Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Global Uniqueness in Determining Polygonal Periodic Structures with a Minimal Number of Incident Plane Waves

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submitted: March 25, 2010

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No. 1498
Berlin 2010

2000 *Mathematics Subject Classification.* 78A46, 35R30.

Key words and phrases. Diffraction gratings, polygonal grating profile, inverse problem, uniqueness.

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

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Abstract

In this paper, we investigate the inverse problem of recovering a two-dimensional perfectly reflecting diffraction grating from the scattered waves measured above the structure. Inspired by a novel idea developed by Bao, Zhang and Zou [to appear in Trans. Amer. Math. Soc.], we present a complete characterization of the global uniqueness in determining polygonal periodic structures using a minimal number of incident plane waves. The idea in this paper combines the reflection principle for the Helmholtz equation and the dihedral group theory. We characterize all periodic polygonal structures that cannot be identified by one incident plane wave, including the resonance case where a Rayleigh frequency is allowed. Furthermore, we show that those unidentifiable gratings provide non-uniqueness examples for appropriately chosen wave number and incident angles. We also indicate and fix a gap in the proof of the main theorem of Elschner and Yamamoto [Z. Anal. Anwend., 26 (2007), 165-177], and generalize the uniqueness results of that paper.

1 Introduction

Diffraction gratings are widely used in many areas of science and technology and have a long history (see the monographs [27] and [5] for the physical and mathematical backgrounds as well as applications). Assume that a time-harmonic (with time variation of the form $\exp(-i\omega t)$, $\omega > 0$) electromagnetic wave is scattered by a perfectly reflecting grating in a homogeneous isotropic lossless medium. Suppose further that the grating is periodic in x_1-direction and constant in x_3-direction. We restrict the diffraction problem to the TE (transverse electric polarization) or TM mode (transverse magnetic polarization), which means that the time-harmonic Maxwell equation can be reduced to a two dimensional scalar Helmholtz equation $(\triangle + k^2)u = 0$ where $u = u(x_1, x_2)$ is the third component of the electric (magnetic) field in the TE (TM) case.

We reformulate the inverse problem according to Kirsch [23] and Bao [4]. Let the cross-section of the diffraction grating in the (x_1, x_2)-plane be given by a Lipschitz curve Λ, which is 2π-periodic with respect to x_1-direction. Suppose that a plane wave given by

$$u^i = \exp(i(\alpha x_1 - \beta x_2)), \quad \text{with } (\alpha, \beta) = k(\sin\theta, \cos\theta)$$

is incident in the (x_1, x_2)-plane upon the grating from the top with a positive constant wave number k and the incident angle $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$. The domain above the grating is denoted by Ω_Λ. Then the total field $u = u(x_1, x_2)$, which can be decomposed as the sum of the incident field u^i and the scattered field u^s, satisfies

$$\Delta u + k^2 u = 0 \qquad \text{in} \qquad \Omega_\Lambda, \tag{1}$$

with the following two kinds of boundary conditions on Λ:

$$\text{(TE mode)} \quad u = 0 \quad \text{or} \quad \text{(TM mode)} \quad \frac{\partial u}{\partial n} = 0, \tag{2}$$

where $\frac{\partial}{\partial n}$ denotes the normal derivative with the normal directed into Ω_Λ.

We require the total field u to be α-quasiperiodic in x_1-direction, i.e.

$$u(x_1 + 2\pi, x_2) = \exp(2i\alpha\pi)u(x_1, x_2) \tag{3}$$

and the scattered field u^s to satisfy the well-known Rayleigh expansion:

$$u^s = \sum_{n\in\mathbb{Z}} A_n \exp(i\alpha_n x_1 + i\beta_n x_2) \qquad \text{for} \quad x_2 > \max\Lambda := \max_{(x_1,x_2)\in\Lambda} x_2, \tag{4}$$

where

$$\alpha_n = n + \alpha,\ \beta_n := \beta_n(\theta, k) = \begin{cases} (k^2 - \alpha_n^2)^{\frac{1}{2}} & \text{if } |\alpha_n| \le k, \\ i(\alpha_n^2 - k^2)^{\frac{1}{2}} & \text{if } |\alpha_n| > k, \end{cases}$$

with $i = \sqrt{-1}$. Here $A_n \in \mathbb{C}(n \in \mathbb{Z})$ are called the Rayleigh coefficients of u^s. Obviously u^s in (4) can be split into a finite sum $\sum_{|\alpha_n|\le k}$ of outgoing plane waves and an infinite sum $\sum_{|\alpha_n|>k}$ of exponentially decreasing functions which are called surface or evanescent waves. Note that the series in (4) and each derivative of it are uniformly convergent on the half space $\{x_2 \ge c\}$ for all $c > \max\Lambda$.

Given a fixed wave number $k > 0$, and one or several incident waves with distinct incident angles θ_i $(i = 1, 2\cdots, N)$, we say that a Rayleigh frequency occurs (the resonance case) if there exist some incident angle $\theta = \theta_i$ and $n \in \mathbb{Z}$ such that $\beta_n(\theta, k) = 0$.

In the following we fix some $b > 0$ and define the admissible class of periodic grating profiles of this paper by

$$\mathcal{A} \ := \ \left\{ \Lambda : \begin{array}{l} \Lambda \text{ is a piecewise linear curve in } \{(x_1, x_2) : x_2 < b\}, \text{ which} \\ \text{is } 2\pi \text{ periodic with respect to } x_1\text{-direction and consists of} \\ \text{a finite number of line segments in each periodic cell.} \end{array} \right\}.$$

The set $\mathcal{A}$ consists of general polygonal grating profiles which are not necessarily defined by the graph of a piecewise linear function. There always exists a solution $u \in H^1_{loc}(\Omega_\Lambda)$ of problem $(1) - (4)$ (see [8] and [14] for the more general transmission problems). The uniqueness to the Dirichlet problem is always true if Λ is given by the graph of a function, e.g., see [23] for C^2 and [17] for Lipschitz functions, whereas this is not true for the Neumann case (see [22]). In this paper we shall focus on the following inverse problem:

(IP): Determine the profile Λ from the knowledge of the near field data $u(x_1, b; k, \theta_j)$ $(j = 1, 2\cdots, N)$ corresponding to N distinct incident plane waves u^{in} with one fixed wave number $k > 0$ and distinct incident angles $\theta_j \in (-\frac{\pi}{2}, \frac{\pi}{2})$ $(j = 1, 2\cdots, N)$.

There are several numerical methods for reconstructing diffraction gratings, e.g., the optimization method ([10], [11], [13] and [17]) and the factorization method ([3] and [25]). Since the uniqueness issue plays an important role in such inverse problems, the purpose of this paper is aimed at giving a complete answer to the uniqueness problem by a minimal number of incident plane waves, within the class of polygonal periodic structures in $\mathbb{R}^2$, and thus improving the existing results developed by Elschner and Yamamoto in [15], [16] and [19]. Note that a class of piecewise linear profiles is always acceptable from a practical viewpoint [28].

If the wave number k is a real number, it is well-known that, for a general periodic grating structure, global uniqueness is impossible by only one incident plane wave (see [4] and [20]). This can also be seen from Section 2 of this paper for the inverse scattering by flat gratings. For other uniqueness results within C^2-smooth functions in $\mathbb{R}^2$, we refer to Bao [4] in the case of a lossy medium (i.e., $\mathrm{Im}k > 0$), Kirsch [24] by using all quasi-periodic incident waves, and Hettlich & Kirsch [20] for a sufficiently small wave number or grating height. See also Ammari [2], Bao & Zhou [7], and Bao, Zhang & Zou [6] for doubly periodic structures in the 3D case. In the special case of piecewise linear periodic structures, making use of the reflection principle developed in [1], [26], [12] and [18] for the inverse scattering problem by bounded obstacles, Elschner, Schmidt and Yamamoto obtained several results on the global uniqueness of (IP) (see [15],[16] and [19]). A recent result, which is shown in [19], states that

- In the inverse Dirichlet problem, two incident waves are enough to uniquely determine a non-flat grating $\Lambda \in \mathcal{A}$, while one incident wave is sufficient if one excludes Rayleigh frequencies.
- In the inverse Neumann problem, four incident waves are enough to uniquely determine a non-flat grating $\Lambda \in \mathcal{A}$, while three incident waves are sufficient if the Rayleigh frequencies are excluded for each incident angle.

We point out that the proofs of the main theorems in [16] and [19] are incomplete, because the identities (2.17) in Section 2.4 of [16] and (12) in Section 2.3 of [19] are not valid if the number of the Dirichlet or Neumann lines is odd. Nevertheless, the main results of [19] indicated above remain true. To fill the gap, instead of using the initial ideas in [16] and [19], we will employ a novel method by combining the reflection principle for the Helmholtz equation with the dihedral group theory, which was first exploited in [6] for proving uniqueness in determining doubly periodic polyhedral structures by scattered electromagnetic waves. In [6], global uniqueness is justified by excluding the unidentifiable gratings in the absence of Rayleigh frequencies. This method seems to be promising since, with the help of group theory, all those unidentifiable periodic gratings by one incident plane wave can be readily found out and characterized.

Motivated by [6], we will apply the same idea to the TE and TM modes of the inverse electromagnetic diffraction problems without excluding the Rayleigh frequencies. We classify all the periodic polygonal structures that cannot be identified by one incident plane wave, which turn out to be extremely exceptional cases since they not only depend on the incident angle θ, but also on the wave number k. Except for these cases, one incident plane wave is always enough to uniquely determine any non-flat grating $\Lambda \in \mathcal{A}$. This paper covers all the existing results in [15],[16] and [19], and contains additional non-uniqueness examples for the inverse Neumann problem. The gaps in [16] and [19] are also filled. The paper is organized as follows.

In Section 2, we exclude the flat gratings from $\mathcal{A}$ by proving that a flat grating cannot be uniquely determined by a fixed number of incident waves in general.

In Sections 3, we make some preliminaries before stating our main theorems, relying on a refinement of the argument in [19] in combination with the idea developed in [6]. The arguments are essentially parallel to those of [6] but with necessary modifications related to the Dirichlet and Neumann boundary conditions. The basic assumption (B) in Section 3, supposing that there exists a Dirichlet or Neumann ray to the inverse problem, has already been justified by Elschner & Yamamoto [19] provided there exist two different gratings Λ_1 and Λ_2 generating the same near field data. Under the assumption (B), the total field can be reduced to a finite sum of propagating modes and is therefore an analytic function in $\mathbb{R}^2$. Two important properties of the set Q of these finitely many propagating directions are that each element of Q has a positive x_2-component except for the incident direction if there is no Rayleigh frequency, and that at most two elements of Q have a vanishing x_2-component if a Rayleigh frequency occurs. Then we introduce a set G, consisting of all reflections with respect to the Dirichlet (or Neumann) rays passing through the origin, which will be proved to be a dihedral group acting on Q. The properties of Q together with the group theory enable us to determine the elements of Q and G, and thus to find out all unidentifiable periodic polygonal structures.

The main uniqueness results (Theorem 2 and Theorem 3) will be shown in Section 4 for the inverse Dirichlet problem and in Section 5 for the inverse Neumann problem. The preliminaries of Section 3 can be viewed as the first step of the proofs of these theorems. Further counterexamples and conclusions for the inverse Neumann problem are presented in Section 5.

2 Uniqueness for flat gratings

The following notations are used throughout the whole paper. For a set A, we denote by $A^{\#}$ the number of elements in A, and for a line segment A_1A_2 with end points $A_1, A_2 \in \mathbb{R}^2$, we denote by $|A_1A_2|$ its length. For a number $a \in \mathbb{C}$, $|a|$ denotes its modulus, and $||x||$ denotes the Euclidean norm of a vector $x \in \mathbb{R}^2$.

