Existence, Uniqueness and Regularity for Solutions of the Conical Diffraction Problem

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Abstract

This paper is devoted to the analysis of two Helmholtz equations in $\mathbb{R}^2$ coupled via quasiperiodic transmission conditions on a set of piecewise smooth interfaces. The solution of this system is quasi–periodic in one direction and satisfies outgoing wave conditions with respect to the other direction. It is shown that Maxwell's equations for the diffraction of a time–harmonic oblique incident plane wave by periodic interfaces can be reduced to problems of this kind. The analysis is based on a strongly elliptic variational formulation of the differential problem in a bounded periodic cell involving nonlocal boundary operators. We obtain existence and uniqueness results for solutions corresponding to electromagnetic fields with locally finite energy. Special attention is paid to the regularity and leading asymptotics of solutions near the edges of the interface.

1 Introduction

We consider a time–harmonic electromagnetic plane wave incident on a general periodic structure in $\mathbb{R}^3$, which is assumed to be infinitely wide and invariant in one spatial direction, say x_3. Such structures are called diffraction gratings in the optics and physics literature. The periodic structure separates two regions with constant dielectric coefficients. Inside the structure, the dielectric coefficient is allowed to be a piecewise constant function. This problem is motivated by several applications in micro–optics, where tools from the semiconductor industry are used to fabricate optical devices with complicated structural features within the lengthscale of optical waves. Such diffractive elements have many technological advantages and can be designed to perform functions unattainable with traditional optical elements. One of the most common geometrical configurations for diffractive optical structures is a periodic pattern etched into the surface of a thin–film layer stack, as shown in Figure 1. Since modern mask–etch fabrication processes yield nonsmooth interface profiles it is important to include this case into the considerations.

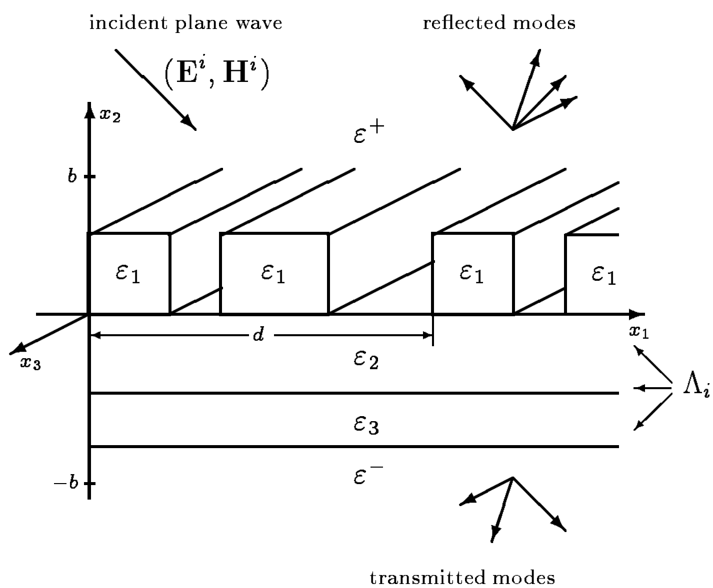

Figure 1: Diffraction of a plane-wave on a so–called binary grating. The period of the grating is generally comparable to the length of the incident wave.

In the engineering community it is widely accepted that theoretical models from scalar geometrical optics are generally not accurate to predict the performance of structures with periods comparable to the wavelength or even to carry out optimal design of new structures. The development and application of this new technology has to rely on accurate mathematical models and numerical codes for solving the full electromagnetic vector–field equations. The electromagnetic theory of gratings has been studied since Rayleigh's time. For an introduction to this problem along with some numerical methods see the collection of articles [25]. By far the largest number of papers in the literature has come from the optics and engineering community, whereas rigorous mathematical results have been obtained only during the last years (see [17], [16] and the references contained therein).

The diffraction by periodic gratings is well understood if the incident wave vector is orthogonal to the x_3–direction, i.e., the incident plane wave given by

$$\mathbf{E}^i = \mathbf{p}\, e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3} e^{-i\omega t}\,, \quad \mathbf{H}^i = \mathbf{q}\, e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3} e^{-i\omega t}\,, \tag{1.1}$$

satisfies the condition $\gamma = 0$. Then the resulting electromagnetic field can be split into the two cases of TE and TM polarization, where either the electric field or the magnetic field is parallel to the x_3–axis. In both cases Maxwell's equations can be reduced to transmission problems for a scalar Helmholtz equation on $\mathbb{R}^2$, giving as solution the x_3–component of the electric or magnetic field, respectively. These solutions u are quasiperiodic in x_1 and satisfy for $|x_2| \to \infty$ the so–called outgoing wave condition, which means that u can be expressed as a sum of bounded outgoing plane waves

$$u = \sum_{n\in\mathbb{Z}} a_n e^{i(2\pi n/d+\alpha)x_1 + i\beta_n |x_2|} \quad \text{with} \;\; (2\pi n/d+\alpha)^2 + \beta_n^2 = k^2\,, \tag{1.2}$$

where k is the refractive index of the homogeneous material above or below the grating, and $\operatorname{Im}\beta_n \geq 0$. We see from (1.2) that in a dielectric medium, i.e. $k^2 > 0$, only a finite number of plane waves in the sum propagate into the far field, the other modes decay exponentially as $|x_2| \to \infty$. The number of propagating modes and the direction of their wave vectors are completely determined by the length of the incident wave, by the period of the grating and by the refractive index of the corresponding material, but the coefficients a_n in (1.2) are unknown. From the engineering point of view, these Rayleigh coefficients are the key feature of any grating since they indicate the energy and phase shift of the propagating modes. However, apart from the trivial case of a layer system, no analytic formulas for these coefficients are available, and various methods for the approximate solution of the classical TE and TM diffraction problems have been proposed. Among the most well known are methods based on Rayleigh or eigenmode expansions, differential and integral methods (cf. [25], [6], [22], [20]), and an analytical continuation method of Bruno & Reitich ([7]). Recently, a finite element method was proposed by Bao & Dobson ([12], [2]), which is based on equivalent variational formulations of the problems in a bounded periodic cell (see also Bonnet-Bendhia & Starling [5]). This approach turned out to be well adapted for the analytical treatment of very general diffraction structures as well as complex materials. Quite complete results on existence, uniqueness and regularity of solutions for non–smooth interfaces and all materials occuring in practice were recently obtained in [16] which extend previous results for the classical diffraction problems by Chen & Friedman [8], Nedelec & Starling [24], Abboud [1], Bao [3], and Dobson [12].

In the recent papers [13], [4] the variational approach was applied to the general case of diffraction in biperiodic structures, which are periodic also in the x_3–direction. The authors obtained a variational equation for the magnetic field $\mathbf{H}$. They investigated existence and uniqueness of H^1–regular solutions and considered the finite element discretization of this equation. These results apply also to the practically important case of so–called conical diffraction, where an incident field is diffracted by a periodic structure, but its wave vector is not orthogonal to the x_3–direction, i.e. $\gamma \neq 0$. Then the components of the diffracted electromagnetic field take the form

$$\sum_{n\in\mathbb{Z}} a_n e^{i(2\pi n/d+\alpha)x_1+i\beta_n|x_2|+i\gamma x_3}\,, \quad \text{where } (2\pi n/d+\alpha)^2+\beta_n^2+\gamma^2=k^2\,. \tag{1.3}$$

Note that the wave vectors of the propagating reflected or transmitted modes lie on the surface of a cone whose axis is parallel to the x_3–direction. Therefore the engineers speak of conical diffraction, which occurs in a variety of technological applications, for example, laser scanners. Due to the simpler geometry compared with biperiodic structures, Maxwell's equations for conical diffraction can be reduced to two–dimensional problems which are closely connected with the classical TE and TM diffraction. To calculate the Rayleigh coefficients under conical incidence, some methods have been proposed which extend the known engineering methods used for the classical problems (cf. [25]). To our knowledge, no rigorous existence and uniqueness results for these equations, especially for structures with non–smooth interfaces, or results on the convergence of the numerical methods are known.

In this paper we extend the approach of [16] to the conical diffraction problem. We obtain a strongly elliptic variational formulation, which allows us to state general existence and uniqueness results and to study the asymptotics and regularity near edges of the grating surface. Note that this formulation can be used successfully to study certain inverse problems for conical diffraction and to develop efficient and reliable numerical methods for solving direct and optimal design problems.

The outline of the paper is as follows. In Section 2 we transform Maxwell's equations to a system of two Helmholtz equations in $\mathbb{R}^2$, with quasiperiodic transmission conditions on the piecewise smooth interfaces, which has to be satisfied by the x_3–components of the electric and magnetic fields. We show that the system admits an equivalent variational formulation in the Sobolev space H^1 on some bounded periodic cell Ω. In Section 3 we prove existence and uniqueness results for variational solutions of the problem under certain assumptions on the grating materials that have a reasonable physical interpretation and are satisfied for any relevant practical application. Finally, in Section 4 we study the singularities of the variational solution to the differential problem near edges of the grating interfaces.

2 Preliminaries

2.1 The Maxwell equations

Suppose that the whole space is filled with non-magnetic material with a permittivity function ε, which in Cartesian coordinates (x_1, x_2, x_3) does not depend on x_3, is periodic in x_1, and homogeneous above and below certain interfaces. In practice, the period d of optical gratings under consideration is comparable with the wavelength $\lambda = 2\pi c/\omega$ of incoming plane optical waves, where c denotes the speed of light. For notational convenience we will change the length scale by a factor of $2\pi/d$, such that the grating becomes 2π- periodic: $\varepsilon(x_1+2\pi, x_2) = \varepsilon(x_1, x_2)$. Note that this is equivalent to multiplying the frequency ω by $d/2\pi$.

The intersection of the upper grating surface with the (x_1, x_2)–plane is denoted in the sequel by Λ_0, the intersection of the lower interface with the (x_1, x_2)–plane will be denoted by Λ_1. We assume that the curves Λ_0 and Λ_1 are simple and 2π–periodic and that $\Lambda_0 > \Lambda_1$ pointwise, i.e., if $(x_1, y_0) \in \Lambda_0$, $(x_1, y_1) \in \Lambda_1$ then $y_0 > y_1$. The material in the region $G^+ \subset \mathbb{R}^3$ above the grating surface $\Lambda_0 \times \mathbb{R}$ has the constant dielectric coefficient $\varepsilon = \varepsilon^+$, whereas the medium in G^- below $\Lambda_1 \times \mathbb{R}$ is homogeneous with $\varepsilon = \varepsilon^-$. The medium in the region G_0 between $\Lambda_0 \times \mathbb{R}$ and $\Lambda_1 \times \mathbb{R}$ is inhomogeneous with $\varepsilon = \varepsilon_0(x_1, x_2)$, and we assume that the function ε_0 is piecewise constant with jumps at certain interfaces Λ_j, $j = 2, \ldots, \ell$.

