TRANSACTIONS OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 366, Number 3, March 2014, Pages 1333–1361
S 0002-9947(2013)05761-3
Article electronically published on October 28, 2013

UNIQUE DETERMINATION OF PERIODIC POLYHEDRAL STRUCTURES BY SCATTERED ELECTROMAGNETIC FIELDS II: THE RESONANCE CASE

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Abstract. This paper is concerned with the unique determination of a three-dimensional polyhedral bi-periodic diffraction grating by the scattered electromagnetic fields measured above the grating. It is shown that the uniqueness by any given incident field fails for seven simple classes of regular polyhedral gratings. Moreover, if a regular bi-periodic polyhedral grating is not uniquely identifiable by a given incident field, then it belongs to a non-empty class of the seven classes whose elements generate the same total field as the original grating when impinged upon by the same incident field. The new theory provides a complete answer to the unique determination of regular bi-periodic polyhedral gratings without any restrictions on Rayleigh frequencies, thus extending our early results (2011) which work under the assumption of no Rayleigh frequencies.

Contents

Received by the editors January 12, 2011 and, in revised form, November 11, 2011 and November 30, 2011.

2010 *Mathematics Subject Classification.* Primary 35R30, 78A46.

Key words and phrases. Inverse electromagnetic scattering, periodic diffraction grating, unique determination, dihedral group.

The research of the first author was supported in part by the NSF grants DMS-0908325, DMS-0968360, and DMS-1211292 and the ONR grants N00014-09-1-0384 and N00014-12-1-0319, a key Project of the Major Research Plan of NSFC (No. 91130004), as well as a special grant from Zhejiang University.

The research of the second author was supported by DMS-0908325.

The research of the third author was substantially supported by Hong Kong RGC grants (Projects 404407 and 405110).

1. Introduction

This is a continuation of our previous work [9] on the unique determination of a bi-periodic diffraction grating in three dimensions by the scattered electromagnetic fields corresponding to some incident plane waves. Throughout the paper, a grating structure S is said to be bi-periodic of period $\Lambda = (\Lambda_1, \Lambda_2)$ if for any point $x = (x_1, x_2, x_3) \in S$, the point $(x_1+n_1\Lambda_1, x_2+n_2\Lambda_2, x_3)$ also belongs to S for all integers n_1 and n_2. We consider such a periodic structure S ruled on a perfect conductor. The medium above S is assumed to be homogenous with a constant dielectric coefficient $\epsilon_0 > 0$ and magnetic permeability $\mu_0 > 0$, and the corresponding region is denoted by Ω. Consider a time-harmonic electromagnetic wave $E^i(x) = se^{iq\cdot x}$ (with time dependence $e^{-i\omega t}$) incident on the grating structure S from above. Due to the solenoidal feature of E^i and its incidence to S from above, the vectors s and q are orthogonal, and the incident direction q can be written as $q = (\alpha_1, \alpha_2, -\beta)$ with $\beta > 0$. Accordingly, the wave number k and the frequency ω are given by

$$k = |q|\,, \quad \omega = k/\sqrt{\epsilon_0\mu_0}\,.$$

For subsequent analysis, we introduce a special vector, $\alpha = (\alpha_1, \alpha_2, 0)$, which is defined by the first two components of q and is parallel to the x_1x_2-plane.

Let E be the total field, the sum of the incident field E^i and scattered field E^s. Then E satisfies the following vector-valued Helmholtz system:

$$\Delta E + k^2 E = 0 \quad \text{in} \quad \Omega, \tag{1}$$

$$\mathrm{div} E = 0 \quad \text{in} \quad \Omega, \tag{2}$$

$$\nu \times E = 0 \quad \text{on} \quad S, \tag{3}$$

where ν is the unit outward normal vector to the surface S.

Noting the bi-periodic structure of the grating, we are only interested in the quasi-periodic solutions E to the system (1)-(3), i.e. $e^{-i\alpha\cdot x}E$ is periodic respectively with period Λ_1 in the x_1-direction and Λ_2 in the x_2-direction; see [11], [15]. We also impose a radiation condition in the x_3-direction by assuming that the scattered field E^s is composed of bounded outgoing plane waves. Then it follows from the knowledge of a fundamental solution to the periodic Helmholtz equation (cf. [11], [15]) that E can be expressed in the form:

$$E(x) = E^i(x) + \sum_{n\in\mathbf{Z}^2} A^n e^{iq^n\cdot x} \text{ for all } x \text{ in } \mathbf{R}^3 \text{ above the highest point on } S, \tag{4}$$

where the A^n's are complex vectors, called *Rayleigh coefficients*, and the q^n's are wave vectors given by

$$q^n = \alpha^n + \alpha + (0, 0, \beta^n) \tag{5}$$

with $\alpha^n = (2\pi n_1/\Lambda_1, 2\pi n_2/\Lambda_2, 0)$ and

$$\beta^n = \begin{cases} \sqrt{k^2 - |\alpha^n + \alpha|^2}, & k^2 \geq |\alpha^n + \alpha|^2\,, \\ i\sqrt{-k^2 + |\alpha^n + \alpha|^2}, & k^2 < |\alpha^n + \alpha|^2\,. \end{cases} \tag{6}$$

We readily observe from (6) that there are only a finite number of propagating plane waves in the scattered field, namely those modes in (4) corresponding to

which the components β^n are real; while the remaining modes decay exponentially along the x_3-direction.

For the sake of convenience, we introduce two index sets,

$$\Xi = \{n \in \mathbf{Z}^2;\ \beta^n > 0\}\,, \quad \Xi^* = \{n \in \mathbf{Z}^2;\ \beta^n = 0\}.$$

Note that the set Ξ^* may not be empty. We denote by E_p the *propagating field*, namely, the part of the total field of E in (4) with those exponentially decaying modes removed:

$$E_p(x) = E^i(x) + \sum_{n\in\Xi} A^n e^{iq^n\cdot x}\,. \tag{7}$$

Different from the total field E in expression (4), the propagating field E_p can be extended to the whole space $\mathbf{R}^3$ naturally, due to the finite number of terms in (7). This fact will be used repeatedly in our analysis.

Given a periodic structure S and an incident field E^i, the forward diffraction problem is to solve system (1)-(4) for the total field E, which has been extensively studied in the literature; see, e.g., [6], [7], [10], [15], [26]. It is known that the solution to the forward problem is not unique in the case of resonance. Throughout this work we assume the existence of a solution to the forward problem (1)-(4), though the solution may not necessarily be unique. Indeed a non-uniqueness example can be drawn in Subsection 3.6.

This work is mainly concerned with an inverse problem associated with the system (1)-(4). For a given incident wave E^i, we assume that the total field E can be measured on a plane Γ_b above the structure S. Our aim is to find out how many incident waves should be sent so that measurements of the resulting total fields on the plane Γ_b can uniquely determine the shape and position of the structure S. It is known that global uniqueness with one incident wave is generally not true [9]. For general periodic grating profiles, the global uniqueness by one or several incident waves remains open. However, when periodic structures are restricted to some special classes, significant progress has been achieved in two dimensions; see [3], [4], [8], [11], [17], [18], [19], [20], [21], and a review of such references in [9].

The situation is much more complicated in three dimensions, for which some important results were made in [9]. For the description of those results, we introduce a new concept. We say that a grating is *regular* if its profile S satisfies the following convexity condition: for any $x \in S$, the ray γ given by $\gamma(t) = x + te_3$ for $t > 0$ lies in the set $\Omega \cup S$, and $\gamma \cap S$ is either empty or an interval. Here we recall that Ω is the domain above S. This convexity condition is not stated explicitly in [9], but is assumed in the arguments there; see the proof of Theorem 4.1 in [9]. When gratings are restricted to such regular bi-periodic polyhedral types, and under the condition that Rayleigh frequencies do not occur, namely the following relation

$$k^2 \neq |\alpha^n + \alpha|^2 \tag{8}$$

holds for all $n \in \mathbf{Z}^2$, it was shown in [9] that corresponding to each incident plane wave, there are three simple classes of unidentifiable gratings such that any regular bi-periodic polyhedral grating can be uniquely determined by the incident field if and only if it belongs to none of the three classes.

Different from all existing results, the theoretical development in [9] is based on the following essential observations and insights: if S is a regular polyhedral grating unidentifiable by the incident field E^i, then the set of perfect planes associated with

the total field E is not empty, and so is the set of perfect planes associated with the propagating field E_p. But it is found that those wave vectors q^n which form E_p in (7) possess some essential symmetry. It is this symmetric property, combined with some application of group theory and other facts about the coefficients A^n appearing in E_p that enables the unique determination of the propagating field E_p and the structure S.

This paper is devoted to the unique determination of regular bi-periodic polyhedral structures for the general and more challenging case where Rayleigh frequencies are allowed to occur, i.e., condition (8) is not assumed. From now on, we shall restrict our study to bi-periodic gratings which are regular and are of polyhedral type. To the best of our knowledge, this work represents the first attempt to study inverse scattering by periodic structures in the resonance case in three dimensions, while the two-dimensional case was investigated in [19], [20]. Although the basic analytical methodologies here follow the ones in our early work [9], the presence of Rayleigh frequencies will lead to four new and more complicated classes of unidentifiable gratings, and this requires much more delicate and technical derivations and treatments as well as some new analysis tools. Moreover, for each new class, except for the last one, we are able to construct a series of concrete examples of grating structures.

The rest of the paper is organized as follows. In Section 2, we introduce some notation, concepts, and tools which are key to subsequent analysis. In Section 3, we show how to start from one perfect plane of the total field to find all possible gratings to which the global uniqueness fails. Finally, we establish the main result about the uniqueness of our inverse scattering problem in Section 4.

2. Preliminaries

We begin with the following conventions and notation:

(1) For any vector $b \in \mathbf{R}^3$, its norm is denoted by $\|b\|$. For convenience, a point $r \in \mathbf{R}^3$ is often viewed as the vector originating from the origin which directs to the point r.

For any $r > 0$ and $y \in \mathbf{R}^3$, we define $B_r(y) = \{x \in \mathbf{R}^3;\ \|x - y\| \le r\}$.

(2) A vector $r \in \mathbf{R}^3$ is said to be parallel to a line l in $\mathbf{R}^3$ with a tangential unit vector ν, if $r \parallel \nu$. For a plane Π in $\mathbf{R}^3$, we denote by ν_Π the unit normal vector to Π. A vector r is said to be parallel to a plane Π in $\mathbf{R}^3$, if $r \perp \nu_\Pi$.

For any two parallel planes Π and Π^* in $\mathbf{R}^3$, their distance is denoted by $\mathrm{dist}(\Pi, \Pi^*)$.

(3) For any $c \in \mathbf{C}^3$ and $r \in \mathbf{R}^3$, the dot product $c \cdot r = 0$ means $\mathrm{Re}(c) \cdot r = 0$ and $\mathrm{Im}(c) \cdot r = 0$. The same conventions will be made for relations $c \,||\, r$, $c \times r$ and $c \perp \Pi$ for any plane Π in $\mathbf{R}^3$.

(4) Let Π be a plane in $\mathbf{R}^3$; we denote by R_Π the reflection with respect to plane Π in $\mathbf{R}^3$. The reflection R_Π is always understood to be acting on points in $\mathbf{R}^3$.

Let Π' be the plane that passes through the origin and is parallel to Π, and R'_Π be the derivative of R_Π, namely the linear part of R_Π. One can see that R'_Π is the reflection with respect to the plane Π'. For a point $r \in \mathbf{R}^3$, $R'_\Pi r$ can also be viewed as the reflection of the vector that initiates from the

origin and points to the point r, with respect to the plane Π'. By natural extension, we apply R'_Π to complex vectors in $\mathbf{C}^3$ as well.

(5) For a set $\mathcal{A}$, we denote by $|\mathcal{A}|$ the number of elements in $\mathcal{A}$.

(6) Let G be a group which acts on a set $\mathcal{A}$. Let $a \in \mathcal{A}$; then $G\{a\}$ means the orbit of a under the action of the group G.

The following concepts about perfect sets and planes are important tools to our subsequent analysis.

Definition 2.1. Let $F : O \to \mathbf{C}^3$ be a given analytic complex vector-valued function in a domain $O \subset \mathbf{R}^3$. $\mathcal{P}_F$ is called the perfect set of F if

$$\mathcal{P}_F = \{x \in O;\ \nu_\Pi \times F\,|_{\Pi \cap B_r(x) \cap O} = 0 \text{ for some } r > 0 \text{ and plane } \Pi \text{ passing through } x\}.$$

The points in $\mathcal{P}_F$ are called perfect points of F.

For any $x \in \mathcal{P}_F$, let Π be a corresponding plane involved in the definition of $\mathcal{P}_F$, and $\widetilde{\Pi}$ the connected component of $\Pi \cap O$ containing x. Then by the analyticity of F and analytic continuation, we have $\nu_\Pi \times F = 0$ on $\widetilde{\Pi}$. In the sequel, such $\widetilde{\Pi}$ will be referred to as a *perfect plane* of F. We also use $\mathcal{P}_F$ to denote the set of perfect planes of F whenever there is no confusion caused.

Note that the electric field E to the system (1)-(3) is analytic in the domain Ω, which leads to the important reflection property of E about a perfect plane; see [24].

Lemma 2.1 (Reflection principle)**.** *Let O be a domain in $\mathbf{R}^3$ which is symmetric with respect to a plane Π, and E be an electric field in O satisfying the vector-valued Helmholtz equations* (1)-(2)*. Assume that $\tilde{\Pi}$ is a connected open subset in $\Pi \cap O$. Then $\tilde{\Pi}$ is a perfect plane of E if and only if the following relation holds:*

$$E(x) + R'_\Pi(E(R_\Pi(x))) = 0 \text{ in } O. \tag{9}$$

Moreover, if $\Gamma \subset O$ or $\Gamma \subset \partial O$ is a perfect plane of E, then $R_\Pi(\Gamma)$ is also a perfect plane of E.

3. Classification of unidentifiable periodic structures

3.1. **Observations and the first class.** We recall some basic notation from Section 1.

$E^i(x) = se^{iq\cdot x}$: the incident electric field;

$E(x)$: the total field;

S: the grating profile of bi-period Λ. S is also often referred to as the grating for the purpose of simplifying notation;

Γ_b: the plane $\{x_3 = b\}$ above the grating S, on which the total field E is measured;

Ω_b: the domain above the plane Γ_b.