Theorem 1 *Let $\Lambda_j = \{x_2 := b_j\}$ where b_j are constants satisfying $|b_j| < b$ $(j = 1, 2)$, and let $u_j := u_j(x;\theta)$ satisfy the corresponding direct diffraction problem (1)-(4) with Dirichlet (or Neumann) boundary condition on Λ_j, j=1,2. If*

$$u_1(x;\theta_m) = u_2(x;\theta_m) \quad \text{on} \quad x_2 = b \tag{5}$$

holds for $2\mathcal{B}^{\#}_{k,b}+1$ incident waves with distinct incident angles $\theta_m \in (-\frac{\pi}{2}, \frac{\pi}{2})$ $(m = 1, 2 \cdots, 2\mathcal{B}^{\#}_{k,b}+1)$, then $b_1 = b_2$. Here

$$\mathcal{B}_{k,b} := \{n \in \mathbb{Z} : |n| < \frac{2bk}{\pi}\}. \tag{6}$$

Proof. Suppose the total field satisfies the Dirichlet boundary condition on Λ_j $(j = 1, 2)$. We shall prove the theorem by contradiction. If $b_1 \neq b_2$, we assume $b > b_2 > b_1$. It is seen from (5) and the uniqueness for the Dirichlet problem that $u_1 = u_2$ in $x_2 > b$. The application of the unique continuation theorem yields that $u_1 = u_2$ in $x_2 \geq b_2$. Setting $u := u_1(x_1, x_2)$, we have $u|_{\Gamma_{b_1}} = u|_{\Gamma_{b_2}} = 0$, which can be written as

$$\begin{aligned} 0 = u(x_1, b_j) &= \exp(i\alpha x_1)(\exp(-i\beta b_j) + A_0 \exp(i\beta b_j)) \\ &\quad + \sum_{n\in\mathbb{Z}\backslash\{0\}} A_n \exp(i\alpha_n x_1)\exp(i\beta_n b_j), \end{aligned}$$

for $j = 1, 2$. Since $\{\exp(i\alpha_n x_1), n \in \mathbb{Z}\}$ is an orthogonal basis of $L^2(0, 2\pi)$, we have that

$$\exp(-i\beta b_j) + A_0 \exp(i\beta b_j) = 0, \text{ and } A_n = 0 \text{ for } n \in \mathbb{Z}\backslash\{0\},$$

from which we arrive at

$$u = \exp(i(\alpha x_1 - \beta x_2)) + A_0 \exp(i(\alpha x_1 + \beta x_2)),$$

with $A_0 = -\exp(-2i\beta b_j)$ for $j = 1, 2$. It is seen from the representation of A_0 that

$$b_2 - b_1 = \frac{\pi}{\beta} m = \frac{\pi}{k\cos\theta} m, \quad \text{for some } m \in \mathbb{Z}.$$

Since $b_2 - b_1 < 2b$, m must belong to $\mathcal{B}_{k,b}$ defined by (6). Obviously, given a fixed $k > 0$ and for each incident angle θ_m, there must exist some $n_m \in \mathcal{B}_{k,b}$, and $n_{m_1} = n_{m_2}$ if and only if $\theta_{m_1} = \theta_{m_2}$ or $\theta_{m_1} = -\theta_{m_2}$. Thus, if (5) holds for $2\mathcal{B}^{\#}_{k,b} + 1$ incident waves with distinct incident angles, then $\mathcal{B}_{k,b}$ contains at least $\mathcal{B}^{\#}_{k,b} + 1$ elements, which is impossible.

If the total field u satisfies the homogeneous Neumann boundary condition on Γ_{b_j}, then u takes the form

$$u = \exp(i(\alpha x_1 - \beta x_2)) + A_0 \exp(i(\alpha x_1 + \beta x_2)) + A_{n_1} \exp(ikx_1) + A_{n_2} \exp(-ikx_1)$$

with $A_0 = \exp(-2i\beta b_j)$ $(j = 1, 2)$ and $A_{n_1}, A_{n_2} \in \mathbb{C}$, which leads to the same consequence as in the Dirichlet case by an analogous argument. □

Remark 1 *For any fixed wave number $k > 0$, if (5) is valid for $\mathcal{B}^{\#}_{k,b} + 1$ incident waves with distinct non-positive (or non-negative) incident angles θ_j $(j = 1, 2\cdots, \mathcal{B}^{\#}_{k,b} + 1)$, then $b_1 = b_2$.*

Remark 2 *Note that $\mathcal{B}^{\#}_{k,b} \to \infty$ as $k \to \infty$ or $b \to \infty$, so that a fixed number of incident waves is not sufficient to uniquely determine an arbitrary flat grating. The corresponding counterexample can be readily constructed from the proof of Theorem 1. In fact, if the number of incident waves is $N \in \mathbb{N}$, then we may choose the wave number $k > N$, the grating profiles $\Lambda_1 = \{x_2 = 0\}, \Lambda_2 = \{x_2 = \pi\}$, and take the incident angles θ_j $(j = 1, 2\cdots, N)$ as follows:*

$$\theta_j > 0, \quad \cos\theta_j = \frac{j}{k}, \quad \text{for } j = 1, 2\cdots, N.$$

In the Dirichlet case, it follows from the proof of Theorem 1 that the total fields $u_j^{(m)}(x)$ corresponding to θ_j $(j = 1, 2\cdots, n)$, Λ_m $(m = 1, 2)$ can be written as

$$\begin{aligned} u_j^{(1)} &= \exp[ik(x_1\cos\theta_j - x_2\sin\theta_j)] - \exp[ik(x_1\cos\theta_j + x_2\sin\theta_j)] \\ u_j^{(2)} &= \exp[ik(x_1\cos\theta_j - x_2\sin\theta_j)] \\ &\quad - \exp[ik(x_1\cos\theta_j + x_2\sin\theta_j)]\exp(-2\pi ik\sin\theta_j). \end{aligned}$$

Moreover, it can be verified from $k\cos\theta_j \in \mathbb{N}$ that

$$u_j^{(1)}(x_1, b; k, \theta_j) = u_j^{(2)}(x_1, b; k, \theta_j), \quad \forall\, b > \pi,\ j = 1, 2\cdots, N.$$

Thus N incident plane waves are not enough to uniquely determine a flat grating in the Dirichlet case. The counterexample for the Neumann case can be constructed analogously. This implies that the global uniqueness by finitely many incoming plane waves is impossible for general periodic gratings.

Before proving our global uniqueness results, we exclude flat gratings by making the following basic assumption for the subsequent analysis:

Basic assumption (A): The admissible class $\mathcal{A}$ does not contain any flat grating.

3 Preliminaries

In this section, we will make some preparations for the proof of the inverse Dirichlet and Neumann problems, which are parallel to those of [6]. Firstly, we introduce the following notations:

1. For two parallel lines l_1 and l_2, we denote by $\mathrm{dist}(l_1, l_2)$ the distance between l_1 and l_2. For two non-parallel lines l_1 and l_2, we denote by $\angle(l_1, l_2)$ the angle formed by l_1 and l_2 that belongs to $(0, \frac{\pi}{2}]$. The distance and angle for rays or line segments can be understood in the same way.

2. Let l be a line in $\mathbb{R}^2$. We denote by R_l the reflection with respect to l in $\mathbb{R}^2$. Let l' be the line that passes through the origin and is parallel to l. We denote by R_l' the reflection with respect to l' in $\mathbb{R}^2$. For any $x \in \mathbb{R}^2$, it is easy to verify that

$$\mathrm{R}_l x = \mathrm{R}_l' x + \mathrm{R}_l O,$$

   where $O = (0, 0) \in \mathbb{R}^2$ is the origin. The reflection R_l' can be represented via an orthogonal matrix such that $\mathrm{R}_l' x \cdot y = x \cdot \mathrm{R}_l' y$. Clearly, $||\mathrm{R}_l O|| = 2\mathrm{dist}(O, l)$.

3. Let G be a group which acts on a set A, and let $d \in A$. We denote by $G\{d\}$ the orbit of d under the action of group G, i.e.

$$G\{d\} = \{a \in A : \exists\ T \in G \text{ such that } a = T(d)\}.$$

   By the group property, we know that for any two elements $a, b \in A$, either $G\{a\} \cap G\{b\} = \emptyset$ or $G\{a\} = G\{b\}$.

4. Let $d \in A$. We denote by G_d the stabilizer subgroup of d in G, i.e.

$$G_d = \{T \in G : T(d) = d\}.$$

   By the orbit-stabilizer theorem and Lagrange's theorem (see e.g. [21]) , we have

$$G\{d\}^{\#} = \frac{G^{\#}}{G_d^{\#}}.$$

The following two lemmas play an important role in this paper; the first one is related to properties of almost periodic functions and can be found in [9] (see also [6] for a new proof), while the second one can be seen in [26], [12] and [18].

Lemma 1 *Let $a_j \in \mathbb{C}$, and $\lambda_j \in \mathbb{R}$ be distinct numbers $(j = 1, 2, \cdots, n)$. If*

$$\lim_{t \to +\infty} \sum_{j=1}^{n} a_j \exp(i\lambda_j t) = 0,$$

then

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

and $a_j = 0, j = 1, 2, \cdots n$.

Lemma 2 (Reflection Principle) *Let Ω be a symmetric domain with respect to a line l, and let $\tilde{l} \subset \Omega$ be a subset of another line such that $\mathrm{R}_l(\tilde{l}) \subset \Omega$. Assume $u \in H^1(\Omega)$ satisfies the Helmholtz equation in Ω, i.e. $\triangle u + k^2 u = 0$.*

1. If $u = 0$ on $l \cap \Omega$, then

$$u(x) + u(\mathrm{R}_l(x)) = 0 \quad in \;\; \Omega.$$

In particular, if $u|_{\tilde{l}} = 0$, then $u|_{\mathrm{R}_l(\tilde{l})} = 0$.

2. If $\frac{\partial u}{\partial n} = 0$ on $l \cap \Omega$, then

$$u(x) - u(\mathrm{R}_l(x)) = 0 \quad in \;\; \Omega.$$

In particular, if $\frac{\partial u}{\partial n}|_{\tilde{l}} = 0$, then $\frac{\partial u}{\partial n}|_{\mathrm{R}_l(\tilde{l})} = 0$.

Definition 1 *Let $S \subset \Omega_\Lambda$ be a straight line starting from one point and leading to infinity in $\{x_2 > b\}$, $b > \max \Lambda$. S is called a Dirichlet ray of u if $u|_S = 0$, while S is called a Neumann ray of u if $\frac{\partial u}{\partial n}|_S = 0$.*

Next we suppose $u(x_1, x_2) \in H^1_{loc}(\Omega_\Lambda)$ is a solution of problem (1)-(4) associated with some grating profile $\Lambda \in \mathcal{A}$. Note that by the standard elliptic regularity theory, u is infinitely smooth up to Λ except for the corner points, and is real-analytic in Ω_Λ. Relying on such an analyticity, we can justify the following basic assumption in either the inverse Dirichlet problem (Section 4) or the inverse Neumann problem (Section 5):

Assumption (B): There exists a Dirichlet ray $S \subset \Omega_\Lambda$ in the Dirichlet case, and a Neumann ray $S \subset \Omega_\Lambda$ in the Neumann case.