The grating is illuminated by a plane wave of the form (1.1) at conical incidence. This wave $(\mathbf{E}^i, \mathbf{H}^i)$ will be diffracted by the grating, and the total fields will be given by

$$\mathbf{E}^{up} = \mathbf{E}^i + \mathbf{E}^{refl}\,, \mathbf{H}^{up} = \mathbf{H}^i + \mathbf{H}^{refl}$$

in the region G^+, by $\mathbf{E}^{int}$ and $\mathbf{H}^{int}$ in G_0, and by

$$\mathbf{E}^{down} = \mathbf{E}^{refr}\,,\ \mathbf{H}^{down} = \mathbf{H}^{refr}$$

in the region G^-. Dropping the factor $e^{-i\omega t}$, the incident, diffracted, and total fields satisfy the time–harmonic Maxwell equations

$$\nabla \times \mathbf{E} = i\omega\mu\mathbf{H} \quad \text{and} \quad \nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E}\,, \tag{2.1}$$

with the everywhere constant magnetic permeability $\mu > 0$. Additionally the tangential components of the total fields are continuous when crossing an interface $\Lambda \times \mathbb{R}$ between two homogeneous media

$$\mathbf{n} \times (\mathbf{E}^1 - \mathbf{E}^2) = 0 \quad \text{and} \quad \mathbf{n} \times (\mathbf{H}^1 - \mathbf{H}^2) = 0 \quad \text{on} \ \ \Lambda \times \mathbb{R}\,, \tag{2.2}$$

where $\mathbf{n}$ is the unit normal to the interface $\Lambda \times \mathbb{R}$. Taking the divergence of (2.1) leads to

$$\nabla \cdot (\varepsilon\mathbf{E}) = 0 \quad \text{and} \quad \nabla \cdot (\mu\mathbf{H}) = 0\,. \tag{2.3}$$

We look for vector fields satisfying (2.1) and (2.2) and possessing locally a finite energy, that is

$$\mathbf{E}\,,\ \mathbf{H}\,,\ \nabla \times \mathbf{E}\,,\ \nabla \times \mathbf{H} \in (L^2_{loc}(\mathbb{R}^3))^3\,. \tag{2.4}$$

Let us make some remarks on the solvability of the diffraction in periodic structures governed by (2.1), (2.2) and on the regularity of solutions:
Though Maxwell's equations are not an elliptic system, the elimination of one of the two fields $\mathbf{E}$ or $\mathbf{H}$ yields a variational formulation for a second order elliptic system. For example, if we integrate the second equation of (2.1) over some bounded domain $\mathbf{\Omega} \subset \mathbb{R}^3$ versus $\varepsilon^{-1}\overline{(\nabla \times \mathbf{F})}$ and the first versus $i\omega\overline{\mathbf{F}}$, then we obtain

$$\int_{\mathbf{\Omega}} \left(\varepsilon^{-1}(\nabla \times \mathbf{H}) \cdot \overline{(\nabla \times \mathbf{F})} - \omega^2\mu\,\mathbf{H} \cdot \overline{\mathbf{F}}\right) - \int_{\partial\mathbf{\Omega}} \varepsilon^{-1}((\nabla \times \mathbf{H}) \times \mathbf{n}) \cdot \overline{\mathbf{F}} = \mathbf{0}\,.$$

Taking into account the divergence equation (2.3) the magnetic field $\mathbf{H}$ satisfies also the equation

$$\int_{\mathbf{\Omega}} \left(\varepsilon^{-1}(\nabla \times \mathbf{H}) \cdot \overline{(\nabla \times \mathbf{F})} + s\,(\nabla \cdot \mu \mathbf{H})\,\overline{(\nabla \cdot \mu \mathbf{F})} - \omega^2 \mu\, \mathbf{H} \cdot \overline{\mathbf{F}}\right) - \int_{\partial \mathbf{\Omega}} \varepsilon^{-1}((\nabla \times \mathbf{H}) \times \mathbf{n}) \cdot \overline{\mathbf{F}} = 0 \tag{2.5}$$

for any parameter $s > 0$. This relation can be used to treat boundary value problems for Maxwell's equations with variational methods; for a discussion of this topic cf. [9], [10]. It is also possible to derive a variational formulation for the general case of diffraction in biperiodic structures if the periodic nature of the problem and the corresponding radiation condition are employed. Here this condition means that the far field is composed of bounded outgoing plane waves which are quasiperiodic in both the x_1– and x_3–directions. The explicit form of this variational equation was given by Dobson [13] and Bao [4], where also the existence of unique solutions $\mathbf{H} \in (H^1_{loc})^3$ is stated, except possibly for a discrete set of frequencies ω.

It is important to mention that there exist solutions of finite energy of the Dirichlet problem for Maxwell's equations, posed with smooth data functions on a polyhedral domain, which are not H^1–regular, see [10] and the literature cited therein. This results from the fact that the energy space of the variational forms for Maxwell's equations consists of square integrable vector fields with square integrable curl and divergence, and only those variational forms give back a solution of the original Maxwell equations. If the variational equation is solvable both in H^1 and in the energy space, then the H^1–solution is only the projection of the corresponding solution from the energy space. In general, the H^1–solution does not satisfy the divergence equations (2.3).

However, in the case of constant permeability μ considered here, the H^1–solution is divergence free. A detailed proof for the biperiodic diffraction is beyond the scope of this paper. Here we consider only the simple case that the wave vector of the incoming field is parallel to the x_2–axis. Due to [13] the domain $\mathbf{\Omega} \subset \mathbb{R}^3$ in (2.5) is a bounded periodic cell, i.e., the cuboid $(0, d_1) \times (-b, b) \times (0, d_2)$ with d_1, d_2 the periods of the diffractive structure in x_1– and x_3–direction, respectively, and b is an arbitrary sufficiently large number (cf. also Subsection 2.3). Taking in (2.5) the test function $\mathbf{F} = \nabla\varphi$ with $\varphi \in H^2(\mathbf{\Omega}) \cap H^1_o(\mathbf{\Omega})$, it can be easily seen that

$$\int_{\mathbf{\Omega}} \left(\varepsilon^{-1}(\nabla \times \mathbf{H}) \cdot \overline{(\nabla \times \mathbf{F})} + s\,(\nabla \cdot \mu \mathbf{H})\,\overline{(\nabla \cdot \mu \mathbf{F})} - \omega^2 \mu \mathbf{H} \cdot \overline{\mathbf{F}}\right) - \int_{\partial \mathbf{\Omega}} \varepsilon^{-1}((\nabla \times \mathbf{H}) \times \mathbf{n}) \cdot \overline{\mathbf{F}} = \int_{\mathbf{\Omega}} \left(s\,\mu^2 (\nabla \cdot \mathbf{H})\,\overline{\Delta\varphi} + \omega^2 \mu (\nabla \cdot \mathbf{H})\,\overline{\varphi}\right) = 0\,.$$

If the number $s > 0$ is chosen such that $\omega^2/s\,\mu$ is not an eigenvalue of the Dirichlet problem for $-\Delta$ in $\mathbf{\Omega}$, then the H^2–regularity for solutions φ of the boundary value problem

$$s\,\mu\,\Delta\varphi + \omega^2\varphi = f \in L^2(\mathbf{\Omega})\,, \quad \varphi|_{\partial\mathbf{\Omega}} = 0\,,$$

shows that $\nabla \cdot \mathbf{H} = 0$ in $\mathbf{\Omega}$ for the H^1–solution $\mathbf{H}$.

Consequently, Maxwell's equation for the biperiodic diffraction problem equipped with the mentioned radiation condition has for all but possibly a discrete set of frequencies ω a unique solution $(\mathbf{E}, \mathbf{H})$ and the components of the magnetic field are H^1–regular.

2.2 The Helmholtz equations

The special situation of conical diffraction allows us to transform Maxwell's equation to a simpler system of two–dimensional Helmholtz equations coupled via transmission conditions at the interfaces. For the following we introduce the piecewise constant function

$$k = \sqrt{\omega^2 \varepsilon \mu}\,, \tag{2.6}$$

where the branch of the square-root is chosen such that $k > 0$ for positive real arguments $\omega^2\varepsilon\mu$ and its branch-cut is $(-\infty, 0)$.

In order for $(\mathbf{E}^i, \mathbf{H}^i)$ to satisfy (2.1) the constant amplitude vector $\mathbf{p}$ must be perpendicular to the wave vector $\mathbf{k} = (\alpha, -\beta, \gamma)$, $\mathbf{p}\cdot\mathbf{k} = 0$, further $\mathbf{k}\cdot\mathbf{k} = (k^+)^2 = \omega^2\mu\varepsilon^+$ and $\mathbf{q} = (\omega\mu)^{-1}\mathbf{k}\times\mathbf{p}$. The wave vector of the incident field can be expressed in terms of the angles of incidence $\Phi_1, \Phi_2 \in (-\pi/2, \pi/2)$ as

$$\mathbf{k} = k^+(\sin\Phi_1\cos\Phi_2, -\cos\Phi_1\cos\Phi_2, \sin\Phi_2)\,.$$

Since the grating is invariant with respect to any translation parallel to the x_3–axis, in view of (1.1) we assume the representation of the total field

$$(\mathbf{E}, \mathbf{H})(x_1, x_2, x_3) = (E, H)(x_1, x_2)\, e^{i\gamma x_3}, \tag{2.7}$$

with $E, H : \mathbb{R}^2 \to \mathbb{C}^3$. Note that numerical methods for solving conical diffraction problems are usually based on (2.7); see [27], [26].

To simplify the notation we define the differential operator

$$\mathrm{curl}_\gamma \bullet = (\nabla, i\gamma)\times\bullet := (\partial_1, \partial_2, i\gamma)\times\bullet\,.$$

Then the Maxwell equations (2.1) for $(\mathbf{E}, \mathbf{H})$ are equivalent to

$$\mathrm{curl}_\gamma E = i\omega\mu H\,,\ \ \mathrm{curl}_\gamma H = -i\omega\varepsilon E \tag{2.8}$$

in each subdomain in which ε is constant. The boundary conditions on the interface between two such subdomains are

$$[(n,0)\times E]_{\Lambda_j\times\mathbb{R}} = [(n,0)\times H]_{\Lambda_j\times\mathbb{R}} = 0 \tag{2.9}$$

where $(n, 0) = (n_1, n_2, 0)$ is the normal vector on the interface and $[(n,0)\times E]_{\Lambda_j\times\mathbb{R}}$ denotes the jump of the function $(n, 0)\times E$ across the interface $\Lambda_j\times\mathbb{R}$. Note that from the identity

$$\int_\Omega \overline{v}\,\mathrm{curl}_\gamma\, u - u\,\overline{\mathrm{curl}_\gamma v} = \int_{\partial\Omega} ((n,0)\times u)\,\overline{v}\,,$$

which holds for any bounded Lipschitz domain $\Omega\subset\mathbb{R}^2$, any functions $u, \mathrm{curl}_\gamma u \in (L^2(\Omega))^3$ and $v \in (H^1(\Omega))^3$, it follows that $(n,0)\times u \in (H^{-1/2}(\partial\Omega))^3$.