We also introduce

$$\Xi_0 = \{n \in \Xi;\ A^n \neq 0\}, \quad \mathcal{Q} = \{q\} \cup \{q^n\}_{n \in \Xi_0}, \tag{10}$$

$$E_p(x) = se^{iq\cdot x} + \sum_{n \in \Xi_0} A^n e^{iq^n \cdot x}, \tag{11}$$

$$\mathcal{P} = \{\Pi;\ \Pi \text{ is a perfect plane of } E_p\}. \tag{12}$$

Now for the incident field E^i, we intend to find all the regular bi-periodic polyhedral structures which cannot be identified by E^i. We start with an assumption, which is the first fundamental fact to be established in the demonstration of our main global uniqueness result in Section 4.

Assumption 1. *There exists a perfect plane of E, which intersects Ω_b and is not perpendicular to the plane $\{x_3 = 0\}$.*

The aim of this section is to show that under Assumption 1, there are seven cases, in each of which we can determine the propagating field E_p, the set of perfect planes $\mathcal{P}$, and the structure of grating S simultaneously. This leads to seven classes of unidentifiable regular polyhedral structures in correspondence to each given incident field E^i.

Next we recall several important observations and results in [9].

Lemma 3.1. *If Π is a perfect plane of E, then Π is also a perfect plane of E_p.*

Lemma 3.1 presents an obvious advantage to working with the perfect planes of the propagating field E_p over the ones of the total field E: the perfect planes of E_p are truly two-dimensional planes in $\mathbf{R}^3$.

Proposition 3.1. *Each vector in $\mathcal{Q}$ except q has a non-negative x_3-component.*

Proposition 3.2. *For each perfect plane Π in $\mathcal{P}$, we have $R'_\Pi \mathcal{Q} = \mathcal{Q}$, $R_\Pi \mathcal{P} = \mathcal{P}$. Moreover, both maps R'_Π: $\mathcal{Q} \to \mathcal{Q}$ and R_Π: $\mathcal{P} \to \mathcal{P}$ are bijective.*

Lemma 3.2. *Let $F = te^{ip\cdot x}$ be one of the Fourier modes of E_p in* (11)*. Then the following two statements hold:*

1. *If Π is a perfect plane in $\mathcal{P}$ such that $R'_\Pi p = p$, then $t \perp \Pi$.*
2. *If Π and Π^* are two perfect planes in $\mathcal{P}$ such that $R'_\Pi p = R'_{\Pi^*} p$, then $\Pi \parallel \Pi^*$.*

We now begin the process of finding all seven classes of unidentifiable gratings corresponding to the incident field $E^i = se^{iq\cdot x}$. Our approach is based on the analysis of the set of perfect planes of E_p, namely $\mathcal{P}$. We know that $\mathcal{P}$ is not empty by Assumption 1 and Lemma 3.1, and that planes of $\mathcal{P}$ are all true planes in $\mathbf{R}^3$.

Clearly $\mathcal{P}$ may have the following three cases:

Case 1. Any two planes in $\mathcal{P}$ are parallel to each other.

Case 2. There are at least two planes in $\mathcal{P}$ that are not parallel to each other; and the intersection line between any two intersecting planes in $\mathcal{P}$ is parallel to the plane $\{x_3 = 0\}$.

Case 3. There are at least two planes in $\mathcal{P}$ that are not parallel to each other; and there exists an intersection line between two intersecting planes in $\mathcal{P}$, which is not parallel to the plane $\{x_3 = 0\}$.

Case 1 was studied in [9], which yields the first unidentifiable class of polyhedral gratings:

$$\mathcal{S}_1(q,r) = \Big\{\text{all planes which are parallel to } \{x_3 = 0\} \text{ and have equal distance } \pi/\beta \text{ between each other, with } r \text{ lying on one of the planes}\Big\},$$

where r is an arbitrary point in $\mathbf{R}^3$.

According to [9], any two gratings belonging to the class $\mathcal{S}_1(q,r)$, say S_1 and S_2, are not distinguishable by the incident wave E^i, since the total fields generated by the incident wave E^i in the domain above S_1 and S_2 respectively are exactly the same.

Cases 2 and 3 above will be studied in detail in Subsections 3.2-3.6 and 3.7-3.9, respectively.

3.2. **Preparations for Case 2.** In this section we study Case 2 classified in Subsection 3.1. In this case, there are at least two planes in $\mathcal{P}$ that are not parallel to each other, and the intersection line between any two intersecting planes in $\mathcal{P}$ is parallel to the plane $\{x_3 = 0\}$. As we shall see, this case leads to five classes of unidentifiable gratings.

Let Π_0 and Π_1 be two planes in $\mathcal{P}$ which are not parallel to each other. We further introduce the following notation:

L: the intersection line between Π_0 and Π_1;

r: an arbitrary but fixed point on L;

ν: the unit tangential vector along L;

Γ: the plane in $\mathbf{R}^3$, which passes through the origin and has a normal ν. For convenience, we assign an orientation to Γ: its normal ν and Γ form a right-handed coordinate system.

P_Γ: the projection from $\mathbf{R}^3$ onto Γ.

T_θ: the rotation on the plane Γ about the origin by angle θ. Clearly T_θ can also be viewed as a rotation in the whole space $\mathbf{R}^3$ about the axis fixed to be the line passing through the origin and parallel to direction ν. In both cases, the rotation is understood to be counterclockwise with respect to the assigned orientation on the plane Γ.

We remark that $\nu \parallel \{x_3 = 0\}$. As a result, Γ is perpendicular to the plane $\{x_3 = 0\}$. Viewing (ν, Γ) as a coordinate system, we can write all vectors in $\mathcal{Q}$ as follows:

$$q = \tau\nu + P_\Gamma q, \quad q^n = \tau_n \nu + P_\Gamma q^n \text{ for all } n \in \Xi_0, \tag{13}$$

where τ and τ_n are constants. It is important to observe that (Lemma 3.4, [9]):

$$\text{for any } p \in \mathcal{Q},\ P_\Gamma p \neq 0.$$

Define

$$\begin{aligned} \mathcal{P}_0 &= \{\Pi;\ \Pi \text{ is a perfect plane of } E_p \text{ and passes through the line } L\}, \\ G &= \text{ the group generated by reflections } \{R'_\Pi;\ \Pi \in \mathcal{P}_0\}. \end{aligned}$$

Lemma 3.3 (cf. [9]). *The set $\mathcal{P}_0$ and group G have the following properties:*

(1) The number of perfect planes in $\mathcal{P}_0$ is finite. In fact $|\mathcal{P}_0| \leq |\mathcal{Q}|$.

(2) The angles formed by any two neighboring planes in $\mathcal{P}_0$ are all equal; G consists of $|\mathcal{P}_0|$ reflections and $|\mathcal{P}_0|$ rotations, and has the structure of a dihedral group of order $2|\mathcal{P}_0|$.

We remark that the proof of Lemma 3.3 is independent of the assumption that L is parallel to the plane $\{x_3 = 0\}$. Thus its conclusions still hold in the case when L is not parallel to the plane $\{x_3 = 0\}$. The same holds for the subsequent Lemma 3.4, (1)-(3).

In the sequel, we denote by G^* the subgroup of G which consists of all its rotations. It is clear that $|G^*| = |\mathcal{P}_0|$. Note that the identity element of both

the groups G and G^* is the rotation by angle 2π. When the domain on which transformations in G act is restricted to the plane Γ, G reduces to a *dihedral group*, which acts only on vectors lying on the plane Γ.

The following important properties of groups G and G^* and the set $\mathcal{P}_0$ can be derived in a similar way to the one in the proof of Lemma 3.6 in [9].

Lemma 3.4. *The following statements hold:*

(1) *For any $T \in G$, $T\mathcal{Q} = \mathcal{Q}$ and $T\nu = \nu$. For any $q^n \in G\{q\}$, $\tau_n = \tau$.*
(2) $|\{R'_\Pi q;\ \Pi \in \mathcal{P}_0\}| = |G^*\{q\}| = |\mathcal{P}_0|$.
(3) $|G\{q\}| = 2|\mathcal{P}_0|$ *or* $|G\{q\}| = |\mathcal{P}_0|$. *If* $|G\{q\}| = 2|\mathcal{P}_0|$, *there exists some* $q^1 \in G\{q\}$ *such that* $G\{q\} = G^*\{q\} \cup G^*\{q^1\}$; *if* $|G\{q\}| = |\mathcal{P}_0|$, *then* $G\{q\} = G^*\{q\}$ *and there exists a plane* Π *in* $\mathcal{P}_0$ *such that* $R'_\Pi q = q$. *Moreover, these results hold when q is replaced by any element in $G\{q\}$.*
(4) *If* $|G\{q\}| = 3$, *there exists at least one element in* $G\{P_\Gamma q\}$ *whose* x_3-*component is negative.*
(5) *If* $|G\{q\}| = 4$ *(resp.* $|G\{q\}| > 4$*), there exist at least two elements in* $G\{P_\Gamma q\}$ *whose* x_3-*components are non-positive (resp. negative).*

With the help of set $G\{q\}$, Case 2 can be further divided into two subcases:

Case 2.1. $\mathcal{Q} = G\{q\}$.

Case 2.2. $\mathcal{Q} \neq G\{q\}$.

For the sake of exposition, we assume that the angle between Π_0 and Π_1 is the minimum one among all angles formed by intersecting planes in $\mathcal{P}$. Here the attainability of the minimum angle is guaranteed by Lemma 3.3. In fact, by Lemma 3.3 (2), the angle between any two intersecting planes in $\mathcal{P}$ can take only values of the form π/m for some positive integers m. By Lemma 3.3 (1), we know that $m \leq |\mathcal{Q}|$. Thus the set of angles formed by all pairs of intersecting planes in $\mathcal{P}$ is finite and the minimum angle can then be realized.

Before we study Cases 2.1 and 2.2 in Subsections 3.3-3.6, we first introduce a transformation that can simplify many of our subsequent derivations. To do so, we fix a point r on the line L, and then introduce the following transformation by the change of variables:

$$\hat{x} = x - r. \tag{14}$$

In terms of the $\hat{x}$-variable, the propagating field $E_p(x)$ in (11) takes the form

$$E_p(x) = E_p(\hat{x} + r) = se^{iq\cdot(\hat{x}+r)} + \sum_{n\in\Xi_0} A^n e^{iq^n\cdot(\hat{x}+r)} \equiv \hat{E}_p(\hat{x})\,.$$

By setting $\hat{s} = se^{iq\cdot r}$ and $\hat{A}^n = A^n e^{iq^n\cdot r}$, we can write $\hat{E}_p(\hat{x})$ as

$$\hat{E}_p(\hat{x}) = \hat{s}e^{iq\cdot\hat{x}} + \sum_{n\in\Xi_0} \hat{A}^n e^{iq^n\cdot\hat{x}}. \tag{15}$$

A significant advantage of the $\hat{x}$-variable over the original x-variable can be seen from the following lemma (see Lemma 3.8, [9]), where we write $\hat{s}$ for $\hat{A}^0$ and q for q^0.

Lemma 3.5. *Let Π be a plane passing through the intersection line L between Π_0 and Π_1. Then $\Pi \in \mathcal{P}_0$ if and only if $R'_\Pi \mathcal{Q} \subset \mathcal{Q}$ and the relation $R'_\Pi \hat{A}^l + \hat{A}^m = 0$ holds whenever $R'_\Pi q^l - q^m = 0$ for $q^l, q^m \in \mathcal{Q}$.*

The next result will facilitate us to divide our analysis of Case 2.1 into different possible subcases.

Lemma 3.6. *Case 2.1 allows only four subcases to occur:*

Case 2.1.1. $|\mathcal{P}_0| = 2$ and $|G\{q\}| = 4$.

Case 2.1.2. $|\mathcal{P}_0| = 3$ and $|G\{q\}| = 3$.

Case 2.1.3. $|\mathcal{P}_0| = 4$ and $|G\{q\}| = 4$.

Case 2.1.4. $|\mathcal{P}_0| = 2$ and $|G\{q\}| = 2$.

Proof. Since the intersection line $L \parallel \{x_3 = 0\}$, the x_3-component of ν is zero. Using the decomposition (13) and Proposition 3.1, we see that all vectors in $G\{P_\Gamma q\}$, except $P_\Gamma q$, have non-negative x_3-components. Then our lemma follows directly from Lemma 3.4 (3)-3.4 (6). □

We shall handle the above four Cases 2.1.1-2.1.4 respectively in Subsections 3.3-3.5.

3.3. **Cases 2.1.1-2.1.2: The second and third classes of unidentifiable gratings.** Cases 2.1.1-2.1.2 were studied in [9], which leads to the second and third classes of unidentifiable gratings corresponding to the given incident field E^i. To describe the second class, we specify the following notation:

r: a point in $\mathbf{R}^3$;

Γ: the plane which passes through the origin with normal $s \times e_3$;

Π_0: the plane which passes through r with normal s;

Π_1: the plane which passes through r with normal $(s \times e_3) \times s$.

Then the set of perfect planes of E_p in (11) is given by

$$\mathcal{P} = \Big\{\text{plane } \Pi;\ \Pi \parallel \Pi_0\Big\} \cup \Big\{\text{plane } \Pi;\ \Pi \parallel \Pi_1,\ \operatorname{dist}(\Pi, \Pi_1) = \frac{m\pi}{\|P_\Gamma q\|} \text{ for some } m \in \mathbf{N}\Big\},$$

which gives rise to the second class of unidentifiable gratings corresponding to the incident E^i:

$$\mathcal{S}_2(s, q, \Lambda, r) = \Big\{\text{regular gratings with profile } S\text{, which are } \Lambda\text{-periodic polyhedral structures such that faces of } S \text{ lie on planes in } \mathcal{P}\Big\}.$$

To describe the third class of unidentifiable gratings, we introduce the following notation:

r, Γ, Π_0: the same as above;

L: the line passing through r with direction $s \times e_3$;

Π_1, Π_2: planes which contain line L and form an angle of $\pi/3$ and $2\pi/3$ with Π_0, respectively.