In fact, the desired ray mentioned above can always be found if there exist two different polygonal periodic structures generating the same near field. We will review this point in our proofs. Recalling the Rayleigh expansion of u^s defined in (4), we introduce the following notations for convenience:

$d = (\alpha, -\beta) = k(\sin\theta, -\cos\theta) = d_\kappa$.

$d_n = (\alpha_n, \beta_n)$ for $n \in \mathbb{Z}$. In particular, $d_0 = (\alpha, \beta)$.

$P := \{n \in \mathbb{Z} : |\alpha_n| \le k, A_n \neq 0\}$, $Q := \{d_i : i = \kappa \text{ or } i \in P\}$.

Obviously, only one element of Q, d, has a negative x_2-component, $-\beta$. Moreover, if Rayleigh frequencies are excluded, all elements of Q but d have a positive x_2-component, and if a Rayleigh frequency occurs, all elements of Q but d have a non-negative x_2-component and at most two elements of Q, say d_n and d_m, have vanishing x_2-components, $\beta_n = \beta_m = 0$. In addition, Q consists of a finite number of upward propagating directions d_i with $i \in P$ as well as of the incident downward direction d, and can be considered as a set of points located on the circle centered at the origin with radius k. By the quasi-periodicity of the solutions, we arrive at

Lemma 3 *If $(-\alpha, \beta) \in Q$, then $2k \sin\theta \in \mathbb{Z}$. If $(\pm k, 0) \in Q$, then $k(1 \mp \sin\theta) \in \mathbb{Z}$. Finally, if $\{(-\alpha, \beta), (k, 0), (-k, 0)\} \subset Q$, then $k(1 + \sin\theta) \in \mathbb{Z}$ and $k(1 - \sin\theta) \in \mathbb{Z}$.*

The following lemma is a direct consequence of assumption (B) in combination with the Rayleigh expansion. See also [15] and [19] for the existing proofs using the properties of almost periodic functions.

Lemma 4 *Under assumption (B), the total field $u = u^i + u^s$ can be reduced to a finite sum of propagating waves, i.e.*

$$u = \exp(ix \cdot d) + \sum_{n \in P} A_n \exp(ix \cdot d_n), \quad \textit{for} \;\; x_2 > \max \Lambda. \tag{7}$$

It follows from Lemma 4 that u can be extended to an analytic function in $\mathbb{R}^2$ by (7), which means that each line segment of Λ can be extended to a Dirichlet (Neumann) ray of u, and each Dirichlet (Neumann) ray can be extended to a Dirichlet (Neumann) line in $\mathbb{R}^2$. Since we have excluded the flat gratings, there exist at least two Dirichlet (Neumann) rays L and S extending the line segements of Λ. Without loss of generality, we assume that one of the corner points on Λ coincides with the origin such that $L \cap S = O$, and then u takes the form

$$u = A_\kappa \exp(ix \cdot d) + \sum_{n \in P} A_n \exp(ix \cdot d_n), \quad \text{for} \;\; x_2 > \max \Lambda,$$

with $A_i \neq 0$ for all $i \in P$ and $A_\kappa = 1$. Define

$$D = \left\{ l : \begin{array}{l} l \text{ is a line that passes through the origin } O. \text{ Furthermore } l \text{ is} \\ \text{a Dirichlet (Neumann) line in the Dirichlet (Neumann) case.} \end{array} \right\}.$$

It is seen from $L, S \in D$ that $D^\# \geq 2$. Since u is analytic in $\mathbb{R}^2$, by the reflection principle, for each $l \in D$, we have that

$$\begin{aligned} &u(x) + u(\mathrm{R}_l x) = 0 \;\; \text{in} \;\; \mathbb{R}^2, \quad \text{in the Dirichlet case;} \qquad \text{or} \\ &u(x) - u(\mathrm{R}_l x) = 0 \;\; \text{in} \;\; \mathbb{R}^2, \quad \text{in the Neumann case,} \end{aligned}$$

so that the relations

$$A_\kappa \exp(ix \cdot d) + \sum_{n \in P} A_n \exp(ix \cdot d_n) \pm A_\kappa \exp(ix \cdot \mathrm{R}_l d) \pm \sum_{n \in P} A_n \exp(ix \cdot \mathrm{R}_l d_n) = 0$$

hold in the whole $\mathbb{R}^2$. By Lemma 1, the above identities imply the following lemma:

Lemma 5 *Under assumption (B), for each $l \in D$ we have*

1. $\mathrm{R}_l Q = Q$ *for both the Dirichlet and Neumann case.*
2. *Assume $n, m \in P \cup \{\kappa\}$. If $\mathrm{R}_l d_n = d_m$, then*

   $$A_n + A_m = 0 \textit{ in the Dirichlet case, and } \; A_n - A_m = 0 \textit{ in the Neumann case.}$$

3. *In the Dirichlet case, $\mathrm{R}_l d_n \neq d_n$ for any $n \in P$, and $\mathrm{R}_l d \neq d$.*

Next we derive some important properties of D by the reflection principle.

Lemma 6 *Under assumption (B), we have that*

1. $D^{\#} \leq Q^{\#}$.

2. *The angles formed by each two neighboring lines of D are all equal.*

Proof. (1) Since $\mathrm{R}_{l_1} d \neq \mathrm{R}_{l_2} d$ for $l_1 \neq l_2$, we have $D^{\#} = \{\mathrm{R}_l d : l \in D\}^{\#}$. It follows from $\mathrm{R}_l d \in Q$ for $l \in D$ that $D^{\#} \leq Q^{\#}$.

(2) Let l_i $(i = 1, 2 \cdots, D^{\#})$ be the elements of D such that there is no Dirichlet line $l \in D$ between two neighboring Dirichlet lines $l_i, l_{i+1} \in D$ with $l_{D^{\#}+1} = l_1$. Let $\varphi_i \in (0, \frac{\pi}{2}]$ $(i = 1, 2 \cdots, D^{\#})$ be the angle formed by $l_i, l_{i+1} \in D$. We next consider the angles φ_1 and φ_2 formed by l_1, l_2, and l_2, l_3 respectively. Since $u = 0$ on l_i $(i = 1, 2, 3)$, by the reflection principle, if $\varphi_2 > \varphi_1$, then $\mathrm{R}_{l_2} l_1 \in D$ is another Dirichlet line of u between l_2 and l_3; if $\varphi_2 < \varphi_1$, then $\mathrm{R}_{l_2} l_3 \in D$ is another Dirichlet line of u between l_1 and l_2. Both cases lead to a contradiction, thus $\varphi_1 = \varphi_2$. By induction we can prove that $\varphi_1 = \varphi_2 = \varphi_i$ $(i = 3, \cdots, D^{\#})$. The Neumann case can be proved similarly. □

From now on, we assume

$$G := \text{the group generated by } \{\mathrm{R}_l : l \in D\}.$$

Let $\mathrm{Rot}(\varphi)$ be the rotation about the origin O by the angle φ, and $\mathrm{Ref}(\varphi)$ be the reflection about the line L through the origin which makes an angle φ with the x_1-axis. The group G has the identity $\mathrm{Rot}(0)$. Every rotation $\mathrm{Rot}(\varphi)$ has the inverse $\mathrm{Rot}(-\varphi)$, and every reflection $\mathrm{Ref}(\varphi)$ is its own inverse. Actually, G is the dihedral group of order $G^{\#} = 2D^{\#}$, since G consists of $D^{\#}$ reflections and $D^{\#}$ rotations. Since all the rotations of G form a subgroup of G, we define

$$G^* := \text{the subgroup of } G \text{ generated by all rotations of } G.$$

For each element $q \in Q, G^*\{q\}^{\#} = D^{\#}$. Since $G^*\{q\}$ consists of the vertices of some regular $G^*\{q\}^{\#}$-sided polygon centered at the origin, if $G^*\{q\}^{\#} \geq 3$, then there exists at least one element of $G^*\{q\}$ having a negative x_2-component.

Lemma 7 *Under assumption (B), we have*

1. *In the Dirichlet case, $G\{d\}^{\#} = 2D^{\#}$; and in the Neumann case, $G\{d\}^{\#} = 2D^{\#}$ or $G\{d\}^{\#} = D^{\#}$. Furthermore, $G\{d\}^{\#} = D^{\#}$ if there exists some $l \in D$ such that $l \parallel Od$, i.e. $\mathrm{R}_l d = d$.*

2. *If $G\{d\}^{\#} = 2D^{\#}$, then there exists some $d_n \in G\{d\}$ with $n \in P$ such that $G\{d\} = G^*\{d\} \cup G^*\{d_n\}$.*

Proof. In the Dirichlet case, it is seen from Lemma 5 (3) that for each $l \in D, \mathrm{R}_l d \neq d$. Thus if $T \in G_d$, then T must be the rotation about the origin by 2π, i.e. $T = \mathrm{Rot}(2\pi)$, implying that $G_d^{\#} = 1$. By the orbit-stabilizer theorem and Lagrange's theorem we have $G\{d\}^{\#} = 2D^{\#}$. Since $G^*\{d\}^{\#} = D^{\#} < G\{d\}^{\#}$, by the group property, there must exist some $d_n \in G\{d\}$ with $n \in P$ such that $G^*\{d_n\} \cap G^*\{d\} = \emptyset$ and $G^*\{d_n\}^{\#} = D^{\#}$. On noting that $G^*\{d_n\}^{\#} + G^*\{d\}^{\#} = G\{d\}^{\#}$, we have $G\{d\} = G^*\{d\} \cup G^*\{d_n\}$. This proves the lemma in the Dirichlet case.

In the Neumann case, it is possible that $\mathrm{R}_l d = d$ for some $l \in D$, leading to the consequence that both R_l and $\mathrm{Rot}(2\pi)$ belong to G_d, i.e., $G_d^{\#} = 2$. Thus it follows from the orbit-stabilizer and Lagrange theorems that $G\{d\}^{\#} = D^{\#}$. If $\mathrm{R}_l d \neq d$ for all $l \in D$, an argument similar to that in the Dirichlet case finishes the proof in the Neumann case. $\square$

Denote a straight line which passes through the origin and makes the angle φ with the positive x_1-axis by

$$L_\varphi \quad := \quad \{(t\cos\varphi, t\sin\varphi) : t \in \mathbb{R}, \varphi \in [0, 2\pi)\}.$$

To generalize the results of [15], we define a special class of rectangular-groove grating profiles by

$$\mathcal{F} \quad := \quad \{\Lambda : \quad \text{each segment of } \Lambda \text{ is parallel to the } x_1\text{- or } x_2\text{-axis. }\} \tag{8}$$

Note that the inverse problems for this class of grating profiles have already been studied in [15].

4 Inverse problem for the Dirichlet boundary condition

Define the following class of polygonal gratings by

$$\mathcal{D}_2(\theta, k) := \left\{ \Lambda \in \mathcal{A} : \begin{array}{l} \text{Each line segment of } \Lambda \text{ is parallel to one of the lines} \\ L_{\frac{\theta}{2}+\frac{\pi}{4}}, L_{\frac{\theta}{2}-\frac{\pi}{4}}, \text{ and its distance to } L_{\frac{\theta}{2}\pm\frac{\pi}{4}} \text{ is some integral} \\ \text{multiple of } \frac{\pi}{k\cos(\frac{\theta}{2}\mp\frac{\pi}{4})}. \text{ In addition, } k(1 \pm \sin\theta) \in \mathbb{Z}. \end{array} \right\}.$$

Suppose A_1A_2 is a line segment of $\Lambda \in \mathcal{D}_2(\theta, k)$ connecting two corner points A_1 and A_2, and $\varphi \in [-\frac{\pi}{2}, \frac{\pi}{2})$ is the angle formed by A_1A_2 and the positive x_1-axis. It follows from the definition of $\mathcal{D}_2(\theta, k)$ that either $\varphi = \frac{\theta}{2} + \frac{\pi}{4}$ or $\varphi = \frac{\theta}{2} - \frac{\pi}{4}$. If $\varphi = \frac{\theta}{2} \pm \frac{\pi}{4}$, then $|A_1A_2| = \frac{\pi}{k\cos(\frac{\theta}{2}\pm\frac{\pi}{4})} n^{\pm}$ for some $n^{\pm} \in \mathbb{N}$. Moreover, $\mathcal{D}_2(\theta, k) \neq \emptyset$ for all k and θ satisfying $k(1 \pm \sin\theta) \in \mathbb{Z}$ (see Lemma 11), and a Rayleigh frequency always occurs in this case.

