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Integral methods for conical diffraction

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Abstract

The paper is devoted to the scattering of a plane wave obliquely illuminating a periodic surface. Integral equation methods lead to a system of singular integral equations over the profile. Using boundary integral techniques we study the equivalence of these equations to the electromagnetic formulation, the existence and uniqueness of solutions under general assumptions on the permittivity and permeability of the materials. In particular, new results for materials with negative permittivity or permeability are established.

1 Introduction

We study the scattering of time-harmonic plane waves by a surface, which in Cartesian coordinates (x, y, z) is periodic in x- and invariant in z-direction and separates two different materials. This is the simplest model of diffraction gratings, which have found several applications in micro-optics, where tools from the semiconductor industry are used to fabricate optical devices with complicated structural features within the length-scale of optical waves. Such diffractive elements have many technological advantages and can be designed to perform functions unattainable with traditional optical elements.

The electromagnetic formulation of the scattering by gratings, which are modeled as infinite periodic structures, can be reduced to a system of Helmholtz equations for the z-components of the electric and magnetic fields in $\mathbb{R}^2$, where the solutions have to be quasiperiodic in one variable, subject to radiation conditions with respect to the other and satisfy certain jump conditions at the interfaces between different materials of the diffraction grating. In the case of classical diffraction, when the incident wave is orthogonal to the z-direction, the system degenerates to independent transmission problems for the two basic polarizations of the incident wave, whereas for the so called conical diffraction the boundary values of the z-components as well as their normal and tangential derivatives at the interfaces are coupled.

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 in [12]. 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 15 years.

In the case of classical diffraction existence and uniqueness results are based on the observation that the weak form of corresponding boundary value problems in a periodic cell satisfies a Gårding inequality if the argument of the in general complex permittivity ε of the non-magnetic grating materials satisfies $0 \le \arg \varepsilon < \pi$ (see [5, 6] and the references contained therein). Here the radiation condition is reformulated as a nonlocal boundary condition imposed on one part of the boundary of the periodic cell. The reduction of conical diffraction to a transmission problem for the system of Helmholtz equations in $\mathbb{R}^2$ goes back to [18] (in the case of one interface) and [4], where results, similar to classical diffraction, have been established by extending the variational approach.

The variational formulation is also used for the numerical solution of periodic diffraction problems with the Finite-Element-Method, which is now accepted also in the optics community. But the most popular numerical methods for grating problems are methods based on Rayleigh or eigenmode expansions, differential and integral methods, which have been developed since 1970. Especially integral equation methods are very efficient for solving the classical diffraction problems in certain scenarios with large ratio period over wavelength, profile curves with corners and gratings with thin coated layers. Various integral formulations have been proposed and implemented, e.g. [10, 13, 14, 7, 15], but a rigorous mathematical and numerical analysis of these methods can not be found in the literature. The mathematical papers dealing with integral formulations of grating problems are mainly concerned with perfectly reflecting gratings or the study of the fundamental solution and radiation conditions.

Recently in [16] an integral equation approach from [10, 13] was extended to conical diffraction, resulting in a system of integral equations over the interface, which contains besides the single and double layer potentials of periodic diffraction also the integral operator with the tangential derivative of the fundamental solution as kernel. It was shown in particular, that this system of singular integral equations generates a strongly elliptic operator if the materials satisfy the assumptions of the variational approach. For the analysis the interface is conformly mapped to a close curve, such that the transformed integral operators are compact perturbations of boundary integral operators for the Laplacian on that curve.

This allows to apply techniques from the method of boundary integral equations to study conical diffraction with quite general assumptions on the permittivity and permeability of the materials. Motivated by recent proposals for the design of optical metamaterials we allow magnetic materials with complex permeability μ, $\arg \mu \in [0, \pi)$, and consider also the case that either ε or μ are negative. Then the variational formulation does not satisfy a Gårding type inequality and strong ellipticity principles do not work. However, the integral formulation can be analyzed by using some more or less standard techniques from singular and second kind integral equations with double layer potentials. We find conditions for the existence and uniqueness of solutions of the integral equation system and for its equivalence to the transmission problem for the Helmholtz equations.

To give an example. Let the profile of the surface in the (x, y)-plane be given by a smooth periodic function $y = f(x)$ and denote the permittivities and permeabilities of the materials above and below the surface by $\varepsilon_\pm$ and $\mu_\pm$, respectively. Then the integral formulation is solvable if $\varepsilon_- \neq -\varepsilon_+$ and $\mu_- \neq -\mu_+$, and its solution generates a solution of the conical diffraction problem. Moreover, the solution is unique except for certain real ε_- and μ_-, where resonances or so called trapped modes can occur.

In the case of profiles with corners the existence of solutions can be guaranteed if the ratios

$$\frac{\varepsilon_+ + \varepsilon_-}{\varepsilon_+ - \varepsilon_-} \quad \text{and} \quad \frac{\mu_+ + \mu_-}{\mu_+ - \mu_-}$$

belong to the essential spectrum of the double layer logarithmic potential in the Sobolev space $H^{1/2}$ on the associated closed curve.

The outline of the paper is as follows. Section 2 is devoted to the conical diffraction by periodic structures and the formulation by partial differential equations. Quasiperiodic potentials for Helmholtz equations and integral operators of periodic diffraction are discussed in Section 3. In Section 4 we derive the system of singular integral equations for conical diffraction and study its equivalence to the differential equations. Conditions for the existence and uniqueness of solutions are obtained in Section 5. In the final Section 6 we briefly discuss the singularities of the solution of the integral equation system.

2 Conical Diffraction

Let Σ be a non self-intersecting curve in the (x, y)-plane which is d-periodic in x-direction. The surface $\Sigma \times \mathbb{R}$ separates two regions $G_\pm \times \mathbb{R} \subset \mathbb{R}^3$ filled with materials of constant electric permittivity $\varepsilon_\pm$ and magnetic permeability $\mu_\pm$, see Fig. 1.

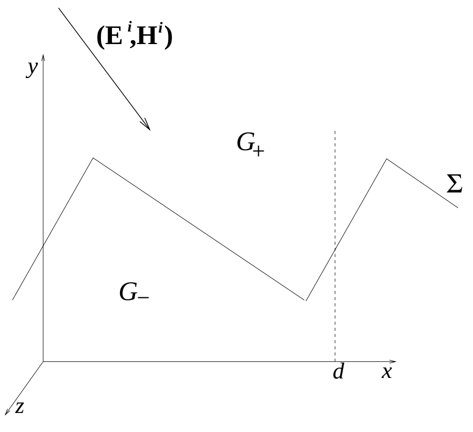

Figure 1: Schematic presentation of a simple grating

The surface is illuminated from $G_+ \times \mathbb{R}$, where $\varepsilon_+, \mu_+ > 0$, by a electromagnetic plane wave at oblique incidence

$$\mathbf{E}^i = \mathbf{p}\, e^{i(\alpha x - \beta y + \gamma z)}\, e^{-i\omega t}\,, \quad \mathbf{H}^i = \mathbf{s}\, e^{i(\alpha x - \beta y + \gamma z)}\, e^{-i\omega t}\,, \tag{2.1}$$

which due to the periodicity of Σ is scattered into a finite number of plane waves in $G_+ \times \mathbb{R}$ and possibly in $G_- \times \mathbb{R}$. The wave vectors of these outgoing modes lie on the surface of a cone whose axis is parallel to the z–axis. Therefore in optics one speaks of conical diffraction, which occurs in a variety of technological applications.

2.1 Maxwell equations

The wave $(\mathbf{E}^i, \mathbf{H}^i)$ is scattered by the surface, and the total fields will be given by

$$\mathbf{E}_+ = \mathbf{E}^i + \mathbf{E}^{refl}\,,\ \mathbf{H}_+ = \mathbf{H}^i + \mathbf{H}^{refl} \qquad \text{in the region } G_+ \times \mathbb{R}\,,$$
$$\mathbf{E}_- = \mathbf{E}^{tran}\,,\ \mathbf{H}_- = \mathbf{H}^{tran} \qquad \text{in the region } G_- \times \mathbb{R}\,.$$

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

$$\boldsymbol{\nabla} \times \mathbf{E} = i\omega\mu\mathbf{H} \quad \text{and} \quad \boldsymbol{\nabla} \times \mathbf{H} = -i\omega\varepsilon\mathbf{E}\,, \tag{2.2}$$

with piecewise constant functions $\varepsilon(x,y) = \varepsilon_\pm$, $\mu(x,y) = \mu_\pm$ for $(x,y) \in G_\pm$. The components of the wave vector $\mathbf{k}_+ = (\alpha, -\beta, \gamma)$ of the incoming field satisfy

$$\beta > 0 \quad \text{and} \quad \alpha^2 + \beta^2 + \gamma^2 = \omega^2\varepsilon_+\mu_+\,,$$

and they are expressed using the incidence angles $|\theta|, |\phi| < \pi/2$

$$(\alpha, -\beta, \gamma) = \omega\sqrt{\varepsilon_+\mu_+}\,(\sin\theta\cos\phi, -\cos\theta\cos\phi, \sin\phi)\,.$$

If the angle $\phi = 0$, then one speaks of classical periodic diffraction, whereas $\phi \neq 0$ characterizes conical diffraction. To be a solution of Maxwell's system above the surface the coefficient vectors $\mathbf{p}, \mathbf{s}$, which determine the polarization of the incident light (2.1), and the wave vector $\mathbf{k}_+$ are connected by certain compatibility relations.

When crossing the surface the tangential components of the total fields are continuous

$$\mathbf{n} \times (\mathbf{E}_+ - \mathbf{E}_-) = 0 \quad \text{and} \quad \mathbf{n} \times (\mathbf{H}_+ - \mathbf{H}_-) = 0 \quad \text{on } \Sigma \times \mathbb{R}\,, \tag{2.3}$$

where $\mathbf{n}$ is the unit normal to the interface $\Sigma \times \mathbb{R}$. Taking the divergence of (2.2) leads to

$$\boldsymbol{\nabla} \cdot (\varepsilon\mathbf{E}) = 0 \quad \text{and} \quad \boldsymbol{\nabla} \cdot (\mu\mathbf{H}) = 0\,. \tag{2.4}$$

We look for vector fields $\mathbf{E}, \mathbf{H}$ satisfying (2.2) and (2.3) such that

$$\mathbf{E}\,,\ \mathbf{H}\,,\ \boldsymbol{\nabla} \times \mathbf{E}\,,\ \boldsymbol{\nabla} \times \mathbf{H} \in \big(L^2_{loc}(\mathbb{R}^3)\big)^3\,, \tag{2.5}$$

i.e. possessing locally a finite energy.

2.2 Helmholtz equations

Since the geometry is invariant with respect to any translation parallel to the z–axis, we make the ansatz for the total field

$$(\mathbf{E}, \mathbf{H})(x,y,z) = (E, H)(x,y)\ \mathrm{e}^{i\gamma z} \tag{2.6}$$

with $E, H : \mathbb{R}^2 \to \mathbb{C}^3$. This transforms the equations in $\mathbb{R}^3$ into a two-dimensional problem. Maxwell's equations (2.2) provide

$$\begin{aligned} E = (E_x, E_y, E_z) &= \frac{i}{\omega\varepsilon}\big(\partial_y H_z - i\gamma H_y, i\gamma H_x - \partial_x H_z, \partial_x H_y - \partial_y H_x\big),\\ H = (H_x, H_y, H_z) &= \frac{1}{i\omega\mu}\big(\partial_y E_z - i\gamma E_y, i\gamma E_x - \partial_x E_z, \partial_x E_y - \partial_y E_x\big). \end{aligned} \tag{2.7}$$

Hence if (2.6) holds, then the condition of locally finite energy (2.5) is satisfied only if the z-components of E, H are H^1- regular, since

$$\begin{aligned} \partial_x E_z &= i\gamma E_x - i\omega\mu H_y\,, \quad & \partial_y E_z &= i\gamma E_y + i\omega\mu H_x\,,\\ \partial_x H_z &= i\gamma H_x + i\omega\varepsilon E_y\,, \quad & \partial_y H_z &= i\gamma H_y - i\omega\varepsilon E_x\,. \end{aligned}$$

Moreover, from (2.7) we derive

$$E_x = \frac{i}{\omega\varepsilon}\big(\partial_y H_z - i\gamma H_y\big) = \frac{i}{\omega\varepsilon}\partial_y H_z + \frac{i\gamma}{\omega^2\varepsilon\mu}\partial_x E_z + \frac{\gamma^2}{\omega^2\varepsilon\mu}E_x\,,$$

implying

$$\frac{\omega^2\varepsilon\mu-\gamma^2}{\omega^2\varepsilon\mu}\,E_x=\frac{i}{\omega\varepsilon}\,\partial_y H_z+\frac{i\gamma}{\omega^2\varepsilon\mu}\,\partial_x E_z, \tag{2.8}$$

and similar relations for E_y, H_x and H_y. Noting $\gamma=\omega\sqrt{\varepsilon_+\mu_+}\,\sin\phi$, we introduce the piecewise constant function

$$\kappa(x,y)=\begin{cases}\sqrt{\varepsilon_+\mu_+-\varepsilon_+\mu_+\sin^2\phi}=\kappa_+\,, & (x,y)\in G_+\,,\\ \sqrt{\varepsilon_-\mu_--\varepsilon_+\mu_+\sin^2\phi}=\kappa_-\,, & (x,y)\in G_-\,,\end{cases} \tag{2.9}$$

where we choose the square root $\sqrt{z}=\sqrt{r}\,e^{\,i\varphi/2}$ for $z=r\,e^{\,i\varphi}$, $0\le\varphi<2\pi$. Thus (2.8) and the other relations give

$$\begin{aligned}\omega^2\kappa^2E_x&=i\gamma\partial_xE_z+i\omega\mu\partial_yH_z, & \omega^2\kappa^2E_y&=i\gamma\partial_yE_z-i\omega\mu\partial_xH_z,\\ \omega^2\kappa^2H_x&=i\gamma\partial_xH_z-i\omega\varepsilon\partial_yE_z, & \omega^2\kappa^2H_y&=i\gamma\partial_yH_z+i\omega\varepsilon\partial_xE_z,\end{aligned} \tag{2.10}$$

implying that under the condition $\kappa\neq 0$, which will be assumed throughout, the components E_z, H_z of the electric and the magnetic field determine the other components, which in general belong only to L^2.

