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INTEGRAL EQUATIONS FOR CONICAL DIFFRACTION BY COATED GRATING

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ABSTRACT. The paper is devoted to integral formulations for the scattering of plane waves by diffraction gratings under oblique incidence. For the case of coated gratings Maxwell's equations can be reduced to a system of four singular integral equations on the piecewise smooth interfaces between different materials. We study analytic properties of the integral operators for periodic diffraction problems and obtain existence and uniqueness results for solutions of the systems corresponding to electromagnetic fields with locally finite energy.

1. Introduction. In this paper we study an integral equation formulation for the numerical simulation of diffraction by optical gratings under oblique incidence, the so-called conical diffraction. We extend an approach developed in [**14**] for classical TE and TM diffraction problems which turned out to be very efficient for solving diffraction problems in certain scenarios with unfavorably large ratio period over wavelength, profile curves with corners and gratings with thin coated layers. A description of the method together with numerical tests for complicated situations is given in [**16**].

The electromagnetic formulation of conical diffraction by gratings, which are modeled as infinite periodic structures, can be reduced to a system of two Helmholtz equations in $\mathbf{R}^2$ coupled by transmission conditions at the interfaces between different materials of the diffraction grating. Using integral equation methods this transmission problem can be transformed to a system of integral equations over the interfaces. We consider here the case of coated gratings, where the interfaces between different materials are separated (see Figure 1 in Section 4). The integral equations are derived by a combination of direct and indirect methods. Due to the oblique incidence the approach leads

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to two integral equations on each interface which contain besides the boundary integrals of the single and double layer potentials also singular integral operators, the tangential derivative of single layer potentials.

The aim of the present paper is to study the basic analytic properties of the derived equations. We analyze mapping properties of the integral operators for periodic diffraction on nonsmooth interfaces and formulate conditions for the equivalence of the integral equation systems with the conical diffraction problem. We establish the strong ellipticity of the integral formulation for all relevant physical parameters, which allows to deduce solvability and uniqueness results and to study the convergence of numerical methods. For the sake of clarity the results are established for the 4×4 systems of singular integral equations corresponding to practically important single-coated gratings, but it will be clear that they are valid for diffraction gratings with any number of coatings, as long as the interfaces between them do not touch.

Grating problems can be treated very efficiently using integral equation methods, if the distribution of the optical materials is relatively simple and the interfaces between them are sufficiently regular. Many different, quite sophisticated formulations for solving the classical diffraction problems have been proposed and implemented, cf., e.g., [**8, 10, 14, 15**]. However, a rigorous mathematical and numerical analysis, comparable to standard boundary integral methods, cannot 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, see [**1, 2, 12**] and the references therein.

The outline of the paper is as follows. Section 2 is devoted to the conical diffraction by periodic structures, where we report on the differential equation formulation and known results. Quasiperiodic potentials for Helmholtz equations and integral operators of periodic diffraction on nonsmooth curves are discussed in Section 3. In Section 4 we derive two systems of singular integral equations for conical diffraction by coated gratings, which are analyzed in Section 5. In particular, it is shown that the integral equations are equivalent to the differential formulation for gratings with non-overhanging profiles or metallic substrate. The analysis of numerical methods for solving the integral equations, which is based on the strong ellipticity, will be discussed elsewhere.

2. Conical diffraction. We consider the scattering of a time-harmonic plane wave incident on a general periodic structure in $\mathbf{R}^3$, which is assumed to be infinitely wide and invariant in one spatial direction. The structure is characterized by the optical index ν of the non-magnetic grating materials, which is supposed to be a piecewise constant function not depending on z and periodic in x in the Cartesian coordinates (x, y, z). The optical index is defined by $\nu = \sqrt{\varepsilon/\varepsilon_0} = c\sqrt{\mu\varepsilon}$, where ε_0, μ are the permittivity, respectively permeability of free space, ε is the dielectric coefficient of the material and c denotes the speed of light. Note that standard optical materials satisfy $\operatorname{Re}\nu > 0$, $\operatorname{Im}\nu \geq 0$. The periodic structure separates two regions with constant optical index, thus the function ν is constant if y is outside a bounded interval.