Then the set of perfect planes of E_p in (11) is given by

$$\mathcal{P} = \Big\{\text{plane } \Pi;\ \exists j \in \{0, 1, 2\} \text{ such that } \Pi \parallel \Pi_j,\ \operatorname{dist}(\Pi, \Pi_j) = \frac{2m\pi}{\sqrt{3}\|P_\Gamma q\|} \text{ for some } m \in \mathbf{N}\Big\},$$

which gives the third class of unidentifiable gratings corresponding to E^i:

$$\mathcal{S}_3(s,q,\Lambda,r) = \Big\{\text{regular gratings with profile } S\text{, which are } \Lambda\text{-periodic polyhedral structures such that faces of } S \text{ lie on planes in } \mathcal{P}\Big\}.$$

We know from [9] that the class $\mathcal{S}_k(s,q,\Lambda,r)$ $(k=2,3)$ corresponds to a unique electric field E_p (see [9] for the formula for E_p in the respective cases), which solves the direct scattering problem (1)-(4) for all gratings in $\mathcal{S}_k$. Thus the system (1)-(4) has a solution $E = E_p$, which is a total field without evanescent modes. We remark that since we may not have uniqueness for the forward problem, we do not exclude the existence of other solutions with evanescent modes. But this fact does not affect our conclusion that any two gratings in $\mathcal{S}_k$ cannot be distinguished by the incident field $E^i(x) = se^{iq\cdot x}$. Thus, the following results hold.

Lemma 3.7. *When Case 2.1.1 (resp. Case 2.1.2) happens, the corresponding grating S belongs to $\mathcal{S}_2(s,q,\Lambda,r)$ (resp. $\mathcal{S}_3(s,q,\Lambda,r)$) for some point $r \in \mathbf{R}^3$. Furthermore, all gratings in $\mathcal{S}_2(s,q,\Lambda,r)$ (resp. $\mathcal{S}_3(s,q,\Lambda,r)$) can generate the same total field $E = E_p$ as the grating S.*

3.4. **Case 2.1.3: The fourth class of unidentifiable gratings.** In this subsection we consider Case 2.1.3 stated in Lemma 3.6, which will lead to the fourth class of unidentifiable gratings corresponding to the given incident field E^i. We first show that both the propagating field E_p and its perfect planes in $\mathcal{P}_0$ are all uniquely determined by E^i.

Lemma 3.8. *In Case 2.1.3, the following statements hold:*

(1) $s \parallel \{x_3 = 0\}$, $L \parallel (s \times e_3)$.

(2) *$\mathcal{P}_0$ consists of four planes. The first one is a plane which is perpendicular to s, denoted by Π_0. The other three planes are $\Pi_1 = T_{\pi/4}\Pi_0$, $\Pi_2 = T_{\pi/2}\Pi_0$, $\Pi_3 = T_{3\pi/4}\Pi_0$.*

(3) *The propagating field $E_p(x)$ in (11) or $\hat{E}_p(\hat{x})$ in (15) can be written as*

$$E_p(x) = s(e^{iq\cdot x} - e^{iq^2\cdot x+(q-q^2)\cdot r}) + T_{\pi/2}s(e^{iq^1\cdot x+(q-q^1)\cdot r} - e^{iq^3\cdot x+(q-q^3)\cdot r}),$$

$$\hat{E}_p(\hat{x}) = \hat{s}(e^{iq\cdot\hat{x}} - e^{iq^2\cdot\hat{x}}) + T_{\pi/2}\hat{s}(e^{iq^1\cdot\hat{x}} - e^{iq^3\cdot\hat{x}}),$$

where $q^j = T_{j\pi/2}q$, $j = 1,2,3$. Moreover, vectors $q^1, q^3 \in \Xi^*$.

Proof. The proof may be divided into three steps.

Step 1. We show that $P_\Gamma q \parallel e_3$. By observing $|G\{q\}| = |\mathcal{P}_0|$, by Lemma 3.4 (3) we have that

$$\begin{aligned}\mathcal{Q} &= G\{q\} = G^*\{q\} = \tau\nu + G^*\{P_\Gamma q\} = \tau\nu + \{P_\Gamma q, T_{\pi/2}P_\Gamma q, T_\pi P_\Gamma q, T_{3\pi/2}P_\Gamma q\}\\ &= \tau\nu + \{P_\Gamma q, T_{\pi/2}P_\Gamma q, -P_\Gamma q, -T_{\pi/2}P_\Gamma q\}.\end{aligned}$$

Recall that the x_3-component of ν is zero. By Proposition 3.1, the x_3-component of $P_\Gamma q$ should be zero as well, or $T_{\pi/2}P_\Gamma q \parallel \{x_3 = 0\}$. It follows that $P_\Gamma q \parallel e_3$.

Step 2. We determine $\mathcal{P}_0$. Note that $|G\{q\}| = |\mathcal{P}_0|$. By Lemma 3.4 (3), there is a plane in $\mathcal{P}_0$, denoted by Π_0, such that $R'_{\Pi_0}q = q$. Since $R'_{\Pi_0}\nu = \nu$, we see $R'_{\Pi_0}P_\Gamma q = P_\Gamma q$. Thus $P_\Gamma q \parallel \Pi_0$. This, combined with the result $P_\Gamma q \parallel e_3$ in Step 1, gives $\Pi_0 \perp \{x_3 = 0\}$. But according to Lemma 3.2, $R'_{\Pi_0}q = q$ also implies $s \perp \Pi_0$, consequently $s \parallel \{x_3 = 0\}$. The direction of the line L or the vector ν is hence

determined. Indeed, since $s \perp \Pi_0$ and $\nu \parallel \Pi_0$, we have $\nu \perp s$. This together with $\nu \perp e_3$ yields $\nu \parallel (s \times e_3)$, which determines ν, hence the direction of the line L.

Now, by Lemma 3.3 (2) we know that planes in $\mathcal{P}_0$ are determined as well: in addition to Π_0, the other three planes are formed by rotating Π_0 by angles $\pi/4$, $\pi/2$ and $3\pi/4$ respectively about the axis L.

Step 3. We determine the coefficients of E_p in (11) or $\hat{E}_p$ in (15). By Lemma 3.4 (2), we have

$$\mathcal{Q} = \{R'_\Pi q : \Pi \in \mathcal{P}_0\} = \{R'_{\Pi_0} q, R'_{\Pi_1} q, R'_{\Pi_2} q, R'_{\Pi_3} q\}.$$

Let $q^j = R'_{\Pi_j} q$, $j = 1, 2, 3$. Then

$$q^j = \tau\nu + T_{j\pi/2} P_\Gamma q = T_{j\pi/2} q, \ j = 1, 2, 3.$$

We can write $\hat{E}_p$ as

$$\hat{E}_p(\hat{x}) = \hat{s} e^{iq\cdot\hat{x}} + \hat{A}^1 e^{iq^1\cdot\hat{x}} + \hat{A}^2 e^{iq^2\cdot\hat{x}} + \hat{A}^3 e^{iq^3\cdot\hat{x}}. \tag{16}$$

Using Lemma 3.5 and the relations $q^j = R'_{\Pi_j} q$ for $j = 1, 2, 3$, we obtain

$$\hat{A}^1 = -R'_{\Pi_1}\hat{s}, \ \hat{A}^2 = -R'_{\Pi_2}\hat{s}, \ \hat{A}^3 = -R'_{\Pi_3}\hat{s}.$$

These equalities can be further simplified by observing that $\hat{s} \perp \Pi_0$ and $\hat{s} \parallel \Pi_2$. As a result,

$$\hat{A}^1 = -R'_{\Pi_1}\hat{s} = T_{\pi/2}\hat{s}, \ \hat{A}^2 = -R'_{\Pi_2}\hat{s} = -s, \ \hat{A}^3 = -R'_{\Pi_3}\hat{s} = -\hat{A}^1,$$

which completes the proof of Lemma 3.8. □

The next lemma shows the determination of the perfect planes of $\hat{E}_p$.

Lemma 3.9. *Let $\hat{E}_p$ and Π_j, $j = 0, 1, 2, 3$, be defined as in Lemma 3.8. Then:*

(1) *The set $\mathcal{P}$ is uniquely determined by the incident field E^i. Specifically, a plane Π belongs to $\mathcal{P}$ if and only if there exists some $j \in \{0, 1, 2, 3\}$ such that $\Pi \parallel \Pi_j$ and the distance between Π and Π_j equals $\frac{m\pi}{\|P_\Gamma q\|}$ for $j = 0, 2$ and $\frac{m\sqrt{2}\pi}{\|P_\Gamma q\|}$ for $j = 1, 3$, where m is some integer.*

(2) *Each face of the grating structure S lies on a plane in $\mathcal{P}$.*

Proof. Consider a plane $\Pi \in \mathcal{P}$; we know $R'_\Pi q \in \mathcal{Q}$ by Proposition 3.2. It follows from Step 3 of the proof of Lemma 3.8 that $\mathcal{Q} = \{R'_{\Pi_0} q, R'_{\Pi_1} q, R'_{\Pi_2} q, R'_{\Pi_3} q\}$. Hence we have $R'_\Pi q = R'_{\Pi_j} q$ for some $j \in \{0, 1, 2, 3\}$. Now by Lemma 3.2 we deduce that $\Pi \parallel \Pi_j$. The rest of the proof can be carried out in the same manner as in the proof of Lemma 3.7 of [9]. □

We are ready to define the fourth class of unidentifiable gratings. Let us first recall some notation:

r: a point in $\mathbf{R}^3$;

L: the line passing through the point r with the direction $s \times e_3$;

Π_0: the plane in $\mathbf{R}^3$ which passes through L and is perpendicular to the plane $\{x_3 = 0\}$;

Π_1, Π_2, Π_3: planes in $\mathbf{R}^3$ which pass through L and form an angle of $\pi/4$, $\pi/2$, $3\pi/4$ respectively, with Π_0.

With the above notation, the set of perfect planes of E_p can be described by

$$\begin{aligned}\mathcal{P} \;=\; \Big\{&\text{plane } \Pi;\ \exists j \in \{0,1,2,3\} \text{ such that } \Pi \parallel \Pi_j, \text{ and for}\\ &j = 0,2,\ \operatorname{dist}(\Pi,\Pi_j) = \frac{m\pi}{\|P_\Gamma q\|} \text{ for some } m \in \mathbf{N},\\ &\text{for } j = 1,3,\ \operatorname{dist}(\Pi,\Pi_j) = \frac{m'\sqrt{2}\pi}{\|P_\Gamma q\|} \text{ for some } m' \in \mathbf{N}\Big\},\end{aligned}$$

which leads to a new class of gratings unidentifiable by the incident field $E^i = se^{iq\cdot x}$:

$$\begin{aligned}\mathcal{S}_4(s,q,\Lambda,r) \;=\; \Big\{&\text{regular gratings with profile } S, \text{ which are } \Lambda\text{-periodic polyhedral}\\ &\text{structures such that faces of } S \text{ lie on planes in } \mathcal{P}\Big\}\end{aligned}$$

for some point $r \in \mathbf{R}^3$. The results of this subsection can be summarized in the following lemma.

Lemma 3.10. *When Case 2.1.3 in Lemma* 3.6 *happens, the corresponding grating S belongs to $\mathcal{S}_4(s,q,\Lambda,r)$ for some $r \in \mathbf{R}^3$. Furthermore, all gratings in $\mathcal{S}_4(s,q,\Lambda,r)$ can generate the same total field $E = E_p$ as the grating S.*

Next we provide an example to show that the class $\mathcal{S}_4(s,q,\Lambda,r)$ is not empty.

Example 1. Consider an incident field $E^i = se^{iq\cdot x}$, with $s = e_2 = (0,1,0)$ and $q = (\alpha_1,\alpha_2,-\beta) = (0,0,-1) = -e_3$. Then we construct some concrete grating profile belonging to the class $\mathcal{S}_4(s,q,\Lambda,0)$ for $\Lambda = (\Lambda_1,\Lambda_2) = (0,2\pi)$. Clearly, the grating should be invariant along the x_1-axis since the period is 0 in that direction.

First, we determine $\mathcal{P}_0$ and E_p according to Lemma 3.8. It is evident that the intersection line of planes in $\mathcal{P}_0$ is the x_1-axis, the plane Π_0 is $\{x_2 = 0\}$, and the other three planes Π_1, Π_2, Π_3 are generated by rotating Π_0 counterclockwise about the x_1-axis by angles $\pi/4, \pi/2, 3\pi/4$, respectively. In addition, the field E_p is determined by

$$E_p(x) = e_2(e^{iq\cdot x} - e^{iq^2\cdot x}) + e_3(e^{iq^1\cdot x} - e^{iq^3\cdot x})$$

with $q^1 = (0,1,0) = e_2$, $q^2 = (0,0,1) = e_3$ and $q^3 = (0,-1,0) = -e_2$. One can easily check by the formulas (5)-(6) that $q^1 = q^{(0,1)}$, $q^2 = q^{(0,0)}$ and $q^3 = q^{(0,-1)}$.

Second, we determine the set of perfect planes of the field E_p by Lemma 3.9. We see that $\mathcal{P}$ consists of four sets of planes: the first two sets contain all planes that are parallel to Π_0 or Π_2 with distance π between any two neighboring parallel planes; the last two sets contain all planes parallel to Π_1 or Π_3 with the distance $\sqrt{2}\pi$ between any two neighboring parallel planes.

Third, we find some Λ-periodic structure in the set $\mathcal{P}$. For each $l \in \mathbf{Z}$, we denote by L_{3l}, L_{3l+1}, L_{3l+2} the lines of forms $\{(\lambda, 2l\pi, 0) : \lambda \in \mathbf{R}\}$, $\{(\lambda, 2l\pi+\pi, \pi) : \lambda \in \mathbf{R}\}$, $\{(\lambda, 2l\pi+\pi, 0) : \lambda \in \mathbf{R}\}$, respectively. For each $m \in \mathbf{Z}$, let Π_m be the plane that contains lines L_m and L_{m+1}, and let F_m be the part on Π_m which lies between lines L_m and L_{m+1}. Then it is easy to see that Π_m belongs to $\mathcal{P}$ for all $m \in \mathbf{Z}$ and that $\bigcup_{m\in\mathbf{Z}} F_m$ forms a $\Lambda-$periodic structure in $\mathcal{P}$.

Finally, we choose the above periodic structure to be our grating profile S in (3). Since all faces of this structure lie on perfect planes of E_p determined in the first step above, the field $E = E_p$ solves the direct scattering problem (1)-(4) associated with

the incident field E^i and the previously specified grating S. By making appropriate shifts, one obtains infinitely many $\Lambda-$periodic structures in $\mathcal{P}$, thus showing the existence of infinitely many gratings in the class $\mathcal{S}_4(s, q, \Lambda, 0)$. It follows that all these gratings generate the same total field $E = E_p$, and hence cannot be identified by the incident field E^i.

3.5. **Case 2.1.4: The fifth class of unidentifiable gratings.** In this subsection we study Case 2.1.4 classified in Lemma 3.6, leading to the fifth class of unidentifiable gratings corresponding to the given incident field E^i. For this purpose, we first show that both the propagating field E_p and the set $\mathcal{P}_0$ are uniquely determined by the incident field E^i and the directional vector ν of the line L.

