theta}) + \mathrm{Rot}_{\pi}(\hat{\theta}^{\perp}) \exp(ik_s x \cdot \mathrm{Rot}_{\pi}(\hat{\theta}))$$
$$+ \mathrm{Ref}_{\Pi_1}(\hat{\theta}^{\perp}) \exp(ix \cdot \boldsymbol{S}) + \mathrm{Ref}_{\Pi_2}(\hat{\theta}^{\perp}) \exp(ix \cdot \mathrm{Rot}_{\pi}(\boldsymbol{S}))$$
$$+ [C^+ \exp(ik_p x_2) - C^- \exp(-ik_p x_2)] e_2,$$

where $\Pi_j = \{x : \nu_{\Pi_j} \cdot x = 0\}$ $(j = 1, 2)$ *with* ν_{Π_j} *defined in equation* (4.12)*,* $\boldsymbol{S} = k_s \, \mathrm{Ref}_{\Pi_1}(\hat{\theta})$ *and the constants* $C^{\pm} \in \mathbb{C}$ *are determined as in Lemma* 4.10.

Since Lemma 4.12 (and also the following Lemmas 4.14 and 4.16) can be proved analogously to Lemma 4.10, we omit the details for the sake of brevity.

Unidentifiable grating profiles in the case $D^{\#} = 3$

Lemma 4.13. *Assume that* **(A1)–(A3)** *hold and* $D^{\#} = 3$*. Then we have*

(1) $\mathcal{P} \subseteq \{\pm k_p e_2\}$ *and*

$$\mathcal{S} = \{\boldsymbol{S}_\kappa, \mathrm{Rot}_{2\pi/3}(\boldsymbol{S}_\kappa), \mathrm{Rot}_{4\pi/3}(\boldsymbol{S}_\kappa)\} = k_s\{\hat{\theta}, \mathrm{Rot}_{2\pi/3}(\hat{\theta}), \mathrm{Rot}_{4\pi/3}(\hat{\theta})\}$$

with

$$\mathrm{Rot}_{2\pi/3}(\hat{\theta}) = \Big(-\frac{1}{2}\sin\theta_1\cos\theta_2 - \frac{\sqrt{3}}{2}\cos\theta_1, \sin\theta_1\sin\theta_2,$$
$$-\frac{\sqrt{3}}{2}\sin\theta_1\cos\theta_2 + \frac{1}{2}\cos\theta_1\Big),$$
$$\mathrm{Rot}_{4\pi/3}(\hat{\theta}) = \Big(-\frac{1}{2}\sin\theta_1\cos\theta_2 + \frac{\sqrt{3}}{2}\cos\theta_1, \sin\theta_1\sin\theta_2,$$
$$\frac{\sqrt{3}}{2}\sin\theta_1\cos\theta_2 + \frac{1}{2}\cos\theta_1\Big).$$

(2) $D = \{\Pi_1, \Pi_2, \Pi_3\}$ *and*

$$\boldsymbol{S}_\kappa \in \Pi_1, \quad \mathrm{Rot}_{2\pi/3}(\boldsymbol{S}_\kappa) \in \Pi_2, \quad \mathrm{Rot}_{4\pi/3}(\boldsymbol{S}_\kappa) \in \Pi_3.$$

Moreover,

$$\Pi_j = \{x : \nu_{\Pi_j} \cdot x = 0\},$$

where the normal directions ν_{Π_j} *corresponding to* Π_j *are given by*

$$\begin{aligned}
\nu_{\Pi_1} &= \hat{\theta} \times e_2 = (\cos\theta_1,\ 0,\ \sin\theta_1\cos\theta_2),\\
\nu_{\Pi_2} &= e_2 \times \mathrm{Rot}_{2\pi/3}(\hat{\theta})\\
&= \left(-\frac{\sqrt{3}}{2}\sin\theta_1\cos\theta_2 + \frac{1}{2}\cos\theta_1, 0, \frac{1}{2}\sin\theta_1\cos\theta_2 + \frac{\sqrt{3}}{2}\cos\theta_1\right),\\
\nu_{\Pi_3} &= e_2 \times \mathrm{Rot}_{4\pi/3}(\hat{\theta})\\
&= \left(\frac{\sqrt{3}}{2}\sin\theta_1\cos\theta_2 + \frac{1}{2}\cos\theta_1, 0, \frac{1}{2}\sin\theta_1\cos\theta_2 - \frac{\sqrt{3}}{2}\cos\theta_1\right).
\end{aligned}$$

(3) $-\frac{3}{2}\sin\theta_1\cos\theta_2 \pm \frac{\sqrt{3}}{2}\cos\theta_1 \in \mathbb{Z},\ |\sqrt{3}\sin\theta_1\cos\theta_2| \le \cos\theta_1,\ \nu_{\Pi_1}\cdot\hat{\theta}^{\perp} = 0.$

Proof. The first assertion follows from Lemma 4.8 (3), while the second assertion can be derived from the proof of Lemma 4.8 (3) in combination with the fact that each Π_j passes through the x_2-axis. To prove the third assertion, making use of the α-quasi-periodicity we see that

$$\begin{aligned}
&\mathrm{Rot}_{2\pi/3}(\hat{\theta}) = \mathbf{S}_n = (\alpha_1 + n_1, \alpha_2 + n_2, \gamma_n) \quad \text{for some } n \in \mathbb{Z}^2, \text{ with } \gamma_n \ge 0,\\
&\mathrm{Rot}_{4\pi/3}(\hat{\theta}) = \mathbf{S}_m = (\alpha_1 + m_1, \alpha_2 + m_2, \gamma_m) \quad \text{for some } m \in \mathbb{Z}^2, \text{ with } \gamma_m \ge 0.
\end{aligned}$$

In view of the components of $\mathrm{Rot}_{2\pi/3}(\hat{\theta}), \mathrm{Rot}_{4\pi/3}(\hat{\theta})$ indicated in the first assertion, we arrive at

$$-\frac{3}{2}\sin\theta_1\cos\theta_2 \pm \frac{\sqrt{3}}{2}\cos\theta_1 \in \mathbb{Z}, \quad |\sqrt{3}\sin\theta_1\cos\theta_2| \le \cos\theta_1.$$

Finally, the relation

$$\nu_{\Pi_1}\cdot\hat{\theta}^{\perp} = 0$$

is a consequence of $\hat{\theta} \in \Pi_1$ and Corollary 4.4 (1). □

Define the third class $U_3 = U_3(\theta_1, \theta_2, k_s, \hat{\theta}^{\perp})$ of unidentifiable grating profiles by

$$U_3 := \Big\{\Lambda \in \mathcal{A}_1 : \text{each face of } \Lambda \text{ lies on a plane given by } \nu_{\Pi_j}\cdot x + \tfrac{4\pi}{k_s\sqrt{3}}m = 0 \text{ for some } m \in \mathbb{Z}, \text{ where } \nu_{\Pi_j}\ (j = 1,2,3) \text{ are defined in Lemma 4.13 (2)}\Big\}$$

if the conditions of Lemma 4.13 (3) are all satisfied, and by $U_3 := \emptyset$ if one of the conditions of Lemma 4.13 (3) is not satisfied.

Lemma 4.14. *Under the assumptions of Lemma* 4.13*, we have* $\Lambda_1, \Lambda_2 \in U_3$*, and the total field* $u = u_1 = u_2$ *takes the form*

$$u = \hat{\theta}^{\perp} \exp(ik_s x \cdot \hat{\theta}) + \mathrm{Rot}_{2\pi/3}(\hat{\theta}^{\perp}) \exp(ik_s x \cdot \mathrm{Rot}_{2\pi/3}(\hat{\theta})) + \mathrm{Rot}_{4\pi/3}(\hat{\theta}^{\perp}) \exp(ik_s x \cdot \mathrm{Rot}_{4\pi/3}(\hat{\theta})) + [C^+ \exp(ik_p x_2) - C^- \exp(-ik_p x_2)]e_2,$$

where the constants $C^{\pm} \in \mathbb{C}$ *are determined as in Lemma* 4.10.

Unidentifiable grating profiles in the case $D^{\#} = 4$

Lemma 4.15. *Assume that* **(A1)–(A3)** *hold and* $D^{\#} = 4$*. Then*

(1) $\mathcal{P} \subseteq \{\pm k_p e_2\}$, $\mathcal{S} = k_s\{\hat{\theta}, \mathrm{Rot}_{\pi/2}(\hat{\theta}), \mathrm{Rot}_{\pi}(\hat{\theta}), \mathrm{Rot}_{3\pi/2}(\hat{\theta})\}$ *with*

$$\hat{\theta} = (0, \sin\theta_1 \sin\theta_2, -\cos\theta_1),$$
$$\mathrm{Rot}_{\pi/2}(\hat{\theta}) = (-\cos\theta_1, \sin\theta_1 \sin\theta_2, 0),$$
$$\mathrm{Rot}_{\pi}(\hat{\theta}) = (0, \sin\theta_1 \sin\theta_2, \cos\theta_1),$$
$$\mathrm{Rot}_{3\pi/2}(\hat{\theta}) = (\cos\theta_1, \sin\theta_1 \sin\theta_2, 0).$$

(2) $\sin\theta_1 \cos\theta_2 = 0$, $\hat{\theta}^{\perp} \in \{x_3 = 0\}$ *and* $k_s \cos\theta_1 \in \mathbb{Z}$.