With the ansatz (2.7) and using the notation (2.6) it is easily seen that the Maxwell equations (2.1), (2.3) for $(\mathbf{E}, \mathbf{H})$ are reduced to the vector Helmholtz equations

$$(\Delta + k^2 - \gamma^2)\,E\ = (\Delta + k^2 - \gamma^2)\,H\ = 0\,. \tag{2.10}$$

We shall assume throughout the paper that the material parameters of the grating fulfil the following conditions

$$k_\gamma^2 := k^2 - \gamma^2 \neq 0 \,,$$
$$k^+ > 0\,,\ \mathrm{Re}\, k^- > 0\,,\ \mathrm{Im}\, k^- \geq 0\,, \tag{2.11}$$
$$\mathrm{Re}\, k_0(x_1,x_2) > 0\,,\ \mathrm{Im}\, k_0(x_1,x_2) \geq 0\,.$$

Note that materials with real k are dielectrics, whereas the case $\mathrm{Im}\, k > 0$ accounts for materials which absorb energy.

Since $k_\gamma^2 \neq 0$, from the 2d-Maxwell equations (2.8) it follows directly that if we know the third components E_3, H_3 of the electric and the magnetic field we can compute the other components by

$$\begin{aligned} E_1 &= \frac{i}{k_\gamma^2}\left(\omega\mu\partial_2 H_3 + \gamma\partial_1 E_3\right), \quad & H_1 &= \frac{i}{k_\gamma^2}\left(-\omega\varepsilon\partial_2 E_3 + \gamma\partial_1 H_3\right), \\ E_2 &= \frac{i}{k_\gamma^2}\left(-\omega\mu\partial_1 H_3 + \gamma\partial_2 E_3\right), \quad & H_2 &= \frac{i}{k_\gamma^2}\left(\omega\varepsilon\partial_1 E_3 + \gamma\partial_2 H_3\right). \end{aligned} \tag{2.12}$$

Thus we obtain the identities

$$\partial_1 E_3 = i\gamma E_1 - i\omega\mu H_2\ , \quad \partial_2 E_3 = i\gamma E_2 + i\omega\mu H_1\ ,$$
$$\partial_1 H_3 = i\gamma H_1 + i\omega\varepsilon E_2\ , \quad \partial_2 H_3 = i\gamma H_2 - i\omega\varepsilon E_1\ ,$$

implying that the condition of locally finite energy (2.4) is satisfied only if the x_3–components of $\mathbf{E}$ and $\mathbf{H}$ are H^1–regular. Therefore we look for solutions $E_3, H_3 \in H^1_{loc}(\mathbb{R}^2)$ of the equations

$$(\Delta + k_\gamma^2)\, E_3 = (\Delta + k_\gamma^2)\, H_3 = 0 \tag{2.13}$$

in each of the domains in which ε is constant. In addition, one has to impose the transmission conditions

$$[E_3]_{\Lambda_j} = [H_3]_{\Lambda_j} = 0\ ,\ \left[\frac{\gamma}{k_\gamma^2}\partial_t H_3 + \frac{\omega\varepsilon}{k_\gamma^2}\partial_n E_3\right]_{\Lambda_j} = \left[\frac{\gamma}{k_\gamma^2}\partial_t E_3 - \frac{\omega\mu}{k_\gamma^2}\partial_n H_3\right]_{\Lambda_j} = 0\ , \tag{2.14}$$

at the interfaces Λ_j, where $\partial_t = n_1\partial_2 - n_2\partial_1$ denotes the tangential derivative. The conditions (2.14) are a direct consequence of (2.9) taking into account the definition of $n = (n_1, n_2, 0)$ and equations (2.12).

It is easy to check that any solution of (2.13), (2.14) gives via (2.12) and (2.7) a solenoidal solution of the Maxwell equations (2.1) – (2.3).

Remark 2.1 In the case $\gamma = 0$ the problem (2.13), (2.14) splits into the known transmission problems for scalar Helmholtz equations corresponding to the TE and TM polarization, respectively. In the engineering literature Maxwell's equations for conical diffraction are mostly reduced to a system of 4 first-order partial differential equations (cf. [27]), a differential problem similar to (2.13), (2.14) in the case of two different materials was recently proposed in [26]. ∎

The periodicity of ε, together with the form of the incident wave, motivates to seek for physical solutions $\mathbf{E}$ and $\mathbf{H}$ which are α quasi–periodic in x_1, i.e., we look for solutions of (2.13), (2.14) satisfying

$$E_3(x_1 + 2\pi, x_2) = e^{2\pi i\alpha}\, E_3(x_1, x_2)\,, \quad H_3(x_1 + 2\pi, x_2) = e^{2\pi i\alpha}\, H_3(x_1, x_2)\,. \tag{2.15}$$

Because the domain is unbounded in the x_2–direction, a radiation condition on the scattering problem must be imposed at infinity, namely that the diffracted fields remain bounded and that they should be representable as superpositions of outgoing waves. Note that this conditions follows immediately from Sommerfeld's radiation condition specified to the quasi–periodic nature of the problem.

In the following we denote by Ω^+ the domain $x_2 > \Lambda_0$, $x_1 \in (0, 2\pi)$, by Ω^- the domain below $x_2 < \Lambda_1$, $x_1 \in (0, 2\pi)$, and let Ω_0 be the intersection of G_0 with $\Lambda_1 < x_2 < \Lambda_0$, $x_1 \in (0, 2\pi)$. We denote the diffracted fields in $\Omega^\pm$ by $E^\pm, H^\pm$. Introduce the coefficients

$$\beta_n^\pm = \beta_n^\pm(\alpha) = \sqrt{(k_\gamma^\pm)^2 - (n+\alpha)^2}, n \in \mathbb{Z} \tag{2.16}$$

where the square-root is defined as in equation (2.6).

Since the α quasi–periodic functions $E_3^\pm, H_3^\pm$ are analytic above Λ_0 resp. below Λ_1, they can be expressed as a sum of outgoing bounded plane waves, i.e., $E_3^\pm, H_3^\pm$ must take the form

$$\begin{aligned} E_3^+ &= \sum_{n\in\mathbb{Z}} A_n^+ e^{i(n+\alpha)x_1 + i\beta_n^+ x_2}, \; H_3^+ = \sum_{n\in\mathbb{Z}} B_n^+ e^{i(n+\alpha)x_1 + i\beta_n^+ x_2}, \quad x_2 > \max \Lambda_0, \\ E_3^- &= \sum_{n\in\mathbb{Z}} A_n^- e^{i(n+\alpha)x_1 - i\beta_n^- x_2}, \; H_3^- = \sum_{n\in\mathbb{Z}} B_n^- e^{i(n+\alpha)x_1 - i\beta_n^- x_2}, \quad x_2 < \min \Lambda_1, \end{aligned} \tag{2.17}$$

with some complex constants $A_n^\pm, B_n^\pm$. More details can be found in [24, 17, 16].

2.3 The variational formulation

To obtain equations being equivalent to (2.13), (2.14), (2.17) we introduce the functions

$$u = \begin{cases} e^{-i\alpha x_1} E_3^+ + p_3 e^{-i\beta x_2} \\ e^{-i\alpha x_1} E_3 \\ e^{-i\alpha x_1} E_3^- \end{cases}, \quad v = \begin{cases} e^{-i\alpha x_1} H_3^+ + q_3 e^{-i\beta x_2} & \text{in } \Omega^+, \\ e^{-i\alpha x_1} H_3 & \text{in } \Omega_0, \\ e^{-i\alpha x_1} H_3^- & \text{in } \Omega^-, \end{cases}$$

which are in view of (2.15) 2π–periodic in x_1. To formulate the differential problem for u and v, we define the operators

$$\begin{aligned} &\nabla_\alpha = \nabla + i(\alpha, 0), \; \Delta_\alpha = \nabla_\alpha \cdot \nabla_\alpha = \Delta + 2i\alpha\partial_{x_1} - \alpha^2, \\ &\partial_{t,\alpha} = n_1\partial_2 - n_2\partial_1 - i\alpha n_2, \; \partial_{n,\alpha} = n \cdot \nabla_\alpha . \end{aligned}$$

Next, we introduce as artificial boundaries two straight lines $\Gamma^\pm = \{(x_1, \pm b) | \, x_1 \in [0, 2\pi]\}$, with $b > 0$ such that $b > \Lambda_0$ and $-b < \Lambda_1$, and set $\Omega = (0, 2\pi) \times (-b, b)$. Let us denote by $H_p^s(\Omega)$, $s \geq 0$, the restriction to Ω of all functions in the Sobolev space $H_{loc}^s(\mathbb{R}^2)$ which are 2π–periodic in x_1.

The diffraction problem can now be formulated as follows. By virtue of (2.10) the functions $u, v \in H_p^1(\Omega)$ have to satisfy the differential equations

$$(\Delta_\alpha + k_\gamma^2)u = (\Delta_\alpha + k_\gamma^2)v = 0 \quad \text{in } \Omega \tag{2.18}$$

and the transmission conditions (2.14) read

$$\left[\frac{\gamma}{k_\gamma^2}\partial_{t,\alpha}u - \frac{\omega\mu}{k_\gamma^2}\partial_{n,\alpha}v\right]_{\Lambda_j} = \left[\frac{\gamma}{k_\gamma^2}\partial_{t,\alpha}v + \frac{\omega\varepsilon}{k_\gamma^2}\partial_{n,\alpha}u\right]_{\Lambda_j} = 0, \quad j = 0, ..., \ell. \tag{2.19}$$

The conditions $[u]_{\Lambda_j} = [v]_{\Lambda_j} = 0$, which have to be imposed in view of equation (2.9), are a consequence of $u, v \in H_p^1(\Omega)$. Moreover, u and v have to satisfy the radiation condition (2.17). which implies representations of the following form in a neighbourhood of Γ^+ and Γ^-, respectively:

$$
\begin{aligned}
u(x_1,x_2) &= \sum_{n\in\mathbb{Z}} A_n^+ e^{inx_1+i\beta_n^+ x_2} + p_3 e^{-i\beta x_2} , \quad v(x_1,x_2) = \sum_{n\in\mathbb{Z}} B_n^+ e^{inx_1+i\beta_n^+ x_2} + q_3 e^{-i\beta x_2} , \\
u(x_1,x_2) &= \sum_{n\in\mathbb{Z}} A_n^- e^{inx_1+i\beta_n^- x_2} , \quad v(x_1,x_2) = \sum_{n\in\mathbb{Z}} B_n^- e^{inx_1+i\beta_n^- x_2} .
\end{aligned}
\tag{2.20}
$$

Let Ω_j, $j = 1, \cdots, m$, be the two-dimensional subdomains of Ω in which ε does not jump. From Green's formula we obtain for $f, g \in H_p^1(\Omega)$ the identities

$$
\int_{\Omega_j} \Delta_\alpha f \, \overline{g} = - \int_{\Omega_j} \nabla_\alpha f \, \overline{\nabla_\alpha g} + \int_{\partial\Omega_j} \partial_{n,\alpha} f \, \overline{g} , \quad \int_{\Omega_j} \nabla_\alpha g \, \overline{\nabla_\alpha^\perp f} = - \int_{\partial\Omega_j} \partial_{t,\alpha} g \, \overline{f} , \tag{2.21}
$$

where we use the notation $\nabla_\alpha^\perp := (-\partial_2 f, \partial_1 f) + i\,(0, \alpha)$.