Let us now give the main results for the inverse Dirichlet problem.

Theorem 2 *Let $\Lambda_1, \Lambda_2 \in \mathcal{A}$ satisfy the basic assumption (A). Furthermore, suppose without loss of generality that one of the profiles Λ_1, Λ_2 has a corner point at the origin. Let $u_j := u_j(x; \theta)$ satisfy the corresponding direct diffraction problem (1)-(4) with Dirichlet boundary condition on Λ_j, $j = 1, 2$. If*

$$u_1(x_1, b; \theta) = u_2(x_1, b; \theta) \quad \textit{for all } x_1 \in (0, 2\pi) \tag{9}$$

holds for one incident wave with the incident angle $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$, then one of the following cases must occur:

(1) $\Lambda_1 = \Lambda_2$. (2) $\Lambda_1, \Lambda_2 \in \mathcal{D}_2(\theta, k)$, and a Rayleigh frequency occurs.

Remark 3 *Assume that $\Lambda \in \mathcal{A}$ has a corner point at the origin. Several results can be obtained directly from Theorem 2.*

1. Given the a priori information that Λ does not belong to $\mathcal{D}_2(\theta, k)$, the data of the total field on Γ_b from one incident wave (with the incident angle θ) are always enough to uniquely determine Λ. In particular, the elements of the class $\mathcal{F}$ defined in (8) do not belong to

$\mathcal{D}_2(\theta, k)$ for any $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$ and $k > 0$, and thus can be uniquely determined by one incident plane wave. This generalizes the result of [15] in the case of the Dirichlet problem.

2. Given a fixed wave number $k > 0$ and an incident angle $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$, if $\mathcal{D}_2(\theta, k) = \emptyset$, then one incident wave with the incident angle θ uniquely determines $\Lambda \in \mathcal{A}$. Note that $\mathcal{D}_2(\theta, k) = \emptyset$ if one of the numbers $\{k(1+\sin\theta), k(1-\sin\theta)\}$ is not an integer. In particular, if Rayleigh frequencies are excluded, then both $k(1+\sin\theta)$ and $k(1-\sin\theta)$ are not integers.

3. If Rayleigh frequencies are allowed, two incident waves are sufficient to uniquely determine $\Lambda \in \mathcal{A}$ since $\mathcal{D}_2(\theta_1, k) \cap \mathcal{D}_2(\theta_2, k) = \emptyset$ for any $\theta_1 \neq \theta_2$. This together with 2. generalizes the results of [19] in the Dirichlet case.

Proof of Theorem 2: Assuming $\Lambda_1 \neq \Lambda_2$, we are going to prove the second assertion. The proof can be decomposed into several steps.

Step 1. It follows from (9) and the uniqueness for the Dirichlet problem (1)-(4) (see [23]) that $u_1(x) = u_2(x)$ in $x_2 > b$. The application of the unique continuation theorem yields that $u_1(x) = u_2(x)$ in the unbounded connected component Ω of $\Omega_{\Lambda_1} \cap \Omega_{\Lambda_2}$. Since $u_i (i = 1, 2)$ is analytic in Ω and $\Lambda_i (i = 1, 2)$ is piecewise linear, if $\Lambda_1 \neq \Lambda_2$, the reflection principle in combination with the path argument developed in [1], [26] and [18] can be utilized for finding the desired Dirichlet ray S involved in the assumption (B) of Section 3. We leave out the proof and only refer to [19] and [18] for the existing proofs.

Next we will proceed using the preliminaries in Section 3. Without loss of generality, we suppose Λ_1 has a corner point at the origin and write u_1 as u for convenience. By Lemma 4, the existence of a Dirichlet ray implies that u can be reduced to a finite sum of propagating waves (7), which is analytic in $\mathbb{R}^2$ and satisfies $u|_L = 0$ on each straight line L extending a segment of $\partial\Omega$. Furthermore, there exist two Dirichlet rays L and S extending two segments of Λ_1 such that $L \cap S = O$. Then we introduce the set D, the dihedral group G and its subgroup G^*, and take into account Lemmas 5-7 in the Dirichlet case.

It is seen from Lemma 7 (1) that $G\{d\}^\# = 2D^\# \geq 4$, and that for any $l \in D, \mathrm{R}_l d \neq d$. We claim that a Rayleigh frequency must occur in this case. In fact, by Lemma 7 (2), there exists some $d_n \in Q$ with $n \in P$ such that $G\{d\} = G^*\{d\} \cup G^*\{d_n\}$. On noting that $G^*\{d_n\}^\# = D^\# \geq 2$ and that $G^*\{d_n\}$ consists of the vertices of a regular $D^\#$-sided polygon centered at the origin, if there is no Rayleigh frequency, there must exist at least one element q of $G^*\{d_n\}$ which has a negative x_2-component. This is impossible since $q \neq d$ and $q \in Q$.

Step 2. It is seen from step 1 that a Rayleigh frequency occurs, thus there are at most three elements of Q having a non-positive x_2-component, $d = (\alpha, -\beta), d_{n_1} = (k, 0)$ and $d_{n_2} = (-k, 0)$ for some $n_1, n_2 \in P$.

Lemma 8 *$D^\#$=2.*

Proof of Lemma 8. In fact, if $D^\# \geq 3$, then $G\{d\}^\# = 2D^\# \geq 6$, and there exists some d_n such that $G\{d\} = G^*\{d\} \cup G^*\{d_n\}$ with $G^*\{d\}^\# = G^*\{d_n\}^\# \geq 3$. Thus there exists at least one element of $G^*\{d_n\}$ having a negative x_2-component, which leads to the result that two elements of $G^*\{d\}$ have a negative x_2-component. However this is impossible. Thus $D^\#$=2. $\square$.

More precisely, we obtain that $D = \{L, S\}$, and by Lemma 6 (2) we know that $S \perp L$.

Without loss of generality, we can assume that

$$L = L_{\varphi_1} \text{ with } \varphi_1 \in [0, \frac{\pi}{2}), \text{ and } S = L_{\varphi_2} \text{ with } \varphi_2 = \varphi_1 - \frac{\pi}{2} \in [-\frac{\pi}{2}, 0).$$

Now the group G takes the form

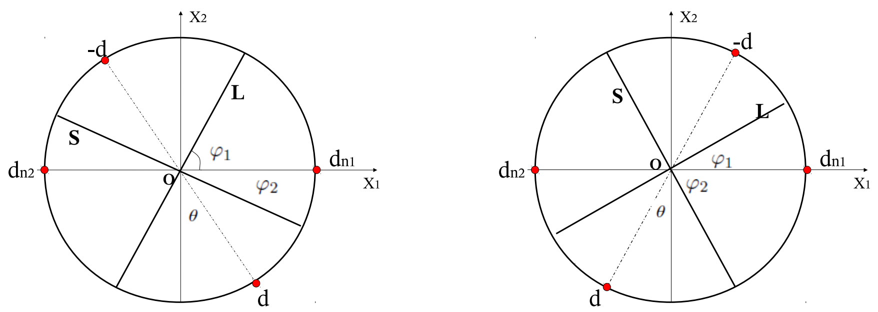
$$G = \{\mathrm{Rot}(\pi), \mathrm{Rot}(2\pi), \mathrm{Ref}(\varphi_1), \mathrm{Ref}(\varphi_2)\}, \tag{10}$$

so that the orbit of d, $G\{d\}$, is given by $G\{d\} = \{d, -d, d_{n_1}, d_{n_2}\}$. Next we are aimed at proving that $L = L_{\frac{\theta}{2}+\frac{\pi}{4}}, S = L_{\frac{\theta}{2}-\frac{\pi}{4}}$.

Lemma 9 *$Q = G\{d\} = \{d, -d, d_{n_1}, d_{n_2}\} = \{(\alpha, -\beta), (-\alpha, \beta), (k, 0), (-k, 0)\}$ and $k\sin(1 \pm \theta) \in \mathbb{Z}$.*

Proof of Lemma 9. If there exists an element $d_n \in Q\backslash\{d, -d, d_{n_1}, d_{n_2}\}$, then $G\{d\} \cap G\{d_n\} = \emptyset$, and $d_n = (\alpha_n, \beta_n)$ has a positive x_2-component, $\beta_n > 0$. This yields that $\mathrm{Rot}(\pi)d_n = (-\alpha_n, -\beta_n) \in Q$ has a negative x_2-component, contradicting the fact that $\mathrm{Rot}(\pi)d_n \in Q$ has a positive x_2-component. Thus $Q = G\{d\} = \{(\alpha, -\beta), (-\alpha, \beta), (k, 0), (-k, 0)\}$, which together with Lemma 3 yields that $k(1 \pm \sin\theta) \in \mathbb{Z}$. $\square$

Figure 1: $D^{\#} = 2, Q = G\{d\} = \{d, -d, d_{n_1}, d_{n_2}\} = \{(\alpha, -\beta), (-\alpha, \beta), (k, 0), (-k, 0)\}$. Left: $\theta > 0$. Right: $\theta < 0$.



Now we can characterize the actions of G on Q by the relations (see Figure 1)

$$\mathrm{Rot}(\pi)d = -d, \mathrm{Rot}(\pi)d_{n_1} = d_{n_2}, \mathrm{R}_S d = \mathrm{Ref}(\varphi_2)d = d_{n_1}, \mathrm{R}_L d = \mathrm{Ref}(\varphi_1)d = d_{n_2}, \tag{11}$$

from which we obtain that

$$\varphi_2 = \frac{\theta}{2} - \frac{\pi}{4} \text{ and } \varphi_1 = \frac{\theta}{2} + \frac{\pi}{4}, \tag{12}$$

i.e., $L = L_{\frac{\theta}{2}+\frac{\pi}{4}}$ and $S = L_{\frac{\theta}{2}-\frac{\pi}{4}}$.

Step 3. We finally complete the proof of the relation $\Lambda_1, \Lambda_2 \in \mathcal{D}_2(\theta, k)$. We introduce the set of all Dirichlet lines by

$$\tilde{D} = \{l : l \text{ is a Dirichlet line of } u \text{ in } \mathbb{R}^2\}.$$

Lemma 10 *1. For each $l \in \tilde{D}$, either $l \parallel L$ or $l \parallel S$.*

2. If $l \parallel L$, then $\mathrm{dist}(l, L) = \dfrac{\pi}{k\cos\varphi_2} n$ for some $n \in \mathbb{N}$, and if $l \parallel S$, then $\mathrm{dist}(l, S) = \dfrac{\pi}{k\cos\varphi_1} m$ for some $m \in \mathbb{N}$.