Lemma 3.11. *If Case 2.1.4 happens, then:*

(1) *$\mathcal{P}_0$ consists of two planes, Π_0 and Π_1, which are perpendicular respectively to vectors $P_\Gamma q - \sqrt{k^2-\tau^2}(e_3 \times \nu)$ and $P_\Gamma q + \sqrt{k^2-\tau^2}(e_3 \times \nu)$.*

(2) *The propagating field E_p in (11) or $\hat{E}_p$ in (15) can be written as*

$$\begin{aligned} E_p(x) =& se^{iq\cdot x} - R'_{\Pi_0} se^{iq^1\cdot x+(q-q^1)\cdot r} + R'_{\Pi_1}(R'_{\Pi_0}s)e^{iq^2\cdot x+(q-q^2)\cdot r} \\ & - R'_{\Pi_1} se^{iq^3\cdot x+(q-q^3)\cdot r}, \\ \hat{E}_p(\hat{x}) =& \hat{s}e^{iq\cdot\hat{x}} - R'_{\Pi_0}\hat{s}e^{iq^1\cdot\hat{x}} + R'_{\Pi_1}(R'_{\Pi_0}\hat{s})e^{iq^2\cdot\hat{x}} - R'_{\Pi_1}\hat{s}e^{iq^3\cdot\hat{x}}, \end{aligned} \tag{17}$$

where $q^1 = \tau\nu + \sqrt{k^2-\tau^2}(e_3 \times \nu)$, $q^3 = \tau\nu - \sqrt{k^2-\tau^2}(e_3 \times \nu)$ and $q^2 = \tau\nu - P_\Gamma q$. Moreover, $q^1, q^3 \in \Xi^*$.

Proof. The proof may be divided into four steps.

Step 1. We determine elements of $G\{q\}$ in terms of q and ν. Note that $|G| = |G\{q\}| = 4$. By Lemma 3.4 (3), we can find $q^1 \in G\{q\}$ such that $G\{q\} = G^*\{q\} \cup G^*\{q^1\}$. Since $|G^*| = |G|/2 = 2$, we have $G^* = \{T_\pi, Id\}$. Thus

$$G^*\{q\} = \{\tau\nu + P_\Gamma q, \tau\nu - P_\Gamma q\},\ G^*\{q^1\} = \{\tau\nu + P_\Gamma q^1, \tau\nu - P_\Gamma q^1\}.$$

By Proposition 3.1 and the assumption that $\nu \parallel \{x_3 = 0\}$, the x_3-component of $P_\Gamma q^1$ should be zero. Therefore, we have $P_\Gamma q^1 \parallel \{x_3 = 0\}$, which yields $P_\Gamma q^1 \parallel (e_3 \times \nu)$ by noting that $P_\Gamma q^1 \perp \nu$. It follows that $P_\Gamma q^1 = \pm\sqrt{k^2 - |q\cdot\nu|^2}(e_3 \times \nu)$ since $\|q^1\|^2 = k^2 = \tau^2 + \|P_\Gamma q^1\|^2 = \tau^2 + \|P_\Gamma q^1\|^2$. We then fix q^1 by letting

$$P_\Gamma q^1 = \sqrt{k^2 - |q\cdot\nu|^2}(e_3 \times \nu)\,.$$

Also, we write $q^2 = \tau\nu - P_\Gamma q$, $q^3 = \tau\nu - P_\Gamma q^1$.

Step 2. It is clear that $\mathcal{P}_0 = \{\Pi_0, \Pi_1\}$ since $|\mathcal{P}_0| = 2$. Let $\Pi \in \{\Pi_0, \Pi_1\}$; we claim that $R'_\Pi q \in \{q^1, q^3\}$. Indeed, by Proposition 3.2, $R'_\Pi\{q, q^1, q^2, q^3\} = \{q, q^1, q^2, q^3\}$. Since $|\mathcal{P}_0| = 2$ and $|G\{q\}| = |G\{q^1\}| = |G\{q^3\}| = 4$, Lemma 3.4 (3) implies that $R'_\Pi q \neq q$, $R'_\Pi q^1 \neq q^1$ and $R'_\Pi q^3 \neq q^3$. Therefore, it suffices to show that the case when $R'_\Pi q = q^2$ and $R'_\Pi q^1 = q^3$ cannot happen. Indeed, if $R'_\Pi q = q^2$ and $R'_\Pi q^1 = q^3$, then $R'_\Pi P_\Gamma q = -P_\Gamma q$ and $R'_\Pi P_\Gamma q^1 = -P_\Gamma q^1$ by using the fact that $R'_\Pi \nu = \nu$. Hence both $P_\Gamma q$ and $P_\Gamma q^1$ are perpendicular to the plane Π. We then have $P_\Gamma q \parallel P_\Gamma q^1$, which implies that either $q = q^1$ or $q = q^2$. This contradiction leads to our claim.

Step 3. We determine the plane Π_0 and Π_1. By the result in Step 2, we can fix Π_0 by letting $R'_{\Pi_0} q = q^1$. Consequently

$$R'_{\Pi_0} q^2 = q^3,\ R'_{\Pi_1} q = q^3,\ R'_{\Pi_1} q^1 = q^2.$$

Using $R'_\Pi \nu = \nu$ for $\Pi = \Pi_0, \Pi_1$ again, we have $R'_{\Pi_0} P_\Gamma q = P_\Gamma q^1$ and $R'_{\Pi_1} P_\Gamma q = P_\Gamma q^3$. Thus

$$\nu_{\Pi_0} \parallel (P_\Gamma q - P_\Gamma q^1),\ \nu_{\Pi_1} \parallel (P_\Gamma q + P_\Gamma q^3).$$

Recalling that $P_\Gamma q^1 = \sqrt{k^2 - \tau^2}(e_3 \times \nu) = -P_\Gamma q^3$, the first part of our lemma follows immediately.

Step 4. We determine the field E_p. We write

$$\hat{E}_p(\hat{x}) = \hat{s} e^{iq\cdot\hat{x}} + \hat{A}^1 e^{iq^1\cdot\hat{x}} + \hat{A}^2 e^{iq^2\cdot\hat{x}} + \hat{A}^3 e^{iq^3\cdot\hat{x}}.$$

A direct application of Lemma 3.5 and the relations $R'_{\Pi_0} q = q^1$, $R'_{\Pi_1} q = q^3$ and $R'_{\Pi_0} q^2 = q^3$ yields

$$\hat{A}^1 = -R'_{\Pi_0}\hat{s},\ \hat{A}^3 = -R'_{\Pi_1}\hat{s},\ \hat{A}^2 = -R'_{\Pi_0}\hat{A}^3 = R'_{\Pi_0}(R'_{\Pi_1}\hat{s}).$$

This completes the proof of Lemma 3.11. □

After obtaining $\mathcal{P}_0$ and E_p, we now proceed to find $\mathcal{P}$. We first present an auxiliary result.

Lemma 3.12. *Let E_p, Π_0, Π_1 be as determined in Lemma* 3.11. *Then the condition stated in Case 2 (cf. Subsection* 3.1*) that the intersection line between any two intersecting planes in $\mathcal{P}$ is parallel to the plane $\{x_3 = 0\}$ implies that $\nu \nparallel s$.*

Proof. We prove by contradiction. Assume $\nu \parallel s$. Then $\hat{s} \parallel s \parallel \Pi_0$ and $\hat{s} \parallel \Pi_1$, implying

$$\hat{A}^1 = -R'_{\Pi_0}\hat{s} = -\hat{s},\ \hat{A}^3 = -R'_{\Pi_1}\hat{s} = -\hat{s},\ \hat{A}^2 = -R'_{\Pi_0}\hat{A}^3 = \hat{s}.$$

Thus we can write

$$\hat{E}_p(\hat{x}) = \hat{s}(e^{iq\cdot\hat{x}} - e^{iq^1\cdot\hat{x}} + e^{iq^2\cdot\hat{x}} - e^{iq^3\cdot\hat{x}}).$$

By the definition of a perfect plane, it is easy to verify that all the planes perpendicular to s are perfect planes of E_p. Let Π be such a plane. Note that Π_0 and Π_1 are two planes in $\mathcal{P}$ which have an intersection line L with $L \parallel \nu \parallel \{x_3 = 0\}$ and $\nu \parallel s$. It is clear that there exists one intersection line, either $\Pi \cap \Pi_0$ or $\Pi \cap \Pi_1$, which is not parallel to the plane $\{x_3 = 0\}$. This contradicts the condition that all intersection lines between planes in $\mathcal{P}$ are parallel to the plane $\{x_3 = 0\}$. □

With the help of Lemma 3.12, we can show the next lemma.

Lemma 3.13. *Let E_p, Π_0, Π_1 be determined as in Lemma* 3.11. *Then*

(1) *The condition that the intersection line between any two intersecting planes in $\mathcal{P}$ is parallel to the plane $\{x_3 = 0\}$ implies that $\nu \nparallel s$. Moreover, $\mathcal{P}$ consists of only two sets of planes: the first set contains only planes parallel to Π_0 with the distance $\frac{\pi}{\|q\cdot\nu_{\Pi_0}\|}$ between any two parallel neighboring planes, while the second set contains only planes parallel to Π_1 with the distance $\frac{\pi}{\|q\cdot\nu_{\Pi_1}\|}$ between any two parallel neighboring planes.*

(2) *Each face of the grating structure S lies on a plane in $\mathcal{P}$.*

Lemma 3.13 enables us to find a new class of unidentifiable gratings. To describe the class, we first recall some notation:

r: a position vector, viewed as a point in $\mathbf{R}^3$;

ν: a non-zero vector in $\mathbf{R}^3$ which is parallel to the plane $\{x_3 = 0\}$;

Γ: the plane in $\mathbf{R}^3$, which passes through the origin with normal ν;

L: the line in $\mathbf{R}^3$ passing through r with direction ν;

Π_0: the plane in $\mathbf{R}^3$ which passes through L with $P_\Gamma q + \sqrt{k^2-\tau^2}(e_3 \times \nu)$ as its normal;

Π_1: the plane in $\mathbf{R}^3$ which passes through L and is perpendicular to Π_0.

With these notation, the set of perfect planes of E_p can be explicitly described by

$$\mathcal{P} = \left\{ \text{plane } \Pi;\ \Pi \parallel \Pi_0 \text{ or } \Pi_1, \text{ and } \operatorname{dist}(\Pi, \Pi_0) = \frac{m\pi}{|q \cdot \nu_{\Pi_0}|} \text{ for some } m \in \mathbf{N} \right.$$
$$\left. \text{or } \operatorname{dist}(\Pi, \Pi_1) = \frac{m'\pi}{|q \cdot \nu_{\Pi_1}|} \text{ for some } m' \in \mathbf{N} \right\}.$$

Now, for the incident field $E^i = se^{iq\cdot x}$, a point $r \in \mathbf{R}^3$ and a non-zero vector $\nu \parallel \{x_3 = 0\}$, we define the fifth class of unidentifiable gratings:

$$\mathcal{S}_5(s, q, \Lambda, r, \nu) = \left\{ \text{regular gratings with profile } S, \text{ which are } \Lambda\text{-periodic polyhedral} \right.$$
$$\left. \text{structures such that faces of } S \text{ lie on planes in } \mathcal{P} \right\}.$$

Using $\mathcal{S}_5(s, q, \Lambda, \nu, r)$, we can summarize results of this subsection in the following lemma.

Lemma 3.14. *When Case 2.1.4 stated in Lemma* 3.6 *happens, the grating S belongs to $\mathcal{S}_5(s, q, \Lambda, \nu, r)$ for some point $r \in \mathbf{R}^3$ and the direction vector $\nu \parallel \{x_3 = 0\}$. Furthermore, all gratings in $\mathcal{S}_5(s, q, \Lambda, \nu, r)$ can generate the same total field $E = E_p$ as the grating S.*

Finally, we give a concrete example of the non-empty class $\mathcal{S}_5(s, q, \Lambda, \nu, r)$.

Example 2. Consider an incident field $E^i = se^{iq\cdot x}$, with $s = (\frac{\sqrt{3}}{2}, 0, \alpha_1)$, $q = (\alpha_1, \alpha_2, -\beta) = (\alpha_1, \frac{1}{2}, -\frac{\sqrt{3}}{2})$, where α_1 is a non-zero real number. Next we construct some grating in the class $\mathcal{S}_5(s, q, \Lambda, \nu, 0)$ for $\Lambda = (\Lambda_1, \Lambda_2) = (0, 2\pi)$ and $\nu = (1, 0, 0)$. Note that $\nu \nparallel s$ and that the grating should be invariant along the x_1-axis.

First, we determine $\mathcal{P}_0$ and E_p according to Lemma 3.11. It is obvious that the intersection line of planes in $\mathcal{P}_0$ is the x_1-axis, and that planes Π_0 and Π_1 are determined by their normals $\nu_{\Pi_0} = (0, \frac{1}{2}, \frac{\sqrt{3}}{2})$, $\nu_{\Pi_1} = (0, -\frac{\sqrt{3}}{2}, \frac{1}{2})$ respectively, and $\Pi_0 \perp \Pi_1$. In addition, the field E_p is determined by

$$E_p(x) = se^{iq\cdot x} - R'_{\Pi_0} se^{iq^1\cdot x} + R'_{\Pi_1}(R'_{\Pi_0} s)e^{iq^2\cdot x} - R'_{\Pi_1} se^{iq^3\cdot x}$$

with $q^1 = (\alpha_1, 1, 0)$, $q^2 = (\alpha_1, -\frac{1}{2}, \frac{\sqrt{3}}{2})$ and $q^3 = (\alpha_1, -1, 0)$. One can check by formulas (5)-(6) that $q^1 = q^{(0,3)}$, $q^2 = q^{(0,2)}$ and $q^3 = q^{(0,1)}$.

Second, we determine the set of perfect planes of the field E_p by Lemma 3.13. It is evident that $\mathcal{P}$ consists of two sets of planes: the first set contains all planes that are parallel to Π_0 with the distance 2π between any two neighboring planes; the second set contains all planes that are parallel to Π_1 with distance $\frac{2\pi}{\sqrt{3}}$ between any two neighboring planes.