The structure is illuminated by an electromagnetic plane wave $\mathbf{e}^{i\omega t}(\mathbf{E}^i, \mathbf{H}^i)$. If the period d of optical gratings under consideration is comparable with the wavelength $\lambda = 2\pi c/\omega$ of the incoming field, then the mathematical model has to rely on Maxwell's equations. We look for solutions $\varepsilon^{i\omega t}(\mathbf{E}, \mathbf{H})$ possessing locally a finite energy, that is,

$$\mathbf{E},\ \mathbf{H},\ \boldsymbol{\nabla} \times \mathbf{E},\ \boldsymbol{\nabla} \times \mathbf{H} \in \left(L^2_{\mathrm{loc}}(\mathbf{R}^3)\right)^3. \tag{2.1}$$

Specified to the case of oblique incidence the following differential problem has been derived in [**6**]:

For notational convenience we will change the length scale by the factor $2\pi/d$, so that the grating becomes 2π-periodic: $\varepsilon(x + 2\pi, y) = \varepsilon(x, y)$. We introduce the piecewise constant function

$$k = \frac{d}{\lambda}\nu \tag{2.2}$$

and denote by $k_\pm$ the values of k above, respectively below, the grating structure. We suppose that $k_+ > 0$ since the structure is illuminated from above. The incoming plane wave has the form

$$\begin{aligned} &(\mathbf{E}^i, \mathbf{H}^i) = (\mathbf{p}, \mathbf{s})\, \varepsilon^{i(\alpha x - \beta y + \gamma z)}, \\ &(\alpha, \beta, \gamma) = k_+(\sin\theta\cos\phi, \cos\theta\cos\phi, \sin\phi), \quad |\theta|, |\phi| < \pi/2, \end{aligned} \tag{2.3}$$

where the angle ϕ characterizes the oblique incidence. In order to be a solution of Maxwell's system above the grating structure the coefficient vectors $\mathbf{p}, \mathbf{s}$ and the wave vector $\mathbf{k} = (\alpha, -\beta, \gamma)$ are connected by certain compatibility relations.

Denote $Z = \nu_+ \sqrt{\varepsilon_0/\mu}$, where ν_+ is the optical index of the material above the grating, introduce

$$\mathbf{E}(x,y,z) = E(x,y)\, e^{i\gamma z}, \quad \mathbf{H}(x,y,z) = Z\, B(x,y)\, e^{i\gamma z}, \quad \mathbf{q} = Z^{-1}\mathbf{s},$$

and assume that everywhere $k^2(x,y) \neq \gamma^2$. It is shown in [**6**] that the condition of locally finite energy (2.1) is satisfied only if the z-components of $\mathbf{E}$ and $\mathbf{H}$ are H^1-regular. Moreover, the time-harmonic Maxwell equations for $\mathbf{E}$ and $\mathbf{H}$ lead to Helmholtz equations for the z-components $E_z, B_z \in H^1_{\mathrm{loc}}(\mathbf{R}^2)$ of E and B

$$(\Delta + k^2 - \gamma^2)\, E_z = (\Delta + k^2 - \gamma^2)\, B_z = 0 \tag{2.4}$$

in each of the domains in which $k(x,y)$ is constant. The Helmholtz equations are coupled by transmission conditions at the interfaces between different materials

$$[E_z] = [B_z] = 0,$$
$$\left[\frac{k^2\, \partial_\nu E_z}{k^2 - \gamma^2}\right] = -\left[\frac{\gamma k_+\, \partial_\tau B_z}{k^2 - \gamma^2}\right], \quad \left[\frac{\partial_\nu B_z}{k^2 - \gamma^2}\right] = \left[\frac{\gamma\, \partial_\tau E_z}{k_+(k^2 - \gamma^2)}\right]. \tag{2.5}$$

Here ∂_ν, ∂_τ are the derivatives in the direction of the normal $\nu = (\nu_1, \nu_2)$, respectively of the tangential vector $\tau = (-\nu_2, \nu_1)$, to the interface in the (x,y)-plane, $\partial_\nu = \nu_1 \partial_1 + \nu_2 \partial_2$, $\partial_\tau = -\nu_2 \partial_1 + \nu_1 \partial_2$, and $[\,\cdot\,]$ denotes the jump of the boundary values if crossing the interface.