It follows from (2.7) and (2.4) that the Maxwell equations (2.2) can be replaced by Helmholtz equations

$$(\Delta+\omega^2\kappa^2)\,E_z\;=(\Delta+\omega^2\kappa^2)\,H_z\;=0 \tag{2.11}$$

in $G_\pm$. The continuity conditions (2.3) on the surface take the form

$$\big[(n,0)\times E\big]_{\Sigma\times\mathbb{R}}=\big[(n,0)\times H\big]_{\Sigma\times\mathbb{R}}=0\,,$$

where $(n,0)=(n_x,n_y,0)$ is the normal vector and $\big[(n,0)\times E\big]_{\Sigma\times\mathbb{R}}$ denotes the jump of the function $(n,0)\times E$ across the interface $\Sigma\times\mathbb{R}$. Since

$$(n,0)\times E=\big(n_yE_z,-n_xE_z,n_xE_y-n_yE_x\big)$$

we conclude that

$$\big[E_z\big]_\Sigma=\big[H_z\big]_\Sigma=0\,.$$

Furthermore, because of $\kappa\neq 0$ relations (2.10) give

$$\begin{aligned}n_xE_y-n_yE_x&=\frac{1}{\omega^2\kappa^2}\Big(i\gamma(n_x\partial_yE_z-n_y\partial_xE_z)-i\omega\mu(n_x\partial_xH_z+n_y\partial_yH_z)\Big),\\ n_xH_y-n_yH_x&=\frac{1}{\omega^2\kappa^2}\Big(i\gamma(n_x\partial_yH_z-n_y\partial_xH_z)+i\omega\varepsilon(n_x\partial_xE_z+n_y\partial_yE_z)\Big),\end{aligned}$$

which implies the jump conditions

$$\Big[\frac{\gamma}{\omega^2\kappa^2}\,\partial_tH_z+\frac{\omega\varepsilon}{\omega^2\kappa^2}\,\partial_nE_z\Big]_\Sigma=\Big[\frac{\gamma}{\omega^2\kappa^2}\,\partial_tE_z-\frac{\omega\mu}{\omega^2\kappa^2}\,\partial_nH_z\Big]_\Sigma=0\,.$$

Here $\partial_n=n_x\partial_x+n_y\partial_y$ and $\partial_t=-n_y\partial_x+n_x\partial_y$ are the normal resp. tangential derivatives on Σ. Introduce $B_z=\sqrt{\mu_+/\varepsilon_+}\,H_z$ and use $\gamma=\omega\sqrt{\varepsilon_+\mu_+}\,\sin\phi$ to rewrite the jump conditions in the form

$$\Big[\frac{\varepsilon\,\partial_nE_z}{\kappa^2}\Big]_\Sigma=-\varepsilon_+\sin\phi\Big[\frac{\partial_tB_z}{\kappa^2}\Big]_\Sigma,\;\Big[\frac{\mu\,\partial_nB_z}{\kappa^2}\Big]_\Sigma=\mu_+\sin\phi\Big[\frac{\partial_tE_z}{\kappa^2}\Big]_\Sigma. \tag{2.12}$$

In addition, the z-components of the incoming field

$$E_z^i(x,y)=p_z\,\mathrm{e}^{i(\alpha x-\beta y)}\,,\;B_z^i(x,y)=q_z\,\mathrm{e}^{i(\alpha x-\beta y)}\,, \tag{2.13}$$

are α-quasiperiodic in x of period d, i.e. satisfy the relation

$$u(x+d,y)=\mathrm{e}^{id\alpha}\,u(x,y)\,.$$

The periodicity of ε and μ, together with the form of the incident wave, motivates to seek for solutions E_z, B_z which are α-quasiperiodic, too. Because the domain is unbounded, a radiation condition on the scattering problem must be imposed at infinity, namely that the diffracted fields remain bounded. This implies the so called outgoing wave condition

$$\begin{aligned}(E_z, B_z)(x, y) &= (E_z^i, B_z^i) + \sum_{n\in\mathbb{Z}} (E_n^+, B_n^+)\, e^{i(\alpha_n x + \beta_n^+ y)}, \qquad y \geq H,\\ (E_z, B_z)(x, y) &= \sum_{n\in\mathbb{Z}} (E_n^-, B_n^-)\, e^{i(\alpha_n x - \beta_n^- y)}, \qquad y \leq -H,\end{aligned} \tag{2.14}$$

where $\Sigma \subset \{(x, y) : |y| < H\}$, and α_n, $\beta_n^\pm$ are given by

$$\alpha_n = \alpha + \frac{2\pi n}{d}\,, \quad \beta_n^\pm = \sqrt{\omega^2\kappa_\pm^2 - \alpha_n^2} \quad \text{with } 0 \leq \arg \beta_n^\pm < \pi\,. \tag{2.15}$$

The Rayleigh coefficients $E_n^\pm, B_n^\pm \in \mathbb{C}$ are the main characteristics of diffraction gratings. In particular, if $\beta_n^\pm \in \mathbb{R}$ (which is possible only for a finite number of indices), then the Rayleigh coefficients indicate the energy and the phase shift of the propagating modes, i.e. of the outgoing plane waves with the wave vectors

$$(\alpha_n, \beta_n^+, \gamma) \text{ in } G_+ \;\text{ and }\; (\alpha_n, -\beta_n^-, \gamma) \text{ in } G_-\,.$$

In view of (2.15) we have to specify the assumptions for the material parameters ε_- and μ_-. In the following it is always assumed that

$$\operatorname{Im}\varepsilon_-, \operatorname{Im}\mu_- \geq 0 \quad \text{unless} \quad \varepsilon_- \text{ and } \mu_- < 0\,, \tag{2.16}$$

which holds for all existing optical (meta)materials.

We will not consider the case $\varepsilon_-, \mu_- < 0$, which corresponds to negative refraction index materials, proposed in [17]. Then $\omega^2\kappa_-^2 - \alpha_n^2 = \omega^2\varepsilon_-\mu_- - \gamma^2 - \alpha_n^2$ can be positive and one has to choose $\beta_n^- = -\sqrt{\omega^2\kappa_-^2 - \alpha_n^2} < 0$.

3 Potential methods

Here we describe some potential-theoretic methods for quasiperiodic Helmholtz equations in $\mathbb{R}^2$ and the mapping properties of the resulting integral operators which have been studied in [16]. They are consequences of well-known properties of the classical logarithmic potentials on closed curves.

3.1 Potentials of periodic diffraction

We assume that Σ is non self-intersecting and given by a piecewise C^2 parametrization

$$\sigma(t) = (X(t), Y(t)), \quad X(t+1) = X(t) + d,\; Y(t+1) = Y(t)\,, \quad t \in \mathbb{R}\,,$$

i.e. the continuous functions X, Y are piecewise C^2 with

$$|\sigma'(t)| = \sqrt{(X'(t))^2 + (Y'(t))^2} > 0\,,$$

and $\sigma(t_1) \neq \sigma(t_2)$ if $t_1 \neq t_2$. Suppose additionally that if Σ has corners, then the angles between adjacent tangents at the corners are strictly between 0 and 2π.

The potentials which provide α-quasiperiodic solutions of the Helmholtz equation

$$\Delta u + k^2 u = 0 \tag{3.1}$$

are based on the quasiperiodic fundamental solution of period d

$$\Psi_{k,\alpha}(P) = \frac{i}{4}\sum_{n\in\mathbb{Z}} H_0^{(1)}\Big(k\sqrt{(X - nd)^2 + Y^2}\Big)\, e^{ind\alpha}\,, \quad P = (X, Y)\,, \tag{3.2}$$

with the Hankel function of the first kind $H_0^{(1)}$ for $\arg k \in (-\pi, \pi)$. The single and double layer potentials are defined by

$$\begin{aligned}\mathcal{S}_{k,\alpha}\varphi(P) &= 2\int_\Gamma \varphi(Q)\, \Psi_{k,\alpha}(P - Q)\, d\sigma_Q\,,\\ \mathcal{D}_{k,\alpha}\varphi(P) &= 2\int_\Gamma \varphi(Q)\, \partial_{n(Q)}\Psi_{k,\alpha}(P - Q)\, d\sigma_Q\,,\end{aligned} \tag{3.3}$$

where Γ is one period of the interface Σ, i.e. $\Gamma = \{\sigma(t) : t \in [t_0, t_0+1]\}$ for some t_0. In (3.3) $d\sigma_Q$ denotes the integration with respect to the arc length and $n(Q)$, $Q \in \Sigma$, is the normal to Σ pointing into G_-. Obviously, for α-quasiperiodic densities φ on Σ the value of the potentials does not depend on the choice of Γ.

The series (3.2) converges uniformly over compact sets in $\mathbb{R}^2 \setminus \bigcup_{n\in\mathbb{Z}} \{(nd, 0)\}$ if

$$k^2 \neq \alpha_n^2 = \Big(\alpha + \frac{2\pi n}{d}\Big)^2 \quad \text{for all} \quad n \in \mathbb{Z}\,. \tag{3.4}$$

Moreover, setting $\beta_n = \sqrt{k^2 - \alpha_n^2}$ (recall that $\operatorname{Im}\beta_n \geq 0$) Poisson's summation formula leads to the representation

$$\Psi_{k,\alpha}(P) = \lim_{N\to\infty} \frac{i}{2d} \sum_{n=-N}^{N} \frac{\mathrm{e}^{\,i\alpha_n X + i\beta_n|Y|}}{\beta_n}\,. \tag{3.5}$$

Define the function spaces

$$H^s_\alpha(\Gamma) = \Big\{ \mathrm{e}^{\,i\alpha X}\, \varphi \circ \sigma :\ \varphi \circ \sigma \in H^s_p(0,1) \Big\}\,, \tag{3.6}$$

where $H^s_p(0,1)$, $s \in \mathbb{R}$, denotes the Sobolev space of 1-periodic functions on the real line and suppose (3.4). For $\varphi \in H_\alpha^{-1/2}(\Gamma)$ and $\psi \in H_\alpha^{1/2}(\Gamma)$ the potentials $u = V_\Gamma\varphi(P)$ resp. $u = K_\Gamma\psi(P)$, $P \notin \Sigma$, are H^1-regular and α-quasiperiodic solutions of the Helmholtz equation (3.1) which satisfy the radiation condition

$$u(x,y) = \sum_{n=-\infty}^{\infty} u_n\, \mathrm{e}^{\,i\alpha_n x + i\beta_n|y|}\,, \quad |y| \geq H\,. \tag{3.7}$$

The potentials provide also the usual representation formulas. Suppose that the α-quasiperiodic function u given in G_+ is locally H^1 such that $\Delta u \in L^2_{loc}(G_+)$, satisfies the Helmholtz equation (3.1) almost everywhere and the radiation condition (3.7). Then

$$\frac{1}{2}\big(\mathcal{S}_{k,\alpha}\partial_n u - \mathcal{D}_{k,\alpha} u\big) = \begin{cases} u & \text{in } G_+, \\ 0 & \text{in } G_-, \end{cases}\,, \tag{3.8}$$

where the normal n points into G_-. Under the same assumptions for a function u in G_- the representation

$$\frac{1}{2}\big(\mathcal{D}_{k,\alpha} u - \mathcal{S}_{k,\alpha}\partial_n u\big) = \begin{cases} 0 & \text{in } G_+, \\ u & \text{in } G_-, \end{cases} \tag{3.9}$$

is valid.