Multiplying the equations (2.18) in each subdomain Ω_j by the constant factors $\omega\varepsilon/k_\gamma^2$ and $\omega\mu/k_\gamma^2$, respectively, the application of the first identity in (2.21) with $\varphi, \psi \in H_p^1(\Omega)$ leads to the equations

$$
\begin{aligned}
&\sum_{j=1}^m \Big(\int_{\Omega_j} \Big(\frac{\omega\varepsilon}{k_\gamma^2} \nabla_\alpha u \, \overline{\nabla_\alpha \varphi} - \omega\varepsilon \, u \, \overline{\varphi} \Big) - \int_{\partial\Omega_j} \frac{\omega\varepsilon}{k_\gamma^2} \, \partial_{n,\alpha} u \, \overline{\varphi} \Big) = 0 , \\
&\sum_{j=1}^m \Big(\int_{\Omega_j} \Big(\frac{\omega\mu}{k_\gamma^2} \, \nabla_\alpha v \, \overline{\nabla_\alpha \psi} - \omega\mu \, v \, \overline{\psi} \Big) - \int_{\partial\Omega_j} \frac{\omega\mu}{k_\gamma^2} \, \partial_{n,\alpha} v \, \overline{\psi} \Big) = 0 .
\end{aligned}
\tag{2.22}
$$

Using the transmission conditions (2.19) at the interfaces and the outgoing wave conditions the equations (2.22) can be transformed to a variational problem for u and v in Ω. We obtain here a formulation in which the integrals over the interfaces disappear, which will be useful for theoretic investigations. Note that the straightforward generalization of the variational formulations for the classical diffraction problems will contain integrals over the interfaces and scalar nonlocal boundary operators. The use of this formulation for numerical approximations will be discussed elsewhere.

The integrals over the interfaces disappear if we use the second identity in (2.21) to obtain the equivalent equations

$$
\begin{aligned}
&\sum_j \Big(\int_{\Omega_j} \Big(\frac{\omega\varepsilon}{k_\gamma^2} \nabla_\alpha u \overline{\nabla_\alpha \varphi} - \frac{\gamma}{k_\gamma^2} \nabla_\alpha v \overline{\nabla_\alpha^\perp \varphi} - \omega\varepsilon u \overline{\varphi} \Big) - \int_{\partial\Omega_j} \Big(\frac{\omega\varepsilon}{k_\gamma^2} \partial_{n,\alpha} u + \frac{\gamma}{k_\gamma^2} \partial_{t,\alpha} v \Big) \overline{\varphi} \Big) = 0 , \\
&\sum_j \Big(\int_{\Omega_j} \Big(\frac{\omega\mu}{k_\gamma^2} \nabla_\alpha v \, \overline{\nabla_\alpha \psi} + \frac{\gamma}{k_\gamma^2} \nabla_\alpha u \overline{\nabla_\alpha^\perp \psi} - \omega\mu v \overline{\psi} \Big) - \int_{\partial\Omega_j} \Big(\frac{\omega\mu}{k_\gamma^2} \partial_{n,\alpha} v - \frac{\gamma}{k_\gamma^2} \partial_{t,\alpha} u \Big) \overline{\psi} \Big) = 0 .
\end{aligned}
\tag{2.23}
$$

Now the boundary integrals on the interfaces in (2.23) annihilate in view of (2.14) and it remains to handle the integrals over the artificial boundaries $\Gamma^\pm$. Introduce the matrix functions

$$
M_n^\pm = \frac{1}{(k_\gamma^\pm)^2} \begin{pmatrix} -i\omega\varepsilon\beta_n^\pm & \pm i\gamma(n+\alpha) \\ \mp i\gamma(n+\alpha) & -i\omega\mu\beta_n^\pm \end{pmatrix} . \tag{2.24}
$$

Then the action of the boundary operators onto the functions u and v satisfying (2.20) can be represented in the form

$$\begin{aligned}\begin{pmatrix}(\omega\varepsilon\partial_{n,\alpha}u+\gamma\partial_{t,\alpha}v)/k_\gamma^2\\(\omega\mu\partial_{n,\alpha}v-\gamma\partial_{t,\alpha}u)/k_\gamma^2\end{pmatrix}(x_1,b)&=-\sum_{n\in\mathbb{Z}}M_n^+\begin{pmatrix}A_n^+\\B_n^+\end{pmatrix}e^{inx_1+i\beta_n^+b}-\frac{i\omega\beta\,e^{-i\beta b}}{k_\gamma^2}\begin{pmatrix}\varepsilon\,p_3\\\mu\,q_3\end{pmatrix},\\\begin{pmatrix}(\omega\varepsilon\partial_{n,\alpha}u+\gamma\partial_{t,\alpha}v)/k_\gamma^2\\(\omega\mu\partial_{n,\alpha}v-\gamma\partial_{t,\alpha}u)/k_\gamma^2\end{pmatrix}(x_1,-b)&=-\sum_{n\in\mathbb{Z}}M_n^-\begin{pmatrix}A_n^-\\B_n^-\end{pmatrix}e^{inx_1-i\beta_n^-b}\,.\end{aligned}\tag{2.25}$$

On the other hand, define the operators $T_\alpha^\pm$ acting on 2π-periodic vector functions on $\mathbb{R}$

$$(T_\alpha^\pm w)(x)=\sum_{n\in\mathbb{Z}}M_n^\pm\hat{w}_ne^{inx}\,,\quad\hat{w}_n=(2\pi)^{-1}\int_0^{2\pi}w(x)\,e^{-inx}\,dx\,.\tag{2.26}$$

In the sequel the action of these operators on boundary values $(u,v)|_{\Gamma^\pm}\in(H_p^{s-1/2}(\Gamma^\pm))^2$ of functions $(u,v)\in(H_p^s(\Omega))^2$ is denoted by $T_\alpha^\pm(u,v)$. Note that an equivalent norm of $H_p^s(\Gamma^\pm)$ is given by

$$\|u\|_{H_p^s(\Gamma^\pm)}=\Big(|\hat{u}_0^\pm|^2+\sum_{n\neq0}|n|^{2s}|\hat{u}_n^\pm|^2\Big)^{1/2}\,,\quad\hat{u}_n^\pm=(2\pi)^{-1}\int_0^{2\pi}u(x,\pm b)\,e^{-inx}\,dx\,.\tag{2.27}$$

Taking into account (2.20) we get

$$\begin{aligned}T_\alpha^+\begin{pmatrix}u\\v\end{pmatrix}&=\sum_{n\in\mathbb{Z}}M_n^+\begin{pmatrix}A_n^+\\B_n^+\end{pmatrix}e^{inx_1+i\beta_n^+b}-\frac{i\omega\beta\,e^{-i\beta b}}{k_\gamma^2}\begin{pmatrix}\varepsilon\,p_3\\\mu\,q_3\end{pmatrix},\\T_\alpha^-\begin{pmatrix}u\\v\end{pmatrix}&=\sum_{n\in\mathbb{Z}}M_n^-\begin{pmatrix}A_n^-\\B_n^-\end{pmatrix}e^{inx_1-i\beta_n^-b}\,.\end{aligned}\tag{2.28}$$

Therefore, combining (2.23), (2.25) and (2.28), the conical diffraction problem (2.18) – (2.20) can now be formulated as follows: Find $u,v\in H_p^1(\Omega)$ such that

$$\begin{aligned}&B(u,v;\varphi,\psi):=\\&\int_\Omega\Big(\frac{\omega\varepsilon}{k_\gamma^2}\nabla_\alpha u\,\overline{\nabla_\alpha\varphi}-\frac{\gamma}{k_\gamma^2}\nabla_\alpha v\,\overline{\nabla_\alpha^\perp\varphi}+\frac{\omega\mu}{k_\gamma^2}\nabla_\alpha v\,\overline{\nabla_\alpha\psi}+\frac{\gamma}{k_\gamma^2}\nabla_\alpha u\,\overline{\nabla_\alpha^\perp\psi}-\omega\varepsilon\,u\overline{\varphi}-\omega\mu\,v\overline{\psi}\Big)\\&+\int_{\Gamma^+}T_\alpha^+\begin{pmatrix}u\\v\end{pmatrix}\cdot\begin{pmatrix}\overline{\varphi}\\\overline{\psi}\end{pmatrix}+\int_{\Gamma^-}T_\alpha^-\begin{pmatrix}u\\v\end{pmatrix}\cdot\begin{pmatrix}\overline{\varphi}\\\overline{\psi}\end{pmatrix}=-\frac{2i\,e^{-i\beta b}}{k_\gamma^2}\int_{\Gamma^+}\Big(\omega\varepsilon\,p_3\,\overline{\varphi}+\omega\mu q_3\,\overline{\psi}\Big),\\&\qquad\forall\varphi,\psi\in H_p^1(\Omega)\,.\end{aligned}\tag{2.29}$$

Since $T_\alpha^\pm$ is a periodic pseudodifferential operator of order 1 (see e.g. [15]), it maps the Sobolev space $(H_p^{1/2}(\Gamma^\pm))^2$ boundedly into $(H_p^{-1/2}(\Gamma^\pm))^2$ and therefore, $B(u,v;\varphi,\psi)$ is a bounded sesquilinear form on $(H_p^1(\Omega))^2$. Setting

$$B(u,v;\varphi,\psi)=\Big(\mathcal{B}\begin{pmatrix}u\\v\end{pmatrix},\begin{pmatrix}\varphi\\\psi\end{pmatrix}\Big)_{L^2(\Omega)\times L^2(\Omega)}\,,$$

the form B obviously generates a bounded linear operator

$$\mathcal{B}:H_p^1(\Omega)\times H_p^1(\Omega)\longrightarrow(H_p^1(\Omega))'\times(H_p^1(\Omega))'\,.\tag{2.30}$$

3 Solvability and regularity of the conical diffraction problem

3.1 First existence and uniqueness results

We are interested in the existence and uniqueness of solutions for ranges of frequencies ω and of incidence angles Φ_1, Φ_2. First we state a uniqueness result generalizing [16, Lemma 3.1] in the case of classical diffraction.

Theorem 3.1 *Suppose that* $\operatorname{Im} k > 0$ *in some subdomain* $\Omega_1 \subset \Omega$ *where* ε *is constant. Then the diffraction problem* (2.18) – (2.20)*, or equivalently, the variational problem* (2.29) *has at most one solution in* $(H_p^1(\Omega))^2$ *for all* $\omega > 0$.

The following theorem establishes existence and uniqueness for all sufficiently small frequencies.

Theorem 3.2 *Choose some maximum incidence angle* $\Phi_0 \in (0, \pi/2)$*, and suppose that* $k^2 > \gamma^2$ *if* k *is real. Assume further that* $(k^-)^2 > \alpha^2 + \gamma^2$ *if* k^- *is real. Then there exists a frequency* $\omega_0 > 0$ *such that the variational problem* (2.29) *admits a unique solution* $(u, v) \in (H_p^1(\Omega))^2$ *for all incidence angles* Φ_1, Φ_2 *with* $|\Phi_1|, |\Phi_2| \le \Phi_0$ *and all frequencies* ω *with* $0 < \omega \le \omega_0$.