Third, we find some Λ-periodic structure in the set $\mathcal{P}$. For each $l \in \mathbf{Z}$, we denote by L_{3l}, L_{3l+1}, L_{3l+2} the lines of the form $\{(\lambda, 4l\pi, 0) : \lambda \in \mathbf{R}\}$, $\{(\lambda, 4l\pi + \pi, -\frac{\sqrt{3}\pi}{3}) : \lambda \in \mathbf{R}\}$, $\{(\lambda, 4l\pi + 2\pi, \frac{2\sqrt{3}\pi}{3}) : \lambda \in \mathbf{R}\}$, respectively. For each $m \in \mathbf{Z}$, let Π_m be the plane that contains lines L_m and L_{m+1}, and F_m be the part on Π_m which lies

between lines L_m and L_{m+1}. Then it is easy to see that Π_m belongs to $\mathcal{P}$ for all $m \in \mathbf{Z}$ and that $\bigcup_{m\in\mathbf{Z}} F_m$ forms a $\Lambda-$periodic structure in $\mathcal{P}$.

Finally, we choose the above periodic structure to be our grating profile S in (3). It follows that the field $E = E_p$ solves the direct scattering problem (1)-(4) associated with the incident field E^i and the grating S. By making appropriate shifts, one obtains infinitely many $\Lambda-$periodic structures in $\mathcal{P}$, thus showing the existence of infinitely many gratings in the class $\mathcal{S}_5(s, q, \Lambda, \nu, 0)$. All these gratings generate the same total field $E = E_p$, and hence cannot be identified by the incident field E^i.

3.6. **Case 2.2: The sixth class of unidentifiable gratings.** So far we have studied all the possibilities in Case 2.1. Now we proceed to study Case 2.2. We show that this case leads to the sixth unidentifiable grating class corresponding to the incident electric field E^i. To demonstrate this, we first present some useful properties about the propagating field E_p and the set of perfect planes that pass through the line L, i.e. $\mathcal{P}_0$.

Lemma 3.15. *When Case 2.2 happens, the following statements hold:*

(1) $s \parallel \{x_3 = 0\}$, $L \parallel (s \times e_3)$;
(2) $\mathcal{P}_0$ *consists of two planes: one is perpendicular to the vector* s, *and is denoted by* Π_0; *the other is perpendicular to* e_3, *and is denoted by* Π_1;
(3) $R'_{\Pi_0} q = q$ *and* $G\{q\} = \{q, R'_{\Pi_1} q\}$;
(4) $\mathcal{Q} \setminus G\{q\} \subset \Xi^*$.

Proof. We divide the proof into the following four steps.

Step 1. We first prove (4) and that $|\mathcal{P}_0| = 2$. For each $q^* \in \mathcal{Q} \setminus G\{q\}$, consider the set $G^*\{q^*\} \subset \mathcal{Q}$ and we see $|G^*\{q^*\}| \geq 2$. According to Proposition 3.1, all its elements have non-negative x_3-components. However, this is possible only if $G^* = \{Id, T_\pi\}$ and $P_\Gamma q^* \parallel \{x_3 = 0\}$ by Lemma 3.4 and the assumption that the x_3-component of ν is zero. Hence $|\mathcal{P}_0| = 2$ and the result (4) follows.

Step 2. We derive some information about the set $\mathcal{P}_0$. As $|\mathcal{P}_0| = 2$, we can write $\mathcal{P}_0 = \{\Pi_0, \Pi_1\}$. Let $q^* \in \mathcal{Q}\backslash G\{q\}$; then $\{R'_{\Pi_0} q^*, R'_{\Pi_1} q^*\} \subset G\{q^*\} \subset \mathcal{Q}\backslash G\{q\} \subset \Xi^*$. This means that vectors $R'_{\Pi_0} q^*$ and $R'_{\Pi_1} q^*$ lie on the plane $\{x_3 = 0\}$. Since q^* also lies on the plane, we see that Π_0 and Π_1 are either parallel or perpendicular to the plane $\{x_3 = 0\}$. Besides, we know that Π_0 and Π_1 are perpendicular since they are the only two planes in $\mathcal{P}$. Thus one of them is parallel to $\{x_3 = 0\}$ and the other is perpendicular to $\{x_3 = 0\}$. Let the plane which is perpendicular to the plane $\{x_3 = 0\}$ be Π_0, and the other be Π_1.

Step 3. We prove (3) and (1). We first establish (3). Note that $\Pi_0 \perp \{x_3 = 0\}$, and the x_3-component of $R'_{\Pi_0} q$ is the same as that of q. But q is the only element in $\mathcal{Q}$ which has a negative x_3-component, so we have $R'_{\Pi_0} q = q$ and it follows by the definition of the group G that $G\{q\} = \{q, R'_{\Pi_1} q\}$. This proves (3). Now, a direct application of Lemma 3.2 yields $s \perp \Pi_0$. Note that $\Pi_0 \perp \{x_3 = 0\}$; we have $s \parallel \{x_3 = 0\}$. Besides, we know $\nu \parallel \Pi_0$, so $s \perp \Pi_0$ also implies that $\nu \perp s$. It then follows that $\nu \parallel (s \times e_3)$ since $\nu \perp e_3$. This proves (1).

Step 4. We prove (2). We know that $\nu_{\Pi_1} \perp s$ since $\Pi_1 \perp \Pi_0$ and $s \parallel \Pi_0$. In addition, since $\Pi_1 \parallel \nu$ and $\nu \parallel (s \times e_3)$, we have $\nu_{\Pi_1} \perp (s \times e_3)$. It then follows that $\nu_{\Pi_1} \perp s \times (s \times e_3)$. We know $s \perp e_3$ from Step 3. Thus $s \times (s \times e_3) \parallel e_3$ and

$\nu_{\Pi_1} \parallel e_3$. This completes the proof of the assertions in (2), hence the proof of the lemma. □

By now, we have obtained some useful information about E_p and $\mathcal{P}_0$ in Lemma 3.15. We continue to determine $\mathcal{P}$ as we did before. For this, we first consider the case with $|\mathcal{Q}| = 4$.

Lemma 3.16. *If $|\mathcal{Q}| = 4$ in Case 2.2, then the propagating field E_p in* (11) *or $\hat{E}_p$ in* (15) *can be written as*

$$E_p(x) = s(e^{iq\cdot x} - e^{iq^2\cdot x+(q-q^2)\cdot r}) + A^1(e^{iq^1\cdot x} - e^{iq^3\cdot x+(q^1-q^3)\cdot r}), \tag{18}$$

$$\hat{E}_p(\hat{x}) = \hat{s}(e^{iq\cdot\hat{x}} - e^{iq^2\cdot\hat{x}}) + \hat{A}^1(e^{iq^1\cdot\hat{x}} - e^{iq^3\cdot\hat{x}}), \tag{19}$$

where $q^2 = R'_{\Pi_1}q = T_\pi q$, $q^1, q^3 \in \Xi^*$ with $R'_{\Pi_0}q^1 = q^3$, and $\hat{A}^1$ is any non-zero vector which is parallel to e_3.

Proof. We know from the previous lemma that $|G\{q\}| = 2$. Since $|\mathcal{Q}| = 4$, we can write $\mathcal{Q} = G\{q\} \cup G\{q^1\}$ with $G\{q\} = \{q, q^2\}$ and $G\{q^1\} = \{q^1, q^3\}$. We also write $\hat{E}_p$ in the form

$$\hat{E}_p(\hat{x}) = \hat{s}e^{iq\cdot\hat{x}} + \hat{A}^1e^{iq^1\cdot\hat{x}} + \hat{A}^2e^{iq^2\cdot\hat{x}} + \hat{A}^3e^{iq^3\cdot\hat{x}}.$$

By the results in Lemma 3.15, the following relations hold:

$$R'_{\Pi_1}q^1 = q^1,\ R'_{\Pi_1}q = q^2,\ R'_{\Pi_0}q^1 = q^3.$$

Now, a direct application of Lemma 3.2 and Lemma 3.5 yields

$$\hat{A}^1 \perp \Pi_1,\ \hat{A}^2 = -R'_{\Pi_1}s,\ \hat{A}^3 = -R'_{\Pi_0}\hat{A}^1.$$

Recalling that $\Pi_1 \parallel s$ and $\Pi_1 \parallel \{x_3 = 0\}$ (see Lemma 3.15), we have $\hat{A}^2 = -R'_{\Pi_1}s = -\hat{s}$ and $\hat{A}^1 \parallel e_3$ from the first two equalities. Besides, by the relation $\Pi_0 \perp e_3$, the last equality, combined with $\hat{A}^1 \parallel e_3$, gives $\hat{A}^3 = -\hat{A}^1$, which leads to (19). □

By Lemma 3.16, it is clear that the electric field E_p is not totally determined in Case 2.2 under the additional assumption that $|\mathcal{Q}| = 4$. In fact, (q^1, q^3) can be any pair in Ξ^* such that $R'_{\Pi_0}q^1 = q^3$, and $\hat{A}^1$ can be any non-zero vector that is parallel to e_3.

Next, we want to find the set of perfect planes of E_p in Lemma 3.16.

Lemma 3.17. *Let E_p, Π_0, Π_1 be defined as in Lemma* 3.16. *Then*

(1) *$\mathcal{P}$ consists of two sets of planes: the first set contains the planes that are parallel to Π_0 with a distance of some multiple of $\frac{\pi}{\|P_\Gamma q^1\|}$; the second set contains the planes that are parallel to Π_1 with a distance of some multiple of $\frac{\pi}{\|P_\Gamma q\|}$.*

(2) *Each face of the grating S lies on a plane in $\mathcal{P}$.*

Proof. Let Π be a plane in $\mathcal{P}$. By the minimum angle assumption made on the planes Π_0 and Π_1, we see that only three cases are possible:

(i) $\Pi \parallel \Pi_0$;

(ii) $\Pi \parallel \Pi_1$;

(iii) $\Pi \perp \Pi_0$ and $\Pi \perp \Pi_1$.

Following similar arguments as in the proof of Lemma 3.13, we can show that Case (i) happens if the distance between Π and Π_0 is of some multiple of $\frac{\pi}{|q^1\cdot\nu_{\Pi_0}|} =$

$\frac{\pi}{\|P_\Gamma q^1\|}$; the same for Case (ii). We claim that Case (iii) is impossible to occur. Indeed, in Case (iii), one has $\Pi \perp \Pi_1$, and $\Pi_1 \parallel \{x_3 = 0\}$, hence $\Pi \perp \{x_3 = 0\}$. Thus the x_3-component of $R'_\Pi q$ is the same as q. But q is the only element in $\mathcal{Q}$ whose x_3-component is negative, hence $R'_\Pi q = q$. This combined with $R'_{\Pi_0} q = q$ in Lemma 3.15 yields $\Pi \parallel \Pi_0$ by Lemma 3.5. But our assumption for Case (iii) is that $\Pi \perp \Pi_0$. This contradiction leads to our claim. The rest of the lemma follows from the same arguments as in the proof of Lemma 3.13. □

We have studied the case with $|\mathcal{Q}| = 4$ in Lemmas 3.16-3.17, and we now turn to the case with $|\mathcal{Q}| > 4$. We start by partitioning the set $\mathcal{Q}$ into pairwise disjoint orbits under the group G's action, that is,

$$\mathcal{Q} = G\{q\} \cup \Big(\bigcup_{1 \le j \le m_0 - 1} G\{q^j\} \Big)$$

for some integer $m_0 > 2$. By Lemma 3.15, we know that $\Pi_1 \parallel \{x_3 = 0\}$ and q^j lies on the plane $\{x_3 = 0\}$ for $1 \le j \le m_0 - 1$. It follows that $R'_{\Pi_1} q^j = q^j$ and $G\{q^j\} = G^*\{q^j\} = \{q^j, R'_{\Pi_0} q^j\}$. Clearly we have $|\mathcal{Q}| = 2m_0$. Following the same steps as those in the proof of Lemmas 3.16-3.17 (for $m_0 = 2$), we can determine E_p and $\mathcal{P}$.

Lemma 3.18. *If $L \parallel \{x_3 = 0\}$, $|G| = 4$, $|G\{q\}| = 2$ and $|\mathcal{Q}| = 2m_0$ for some integer $m_0 > 2$, then the following statements hold:*

(1) *$\hat{E}_p$ can be written as*

$$\hat{E}_p(\hat{x}) = \hat{s}(e^{iq\cdot\hat{x}} - e^{iq^{m_0}\cdot\hat{x}}) + \sum_{1 \le j \le m_0 - 1} \hat{A}^j (e^{iq^j\cdot\hat{x}} - e^{iq^{j+m_0}\cdot\hat{x}}) \tag{20}$$

where each q^j is a vector in $\Xi^* \cap \Xi_0$ such that $q^{j+m_0} =: R'_{\Pi_1} q^j$ also belongs to $\Xi^* \cap \Xi_0$. Here each $\hat{A}^j$ is a non-zero vector that is parallel to e_3.

(2) *There are two sets of perfect planes in $\mathcal{P}$. The first set contains planes that are parallel to Π_0 with a distance of some multiple of $\frac{\pi}{\|P_\Gamma q^j\|}$ for all $1 \le j \le m_0 - 1$; the second set contains planes that are parallel to Π_1 with a distance of some multiple of $\frac{\pi}{\|P_\Gamma q\|}$.*

(3) *Each face of the grating structure S lies on some plane in $\mathcal{P}$.*

We note that compared with the case of $|\mathcal{Q}| = 4$, the presence of additional modes in the case $|\mathcal{Q}| = 2m_0$ ($m_0 > 2$) requires more stringent conditions on the distance between planes in $\mathcal{P}$ which are parallel to Π_0.

Now, we are ready to define the sixth class of unidentifiable gratings. Recall that

r: a point in $\mathbf{R}^3$;

L: the line in $\mathbf{R}^3$ which passes through the point r and has direction $s \times e_3$;

Π_0: the plane in $\mathbf{R}^3$ which passes through L with normal $s/\|s\|$; here $s \perp e_3$.

Π_1: the plane in $\mathbf{R}^3$ which passes through L and is perpendicular to Π_0.