3.2 Boundary integrals for periodic diffraction

Boundary integral operators are restriction of $\mathcal{S}_{k,\alpha}$ and $\mathcal{D}_{k,\alpha}$ to the profile curve Σ. The potentials provide the usual jump relations of classical potential theory. The single layer potential is continuous across Σ

$$(\mathcal{S}_{k,\alpha}\varphi)^+(P) = (\mathcal{S}_{k,\alpha}\varphi)^-(P) = V_{k,\alpha}\varphi(P)\,,$$

where the upper sign $+$ resp. $-$ denotes the limits of the potentials for points in $G_\pm$ tending in non-tangential direction to $P \in \Sigma$, and

$$V_{k,\alpha}\varphi(P) = 2\int_\Gamma \Psi_{k,\alpha}(P-Q)\,\varphi(Q)\,d\sigma_Q\,, \quad P \in \Sigma\,. \tag{3.10}$$

The double layer potential has a jump if crossing Γ:

$$\big(\mathcal{D}_{k,\alpha}\varphi\big)^+ = K_{k,\alpha}\varphi - \varphi, \quad \big(\mathcal{D}_{k,\alpha}\varphi\big)^- = K_{k,\alpha}\varphi + \varphi \tag{3.11}$$

with the boundary double layer potential

$$K_{k,\alpha}\varphi(P) = 2\int_\Gamma \varphi(Q)\,\partial_{n(Q)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q + (\delta(P)-1)\varphi(P)\,. \tag{3.12}$$

Here $\delta(P) \in (0,2)$, $P \in \Sigma$, denotes the ratio of the angle in G_+ at P and π, i.e. $\delta(P) = 1$ outside corner points of Σ. The normal derivative of $\mathcal{S}_{k,\alpha}\varphi$ at Σ exists outside corners and has the limits

$$\big(\partial_n\mathcal{S}_{k,\alpha}\varphi\big)^+ = L_{k,\alpha}\varphi + \varphi, \quad \big(\partial_n\mathcal{S}_{k,\alpha}\varphi\big)^- = L_{k,\alpha}\varphi - \varphi, \tag{3.13}$$

where we denote

$$L_{k,\alpha}\varphi(P) = 2\int_\Gamma \varphi(Q)\,\partial_{n(P)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q\,, \quad P\in\Sigma\,. \tag{3.14}$$

In the following we consider also operators of the form

$$2\int_\Gamma \varphi(Q)\,\partial_{t(Q)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q = -2\int_\Gamma \Psi_{k,\alpha}(P-Q)\,\partial_t\varphi(Q)\,d\sigma_Q\,, \tag{3.15}$$

where φ has a α-quasiperiodic extension to Σ. If $P\notin\Sigma$, then equality (3.15) follows from integration by parts and the quasi-periodicity

$$\varphi(\sigma(t_0+1)) = e^{id\alpha}\varphi(\sigma(t_0))\,,\ \Psi_{k,\alpha}(P-\sigma(t_0+1)) = e^{-id\alpha}\Psi_{k,\alpha}(P-\sigma(t_0))$$

at the end points of Γ. If $P\in\Sigma$, then the integral on the left of (3.15) is defined as the principal value integral

$$H_{k,\alpha}\varphi(P) = 2\lim_{\delta\to0}\int_{\Gamma\setminus\Gamma(P,\delta)} \varphi(Q)\,\partial_{t(Q)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q\,, \tag{3.16}$$

where $\Gamma(P,\delta)$ is the subarc of Γ of length 2δ with the mid point P. Let us denote the integral operator

$$\mathcal{H}_{k,\alpha}\varphi(P) = 2\int_\Gamma \varphi(Q)\,\partial_{t(Q)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q = -\mathcal{S}_{k,\alpha}\big(\partial_t\varphi\big)(P)\,, \quad P\notin\Sigma\,,$$

which satisfies for $P\in\Sigma$ the relation

$$(\mathcal{H}_{k,\alpha}\varphi)^+(P) = (\mathcal{H}_{k,\alpha}\varphi)^-(P) = H_{k,\alpha}\varphi(P) = -V_{k,\alpha}\big(\partial_t\varphi\big)(P)\,, \tag{3.17}$$

with the singular integral operator $H_{k,\alpha}$ defined by (3.16). Finally, for $P\in\Sigma$ we also define the singular integral operator

$$J_{k,\alpha}\varphi(P) = 2\int_\Gamma \varphi(Q)\,\partial_{t(P)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q = \partial_t\big(V_{k,\alpha}\varphi\big)(P)\,. \tag{3.18}$$

Mapping properties of the boundary integral operators for the quasiperiodic Helmholtz equation in the function spaces $H^s_\alpha(\Gamma)$ have been studied in [16]. In particular, the operators

$$V_{k,\alpha}: H^{-1/2}_\alpha(\Gamma)\to H^{1/2}_\alpha(\Gamma),\ H_{k,\alpha},\, K_{k,\alpha}: H^{1/2}_\alpha(\Gamma)\to H^{1/2}_\alpha(\Gamma),\ J_{k,\alpha},\, L_{k,\alpha}: H^{-1/2}_\alpha(\Gamma)\to H^{-1/2}_\alpha(\Gamma)$$

are bounded, and $V_{k,\alpha}$, $H_{k,\alpha}$ and $J_{k,\alpha}$ are Fredholm operators with index 0.

The single layer potential operator $V_{k,\alpha}$ is invertible if and only if the homogeneous Dirichlet problems in the domains G_+ and G_-

$$\Delta u + k^2 u = 0\,, \quad u|_\Sigma = 0 \ \text{ and } u \text{ satisfies (3.7)}\,, \tag{3.19}$$

have only the trivial solution.

Remark 3.1. *Well-known sufficient conditions for the unique solvability of* (3.19) *in G_+ (and consequently in G_-) are*

– $\operatorname{Im} k^2 > 0$ *or* $\operatorname{Re} k^2 < 0$;

– *the profile curve Σ is non-overhanging, i.e. $n_y(Q)\le 0$ for all $Q\in\Sigma$.*

In the following we consider also equations with transposed operators. For the physical interpretation we need that their kernel functions satisfy a radiation condition similar to (3.7). To this end we introduce the bilinear form

$$[\varphi,\psi]_\Gamma = \int_\Gamma \varphi\,\psi\,d\sigma\,, \tag{3.20}$$

which extends to a duality between the spaces $H^s_\alpha(\Gamma)$ and $H^{-s}_{-\alpha}(\Gamma)$, see (3.6). Then, for bounded $A: H^s_\alpha(\Gamma)\to H^t_\alpha(\Gamma)$ the transposed A' with respect to (3.20) maps $H^{-t}_{-\alpha}(\Gamma)$ into $H^{-s}_{-\alpha}(\Gamma)$. From the relation

$$\Psi_{k,-\alpha}(P) = \Psi_{k,\alpha}(-P) \quad \text{for all } P\in\mathbb{R}^2$$

one easily concludes that the integral operators associated with $\Psi_{k,\alpha}$ and $\Psi_{k,-\alpha}$ are connected by

$$\big(V_{k,\alpha}\big)' = V_{k,-\alpha}\,,\ \big(K_{k,\alpha}\big)' = L_{k,-\alpha}\,,\ \big(H_{k,\alpha}\big)' = J_{k,-\alpha}\,. \tag{3.21}$$

3.3 Boundary integrals for the Laplacian

The mapping properties mentioned above follow from the close connection of the boundary integral operators on Γ with corresponding operators for the Laplacian on the simple closed curve

$$\widetilde{\Gamma} = \left\{ \mathrm{e}^{-Y(t)} \big(\cos X(t), \sin X(t) \big) : t \in [0,1] \right\}, \tag{3.22}$$

which is the image of Γ under the conformal mapping $\mathrm{e}^{i\zeta}$, $\zeta \in \mathbb{C}$. Note that $\widetilde{\Gamma}$ has the same smoothness as Γ and additionally, if Σ has corners, then the angles at corner points of Σ in G_+ and interior angles at the corresponding corner points of $\widetilde{\Gamma}$ coincide.

On $\widetilde{\Gamma}$ we consider boundary integral operators corresponding to the fundamental solution of the Laplacian $\gamma(x) = -\log|x|/2\pi$. The operators $\widetilde{V}$, $\widetilde{K}$, $\widetilde{L}$, $\widetilde{H}$, and $\widetilde{J}$ are defined as in (3.10), (3.12), (3.14) (3.16), and (3.18) with Γ and $\Psi_{k,\alpha}$ replaced by $\widetilde{\Gamma}$ and γ, and n is the exterior normal to $\widetilde{\Gamma}$.

For completeness we give some properties of the operators in the energy spaces $H^{\pm 1/2}(\widetilde{\Gamma})$, where $H^s(\widetilde{\Gamma})$ denotes the usual Sobolev space over the close curve $\widetilde{\Gamma}$ (cf. [8]): The operators $\widetilde{V} : H^{-1/2}(\widetilde{\Gamma}) \to H^{1/2}(\widetilde{\Gamma})$, and $\widetilde{K}, \widetilde{H} : H^{1/2}(\widetilde{\Gamma}) \to H^{1/2}(\widetilde{\Gamma})$ are bounded. With respect to the L_2-duality the operators $\widetilde{L}$ and $\widetilde{J}$ are the adjoints of $\widetilde{K}$ and $\widetilde{H}$, respectively, i.e. $\widetilde{L} = \widetilde{K}'$, $\widetilde{J} = \widetilde{H}'$, whereas $\widetilde{V}$ is symmetric. Denote by $\mathcal{C}$ the set of constant functions and by $\widetilde{I}$ the identity operator on $\widetilde{\Gamma}$. Then $\ker(\widetilde{I} + \widetilde{K}) = \ker H = \mathcal{C}$. Moreover, the operator $\widetilde{I} - \widetilde{K}$ is invertible, $\widetilde{V}$ and $\widetilde{H} = -\widetilde{V}\partial_t$ are Fredholm operators with index 0. Among the interesting relations between the integral operators we mention

$$\widetilde{V}\widetilde{K}' = \widetilde{K}\widetilde{V}\,, \quad \widetilde{H}\widetilde{V} = -\widetilde{V}\widetilde{H}'\,, \quad \widetilde{H}\widetilde{K} = -\widetilde{K}\widetilde{H}\,, \quad \widetilde{K}^2 - \widetilde{H}^2 = \widetilde{I}\,. \tag{3.23}$$

The last two equations follow from the representation

$$\frac{1}{\pi i} \int_{\widetilde{\Gamma}} \frac{\varphi(t)dt}{t - (x+iy)} = -\widetilde{K}\varphi(x,y) + i\widetilde{H}\varphi(x,y) \quad \text{for } (x,y) \in \widetilde{\Gamma}\,,$$

of the Cauchy singular integral, see [11].

Defining the isomorphisms $M : H^s_\alpha(\Gamma) \to H^s_\alpha(\Gamma)$ and $\vartheta^*_\alpha : H^s(\widetilde{\Gamma}) \to H^s_\alpha(\Gamma)$ by

$$M\varphi(P) = \mathrm{e}^{Y} \varphi(P)\,, \quad \vartheta^*_\alpha \varphi(P) = \mathrm{e}^{i\alpha X} \varphi(\vartheta(P))\,, \quad P = (X,Y) \in \Gamma$$

where $\vartheta : \Gamma \ni P = (X,Y) \to \mathrm{e}^{-Y}(\cos X, \sin X) \in \widetilde{\Gamma}$, one can show by using the asymptotics of the fundamental solution $\Psi_{k,\alpha}$ that the differences

$$\begin{aligned} V_{k,\alpha} - \vartheta^*_\alpha \widetilde{V} (\vartheta^*_\alpha)^{-1} M &: H^{-1/2}_\alpha(\Gamma) \to H^{1/2}_\alpha(\Gamma)\,, \\ X_{k,\alpha} - \vartheta^*_\alpha \widetilde{X} (\vartheta^*_\alpha)^{-1} &: H^{1/2}_\alpha(\Gamma) \to H^{1/2}_\alpha(\Gamma)\,, \\ Y_{k,\alpha} - M^{-1}\vartheta^*_\alpha \widetilde{Y} (\vartheta^*_\alpha)^{-1} M &: H^{-1/2}_\alpha(\Gamma) \to H^{-1/2}_\alpha(\Gamma)\,, \end{aligned} \tag{3.24}$$

are compact operators, where X stands for K or H and Y for L or J.

4 Integral formulation

Here we derive the system of integral equations for conical diffraction in the case of one surface and study the equivalence to the electromagnetic formulation.

4.1 Integral equation

Denoting the components of the total fields

$$E_z = \begin{cases} u_+ + E^i_z \\ u_- \end{cases}, \quad B_z = \begin{cases} v_+ + B^i_z & \text{in } G_+, \\ v_- & \text{in } G_-\,. \end{cases}$$

the transmission problem described in Subsection 2.2 can be formulated as follows. We seek H^1-regular α-quasiperiodic functions $u_\pm, v_\pm$ such that

$$\Delta u_\pm + \omega^2 \kappa_\pm^2 u_\pm = \Delta v_\pm + \omega^2 \kappa_\pm^2 v_\pm = 0 \quad \text{in } G_\pm, \tag{4.1}$$

subject to the transmission conditions on Σ

$$
\begin{aligned}
u_- &= u_+ + E_z^i, \quad \frac{\varepsilon_-\,\partial_n u_-}{\kappa_-^2} - \frac{\varepsilon_+\partial_n(u_+ + E_z^i)}{\kappa_+^2} = \varepsilon_+ \sin\phi\Big(\frac{1}{\kappa_+^2} - \frac{1}{\kappa_-^2}\Big)\partial_t v_-, \\
v_- &= v_+ + B_z^i, \quad \frac{\mu_-\partial_n v_-}{\kappa_-^2} - \frac{\mu_+\partial_n(v_+ + B_z^i)}{\kappa_+^2} = -\mu_+ \sin\phi\Big(\frac{1}{\kappa_+^2} - \frac{1}{\kappa_-^2}\Big)\partial_t u_-,
\end{aligned}
\tag{4.2}
$$

and satisfying the outgoing wave condition

$$
\begin{aligned}
(u_+, v_+)(x,y) &= \sum_{n=-\infty}^{\infty} (u_n^+, v_n^+)\, \mathrm{e}^{i(\alpha_n x + \beta_n^+ y)} \qquad \text{for } y \geq H, \\
(u_-, v_-)(x,y) &= \sum_{n=-\infty}^{\infty} (u_n^-, v_n^-)\, \mathrm{e}^{i(\alpha_n x - \beta_n^- y)} \qquad \text{for } y \leq -H,
\end{aligned}
\tag{4.3}
$$

with α_n and $\beta_n^\pm$ given in (2.15) and $u_n^\pm, v_n^\pm \in \mathbb{C}$.

There exist different ways to transform (4.1) - (4.3) to integral equations. We combine here the direct and indirect approach as proposed in [10, 13] for the case of classical diffraction ($\phi = 0$).