Remark 3.1 By Snell's law the condition $(k^-)^2 > \alpha^2 + \gamma^2$ is necessary that the incident wave will be transmitted to the lower region. Hence, the assumptions of Theorem 3.2 have a reasonable physical interpretation and are satisfied for any relevant application. ∎

Further solvability results in the case of arbitrary frequencies will be presented in the next paragraph. To prove the above theorems, it is convenient to reformulate the principal part of the variational form (2.29) as follows. We have

$$\begin{aligned} B_1(u, v; \varphi, \psi) &:= \int_\Omega \Big(\frac{\omega\varepsilon}{k_\gamma^2} \nabla_\alpha u \, \overline{\nabla_\alpha \varphi} - \frac{\gamma}{k_\gamma^2} \nabla_\alpha v \, \overline{\nabla_\alpha^\perp \varphi} + \frac{\omega\mu}{k_\gamma^2} \nabla_\alpha v \, \overline{\nabla_\alpha \psi} + \frac{\gamma}{k_\gamma^2} \nabla_\alpha u \, \overline{\nabla_\alpha^\perp \psi} \Big) \\ &= \int_\Omega D(\partial_{1,\alpha} u, \partial_{1,\alpha} v, \partial_2 u, \partial_2 v)^T \cdot \overline{(\partial_{1,\alpha}\varphi, \partial_{1,\alpha}\psi, \partial_2\varphi, \partial_2\psi)^T} \end{aligned} \tag{3.1}$$

with the matrix D given by

$$D = \frac{1}{k_\gamma^2} \begin{pmatrix} \omega\varepsilon & 0 & 0 & -\gamma \\ 0 & \omega\mu & \gamma & 0 \\ 0 & \gamma & \omega\varepsilon & 0 \\ -\gamma & 0 & 0 & \omega\mu \end{pmatrix} .$$

Taking the unitary matrix

$$\mathcal{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} I & iI \\ iI & I \end{pmatrix} \quad \text{with} \quad \mathcal{U}^* = \mathcal{U}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} I & -iI \\ -iI & I \end{pmatrix} , \tag{3.2}$$

where I denotes the two–dimensional identity matrix, we obtain

$$\mathcal{U}^{-1} D \mathcal{U} = \begin{pmatrix} N^- & 0 \\ 0 & N^+ \end{pmatrix}, \quad \text{where} \quad N^\pm = \frac{1}{k_\gamma^2} \begin{pmatrix} \omega\varepsilon & \pm i\gamma \\ \mp i\gamma & \omega\mu \end{pmatrix}. \tag{3.3}$$

Introducing the differential operators

$$\partial_\alpha^+ := \frac{1}{\sqrt{2}}(-i\partial_{1,\alpha} + \partial_2), \quad \partial_\alpha^- := \frac{1}{\sqrt{2}}(\partial_{1,\alpha} - i\partial_2),$$

we get from (3.2) and (3.3) that the representation

$$B_1(u,v;\varphi,\psi) = \int\limits_\Omega \left(N^+ \partial_\alpha^+ \binom{u}{v} \cdot \overline{\partial_\alpha^+ \binom{\varphi}{\psi}} + N^- \partial_\alpha^- \binom{u}{v} \cdot \overline{\partial_\alpha^- \binom{\varphi}{\psi}} \right) \tag{3.4}$$

holds. To study the form B_1, the following lemma is needed. We shall write $N > 0$ if the matrix N is positive definite and $N \geq 0$ if it is non–negative.

Lemma 3.1 *(i) If* $\operatorname{Im} k^2 > 0$ *or* $k^2 \neq \gamma^2$ *for real* k*, then* $\operatorname{Re}(iN^\pm) \geq 0$.
(ii) Suppose that $\operatorname{Im} k^2 > 0$ *or* $k^2 > \gamma^2$ *if* k *is real. Then* $\operatorname{Re}(\theta N^\pm) > 0$ *with* $\theta = (i+\delta)/|i+\delta|$ *and* $\delta > 0$ *sufficiently small.*

Proof. We have

$$\operatorname{Re}(\theta N^\pm) = \begin{pmatrix} (\omega\mu)^{-1} \operatorname{Re}(\theta k^2/k_\gamma^2) & \pm i\gamma \operatorname{Re}(\theta/k_\gamma^2) \\ \mp i\gamma \operatorname{Re}(\theta/k_\gamma^2) & \omega\mu \operatorname{Re}(\theta/k_\gamma^2) \end{pmatrix}.$$

If k is real, then obviously (i) holds with $\operatorname{Re}(iN^\pm) = 0$. In the case of nonreal k, $\operatorname{Re}(\theta N^\pm) \geq 0$ if and only if the following two conditions are satisfied:

$$\begin{aligned} \operatorname{Re}(\theta k^2/k_\gamma^2) &= \operatorname{Re}\theta + \gamma^2 \operatorname{Re}(\theta/k_\gamma^2) \geq 0\,, \\ \det(\theta N^\pm) &= (\operatorname{Re}\theta + \gamma^2 \operatorname{Re}(\theta/k_\gamma^2)) \operatorname{Re}(\theta/k_\gamma^2) - \gamma^2 \left(\operatorname{Re}(\theta/k_\gamma^2)\right)^2 \\ &= \operatorname{Re}\theta \operatorname{Re}(\theta/k_\gamma^2) \geq 0. \end{aligned} \tag{3.5}$$

These conditions are equivalent to

$$\operatorname{Re}\theta \geq 0, \quad \operatorname{Re}\theta \operatorname{Re} k_\gamma^2 + \operatorname{Im}\theta \operatorname{Im} k_\gamma^2 \geq 0. \tag{3.6}$$

Consequently, for $\operatorname{Im} k^2 > 0$, (3.6) is satisfied with $\theta = i$ which proves (i). Moreover, (3.5) and (3.6) hold with strict inequalities if $\operatorname{Im} k^2 > 0$ and $\theta = (i+\delta)/|i+\delta|$ with $\delta > 0$ sufficiently small, or if $k^2 > \gamma^2$ and $\operatorname{Re}\theta > 0$. Thus (ii) is proved. ∎

To examine the terms in (2.29) coming from the boundary operators $T_\alpha^\pm$, we need the following lemma. Consider the matrices

$$M^\pm := \frac{1}{k_\gamma^2} \begin{pmatrix} -i\omega\varepsilon(k_\gamma^2 - \alpha^2)^{1/2} & \pm i\gamma\alpha \\ \mp i\gamma\alpha & -i\omega\mu(k_\gamma^2 - \alpha^2)^{1/2} \end{pmatrix}.$$

Note that the matrices $M_n^\pm$ defined in (2.24) are obtained from $M^\pm$ by replacing α with $\alpha + n$.

Lemma 3.2 *(i) If* $\operatorname{Im} k^2 > 0$*, then* $\operatorname{Re}(iM^{\pm}) > 0$.
(ii) For $k \in \mathbb{R}$ *and* $k^2 \neq \gamma^2$*, we have* $\operatorname{Re}(iM^{\pm}) \geq 0$.
(iii) Suppose that $k^2 > \alpha^2 + \gamma^2$*. Then* $\operatorname{Re}(\theta M^{\pm}) > 0$ *with* $\theta = (i+\delta)/|i+\delta|$ *and* $\delta > 0$ *sufficiently small.*

Proof. (i) We have

$$L^{\pm} := \operatorname{Re}(iM^{\pm}) = \begin{pmatrix} (\omega\mu)^{-1} \operatorname{Re}(k^2(k_\gamma^2 - \alpha^2)^{1/2} k_\gamma^{-2}) & \mp i\alpha\gamma \operatorname{Im} k_\gamma^{-2} \\ \pm i\alpha\gamma \operatorname{Im} k_\gamma^{-2} & \omega\mu \operatorname{Re}((k_\gamma^2 - \alpha^2)^{1/2} k_\gamma^{-2}) \end{pmatrix}.$$

Since

$$0 < \arg k_\gamma^2 \leq \arg(k_\gamma^2 - \alpha^2) < \pi$$

implies the relation

$$-\pi/2 < -(\arg k_\gamma^2)/2 \leq \arg((k_\gamma^2 - \alpha^2)^{1/2} k_\gamma^{-2}) < \pi/2,$$

the elements on the main diagonal of $L^{\pm}$ are positive. Thus it remains to verify that

$$\begin{aligned} \det L^{\pm} = & \Big(\operatorname{Re}(k_\gamma^2 - \alpha^2)^{1/2} + \gamma^2 \operatorname{Re}((k_\gamma^2 - \alpha^2)^{1/2} k_\gamma^{-2})\Big) \operatorname{Re}((k_\gamma^2 - \alpha^2)^{1/2} k_\gamma^{-2}) \\ & -\gamma^2\alpha^2 \Big(\operatorname{Im} k_\gamma^{-2}\Big)^2 > 0\,, \end{aligned}$$

which is obviously a consequence of the inequality

$$\Big(\operatorname{Re}((k_\gamma^2 - \alpha^2)^{1/2} k_\gamma^{-2})\Big)^2 \; > \; \alpha^2 \, \Big(\operatorname{Im} k_\gamma^{-2}\Big)^2. \tag{3.7}$$

To prove (3.7), we set $k_\gamma^2 = ia + b, a > 0, b \in \mathbb{R}$, and $c = b - \alpha^2$ so that this estimate is equivalent to

$$A := (\operatorname{Re}[(ia+c)^{1/2}(b - ia)])^2 \; > \; \alpha^2 a^2. \tag{3.8}$$

Let $\phi = \arg(ia + c) \in (0, \pi)$. Then

$$\begin{gathered} \sin\phi = a\,(a^2 + c^2)^{-1/2}\,, \quad \cos\phi = c\,(a^2+c^2)^{-1/2}\,, \\ \sin^2(\phi/2) = (1 - \cos\phi)/2 = \{1 - c(a^2+c^2)^{-1/2}\}/2\,, \end{gathered}$$

and we obtain from

$$\begin{aligned} \operatorname{Re}[(ia+c)^{1/2}(b-ia)] \; &= \; (a^2+c^2)^{1/4} \operatorname{Re}[(\cos\frac{\phi}{2} + i\,\sin\frac{\phi}{2})(b - ia)] \\ &= \; (a^2+c^2)^{1/4}\,(b\cos\frac{\phi}{2} + a\sin\frac{\phi}{2}) \end{aligned}$$

the inequality

$$\begin{aligned} A \; &= \; (a^2+c^2)^{1/2}\,(b^2\cos^2\frac{\phi}{2} + a^2\sin^2\frac{\phi}{2} + ab\sin\phi) \\ &\geq \; (a^2+c^2)^{1/2}\,(a^2\sin^2\frac{\phi}{2} + ab\sin\phi) = a^2\,((a^2+c^2)^{1/2} - c)/2 + a^2 b \; =: \; B\,. \end{aligned}$$

To verify (3.8), we have to show that $B > \alpha^2 a^2 = a^2(b-c)$. This is obvious for $c \geq 0$ and follows from the estimate $(a^2+c^2)^{1/2} + |c| \geq 2\,|c|$ for $c < 0$.

(ii) For $k_\gamma^2 \leq \alpha^2$ we have $L^\pm = 0$, whereas $L^\pm$ is a diagonal matrix with positive entries if $k_\gamma^2 > \alpha^2$.