With these notation, we conclude that

$$\begin{aligned}\mathcal{P} \;=\; \Big\{&\text{plane } \Pi;\ \exists j \in \{0,1\} \text{ such that } \Pi \parallel \Pi_j, \text{ and for } j=0,\\ &\operatorname{dist}(\Pi,\Pi_0) = \frac{m\pi}{|q^n \cdot \nu_{\Pi_0}|} \text{ for some } m \in \mathbf{N} \text{ and for all } q^n \in \Xi^* \cap \Xi_0\\ &\text{satisfying } R'_{\Pi_1} q^n \in \Xi^*;\ \text{for } j=1,\ \operatorname{dist}(\Pi,\Pi_1) = \frac{m\pi}{|q \cdot \nu_{\Pi_1}|}\\ &\text{for some } m \in \mathbf{N}\Big\}\ ,\end{aligned}$$

which leads us to the sixth class of unidentifiable gratings for the incident field $E^i = se^{iq\cdot x}$ and each point $r \in \mathbf{R}^3$:

$$\begin{aligned}\mathcal{S}_6(s,q,\Lambda,r) \;=\; \Big\{&\text{regular gratings with profile } S, \text{ which are regular } \Lambda\text{-periodic}\\ &\text{polyhedral structures such that faces of } S \text{ lie on planes in } \mathcal{P}\Big\}.\end{aligned}$$

In summary, the major result of this subsection can be stated in the following lemma.

Lemma 3.19. *When Case 2.2 happens, the corresponding grating S belongs to $\mathcal{S}_6(s,q,\Lambda,r)$ for some $r \in \mathbf{R}^3$. Furthermore, all gratings in $\mathcal{S}_6(s,q,\Lambda,r)$ can generate the same total field $E = E_p$ as the grating S.*

Finally, we give a concrete example of the non-empty class $\mathcal{S}_6(s,q,\Lambda,r)$.

Example 3. Consider an incident field $E^i = se^{iq\cdot x}$, with $s = e_2 = (0,1,0)$ and $q = (\alpha_1,\alpha_2,-\beta) = (0,0,-1)$. We next construct some grating in the class $\mathcal{S}_6(s,q,\Lambda,0)$ for $\Lambda = (\Lambda_1,\Lambda_2) = (0,2\pi)$. It is clear that the grating should be invariant along the x_1-axis.

First, we determine $\mathcal{P}_0$ and E_p according to Lemmas 3.15-3.16. Clearly, the intersection line of planes in $\mathcal{P}_0$ is the x_1-axis, and Π_0 and Π_1 are respectively the planes $\{x_2 = 0\}$ and $\{x_3 = 0\}$. In addition, the field E_p is determined by

$$E_p(x) = s(e^{iq\cdot x} - e^{iq^2\cdot x}) + A^1(e^{iq^1\cdot x} - e^{iq^3\cdot x})$$

with $q^1 = (0,1,0)$, $q^2 = (0,0,1)$ and $q^3 = (0,-1,0)$. Here A^1 can be any non-zero vector which is parallel to e_3. One can check by formulas (5)-(6) that $q^1 = q^{(0,1)}$, $q^2 = q^{(0,0)}$ and $q^3 = q^{(0,-1)}$.

Second, we determine the set of perfect planes of the field E_p by Lemma 3.17. It is evident that $\mathcal{P}$ consists of two sets of planes: the first set contains all planes parallel to Π_0 with the neighboring distance $\frac{m\pi}{\|q^1\cdot\nu_{\Pi_0}\|} = m\pi$; the second set contains all planes parallel to Π_1 with the neighboring distance $\frac{m\pi}{\|q\cdot\nu_{\Pi_1}\|} = m\pi$.

Third, we try to find some Λ-periodic structure in the set $\mathcal{P}$. For each $l \in \mathbf{Z}$, we denote by L_{4l}, L_{4l+1}, L_{4l+2}, L_{4l+3} the lines of the form $\{(\lambda, 2l\pi, 0) : \lambda \in \mathbf{R}\}$, $\{(\lambda, 2l\pi+\pi, 0) : \lambda \in \mathbf{R}\}$ $\{(\lambda, 2l\pi+\pi, \pi) : \lambda \in \mathbf{R}\}$, $\{(\lambda, 2l\pi+2\pi, \pi) : \lambda \in \mathbf{R}\}$, respectively. For each $m \in \mathbf{Z}$, let Π_m be the plane that contains lines L_m and L_{m+1}, and F_m be the part on Π_m which lies between L_m and L_{m+1}. Then it is clear that Π_m belongs to $\mathcal{P}$ for all $m \in \mathbf{Z}$ and that $\bigcup_{m\in\mathbf{Z}} F_m$ forms a $\Lambda-$periodic structure in $\mathcal{P}$.

Finally, we choose the above periodic structure to be our grating profile S in (3). As we argued in Examples 1-2, by making appropriate shifts one can obtain

infinitely many $\Lambda-$periodic structures in $\mathcal{P}$ and hence infinitely many gratings in the class $\mathcal{S}_6(s, q, \Lambda, 0)$. All these gratings can generate the same total field $E = E_p$, hence cannot be identified by the incident field E^i.

We remark that based on the results in Lemma 3.16, the above example illustrates the non-uniqueness of the direct scattering problem.

3.7. **Preparations for Case 3.** We have studied Cases 1 and 2 for the set $\mathcal{P}$ of perfect planes of E_p classified in Subsection 3.1. Next, we investigate the last possible case, Case 3, and demonstrate that this case leads to the final class of unidentifiable gratings.

Our analysis is similar to the one in Subsection 3.2. Let Π_0, Π_1 be two planes in $\mathcal{P}$ such that the following two conditions are satisfied: first, their intersection line L is not parallel to the plane $\{x_3 = 0\}$; second, the angle between them is the smallest one among those between intersecting planes in $\mathcal{P}$ whose intersection lines are not parallel to the plane $\{x_3 = 0\}$. Here again the existence of minimum angle is guaranteed by Lemma 3.3 of Subsection 3.2. Also, we choose the direction vector of L, ν, to be the one with unit length and positive x_3-component, and define the plane Γ, the projection P_Γ, the set $\mathcal{P}_0$ and the groups G and G^* as before.

We claim that Γ does not coincide with the plane $\{x_3 = 0\}$. Otherwise, both planes Π_0 and Π_1 would be perpendicular to the plane $\{x_3 = 0\}$. Consider the vectors $R'_{\Pi_0} q$ and $R'_{\Pi_1} q$: as the x_3-component of vector q is negative, so are the x_3-components of $R'_{\Pi_0} q$ and $R'_{\Pi_1} q$. Noting that both $R'_{\Pi_0} q$ and $R'_{\Pi_1} q$ belong to $\mathcal{Q}$, we can conclude from Proposition 3.1 that $R'_{\Pi_0} q = R'_{\Pi_1} q$. It then follows from Lemma 3.5 that $\Pi_0 \parallel \Pi_1$, which contradicts our assumption that Π_0 and Π_1 intersect, and thus proves our assertion. We shall use the fact that Γ does not coincide with the plane $\{x_3 = 0\}$ in the proofs of Lemmas 3.22 and 3.25.

We now recall two lemmas from [9] that are fundamental to our subsequent analysis.

Lemma 3.20. *When Case 3 for the set $\mathcal{P}$ of perfect planes of E_p classified in Subsection* 3.1 *occurs, there exists a plane $\Pi^* \in \mathcal{P}$ such that $\Pi^* \nparallel L$. As a result, we have $\Pi^* \nparallel \Pi_0$ and $\Pi^* \nparallel \Pi_1$.*

Lemma 3.21. *When Case 3 occurs it holds that*

$$q + \sum_{n \in \Xi_0} q^n = 0\,, \tag{21}$$

$$\tau + \sum_{n \in \Xi_0} \tau_n = 0\,, \tag{22}$$

$$\tau_n \geq 0 \quad \forall\, q^n \in \mathcal{Q} \setminus G\{q\}\,. \tag{23}$$

We shall separate our next analysis based on $\tau = 0$ or $\tau \neq 0$, and study

Case 3.1. $\tau = 0$,

and

Case 3.2. $\tau \neq 0$

in Subsections 3.8-3.9 respectively, and show that both cases lead to the seventh class of unidentifiable gratings.

3.8. **Case 3.1: The seventh class of unidentifiable gratings.**

Lemma 3.22. *If Case 3.1 happens, then*

(1) $s \parallel \nu$.

(2) *Let* $q^1 = k\frac{s\times e_3}{\|s\times e_3\|}$. *Then the propagating field* E_p *in* (11) *or* $\hat{E}_p$ *in* (15) *can be written as*

$$E_p(x) = s(e^{iq\cdot x} - e^{iq^1\cdot x+(q-q^1)\cdot r} + e^{-iq\cdot x+2q\cdot r} - e^{-iq^1\cdot x+(q+q^1)\cdot r}), \tag{24}$$

$$\hat{E}_p(\hat{x}) = \hat{s}(e^{iq\cdot\hat{x}} - e^{iq^1\cdot\hat{x}} + e^{-iq\cdot\hat{x}} - e^{-iq^1\cdot\hat{x}}). \tag{25}$$

(3) $\mathcal{P}_0$ *consists of two planes. One is perpendicular to the vector* $q - q^1$, *and is denoted by* Π_0; *the other is perpendicular to the vector* $q + q^1$, *and is denoted by* Π_1.

Proof. We divide the proof into the following five steps.

Step 1. Since $\tau = 0$, using Lemma 3.21 and Lemma 3.4 (1), we know $\tau_n = 0$ for all $q^n \in \mathcal{Q}$. Hence all elements in $\mathcal{Q}$ lie on the plane Γ.

Step 2. We claim that $|\mathcal{P}_0| = 2$. We assume otherwise that $|\mathcal{P}_0| > 2$. Consider the set $\mathcal{Q}$; we can write it as the union of pairwise disjoint orbits $G^*\{p\}$ for $p \in \mathcal{Q}$. Recall that the plane Γ does not coincide with the plane $\{x_3 = 0\}$. Since $|\mathcal{P}_0| > 2$, there exists at least one element in each orbit $G^*\{p\}$ whose x_3-component is negative. But q is the only element in $\mathcal{Q}$ whose x_3-component is negative. So we get $\mathcal{Q} = G^*\{q\}$, hence $G\{q\} = G^*\{q\}$. It is clear that vectors in $\mathcal{Q}$ can span the plane Γ. By Proposition 3.2, we have $R'_{\Pi^*}\Gamma = \Gamma$. As a result, either $\Pi^* \parallel \Gamma$ or $\Pi^* \perp \Gamma$. However, $\Pi^* \perp \Gamma$ implies that $\Pi^* \parallel L$, which contradicts Lemma 3.20. So we have $\Pi^* \parallel \Gamma$. It follows by using the assumption $\tau = 0$ that $R'_{\Pi^*}q = q$. On the other hand, it follows from $G\{q\} = G^*\{q\}$ and Lemma 3.4 (3) that there exists Π in $\mathcal{P}_0$ such that $R'_\Pi q = q$. Then, by Lemma 3.2, $\Pi \parallel \Pi^*$, which contradicts Lemma 3.20. The claim is verified.

Step 3. We show that $\mathcal{Q} = G\{q\} = G^*\{q\} \cup G^*\{q^1\} = \{q, -q\} \cup \{q^1, -q^1\}$ for some q^1 in $\mathcal{Q}$. Indeed, since $|\mathcal{P}_0| = 2$, we can write $\mathcal{P}_0 = \{\Pi_0, \Pi_1\}$ and $G^* = \{T_\pi, Id\}$. By the result in Step 1, all elements in $\mathcal{Q}$ lie on the plane Γ, so we have $G^*\{p\} = \{p, -p\}$ for each $p \in \mathcal{Q}$. This together with Proposition 3.1 yields that each orbit $G^*\{p\}$ for $p \in \mathcal{Q}\backslash G^*\{q\}$ lies on the plane $\{x_3 = 0\}$ and hence on the intersection line between plane Γ and $\{x_3 = 0\}$. Note that all elements in $\mathcal{Q}$ have the same length. It follows that there is at most one such orbit in $\mathcal{Q}$. We next show the existence of such an orbit. If it is not the case, then $\mathcal{Q} = G^*\{q\} = \{q, -q\}$; hence $G\{q\} = G^*\{q\}$. By Lemma 3.4 (3), there is a plane in $\mathcal{P}_0$, say Π_0, such that $R'_{\Pi_0}q = q$. Then $R'_{\Pi_1}q = -q$. On the other hand, let Π^* be the plane in Lemma 3.20; then we obtain by Proposition 3.2 that $R'_{\Pi^*}\{q, -q\} = \{q, -q\}$. So either $R'_{\Pi^*}q = q$ or $R'_{\Pi^*}q = -q$. Then one can deduce from Lemma 3.2 that either $\Pi^* \parallel \Pi_0$ or $\Pi^* \parallel \Pi_1$. But this contradicts Lemma 3.20, which shows that we can write $\mathcal{Q} = G^*\{q\} \cup G^*\{q^1\}$ for some q^1 in $\mathcal{Q}$.

Now we show that $G^*\{q\} \cup G^*\{q^1\} = G\{q\}$. In fact, since vectors in the set $G^*\{q\} \cup G^*\{q^1\}$ span the plane Γ, we can apply the same argument as in Step 2 to show that $\Pi^* \parallel \Gamma$ and $R'_{\Pi^*}q = q$. Let Π be a plane in $\mathcal{P}_0$. It is implied by Lemma 3.2 that $R'_\Pi q \neq q$, for otherwise one has $\Pi \parallel \Pi^*$, which contradicts Lemma 3.20. Thus we can conclude by Lemma 3.4 (3) that $G\{q\} \neq G^*\{q\}$, hence it follows that $G\{q\} = G^*\{q\} \cup G^*\{q^1\}$.

Step 4. It is clear by Proposition 3.1 that $q^1 \parallel \{x_3 = 0\}$, or equivalently $q^1 \in \Xi^*$. We claim that $R'_\Pi q \in \{q^1, -q^1\}$ for $\Pi \in \mathcal{P}_0$. Indeed, by Proposition 3.2, $R'_\Pi\{q, q^1, -q, -q^1\} = \{q, q^1, -q, -q^1\}$. Note that $|G| = |G\{q\}| = 4$ and $G\{q\} = G\{q^1\} = G\{-q^1\}$. By Lemma 3.4 (3) we have $R'_\Pi q \neq q$, $R'_\Pi q^1 \neq q^1$ and $R'_\Pi q^3 \neq q^3$. So it suffices to show that the case with $R'_\Pi q = -q$ and $R'_\Pi q^1 = -q^1$ cannot occur. In fact, the equalities $R'_\Pi q = -q$ and $R'_\Pi q^1 = -q^1$ would imply that both q and q^1 are perpendicular to the plane Π, and hence are parallel to each other, which is impossible since $q^1 \parallel \{x_3 = 0\}$ and $q \nparallel \{x_3 = 0\}$. This contradiction proves our claim.