In order to represent $u_\pm$ and $v_\pm$ as layer potentials we assume in what follows that the parameters are such that $\beta_n^\pm \neq 0$ for all n. Since $\arg \kappa_- \in [0, \pi)$ (see (2.16)) the boundary integral operators corresponding to the fundamental solution $\Psi_{\omega\kappa_\pm,\alpha}$ are well defined and by (3.8), (3.9) we can write

$$
\begin{aligned}
u_+ &= \frac{1}{2}\big(\mathcal{S}_\alpha^+\partial_n u_+ - \mathcal{D}_\alpha^+ u_+\big), \qquad v_+ = \frac{1}{2}\big(\mathcal{S}_\alpha^+\partial_n v_+ - \mathcal{D}_\alpha^+ v_+\big) \qquad \text{in } G_+\,, \\
E_z^i &= \frac{1}{2}\big(\mathcal{D}_\alpha^+ E_z^i - \mathcal{S}_\alpha^+\partial_n E_z^i\big), \qquad B_z^i = \frac{1}{2}\big(\mathcal{D}_\alpha^+ B_z^i - \mathcal{S}_\alpha^+\partial_n B_z^i\big) \qquad \text{in } G_-\,.
\end{aligned}
$$

Here we denote by $\mathcal{S}_\alpha^\pm$ the single layer potential defined on Γ with the fundamental solution $\Psi_{\omega\kappa_\pm,\alpha}$. Correspondingly $\mathcal{D}_\alpha^\pm$ is the double layer potential over Γ with the normal derivative of $\Psi_{\omega\kappa_\pm,\alpha}$ as kernel function. Taking the limits on Σ the jump relations (3.11) lead to

$$
\begin{aligned}
V_\alpha^+\partial_n(u_+ + E_z^i) - \big(I + K_\alpha^+\big)\,(u_+ + E_z^i) &= 2E_z^i|_\Sigma\,, \\
V_\alpha^+\partial_n(v_+ + B_z^i) - \big(I + K_\alpha^+\big)\,(v_+ + B_z^i) &= 2B_z^i|_\Sigma\,,
\end{aligned}
\tag{4.4}
$$

where $V_\alpha^\pm$ denote the single layer potential operators

$$
V_\alpha^\pm\varphi(P) = 2\int_\Gamma \varphi(Q)\,\Psi_{\omega\kappa_\pm,\alpha}(P-Q)\,d\sigma_Q\,, \quad P \in \Sigma\,,
\tag{4.5}
$$

and the operators $K_\alpha^\pm$ and $L_\alpha^\pm$ are defined analogously.

The solutions in G_- are sought as single layer potentials

$$
u_- = \mathcal{S}_\alpha^- w\,, \quad v_- = \mathcal{S}_\alpha^-\tau
\tag{4.6}
$$

with certain auxiliary densities $w, \tau \in H_\alpha^{-1/2}(\Gamma)$. Since by (3.13)

$$
u_-|_\Sigma = V_\alpha^- w,\ \partial_n u_-|_\Sigma = (L_\alpha^- - I)w, \quad v_-|_\Sigma = V_\alpha^-\tau,\ \partial_n v_-|_\Sigma = (L_\alpha^- - I)\tau,
$$

we see from (4.4) that the transmission conditions (4.2) are valid, when the unknows w, τ satisfy the equations

$$
\begin{aligned}
&\frac{\varepsilon_-\kappa_+^2}{\varepsilon_+\kappa_-^2}V_\alpha^+(L_\alpha^- - I)w - \big(I + K_\alpha^+\big)\,V_\alpha^- w - \sin\phi\Big(1 - \frac{\kappa_+^2}{\kappa_-^2}\Big)V_\alpha^+\partial_t V_\alpha^-\tau = 2E_z^i, \\
&\frac{\mu_-\kappa_+^2}{\mu_+\kappa_-^2}V_\alpha^+(L_\alpha^- - I)\tau - \big(I + K_\alpha^+\big)\,V_\alpha^-\tau + \sin\phi\Big(1 - \frac{\kappa_+^2}{\kappa_-^2}\Big)V_\alpha^+\partial_t V_\alpha^- w = 2B_z^i.
\end{aligned}
$$

Noting $V_\alpha^+\partial_t = -H_\alpha^+$ (see (3.17)) and introducing the coefficients

$$
a = \frac{\varepsilon_-\kappa_+^2}{\varepsilon_+\kappa_-^2}\,,\ b = \frac{\mu_-\kappa_+^2}{\mu_+\kappa_-^2}\,,\ c = \sin\phi\Big(1 - \frac{\kappa_+^2}{\kappa_-^2}\Big),
\tag{4.7}
$$

we obtain the system of singular integral equations on Γ

$$\mathcal{A}\begin{pmatrix} w \\ \tau \end{pmatrix} = -2\begin{pmatrix} E_z^i \\ B_z^i \end{pmatrix} \tag{4.8}$$

with the operator matrix

$$\mathcal{A} = \begin{pmatrix} (I+K_\alpha^+)V_\alpha^- + aV_\alpha^+(I-L_\alpha^-) & -c\,H_\alpha^+V_\alpha^- \\ c\,H_\alpha^+V_\alpha^- & (I+K_\alpha^+)V_\alpha^- + b\,V_\alpha^+(I-L_\alpha^-) \end{pmatrix}. \tag{4.9}$$

Recall that we have assumed (2.16), $\kappa_-^2 \neq 0$ and $\omega^2\kappa_\pm^2 - \alpha_n^2 \neq 0$ for all n, which implies that $\mathcal{A}$ maps $\big(H_\alpha^{-1/2}(\Gamma)\big)^2$ boundedly into $\big(H_\alpha^{1/2}(\Gamma)\big)^2$.

4.2 Equivalence

It is evident from (4.6) that any solution of (4.1) - (4.3) provides a solution of the integral equations (4.8) if the operator V_α^- is invertible.

Lemma 4.1. *Let $w,\tau \in H_\alpha^{-1/2}(\Gamma)$ be a solution of* (4.8) *and assume* $\ker V_\alpha^+ = \{0\}$*. Then the functions*

$$\begin{aligned} u_+ &= \frac{1}{2}\left(a\,\mathcal{S}_\alpha^+(L_\alpha^- - I)w - \mathcal{D}_\alpha^+V_\alpha^- w + c\,\mathcal{H}_\alpha^+V_\alpha^-\tau\right), \\ v_+ &= -\frac{1}{2}\left(c\,\mathcal{H}_\alpha^+V_\alpha^- w + b\,\mathcal{S}_\alpha^+(L_\alpha^- - I)\tau + \mathcal{D}_\alpha^+V_\alpha^-\tau\right), \end{aligned} \tag{4.10}$$

with the coefficients a, b, c given by (4.7) *and*

$$u_- = \mathcal{S}_\alpha^- w\,,\ v_- = \mathcal{S}_\alpha^-\tau\,, \tag{4.11}$$

are a solution of the transmission problem (4.1) - (4.3).

Proof. For any densities $w,\tau \in H_\alpha^{-1/2}(\Gamma)$ the single layer potentials u_-, v_- are quasi-periodic solutions of $\Delta u + \omega^2\kappa_-^2 u = 0$ in G_- and satisfy the outgoing wave condition (4.3). Moreover, since $u_-|_\Gamma, v_-|_\Gamma \in H_\alpha^{1/2}(\Gamma)$, $\partial_n u_-, \partial_n v_- \in H_\alpha^{-1/2}(\Gamma)$, the functions

$$\begin{aligned} u_+ &= \frac{1}{2}\left(\mathcal{S}_\alpha^+\Big(a\,\partial_n u_- - c\,\partial_t v_-\Big) - \mathcal{D}_\alpha^+ u_-\right), \\ v_+ &= \frac{1}{2}\left(\mathcal{S}_\alpha^+\Big(b\,\partial_n v_- + c\,\partial_t u_-\Big) - \mathcal{D}_\alpha^+ v_-\right) \end{aligned} \tag{4.12}$$

are H^1 regular solutions of $\Delta u + \omega^2\kappa_+^2 u = 0$ in G_+, satisfy (4.3) and have the boundary values

$$\begin{aligned} u_+|_\Gamma &= \frac{1}{2}\left(V_\alpha^+\Big(a\,\partial_n u_- - c\,\partial_t v_-\Big) + (I - K_\alpha^+)u_-\right), \\ v_+|_\Gamma &= \frac{1}{2}\left(V_\alpha^+\Big(b\,\partial_n v_- + c\,\partial_t u_-\Big) + (I - K_\alpha^+)v_-\right). \end{aligned}$$

Since $\partial_n u_-|_\Gamma = (L_\alpha^+ - I)w$, $H_\alpha^+V_\alpha^- w = -V_\alpha^+\,\partial_t u_-$, and w,τ satisfy (4.8), it follows that

$$\begin{aligned} a\,V_\alpha^+\partial_n u_- + (I-K_\alpha^+)u_- - c\,V_\alpha^+\partial_t v_- &= 2(u_- - E_z^i)|_\Gamma\,. \\ b\,V_\alpha^+\partial_n v_- - (I-K_\alpha^+)v_- + c\,V_\alpha^+\partial_t u_- &= 2(v_- - B_z^i)|_\Gamma\,. \end{aligned}$$

This gives $u_+ + E_z^i = u_-$ and $v_+ + B_z^i = v_-$ on Σ. Since by (3.8)

$$\mathcal{D}_\alpha^+ E_z^i = \mathcal{S}_\alpha^+\partial_n E_z^i\,, \quad \mathcal{D}_\alpha^+ B_z^i = \mathcal{S}_\alpha^+\partial_n B_z^i \quad \text{in } G_+\,,$$

formulas (4.12) transform to

$$\begin{aligned} u_+ &= \frac{1}{2}\left(\mathcal{S}_\alpha^+\Big(a\,\partial_n u_- - c\,\partial_t v_-\Big) - \mathcal{D}_\alpha^+ u_+ - \mathcal{S}_\alpha^+\partial_n E_z^i\right), \\ v_+ &= \frac{1}{2}\left(\mathcal{S}_\alpha^+\Big(b\,\partial_n v_- + c\,\partial_t u_-\Big) - \mathcal{D}_\alpha^+ v_+ - \mathcal{S}_\alpha^+\partial_n B_z^i\right). \end{aligned}$$

Again by (3.8) we obtain that in G_+

$$\begin{aligned} \mathcal{S}_\alpha^+\Big(a\,\partial_n u_- - c\,\partial_t v_-\Big) &= \mathcal{S}_\alpha^+\partial_n(u_+ + E_z^i). \\ \mathcal{S}_\alpha^+\Big(b\,\partial_n v_- + c\,\partial_t u_-\Big) &= \mathcal{S}_\alpha^+\partial_n(v_+ + B_z^i)\,, \end{aligned}$$

which shows that conditions (4.2) are satisfied if $\ker V_\alpha^+ = \{0\}$. □

5 Existence and Uniqueness of Solutions

Here we obtain conditions that the operator matrix $\mathcal{A}$ defined by (4.9) is a Fredholm mapping with index 0. Then we show that the system (4.8) is always solvable and describe cases where the solution is unique. For the following we denote by $\Phi_0(X)$ the set of bounded Fredholm operators of index 0 in the space X.

5.1 Fredholmness

Theorem 5.1. *The matrix* $\mathcal{A} : \big(H_\alpha^{-1/2}(\Gamma)\big)^2 \to \big(H_\alpha^{1/2}(\Gamma)\big)^2$ *is a Fredholm operator with index* 0 *if*

$$(\varepsilon_+ + \varepsilon_-)\widetilde{I} + (\varepsilon_+ - \varepsilon_-)\widetilde{K}\,,\ (\mu_+ + \mu_-)\widetilde{I} + (\mu_+ - \mu_-)\widetilde{K} \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma})\big). \tag{5.1}$$

Here $\widetilde{K}$ is the double layer logarithmic potential on the closed curve $\widetilde{\Gamma}$ introduced in 3.3. Note that for sufficiently smooth $\widetilde{\Gamma}$, for example C^2, the operator $\widetilde{K}$ is compact in $H^{1/2}(\widetilde{\Gamma})$. Hence, if the profile curve Σ is sufficiently smooth, then the operator matrix $\mathcal{A}$ is Fredholm with index 0 if $\varepsilon_- \neq -\varepsilon_+$ and $\mu_- \neq -\mu_+$.

The study of Fredholm properties of the operator $\lambda\widetilde{I} + \widetilde{K}$ on non-smooth curves $\widetilde{\Gamma}$ has a long history. A excellent overview is given in [9, §4.1], where also higher dimensional cases and double layer potentials of other equations are discussed. Unfortunately, the results on the essential spectrum and Fredholm domain of double layer potentials cannot be applied directly, since they were obtained mainly for (weighted) spaces of continuous and Hölder-continuous functions and L_p spaces. But due to the relations (3.23) it is simple to get conditions in the "energy" space $H^{1/2}(\widetilde{\Gamma})$, which are sufficient for the Fredholmness of $\mathcal{A}$.

Lemma 5.1. *For any* $\lambda \notin (-1, 1)$ *the operator* $\lambda\widetilde{I} + \widetilde{K} \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma})\big)$.

This result for space dimension $n \geq 3$ and Lipschitz domains was proved in [3]. For $n = 2$ one needs a slight modification of the proof due to the fact that the gradient of the single layer logarithmic potential does not belong to $L_2(\mathbb{R}^2)$. This holds however for the gradient of the double layer logarithmic potential, which gives together with the application of Thm. 12 in [9, Chapter 1] that in the quotient space over the constants $H^{1/2}(\widetilde{\Gamma}) / \mathcal{C}$ the induced operator $\lambda\widetilde{I} + \widetilde{K}$ is invertible if $\lambda \notin [-1, 1]$.

Thus, if the grating profile Σ has corners, then by Lemma 5.1 the matrix $\mathcal{A}$ is Fredholm with index 0 for $\varepsilon_-, \mu_- \notin (-\infty, 0]$. It should be noted however, that for piecewise C^2 curves one could expect the existence of $\rho < 1$ depending on the angles of $\widetilde{\Gamma}$, such that $\lambda\widetilde{I} + \widetilde{K} \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma})\big)$ if $\lambda \notin (-\rho, \rho)$. For example, in the space $C(\widetilde{\Gamma})$ the parameter ρ is equal to $\max|\pi - \alpha_s|/\pi$, where the maximum is taken over all interior angles α_s of $\widetilde{\Gamma}$, but for Sobolev spaces the answer is unknown.