(iii) Since

$$L^\pm := \mathrm{Re}\,(\theta M^\pm) = \begin{pmatrix} (\omega\mu)^{-1}\; k^2(k_\gamma^2-\alpha^2)^{1/2}k_\gamma^{-2}\;\mathrm{Im}\,\theta & \mp i\alpha\gamma\; k_\gamma^{-2}\;\mathrm{Re}\,\theta \\ \pm i\alpha\gamma\; k_\gamma^{-2}\;\mathrm{Re}\,\theta & \omega\mu\;(k_\gamma^2-\alpha^2)^{1/2}k_\gamma^{-2}\;\mathrm{Im}\,\theta \end{pmatrix},$$

we have $L^\pm > 0$ if and only if the conditions $\mathrm{Im}\,\theta > 0$ and

$$\det L^\pm = k^2\;(k^2-\alpha^2-\gamma^2)\;(\mathrm{Im}\,\theta)^2 \;-\; \alpha^2\gamma^2\;(\mathrm{Re}\,\theta)^2 > 0$$

are satisfied. Setting $\theta = (i+\delta)/|i+\delta|$ with $\delta > 0$ sufficiently small, we get the result. ∎

We are now in the position to prove Theorems 3.1 and 3.2.

Proof of Theorem 3.1. Suppose that $u, v \in H_p^1(\Omega)$ satisfy (cf. (2.29) and (3.4))

$$\begin{aligned} 0 &= B(u,v;u,v) \\ &= \int_\Omega \Big(N^+\partial_\alpha^+\binom{u}{v}\cdot\overline{\partial_\alpha^+\binom{u}{v}} + N^-\partial_\alpha^-\binom{u}{v}\cdot\overline{\partial_\alpha^-\binom{u}{v}} - \omega\varepsilon\,|u|^2 - \omega\mu\,|v|^2\Big) \\ &\quad + \sum_{n\in\mathbb{Z}} \Big(M_n^+\binom{\hat{u}_n^+}{\hat{v}_n^+}\cdot\overline{\binom{\hat{u}_n^+}{\hat{v}_n^+}} + M_n^-\binom{\hat{u}_n^-}{\hat{v}_n^-}\cdot\overline{\binom{\hat{u}_n^-}{\hat{v}_n^-}}\Big), \end{aligned} \tag{3.9}$$

where $\hat{u}_n^\pm, \hat{v}_n^\pm$ denote the Fourier coefficients of u, v on $\Gamma^\pm$. Now Lemma 3.1 (i) implies $\mathrm{Re}\,(iN^\pm) \geq 0$ and Lemma 3.2 (i), (ii) (with α replaced by $\alpha + n$) yields $\mathrm{Re}\,(iM_n^\pm) \geq 0$ for all $n \in \mathbb{Z}$. Furthermore, $\mathrm{Re}\,(i\omega\mu) = 0$, $\mathrm{Re}\,(i\omega\varepsilon) = -(\omega\mu)^{-1}\;\mathrm{Im}\,k^2 < 0$ in Ω_1, and $\mathrm{Re}\,(i\omega\varepsilon) \leq 0$ in Ω in view of (2.11). Hence it follows from (3.9) that

$$0 = \mathrm{Re}\,(iB(u,v;u,v)) \;\geq\; (\omega\mu)^{-1}\int_\Omega (\mathrm{Im}\,k^2)\,|u|^2$$

which implies $u = 0$ in Ω_1. Inserting this into (3.9) gives

$$\begin{aligned} \mathrm{Re}\,(iB(u,v;u,v)) &\geq \mathrm{Re}\int_{\Omega_1} i\Big(N^+\partial_\alpha^+\binom{0}{v}\cdot\overline{\partial_\alpha^+\binom{0}{v}} + N^-\partial_\alpha^-\binom{0}{v}\cdot\overline{\partial_\alpha^-\binom{0}{v}}\Big) \\ &= \int_{\Omega_1} \omega\mu\,\mathrm{Im}\,(-k_\gamma^{-2})\,(|\partial_\alpha^+ v|^2 + |\partial_\alpha^- v|^2)/2 \;\geq\; c\int_{\Omega_1} |\nabla_\alpha v|^2 \end{aligned}$$

with some positive constant c. Hence $\nabla_\alpha v = 0$ in Ω_1, or equivalently, $z := v\,\exp(i\alpha x_1) = \mathit{const}$ in Ω_1. Since z satisfies the Helmholtz equation $\Delta z + k_\gamma^2 z = 0$ in Ω_1 with $k_\gamma^2 \neq 0$, we get $z = 0$ and thus $v = 0$ in Ω_1.

Consider now an adjacent subdomain Ω_2 (where ε is constant) with joint boundary Σ. Then obviously

$$u|_\Sigma^+ = v|_\Sigma^+ = 0, \quad \partial_t u|_\Sigma^+ = \partial_t v|_\Sigma^+ = 0, \quad \partial_n u|_\Sigma^+ = \partial_n v|_\Sigma^+ = 0, \tag{3.10}$$

and the first relation implies $u|_\Sigma^- = v|_\Sigma^- = 0$ because of $[u]_\Sigma = [v]_\Sigma = 0$. Here the plus resp. minus sign denotes the limit as Σ is approached from Ω_1 resp. Ω_2. Moreover, $[\partial_t u]_\Sigma = [\partial_t v]_\Sigma = 0$, and then the transmission conditions (2.19) on Σ together with (3.10) imply $\partial_n u|_\Sigma^- = \partial_n v|_\Sigma^- = 0$. Therefore u, v satisfy homogeneous Helmholtz equations in Ω_2 with the boundary conditions $u = v = \partial_n u = \partial_n v = 0$ on some part of the boundary so that u and v must vanish in Ω_2. Proceeding in this manner, we finally obtain $u = v = 0$ in Ω. ∎

Proof of Theorem 3.2. We choose $\theta = (i+\delta)/|i+\delta|$ as in Lemmas 3.1 and 3.2 and show that the form $\mathrm{Re}\,(\theta B)$ is coercive for all sufficiently small $\omega > 0$. Recall that $k^2 = \omega^2\mu\varepsilon$ and that $(\alpha,\beta,\gamma) = k^+(\sin\Phi_1\cos\Phi_2,\, \cos\Phi_1\cos\Phi_2,\, \sin\Phi_2)$, where k satisfies the conditions (2.11). Using (3.4), we obtain from Lemma 3.1 (ii) applied to the matrices $\omega N^\pm$ (which are independent of ω)

$$\mathrm{Re}\,(\theta B_1(u,v;u,v)) \ge c\omega^{-1}\int_\Omega (|\nabla_\alpha u|^2 + |\nabla_\alpha v|^2), \quad u,v \in H_p^1(\Omega), \tag{3.11}$$

where c is a positive constant not depending on ω. Consider the matrices

$$N_n^\pm = \frac{1}{(k_\gamma^\pm)^2}\begin{pmatrix} \omega\varepsilon^\pm|n| & \pm i\gamma n \\ \mp i\gamma n & \omega\mu|n| \end{pmatrix}, \quad n \neq 0.$$

Applying Lemma 3.1 (ii) to the matrices $\omega|n|^{-1}N_n^\pm$, which are independent of n and ω, gives

$$\mathrm{Re}\,(\theta N_n^\pm \xi\cdot\overline{\xi}) \ge c\,|n|\,\omega^{-1}|\xi|^2\,, \quad \xi \in \mathbb{C}^2, \quad n \neq 0\,, \tag{3.12}$$

with $c > 0$ not depending on n and ω. Furthermore, since

$$|\beta_n^\pm - i|n|\,| = |(k_\gamma^\pm)^2 - 2\alpha n - \alpha^2|\,|\beta_n^\pm + i|n|\,|^{-1} \le c_1\omega,$$

we have the estimate

$$||M_n^\pm - N_n^\pm||_{\mathbb{C}^2\to\mathbb{C}^2} \le c, \quad n \neq 0,$$

with positive constants c, c_1 not depending on $n, n \neq 0$, and $\omega, 0 < \omega \le \omega_0$. Together with (3.12), this implies the uniform estimate

$$\mathrm{Re}\,(\theta M_n^\pm\xi\cdot\overline{\xi}) + c_1|\xi|^2 \ge c\,|n|\,\omega^{-1}|\xi|^2, \quad \xi\in\mathbb{C}^2, \quad n\neq 0, \quad \omega\in(0,\omega_0]. \tag{3.13}$$

From Lemma 3.2 (i), (iii) applied to the matrices $M_0^\pm$, we further get the inequality

$$\mathrm{Re}\,(\theta M_0^\pm\xi\cdot\overline{\xi}) \ge c\,|\xi|^2, \quad \xi\in\mathbb{C}^2, \tag{3.14}$$

where $c > 0$ does not depend on ω. Finally, we have the obvious uniform bound

$$\Big|\int_\Omega (\omega\varepsilon|u|^2 + \omega\mu|v|^2)\Big| \le c_0\,\omega\int_\Omega (|u|^2 + |v|^2)\,. \tag{3.15}$$

Combining the estimates (3.11), (3.13) – (3.15) and (2.27) gives, for $0 < \omega \le \omega_0$, ω_0 sufficiently small, and all $u, v \in H_p^1(\Omega)$

$$\begin{aligned} &\mathrm{Re}\,(\theta B(u,v;u,v)) + c_0\,\omega\int_\Omega (|u|^2+|v|^2) \\ &\ge c\Big(\int_\Omega (|\nabla_\alpha u|^2 + |\nabla_\alpha v|^2) + \|u\|^2_{H^{1/2}(\Gamma^+)} + \|v\|^2_{H^{1/2}(\Gamma^+)} + \|u\|^2_{H^{1/2}(\Gamma^-)} + \|v\|^2_{H^{1/2}(\Gamma^-)}\Big). \end{aligned} \tag{3.16}$$

Since the square root of the last expression is an equivalent norm on $(H_p^1(\Omega))^2$ (see e.g. the proof of [16, Theorem 3.1]), estimate (3.16) finishes the proof. ∎

3.2 Strong ellipticity of the variational form and further solvability results

We call a bounded sesquilinear form $a(\cdot,\cdot)$ given on some Hilbert space X strongly elliptic if there exists a complex number θ, $|\theta| = 1$, a constant $c > 0$ and a compact form $q(\cdot,\cdot)$ such that

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

The following theorem establishes the strong ellipticity of the form (2.29) and leads, together with Theorems 3.1 and 3.2, to solvability results for the conical diffraction problem if ω is not small.

Theorem 3.3 *Assume $k^2 > \gamma^2$ if k is real. Then the sesquilinear form B defined in* (2.29) *is strongly elliptic over $(H_p^1(\Omega))^2$.*

Proof. Consider an arbitrary but fixed number $\omega > 0$ and choose $\theta = (i+\delta)/|i+\delta|$ as in Lemma 3.1. Then estimate (3.11) can be written

$$\mathrm{Re}\,(\theta\, B_1(u,v;u,v)) \geq c \int_\Omega (|\nabla_\alpha u|^2 + |\nabla_\alpha v|^2). \tag{3.17}$$

Furthermore, from (2.27) and (3.13) we obtain

$$\mathrm{Re} \int_{\Gamma^\pm} \theta\, T_\alpha^\pm \binom{u}{v} \cdot \binom{\overline{u}}{\overline{v}} \;\geq\; c(\|u\|_{H^{1/2}(\Gamma^\pm)}^2 + \|v\|_{H^{1/2}(\Gamma^\pm)}^2) \tag{3.18}$$

for all $u, v \in H_p^1(\Omega)$ whose nth Fourier coefficients on $\Gamma^\pm$ vanish for all $|n| \leq n_0$, where n_0 is chosen sufficiently large. Since these functions build up a space of finite codimension, (3.17) and (3.18) imply that θB is coercive modulo a compact form. ∎

Note that under the assumptions of the preceding theorem the operator $\mathcal{B}$ defined in (2.30) is always a Fredholm operator with index 0. Together with Theorem 3.1, this implies the following existence and uniqueness result.