Step 5. By the result in Step 4, we can fix Π_0 and Π_1 by letting

$$R'_{\Pi_0} q = q^1,\ R'_{\Pi_1} q = -q^1.$$

It then follows that $R'_{\Pi_0}(-q) = -q^1$ and $R'_{\Pi_1} q^1 = -q$. We write

$$\hat{E}_p(\hat{x}) = \hat{s} e^{iq\cdot\hat{x}} + \hat{A}^1 e^{iq^1\cdot\hat{x}} + \hat{A}^2 e^{-iq\cdot\hat{x}} + \hat{A}^3 e^{-iq^1\cdot\hat{x}}.$$

A direct application of Lemma 3.5 yields that

$$\hat{A}^1 = -R'_{\Pi_0}\hat{s},\ \hat{A}^3 = -R'_{\Pi_1}\hat{s},\ \hat{A}^2 = -R'_{\Pi_1}\hat{A}^1. \tag{26}$$

To simplify the equalities above, we observe that $\hat{s} \parallel \nu$. Indeed, recall that $\Pi^* \parallel \Gamma$ (see the second paragraph in Step 3). By the result in Step 1, we have $R'_{\Pi^*} q = q$. Referring to Lemma 3.2, this implies that $s \perp \Pi^*$, hence $s \perp \Gamma$. Therefore we have $s \parallel \nu$, so $\hat{s} \parallel \nu$. As a result we conclude from equalities in (26) that $\hat{A}^1 = \hat{A}^3 = -\hat{s},\ \hat{A}^2 = \hat{s}$.

Finally, recall that q^1 lies on the plane Γ, so $q^1 \perp \nu$. But $\nu \parallel s$, leading to the fact that $q^1 \perp s$. This combined with $q^1 \perp e_3$ yields $q^1 \parallel (s \times e_3)$. Since $\|q\| = k$, we see $q^1 = \pm k \frac{s\times e_3}{\|s\times e_3\|}$. We can fix q^1 by letting $q^1 = k\frac{s\times e_3}{\|s\times e_3\|}$. Then the rest of the lemma follows. □

We remark that in the proof of Lemma 3.22, the condition that the intersection line L is not parallel to the plane $\{x_3 = 0\}$ and the minimum angle assumptions are not used. In fact, Π_0 and Π_1 may be any two planes in $\mathcal{P}$ which have the intersection line L. What we have used is the condition that $\tau = 0$ and that there exists a plane in $\mathcal{P}$ not parallel to the line L. We shall use this fact in the proof of Lemma 3.26.

So far, we have determined the propagating field E_p in terms of vectors s and q. The set of perfect planes of E_p can be determined as well. By the same approach as in the proof of Lemma 3.17, we can show the following result.

Lemma 3.23. *Let E_p, Π_0, Π_1 be determined as in Lemma 3.22. Then*

(1) *$\mathcal{P}$ consists of three sets of planes: the first set consists of planes that are parallel to Π_0 with a distance of some multiple of $\frac{\pi}{\|q\cdot\nu_{\Pi_0}\|}$; the second set consists of planes that are parallel to Π_1 with a distance of some multiple of $\frac{\pi}{\|q\cdot\nu_{\Pi_1}\|}$; the last set consists of planes that are perpendicular to s.*
(2) *Each face of the grating structure S lies on a plane in $\mathcal{P}$.*

Lemma 3.23 enables us to find a new class of unidentifiable gratings. To describe the class explicitly, we specify

r: a point in $\mathbf{R}^3$;

L: the line in $\mathbf{R}^3$ which contains r and has direction ν with $\nu \parallel s$;

Γ: the plane in $\mathbf{R}^3$ which passes through the origin with normal ν;
Π_0: the plane in $\mathbf{R}^3$ which passes through L with normal $q - k\frac{s\times e_3}{\|s\times e_3\|}$;
Π_1: the plane in $\mathbf{R}^3$ which passes through L and is perpendicular to Π_0.
With the notation, the set of perfect planes of E_p is given by

$$\mathcal{P} = \Big\{\text{plane } \Pi;\ \text{either } \Pi \perp s \text{ or } \exists j \in \{0,1\} \text{ such that } \Pi \parallel \Pi_j \text{ and } \operatorname{dist}(\Pi, \Pi_j) = \frac{m\pi}{\|q\cdot \nu_{\Pi_j}\|} \text{ for some } m \in \mathbf{N}\Big\}.$$

Now, for the incident field $E^i = se^{iq\cdot x}$ and a point $r \in \mathbf{R}^3$ we can define the seventh class of unidentifiable gratings:

$$\mathcal{S}_7(s,q,\Lambda,r,\nu) = \Big\{\text{regular gratings with profile } S\text{, which are } \Lambda\text{-periodic polyhedral structures such that faces of } S \text{ lie on planes in } \mathcal{P}\Big\}.$$

We summarize the above results in the following lemma.

Lemma 3.24. *If Case 3.1 happens, then the grating S belongs to $\mathcal{S}_7(s,q,\Lambda,r)$ for some point $r \in \mathbf{R}^3$. Furthermore, all gratings in $\mathcal{S}_7(s,q,\Lambda,r)$ can generate the same total field $E = E_p$ as the grating S.*

3.9. **Case 3.2: The seventh class of unidentifiable gratings.** Finally, we investigate Case 3.2. We have the following results.

Lemma 3.25. *In Case 3.2, $|G\{q\}| = |\mathcal{P}_0| = 2$.*

Proof. We prove the lemma in six steps: we show $|G\{q\}| \neq 3$ in Steps 1-4, then $|G\{q\}| \leq 3$ in Step 5, and finally $|G\{q\}| = |\mathcal{P}_0| = 2$ in Step 6.

Step 1. To show that $|G\{q\}| \neq 3$, we assume otherwise that $|G\{q\}| = 3$. First, note that $\tau_n = \tau$ for all $q^n \in G\{q\}$. We have by using (22) that

$$3\tau + \sum_{q^n \in \mathcal{Q}\setminus G\{q\}} \tau_n = 0. \tag{27}$$

Since $\tau_n \geq 0$ for all $q^n \in \mathcal{Q}\setminus G\{q\}$ by using (23), we see that $\tau < 0$ and there exists some $q^m \in \mathcal{Q}\setminus G\{q\}$ such that $\tau_m > 0$.

Step 2. We claim $\mathcal{Q} = G\{q\} \cup G\{q^m\}$ and $|G\{q^m\}| = 3$. Indeed, since $|G\{q\}| = 3$, Lemma 3.4 (3) implies that $|\mathcal{P}_0| = 3$ and that either $|G\{q^m\}| = 3$ or $|G\{q^m\}| = 6$. Then equation (27) yields

$$3\tau + 3\tau_m \leq \tau + \sum_{q^n \in G\{q\}} \tau_n + \sum_{q^n \in G\{q^m\}} \tau_n \leq \tau + \sum_{q^n \in \mathcal{Q}} \tau_n = \tau + \sum_{n \in \Xi_0} \tau_n = 0.$$

Thus we have $\tau + \tau_m \leq 0$. Define

$$d_0 = \min\{x_3;\ x = (x_1, x_2, x_3) \in \Gamma \text{ and } \|x\| \leq \|P_\Gamma q\|\}.$$

Recall that $\Gamma \neq \{x_3 = 0\}$. It is clear that $d_0 < 0$. We can find $q^{n_1} \in G\{q\}\setminus\{q\}$ such that the x_3-component of $P_\Gamma q^{n_1}$ is less than or equal to $-d_0/2$. Since $\|q^m\| = \|q\| = k$ and $\tau + \tau_m \leq 0$, we have $\|P_\Gamma q^m\| \geq \|P_\Gamma q\|$. Therefore we can find $q^{n_2} \in G\{q^m\}$

such that its x_3-component of $P_\Gamma q^{n_2}$ is less than or equal to $d_0/2$. Now, consider the x_3-component of of the vector

$$q^{n_1} + q^{n_2} = (\tau + \tau_m)\nu + P_\Gamma q^{n_1} + P_\Gamma q^{n_2},$$

which is non-negative by Proposition 3.1. Note that the x_3-component of ν is positive. The following three conditions hold:

(1) $\tau + \tau_m = 0$ and $\|P_\Gamma q\| = \|P_\Gamma q^m\|$.

(2) The x_3-component of $P_\Gamma q^{n_1}$ is equal to $-d_0/2$.

(3) The x_3-component of $P_\Gamma q^{n_2}$ is equal to $d_0/2$.

It follows from condition (1) and equations (22)-(23) in Lemma 3.21 that $|G\{q^m\}| = 3$ and $\tau_n = 0$ for all $q^n \in \mathcal{Q} \setminus (G\{q\} \cup G\{q^m\})$. Now we take $q^n \in \mathcal{Q} \setminus (G\{q\} \cup G\{q^m\}$. Since $\Gamma \neq \{x_3 = 0\}$, one can show, by a similar proof to that of Lemma 3.4 (4), that at least one element from the set

$$G^*\{q^n\} = \tau_n \nu + \{P_\Gamma q^n, T_{2\pi/3} P_\Gamma q^n, T_{4\pi/3} P_\Gamma q^n\} = \{P_\Gamma q^n, T_{2\pi/3} P_\Gamma q^n, T_{4\pi/3} P_\Gamma q^n\}$$

has a negative x_3-component. This is impossible according to Proposition 3.1. Thus the set $\mathcal{Q} \setminus (G\{q\} \cup G\{q^m\})$ is empty, and our claim is proved.

Step 3. We show that $G\{q^m\} = -G\{q\}$. Indeed, let V_1 and V_2 be the two vectors on the plane Γ such that $\|V_1\| = \|V_2\| = \|P_\Gamma q\|$, $V_1 \parallel \{x_3 = 0\}$ and the x_3-component of V_2 is d_0. It is clear that $V_1 \perp V_2$ and the set $\{\nu, V_1, V_2\}$ forms an orthogonal basis in $\mathbf{R}^3$. By using the conditions (2) and (3) in Step 2, $G\{q\}$ and $G\{q^m\}$ can be written as:

$$G\{q\} = \tau\nu + \{V_2, T_{2\pi/3} V_2, T_{4\pi/3} V_2\},$$
$$G\{q^m\} = \tau_m \nu + \{-V_2, -T_{2\pi/3} V_2, -T_{4\pi/3} V_2\} = -\tau\nu + \{-V_2, -T_{2\pi/3} V_2, -T_{4\pi/3} V_2\}.$$

The conclusion that $G\{q^m\} = -G\{q\}$ now follows.

Step 4. Let $G\{q\} = \{q, q^1, q^2\}$; then $\mathcal{Q} = \{q, q^1, q^2, -q, -q^1, -q^2\}$. Clearly both q^1 and q^2 lie on the plane $\{x_3 = 0\}$ by Proposition 3.1. Since $|\mathcal{P}_0| = |G\{q\}| = 3$, we write $\mathcal{P}_0 = \{\Pi_0, \Pi_1, \Pi_2\}$. By Lemma 3.4 (3) there exists a plane from $\mathcal{P}_0$, say Π_0, such that $q = R'_{\Pi_0} q$. Then $G\{q\} = \{R'_{\Pi_0} q, R'_{\Pi_1} q, R'_{\Pi_2} q\}$, and hence $\{R'_{\Pi_1} q, R'_{\Pi_2} q\} = \{q^1, q^2\}$. Now, we fix q^1, q^2 by letting $q^1 = R'_{\Pi_2} q$, $q^2 = R'_{\Pi_1} q$. Then it is easy to check that $q^1 = R'_{\Pi_1} q^1$ and $q^2 = R'_{\Pi_2} q^2$.

Let Π^* be the perfect plane in Lemma 3.20. By Proposition 3.2 we have

$$R'_{\Pi^*}\{q, q^1, q^2, -q, -q^1, -q^2\} = \{q, q^1, q^2, -q, -q^1, -q^2\}.$$

Then the following four cases may happen:

(1) $R'_{\Pi^*} q \in \{q, q^1, q^2\}$. Recall in Step 4 that $\{q, q^1, q^2\} = \{R'_{\Pi_0} q, R'_{\Pi_1} q, R'_{\Pi_2} q\}$. By Lemma 3.2, this implies that Π^* is parallel to one of the planes in $\{\Pi_0, \Pi_1, \Pi_2\}$ if $R'_{\Pi^*} q \in \{q, q^1, q^2\}$. This contradicts Lemma 3.20.

(2) $R'_{\Pi^*} q = -q$. In this case, $R'_{\Pi^*}\{q^1, q^2, -q^1, -q^2\} = \{q^1, q^2, -q^1, -q^2\}$. So R'_{Π^*} maps the plane $\{x_3 = 0\}$ to itself. Therefore, either $\Pi^* \perp \{x_3 = 0\}$ or $\Pi^* \parallel \{x_3 = 0\}$. But it follows from $R'_{\Pi^*} q = -q$ that $q \perp \Pi^*$, so we have $\Pi^* \parallel \{x_3 = 0\}$. We now have that $R'_{\Pi^*} q^1 = q^1$, since q^1 lies on the plane $\{x_3 = 0\}$. This together with the relation $R'_{\Pi_1} q^1 = q^1$ in Step 4 yields $\Pi_1 \parallel \Pi^*$ by using Lemma 3.2, which contradicts Lemma 3.20.

(3) $R'_{\Pi^*} q = -q^1$. In this case, $R'_{\Pi^*}\{q^2, -q^2\} = \{q^2, -q^2\}$. Since $R'_{\Pi^*} q^2 = q^2$ would imply $\Pi^* \parallel \Pi_2$, which contradicts Lemma 3.20, we have $R'_{\Pi^*} q^2 = -q^2$. As a result, $q^2 \perp \Pi^*$. Recall in Step 4 that q^2 lies on the plane

$\{x_3 = 0\}$, so $\Pi^* \perp \{x_3 = 0\}$. It then follows that the x_3-component of $R'_{\Pi^*}q$ is the same as q and hence is negative. Thus it is impossible to have $R'_{\Pi^*}q = -q^1$, since the x_3-component of q^1 is zero (see Step 4). This contradiction shows that we cannot have $R'_{\Pi^*}q = -q^1$.

(4) $R'_{\Pi^*}q = -q^2$. This case can be excluded by the same method as we do for $R'_{\Pi^*}q = -q^1$.

We have shown that all four cases are impossible, and hence have established the assertion that $|G\{q\}| \neq 3$.