(3) $D = \{\Pi_1, \Pi_2, \Pi_3, \Pi_4\}$ *with*

$$\Pi_1 = \{x_1 = 0\}, \qquad \Pi_2 = \{x_1 = x_3\},$$
$$\Pi_3 = \{x_3 = 0\}, \qquad \Pi_4 = \{x_1 = -x_3\}.$$

Proof. By Lemma 4.8 (4), we have $\mathcal{P} \subseteq \{\pm k_p e_2\}$ and

$$\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_{\pi/2}(\mathbf{S}_\kappa), \mathrm{Rot}_{\pi}(\mathbf{S}_\kappa), \mathrm{Rot}_{3\pi/2}(\mathbf{S}_\kappa)\} = k_s\{\hat{\theta}, \mathrm{Rot}_{\pi/2}(\hat{\theta}), \mathrm{Rot}_{\pi}(\hat{\theta}), \mathrm{Rot}_{3\pi/2}(\hat{\theta})\}.$$

Analogously to the proof of Lemma 4.13 (2), one can verify that each element from $\mathcal{S}$ lies on some perfect plane in D. This implies that $\mathbf{S}_\kappa, \mathrm{Rot}_{\pi}(\mathbf{S}_\kappa) \in \{x_1 = 0\}$ and $\mathrm{Rot}_{\pi/2}(\hat{\theta}), \mathrm{Rot}_{3\pi/2}(\hat{\theta}) \in \{x_3 = 0\}$. By Lemma 4.2, without loss of generality, we may assume that

$$\Pi_1 = \{x_1 = 0\}, \quad \Pi_2 = \{x_1 = x_3\}, \quad \Pi_3 = \{x_3 = 0\}, \quad \Pi_4 = \{x_1 = -x_3\}.$$

The relations $\sin\theta_1 \cos\theta_2 = 0$ and $\hat{\theta}^{\perp} \in \{x_3 = 0\}$ follow from $\mathbf{S}_\kappa \in \{x_1 = 0\}$ and Corollary 4.4 (1), while $k_s \cos\theta_1 \in \mathbb{Z}$ is derived from the α-quasi-periodicity of u. □

Define the fourth class $U_4 = U_4(\theta_1, \theta_2, k_s, \hat{\theta}^\perp)$ of unidentifiable grating profiles by

$$U_4 = \Big\{\Lambda \in \mathcal{A}_1 : \text{each face of } \Lambda \text{ lies on a plane defined by } x_3 + \tfrac{\pi}{k_s} m = 0,\\ x_3 + \tfrac{\pi}{k_s} m = 0, \text{ or } x_3 \pm x_1 + \tfrac{2\pi}{k_s} m = 0 \text{ for some } m \in \mathbb{Z}\Big\}$$

if $k_s \cos\theta_1 \in \mathbb{Z}$, $\sin\theta_1 \cos\theta_2 = 0$ and $\hat{\theta}^\perp \in \{x_3 = 0\}$, and by $U_4 := \emptyset$ if one of the relations in Lemma 4.15 (2) is not satisfied.

Lemma 4.16. *Under the assumptions of Lemma* 4.15*, we have* $\Lambda_1, \Lambda_2 \in U_4$*, and the total field* $u = u_1 = u_2$ *takes the form*

$$\begin{aligned} u = {} & \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta}) + \mathrm{Rot}_{\pi/2}(\hat{\theta}^\perp) \exp(ik_s x \cdot \mathrm{Rot}_{\pi/2}(\hat{\theta})) \\ & + \mathrm{Rot}_{\pi}(\hat{\theta}^\perp) \exp(ik_s x \cdot \mathrm{Rot}_{\pi}(\hat{\theta})) \\ & + \mathrm{Rot}_{3\pi/2}(\hat{\theta}^\perp) \exp(ik_s x \cdot \mathrm{Rot}_{3\pi/2}(\hat{\theta})) \\ & + [C^+ \exp(ik_p x_2) - C^- \exp(-ik_p x_2)] e_2, \end{aligned}$$

where the constants $C^\pm \in \mathbb{C}$ *are determined as in Lemma* 4.10.

4.4 Unidentifiable grating profiles which vary in both the x_1 and x_2 directions

Throughout this section we assume $\Lambda_1, \Lambda_2 \in \mathcal{A}_2$, that is, Λ_j is not constant in x_2 and varies in x_1 and x_2 2π-periodically. In this case, there always exists a corner point of Λ_1 where at least three faces of Λ_1, $\Theta_1, \Theta_2, \dots, \Theta_N$ $(N \geq 3)$, meet together. This corner point is supposed to coincide with the origin O without loss of generality. Let Π_j $(j = 1, 2, \dots, N)$ be the perfect planes obtained by extending the faces Θ_j. These planes form at least N intersection lines that pass through O, which we denote by $l_1, l_2, \dots, l_N$ respectively. Without loss of generality, we assume

$$l_1 = \Pi_1 \cap \Pi_2, \quad l_2 = \Pi_2 \cap \Pi_3, \quad l_3 = \Pi_3 \cap \Pi_1.$$

Furthermore we suppose that l_j $(j = 1, 2, 3)$ are three non-coplanar lines in $\mathbb{R}^3$. Recalling the set D_l defined in (4.2), we obtain three equiangular systems of perfect planes D_{l_j} $(j = 1, 2, 3)$. Define

$$\begin{aligned} \mathcal{D} &= \{\Pi : \Pi \in D_{l_1} \cup D_{l_2} \cup D_{l_3}\}, \\ \mathcal{L} &= \{l : \exists\, \Pi, \tilde{\Pi} \in \mathcal{D} \text{ such that } l = \Pi \cap \tilde{\Pi}\}. \end{aligned}$$

The set $\mathcal{D}$ consists of all perfect planes passing through l_1, l_2 or l_3, whereas $\mathcal{L}$ consists of all intersection lines of any two planes from $\mathcal{D}$. Evidently, each element in $\mathcal{D}$ and $\mathcal{L}$ passes through the origin O.

Lemma 4.17. (1) *In the case of the boundary conditions of the third kind, the incident direction* $\boldsymbol{S}_\kappa = k_s\hat{\theta}$ *satisfies* $\boldsymbol{S}_\kappa \notin l$ *for all* $l \in \mathcal{L}$.

(2) $\mathrm{Ref}_\Pi(\mathcal{S}) = \mathcal{S}$ *and* $\mathrm{Ref}_\Pi(\mathcal{P}) = \mathcal{P}$ *for all* $\Pi \in \mathcal{D}$.

Proof. See Corollary 4.4 (2) and Lemma 4.3. □

We proceed to determine the finite number of the propagating directions of the total field and the perfect planes passing through O, relying on the above Lemma 4.17, and the reflectional and rotational invariance of the total field (Lemma 4.3 and Lemma 4.6). As one would expect, the arguments in this section will be more complicated than those in Section 4.3, because the grating profiles from $\mathcal{A}_2$ vary in both the x_1 and x_2 directions. Analogously to Lemmas 4.9,4.11,4.13 and 4.15, we establish the following lemma for $\Lambda_1, \Lambda_2 \in \mathcal{A}_2$, from which the fifth class of unidentifiable grating profiles can be derived (see Lemma 4.21).

Lemma 4.18. *Under the assumptions* **(A1)–(A2)** *and* $\Lambda_1, \Lambda_2 \in \mathcal{A}_2$*, we have:*

(1) *All points of* $\mathcal{S}$ *lie on one perfect plane in* $\mathcal{D}$*. Without loss of generality, we may assume that* $\mathcal{S} \subset \Pi_3$.

(2) $\mathcal{S} = \{\pm k_s\hat{\theta}, \pm\boldsymbol{S}\}$ *with* $\boldsymbol{S} = (y_1, y_2, 0) \in \mathbb{R}^3$*, where* $y_1, y_2 \in \mathbb{R}$ *satisfy*

$$y_1^2 + y_2^2 = k_s^2, \quad (\hat{\theta} \times \hat{\theta}^\perp) \cdot (y_1, y_2, 0) = 0.$$

(3) $\mathcal{D} = \{\Pi_1, \Pi_2, \Pi_3\}$ *with* $\Pi_1 \perp \Pi_2, \Pi_2 \perp \Pi_3, \Pi_3 \perp \Pi_1$*. Furthermore, the normal directions* ν_{Π_j} *corresponding to* Π_j $(j = 1, 2, 3)$ *are given by*

$$\nu_{\Pi_3} = \hat{\theta} \times \hat{\theta}^\perp, \quad \nu_{\Pi_1} = \boldsymbol{S} - \boldsymbol{S}_\kappa, \quad \nu_{\Pi_2} = \boldsymbol{S} + \boldsymbol{S}_\kappa.$$

(4) $\pm y_1 - k_s \sin\theta_1 \cos\theta_2 \in \mathbb{Z}$, $\pm y_2 - k_s \sin\theta_1 \sin\theta_2 \in \mathbb{Z}$.

(5) *If* $\hat{\theta} \times \hat{\theta}^\perp$ *is parallel to the plane* $\{x_3 = 0\}$*, then*

$$\mathcal{P} \subseteq \{\pm k_p(\hat{\theta} \times \hat{\theta}^\perp)/\|\hat{\theta} \times \hat{\theta}^\perp\|\};$$

otherwise $\mathcal{P} = \emptyset$.

Proof. We decompose the proof into three steps.

Step 1. Prove Lemma 4.18 if one of the lines l_j $(j = 1, 2, 3)$ is parallel to the plane $\{x_3 = 0\}$.

Without loss of generality, we may assume $l_1 \| \{x_3 = 0\}$. Two cases need to be considered.

Case (i): l_1 coincides with the x_2-axis.