Corollary 3.1 *Suppose that $k^2 > \gamma^2$ if $k \in \mathbb{R}$ and that* $\mathrm{Im}\, k > 0$ *on some subdomain of Ω. Then the variational problem* (2.29) *has a unique solution in $(H_p^1(\Omega))^2$ for all $\omega > 0$.*

We finally study the solvability of the diffraction problem for arbitrary ω when k is real in the whole domain Ω. Introduce the set of exceptional values (the Rayleigh frequencies)

$$\mathcal{R}(\varepsilon) = \left\{(\omega, \Phi_1, \Phi_2) : \exists\, n \in \mathbb{Z} \text{ such that } (k_\gamma^\pm)^2 = (n+\alpha)^2\right\},$$

corresponding to physically anomalous behaviour first observed by Wood.

Corollary 3.2 *Assume that $k^2 > \gamma^2$ everywhere in Ω and $(k^-)^2 > \alpha^2 + \gamma^2$.*
(i) The diffraction problem (2.29) is solvable in $(H_p^1(\Omega))^2$ for any frequency ω.
(ii) For all but a countable set of frequencies ω_j, $\omega_j \to \infty$, the operator

$$\mathcal{B} : H_p^1(\Omega) \times H_p^1(\Omega) \longrightarrow (H_p^1(\Omega))' \times (H_p^1(\Omega))'$$

is invertible.

Proof. It follows from Theorem 3.3 that the operator $\mathcal{B}$ defined in (2.30) is Fredholm with index 0 for any $\omega > 0$. Moreover, the inequality

$$\mathrm{Re}\, iB(u,v;u,v) \geq iM_0^+ \begin{pmatrix} \hat{u}_0^+ \\ \hat{v}_0^+ \end{pmatrix} \cdot \overline{\begin{pmatrix} \hat{u}_0^+ \\ \hat{v}_0^+ \end{pmatrix}} = \omega\beta(\varepsilon^+ |\hat{u}_0^+|^2 + \mu |\hat{v}_0^+|^2)$$

(cf. the proofs of Lemmas 3.1 and 3.2) shows that the right–hand side of (2.29) is orthogonal to the kernel of the adjoint operator $\mathcal{B}^*$ given by

$$\left(\mathcal{B}^* \begin{pmatrix} u \\ v \end{pmatrix}, \begin{pmatrix} \varphi \\ \psi \end{pmatrix}\right)_{L^2(\Omega)\times L^2(\Omega)} := \overline{B(\varphi,\psi;u,v)}\,.$$

Furthermore, by Theorem 3.2 $\mathcal{B}$ is invertible for small ω and, for any fixed incident angles $\Phi_1, \Phi_2 \in (-\pi/2, \pi/2)$, the definition (2.26) of $T_\alpha^\pm$ implies that $\mathcal{B}$ is an analytic operator function in $\omega \in \mathbb{R}^+ \backslash \mathcal{R}(\varepsilon)$ with an algebroid branching point at any $\omega \in \mathcal{R}(\varepsilon)$. Thus *(ii)* follows as in the proof of [16, Theorem 3.3] in the case of the classical diffraction problem. ∎

Remark 3.2 If for $(\omega^0, \Phi_1^0, \Phi_2^0) \notin \mathcal{R}(\varepsilon)$ the diffraction problem is uniquely solvable, then the solution depends analytically on ω, Φ_1, Φ_2 in a neighbourhood of this point. This follows immediately from the fact that the inverse of an analytic operator function is also analytic.

4 Singularities of solutions to the diffraction problem

We will restrict ourselves to the case when ε is constant in some neighbourhood below the grating surface Λ_0 and that the other interfaces $\Lambda_j, j = 1, ..., \ell$, do not intersect and are smooth. Since the regularity of the solution is a local problem, we may simplify the notation further by assuming that $\Omega_0 = \emptyset$.

Consider the transmission problem (2.18), (2.19), or equivalently, the variational problem (2.29). If the grating profile is (infinitely) smooth, then standard regularity theory shows that any solution $(u,v) \in (H_p^1(\Omega))^2$ of (2.29) satisfies $(u,v)|_{\Omega^\pm} \in (H_p^s(\Omega^\pm))^2$ for arbitrary $s > 1$. For non–smooth Λ_0, this is not true, even for $s = 2$, due to the singularities at the corner points.

We are interested in the leading singularities of the transmission problem in the case when Λ_0 is a curved polygon, i.e. Λ_0 is smooth with the exception of a finite number of corner points. We may assume without loss of generality that O is a corner point of Λ_0 and that Ω^+ coincides with the sector $S = \{(r,\phi) : 0 < r < \infty, |\phi| < \delta/2\}$ with angle $\delta \in (0, 2\pi)\backslash\{\pi\}$ in a neighbourhood of this point, whereas Λ_0 is locally given by

$\partial S = \{\phi = -\delta/2\} \cup \{\phi = \delta/2\}$. Here (r, ϕ) denote polar coordinates centered at O. To determine the corner singularities at O with Kondratiev's method [19] (see also [21], [23] and, in particular, [18], [28], [11] in the case of transmission problems), one applies Mellin transformation with respect to the radial variable to the model problem

$$\Delta u = \Delta v = 0 \quad \text{in} \quad \mathbb{R}^2 \backslash \partial S ,$$

$$[u]_{\partial S} = [v]_{\partial S} = 0 , \quad \Big[\frac{\gamma}{k_\gamma^2}\partial_t u - \frac{\omega\mu}{k_\gamma^2}\partial_n v\Big]_{\partial S} = \Big[\frac{\gamma}{k_\gamma^2}\partial_t v + \frac{\omega\varepsilon}{k_\gamma^2}\partial_n u\Big]_{\partial S} = 0 ,$$

which results from (2.18), (2.19) by neglecting all lower order terms. Since $\partial_n = \pm r^{-1}\partial/\partial\phi$, $\partial_t = \mp\partial/\partial r$ on $\{\phi = \pm\delta/2\}$, we arrive at the following eigenvalue problem for a system of two ordinary differential equations:

$$U'' + \lambda^2 U = V'' + \lambda^2 V = 0, \quad \phi \in (-\delta/2, \delta/2) \cup (\delta/2, 2\pi - \delta/2) , \tag{4.1}$$

$$[U]_{\phi=\pm\delta/2} = [V]_{\phi=\pm\delta/2} = 0 , \tag{4.2}$$

$$\Big[\frac{\gamma\lambda}{k_\gamma^2}U + \frac{\omega\mu}{k_\gamma^2}V'\Big]_{\phi=\pm\delta/2} = \Big[\frac{\gamma\lambda}{k_\gamma^2}V - \frac{\omega\varepsilon}{k_\gamma^2}U'\Big]_{\phi=\pm\delta/2} = 0 . \tag{4.3}$$

We are looking for complex numbers $\lambda, 0 < \text{Re}\,\lambda < 1$, such that this problem has a non–trivial solution $(U(\phi), V(\phi))$. Obviously, the general solution of (4.1) takes the form

$$(U, V) = \begin{cases} A^+ \cos\lambda\phi + B^+ \sin\lambda\phi , & \phi \in (-\delta/2, \delta/2) , \\ A^- \cos\lambda(\phi - \pi) + B^- \sin\lambda(\phi - \pi) , & \phi \in (\delta/2, 2\pi - \delta/2) , \end{cases}$$

where the vectors $A^\pm = (A_1^\pm, A_2^\pm), B^\pm = (B_1^\pm, B_2^\pm)$ are to be determined from the transmission conditions (4.2). This leads to an 8×8 linear system in the unknowns $A_j^\pm$, $B_j^\pm$, $j = 1, 2$. The following observation reduces its dimension by half. Introduce the terms

$$(U_e, V_e) = \begin{cases} A^+ \cos\lambda\phi , & \phi \in (-\delta/2, \delta/2) , \\ A^- \cos\lambda(\phi - \pi) , & \phi \in (\delta/2, 2\pi - \delta/2) \end{cases}$$

and $(U_o, V_o) = (U, V) - (U_e, V_e)$, which are even and odd functions, respectively, about $\phi = 0$ and $\phi = \pi$.

Lemma 4.1 *If (U, V) is a solution of problem (4.1) – (4.3), then both the terms (U_o, V_e) and (U_e, V_o) solve this problem.*

Proof. The first relation of (4.3) implies

$$0 = \Big[\frac{\gamma\lambda}{k_\gamma^2}U + \frac{\omega\mu}{k_\gamma^2}V'\Big]_{\phi=\pm\delta/2} = \Big[\frac{\gamma\lambda}{k_\gamma^2}(U_e \pm U_o) + \frac{\omega\mu}{k_\gamma^2}(V_o' \mp V_e')\Big]_{\phi=\delta/2} ,$$

which gives

$$\Big[\frac{\gamma\lambda}{k_\gamma^2}U_e + \frac{\omega\mu}{k_\gamma^2}V_o'\Big]_{\phi=\delta/2} = \Big[\frac{\gamma\lambda}{k_\gamma^2}U_o + \frac{\omega\mu}{k_\gamma^2}V_e'\Big]_{\phi=\delta/2} = 0 .$$

The corresponding relations on $\{\phi = -\delta/2\}$ are then automatically satisfied. The verification of the other transmission conditions is analogous. ∎

Suppose now that (U_o, V_e) is a non–trivial solution of (4.1) – (4.3) corresponding to the eigenvalue λ, $0 < \mathrm{Re}\,\lambda < 1$. Then we obtain the linear system

$$\begin{aligned}
A_2^+ \cos\frac{\lambda\delta}{2} \;-\; A_2^- \cos\lambda(\pi-\frac{\delta}{2}) &= 0\\
B_1^+ \sin\frac{\lambda\delta}{2} \;+\; B_1^- \sin\lambda(\pi-\frac{\delta}{2}) &= 0\\
\frac{\gamma A_2^+ - \omega\varepsilon^+ B_1^+}{(k_\gamma^+)^2} \cos\frac{\lambda\delta}{2} \;-\; \frac{\gamma A_2^- - \omega\varepsilon^- B_1^-}{(k_\gamma^-)^2} \cos\lambda(\pi-\frac{\delta}{2}) &= 0\\
\frac{\gamma B_1^+ - \omega\mu A_2^+}{(k_\gamma^+)^2} \sin\frac{\lambda\delta}{2} \;+\; \frac{\gamma B_1^- - \omega\mu A_2^-}{(k_\gamma^-)^2} \sin\lambda(\pi-\frac{\delta}{2}) &= 0
\end{aligned} \tag{4.4}$$