The proof of Theorem 5.1 follows from Lemmas 5.2, 5.3 and 5.4 given below. As in 3.3 we associate to $\mathcal{A}$ boundary integral operators for the Laplacian, more precisely, we consider the 2×2 matrix

$$\widetilde{\mathcal{A}} = \begin{pmatrix} (\widetilde{I} + \widetilde{K})\widetilde{V} + a\widetilde{V}(\widetilde{I} - \widetilde{L}) & -c\,\widetilde{H}\widetilde{V} \\ c\,\widetilde{H}\widetilde{V} & (\widetilde{I} + \widetilde{K})\widetilde{V} + b\,\widetilde{V}(\widetilde{I} - \widetilde{L}) \end{pmatrix}$$

with the coefficients a, b and c given by (4.7). From (3.24) and (4.9) it follows immediately that the difference

$$\mathcal{A} - \begin{pmatrix} \vartheta_\alpha^* & 0 \\ 0 & \vartheta_\alpha^* \end{pmatrix} \widetilde{\mathcal{A}} \begin{pmatrix} (\vartheta_\alpha^*)^{-1}M & 0 \\ 0 & (\vartheta_\alpha^*)^{-1}M \end{pmatrix} : \big(H_\alpha^{-1/2}(\Gamma)\big)^2 \to \big(H_\alpha^{1/2}(\Gamma)\big)^2$$

is compact, which provides

Lemma 5.2. $\mathcal{A} : \big(H_\alpha^{-1/2}(\Gamma)\big)^2 \to \big(H_\alpha^{1/2}(\Gamma)\big)^2$ *is Fredholm if and only if* $\widetilde{\mathcal{A}} : \big(H^{-1/2}(\widetilde{\Gamma})\big)^2 \to \big(H^{1/2}(\widetilde{\Gamma})\big)^2$ *is Fredholm and* $\operatorname{ind}\mathcal{A} = \operatorname{ind}\widetilde{\mathcal{A}}$.

By using the relation $\widetilde{K}\widetilde{V} = \widetilde{V}\widetilde{L}$ we can write

$$\widetilde{\mathcal{A}} = \widetilde{\mathcal{A}}_0 \begin{pmatrix} \widetilde{V} & 0 \\ 0 & \widetilde{V} \end{pmatrix} \quad \text{with} \quad \widetilde{\mathcal{A}}_0 = \begin{pmatrix} (1+a)\widetilde{I} + (1-a)\widetilde{K} & -c\,\widetilde{H} \\ c\,\widetilde{H} & (1+b)\widetilde{I} + (1-b)\widetilde{K} \end{pmatrix}.$$

The single layer logarithmic potential $\widetilde{V} : H^{-1/2}(\widetilde{\Gamma}) \to H^{1/2}(\widetilde{\Gamma})$ is Fredholm with index 0, hence it remains to study Fredholm properties of $\widetilde{\mathcal{A}}_0$.

Lemma 5.3. *Let* $c = \sin\phi\,(1 - \kappa_+^2/\kappa_-^2) = 0$. *Then* $\widetilde{\mathcal{A}}_0 \in \Phi_0\big(\big(H^{1/2}(\widetilde{\Gamma})\big)^2\big)$ *if condition* (5.1) *holds.*

Proof. $\widetilde{\mathcal{A}}_0$ is diagonal and therefore Fredholm with index 0 if and only if

$$(1+a)\widetilde{I}+(1-a)\widetilde{K}\,,\ (1+b)\widetilde{I}+(1-b)\widetilde{K}\in\Phi_0\big(H^{1/2}(\widetilde{\Gamma})\big)\,.$$

This is (5.1) when $\kappa_+^2=\kappa_-^2$. If otherwise $\phi=0$, then

$$a=\frac{\mu_+}{\mu_-}\,,\ b=\frac{\varepsilon_+}{\varepsilon_-}\,,$$

and (5.1) follows from the simple observation that $\widetilde{I}+\lambda\widetilde{K}\in\Phi_0\big(H^{1/2}(\widetilde{\Gamma})\big)$ implies $\widetilde{I}-\lambda\widetilde{K}\in\Phi_0\big(H^{1/2}(\widetilde{\Gamma})\big)$, which is due to $\widetilde{K}\widetilde{H}=-\widetilde{H}\widetilde{K}$, see (3.23). □

Lemma 5.4. *The assertion of Lemma* 5.3 *is also valid in the case* $c\neq 0$.

Proof. Since the relation $A\in\Phi_0(X)$ is equivalent to the existence of a compact perturbation T such that $A+T$ is invertible in X, we can apply a method to check the invertibility of operator matrices.

It is easy to see that the operator $\widetilde{H}_1=\widetilde{H}+\mathrm{j}$ with the rank 1 operator

$$\mathrm{j}u=(u,e)_{L_2(\widetilde{\Gamma})}\,e\,,\qquad e=1\in\mathcal{C}\,,$$

is invertible in $H^{1/2}(\widetilde{\Gamma})$. Instead of $\widetilde{\mathcal{A}}_0$ we consider the perturbed matrix

$$\widetilde{\mathcal{A}}_1=\begin{pmatrix}(1+a)\widetilde{I}+(1-a)\widetilde{K} & -c\,\widetilde{H}_1\\ c\,\widetilde{H}_1 & (1+b)\widetilde{I}+(1-b)\widetilde{K}\end{pmatrix}.$$

with invertible off-diagonal elements. Using the abbreviation

$$A_\pm=(1+a)\widetilde{I}\pm(1-a)\widetilde{K}\,,\quad B_\pm=(1+b)\widetilde{I}\pm(1-b)\widetilde{K}\,,$$

we transform

$$\begin{aligned}\widetilde{\mathcal{A}}_1&=\begin{pmatrix}A_+ & -c\,\widetilde{H}_1\\ c\,\widetilde{H}_1 & B_+\end{pmatrix}\begin{pmatrix}-(c\,\widetilde{H}_1)^{-1}B_+ & \widetilde{I}\\ \widetilde{I} & 0\end{pmatrix}\begin{pmatrix}0 & \widetilde{I}\\ I & (c\,\widetilde{H}_1)^{-1}B_+\end{pmatrix}\\ &=\begin{pmatrix}-A_+(c\,\widetilde{H}_1)^{-1}B_+-c\,\widetilde{H}_1 & A_+\\ 0 & c\,\widetilde{H}_1\end{pmatrix}\begin{pmatrix}0 & \widetilde{I}\\ \widetilde{I} & (c\,\widetilde{H}_1)^{-1}B_+\end{pmatrix}.\end{aligned}$$

Now the relation $\widetilde{H}\widetilde{K}=-\widetilde{K}\widetilde{H}$ implies

$$\widetilde{H}_1A_+=A_-\widetilde{H}_1+(1-a)\,\mathrm{j}\,(\widetilde{K}-\widetilde{I})\,,$$

and therefore we get

$$\widetilde{\mathcal{A}}_1=\begin{pmatrix}-(c\,\widetilde{H}_1)^{-1}\big(A_-B_++(c\,\widetilde{H}_1)^2\big)+\mathrm{j}_1 & A_+\\ 0 & c\,\widetilde{H}_1\end{pmatrix}\begin{pmatrix}0 & \widetilde{I}\\ \widetilde{I} & (c\,\widetilde{H}_1)^{-1}B_+\end{pmatrix}$$

with another rank 1 operator j_1. Hence, $\widetilde{\mathcal{A}}_1$ is Fredholm with index 0 if this is true for $A_-B_++(c\,\widetilde{H}_1)^2$, and consequently for

$$A_-B_++c^2\widetilde{H}^2=\big((1+a)(1+b)-c^2\big)\widetilde{I}+2(a-b)\widetilde{K}-\big((1-a)(1-b)-c^2\big)\widetilde{K}^2\,,$$

where we make use of $\widetilde{H}^2=\widetilde{K}^2-\widetilde{I}$. Now (4.7), (2.9) and simple computations give

$$\begin{aligned}(1+a)(1+b)-c^2&=\frac{1}{\varepsilon_+\mu_+\kappa_-^4}\Big(\kappa_+^2\kappa_-^2(\varepsilon_+\mu_-+\varepsilon_-\mu_++2\varepsilon_+\mu_+\sin^2\phi)\\ &\qquad+(\varepsilon_+\mu_+-\varepsilon_+\mu_+\sin^2\phi)\kappa_-^4+(\varepsilon_-\mu_--\varepsilon_+\mu_+\sin^2\phi)\kappa_+^4\Big)\\ &=\frac{\kappa_+^2}{\varepsilon_+\mu_+\kappa_-^2}\big(\varepsilon_++\varepsilon_-\big)\big(\mu_++\mu_-\big)\,,\\ (1-a)(1-b)-c^2&=\frac{\kappa_+^2}{\varepsilon_+\mu_+\kappa_-^2}\big(\varepsilon_+-\varepsilon_-\big)\big(\mu_+-\mu_-\big)\,,\\ a-b&=\frac{\kappa_+^2}{\varepsilon_+\mu_+\kappa_-^2}\big(\varepsilon_-\mu_+-\varepsilon_+\mu_-\big).\end{aligned}$$

Thus we get the explicit representation

$$A_-B_++c^2\widetilde{H}^2=\frac{\kappa_+^2}{\varepsilon_+\mu_+\kappa_-^2}\big((\varepsilon_++\varepsilon_-)\widetilde{I}-(\varepsilon_+-\varepsilon_-)\widetilde{K}\big)\big((\mu_++\mu_-)\widetilde{I}+(\mu_+-\mu_+)\widetilde{K}\big),$$

which completes the proof. □

5.2 Uniqueness

Theorem 5.2. *Assume* $\operatorname{Im}\varepsilon_- \geq 0$ *and* $\operatorname{Im}\mu_- \geq 0$ *with* $\operatorname{Im}(\varepsilon_- + \mu_-) > 0$*, which implies that* $\arg\kappa_-^2 \in (0, 2\pi)$*. If* $\ker V_\alpha^+ = \{0\}$ *and* $\arg\kappa_-^2 \in (0, 3\pi/2)$*, then the system (4.8) has at most one solution. The assertion is valid also in the case* $\arg\kappa_-^2 \in [3\pi/2, 2\pi)$ *if additionally* $\ker V_\alpha^- = \{0\}$.

Proof. Let w, τ be a solution of (4.8) with the right-hand side $E_z^i = B_z^i = 0$. Then in view of Lemma 4.1 the functions $u = u_\pm|_{G_\pm}$ and $v = v_\pm|_{G_\pm}$, given by (4.10) and (4.11), satisfy (4.1), (4.3) and the transmission condition

$$\Big[\frac{\varepsilon}{\varepsilon_+\kappa^2}\,\partial_n u + \frac{\sin\phi}{\kappa^2}\,\partial_t v\Big]_\Sigma = \Big[\frac{\mu}{\mu_+\kappa^2}\,\partial_n v - \frac{\sin\phi}{\kappa^2}\,\partial_t u\Big]_\Sigma = 0\,. \tag{5.2}$$

Our aim is to obtain a variational equality for u and v in a periodic cell Ω_H, which has in x-direction the width d, is bounded by the straight lines $\{y = \pm H\}$ and contains Γ. We multiply the Helmholtz equations (4.1) respectively with

$$\frac{\varepsilon}{\varepsilon_+\kappa^2}\,\overline{u} \quad \text{and} \quad \frac{\mu}{\mu_+\kappa^2}\,\overline{v}\,,$$

and apply Green's formula in the subdomains $\Omega_H \cap G_\pm$. Then by using (5.2)

$$\int\limits_{\Omega_H} \frac{\varepsilon}{\varepsilon_+}\Big(\frac{1}{\kappa^2}|\nabla u|^2 - \omega^2\,|u|^2\Big) + \sin\phi\Big(\frac{1}{\kappa_+^2} - \frac{1}{\kappa_-^2}\Big)\int\limits_\Gamma \partial_t v\,\overline{u} - \frac{1}{\kappa_+^2}\int\limits_{\Gamma(H)} \partial_n u\,\overline{u} - \frac{\varepsilon_-}{\varepsilon_+\kappa_-^2}\int\limits_{\Gamma(-H)} \partial_n u\,\overline{u} = 0\,, \tag{5.3}$$

$$\int\limits_{\Omega_H} \frac{\mu}{\mu_+}\Big(\frac{1}{\kappa^2}|\nabla v|^2 - \omega^2\,|v|^2\Big) - \sin\phi\Big(\frac{1}{\kappa_+^2} - \frac{1}{\kappa_-^2}\Big)\int\limits_\Gamma \partial_t u\,\overline{v} - \frac{1}{\kappa_+^2}\int\limits_{\Gamma(H)} \partial_n v\,\overline{v} - \frac{\mu_-}{\mu_+\kappa_-^2}\int\limits_{\Gamma(-H)} \partial_n v\,\overline{v} = 0\,, \tag{5.4}$$

where $\Gamma(\pm H)$ denotes the upper resp. lower straight boundary of Ω_H. Using the notation $\nabla^\perp = (\partial_y, -\partial_x)$ and Green's formula the integral over Γ equals

$$\int\limits_\Gamma \partial_t v\,\overline{u} = \int\limits_{\Gamma(\pm H)} \partial_x v\,\overline{u} \mp \int\limits_{\Omega_H\cap G_\pm} \nabla v\cdot\nabla^\perp\overline{u}\,,$$

and (4.3) gives

$$\int\limits_{\Gamma(\pm H)} \partial_n u\,\overline{u} = i\sum_{n\in\mathbb{Z}} \beta_n^\pm |u_n^\pm|^2\;\mathrm{e}^{-2H\operatorname{Im}\beta_n^\pm}\,, \qquad \int\limits_{\Gamma(\pm H)} \partial_x v\,\overline{u} = i\sum_{n\in\mathbb{Z}} \alpha_n v_n^\pm\,\overline{u_n^\pm}\;\mathrm{e}^{-2H\operatorname{Im}\beta_n^\pm}\,.$$