Since l_j $(j = 1,2,3)$ are non-coplanar straight lines and $l_1 = \Pi_1 \cap \Pi_2$, the plane Π_3 cannot pass through the x_2-axis. Recall that in this case the sets D_{l_1} and $G_{l_1,\mathbf{S}_\kappa}$ (defined in (4.2) and (4.3)) are denoted by D and $G_{\mathbf{S}_\kappa}$, respectively, and that $G_{\mathbf{S}_\kappa} \subset \Pi := \{x_2 = k_s \sin\theta_1 \sin\theta_2\}$. It is seen from Lemma 4.8 (1) that $2 \le D^\# \le 4$. Based on Lemmas 4.8, 4.9, 4.13 and 4.15, we shall prove that $D^\# = 2$ and that each plane from D does not pass through $\mathbf{S}_\kappa$.

We first exclude the cases $D^\# = 3$ and $D^\# = 4$. In either of the cases, by Lemma 4.8, we have $\mathcal{S} = G_{\mathbf{S}_\kappa} \subset \Pi$. As $\mathrm{Ref}_{\Pi_3}(\mathcal{S}) = \mathcal{S}$, we know that either $\Pi_3 = \Pi$ or $\Pi_3 \perp \Pi$ holds. However, $\Pi_3 = \Pi$ together with Lemmas 4.13 and 4.15 would lead to the fact that each element of $G_{\mathbf{S}_\kappa}$ belongs to two different perfect planes of $\mathcal{D}$, one of which is Π_3 and the other one belongs to D, contradicting Corollary 4.4 (2). Moreover, $\Pi_3 \perp \Pi$ in combination with $O \in l_1, l_1 \perp \Pi$, $O \in \Pi_3$ would result in $l_1 \subset \Pi_3$, contradicting the assumption that l_1 does not lie on Π_3.

Thus $D^\# = 2$, and consequently $\mathcal{S} = \{\mathcal{S}_\kappa, \mathrm{Rot}_\pi(\mathcal{S}_\kappa)\} \cup Q_s$ by Lemma 4.8. We claim that $Q_s \neq \emptyset$. In fact, if $Q_s = \emptyset$, then $\mathcal{S}$ would only consist of two elements, $\mathbf{S}_\kappa$ and $\mathrm{Rot}_\pi(\mathbf{S}_\kappa)$. Since $\mathrm{Ref}_{\Pi_j}(\mathcal{S}) = \mathcal{S}$ for $j = 1,2,3$, there exist a point in $\mathcal{S}$ lying on two planes from $\{\Pi_1, \Pi_2, \Pi_3\}$, which is impossible due to Corollary 4.4 (2).

Next, we exclude the case that one plane of D passes through $\mathbf{S}_\kappa$ when $D^\# = 2$. Clearly, $D = \{\Pi_1, \Pi_2\}$ with $\Pi_1 \perp \Pi_2$. Assume $\mathcal{S}_\kappa \in \Pi_1$ without loss of generality. Since $Q_s \neq \emptyset$, it follows from Lemma 4.8 (2) that

$$\Pi_1 = \{x_1 = 0\}, \quad \Pi_2 = \{x_3 = 0\} \quad \text{and} \quad \sin\theta_1 \cos\theta_2 = 0.$$

Now we consider the straight line $l_2 = \Pi_2 \cap \Pi_3$, which lies on the plane $\{x_3 = 0\}$. We deduce from the previous argument in case (i) that $D^\#_{l_2} = 2$, which leads to $D_{l_2} = \{\Pi_2, \Pi_3\}$ with $\Pi_2 \perp \Pi_3$. Since $O \in \Pi_j$ $(j = 1,2,3)$, it follows that the straight line $l_3 = \Pi_3 \cap \Pi_1$ coincides with the x_3-axis. Thus, by Lemma 4.6 and equation (4.3), the elements in $G_{l_3,\mathbf{S}_\kappa}$ have the same x_3-component $-\gamma$ as $\mathbf{S}_\kappa$. However, this only happens if the set $G_{l_3,\mathbf{S}_\kappa}$ consists of one element $\mathbf{S}_\kappa$, or equivalently, $\mathbf{S}_\kappa \in l_3 \in \Pi_1 \cap \Pi_3$, which contradicts Corollary 4.4 (2).

Therefore, we have proved that $D = \{\Pi_1, \Pi_2\}$ with $\Pi_1 \perp \Pi_2$, and that neither Π_1 nor Π_2 goes through $\mathbf{S}_\kappa$. It follows from Lemma 4.11 that

$$\mathcal{S} = \{\mathbf{S}_\kappa, \mathrm{Rot}_\pi(\mathbf{S}_\kappa), \mathbf{S}, \mathrm{Rot}_\pi(\mathbf{S})\} \subset \Pi,$$

where $\mathbf{S}$ is defined in Lemma 4.11 (1). We claim that $\Pi = \Pi_3$. Actually, it is seen from $\mathrm{Ref}_{\Pi_3}(\mathcal{S}) = \mathcal{S}$ that $\mathrm{Ref}_{\Pi_3}(\Pi) = \Pi$. Thus, either $\Pi_3 \perp \Pi$ or $\Pi_3 = \Pi$ holds. If $\Pi_3 \perp \Pi$, then $l_1 \subset \Pi_3$ since $O \in l_1$, $l_1 \perp \Pi$ and $O \in \Pi_3$. This is impossible because l_1 does not lie on Π_3. Thus it holds that $\Pi = \Pi_3$, leading to

$$\mathcal{S} \subset \Pi_3, \quad \mathbf{S}_\kappa^\perp \in \Pi_3, \quad \Pi_3 = \{x_2 = 0\}, \quad \alpha_2 = k_s \sin\theta_1 \sin\theta_2 = 0,$$
$$\hat{\theta} \times \hat{\theta}^\perp \| e_2, \quad \Pi_1 \perp \Pi_3, \quad \Pi_2 \perp \Pi_3.$$

In view of Lemma 4.11, we conclude from the above analysis that

(I) $\mathcal{S} = k_s\{(\sin\theta_1\cos\theta_2, 0, -\cos\theta_1), (-\sin\theta_1\cos\theta_2, 0, \cos\theta_1), \pm e_1\} \subset \Pi_3$, $\Pi_3 = \{x_2 = 0\}$.

(II) $\mathcal{D} = \{\Pi_1, \Pi_2, \Pi_3\}$ with $\Pi_1 \perp \Pi_2, \Pi_2 \perp \Pi_3, \Pi_3 \perp \Pi_1$. Moreover, the normal directions ν_j corresponding to Π_j are given by

$$\nu_{\Pi_1} = (1 - \sin\theta_1\cos\theta_2, 0, \cos\theta_1),$$
$$\nu_{\Pi_2} = (1 + \sin\theta_1\cos\theta_2, 0, -\cos\theta_1),$$
$$\nu_{\Pi_3} = \hat{\theta} \times \hat{\theta}^\perp.$$

(III) $k_s(\sin\theta_1\cos\theta_2 \pm 1) \in \mathbb{Z}$, $\sin\theta_1\sin\theta_2 = 0$, $\hat{\theta}^\perp \in \Pi_3$, $\mathcal{P} \subseteq \{\pm k_p e_2\}$.

This completes the proof of Lemma 4.18 when l_1 coincides with the x_2-axis.

Case (ii): The line $l_1 \subset \{x_3 = 0\}$ does not coincide with the x_2-axis.

Via a coordinate rotation around the x_3-axis, one can carry over the argument from case (i) to this case. Note that the third component of each point $x \in \mathbb{R}^3$ remains invariant under such a rotation.

Step 2. Prove Lemma 4.18 if none of the lines l_j $(j = 1, 2, 3)$ is parallel to the plane $\{x_3 = 0\}$.

Let $\nu_{l_1} = (\nu_1, \nu_2, \nu_3) \in S^2$ be a vector parallel to the line $l_1 = \Pi_1 \cap \Pi_2$. Since $\nu_{l_1} \nparallel \{x_3 = 0\}$, we may assume $\nu_3 > 0$. Define

$$\Pi_j^* := \{\text{the plane passing through the origin that is orthogonal to } l_j\}$$

and

$$T_{l_1,\mathbf{S}_\kappa} := \big\{\mathbf{S}_n \in \mathcal{S} : \mathbf{S}_n \text{ can be obtained by applying one or several reflections from the set } \{\mathrm{Ref}_\Pi : \Pi \in D_{l_1}\} \text{ to } \mathbf{S}_\kappa\big\}.$$

By Lemma 4.5, we have $G_{l_1,\mathbf{S}_\kappa} \subseteq T_{l_1,\mathbf{S}_\kappa}$. Let H_1 be the projection operator from $\mathbb{R}^3$ to Π_1^*. Then

$$\begin{aligned} \mathbf{S}_\kappa &= \eta\, \nu_{l_1} + H_1(\mathbf{S}_\kappa) \quad \text{with} \quad \eta = \mathbf{S}_\kappa \cdot \nu_{l_1}, \\ \mathbf{S}_n &= \eta_n\, \nu_{l_1} + H_1(\mathbf{S}_n) \quad \text{with} \quad \eta_n = \mathbf{S}_n \cdot \nu_{l_1}. \end{aligned} \tag{4.14}$$

The following lemma has been proved in [9] using the dihedral group theory. Here we present another proof using the reflectional and rotational invariance of $\mathcal{S}$ for the reader's convenience.