Proof of Lemma 10. By the reflection principle and Lemma 1, we know that for each $l \in \tilde{D}$, $\mathrm{R}_l' d \in Q$. If $\mathrm{R}_l' d = d_{n_1}$, then $l \parallel S$; if $\mathrm{R}_l' d = d_{n_2}$, then $l \parallel L$.

We next assume that $l \parallel L$. It is seen from (11) that $\mathrm{R}_l' d = (-k, 0)$ and $\mathrm{R}_l'(-d) = (k, 0)$. By Lemma 5 (2) we can write the total field u as

$$u = \exp(ix \cdot d) + \exp(-ix \cdot d) - \exp(ikx_1) - \exp(-ikx_1), \tag{13}$$

and making use of $\mathrm{R}_l x = \mathrm{R}_l' x + \mathrm{R}_l O$, we can write $u(\mathrm{R}_l(x))$ as

$$\begin{aligned} u(\mathrm{R}_l(x)) &= \exp(i\mathrm{R}_l O \cdot d)\exp(-ikx_1) + \exp(-i\mathrm{R}_l O \cdot d)\exp(ikx_1) \\ &\quad - \exp(ix \cdot d) - \exp(-ix \cdot d). \end{aligned}$$

The application of the reflection principle to the line l yields that

$$1 = \exp(i\mathrm{R}_l O \cdot d) = \exp(-i\mathrm{R}_l O \cdot d). \tag{14}$$

On noting that

$$|\mathrm{R}_l O \cdot d| = ||\mathrm{R}_l O|| \cdot ||d|| \cos\angle(\mathrm{R}_l O, d) = 2\mathrm{dist}(l, L) k \cos\varphi_2,$$

we obtain from (14) and (12) that

$$\mathrm{dist}(l, L) = \frac{\pi}{k\cos\varphi_2} n = \frac{\pi}{k\cos(\frac{\theta}{2} - \frac{\pi}{4})} n, \quad \text{for some } n \in \mathbb{N}.$$

The case when $l \parallel S$ can be proved analogously. □

Since u can be extended to an analytic function defined on the whole plane $\mathbb{R}^2$, each line segment of Λ_1 can be extended to an element of $\tilde{D}$. This gives rise to the relation $\Lambda_1 \in \mathcal{D}_2(\theta, k)$. On noting that the Dirichlet ray S of u_1 in the assumption (B) is also a Dirichlet ray of u_2, we can prove $\Lambda_2 \in \mathcal{D}_2(\theta, k)$ in an analogous manner. The proof is thus complete. □

It follows from the proof of Theorem 2 that each grating from $\mathcal{D}_2(\theta, k)$ generates the same total field of the form (13), thus providing non-uniqueness examples for the inverse Dirichlet problem. In the following, we will show that, for each angle θ satisfying $k(1 \pm \sin\theta) \in \mathbb{Z}$, the corresponding counterexample to uniqueness with one incident wave can be constructed. To do this, we only need to show the following lemma.

Lemma 11 *For all k and θ satisfying $k(1 \pm \sin\theta) \in \mathbb{Z}$, $\mathcal{D}_2(\theta, k) \neq \emptyset$.*

Proof. Let $\varphi_1 = \frac{\theta}{2} + \frac{\pi}{4}$ and $\varphi_2 = \frac{\theta}{2} - \frac{\pi}{4}$, and let Λ_i be the 2π periodic extensions of $\Lambda_i|_{(0,2\pi)} (i = 1, 2)$ defined by

$$\Lambda_1 : x_2 = \begin{cases} x_1 \tan\varphi_1 & x_1 \in (0, T_1), \\ (x_1 - 2\pi)\tan\varphi_2 & x_1 \in [T_1, 2\pi) \end{cases} \quad \text{with } T_1 = \frac{2\pi\tan\varphi_2}{\tan\varphi_2 - \tan\varphi_1},$$

$$\Lambda_2 : x_2 = \begin{cases} x_1 \tan\varphi_2 & x_1 \in (0, T_2), \\ (x_1 - 2\pi)\tan\varphi_1 & x_1 \in [T_2, 2\pi) \end{cases} \quad \text{with } T_2 = \frac{2\pi\tan\varphi_1}{\tan\varphi_1 - \tan\varphi_2}.$$

Then the distance between two neighboring line segments that are parallel to L_{φ_2} (or L_{φ_1}) is $2\pi\cos\varphi_1$ (or $2\pi\sin\varphi_1$). To fulfil the conditions imposed on the elements of $\mathcal{D}_2(\theta,k)$, we have to check that

$$2\pi\cos\varphi_1 = \frac{\pi}{k\cos\varphi_1}n \text{ for some } n\in\mathbb{Z}, \quad \text{and} \quad 2\pi\sin\varphi_1 = \frac{\pi}{k\cos\varphi_2}m \text{ for some } m\in\mathbb{Z},$$

or equivalently,

$$2k\cos^2(\frac{\theta}{2}+\frac{\pi}{4})\in\mathbb{Z} \quad \text{and} \quad 2k\sin^2(\frac{\theta}{2}+\frac{\pi}{4})\in\mathbb{Z}$$

by using $\varphi_1-\varphi_2=\frac{\pi}{2}$. Noting that

$$2k\cos^2(\frac{\theta}{2}+\frac{\pi}{4}) = k(1-\sin\theta) \qquad 2k\sin^2(\frac{\theta}{2}+\frac{\pi}{4}) = k(1+\sin\theta),$$

and $k(1\pm\sin\theta)\in\mathbb{Z}$, we have justified that both Λ_1 and Λ_2 belong to $\mathcal{D}_2(\theta,k)$. □

Taking $\theta=0$ and $k=1$, or $\theta=\pi/6$ and $k=2$, we can obtain two examples which are the same as those of [16, Remark 1]. The argument indicated above gives a general method for constructing such counterexamples as well as the elements of $\mathcal{D}_2(\theta,k)$. Essentially, if Λ is 2π-periodic with respect to x_1-direction and lies on the quadratic grid generated by the 2π-periodic extensions of $\{x_2 = x_1\tan(\frac{\theta}{2}\pm\frac{\pi}{4})\}$, then $\Lambda\in\mathcal{D}_2(\theta,k)$.

Remark 4 *From the proof of Theorem 3, we observe that the number of Dirichlet rays is always two, an even number, so that the proofs in [16] and [19] appear to be correct in the Dirichlet case. However in the Neumann case, as we will show in the next section, the number of Neumann rays may be two, three or four, implying that a more detailed analysis must be involved.*

5 Inverse problem for the Neumann boundary condition

Before we state our main theorem, we define the following three classes of polygonal periodic structures by

$$\mathcal{N}_2(\theta,k) := \left\{ \Lambda\in\mathcal{A} : \begin{array}{l} \text{Each line segment of } \Lambda \text{ is parallel to one of the lines } L_\theta, \\ L_{\theta+\frac{\pi}{2}}, \text{ and its distance to } L_\theta \text{ is some integral multiple} \\ \text{of } \frac{\pi}{k}. \text{ In addition, } 2k\sin\theta\in\mathbb{Z}. \end{array} \right\},$$

$$\mathcal{N}_3(\theta,k) := \left\{ \Lambda\in\mathcal{A} : \begin{array}{l} \text{Each line segment of } \Lambda \text{ is parallel to one of the lines } L_{\theta-\frac{\pi}{6}}, \\ L_{\theta+\frac{\pi}{6}}, L_{\theta+\frac{\pi}{2}}, \text{ and its distance to } L_{\theta-\frac{\pi}{6}} \text{ (or } L_{\theta+\frac{\pi}{6}}, L_{\theta+\frac{\pi}{2}} \text{)} \\ \text{is some integral multiple of } \frac{2\pi}{k\sqrt{3}}. \text{ Moreover, } \theta\in[-\frac{\pi}{6},\frac{\pi}{6}] \\ \text{and } k\sqrt{3}\sin(\frac{\pi}{6}\pm\theta)\in\mathbb{Z}. \end{array} \right\},$$

$$\mathcal{N}_4(0,k) := \left\{ \Lambda\in\mathcal{A} : \begin{array}{l} \text{Each line segment of } \Lambda \text{ is parallel to one of the lines } L_{-\frac{\pi}{4}}, \\ L_{-\frac{\pi}{2}}, L_{\frac{\pi}{4}}, L_0, \text{ and its distance to } L_0 \text{ (or } L_{-\frac{\pi}{2}}) \text{ is some} \\ \text{integral multiple of } \frac{\pi}{k}, \text{ and the distance to } L_{\pm\frac{\pi}{4}} \text{ is some} \\ \text{integral multiple of } \frac{\sqrt{2}\pi}{k}. \text{ In addition } k\in\mathbb{Z}. \end{array} \right\}.$$

Theorem 3 *Let Λ_1, $\Lambda_2 \in \mathcal{A}$ satisfy the basic assumption (A). Furthermore, suppose without loss of generality that one of the profiles Λ_1, Λ_2 has a corner point at the origin. Let $u_j := u_j(x;\theta)$ satisfy the corresponding direct diffraction problem (1)-(4) with the Neumann boundary condition on Λ_j, j=1,2. If*

$$u_1(x_1, b; \theta) = u_2(x_1, b; \theta) \quad \text{for all } x_1 \in (0, 2\pi) \tag{15}$$

holds for one incident plane wave with the incident angle $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$, then one of the following four cases must occur:

(1) $\Lambda_1 = \Lambda_2$.

(2) $\Lambda_1, \Lambda_2 \in \mathcal{D}_2(\theta, k)$ *or* $\Lambda_1, \Lambda_2 \in \mathcal{N}_2(\theta, k)$.

(3) $\Lambda_1, \Lambda_2 \in \mathcal{N}_3(\theta, k)$ *with $\theta \in [-\frac{\pi}{6}, \frac{\pi}{6}]$. In this case, a Rayleigh frequency occurs if $\theta = \frac{\pi}{6}$ or $\theta = -\frac{\pi}{6}$.*

(4) $\Lambda_1, \Lambda_2 \in \mathcal{N}_4(0, k)$, $\theta = 0$, *and a Rayleigh frequency occurs.*

Proof. Assuming $\Lambda_1 \neq \Lambda_2$, we shall prove that one of the cases (2), (3) and (4) must happen.

Step 1. We can repeat step 1 of the proof of Theorem 2 to justify assumption (B) in the Neumann case (see [19] for the details). We suppose the origin is one of the corner points of Λ_1 and write u_1 as u. By Lemma 4, the existence of the Neumann ray implies that u can be reduced to a finite sum of propagating waves (7) which is an analytic function in $\mathbb{R}^2$, thus each line segment of Λ_1 can be extended to a Neumann line of u in $\mathbb{R}^2$. In addition, there exist two Neumann rays L and S such that $L \cap S = O$. As in Section 4, one can introduce the set D with $D^{\#} \geq 2$, the dihedral group G and its subgroup G^*, and then justify Lemmas 5-7 in the Neumann case.

By Lemma 7 (1) and (2), $G\{d\}^{\#}$ is either $2D^{\#}$ or $D^{\#}$. If $G\{d\}^{\#} = 2D^{\#}$, there exists some $d_n \in G\{d\}$ with $n \in P$ such that $G\{d\} = G^*\{d\} \cup G^*\{d_n\}$. If $G\{d\}^{\#} = D^{\#}$, then $G\{d\} = G^*\{d\}$ and there exists an Neumann ray $l \in D$ such that $l \parallel Od$, i.e. $\mathrm{R}_l d = d$. The next lemma connects the elements of $G\{d\}$ with the elements of D.