We may assume that

$$\sin\frac{\lambda\delta}{2}\cos\frac{\lambda\delta}{2}\sin\lambda(\pi-\frac{\delta}{2})\cos\lambda(\pi-\frac{\delta}{2}) \;\neq\; 0,$$

since otherwise it can easily be checked that (4.4) admits only the trivial solution if $\lambda \notin \mathbb{Z}$. Then (4.4) is equivalent to the 2×2 system

$$\begin{aligned}
& A_2^- \,\gamma\omega\mu((k^-)^2-(k^+)^2)\,\cos\lambda(\pi-\frac{\delta}{2})\,\sin\frac{\lambda\delta}{2}\\
& = -B_1^- \left((k^+)^2(k_\gamma^-)^2\,\sin\lambda(\pi-\frac{\delta}{2})\,\cos\frac{\lambda\delta}{2} \;+\; (k^-)^2(k_\gamma^+)^2\,\cos\lambda(\pi-\frac{\delta}{2})\,\sin\frac{\lambda\delta}{2}\right)\\
& A_2^- \left(\omega\mu(k_\gamma^-)^2\,\cos\lambda(\pi-\frac{\delta}{2})\,\sin\frac{\lambda\delta}{2} \;+\; \omega\mu(k_\gamma^+)^2\sin\lambda(\pi-\frac{\delta}{2})\,\cos\frac{\lambda\delta}{2}\right)\\
& = -B_1^-\,\gamma((k^-)^2-(k^+)^2)\,\sin\lambda(\pi-\frac{\delta}{2})\,\cos\frac{\lambda\delta}{2}\;,
\end{aligned} \tag{4.5}$$

where we have used the relation $\omega\varepsilon = k^2/\omega\mu$. With the abbreviation

$$c := -\cos\frac{\lambda\delta}{2}\,\sin\lambda(\pi-\frac{\delta}{2})\Big/\sin\frac{\lambda\delta}{2}\,\cos\lambda(\pi-\frac{\delta}{2})$$

we see that the determinant D of (4.5) takes the form

$$D = \omega\mu\,\det\begin{pmatrix} \gamma((k^-)^2-(k^+)^2) & (k^-)^2(k_\gamma^+)^2 - c\,(k^+)^2(k_\gamma^-)^2\\ c^{-1}(k_\gamma^-)^2-(k_\gamma^+)^2 & -\gamma((k^-)^2-(k^+)^2)\end{pmatrix}.$$

Moreover, we have $D=0$ if and only if

$$c^2 \,+\, (k^-/k^+)^2 \,-\, c(1+(k^-/k^+)^2) \,=\, 0,$$

that is, $c=1$ or $c=(k^-/k^+)^2$. Note that $c=1$ is equivalent to $\sin\lambda\pi=0$, i.e., $\lambda\in\mathbb{Z}$. We may assume in the following that $k^-\neq k^+$, since otherwise the transmission conditions (2.19) would reduce to $[\partial_n(u,v)]_{\Lambda_0}=0$ implying $(u,v)\in(H_p^2(\Omega))^2$. Thus we have $D=0$ if and only if

$$(k^-/k^+)^2 = -\tan\lambda(\pi-\delta/2)/\tan(\lambda\delta/2),$$

or equivalently,

$$\frac{\sin(\pi-\delta)\lambda}{\sin\pi\lambda} \;=\; \frac{(k^-)^2+(k^+)^2}{(k^-)^2-(k^+)^2}\,, \tag{4.6}$$

and solving the corresponding system (4.4), we obtain that (4.1) – (4.3) has the one–dimensional eigenspace spanned by

$$(U^0, V^0) = \begin{cases} \Big(\frac{\omega\mu\gamma}{(k^+)^2}\, \cos\lambda(\pi - \frac{\delta}{2})\, \sin\lambda\phi\,,\ \cos\lambda(\pi - \frac{\delta}{2})\, \cos\lambda\phi\Big)\,, & \phi \in (-\frac{\delta}{2}, \frac{\delta}{2})\,, \\ \Big(\frac{\omega\mu\gamma}{(k^-)^2}\, \cos\frac{\lambda\delta}{2}\, \sin\lambda(\phi - \pi)\,,\ \cos\frac{\lambda\delta}{2}\, \cos\lambda(\phi - \pi)\Big)\,, & \phi \in (\frac{\delta}{2}, 2\pi - \frac{\delta}{2})\,. \end{cases} \tag{4.7}$$

If (U_e, V_o) is a non–trivial solution of (4.1) – (4.3) corresponding to the eigenvalue λ, then analogous considerations lead to the transcendental equation

$$(k^+/k^-)^2 = -\tan\lambda(\pi - \delta/2)/\tan(\lambda\delta/2),$$

or equivalently,

$$\frac{\sin(\pi - \delta)\lambda}{\sin\pi\lambda} = -\frac{(k^-)^2 + (k^+)^2}{(k^-)^2 - (k^+)^2}\,, \tag{4.8}$$

and in this case the corresponding eigenspace is spanned by

$$(U^0, V^0) = \begin{cases} \Big(\frac{\omega\mu\gamma}{(k^+)^2}\, \sin\lambda(\frac{\delta}{2} - \pi)\, \cos\lambda\phi\,,\ \sin\lambda(\pi - \frac{\delta}{2})\, \sin\lambda\phi\Big)\,, & \phi \in (-\frac{\delta}{2}, \frac{\delta}{2})\,, \\ \Big(\frac{\omega\mu\gamma}{(k^-)^2}\, \sin\frac{\lambda\delta}{2}\, \cos\lambda(\phi - \pi)\,,\ \sin\frac{\lambda\delta}{2}\, \sin\lambda(\pi - \phi)\Big)\,, & \phi \in (\frac{\delta}{2}, 2\pi - \frac{\delta}{2})\,. \end{cases} \tag{4.9}$$

Combining (4.6) and (4.8) we obtain the equation

$$g(\lambda) := \frac{\sin(\pi - \delta)\lambda}{\sin\pi\lambda} = \sigma C,\ \sigma = \pm 1,\ C := \frac{c_0 + 1}{c_0 - 1},\ c_0 := \Big(\frac{k^-}{k^+}\Big)^2 \neq 1. \tag{4.10}$$

The transcendental equation (4.10) occurs already in [28, 11] where transmission problems for scalar Laplace and Helmholtz equations are studied. A discussion of its zeroes is given in the following lemma which generalizes [11, Lemma 6.2].

Lemma 4.2 *For $|k^-| \neq k^+$ equation (4.10) has exactly one simple root in the strip $0 < \operatorname{Re}\lambda < 1$. If $|k^-| = k^+$, then (4.10) has no root in that strip.*

Proof. Since $C = |c_0 - 1|^{-2}(|c_0|^2 - 1 - 2i\operatorname{Im} c_0)$, we observe that $C \notin [0,1]$, $\operatorname{Re} C > 0$ for $|k^-| > k^+$, $\operatorname{Re} C < 0$ for $|k^-| < k^+$ and that $\operatorname{Re} C = 0$ for $|k^-| = k^+$.

Let $\lambda = \kappa + i\xi$, $0 \leq \kappa < 1$, $\xi \in \mathbb{R}$, and suppose first that $0 < \delta < \pi$. For $\kappa = 0$, $g(\lambda)$ traverses the segment $[0, 1 - \delta/\pi]$ twice as ξ runs from $-\infty$ to $+\infty$, whereas for $\kappa \in (0,1)$ the circle of centre $(\sin(\pi - \delta)\kappa/2\sin\pi\kappa,\ 0)$ and diameter $d_\kappa = \sin(\pi - \delta)\kappa/\sin\pi\kappa$ is traversed. Note that $d_\kappa \to \infty$ as $\kappa \to 1-$. Applying the Argument Principle to the function $g(\lambda) - \sigma C$ and calculating the change in argument of this function on the boundary of the rectangles $[0, 1 - \epsilon] \times [-iN, iN]$ as $N \to \infty$ and $\epsilon \to 0+$, we then obtain that in $0 < \operatorname{Re}\lambda < 1$ (4.10) has exactly one root of multiplicity one if $\operatorname{Re}\sigma C > 0$ and no zero if $\operatorname{Re}\sigma C \leq 0$. In the case $\pi < \delta < 2\pi$ analogous considerations yield the reverse statement, that is, (4.10) has exactly one simple root in the strip $0 < \operatorname{Re}\lambda < 1$ if $\operatorname{Re}\sigma C < 0$, whereas it has no root there if $\operatorname{Re}\sigma C \geq 0$. ∎

Denote by λ^0 the unique zero of (4.10) in the strip $0 < \mathrm{Re}\lambda < 1$ if it exists. Kondratiev's method of local Mellin transformation and the above discussion imply the following result on the leading singularities of the diffraction problem. Note that, by virtue of Lemma 4.2, Green's function of the eigenvalue problem (4.1) – (4.3) has a simple pole at λ^0; compare the proof of [14, Lemma XIX.4.6].

Theorem 4.1 *Let χ be a smooth cut–off function near the corner point O. Then any solution $(u, v) \in (H_p^1(\Omega))^2$ of* (2.29) *admits the decomposition*

$$\chi(u, v) = (C_1, C_2) + C_3 r^{\lambda^0}(U^0, V^0) + (u_1, v_1), \tag{4.11}$$

where C_j $(j = 1, 2, 3)$ are certain complex constants, and (U^0, V^0) is given by (4.7) *resp.* (4.9) *if λ^0 solves equation* (4.10) *with $\sigma = +1$ resp. $\sigma = -1$. The remainder term in* (4.11) *satisfies*

$$(u_1, v_1)|_{\Omega^\pm} \in (H^{2-\epsilon}(\Omega^\pm))^2 \quad \textit{for all} \quad \epsilon > 0.$$

Remark 4.1 (*i*) Note that (4.10) is the same transcendental equation as in the case of classical diffraction, i.e. for $\gamma = 0$. This result is as expected, since γ only enters the data of the original boundary value problem for Maxwell's equations in a smooth manner; see Section 2.2. To our knowledge, there is no direct approach to the singularities of solutions to transmission problems for the Maxwell equations so far; see, however, [10] for the Dirichlet and Neumann problems.
(*ii*) The term $r^{\lambda^0}(U^0, V^0)$ occurring in (4.11) only depends on the geometry of the domain near the corner point O, whereas the constants C_j are of global nature depending, in particular, on the incoming wave. They are uniquely determined if the variational solution of the diffraction problem is unique. For $\gamma = 0$, (4.7) and (4.9) imply $U^0 = 0$, which corresponds to the fact that u then solves the classical TE diffraction problem and satisfies $u \in H_p^2(\Omega)$; compare [16, Corollary 3.1]. For $\gamma \neq 0$ and $|k^-| = k^+$, the second term in (4.11) vanishes in view of Lemma 4.2.
(*iii*) Using the above considerations, it can be shown that the higher order terms in the asymptotical development of u and v have the same form as in the case of the classical TM diffraction problem; see [16, Section 3.3].
(*iv*) From (2.12), (4.11) and the representations (4.7), (4.9) it is easy to derive the main asymptotics of the x_1– and x_2–components of the electric field $\mathbf{E}$ which are not H^1–regular near the edges of the grating interfaces.

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