Lemma 4.19. *We have* $\eta_n = \eta$ *for all* $\mathbf{S}_n \in T_{l_1,\mathbf{S}_\kappa}$, $\eta_n \geq 0$ *for all* $\mathbf{S}_n \in \mathcal{S}\backslash T_{l_1,\mathbf{S}_\kappa}$, *and*

$$\eta + \sum_{n \in S,\, n \neq \kappa} \eta_n = 0.$$

Proof of Lemma 4.19. Since the perfect planes in D_{l_1} form an equiangular system of planes in $\mathbb{R}^3$ (see Lemma 4.2), there holds $\eta_n = \eta$ for all $\mathbf{S}_n \in T_{l_1,\mathbf{S}_\kappa}$. Then we see that

$$G_{l_1,\mathbf{S}_n} = \{\eta_n\, \nu_{l_1} + H_1(\mathrm{Rot}_{l_1,2m\pi/D^{\#}_{l_1}}(\mathbf{S}_n)) : m = 1, 2, \ldots, D^{*}_{l_1}\},$$

where the set

$$\{H_1(\mathrm{Rot}_{l_1,2m\pi/D^{\#}_{l_1}}(\mathbf{S}_n)) : m = 1, 2, \ldots, D^{*}_{l_1}\}$$

consists of the $D^{\#}_{l_1}$ vertices of some regular polygon lying on Π^*_1 centered at the origin. Thus, if we have $\eta_n < 0$ for some $\mathbf{S}_n \in \mathcal{S}\backslash T_{l_1,\mathbf{S}_\kappa}$, then there exists at least one element in $G_{l_1,\mathbf{S}_n}$ whose x_3-components are negative, which is impossible since $\mathbf{S}_\kappa \notin G_{l_1,\mathbf{S}_n}$. Thus $\eta_n \geq 0$ for all $\mathbf{S}_n \in \mathcal{S}\backslash T_{l_1,\mathbf{S}_\kappa}$. To verify the last assertion, we let $A = \sum_{n \in S} \mathbf{S}_n$. Then, by Lemma 4.6, we see that

$$\mathrm{Rot}_{l_j,2\pi/D^{\#}_{l_j}}(A) = A \quad \text{for} \quad j = 1, 2, 3.$$

Since l_j $(j = 1, 2, 3)$ are three different non-coplanar straight lines, we obtain $A = 0$, and thus

$$\nu_{l_1} \cdot A = \eta + \sum_{n \in S,\, n \neq \kappa} \eta_n = 0. \qquad \square$$

To proceed with the proof of Lemma 4.18, it suffices to consider the following cases:

Case (a) $\mathcal{S}_\kappa$ belongs to one of the planes Π^*_j $(j = 1, 2, 3)$,

Case (b) $\mathcal{S}_\kappa \notin \Pi^*_j$ for all $j = 1, 2, 3$.

We finish this step by studying case (a) and exclude case (b) in the next step. As we will see in the following, case (a) leads to the desired results in Lemma 4.18.

Without loss of generality, we assume $\mathbf{S}_\kappa \in \Pi^*_1$. Since $l_1 \perp \Pi^*_1$, we have $\eta = 0$, and thus by Lemma 4.19, $\eta_n = 0$ for all $\mathbf{S}_n \in T_{l_1,\mathbf{S}_\kappa}$. Furthermore, we obtain from the last assertion of Lemma 4.19 that $\eta_n = 0$ for all $\mathbf{S}_n \in \mathcal{S}$, which leads to $\mathcal{S} \subset \Pi^*_1$. Thus Lemma 4.18 (1) is proved in case (a).

Lemma 4.20. $\mathcal{D} = \{\Pi_1, \Pi_2, \Pi_3\}$, *and the planes* Π_j $(j = 1, 2, 3)$ *are perpendicular to each other.*

Proof of Lemma 4.20. Since $G_{l_1,\mathbf{S}_\kappa} \subset \mathcal{S} \in \Pi_1^*$, using the fact that $\mathbf{S}_\kappa$ is the only component in $\mathcal{S}$ whose x_3-component is negative, one can readily prove that $2 \le D^\#_{l_l} \le 4$ and that $G_{l_1,\mathbf{S}_\kappa} = \mathcal{S}$ if $D^\#_{l_l} = 3$ or $D^\#_{l_l} = 4$; see the proof of Lemma 4.8 above. However, both of the cases $D^\#_{l_l} = 3$ and $D^\#_{l_l} = 4$ can be excluded, since either of them would imply that $\Pi_3 = \Pi_1^*$ and that each point from $\mathcal{S}$ lies on two different perfect planes in D_{l_1} (see the arguments in Step 1, case (i)). This contradicts Corollary 4.4 (2). Thus we have $D^\#_{l_1} = 2$, leading to $D_{l_1} = \{\Pi_1, \Pi_2\}$ with $\Pi_1 \perp \Pi_2$. By the rotational invariance, we further obtain that

$$\mathrm{Rot}_{l_1,\pi}(\mathbf{S}_n) = -\mathbf{S}_n \in \mathcal{S} \quad \text{for} \quad \mathbf{S}_n \in \mathcal{S}.$$

This implies that

$$\mathcal{S} \subset \{\pm k_s \hat{\theta}\} \cup \tilde{Q}_s \subset \Pi_1^*, \quad \tilde{Q}_s = \{\pm(\alpha_n^{(1)}, \alpha_n^{(2)}, 0) : |\alpha_n|^2 = k_s^2\}. \tag{4.15}$$

Using an argument similar to case (i) of Step 1, we see that $\tilde{Q}_s \neq \emptyset$, which together with $\mathrm{Ref}_{\Pi_3}(\mathcal{S}) = \mathcal{S}$ and $\mathcal{S} \subset \Pi_1^*$ yields $\mathrm{Ref}_{\Pi_3}(\Pi_1^*) = \Pi_1^*$. Hence, either $\Pi_3 \perp \Pi_1^*$ or $\Pi_3 = \Pi_1^*$ holds. However, the orthogonality $\Pi_3 \perp \Pi_1^*$ in combination with $O \in \Pi_3 \cap \Pi_1^*$, $l_1 \perp \Pi_1^*$ would lead to $l_1 \subset \Pi_3$. This implies that

$$\Pi_1 \cap \Pi_2 \cap \Pi_3 = l_1,$$

which is impossible since l_j are three non-coplanar lines. Thus $\Pi_3 = \Pi_1^*$ and Π_3 is perpendicular to both Π_1 and Π_2. □

From $\Pi_1^* = \Pi_3$ and Corollary 4.4 (1), we see that $\hat{\theta} \in \Pi_3$ and $\hat{\theta}^\perp \in \Pi_3$. Thus we may write the normal direction to Π_3 as

$$\nu_{\Pi_3} = \hat{\theta} \times \hat{\theta}^\perp.$$

Moreover, using Corollary 4.4 (2), we have $\hat{\theta} \notin \Pi_j$ for $j = 1, 2$, which allows us to assume (see Figure 6)

$$\begin{aligned} \mathrm{Ref}_{\Pi_1}(\mathbf{S}_\kappa) &= \mathbf{S}, \\ \mathrm{Ref}_{\Pi_1}(-\mathbf{S}_\kappa) &= -\mathbf{S}, \\ \mathrm{Ref}_{\Pi_2}(\mathbf{S}_\kappa) &= -\mathbf{S}, \quad \text{for some } \mathbf{S} \in \tilde{Q}_s. \end{aligned} \tag{4.16}$$

We claim that $\mathcal{S} = \{\pm k_s \hat{\theta}, \pm \mathbf{S}\}$ holds. In fact, if there exists some $n \in \mathbb{Z}^2$ such that $\{\pm \mathbf{S}_n\} \subset (\tilde{Q}_s \cap \mathcal{S}) \setminus \{\pm \mathbf{S}\} \subset \Pi_3$, then the plane Π_3 passes through at least four points $\pm\mathbf{S}, \pm\mathbf{S}_n$, all of which lie on the plane $\{x_3 = 0\}$. This implies that $\Pi_3 = \{x_3 = 0\}$, and that the lines $l_2 = \Pi_2 \cap \Pi_3$, $l_3 = \Pi_3 \cap \Pi_1$ are both parallel to $\{x_3 = 0\}$, contradicting our assumptions in Step 2.

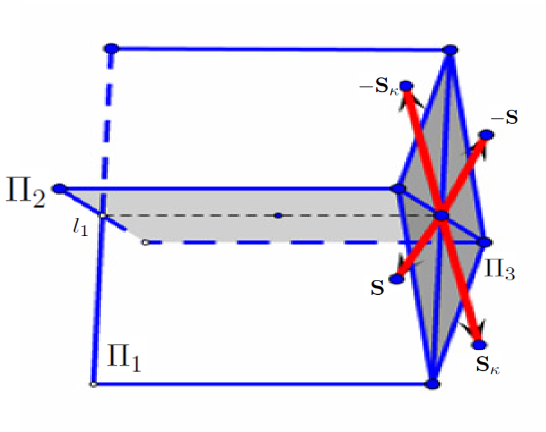

Figure 6. $\mathcal{S} = \{\pm\mathbf{S}_\kappa, \pm\mathbf{S}\}$, $\mathcal{D} = \{\Pi_1, \Pi_2, \Pi_3\}$, $l_1 = \Pi_1 \cap \Pi_2$.

Assuming $\mathbf{S} = (y_1, y_2, 0)$, we know from $\mathbf{S} \in \mathcal{S} \subset B_{k_s}(O)$ and $\mathbf{S} \in \Pi_3$ that

$$y_1^2 + y_2^2 = k_s^2, \quad (\hat{\theta} \times \hat{\theta}^{\perp}) \cdot (y_1, y_2, 0) = 0.$$

This finishes the proof of Lemma 4.18 (2). The third assertion follows directly from equation (4.16), while the fourth one can be easily derived from the α-quasi-periodicity.