Hence (5.3) and (5.4) can be rewritten in the form

$$\begin{aligned}
&\int\limits_{\Omega_H} \Big(\frac{\varepsilon}{\varepsilon_+\kappa^2}|\nabla u|^2 - \frac{\sin\phi}{\kappa^2}\nabla v\cdot\nabla^\perp\overline{u} - \frac{\omega^2\varepsilon}{\varepsilon_+}\,|u|^2\Big)\\
&= \frac{i}{\kappa_+^2}\sum_{n\in\mathbb{Z}}\Big(\beta_n^+ u_n^+ - \alpha_n\sin\phi\, v_n^+\Big)\overline{u_n^+}\;\mathrm{e}^{-2H\operatorname{Im}\beta_n^+} + \frac{i}{\kappa_-^2}\sum_{n\in\mathbb{Z}}\Big(\frac{\varepsilon_-\beta_n^-}{\varepsilon_+}\,u_n^- - \alpha_n\sin\phi\, v_n^-\Big)\overline{u_n^-}\;\mathrm{e}^{-2H\operatorname{Im}\beta_n^-}\,,\\
&\int\limits_{\Omega_H} \Big(\frac{\mu}{\mu_+\kappa^2}|\nabla v|^2 + \frac{\sin\phi}{\kappa^2}\nabla u\cdot\nabla^\perp\overline{v} - \frac{\omega^2\mu}{\mu_+}\,|v|^2\Big)\\
&= \frac{i}{\kappa_+^2}\sum_{n\in\mathbb{Z}}\Big(\beta_n^+ v_n^+ + \alpha_n\sin\phi\, u_n^+\Big)\overline{v_n^+}\;\mathrm{e}^{-2H\operatorname{Im}\beta_n^+} + \frac{i}{\kappa_-^2}\sum_{n\in\mathbb{Z}}\Big(\frac{\mu_-\beta_n^-}{\mu_+}\,v_n^- + \alpha_n\sin\phi\, u_n^-\Big)\overline{v_n^-}\;\mathrm{e}^{-2H\operatorname{Im}\beta_n^-}\,.
\end{aligned} \tag{5.5}$$

To write the quadratic forms in (5.5) more compactly we introduce the 4×4 matrix B and the vector U

$$B = \frac{1}{\kappa^2}\begin{pmatrix} \varepsilon/\varepsilon_+ & 0 & 0 & -\sin\phi \\ 0 & \mu/\mu_+ & \sin\phi & 0 \\ 0 & \sin\phi & \varepsilon/\varepsilon_+ & 0 \\ -\sin\phi & 0 & 0 & \mu/\mu_+ \end{pmatrix}, \quad U = \begin{pmatrix} \partial_x u \\ \partial_x v \\ \partial_y u \\ \partial_y v \end{pmatrix},$$

which allow to write the left of (5.5) in the form

$$\int\limits_{\Omega_H} \Big(BU\cdot\overline{U} - \frac{\omega^2\varepsilon}{\varepsilon_+}\,|u|^2 - \frac{\omega^2\mu}{\mu_+}\,|v|^2\Big).$$

Noting that $\operatorname{Im}\beta_n^- > 0$ for all n and $\operatorname{Im}\beta_n^+ > 0$ for almost all n we see that, if $H \to \infty$, then the right-hand side of (5.5) tends to

$$\sum_{\beta_n^+ \geq 0} M_n \begin{pmatrix} u_n^+ \\ v_n^+ \end{pmatrix} \cdot \overline{\begin{pmatrix} u_n^+ \\ v_n^+ \end{pmatrix}}, \quad \text{where } M_n = \frac{i}{\kappa_+^2} \begin{pmatrix} \beta_n^+ & -\alpha_n \sin\phi \\ \alpha_n \sin\phi & \beta_n^+ \end{pmatrix}.$$

Hence (5.5) states that

$$\int_{\Omega_H} \Big(BU \cdot \overline{U} - \frac{\omega^2 \varepsilon}{\varepsilon_+} |u|^2 - \frac{\omega^2 \mu}{\mu_+} |v|^2 \Big) \longrightarrow \sum_{\beta_n^+ \geq 0} M_n \begin{pmatrix} u_n^+ \\ v_n^+ \end{pmatrix} \cdot \overline{\begin{pmatrix} u_n^+ \\ v_n^+ \end{pmatrix}}$$

when $H \to \infty$. Obviously, if $\beta_n^+ \geq 0$, then $\operatorname{Re}(iM_n) \leq 0$. On the other side, the assumption $\operatorname{Im}\varepsilon_-, \operatorname{Im}\mu_- \geq 0$ implies

$$\operatorname{Re}\Big(-i \int_{\Omega_H} \Big(\frac{\omega^2 \varepsilon}{\varepsilon_+} |u|^2 + \frac{\omega^2 \mu}{\mu_+} |v|^2 \Big) \Big) = \omega^2 \int_{\Omega_H \cap G_-} \Big(\frac{\operatorname{Im}\varepsilon_-}{\varepsilon_+} |u|^2 + \frac{\operatorname{Im}\mu_-}{\mu_+} |v|^2 \Big) \geq 0 ,$$

and in addition

$$\operatorname{Re} \int_{\Omega_H} i\, BU \cdot \overline{U} \geq 0 , \tag{5.6}$$

which can be shown similar to [4]. Taking the unitary matrix

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

where I denotes the 2×2 identity matrix, we obtain

$$i\mathcal{U}^{-1} B \mathcal{U} = \begin{pmatrix} N^+ & 0 \\ 0 & N^- \end{pmatrix}, \quad \text{where} \quad N^\pm = \frac{1}{\kappa^2} \begin{pmatrix} i\varepsilon/\varepsilon_+ & \pm \sin\phi \\ \mp \sin\phi & i\mu/\mu_+ \end{pmatrix}.$$

Introducing the differential operators

$$\partial^+ = \frac{1}{\sqrt{2}} (\partial_x - i\partial_y) , \quad \partial^- = \frac{1}{\sqrt{2}} (\partial_y - i\partial_x) ,$$

we get

$$\int_{\Omega_H} i\, BU \cdot \overline{U} = \int_{\Omega_H} \left(N^+ \partial^+ \begin{pmatrix} u \\ v \end{pmatrix} \cdot \overline{\partial^+ \begin{pmatrix} u \\ v \end{pmatrix}} + N^- \partial^- \begin{pmatrix} u \\ v \end{pmatrix} \cdot \overline{\partial^- \begin{pmatrix} u \\ v \end{pmatrix}} \right).$$

Note that $\operatorname{Re} N^\pm = 0$ in $\Omega_H \cap G_+$. Thus it remains to consider the real part of the matrices in G_-

$$\operatorname{Re} N^\pm = \begin{pmatrix} -\operatorname{Im} \dfrac{\varepsilon_-}{\varepsilon_+ \kappa_-^2} & \pm i \operatorname{Im} \dfrac{\sin\phi}{\kappa_-^2} \\ \mp i \operatorname{Im} \dfrac{\sin\phi}{\kappa_-^2} & -\operatorname{Im} \dfrac{\mu_-}{\mu_+ \kappa_-^2} \end{pmatrix},$$

which is nonnegative if and only if the inequalities

$$-\operatorname{Im} \frac{\varepsilon_-}{\kappa_-^2} \geq 0 \quad \text{and} \quad \operatorname{Im} \frac{\varepsilon_-}{\kappa_-^2} \operatorname{Im} \frac{\mu_-}{\kappa_-^2} - \varepsilon_+ \mu_+ \sin^2\phi \Big(\operatorname{Im} \frac{1}{\kappa_-^2} \Big)^2 \geq 0 \tag{5.7}$$

are valid. Let us denote $\phi_\varepsilon = \arg \varepsilon_-$, $\phi_\mu = \arg \mu_-$, $\phi_\kappa = \arg \kappa_-^2$. The assumptions

$$\phi_\varepsilon, \phi_\mu \in [0, \pi] \quad \text{and} \quad \phi_\kappa \in (0, 2\pi) ,$$

together with $\kappa_-^2 = \varepsilon_- \mu_- - \varepsilon_+ \mu_+ \sin^2\phi$ lead to $0 < \phi_\kappa - \phi_\varepsilon, \phi_\kappa - \phi_\mu \leq \pi$, which gives

$$-\operatorname{Im} \frac{\varepsilon_-}{\kappa_-^2} = \Big| \frac{\varepsilon_-}{\kappa_-^2} \Big| \sin(\phi_\kappa - \phi_\varepsilon) \geq 0.$$

Using

$$\operatorname{Im} \frac{\varepsilon_+ \mu_+ \sin^2 \phi}{\kappa_-^2} = \operatorname{Im} \frac{\varepsilon_- \mu_-}{\kappa_-^2} \,,$$

the second inequality in (5.7) is equivalent to

$$\sin(\phi_\varepsilon - \phi_\kappa) \sin(\phi_\mu - \phi_\kappa) + \sin(\phi_\varepsilon + \phi_\mu - \phi_\kappa) \sin \phi_\kappa = \sin \phi_\varepsilon \sin \phi_\mu \geq 0 \,,$$

which establishes (5.6).

Hence the solution u, v of the homogeneous problem satisfies

$$\int_{\Omega_H \cap G_-} \Big(\frac{\operatorname{Im} \varepsilon_-}{\varepsilon_+} \, |u|^2 + \frac{\operatorname{Im} \mu_-}{\mu_+} \, |v|^2 \Big) = 0 \,,$$

$$\int_{\Omega_H \cap G_-} \left(\operatorname{Re} N^+ \partial^+ \begin{pmatrix} u \\ v \end{pmatrix} \cdot \overline{\partial^+ \begin{pmatrix} u \\ v \end{pmatrix}} + \operatorname{Re} N^- \partial^- \begin{pmatrix} u \\ v \end{pmatrix} \cdot \overline{\partial^- \begin{pmatrix} u \\ v \end{pmatrix}} \right) = 0.$$

If $\operatorname{Im} \varepsilon_-, \operatorname{Im} \mu_- > 0$, then $u_- = v_- = 0$ in G_-. If otherwise, for example, $\operatorname{Im} \varepsilon_- = 0$, then $\sin \phi_\kappa \neq 0$ and $v_- = 0$. Hence

$$\int_{\Omega_H \cap G_-} \left(\operatorname{Re} N^+ \partial^+ \begin{pmatrix} u \\ 0 \end{pmatrix} \cdot \overline{\partial^+ \begin{pmatrix} u \\ 0 \end{pmatrix}} + \operatorname{Re} N^- \partial^- \begin{pmatrix} u \\ 0 \end{pmatrix} \cdot \overline{\partial^- \begin{pmatrix} u \\ 0 \end{pmatrix}} \right)$$
$$= -2 \operatorname{Im} \frac{\varepsilon_-}{\varepsilon_+ \kappa_-^2} \int_{\Omega_H \cap G_-} |\nabla u|^2 = \frac{2 \varepsilon_- \sin \phi_\kappa}{\varepsilon_+ |\kappa_-^2|} \int_{\Omega_H \cap G_-} |\nabla u|^2 = 0 \,,$$

and together with $\Delta u_- + \kappa_-^2 u_- = 0$ this implies $u_- = 0$. By (4.11) we get $w = \tau = 0$ if the single layer potential V_α^- with the fundamental solution $\Psi_{\omega\kappa_-,\alpha}$ is invertible. Due to Remark 3.1 this is always true if $\arg \kappa_-^2 \in (0, 3\pi/2)$. □

5.3 Existence of solutions

It follows from Theorem 5.1 that under (5.1) and the conditions of Theorem 5.2 the integral equation system (4.8) has a unique solution $w, \tau \in H_\alpha^{-1/2}(\Gamma)$. Moreover, due to Lemma 4.1 the functions $u_\pm$ and $v_\pm$ from (4.10), (4.11) are a solution of the diffraction problem (4.1) - (4.3), which is unique if $V_\alpha^- = \{0\}$ is invertible.

Let us consider the remaining case of real ε_- and μ_-, where $\mathcal{A}$ can possess a nontrivial kernel. To show that the right-hand side of (4.8) is in the range of $\mathcal{A}$ we define in accordance with (3.20) the bilinear form

$$\big[W, \Phi\big] = \big[w, \varphi\big]_\Gamma + \big[\tau, \psi\big]_\Gamma \tag{5.8}$$

for $W = (w, \tau) \in \big(H_\alpha^s(\Gamma)\big)^2$, $\Phi = (\varphi, \psi) \in \big(H_{-\alpha}^{-s}(\Gamma)\big)^2$. In view of (3.21) the operator matrix transposed to $\mathcal{A}$ is given by

$$\mathcal{A}' = \begin{pmatrix} V_{-\alpha}^-\big(I + L_{-\alpha}^+\big) + a\big(I - K_{-\alpha}^-\big)V_{-\alpha}^+ & c\, V_{-\alpha}^- J_{-\alpha}^+ \\ -c\, V_{-\alpha}^- J_{-\alpha}^+ & V_{-\alpha}^-\big(I + L_{-\alpha}^+\big) + b\,\big(I - K_{-\alpha}^-\big)V_{-\alpha}^+ \end{pmatrix}$$

(see (4.5) for the definition of the integral operators, corresponding now to the fundamental solution $\Psi_{\omega\kappa_\pm,-\alpha}$). Note that the range of $\mathcal{A}$ is orthogonal to the kernel of $\mathcal{A}'$ with respect to (5.8).

Theorem 5.3. *Suppose* (5.1) *and let the material parameters ε_- and μ_- be real and at least one of them be positive. If V_α^- is invertible, then there exists a solution $w, \tau \in H_\alpha^{-1/2}(\Gamma)$ of the system* (4.8).