Lemma 12 *In the Neumann case, we have*

(1) $G\{d\}^{\#} \neq 2D^{\#}$ *if either Rayleigh frequencies are excluded, or* $D^{\#} \geq 3$.

(2) $G\{d\} = G^*\{d\} = Q$ *if either $D^{\#} \geq 3$, or $D^{\#} = 2$ and Rayleigh frequencies are excluded.*

Proof of Lemma 12. The proof of (1) is similar to that of Lemma 8 in the Dirichlet case. To prove the second assertion, by assertion (1) and Lemma 7 (1) and (2), we know that $G\{d\} = G^*\{d\}$ if either $D^{\#} \geq 3$, or $D^{\#} = 2$ and Rayleigh frequencies are excluded. It remains to prove that $Q = G\{d\}$. If there exists an element $d_n \in Q \backslash G\{d\}$ with a non-negative x_2-component, then $G^*\{d_n\} \cap G^*\{d\} = \emptyset$. If $G^*\{d_n\}^{\#} = D^{\#} \geq 3$, then there exists at least one element of $G^*\{d_n\}$ having a negative x_2-component. The other case when $D^{\#} = 2$ and Rayleigh frequencies are excluded would lead to the same consequence. Both cases are impossible since $G^*\{d_n\} \subset Q$ and each element of $G^*\{d_n\}$ has a non-negative x_2-component. Thus $Q = G\{d\}$. $\square$

We proceed with the proof by considering the possible numbers of elements of D separately.

Step 2. $D^{\#} = 2$.

It is seen from the first step and Lemma 6 (2) that $D = \{L, S\}$ with $L \perp S$. Without loss of generality, we can assume

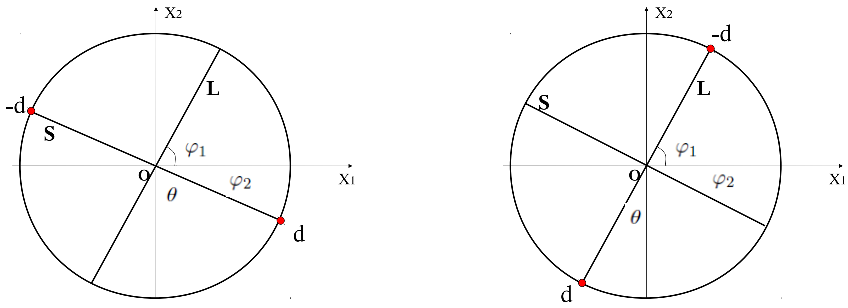
$$L = L_{\varphi_1} \text{ with } \varphi_1 \in [0, \frac{\pi}{2}), \quad S = L_{\varphi_2} \text{ with } \varphi_2 = \varphi_1 - \frac{\pi}{2} \in [-\frac{\pi}{2}, 0). \tag{16}$$

Then, we need to discuss the following two cases.

Case (a): Rayleigh frequencies are excluded.

By the above Lemma 12 (2), we have $G\{d\}^{\#} = G^*\{d\}^{\#} = D^{\#} = 2$. More specifically, $Q = G\{d\} = \{d, -d\}, D = \{L, S\}, G = \{\mathrm{Rot}(2\pi), \mathrm{Rot}(\pi), \mathrm{R}_L, \mathrm{R}_S\}$ and $L \perp S$ (see Figure 2).

Figure 2: $D^{\#} = 2, Q = G\{d\} = \{d, -d\} = \{(\alpha, -\beta), (-\alpha, \beta)\}$. Left: $\theta > 0$. Right: $\theta < 0$.



By Lemma 5, we know that u takes the form

$$u = \exp(ix \cdot d) + \exp(-ix \cdot d).$$

If $\theta \in [0, \frac{\pi}{2})$, then $S \parallel Od$ and $\mathrm{R}_S d = d$, which implies that $\varphi_1 = \theta, \varphi_2 = \theta - \frac{\pi}{2}$, or equivalently, $L = L_\theta, S = L_{\theta - \frac{\pi}{2}}$. If $\theta \in [-\frac{\pi}{2}, 0)$, then $L \parallel Od$ and $\mathrm{R}_L d = d$, which implies that $\varphi_2 = \theta, \varphi_1 = \theta + \frac{\pi}{2}$, or equivalently, $S = L_\theta, L = L_{\theta + \frac{\pi}{2}}$. On noting that $L_{\theta + \frac{\pi}{2}} = L_{\theta - \frac{\pi}{2}}$ and $(d, -d) \in Q$, by repeating the argument in step 3 of Theorem 2, we have $\Lambda_1, \Lambda_2 \in \mathcal{N}_2(\theta, k)$.

Case (b): A Rayleigh frequency occurs.

If $G\{d\}^{\#} = 2D^{\#} = 4$, then we can carry over steps 2 and 3 of the proof of Theorem 2 to prove that $\Lambda_1, \Lambda_2 \in \mathcal{D}_2(\theta, k)$, so that by Lemma 5 (2) the total field u takes the form

$$u = \exp(ix \cdot d) + \exp(-ix \cdot d) + \exp(ikx_1) + \exp(-ikx_1).$$

If $G\{d\}^{\#} = D^{\#} = 2$, then one of the lines $\{S, L\}$ must pass through d. Considering the case of a Rayleigh frequency, we have that $L = L_0, S = L_{-\frac{\pi}{2}}$ and $\theta = 0$, and u takes the form

$$u = \exp(-ikx_2) + \exp(ikx_2) + \exp(ikx_1) + \exp(-ikx_1).$$

Similar to the Dirichlet case, we can derive that $\Lambda_1, \Lambda_2 \in \tilde{\mathcal{N}}_2(0, k)$, where

$$\tilde{\mathcal{N}}_2(0,k) := \left\{ \Lambda \in \mathcal{A} : \begin{array}{l} \text{Each line segment of } \Lambda \text{ is parallel to one of the lines} \\ L_0, L_{\frac{\pi}{2}}, \text{ and its distance to } L_0 \text{ (or } L_{\frac{\pi}{2}}) \text{ is an integral} \\ \text{multiple of } \frac{\pi}{k}. \text{ In addition, } k \in \mathbb{Z}. \end{array} \right\}.$$

Note that $\tilde{\mathcal{N}_2}(0,k)$ is a subset of $\mathcal{N}_2(0,k) \cap \mathcal{N}_4(0,k)$.

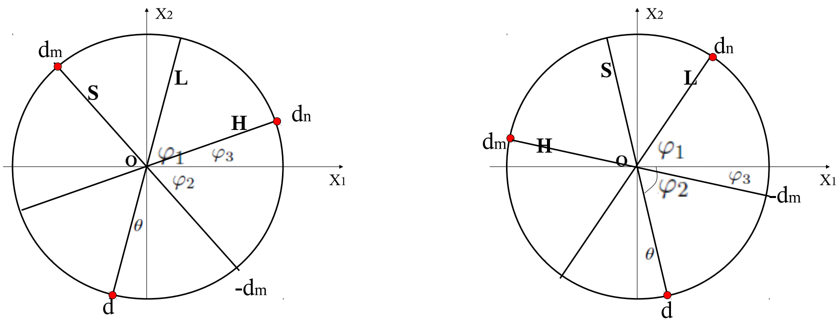
Step 3. $D^{\#} = 3$.

By Lemma 12, we only need to consider the case of $G\{d\}^{\#} = D^{\#}$ by assuming that $Q = G\{d\} = G^*\{d\} = \{d, d_n, d_m\}, D = \{L, S, H\}$ with $L = L_{\varphi_1}, S = L_{\varphi_2}, H = L_{\varphi_3}$. Since L, S and H form an equiangular system of lines, without loss of generality we can suppose that $\varphi_1 \in [0, \frac{\pi}{2}), \varphi_2 \in [-\frac{\pi}{2}, 0), \varphi_3 \in [-\frac{\pi}{2}, \frac{\pi}{2})$ with

$$\varphi_2 < \varphi_3 < \varphi_1 \text{ and } \varphi_1 - \varphi_3 = \varphi_3 - \varphi_2 = \frac{\pi}{3}. \tag{17}$$

Since $\varphi_2 \geq -\frac{\pi}{2}$ and $\varphi_1 < \frac{\pi}{2}$, we have that $-\frac{\pi}{6} \leq \varphi_3 < \frac{\pi}{6}$. We complete this step by discussing the following two cases: (1) $-\frac{\pi}{6} \leq \varphi_3 \leq 0$; (2) $0 < \varphi_3 < \frac{\pi}{6}$.

Figure 3: $D^{\#} = 3, Q = G\{d\} = \{d, d_n, d_m\}$. Right: $-\frac{\pi}{6} < \varphi_3 < 0, 0 < \theta < \frac{\pi}{6}$. Left: $\frac{\pi}{6} > \varphi_3 > 0, -\frac{\pi}{6} < \theta < 0$.



Case (1): $-\frac{\pi}{6} \leq \varphi_3 \leq 0$.

It follows from (17) that $\frac{\pi}{6} \leq \varphi_1 \leq \frac{\pi}{3}, -\frac{\pi}{2} \leq \varphi_2 \leq -\frac{\pi}{3}$. Recalling that one of the lines $\{L, S, H\}$ must be parallel to Od, and that the x_2-components of d_m and d_n are all non-negative, we have that $S \parallel Od$, and

$$\theta = \varphi_2 + \frac{\pi}{2} = \varphi_3 + \frac{\pi}{6} = \varphi_1 - \frac{\pi}{6} \tag{18}$$

which results in $0 \leq \theta \leq \frac{\pi}{6}$. Without loss of generality we can assume (see Figure 3 Right)

$$H \parallel Od_m \text{ with } d_m := (\alpha_m, \beta_m) = (k \sin\theta + m, \beta_m) \text{ for some } m \in \mathbb{Z}, \tag{19}$$

$$L \parallel Od_n \text{ with } d_n := (\alpha_n, \beta_n) = (k \sin\theta + n, \beta_n) \text{ for some } n \in \mathbb{Z}. \tag{20}$$

It follows from (18) that $\varphi_1 = \theta + \frac{\pi}{6}, \varphi_3 = \theta - \frac{\pi}{6}$, leading to

$$-d_m = k(\cos\varphi_3, \sin\varphi_3) = k(\cos(\theta - \frac{\pi}{6}), \sin(\theta - \frac{\pi}{6})), \tag{21}$$

$$d_n = k(\cos\varphi_1, \sin\varphi_1) = k(\cos(\theta + \frac{\pi}{6}), \sin(\theta + \frac{\pi}{6})). \tag{22}$$

In view of (19)-(22), we arrive at

$$k\cos(\theta - \frac{\pi}{6}) + k\sin\theta \in \mathbb{Z}, \; k\cos(\theta + \frac{\pi}{6}) - k\sin\theta \in \mathbb{Z},$$

from which $k\sqrt{3}\sin(\frac{\pi}{6} \pm \theta) \in \mathbb{Z}$ can be obtained.

We next proceed in the same way as in step 3 of Theorem 2 to prove that $\Lambda_1, \Lambda_2 \in \mathcal{N}_3(\theta, k)$. Define

$$\tilde{N} = \{l : l \text{ is a Neumann line of } u \text{ in } \mathbb{R}^2\}.$$

By the reflection principle and Lemma 1, for each $l \in \tilde{N}$, $\mathrm{R}_l'd \in Q = \{d, d_n, d_m\}$. If $\mathrm{R}_l'd = d$, then $l \parallel S$; if $\mathrm{R}_l'd = d_m$, then $l \parallel L$; and if $\mathrm{R}_l'd = d_n$, then $l \parallel H$.