Next we shall prove that $\mathcal{P} = \emptyset$. The elements in $\mathcal{P}$ can be written as

$$\mathbf{P}_n = \tau_n \nu_{l_1} + H_1(\mathbf{P}_n) \quad \text{with } \tau_n = \mathbf{P}_n \cdot \nu_{l_1} \text{ for } n \in P,$$

where $\nu_{l_1} \in S^2$ is defined at the beginning of Step 2. In contrast to $\mathcal{S}$, all the elements in $\mathcal{P}$ are located in $B_{k_p}(O) \cap \{x_3 \geq 0\}$. Similar to Lemma 4.19, it holds that $\tau_n \geq 0$ for all $\mathbf{P}_n \in \mathcal{P}$ and $\sum_{n\in P} \tau_n = 0$, leading to $\tau_n = 0$ for all $\mathbf{P}_n \in \mathcal{P}$. Hence, $\mathcal{P} \subset \Pi_1^*$. Arguing similarly, one obtains $\mathcal{P} \subset \Pi_j^*$ for $j = 2, 3$. Since

$$\Pi_1^* \cap \Pi_2^* \cap \Pi_3^* = O$$

and $|\mathbf{P}_n| = k_p^2$, we arrive at $\mathcal{P} = \emptyset$.

In summary, Lemma 4.18 holds in case (a). It only remains to exclude case (b).

Step 3. To prove that case (b) cannot happen.

Assume none of the lines l_j $(j = 1, 2, 3)$ is parallel to $\{x_3 = 0\}$ and $\mathbf{S}_\kappa \notin \Pi_j^*$ for each $j = 1, 2, 3$. From Lemma 4.19 we see that $\eta = \mathcal{S}_\kappa \cdot \nu_{l_1} < 0$, since if this were not true, there would hold that $\eta_n = 0$ for all $\mathbf{S}_n \in \mathcal{S}$ leading to $\mathbf{S}_\kappa \subseteq \Pi_1^*$.

We claim that $\mathbf{S}_\kappa$ must belong to some perfect plane in D_{l_1}. Otherwise, the set $T_{l_1,\mathcal{S}_\kappa}$ would contain at least four elements obtained by reflecting and rotating $\mathbf{S}_\kappa$ with respect to the perfect planes in D_{l_1}; note that $D^{\#}_{l_1} \geq 2$. Using the decomposition (4.14), the first assertion of Lemma 4.19 and $\eta < 0$, we see that then at least two elements of $T_{l,\mathcal{S}_\kappa}$ would have negative x_3-components. This contradicts Remark 4.1.

Thus we may assume $\mathbf{S}_\kappa \in \tilde{\Pi}_1$ for some $\tilde{\Pi}_1 \in D_{l_1}$. For the same reason, one obtains that $\mathbf{S}_\kappa \in \tilde{\Pi}_j$ for some $\tilde{\Pi}_j \in D_{l_j}$, $j = 2, 3$. Therefore,

$$\mathbf{S}_\kappa \in \tilde{\Pi}_1 \cap \tilde{\Pi}_2 \cap \tilde{\Pi}_3.$$

However, recalling that $l_j \subset \tilde{\Pi}_j$ for $j = 1, 2, 3$ and that l_j are three non-coplanar lines passing through O, we see that the set $\{\tilde{\Pi}_1, \tilde{\Pi}_2, \tilde{\Pi}_3\}$ contains at least two different perfect planes which both pass through the direction $\mathbf{S}_\kappa$. This contradicts Corollary 4.4 (2). The proof of Lemma 4.18 is thus complete. □

Introduce the fifth class $U_5 = U_5(\theta_1, \theta_2, k_s, \hat{\theta}^\perp)$ of unidentifiable grating profiles by setting

$$U_5 = \big\{\Lambda \in \mathcal{A}_2 : \text{each face of } \Lambda \text{ lies on a plane defined by } \nu_{\Pi_j} \cdot x + 2m\pi/k_s = 0 \text{ for some } m \in \mathbb{Z},\ j = 1, 2, \text{ or on a plane given by } \nu_{\Pi_3} \cdot x + C = 0 \text{ for some } C \in \mathbb{R}, \text{ where } \nu_{\Pi_j}\ (j = 1, 2, 3) \text{ are defined in Lemma 4.18 (3)}\big\}$$

if $\pm y_1 - k_s \sin\theta_1 \cos\theta_2 \in \mathbb{Z}$ and $\pm y_2 - k_s \sin\theta_1 \sin\theta_2 \in \mathbb{Z}$, and by $U_5 := \emptyset$ otherwise. Here y_j $(j = 1, 2)$ satisfy the relations of Lemma 4.18 (2).

The following lemma can be derived in a way similar to the proof of Lemma 4.8.

Lemma 4.21. *Assume that* **(A1)–(A2)** *hold and* $\Lambda_1, \Lambda_2 \in \mathcal{A}_2$. *Then* $\Lambda_1, \Lambda_2 \in U_5$, *and the total field* $u = u_1 = u_2$ *takes the form*

$$\begin{aligned} u = {}& \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta}) - \hat{\theta}^\perp \exp(-ik_s x \cdot \hat{\theta}) \\ & + \mathrm{Ref}_{\Pi_1}(\hat{\theta}^\perp) \exp(ix' \cdot y') - \mathrm{Ref}_{\Pi_1}(\hat{\theta}^\perp) \exp(-ix' \cdot y') \\ & + c\big[(\hat{\theta} \times \hat{\theta}^\perp) \exp(ik_p x \cdot (\hat{\theta} \times \hat{\theta}^\perp)) \\ & \qquad - (\hat{\theta} \times \hat{\theta}^\perp) \exp(-ik_p x \cdot (\hat{\theta} \times \hat{\theta}^\perp))\big], \end{aligned}$$

where $c \in \mathbb{C}$ *is an arbitrary constant if* $\hat{\theta} \times \hat{\theta}^\perp$ *is parallel to the plane* $\{x_3 = 0\}$ *and the functions* $\exp\big(\pm ik_p x \cdot (\hat{\theta} \times \hat{\theta}^\perp)\big)$ *are* α*-quasi-periodic in both* x_1 *and* x_2; *otherwise* $c = 0$. *Here* $y' = (y_1, y_2)$ *and* Π_1 *are given by Lemma* 4.18 (2) *and* (3) *respectively.*

4.5 Proof of Theorem 2.1 and non-uniqueness examples

Combining Lemmas 4.10, 4.12, 4.14, 4.16 and 4.21 yields Theorem 2.1 for the incident shear wave under the boundary conditions of the third kind. We present an additional remark concerning Theorem 2.1.

Remark 4.22. (i) The unidentifiable grating classes U_2, U_4 and U_5 are empty if the Rayleigh frequencies of the shear part are excluded. Thus, under the additional assumption that $\pi_s = \emptyset$, the assertion (2.17) of Theorem 2.1 takes the form

$$\text{either } \Lambda_1 = \Lambda_2 \text{ or } \Lambda_1, \Lambda_2 \in U_j \quad \text{for some } j \in \{1, 3\}.$$

(ii) All the unidentifiable grating profile classes U_j $(j = 1, 2, 3, 4, 5)$ are determined by the incident shear wave of the form (2.2). More precisely, the sets U_j for $j = 1, 3, 4, 5$ depend on the incident angles θ_1, θ_2, the shear wave number k_s and the vector $\hat{\theta}^\top$, while the set U_2 only depends on θ_1, θ_2 and k_s.

Each set U_j is not empty and contains at least two elements provided the corresponding conditions imposed on θ_1, θ_2, k_p and $\hat{\theta}^\perp$ are fulfilled. The grating profiles from $U_3 \in \mathcal{A}_1$ will be presented in the following Example 3, which then generate the corresponding three-dimensional non-uniqueness examples. The grating profiles from $U_j \in \mathcal{A}_1$ $(j = 1, 2, 4)$ and their corresponding counterexamples can be constructed analogously. We remark that, in the 2D case, there only exists one unidentifiable class $\mathcal{D}_2$ for the incident shear wave under the third kind of boundary conditions (see [15, Theorem 7]). This class can be also derived from the set $U_2(\theta_1, \theta_2, k_s)$ by assuming that all elastic waves are propagating perpendicular to the x_2-axis, where the three-dimensional problem can be reduced to a problem of plane elasticity in the (x_1, x_3)-plane. Such a reduction is impossible for the other classes U_j $(j = 1, 3, 4, 5)$, because the incident direction $\hat{\theta}$ and the vector $\hat{\theta}^\perp$ would both belong to some perfect plane in any of these cases (see Corollary 4.4), contradicting the fact that $\hat{\theta}^\perp$ lies on the (x_1, x_3)-plane.

Next we shall present two counterexamples for illustrating that one incident shear wave cannot uniquely determine a bi-periodic structure in the case of the boundary conditions of the third kind. Moreover, we will construct grating profiles from the unidentifiable set U_5 which vary in both the x_1 and x_2 directions with period 2π.