Proof. The range of $\mathcal{A}$ is closed, hence it suffices to show that

$$\big[E_z^i, \varphi\big]_\Gamma + \big[B_z^i, \psi\big]_\Gamma = 0 \quad \text{for all } \Phi = (\varphi, \psi) \in \big(H_{-\alpha}^{-1/2}(\Gamma)\big)^2 \quad \text{with } \mathcal{A}'\Phi = 0 \,.$$

The functions $u_+ = \mathcal{S}_{-\alpha}^+ \varphi$, $v_+ = \mathcal{S}_{-\alpha}^+ \psi$ in G_+ and

$$\begin{aligned} u_- &= -\frac{1}{2} \left(\mathcal{S}_{-\alpha}^- \Big(\frac{1}{a}\,(I + L_{-\alpha}^+)\varphi + \frac{c}{a}\, J_{-\alpha}^+ \psi \Big) - \mathcal{D}_{-\alpha}^- V_{-\alpha}^+ \varphi \right), \\ v_- &= -\frac{1}{2} \left(\mathcal{S}_{-\alpha}^- \Big(\frac{1}{b}\,(I + L_{-\alpha}^+)\psi - \frac{c}{b}\, J_{-\alpha}^+ \varphi \Big) - \mathcal{D}_{-\alpha}^- V_{-\alpha}^+ \psi \right) \end{aligned} \tag{5.9}$$

in G_- are $-\alpha$-quasiperiodic of period d, satisfy the Helmholtz equations (4.1) and the outgoing wave condition (4.3) with α replaced by $-\alpha$:

$$\begin{aligned}(u_+,v_+)(x,y) &= \sum_{n=-\infty}^{\infty} (u_n^+,v_n^+)\,\mathrm{e}^{\,i(-\alpha_n x+\beta_n^+ y)} \quad \text{for } y\ge H,\\ (u_-,v_-)(x,y) &= \sum_{n=-\infty}^{\infty} (u_n^-,v_n^-)\,\mathrm{e}^{\,i(-\alpha_n x-\beta_n^- y)} \quad \text{for } y\le -H,\end{aligned} \tag{5.10}$$

the numbers α_n and $\beta_n^\pm$ are given in (2.15). The functions u_-, v_- have the boundary values

$$\begin{aligned} u_-|_\Gamma &= -\frac12\left(V_{-\alpha}^-\Big(\frac1a\,(I+L_{-\alpha}^+)\varphi+\frac ca\,J_{-\alpha}^+\psi\Big)-(I+K_{-\alpha}^-)V_{-\alpha}^+\varphi\right),\\ v_-|_\Gamma &= -\frac12\left(V_{-\alpha}^-\Big(\frac1b\,(I+L_{-\alpha}^+)\psi-\frac cb\,J_{-\alpha}^+\varphi\Big)-(I+K_{-\alpha}^-)V_{-\alpha}^+\psi\right),\end{aligned}$$

by using $\mathcal{A}'\Phi=0$ we get

$$u_-|_\Gamma = V_{-\alpha}^+\varphi = u_+|_\Gamma\,,\quad v_-|_\Gamma = V_{-\alpha}^+\psi = v_+|_\Gamma\,.$$

Now (5.9) and (3.8) imply that

$$\begin{aligned}\mathcal{S}_{-\alpha}^-\Big(\frac1a\,(I+L_{-\alpha}^+)\varphi+\frac ca\,J_{-\alpha}^+\psi\Big) &= \mathcal{S}_{-\alpha}^-\partial_n u_-\,,\\ \mathcal{S}_{-\alpha}^-\Big(\frac1b\,(I+L_{-\alpha}^+)\psi-\frac cb\,J_{-\alpha}^+\varphi\Big) &= \mathcal{S}_{-\alpha}^-\partial_n v_-\,,\end{aligned}$$

and since $V_{-\alpha}^- = (V_\alpha^-)'$ is invertible, this gives the jump relations

$$\Big[\frac{\varepsilon}{\kappa^2}\partial_n u+\frac{\varepsilon_+\sin\phi}{\kappa^2}\,\partial_t v\Big]_\Sigma = \Big[\frac{\mu}{\kappa^2}\partial_n v-\frac{\mu_+\sin\phi}{\kappa^2}\,\partial_t u\Big]_\Sigma = 0\,. \tag{5.11}$$

We proceed as in the proof of Lemma 5.2 and obtain the same variational equalities (5.3), (5.4) over the periodic cell Ω_H, but now for the $-\alpha$-quasiperiodic functions u and v. Since $\varepsilon_-,\mu_-\in\mathbb{R}$ and $\operatorname{Re}\beta_n^\pm=0$ for almost all n, the imaginary parts of (5.3), (5.4) are equal to

$$\begin{aligned}\sin\phi\Big(\frac{1}{\kappa_+^2}-\frac{1}{\kappa_-^2}\Big)\operatorname{Im}\int_\Gamma \partial_t v\,\overline{u} - \frac{1}{\kappa_+^2}\sum_{\beta_n^+>0}\beta_n^+|u_n^+|^2 - \frac{\varepsilon_-}{\varepsilon_+\kappa_-^2}\sum_{\beta_n^->0}\beta_n^-|u_n^-|^2 &= 0,\\ -\sin\phi\Big(\frac{1}{\kappa_+^2}-\frac{1}{\kappa_-^2}\Big)\operatorname{Im}\int_\Gamma \partial_t u\,\overline{v} - \frac{1}{\kappa_+^2}\sum_{\beta_n^+>0}\beta_n^+|v_n^+|^2 - \frac{\mu_-}{\mu_+\kappa_-^2}\sum_{\beta_n^->0}\beta_n^-|v_n^-|^2 &= 0.\end{aligned}$$

Note that if ε_- and μ_- have different signs, then $\kappa_-^2<0$ and $\operatorname{Re}\beta_n^-=0$ for all n. Because of

$$\operatorname{Im}\int_\Gamma \partial_t v\,\overline{u} = \operatorname{Im}\int_\Gamma \partial_t u\,\overline{v}$$

we derive $u_n^+=v_n^+=0$ if $\beta_n^+>0$ and $u_n^-=v_n^-=0$ if $\beta_n^->0$. The Rayleigh coefficients u_n^+, v_n^+ can be computed by the formula

$$u_n^+ = \frac1d\int_0^d u_+(X,H)\,\mathrm{e}^{i\alpha_n X-i\beta_n^+H}\,dX = \frac2d\int_\Gamma\varphi(Q)\,d\sigma_Q\int_0^d \Psi_{\omega\kappa_+,-\alpha}((X,H)-Q)\,\mathrm{e}^{i\alpha_n X-i\beta_n^+H}\,dX\,.$$

From (3.5) we obtain for $Q=(x,y)$

$$\int_0^d \Psi_{\omega\kappa_+,-\alpha}((X,H)-Q)\,\mathrm{e}^{i\alpha_n X-i\beta_n^+H}\,dX = \frac{i}{2\beta_n^+}\,\mathrm{e}^{i\alpha_n x-i\beta_n^+ y}\,,$$

which gives for $n=0$

$$u_0^+ = \frac{i}{d\beta}\int_\Gamma\varphi(Q)\,\mathrm{e}^{\,i\alpha x-\beta y}\,d\sigma_Q\,,\quad v_0^+ = \frac{i}{d\beta}\int_\Gamma\psi(Q)\,\mathrm{e}^{\,i\alpha x-\beta y}\,d\sigma_Q\,.$$

By (2.13) the components of the incoming field E_z^i and B_z^i are multiples of $\mathrm{e}^{\,i\alpha x-\beta y}$, hence

$$\big[E_z^i,\varphi\big]_\Gamma = \big[B_z^i,\psi\big]_\Gamma = 0$$

because of $u_0^+=v_0^+=0$. □

6 Singularities of Solutions to the Diffraction Problem

We are interested in the leading singularities of the solution $w, \tau \in H_\alpha^{-1/2}(\Gamma)$ of the integral equation system (4.8) in the case when Σ is a curved polygon, i.e. Σ is smooth with the exception of a finite number of corner points. It is well known that w and τ in a neighborhood ω of a corner point P of Σ allow decompositions of the type

$$f(Q)\chi(Q) = \chi(Q) \sum_{0<\mathrm{Re}\,\lambda<1} \sum_{l=0}^{k_\lambda - 1} c_{\lambda l} |Q-P|^{\lambda-1} \log^l |Q-P| + f_0(Q)\,, \quad Q \in \Sigma\,, \tag{6.1}$$

where χ is a cut-off function with support in ω, $f_0 \in H^{1/2}(\Sigma \cap \omega)$, the exponents λ are roots of multiplicity k_λ of certain transcendental equations and $c_{\lambda l} \in \mathbb{C}$, see [2]. Denote by Λ_ρ, $0 < \rho \le 1$, the strip $\{\,0 < \mathrm{Re}\,z < \rho\}$ in the complex plane. To determine the exponents $\lambda \in \Lambda_1$ we assume without loss of generality that G_+ coincides with a sector S with angle $\delta \in (0, 2\pi)\backslash\{\pi\}$ in a neighborhood of this point. Let $S = \{(r,\xi) : 0 < r < \infty, |\xi| < \delta/2\}$, where (r,ξ) denote polar coordinates centered at P, and Σ is locally given by $\partial S = \{\xi = -\delta/2\} \cup \{\xi = \delta/2\}$.

Since by (4.11)

$$w = (V_\alpha^-)^{-1} u_-|_\Gamma\,,\ \tau = (V_\alpha^-)^{-1} v_-|_\Gamma\,, \tag{6.2}$$

the exponents λ at corner points are determined from the behavior of $u_-|_\Gamma, v_-|_\Gamma$ and from the singularity of solutions of the integral equation

$$V_\alpha^- \varphi = \psi \tag{6.3}$$

at this point. The solution of (6.3) has even for smooth ψ in the neighborhood of P one exponent in the strip Λ_1 given by $\lambda = \min(\pi/\delta, \pi/(2\pi - \delta))$. This result was obtained in [2] based on Mellin symbol calculus of the localized integral operator. The same technique applied to the localized operator matrix $\mathcal{A}$ should provide the other exponents in Λ_1 caused by the singularity of $u_-|_\Gamma, v_-|_\Gamma$.

Here we follow the method from [4] to study directly the singularities of the solution E_z, B_z of the Helmholtz system (2.11) with the transmission conditions (2.12) near the corner point P. To determine the corner singularities at P with Kondratiev's method, one considers the model problem

$$\begin{aligned} &\Delta u = \Delta v = 0 \quad \text{in} \quad \mathbb{R}^2 \backslash \partial S\,, \\ &\big[u\big]_{\partial S} = \big[v\big]_{\partial S} = 0\,, \quad \Big[\frac{\varepsilon}{\kappa^2}\,\partial_n u + \frac{\varepsilon_+ \sin\phi}{\kappa^2}\,\partial_t u\Big]_{\partial S} = \Big[\frac{\mu}{\kappa^2}\,\partial_n v - \frac{\mu_+ \sin\phi}{\kappa^2}\,\partial_t u\Big]_{\partial S} = 0. \end{aligned}$$

which results from (4.1), (4.2) by neglecting all lower order terms, and seeks solutions of the form $u = r^\lambda U(\xi)$, $v = r^\lambda V(\xi)$. Since $\partial_n = \pm r^{-1}\partial/\partial\xi$, $\partial_t = \mp\partial/\partial r$ on $\{\xi = \pm\delta/2\}$, we arrive at the following eigenvalue problem for a system of two ordinary differential equations:

$$U'' + \lambda^2 U = V'' + \lambda^2 V = 0, \quad \xi \in (-\delta/2, \delta/2) \cup (\delta/2, 2\pi - \delta/2)\,, \tag{6.4}$$

$$\big[U\big]_{\xi=\pm\delta/2} = \big[V\big]_{\xi=\pm\delta/2} = \Big[\frac{\varepsilon}{\kappa^2}\,U' - \frac{\varepsilon_+ \sin\phi}{\kappa^2}\,\lambda V\Big]_{\xi=\pm\delta/2} = \Big[\frac{\mu}{\kappa^2}\,V' + \frac{\mu_+ \sin\phi}{\kappa^2}\,\lambda U\Big]_{\xi=\pm\delta/2} = 0. \tag{6.5}$$

We are looking for complex numbers $\lambda \in \Lambda_1$ such that this problem has a non–trivial solution $(U(\xi), V(\xi))$. Obviously, the general solution of (6.4) takes the form

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

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 (6.5). 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

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

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

Lemma 6.1. ([4]) *If (U,V) is a solution of problem* (6.4), (6.5)*, then both the pairs (U_o, V_e) and (U_e, V_o) solve this problem.*

Suppose that (U_o, V_e) is a non-trivial solution of (6.4), (6.5) corresponding to the eigenvalue λ. Then we obtain the linear system

$$\begin{aligned} A_2^+ \cos\frac{\lambda\delta}{2} - A_2^- \cos\lambda\big(\pi-\frac{\delta}{2}\big) &= 0 \\ B_1^+ \sin\frac{\lambda\delta}{2} + B_1^- \sin\lambda\big(\pi-\frac{\delta}{2}\big) &= 0 \\ \frac{\varepsilon_+ \sin\phi\, A_2^+ - \varepsilon_+ B_1^+}{\kappa_+^2}\cos\frac{\lambda\delta}{2} - \frac{\varepsilon_+ \sin\phi\, A_2^- - \varepsilon_- B_1^-}{\kappa_-^2}\cos\lambda\big(\pi-\frac{\delta}{2}\big) &= 0 \\ \frac{\mu_+ \sin\phi\, B_1^+ - \mu_+ A_2^+}{\kappa_+^2}\sin\frac{\lambda\delta}{2} + \frac{\mu_+ \sin\phi\, B_1^- - \mu_- A_2^-}{\kappa_-^2}\sin\lambda\big(\pi-\frac{\delta}{2}\big) &= 0 \end{aligned} \tag{6.6}$$