It follows from Lemma 5 (2) that

$$u = \exp(ix \cdot d) + \exp(ix \cdot d_n) + \exp(ix \cdot d_m). \tag{23}$$

Without loss of generality, we may assume that $l \parallel S$. Making use of $\mathrm{R}_l x = \mathrm{R}_l' x + \mathrm{R}_l O, \mathrm{R}_l' d = d, \mathrm{R}_l' d_m = d_n$, we derive that

$$u(\mathrm{R}_l x) = \exp(ix \cdot d) + \exp(ix \cdot d_m)\exp(i\mathrm{R}_l O \cdot d_n) + \exp(ix \cdot d_n)\exp(i\mathrm{R}_l O \cdot d_m).$$

The application of the reflection principle to the line l leads to $\exp(i\mathrm{R}_l O \cdot d_n) = \exp(i\mathrm{R}_l O \cdot d_m) = 1$, from which we get

$$\mathrm{dist}(l, S) = \frac{2\pi}{k\sqrt{3}} n_1, \text{ for some } n_1 \in \mathbb{Z},$$

because $|\mathrm{R}_l O \cdot d_n| = |\mathrm{R}_l O \cdot d_m| = 2 \cdot \mathrm{dist}(l, S) k \cos\frac{\pi}{6}$. Analogously, we can prove that

$$\begin{aligned}
\mathrm{dist}(l, L) &= \frac{2\pi}{k\sqrt{3}} n_2, \text{ for some } n_2 \in \mathbb{Z} \text{ if } l \parallel L, \\
\mathrm{dist}(l, H) &= \frac{2\pi}{k\sqrt{3}} n_3, \text{ for some } n_3 \in \mathbb{Z} \text{ if } l \parallel H.
\end{aligned}$$

Since each line segment of Λ_1 can be extended to an element of $\tilde{N}$, we have proved that $\Lambda_1 \in \mathcal{N}_3(\theta, k)$. The relation $\Lambda_2 \in \mathcal{N}_3(\theta, k)$ can be proved likewise.

Case (2): $\frac{\pi}{6} > \varphi_3 > 0$ (see Figure 3 Left).

Analogously to case (1), we obtain from $L \parallel Od$, $-\frac{\pi}{6} < \theta < 0$ and $\theta = \varphi_1 - \frac{\pi}{2} = \varphi_3 - \frac{\pi}{6} = \varphi_2 + \frac{\pi}{6}$ that $\Lambda_1, \Lambda_2 \in \mathcal{N}_3(\theta, k)$ with $k\sqrt{3}\sin(\frac{\pi}{6} \pm \theta) \in \mathbb{Z}$.

It is obvious that a Rayleigh frequency only occurs when $\varphi_3 = 0$, leading to $\varphi_1 = \frac{\pi}{3}$ and $\varphi_2 = -\frac{\pi}{3}$. In this case, $L \parallel Od$ implies that $\theta = -\frac{\pi}{6}$, while $S \parallel Od$ implies that $\theta = \frac{\pi}{6}$.

Step 4. $D^\# \geq 4$.

In this case, by Lemma 12 we have $Q^\# = G^*\{d\}^\# = G\{d\}^\# = D^\# \geq 4$, implying that a Rayleigh frequency occurs. Since there are at most one element of Q having a negative x_2-component, and at most two elements of Q having a vanishing x_2-component, we have that $D^\# = 4$. Taking account of the Rayleigh frequency, we know that one element of D must be parallel to the x_1-axis, thus by Lemma 6 (2) $Q = G^*\{d\} = \{(0, -k), (0, k), (k, 0), (-k, 0)\}$, which means $\theta = 0$, and u takes the form

$$u(x) = \exp(-ikx_2) + \exp(ikx_2) + \exp(ikx_1) + \exp(-ikx_1). \tag{24}$$

By the α-quasi-periodicity of $u(x)$, k must be a positive integer. Repeating step 3 in the proof of Theorem 2 leads to the relation $\Lambda_1, \Lambda_2 \in \mathcal{N}_4(0, k)$.

The proof of Theorem 3 is thus complete. □

From the above proof, it follows that each element of $\mathcal{N}_3(\theta, k)$ (or $(\mathcal{N}_4(0, k))$) can generate the same total field of the form (23) (or (24)). Thus non-uniqueness examples could be constructed for the inverse Neumann problem by the elements of $\mathcal{N}_3(\theta, k)$ and $\mathcal{N}_4(0, k)$.

Counterexample 1 Let $\theta = 0$ (orthogonal incidence) and $k = 2\sqrt{3}$. We can check that the Rayleigh frequency is excluded in this case. Let $\Lambda_1|_{(-\pi,\pi)}$ and $\Lambda_2|_{(-\pi,\pi)}$ be defined by the following piecewise linear functions:

$$\Lambda_1 : x_2 = \begin{cases} x_1\sqrt{3}/3 & x_1 \in (0,\pi), \\ -x_1\sqrt{3}/3 & x_1 \in (-\pi, 0]; \end{cases} \quad \Lambda_2 : x_2 = \begin{cases} -x_1\sqrt{3}/3 & x_1 \in (0,\pi), \\ x_1\sqrt{3}/3 & x_1 \in (-\pi, 0]. \end{cases}$$

Let Λ_i be the 2π-periodic extensions of $\Lambda_i|_{(0,2\pi)} (i = 1, 2)$. We can see that both Λ_1 and Λ_2 belong to $\mathcal{N}_3(0, 2\sqrt{3})$. Then the finite Rayleigh expansion

$$u(x) = \exp(-i2\sqrt{3}x_2) + \exp(i(3x_1 + \sqrt{3}x_2)) + \exp(i(-3x_1 + \sqrt{3}x_2))$$

satisfies the Helmholtz equation and the homogeneous Neumann boundary condition on both Λ_1 and Λ_2. Thus one incident wave is not sufficient to uniquely determine Λ.

One can also construct another example with a non-zero incident angle θ and an appropriately chosen k such that $|\theta| \le \frac{\pi}{6}$ and $k\sqrt{3}\sin(\theta \pm \frac{\pi}{6}) \in \mathbb{Z}$. For instance, taking $k = \frac{\sqrt{28}}{3}$ and $\theta \in (0, \frac{\pi}{6})$ with $\sin\theta = \sqrt{\frac{1}{28}}$, $\cos\theta = \sqrt{\frac{27}{28}}$, we have $k\sqrt{3}\sin(\theta \pm \frac{\pi}{6}) \in \mathbb{Z}$. Then the corresponding example can be constructed in the same way as in Counterexample 1. Next we give an example of a grating from $\mathcal{N}_3(k, \theta)$ in the presence of a Rayleigh frequency.

Counterexample 2: Two incident waves are not sufficient to uniquely determine a grating profile $\Lambda \in \mathcal{A}$.

Let $\Lambda_1|_{(0,2\pi)}$ and $\Lambda_2|_{(0,2\pi)}$ be defined by the following piecewise linear functions:

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

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

and let Λ_i be the 2π-periodic extensions of $\Lambda_i|_{(0,2\pi)} (i = 1, 2)$. Set $k = 2$ and $\theta = \frac{\pi}{6}$ or $-\frac{\pi}{6}$. One can check that $\Lambda_1, \Lambda_2 \in \mathcal{N}_3(\frac{\pi}{6}, 2) \cap \mathcal{N}_3(-\frac{\pi}{6}, 2)$ and the finite Rayleigh expansions

$$\begin{aligned} u(x) &= \exp(i(x_1 - \sqrt{3}x_2)) + \exp(i(x_1 + \sqrt{3}x_2)) + \exp(-2ix_1), \\ u(x) &= \exp(-i(x_1 + \sqrt{3}x_2)) + \exp(-i(x_1 - \sqrt{3}x_2)) + \exp(2ix_1) \end{aligned}$$

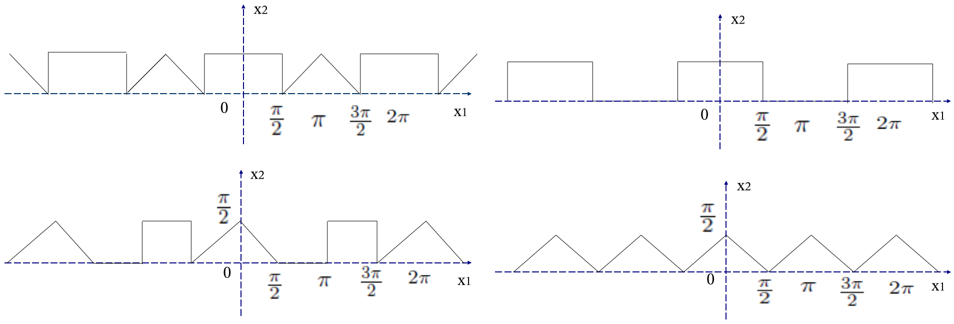
all satisfy the Helmholtz equation and the homogeneous Neumann boundary condition on both Λ_1 and Λ_2.

Counterexample 3 We construct another non-uniqueness example for the inverse Neumann problem by describing the elements in $\mathcal{N}_4(0, k)$.

Set $k = 4, \theta = 0$, then $\alpha = k\sin\theta = 0, \beta = k = 4$. One can see that each grating shown in Figure 4 is an element of $\mathcal{N}_4(0, 4)$. It follows from the proof of Theorem 3 that the gratings indicated in Figure 4 generate the same total field $u(x)$ of the form (24) with $k = 4$, i.e.,

$$u(x) = \exp(-4ix_2) + \exp(4ix_2) + \exp(-4ix_1) + \exp(-4ix_1). \tag{25}$$

Figure 4: $\Lambda \in \mathcal{N}_4(0,k)$ with $k=4$.



.

In fact, we can verify that the function u defined in (25) satisfies the Helmholtz equation, the quasi-periodicity condition and the Rayleigh expansion. Furthermore u satisfies the homogeneous Neumann boundary condition on the following lines:

(1) $x_2 = \frac{\pi}{4}n_1$ for all $n_1 \in \mathbb{Z}$, (2) $x_1 = \frac{\pi}{4}n_2$ for all $n_2 \in \mathbb{Z}$,

(3) $x_2 = x_1 + \frac{\pi}{2}n_3$ for all $n_3 \in \mathbb{Z}$, (4) $x_2 = -x_1 + \frac{\pi}{2}n_4$ for all $n_4 \in \mathbb{Z}$.

Essentially, if each line segment of Λ lies on the grid generated by the above straight lines, then $\Lambda \in \mathcal{N}_4(0,k)$, and thus generates the same total field of the form (25).