Example 1. Set $\theta_1 = \pi/6$, $\theta_2 = 0$, $k_s = 4$, so that the incident shear wave u^{in} is given by

$$u_s^{\text{in}} = (\sqrt{3}, 0, 1/2)^\top \exp(i2(x_1 - \sqrt{3}x_3)).$$

Define seven planes Γ_j $(j = 1, 2, \ldots, 7)$ by (see Figure 7 for their cross sections in the (x_1, x_3)-plane)

$$\Gamma_1 = \{x : x_3 = f_1(x_1) := \sqrt{3}x_1\},$$
$$\Gamma_2 = \{x : x_3 := f_2(x_1) = -(x_1 - 2\pi)\sqrt{3}/3\},$$
$$\Gamma_3 = \{x : x_3 = f_3(x_1) := -x_1\sqrt{3}/3\},$$
$$\Gamma_4 = \{x : x_3 := f_4(x_1) = \sqrt{3}(x_1 - \pi)\},$$
$$\Gamma_5 = \{x : x_3 = f_5(x_1) := -x_1\sqrt{3}/3 + \sqrt{3}\pi\},$$
$$\Gamma_6 = \{x : x_3 := f_6(x_1) = \sqrt{3}(x_1 + \pi)\},$$
$$\Gamma_7 = \{x : x_3 = f_7(x_1) := -x_1\sqrt{3}/3 + 4\sqrt{3}\pi/3\},$$

four truncated prisms L_1, L_2, T_1, T_2 by

$$L_1 = \{x : f_3(x_1) < x_3 < f_5(x_1),\ x_1 \in (0, 3\pi/4), x_2 \in [-\pi, \pi]\},$$
$$L_2 = \{x : f_4(x_1) < x_3 < f_1(x_1),\ x_1 \in (3\pi/4, \pi), x_2 \in [-\pi, \pi]\},$$
$$T_1 = \{x : f_1(x_1) < x_3 < f_6(x_1),\ x_1 \in (0, \pi/4), x_2 \in [-\pi, \pi]\},$$
$$T_2 = \{x : f_2(x_1) < x_3 < f_7(x_1),\ x_1 \in (\pi/4, \pi), x_2 \in [-\pi, \pi]\},$$

and two polyhedral surfaces F_1, F_2 (consisting of four faces) by

$$F_1 : x_3 = \begin{cases} f_5(x_1), & x' \in (0, 3\pi/4) \times (0, \pi), \\ f_1(x_1), & x' \in (3\pi/4, \pi) \times (0, \pi), \\ f_3(x_1), & x' \in (0, 3\pi/4) \times (-\pi, 0), \\ f_4(x_1), & x' \in (3\pi/4, \pi) \times (-\pi, 0), \end{cases}$$

$$F_2 : x_3 = \begin{cases} f_6(x_1), & x' \in (0, 3\pi/4) \times (0, \pi), \\ f_7(x_1), & x' \in (\pi/4, \pi) \times (0, \pi), \\ f_1(x_1), & x' \in (0, \pi/4) \times (-\pi, 0), \\ f_2(x_1), & x' \in (\pi/4, \pi) \times (-\pi, 0). \end{cases}$$

Now let the restriction of the grating profiles to $(0, \pi) \times (-\pi, \pi)$ be defined by

$$\Lambda_1|_{(0,\pi)\times(-\pi,\pi)} = F_2 \cup \{(T_1 \cup T_2) \cap \{x_2 = 0\}\} \cup \{(T_1 \cup T_2) \cap \{x_2 = \pi\}\},$$
$$\Lambda_2|_{(0,\pi)\times(-\pi,\pi)} = F_1 \cup \{(L_1 \cup L_2) \cap \{x_2 = 0\}\} \cup \{(L_1 \cup L_2) \cap \{x_2 = \pi\}\},$$

and let Λ_j $(j = 1, 2)$ be the π-periodic resp. 2π-periodic extensions of the restriction $\Lambda_j|_{(0,\pi)\times(-\pi,\pi)}$ along the x_1 resp. x_2 direction; see Figure 7.

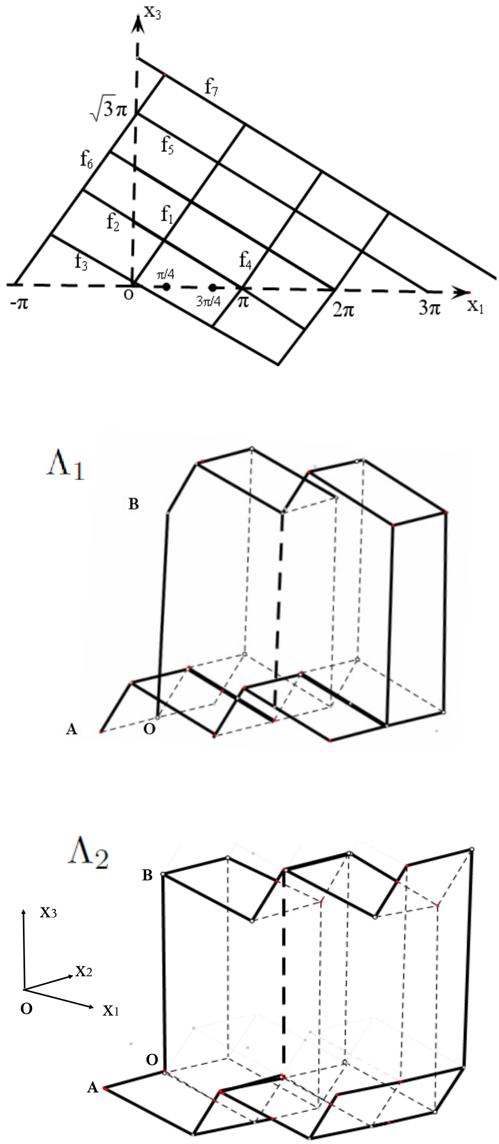

Figure 7. Top: The cross sections of f_j for $j = 1, 2, \ldots, 7$; Middle: The restriction of Λ_1 to $(0, 2\pi) \times (-\pi, \pi)$; Bottom: The restriction of Λ_2 to $(0, 2\pi) \times (-\pi, \pi)$. $A = (0, -\pi, 0)$, $B = (0, 0, \sqrt{3}\pi)$.

Then one can check that $\Lambda_1, \Lambda_2 \in \mathcal{A}_2$, and that the total field of the form

$$u(x) = (\sqrt{3}/2, 0, 1/2)^\top \exp(i2(x_1 - \sqrt{3}x_3)) - e_3 \exp(i4x_1) \\ + (-\sqrt{3}/2, 0, -1/2)^\top \exp(i2(-x_1 + \sqrt{3}x_3)) + e_3 \exp(-i4x_1)$$

satisfies the α-quasi-periodicity condition (2.7) with $\alpha = (2, 0)$, the Rayleigh expansion (2.10) and the third kind boundary conditions on both Λ_1 and Λ_2 as well as the Navier equation

$$(\Delta^* + \omega^2)u = 0 \quad \text{in } \mathbb{R}^3, \quad \text{with } \omega/\sqrt{\mu} = 4.$$

In fact, the above defined total field only consists of propagating modes of the shear part, with four propagating directions

$$\hat{\theta}_0 = \hat{\theta} = \left(\frac{1}{2}, 0, -\frac{\sqrt{3}}{2}\right),\ \hat{\theta}_1 = \left(-\frac{1}{2}, 0, \frac{\sqrt{3}}{2}\right),\ \hat{\theta}_2 = (1, 0, 0),\ \hat{\theta}_3 = (-1, 0, 0),$$

lying on the perfect plane $\Pi_3 = \{x_2 = 0\}$. The other two perfect planes which pass through the origin are given by

$$\Pi_1 = \{x_3 = \sqrt{3}x_1\}, \quad \Pi_2 = \left\{x_3 = -\frac{\sqrt{3}}{3}x_1\right\}.$$

One may check that the set $\mathcal{S} := \{\hat{\theta}_j : j = 0, 1, 2, 3\}$ remains invariant under the reflections with respect to Π_j $(j = 1, 2, 3)$ and the rotations by the angle π with respect to the straight lines $l_1 := \Pi_1 \cap \Pi_2$, $l_2 := \Pi_2 \cap \Pi_3$ and $l_3 := \Pi_3 \cap \Pi_1$.

Thus one incident shear wave cannot uniquely determine a bi-periodic structure in the case of the boundary conditions of the third kind. Note that the grating profiles Λ_1 and Λ_2 contain faces vertical to $\{x_3 = 0\}$, so that they are not polyhedral graphs. Next we present a non-uniqueness example for bi-periodic graphs $\Lambda_1, \Lambda_2 \in \mathcal{A}_2$. To do this, the following lemma is needed.

Lemma 4.23. *Let u satisfy the Navier equation $(\Delta^* + \omega^2)u = 0$ in a domain $\Omega \subset \mathbb{R}^3$ and the boundary conditions of the third kind on $\Gamma := \partial\Omega$. Let $\mathcal{R}$ be a rotation acting on the whole space $\mathbb{R}^3$ around the origin, and write $\Omega^* = \mathcal{R}(\Omega)$, $\Gamma^* := \mathcal{R}(\Gamma)$. Then the function $u^*(x) := \mathcal{R}[u(\mathcal{R}x)]$ satisfies the same Navier equation in Ω^* and the third kind boundary conditions on Γ^*.*

Proof. See Elschner & Yamamoto [20]. □

Example 2. Let $\mathcal{R}$ denote the rotation around the x_1-axis by $\pi/3$ which rotates the positive x_3-axis towards the positive x_2-axis. Such a rotation can be represented by the 3×3 orthogonal matrix

$$\mathcal{R} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & \sqrt{3}/2 \\ 0 & -\sqrt{3}/2 & 1/2 \end{pmatrix}, \quad \text{with } \varphi = \pi/3.$$

Let θ_1, θ_2, k_s be given as in Example 1, so that $\hat{\theta} = (1/2, 0, -\sqrt{3}/2)^\top$. Now, define a new incident direction $\hat{\theta}^*$ by

$$\hat{\theta}^* = (\sin\theta_1^* \cos\theta_2^*, \sin\theta_1^* \sin\theta_2^*, -\cos\theta_1^*) := \mathcal{R}(\hat{\theta}) = (1/2, -3/4, -\sqrt{3}/4),$$

with the incident angles $\theta_1^* \in [0, \pi/2)$, $\theta_2^* \in [0, 2\pi)$ satisfying

$$\cos\theta_1^* = \sqrt{3}/4, \quad \cos\theta_2^* = 2\sqrt{13}/13, \quad \sin\theta_2^* = -3\sqrt{13}/13. \tag{4.17}$$