We may assume that

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

since otherwise it can easily be checked that (6.6) admits only the trivial solution if $\lambda \notin \mathbb{Z}$. Then (6.6) is equivalent to the 2×2 system

$$\begin{aligned} &\varepsilon_+ \sin\phi\Big(\frac{1}{\kappa_+^2} - \frac{1}{\kappa_-^2}\Big)A_2^- + \Big(\cot\frac{\lambda\delta}{2}\tan\lambda\big(\pi-\frac{\delta}{2}\big)\frac{\varepsilon_+}{\kappa_+^2} + \frac{\varepsilon_-}{\kappa_-^2}\Big)B_1^- = 0\,, \\ &\Big(\tan\frac{\lambda\delta}{2}\cot\lambda\big(\pi-\frac{\delta}{2}\big)\frac{\mu_+}{\kappa_+^2} + \frac{\mu_-}{\kappa_-^2}\Big)A_2^- + \mu_+ \sin\phi\Big(\frac{1}{\kappa_+^2} - \frac{1}{\kappa_-^2}\Big)B_1^- = 0\,. \end{aligned} \tag{6.7}$$

With the abbreviation

$$\eta = \cot\frac{\lambda\delta}{2}\tan\lambda\big(\pi-\frac{\delta}{2}\big) \tag{6.8}$$

the determinant D_o of the matrix of (6.7) takes the form

$$\begin{aligned} D_o &= \frac{\varepsilon_+\mu_+\sin^2\phi - \varepsilon_+\mu_+}{\kappa_+^4} + \frac{\varepsilon_+\mu_+\sin^2\phi - \varepsilon_-\mu_-}{\kappa_-^4} - \frac{2\varepsilon_+\mu_+\sin^2\phi + \eta\,\varepsilon_+\mu_- + \eta^{-1}\,\varepsilon_-\mu_+}{\kappa_+^2\kappa_-^2} \\ &= -\frac{\kappa_+^2 + \kappa_-^2 + 2\varepsilon_+\mu_+\sin^2\phi + \eta\,\varepsilon_+\mu_- + \eta^{-1}\,\varepsilon_-\mu_+}{\kappa_+^2\kappa_-^2} = -\frac{(\varepsilon_+ + \eta^{-1}\,\varepsilon_-)(\mu_+ + \eta\,\mu_-)}{\kappa_+^2\kappa_-^2}\,. \end{aligned}$$

Thus a nontrivial solution of (6.6) exists if

$$(\eta\,\varepsilon_+ + \varepsilon_-)(\mu_+ + \eta\,\mu_-) = 0\,.$$

Note that the cases $\varepsilon_- = \pm\varepsilon_+$, $\mu_- = \pm\mu_+$ can be excluded, since they are not of interest. Indeed, from $\eta = \pm 1$ and (6.8) we see that $\eta = 1$ implies $\sin\lambda\pi = 0$, whereas $\eta = -1$ implies $\sin\lambda(\pi+\delta) = 0$ and hence the corresponding roots λ do not belong to the strip Λ_1.

In the other case, if (U_e, V_o) is a non-trivial solution of (6.4), (6.5) for an eigenvalue $\lambda \in \Lambda_1$, then analogous considerations lead to the equivalent equation

$$(\varepsilon_+ + \eta\,\varepsilon_-)(\eta\,\mu_+ + \mu_-) = 0\,.$$

Hence a non-trivial solution (U, V) of (6.4), (6.5) exists, if

$$(\varepsilon_+ + \eta\,\varepsilon_-)(\eta\,\varepsilon_+ + \varepsilon_-)(\mu_+ + \eta\,\mu_-)(\eta\,\mu_+ + \mu_-) = 0\,,$$

which by (6.8) leads to the two transcendental equations

$$\Big(\frac{\sin\lambda(\pi-\delta)}{\sin\lambda\pi}\Big)^2 = \Big(\frac{1+\zeta}{1-\zeta}\Big)^2, \quad \text{with } \zeta = \frac{\varepsilon_-}{\varepsilon_+}\,,\ \frac{\mu_-}{\mu_+}\,. \tag{6.9}$$

Recall that we seek solutions $\lambda \in \Lambda_1$ and that we have to consider the equation only if $\zeta \neq \pm 1$.

Equations with the function

$$g_\delta(\lambda) = \frac{\sin\lambda(\pi-\delta)}{\sin\lambda\pi} \tag{6.10}$$

occurs already at different places where transmission problems for scalar Laplace and Helmholtz equations are studied. It was shown in [1] that the function

$$(g_\delta(\lambda))^2 - C \tag{6.11}$$

with $C > 0$ has a unique root in Λ_1, which is real, simple and greater than 1/2. The case $\delta = \pi/2, 3\pi/2$ was studied in [5], where the existence of a unique simple root in Λ_1 for any fixed $C \in \mathbb{C}$, $\operatorname{Re} C \neq 0$, was established. Moreover, it was shown that for any $\epsilon > 0$ one can find C such that the corresponding root of (6.11) belongs to Λ_ϵ. In the following we correct a statement of [4] where it was erroneously claimed that the same result is valid also for all other angles $\delta \in (0, 2\pi)\backslash\{\pi\}$.

Obviously, in order to study the solutions of (6.9) we can restrict to the case $0 < \delta < \pi$. Then g_δ maps rectangles of the form $R_{\epsilon,N} = (\epsilon, 1-\epsilon) \times (-iN, iN)$ conformly onto simply connected domains, which are symmetric with respect to the x-axis and are contained in the unbounded domain

$$\Omega_\delta = g_\delta(\Lambda_1) = \Big\{ x + iy : x > \cos\delta \, \frac{\sinh \xi(\pi-\delta)}{\sinh \xi\pi} \, , \; y = \sin\delta \, \frac{\cosh \xi(\pi - \delta)}{\sinh \xi\pi} \, , \; \xi \in (-\infty, \infty) \Big\}.$$

Moreover, $g_\delta\big(R_{\epsilon,N}\big)$ approach Ω_δ as $N \to \infty$ and $\epsilon \to 0$. Thus, if $z \in \Omega_\delta$, then due to the Argument Principle the equation $g_\delta(\lambda) = z$ has a unique simple root $\lambda \in \Lambda_1$.

Hence, in order to determine the number of solutions of the equation

$$(g_\delta(\lambda))^2 - z^2 = 0 \, , \quad z \neq 0 \, , \tag{6.12}$$

in the strip Λ_1, we have to decide whether for given $\delta \in (0, \pi)$ the points $\pm z \in \Omega_\delta$.

Lemma 6.2. *Any root $\lambda \in \Lambda_1$ of* (6.12) *is simple. If $0 < \delta \le \pi/2$, then* (6.12) *has a unique solution if*

$$z \in \Omega_\delta \cup (-\Omega_\delta) = \Big\{ x + iy : |x| > \cos\delta \, \frac{\sinh \xi(\pi-\delta)}{\sinh \xi\pi} \, , \; y = \sin\delta \, \frac{\cosh \xi(\pi-\delta)}{\sinh \xi\pi} \, , \; \xi \in (-\infty, \infty) \Big\}, \tag{6.13}$$

otherwise there is no solution in Λ_1. In the case $\pi/2 < \delta \le \pi$ the equation (6.12) *is always solvable in Λ_1, the solution is unique if*

$$z \in \Big\{ x + iy : |x| \ge -\cos\delta \, \frac{\sinh \xi(\pi-\delta)}{\sinh \xi\pi} \, , \; y = \sin\delta \, \frac{\cosh \xi(\pi-\delta)}{\sinh \xi\pi} \, , \; \xi \in (-\infty, \infty) \Big\}, \tag{6.14}$$

otherwise there exist two solutions in Λ_1.

Remark 6.1. If $\pi < \delta < 2\pi$, then the assertion of Lemma 6.2 holds with δ replaced by $\delta_1 = 2\pi - \delta$.

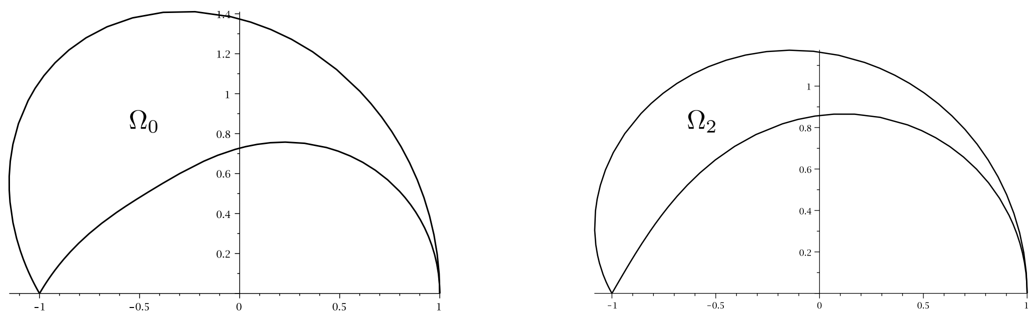

Figure 2: Exceptional domains for $\delta = \pi/3$ and $\delta = 2\pi/3$. If $\zeta = \varepsilon_-/\varepsilon_+$ or μ_-/μ_+ belongs to Ω_0 or Ω_2, then there exists correspondingly 0 or 2 eigenvalues in Λ_1

In order to determine the eigenvalues $\lambda \in \Lambda_1$ of (6.4), (6.5) we have to apply Lemma 6.2 with

$$z = \frac{1+\zeta}{1-\zeta} \, ,$$

where ζ takes the values $\varepsilon_-/\varepsilon_+$ and μ_-/μ_+ if they are different from ± 1. It can be easily checked that the fractional-linear transformation $\zeta = (z-1)/(z+1)$ maps $\partial\Omega_\delta \cup \partial(-\Omega_\delta)$ to the closed curves $\Sigma_\pm$ given by

$$\zeta = \frac{\big(\sin\delta + i \sinh \xi(2\pi - \delta)\big)\big(\sin\delta + i\sinh \xi\delta\big)}{\big(\cosh \xi(2\pi-\delta) \pm \cos\delta\big)\big(\cosh \xi\delta \mp \cos\delta\big)} \, , \quad \xi \in (-\infty, \infty) \, .$$

The curves intersect the real axis at the points $x = \pm 1$ and the domain enclosed by them corresponds to the exceptional domain mentioned in Lemma 6.2, i.e. the domain with no eigenvalues in Λ_1 if $0 < \delta \le \pi/2$ or with two eigenvalues when $\pi/2 < \delta < \pi$. In Figure 2 these domains with $\operatorname{Im}\zeta \ge 0$ are shown for the angles $\delta = \pi/3$ and $\delta = 2\pi/3$. Note that for $\delta = \pi/2$ both curves coincide with $|\zeta| = 1$.

Similarly one can study the existence of eigenvalues $\lambda \in \Lambda_{1/2}$ of (6.4), (6.5), which implies that the solutions of (4.8) $w, \tau \notin L_2(\Sigma)$ as well as the gradients $\nabla E_z|_\Sigma, \nabla B_z|_\Sigma \notin L_2(\Sigma)$ for the solution of (2.11), (2.12). We have

$$g_\delta(1/2 + i\xi) = \cos\delta/2\,\frac{\cosh\xi(\pi-\delta)}{\cosh\xi\pi} + i\sin\delta/2\,\frac{\sinh\xi(\pi-\delta)}{\cosh\xi\pi}\,, \quad \xi \in (-\infty,\infty)\,,$$

which shows that the transcendental equation (6.12) can have at most one solution $\lambda \in \Lambda_{1/2}$. Because of

$$\frac{g_\delta(1/2+i\xi)-1}{g_\delta(1/2+i\xi)+1} = -\frac{(\sin\delta/2 - i\sinh\xi(2\pi-\delta))(\sin\delta/2 + i\sinh\xi\delta)}{(\cos\delta/2 + \cosh\xi(2\pi-\delta))(\cos\delta/2+\cosh\xi\delta)}$$

and

$$\frac{-g_\delta(1/2+i\xi)-1}{-g_\delta(1/2+i\xi)+1} = -\frac{(\sin\delta/2 + i\sinh\xi(2\pi-\delta))(\sin\delta/2 - i\sinh\xi\delta)}{(\cos\delta/2 - \cosh\xi(2\pi-\delta))(\cos\delta/2-\cosh\xi\delta)}$$

the fractional-linear function $(z-1)/(z+1)$ maps the graphs of $g_\delta(1/2+i\xi)$ and $-g_\delta(1/2+i\xi)$ into a closed curve in the halfplane $\operatorname{Re}\zeta < 0$, and its interior determines the values of ζ such than an eigenvalue $\lambda \in \Lambda_{1/2}$ of (6.4), (6.5) exists. The curves with $\operatorname{Im}\zeta \ge 0$ are shown for the angles $\delta = \pi/3$ and $\delta = 2\pi/3$ in Fig. 3.

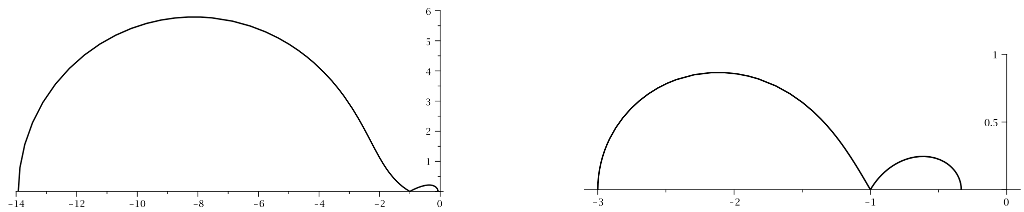

Figure 3: If $\zeta = \varepsilon_-/\varepsilon_+$ or μ_-/μ_+ is below the curves corresponding to $\delta = \pi/3$ (left) and $\delta = 2\pi/3$ (right), then $w, \tau \notin L_2(\Sigma)$

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