We finish this section by studying the minimal number of incident waves that are needed to uniquely determine $\Lambda \in \mathcal{A}$. We introduce the following classes of unidentifiable gratings by defining

$$\mathcal{T}_2(\theta,k) := \mathcal{N}_2(\theta,k) \cup \mathcal{D}_2(\theta,k), \mathcal{T}(\theta,k) := \mathcal{T}_2(\theta,k) \cup \mathcal{N}_3(\theta,k) \cup \mathcal{N}_4(\theta,k),$$

with the convention that $\mathcal{N}_4(\theta,k) = \emptyset$ for $\theta \neq 0$. In view of Theorem 3, we have the following result:

Corollary 4 *Under the conditions of Theorem 3, if (15) holds for M incident waves with distinct incident angles θ_i $(i = 1, 2\cdots, M)$ such that $\mathcal{T}(\theta_1,k) \cap \mathcal{T}(\theta_2,k) \cap \cdots \cap \mathcal{T}(\theta_M,k) = \emptyset$, then $\Lambda_1 = \Lambda_2$.*

To determine the intersection of those unidentifiable sets for different incident angles, we need the following lemma:

Lemma 13 *Let $\theta_i \in (-\frac{\pi}{2}, \frac{\pi}{2})(i = 1, 2, 3, 4)$ be distinct incident angles and k be a fixed wave number.*
(1) $\mathcal{N}_2(\theta_1,k) \cap \mathcal{N}_2(\theta_2,k) \neq \emptyset$ if and only if $\theta_1 \in (0, \frac{\pi}{2}), \theta_2 \in (-\frac{\pi}{2}, 0)$ satisfy

$$\theta_1 - \theta_2 = \frac{\pi}{2}, 2k\sin\theta_1 \in \mathbb{Z} \text{ and } 2k\sin\theta_2 \in \mathbb{Z}.$$

(2) $\mathcal{N}_2(\theta_1,k) \cap \mathcal{N}_2(\theta_2,k) \cap \mathcal{D}_2(\theta_3,k) \neq \emptyset$ if and only if $\theta_1 \in (0, \frac{\pi}{2}), \theta_2 \in (-\frac{\pi}{2}, 0)$ satisfy

$$\theta_2 = \theta_1 - \frac{\pi}{2}, \ \ \theta_3 = 2\theta_1 - \frac{\pi}{2} = 2\theta_2 + \frac{\pi}{2}, \tag{26}$$

$$2k\sin\theta_1 \in \mathbb{Z}, \ \ 2k\sin\theta_2 \in \mathbb{Z}, \ \ \ k(1 \pm \sin\theta_3) \in \mathbb{Z}. \tag{27}$$

(3) $\mathcal{D}_2(\theta_1,k) \cap \mathcal{D}_2(\theta_2,k) = \emptyset, \ \mathcal{T}_2(\theta_1,k) \cap \mathcal{N}_3(\theta_2,k) = \emptyset$.
(4) $\mathcal{T}(\theta_1,k) \cap \mathcal{T}(\theta_2,k) \cap \mathcal{T}(\theta_3,k) \cap \mathcal{T}(\theta_4,k) = \emptyset$.

The above lemma can be derived from the definitions of $\mathcal{D}_2(\theta,k),\mathcal{N}_2(\theta,k)$, $\mathcal{N}_3(\theta,k)$ and $\mathcal{N}_4(\theta,k)$. Next we are mainly concerned with the elements of $\mathcal{N}_2(\theta_1,k)\cap\mathcal{N}_2(\theta_2,k)\cap\mathcal{D}_2(\theta_3,k)$. For this purpose, we set $\lambda=2k$. Then, by (27), λ belongs to the set K defined by

$$K \;:=\; \left\{\lambda>0: \begin{array}{l}\text{There exists } \theta_1\in(0,\frac{\pi}{2}) \text{ such that } \lambda\sin\theta_1\in\mathbb{Z},\\ \lambda\cos\theta_1\in\mathbb{Z},\; \lambda(2\cos^2\theta_1-1)\in\mathbb{Z} \text{ and } \lambda\in\mathbb{Z}.\end{array}\right\}. \tag{28}$$

Lemma 14 *We have* $\min K=25$.

Proof. Suppose $n_1,n_2\in\mathbb{Z},N\in\mathbb{N}$ are coprime numbers such that

$$\sin\theta_1=\frac{n_1}{N},\cos\theta_1=\frac{n_2}{N} \text{ with } n_1^2+n_2^2=N^2,$$

i.e. (n_1,n_2,N) is a primitive Pythagorean triple. It is well-known that the smallest value of N is 5. Since $\lambda\sin\theta_1\in\mathbb{Z}$, we may assume that $\lambda=N\eta$ for some $\eta\in\mathbb{N}$. Then it is seen from the relation

$$\lambda(2\cos^2\theta_1-1)=2\eta\frac{n_2^2}{N}-\lambda\in\mathbb{Z},\quad \lambda\in\mathbb{Z},$$

that $2\eta\frac{n_2^2}{N}\in\mathbb{Z}$. If N is an odd number, we arrive at $\eta=Nm$ for some $m\in\mathbb{Z}$ since n_2 and N are coprime. Hence $\lambda=mN^2$ with some $m,N\in\mathbb{Z}$, implying that the smallest λ is 25 by taking $m=1$. If N is an even number, then N must be greater than 10, implying that $\lambda\geq\frac{N^2}{2}$ which is greater than 25. Thus $\min K=25$. $\square$

If $\Lambda_1\neq\Lambda_2$ but $\Lambda_1,\Lambda_2\in\mathcal{N}_2(\theta_1,k)\cap\mathcal{N}_2(\theta_2,k)\cap\mathcal{D}_2(\theta_3,k)$, then for each incident wave $u^{in}(x)=\exp\left(ik(x_1\sin\theta_i-x_2\cos\theta_i)\right)$ $(i=1,2,3)$, the total fields $u_j^{(i)}(x)$ corresponding to Λ_j $(j=1,2)$ with the homogeneous Neumann boundary conditions coincide in the whole $\mathbb{R}^2$. More precisely, according to the second step in the proof of Theorem 3, these total fields take the following forms:

$$u_1^{(1)}=u_2^{(1)}=\exp(ik(x_1\sin\theta_1-x_2\cos\theta_1))+\exp(ik(-x_1\sin\theta_1+x_2\cos\theta_1)),$$

for the incident wave with incident angle $\theta_1\in(0,\frac{\pi}{2})$,

$$u_1^{(2)}=u_2^{(2)}=\exp(ik(x_1\sin\theta_2-x_2\cos\theta_2))+\exp(ik(-x_1\sin\theta_2+x_2\cos\theta_2)),$$

for $\theta_2=\theta_1-\frac{\pi}{2}\in(-\frac{\pi}{2},0)$, and

$$\begin{aligned}u_1^{(3)}=u_2^{(3)} \;&=\; \exp(ik(x_1\sin\theta_3-x_2\cos\theta_3))+\exp(ikx_1)\\ &\quad+\exp(ik(-x_1\sin\theta_3+x_2\cos\theta_3))+\exp(-ikx_1)\end{aligned}$$

for $\theta_3=2\theta_1-\frac{\pi}{2}=2\theta_2+\frac{\pi}{2}$. Note that a Rayleigh frequency occurs for θ_3. In this way, non-uniqueness examples for illustrating that three incident waves are not sufficient to determine Λ can be constructed (see the following counterexample).

Counterexample 4 Let $\Lambda_i|_{(0,2\pi)}$ $(i=1,2)$ be defined by the following functions:

$$\Lambda_1: x_2=\left\{\begin{array}{ll}(x_1-2\pi)\tan\theta_2 & x_1\in[T_1,2\pi),\\ x_1\tan\theta_1 & x_1\in[0,T_1)\end{array}\right. \text{ with } T_1=\frac{2\pi\tan\theta_2}{\tan\theta_2-\tan\theta_1}, \tag{29}$$

$$\Lambda_2: x_2=\left\{\begin{array}{ll}(x_1-2\pi)\tan\theta_1 & x_1\in[T_2,2\pi),\\ x_1\tan\theta_2 & x_1\in[0,T_2)\end{array}\right. \text{ with } T_2=\frac{2\pi\tan\theta_1}{\tan\theta_1-\tan\theta_2}, \tag{30}$$

and let Λ_i be the 2π-periodic extensions of $\Lambda_i|_{(0,2\pi)}$ $(i=1,2)$. Let $k=\frac{25}{2}$, choose θ_j satisfying

$$\sin\theta_1=\frac{4}{5},\quad \sin\theta_2=-\frac{3}{5}\ \text{ and }\ \sin\theta_3=\frac{7}{25},$$

and set

$$\begin{aligned} u^{(1)}(x) &= 2\cos(10x_1-\frac{15}{2}x_2),\quad u^{(2)}(x)=2\cos(\frac{15}{2}x_1+10x_2),\\ u^{(3)}(x) &= 2\cos(\frac{7}{2}x_1-12x_2)+2\cos(\frac{25}{2}x_1). \end{aligned}$$

So we obtain the counterexample already presented in [19]. Next we give another example by taking $k=\frac{169}{2}$, $\sin\theta_1=\frac{12}{13}$ (or equivalently $\theta_1=\arcsin\frac{12}{13}$). Set

$$\begin{aligned} &\theta_1=\arcsin\frac{12}{13}, && u^{(1)}(x)=2\cos(78x_1-\frac{65}{2}x_2),\\ &\theta_2=\arcsin\frac{12}{13}-\frac{\pi}{2}, && u^{(2)}(x)=2\cos(\frac{65}{2}x_1+78x_2),\\ &\theta_3=2\arcsin\frac{12}{13}-\frac{\pi}{2}, && u^{(3)}(x)=2\cos(\frac{119}{2}x_1-60x_2)+2\cos(\frac{169}{2}x_1). \end{aligned}$$

It can be verified that each $u^{(j)}(x)$ $(j=1,2,3)$ satisfies the Helmholtz equation in the whole plane, the quasi-periodicity condition and the homogeneous Neumann boundary condition on both grating profiles Λ_1 and Λ_2 defined by (29) and (30) with $\tan\theta_1=\frac{12}{5}$ and $\tan\theta_2=-\frac{5}{12}$. Combining Theorem 3 with Corollary 4 and Lemmas 13 and 14, we determine the minimal number of incident plane waves that can identify Λ uniquely.

Corollary 5 *Suppose that the assumptions of Theorem 3 are satisfied.*

1. If (15) holds for three incident waves with distinct incident angles, then either $\Lambda_1=\Lambda_2$, *or*

$$\Lambda_1,\Lambda_2\in\mathcal{N}_2(\theta,k)\cap\mathcal{N}_2(\theta-\frac{\pi}{2},k)\cap\mathcal{D}_2(2\theta-\frac{\pi}{2},k)$$

with some incident angle $\theta\in(0,\frac{\pi}{2})$. *Moreover,* $2k\sin\theta\in\mathbb{Z}, 2k\cos\theta\in\mathbb{Z}, 4k(\cos^2\theta-1)\in\mathbb{Z}$, $2k\geq 25$ *and* $2k\in\mathbb{Z}$. *In addition, a Rayleigh frequency occurs for the incident angle* $2\theta-\frac{\pi}{2}$.

In particular, we have $\Lambda_1=\Lambda_2$ *if one of the following cases occurs:*

(a) Rayleigh frequencies are excluded for each incident angle.

(b) The incident angles are all positive or negative; or one of the incident angles is $\frac{\pi}{4}$, $-\frac{\pi}{4}$ *or* 0.

(c) The wave number k *is less than* $\frac{25}{2}$.

2. If (15) holds for four incident waves with distinct incident angles, then Λ_1 *and* Λ_2 *must be identical.*

3. Given the a priori information that $\Lambda\in\mathcal{A}$ *has a corner point at the origin and is not an element of* $\mathcal{T}(\theta,k)$, *the near field data* $u(x_1,b;\theta)$ *from one incident wave with the incident angle* θ *are enough to identify* Λ *uniquely.*

4. Given the a priori information that Λ_1 and Λ_2 belong to the class $\mathcal{F}$ defined in (8), if (15) holds for one incident wave with the incident angle θ, then either $\Lambda_1 = \Lambda_2$ or $\Lambda_1, \Lambda_2 \in \mathcal{N}_2(\theta, k) \cup \mathcal{N}_4(\theta, k)$ with $\theta = 0$. This implies that one incident wave with a non-zero incident angle uniquely determines each element of $\mathcal{F}$.

The above corollary can be regarded as a generalization of the results in [19] and [15] in the case of Neumann boundary conditions.

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