Define two new grating profiles $\Lambda_j^* := \mathcal{R}(\Lambda_j)$ for $j = 1, 2$. Then we see that Λ_j^* are graphs given by certain piecewise linear functions over $\mathbb{R}^2$. Furthermore, since the two points A and B (as indicated in Figure 7) satisfy $|AB| = 2\pi$ and the angle formed by the line segments AB and AO is $\pi/3$, we see that $|\mathcal{R}(A)\mathcal{R}(B)| = 2\pi$ and the line segment $\mathcal{R}(AB)$ is parallel to e_2 in the new coordinate system. This implies that the profiles Λ_j^* are still 2π-periodic with respect to both x_1 and x_2 after the rotation. Thus $\Lambda_1^*, \Lambda_2^* \in \mathcal{A}_2$. Using the above representation matrix for $\mathcal{R}$, by simple calculations we obtain that

$$\begin{aligned} \mathcal{R}[u(\mathcal{R}x)] = (\sqrt{3}/2, \sqrt{3}/4, 1/4)^\top \exp[i(2x_1 - 3x_2 - \sqrt{3}x_3)] \\ + (-\sqrt{3}/2, -\sqrt{3}/4, -1/4)^\top \exp[-i(2x_1 - 3x_2 - \sqrt{3}x_3)] \\ - (0, \sqrt{3}/2, 1/2)^\top \exp(i4x_1) \\ + (0, \sqrt{3}/2, 1/2)^\top \exp(-i4x_1). \end{aligned}$$

By Lemma 4.23, we see that the function $u^* := \mathcal{R}[u(\mathcal{R}x)]$ satisfies the Navier equation and the third kind boundary conditions on both Λ_1^* and Λ_2^*. One may further check that u^* is the total field corresponding to the incident shear wave $u_s^{\mathrm{in}^*}$ given by

$$u_s^{\mathrm{in}^*} := (\sqrt{3}/2, \sqrt{3}/4, 1/4)^\top \exp[i(2x_1 - 3x_2 - \sqrt{3}x_3)].$$

In this case, $k_s = 4$ and the incident angles θ_1^*, θ_2^* are defined by (4.17). In addition, $u^* - u_s^{\mathrm{in}^*}$ satisfies the α-quasi-periodic radiation condition with $\alpha = (2, -3)$.

Finally, we present an example from U_3 for illustrating that two incident shear waves are not sufficient to uniquely determine a grating profile $\Lambda \in \mathcal{A}$ under the boundary conditions of third kind.

Example 3. Let $\Lambda_1|_{(0,2\pi)\times\mathbb{R}}$ and $\Lambda_2|_{(0,2\pi)\times\mathbb{R}}$ be defined by the following functions:

$$\Lambda_1|_{(0,2\pi)\times\mathbb{R}} : x_3 = \begin{cases} \sqrt{3}x_1, & x_1 \in (0, \frac{\pi}{3}),\ x_2 \in \mathbb{R}, \\ \sqrt{3}\pi/3, & x_1 \in [\frac{\pi}{3}, \frac{5\pi}{3}],\ x_2 \in \mathbb{R}, \\ -\sqrt{3}x_1 + 2\sqrt{3}\pi, & x_1 \in (\frac{5\pi}{3}, 2\pi),\ x_2 \in \mathbb{R}, \end{cases}$$

$$\Lambda_2|_{(0,2\pi)\times\mathbb{R}} : x_3 = \begin{cases} -\sqrt{3}x_1, & x_1 \in (0, \frac{\pi}{3}),\ x_2 \in \mathbb{R}, \\ -\sqrt{3}\pi/3, & x_1 \in [\frac{\pi}{3}, \frac{5\pi}{3}],\ x_2 \in \mathbb{R}, \\ \sqrt{3}x_1 - 2\sqrt{3}\pi, & x_1 \in (\frac{5\pi}{3}, 2\pi),\ x_2 \in \mathbb{R}, \end{cases}$$

and let Λ_i be the 2π-periodic extensions of $\Lambda_i|_{(0,2\pi)\times\mathbb{R}} (i = 1, 2)$ along x_1. Set $k_s = 2$, $\theta_2 = 0$, and $\theta_1 = \frac{\pi}{6}$ or $\theta_1 = -\frac{\pi}{6}$. Then we have two incident directions $\hat{\theta}_1 := (1/2, 0, -\sqrt{3}/2)$, $\hat{\theta}_2 := (-1/2, 0, -\sqrt{3}/2)$, both of them lying on the (x_1, x_3)-plane. Set $\hat{\theta}^\perp := e_2^\top$, where $e_2 = (0, 1, 0)$. One can check that

$$\Lambda_1, \Lambda_2 \in U_3(\pi/6, 0, 2, e_2^\top) \cap U_3(-\pi/6, 0, 2, e_2^\top),$$

and that the finite Rayleigh expansions

$$u(x) = (0, 1, 0)^\top \left[\exp(i(x_1 - \sqrt{3}x_3)) + \exp(i(x_1 + \sqrt{3}x_3)) + \exp(-2ix_1)\right],$$
$$u(x) = (0, 1, 0)^\top \left[\exp(-i(x_1 + \sqrt{3}x_3)) + \exp(-i(x_1 - \sqrt{3}x_3)) + \exp(2ix_1)\right]$$

all satisfy the Helmholtz equation $(\Delta + k_s^2)u = 0$ in $\mathbb{R}^3$ with $k_s = 2$ and the third kind boundary conditions on both Λ_1 and Λ_2.

5 Inverse scattering of an incident pressure wave under the boundary conditions of the fourth kind

The aim of this section is to establish Theorem 2.2 and to give some further remarks on the uniqueness in problem (IP) under the fourth kind boundary conditions. We make the following assumptions throughout this section:

(A4) The incident wave is the incident pressure wave defined in (2.1), i.e.,

$$u^{\text{in}} := \hat{\theta} \exp(ik_p x \cdot \hat{\theta})$$

with $\hat{\theta} = (\sin\theta_1 \cos\theta_2, \sin\theta_1 \sin\theta_2, -\cos\theta_1)$, $\theta_1 \in [0, \frac{\pi}{2})$, $\theta_2 \in [0, 2\pi)$.

(A5) The total fields $u_j(x)$ $(j = 1, 2)$ satisfy problem (DP) corresponding to the different grating profiles Λ_j under the boundary conditions of the fourth kind and fulfill the relation (3.3).

By Lemma 3.5 (2), we write the total field $u = u_1 = u_2$ as

$$u = \sum_{n\in P} A_{p,n}\mathbf{P}_n^{\top} \exp(ix\cdot\mathbf{P}_n) + \sum_{n\in S} A_{s,n}\mathbf{S}_n^{\perp} \exp(ix\cdot\mathbf{S}_n) \quad \text{in } \mathbb{R}^3,$$

where

$$P := \{n \in \mathbb{Z}^2 : |\alpha_n| \le k_p, A_{p,n} \neq 0\} \cup \{\kappa\},$$
$$S := \{n \in \mathbb{Z} : |\alpha_n| \le k_s, A_{s,n} \neq 0\},$$

with $\mathbf{P}_\kappa = k_p\hat{\theta}$, $A_{p,\kappa} = 1/k_p$. Let the sets $\mathcal{P}$, $\mathcal{S}$, $\mathbf{P}_n$ ($n \in P\backslash\{\kappa\}$), $\mathbf{S}_n$ ($n \in S$), π_p, π_s be defined as in Section 4. Then, the third components of the elements in $\mathcal{P}\backslash\{\mathbf{P}_\kappa\}$ and $\mathcal{S}$ are all non-negative, while that of $\mathbf{P}_\kappa$ is negative.

Without loss of generality, let the origin O be located at the intersection line l of two perfect planes Π_1 and Π_2, where Π_j $(j = 1, 2)$ are obtained by extending two faces of $\Lambda_1 \cup \Lambda_2$. Introduce the set D_l consisting of all perfect planes of u that pass through the line l, which is also an equiangular system of planes in $\mathbb{R}^3$. Analogous to Lemma 4.3 and Corollary 4.4, we have

Lemma 5.1. *Assume $\Pi \in D_l$ in the case of the boundary conditions of the fourth kind. Then we have:*

(1) $\mathrm{Ref}_\Pi(\mathcal{P}) = \mathcal{P}$, $\mathrm{Ref}_\Pi(\mathcal{S}) = \mathcal{S}$.

(2) *If* $\mathrm{Ref}_\Pi(\mathbf{P}_n) = \mathbf{P}_m$ *for some* $n, m \in P$, *then* $A_{p,n} = -A_{p,m}$.

(3) *If* $\mathrm{Ref}_\Pi(\mathbf{S}_n) = \mathbf{S}_m$ *for some* $n, m \in S$, *then* $A_{s,n}\,\mathrm{Ref}_\Pi(\mathbf{S}_n^{\perp}) = -A_{s,m}\,\mathbf{S}_m^{\perp}$.

(4) *If* $\mathrm{Ref}_\Pi(\mathbf{S}_n) = \mathbf{S}_n$, *then* $\mathbf{S}_n^{\perp} = -\mathrm{Ref}_\Pi(\mathbf{S}_n^{\perp})$, *i.e.,* $\mathbf{S}_n \in \Pi$ *implies that* $\mathbf{S}_n^{\perp} \perp \Pi$.