Step 5. We show that $|G\{q\}| \leq 3$. By contradiction we assume $|G\{q\}| > 3$. Consider the set $G\{P_\Gamma q\}$. By Lemma 3.4 there exist at least two elements in $G\{P_\Gamma q\}$ whose x_3-components are non-positive. Note that $G\{q\} = \tau\nu + G\{P_\Gamma q\}$ and that the x_3-component of ν is positive. We have $\tau > 0$, for otherwise $G\{q\}$ would contain at least two elements whose x_3-components are negative, which contradicts Proposition 3.1. But then equality (27) and inequality (23) cannot be satisfied simultaneously. This contradiction proves that $|G\{q\}| \leq 3$.

Step 6. Now we have $|G\{q\}| < 3$. It is clear that $|G\{q\}| > 1$, so $|G\{q\}| = 2$. By Lemma 3.4 (3) we have either $|\mathcal{P}_0| = |G\{q\}|$ or $|\mathcal{P}_0| = |G\{q\}|/2$, leading to the fact that $|\mathcal{P}_0| = 2$, and the lemma is proved. □

Lemma 3.26. *If Case 3.2 happens, then the grating S belongs to $\mathcal{S}_7(s, q, \Lambda, r)$ for some point $r \in \mathbf{R}^3$.*

Proof. By Lemma 3.25, we know $|G\{q\}| = |\mathcal{P}_0| = 2$. Then $\mathcal{P}_0 = \{\Pi_0, \Pi_1\}$ and $\Pi_0 \perp \Pi_1$. Let Π^* be the perfect plane in Lemma 3.20. We claim that Π^* is perpendicular to both planes Π_0 and Π_1. Indeed, assume otherwise that $\Pi^* \not\perp \Pi_0$. Let $\tilde{L}$, $\tilde{\mathcal{P}}_0$, $\tilde{G}$ denote the line of intersection between Π^* and Π_0, the set of perfect planes in $\mathcal{P}$ which pass through the line $\tilde{L}$, and the group generated by reflections $\{R'_\Pi : \Pi \in \tilde{\mathcal{P}}_0\}$, respectively. As $\Pi^* \not\perp \Pi_0$, we see that $|\tilde{\mathcal{P}}_0| \geq 3$, and $|\tilde{G}| \geq 6$. By the minimum angle assumption on planes Π_0 and Π_1, it is clear that $\tilde{L} \parallel \{x_3 = 0\}$. Similarly to Lemma 3.6, one can show only two cases are possible: (i) $|\tilde{\mathcal{P}}_0| = |\tilde{G}\{q\}| = 3$; (ii) $|\tilde{\mathcal{P}}_0| = |\tilde{G}\{q\}| = 4$. By the remark at the end of Subsection 3.4, we can apply the same arguments as in Subsection 3.4 to work out all perfect planes in $\mathcal{P}$. By the description of the set $\mathcal{P}$ there, the intersection lines of planes in $\mathcal{P}$ are all parallel to $\tilde{L}$ in both cases. In particular, we have $L \parallel \tilde{L}$. This is impossible since $\tilde{L} \parallel \{x_3 = 0\}$, while $L \nparallel \{x_3 = 0\}$. This contradiction proves that $\Pi^* \perp \Pi_0$. Similarly, we can show that $\Pi^* \perp \Pi_1$, and hence prove our claim.

Now, we know that $\Pi^* \perp \Pi_0$, $\Pi^* \perp \Pi_1$ and $\Pi_0 \perp \Pi_1$. Then the vectors ν, ν_{Π_0} and ν_{Π_1} form an orthogonal basis of $\mathbf{R}^3$. We can write $q = \tau\nu + P_\Gamma q = \tau\nu + \tau_0\nu_{\Pi_0} + \tau_1\nu_{\Pi_1}$ where τ_0 and τ_1 are real numbers. Since $|G\{q\}| = |\mathcal{P}_0| = 2$, by Lemma 3.4 (3) there exists a plane in $\mathcal{P}_0$, say Π_0, such that $R'_{\Pi_0}q = q$. But $R'_{\Pi_0}q = R'_{\Pi_0}(\tau\nu + \tau_0\nu_{\Pi_0} + \tau_1\nu_{\Pi_1}) = \tau\nu - \tau_0\nu_{\Pi_0} + \tau_1\nu_{\Pi_1}$. So we have $\tau_0 = 0$, and hence $q = \tau\nu + \tau_1\nu_{\Pi_1}$.

Finally, let $\tilde{L}$, $\tilde{\nu}$, $\tilde{\Gamma}$, $\tilde{\mathcal{P}}_0$, $\tilde{G}$ denote the line of intersection between Π^* and Π_1, the direction of $\tilde{L}$, the plane passing through the origin with normal $\tilde{\nu}$, the set of perfect planes in $\mathcal{P}$ which pass through the line $\tilde{L}$, and the group generated by reflections $\{R'_\Pi : \Pi \in \tilde{\mathcal{P}}_0\}$, respectively. Then $\tilde{\nu} = \nu_{\Pi_0}$ and the plane $\tilde{\Gamma}$ is spanned by vectors ν and ν_{Π_1}. It follows that the decomposition for the vector q in the coordinate system $(\tilde{\nu}, \tilde{\Gamma})$ is given by $q = \tilde{\tau} \cdot \tilde{\nu} + P_{\tilde{\Gamma}}q$ with $\tilde{\tau} = 0$. Thus we are now in the same

situation as in Lemma 3.22 in Subsection 3.8. Note that here Π_0 plays the role of the plane Π^* in Lemma 3.20. By the remark after the proof of Lemma 3.22, we can apply the same arguments to work out E_p and $\mathcal{P}_0$. This leads to the conclusion that the grating S belongs to $\mathcal{S}_7(s, q, \Lambda, r)$. Hence our proof is completed. □

3.10. **Summary on all the classes of unidentifiable gratings.** Summing up results in Subsections 3.1-3.7, especially Lemmas 3.6, 3.7, 3.10, 3.14, 3.19, 3.22, 3.24, 3.26, we obtain the following conclusion.

Theorem 3.1. *Let S be a regular polyhedral grating with bi-period Λ, $E^i(x) = se^{iq\cdot x}$ be an incident field, and E be a solution to the direct scattering problems* (1)-(4). *Then under Assumption* 1, *seven possibilities may happen: S belongs to one of the seven classes $\mathcal{S}_1(q, r)$, $\mathcal{S}_2(s, q, r, \Lambda)$, $\mathcal{S}_3(s, q, r, \Lambda)$, $\mathcal{S}_4(s, q, r, \Lambda)$, $\mathcal{S}_5(s, q, r, \nu, \Lambda)$, $\mathcal{S}_6(s, q, r, \Lambda)$ and $\mathcal{S}_7(s, q, r, \Lambda)$.*

We have found seven classes of unidentifiable gratings corresponding to each incident field. Now, a natural question arises: when is each class of gratings non-empty? From the description of the set $\mathcal{P}$ in each case, we see that there may not exist a grating structure of period Λ, whose faces lie on planes in $\mathcal{P}$. Besides, vectors q^j appearing in the formula of each E_p may not be the wave vectors defined by (5)-(6). Consequently, the corresponding class of unidentifiable gratings may be an empty set. On the other hand, we do have examples for non-empty classes, as shown in the previous subsections. Thus, certain conditions on s, q and Λ (and ν in $\mathcal{S}_5$) should be satisfied to guarantee the existence of each class. Although the analysis tools developed in this work shed some light for deriving the complete conditions that ensure such an existence, the study is on-going and will be reported elsewhere. In fact, for a given class with Λ, s and q, we can first calculate the corresponding E_p and $\mathcal{P}$, and then solve equations (5)-(6) with wave vectors q^j in E_p for the integer index $n = (n_1, n_2)$. This leads to a set of algebraic equations. In addition, one also needs to find a grating structure of period Λ in $\mathcal{P}$, which gives another set of equations. The class is non-empty if these two sets of equations are held simultaneously; otherwise we denote the corresponding class to be the empty set. A simple condition that is necessary for the existence of a grating structure of bi-period Λ in $\mathcal{P}$ in the case corresponding to the second, third, fourth, fifth and the sixth class is that the line of intersection of planes in $\mathcal{P}_0$, namely L, should be parallel to either e_1 or e_2. Thus $\nu = e_1$ or $\nu = e_2$ in each class. This is true especially for the class $\mathcal{S}_5(s, q, r, \nu, \Lambda)$. For this reason, we can refine the fifth unidentifiable class as

$$\mathcal{S}_5(s, q, r, \Lambda) = \mathcal{S}_5(s, q, r, e_1, \Lambda) \cup \mathcal{S}_5(s, q, r, e_2, \Lambda).$$

In the two-dimensional case, i.e., when gratings considered are invariant in one axis and periodic in the other, one can refer to [20] for the necessary and sufficient condition to ensure the existence of each unidentifiable grating class.

4. Unique determination of periodic polyhedral gratings

In this section we apply the theory developed in the previous sections on the classification of unidentifiable gratings in correspondence to one incident field for the unique determination of regular polyhedral gratings by scattered fields.

Theorem 4.1. *Let $E^i = se^{iq\cdot x}$ be a given incident electric field, S_1 and S_2 be two regular bi-periodic polyhedral gratings with period Λ, and E_1 and E_2 be respectively*

the solution to the forward scattering problem (1)-(4) associated with S_1 and S_2. If $\Gamma_b = \{x_3 = b\}$ is a plane located above both S_1 and S_2, then

$$E_1 = E_2 \quad \text{on } \Gamma_b \tag{28}$$

implies that both S_1 and S_2 belong to one of the seven classes of gratings $\mathcal{S}_1(q,r)$, $\mathcal{S}_2(s,q,r,\Lambda)$, $\mathcal{S}_3(s,q,r,\Lambda)$, $\mathcal{S}_4(s,q,r,\Lambda)$, $\mathcal{S}_5(s,q,r,\Lambda)$, $\mathcal{S}_6(s,q,r,\Lambda)$ and $\mathcal{S}_7(s,q,r,\Lambda)$.

Proof. Assume that (28) is true for two different grating profiles S_1 and S_2. We only need to show that $E_1 = E_2$ in the domain above the measurement plane $\{x_3 = b\}$. The rest can be carried out in the same way as that of [9] with the help of Theorem 3.1. For this purpose, we recall the following expansions:

$$E_1(x) = E^i(x) + \sum_{n\in\mathbf{Z}^2} A_1^n e^{iq^n\cdot x}, \quad E_2(x) = E^i(x) + \sum_{n\in\mathbf{Z}^2} A_2^n e^{iq^n\cdot x}.$$

It suffices to show that $A_1^n = A_2^n$ for all $n \in \mathbf{Z}^2$. To see this, we have by (28) that

$$(E_1 - E_2)|_{x_3=b} = \sum_{n\in\mathbf{Z}^2} (A_1^n - A_2^n) e^{i\beta^n\cdot b} e^{i\alpha^n\cdot x} = 0.$$

Noting that $\{e^{i\alpha^n\cdot x}\}_{n\in\mathbf{Z}^2}$ is an orthogonal family in $L^2((0,\Lambda_1)\times(0,\Lambda_2))$ of variables x_1 and x_2, we immediately get the desired result. This completes the proof. □

Theorem 4.1 immediately leads to the following corollary.

Corollary 4.1. *Let S be a regular polyhedral grating of bi-period Λ. Consider a plane $\Gamma_b = \{x_3 = b\}$ located above S. Then the measurement of the total field E on Γ_b corresponding to the incident field E^i determines S uniquely if the following condition holds:*

There are two faces of S which do not form an angle of $\pi/4$, $\pi/3$, $\pi/2$ or $2\pi/3$.

It follows from Corollary 4.1 that a general regular polyhedral grating structure can be uniquely determined by one incident plane wave. Furthermore, only regular polyhedral gratings of very special structures may require more incident waves for their unique determination.

Now we give a simple condition that guarantees the unique determination by two incident waves for those special structures. Let S be a regular polyhedral grating of bi-period Λ, which is not an entire plane in $\mathbf{R}^3$, and let $E^{i,1} = s_1 e^{iq_1\cdot x}$ and $E^{i,2} = s_2 e^{iq_2\cdot x}$ be two incident fields. Then we define

$$\mathcal{S}_1 = \bigcup_{j=2}^{j=7} \bigcup_{r\in\mathbf{R}^3} \mathcal{S}_j(s_1,q_1,\Lambda,r)), \quad \mathcal{S}_2 = \bigcup_{j=2}^{j=7} (\bigcup_{r\in\mathbf{R}^3} \mathcal{S}_j(s_2,q_2,\Lambda,r)).$$

It is clear that S can be uniquely determined by $E^{i,1}$ and $E^{i,2}$ if and only if S does not belong to $\mathcal{S}_1 \cap \mathcal{S}_2$. Consider the case $S \in \mathcal{S}_1$, and denote the set of the normals to the faces on S by N_1. By our construction of the unidentifiable classes, we have

$$\begin{aligned} N_1 \subset M_1 \quad = \quad & \Big\{\lambda s_1, \lambda T_{\frac{\pi}{4}} s_1, \lambda T_{\frac{\pi}{3}} s_1, \lambda T_{\frac{\pi}{2}} s_1, \lambda(P_\Gamma q_1 \pm \sqrt{k^2-\tau^2}(e_3\times\nu)), \\ & \lambda(q_1 \pm k\frac{s_1\times e_3}{\|s_1\times e_3\|}); \\ & \lambda\in\mathbf{R}\backslash\{0\}, \nu = e_1 \text{ or } e_2\Big\}, \end{aligned}$$

where Γ is a plane passing through the origin with normal ν, T_θ denotes the rotation on the plane Γ about the origin by angle θ, and $P_\Gamma q$ and τ are defined as in (13). Similarly, in the case $S \in \mathcal{S}_2$, denote the set of the normals to the faces on S by N_2. Then

$$\begin{aligned} N_2 \subset M_2 \quad = \quad & \Big\{\lambda s_2, \lambda T_{\frac{\pi}{4}} s_2, \lambda T_{\frac{\pi}{3}} s_2, \lambda T_{\frac{\pi}{2}} s_2, \lambda(P_\Gamma q_2 \pm \sqrt{k^2-\tau^2}(e_3 \times \nu)), \\ & \lambda(q_2 \pm k \frac{s_2 \times e_3}{\|s_2 \times e_3\|}); \\ & \lambda \in \mathbf{R}\backslash\{0\}, \nu = e_1 \text{ or } e_2\Big\}. \end{aligned}$$

If we choose $E^{i,1}$ and $E^{i,2}$ in such a way that $M_1 \cap M_2 = \emptyset$, then $\mathcal{S}_1 \cap \mathcal{S}_2 = \emptyset$. It follows that S can be uniquely determined by the two incident waves $E^{i,1}$ and $E^{i,2}$.

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