(5) *Two different perfect planes from D_l cannot pass through the same point of $\mathcal{S}$, while no perfect plane from D_l can pass through a point of $\mathcal{P}$.*

Using the reflection principle under the boundary conditions of the fourth kind, we see that Lemma 4.5, Lemma 4.6 and Corollary 4.3 are still true. Now we are in a position to derive the unidentifiable grating profiles corresponding to an incident pressure wave.

Lemma 5.2. *Under the assumptions* **(A4)** *and* **(A5)**, *we have $\Lambda_1, \Lambda_2 \in \mathcal{A}_1$ and $D^{\#} = 2$.*

Proof. Assume $\Lambda_1 \in \mathcal{A}_2$ or $\Lambda_2 \in \mathcal{A}_2$. Then, applying the reflectional and rotational invariance to the finite number of propagating directions of the compressional part and arguing as in Lemma 4.18 (1), we know that the points in $\mathcal{P}$ are located on some perfect plane from D_l, which contradicts Lemma 5.1 (5). Thus

$\Lambda_1, \Lambda_2 \in \mathcal{A}_1$. Analogously to Lemma 4.8 (1), we can verify that $2 \le D^\# \le 4$. Moreover, if $D^\# = 3$ or $D^\# = 4$, then $\mathcal{P} = G_{\mathbf{P}_\kappa}$ and each perfect plane from D goes through a point in $\mathcal{P}$, which is impossible due to Lemma 5.1 (5). Thus we get $D^\# = 2$. □

Combining Lemma 5.1 (5), Lemma 5.2 and Lemma 4.11, we may determine the elements of $\mathcal{P}$, $\mathcal{S}$ and D as follows.

Lemma 5.3. *Suppose that the conditions in Lemma* 5.2 *hold. Then*

(1) $s\mathcal{P} = \{\mathbf{P}_\kappa, \mathrm{Rot}_\pi(\mathbf{P}_\kappa), \mathbf{P}, \mathrm{Rot}_\pi(\mathbf{P})\}$, *where* $\mathbf{P}$ *and* $\mathrm{Rot}_\pi(\mathbf{P})$ *are given by*

$$\mathbf{P} = k_p\Big(\sqrt{1-\sin^2\theta_1\sin^2\theta_2}, \sin\theta_1\sin\theta_2, 0\Big),$$
$$\mathrm{Rot}_\pi(\mathbf{P}) = k_p\Big(-\sqrt{1-\sin^2\theta_1\sin^2\theta_2}, \sin\theta_1\sin\theta_2, 0\Big).$$

(2) $D = \{\Pi_1, \Pi_2\}$ *with* $\Pi_1 \perp \Pi_2$. *Moreover, the normal directions* ν_{Π_j} *corresponding to* Π_j *(j=1,2) are given by*

$$\nu_{\Pi_1} = \Big(\sqrt{1-\sin^2\theta_1\sin^2\theta_2} - \sin\theta_1\cos\theta_2, 0, \cos\theta_1\Big), \tag{5.1}$$
$$\nu_{\Pi_2} = \Big(-\sqrt{1-\sin^2\theta_1\sin^2\theta_2} - \sin\theta_1\cos\theta_2, 0, \cos\theta_1\Big). \tag{5.2}$$

(3) $k_p(\sin\theta_1\cos\theta_2 \pm \sqrt{1-\sin^2\theta_1\sin^2\theta_2}) \in \mathbb{Z}$.

(4) $\mathcal{S} = \emptyset$.

Proof. The assertions (1), (2) and (3) can be proved analogously to those of Lemma 4.11. In addition, it follows from Lemma 4.11 (4) that $\mathcal{S} \subset \{\pm k_s e_2\}$. Since both planes Π_1 and Π_2 pass through the x_2-axis, by Lemma 5.1 (5) we arrive at $\mathcal{S} = \emptyset$. □

Based on Lemma 5.3 and the arguments used in the proofs of Lemma 4.8 and Theorem 2.1, we can establish Theorem 2.2 under the boundary conditions of the fourth kind. The following results can be obtained directly from Theorem 2.2.

Remark 5.4. Let u be a solution to (DP) for the incident pressure wave (2.1) fulfilling the boundary conditions of the fourth kind on $\Lambda \in \mathcal{A}$.

(i) Given the a priori information that we have $\Lambda \notin U_2(\theta_1, \theta_2, k_p)$, the near-field data corresponding to the incident pressure wave with the incident angles $\theta_1 \in [0, \pi/2)$, $\theta_2 \in [0, 2\pi)$ are always enough to uniquely determine Λ.

(ii) If the compressional wave number and the incident angles do not satisfy one of the conditions

$$k_p\Big(\sin\theta_1\cos\theta_2 \pm \sqrt{1-\sin^2\theta_1\sin^2\theta_2}\Big) \in \mathbb{Z}$$

(for instance, if the Rayleigh frequencies of the compressional part are excluded, i.e., $\pi_p = \emptyset$), then $U_2(\theta_1, \theta_2, k_p) = \emptyset$, and hence Λ can be uniquely identified by one incident pressure wave.

(iii) Consider two incident pressure waves of the form

$$u^{\text{in}} = (\hat{\theta})\exp(ik_p x\cdot\hat{\theta}), \quad u^{\text{in}^*} = (\hat{\theta}^*)\exp(ik_p x\cdot\hat{\theta}^*),$$

with the incident directions $\hat{\theta}$ and $\hat{\theta}^*$ defined by

$$\hat{\theta} = (\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2, -\cos\theta_1),$$
$$\hat{\theta}^* = (\sin\theta_1^*\cos\theta_2, \sin\theta_1^*\sin\theta_2, -\cos\theta_1^*),$$

where $\theta_1, \theta_1^* \in [0, \pi/2)$, $\theta_2 \in [0, 2\pi)$ satisfy $\theta_1 \neq \theta_1^*$. Then the grating profile Λ can always be uniquely identified by the near-field data corresponding to these two incident pressures waves, because

$$U_2(\theta_1, \theta_2, k_p) \cap U_2(\theta_1^*, \theta_2, k_p) = \emptyset \quad \text{for } \theta_1^* \neq \theta_1.$$

We next construct two grating profiles from $U_2(\theta_1, \theta_2, k_p)$ and present a corresponding non-uniqueness example for our inverse grating diffraction problem.

Example 4. One incident pressure wave is not enough to uniquely determine a grating profile $\Lambda \in \mathcal{A}$ under the boundary conditions of the fourth kind.

Set $\theta_1 = -\pi/6$, $\theta_2 = 0$, $k_p = 2$. Thus the incident pressure wave is given by

$$u_p^{\text{in}} = \hat{\theta}^\top \exp(i2x\cdot\hat{\theta}) \quad \text{with } \hat{\theta} = (-1/2, 0, -\sqrt{3}/2).$$

Let the restriction of two grating profiles Λ_1 and Λ_2 to $(0, 2\pi)\times\mathbb{R}$ be defined by

$$\Lambda_1|_{(0,2\pi)\times\mathbb{R}} : x_3 = \begin{cases} x_1\sqrt{3}/3, & x' \in (0, 3\pi/2)\times\mathbb{R}, \\ -(x_1 - 2\pi)\sqrt{3}\pi, & x' \in (3\pi/2, 2\pi)\times\mathbb{R}, \end{cases}$$

$$\Lambda_2|_{(0,2\pi)\times\mathbb{R}} : x_3 = \begin{cases} -x_1\sqrt{3}, & x' \in (0, \pi/2)\times\mathbb{R}, \\ (x_1 - 2\pi)\sqrt{3}/3\pi, & x' \in (\pi/2, 2\pi)\times\mathbb{R}, \end{cases}$$

and let Λ_j be the 2π-periodic extensions of $\Lambda_j|_{(0,2\pi)\times\mathbb{R}}$ along the x_1-direction; see Figure 8. Then we see that

$$\Lambda_1, \Lambda_2 \in U_2(-\pi/6, 0, 2),$$

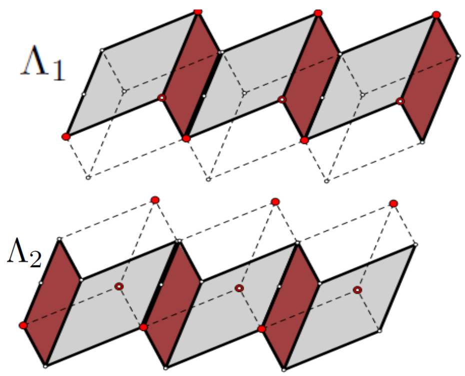

Figure 8. $\Lambda_1, \Lambda_2 \in U_2(\theta_1, \theta_2, k_p)$ with $\theta_1 = -\pi/6$, $\theta_2 = 0$, $k_p = 2$.

and the total fields

$$u_1 = u_2 = (-1/2, 0, -\sqrt{3}/2)^\top \exp(-x_1 - \sqrt{3}x_3) + (1/2, 0, \sqrt{3}/2)^\top \exp(x_1 + \sqrt{3}x_3) + (1, 0, 0)^\top \exp(-2ix_1) - (1, 0, 0)^\top \exp(2ix_1)$$

satisfy the Navier equation in $\mathbb{R}^3$ as well as the boundary conditions of the fourth kind on both Λ_1 and Λ_2. Moreover, the scattered fields $u_j - u_p^{\text{in}}$ satisfy the α-quasi-periodic Rayleigh expansion (2.10) with $\alpha = (-1, 0)$.

Acknowledgments. The authors would like to thank Professor Jun Zou at the Chinese University of Hong Kong and Hai Zhang at the Michigan State University for sending us the manuscripts [8, 9], and the anonymous reviewer for valuable suggestions improving the paper.

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Received March 26, 2011; revised June 1, 2011.

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