The z-components of the incoming field $E^i_z(x,y) = p_z \mathbf{e}^{i(\alpha x - \beta y)}$, $B^i_z(x,y) = q_z \mathbf{e}^{i(\alpha x - \beta y)}$, are α-quasiperiodic functions, i.e., satisfy the relation $u(x + 2\pi, y) = \varepsilon^{2\pi i \alpha} u(x,y)$. Therefore, E_z, B_z have to be α-quasiperiodic, too. Moreover, the scattered field has to satisfy below and above the inhomogeneous grating structure a radiation condition which is known as outgoing wave condition

$$(E_z, B_z)(x,y) - (E^{(i)}_z, B^{(i)}_z)(x,y) = \sum_{n=-\infty}^{\infty} (E^+_n, B^+_n)\mathbf{e}^{\,i(\alpha_n x + \beta^+_n y)}, \quad y \to +\infty,$$
$$(E_z, B_z)(x,y) = \sum_{n=-\infty}^{\infty} (E^-_n, B^-_n)\mathbf{e}^{\,i(\alpha_n x - \beta^-_n y)}, \quad y \to -\infty, \tag{2.6}$$

with the so-called Rayleigh coefficients $E_n^{\pm}, B_n^{\pm} \in \mathcal{C}$, and

$$\alpha_n = \alpha + n, \quad \beta_n^{\pm} = \sqrt{k_{\pm}^2 - \gamma^2 - \alpha_n^2} \quad \text{with } 0 \le \arg \beta_n^{\pm} < \pi, \quad n \in \mathbf{Z}.$$

The Rayleigh coefficients $E_n^{\pm}, B_n^{\pm}$ for $\beta_n^{\pm} \in \mathbf{R}$ are the main characteristics of diffraction gratings. They indicate the efficiency and the phase shift of the finite number of propagating modes, i.e., of the outgoing plane waves

$$\sum_{\beta_n^{\pm} \in \mathbf{R}} (E_n^{\pm}, B_n^{\pm}) \mathbf{e}^{i\alpha_n x + i\beta_n^{\pm}|y| + i\gamma z}, \quad |y| \to \infty.$$

Since the wave vectors of the propagating reflected or transmitted modes lie on the surface of a cone whose axis is parallel to the z-direction, one speaks of conical diffraction.

Under the assumption, that the interfaces between different materials are Lipschitz and that the material parameters of the grating fulfill the condition

$$\arg\left(k^2(x,y) - \gamma^2\right) \in [0, \pi) \tag{2.7}$$

the following existence and uniqueness results for the conical diffraction problem have been proved in [**6**]:

– The conical diffraction problem (2.4)–(2.6) has at least one solution (E_z, B_z) which is H^1-regular near the interfaces.

– If for some grating material $\operatorname{Im} k > 0$, then this solution is unique.

– Suppose that the optical index of the materials are real and fixed for all frequencies ω. If $k_-^2 > \alpha^2 + \gamma^2$, then for all but a countable set of frequencies ω_j, $\omega_j \to \infty$, the solutions are unique.

3. Integral representations. Here we collect analytic properties of the integral representation for solutions and of boundary integral operators for quasiperiodic Helmholtz equations.

3.1. Quasi-periodic potentials. Suppose that Σ is the intersection of the interface between two different materials and the (x, y)-plane. In the following we assume that Σ is non self-intersecting and given by a regular parametrization

$$\begin{aligned} \sigma(t) &= (X(t), Y(t)), \\ X(t+1) &= X(t) + 2\pi, \\ Y(t+1) &= Y(t), \\ t &\in \mathbf{R}, \end{aligned} \tag{3.1}$$

i.e., the functions X, Y have piecewise continuous derivatives and

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

Concerning the smoothness of Σ we will restrict for simplicity to the two cases:

– Σ is smooth, i.e., $X, Y \in C^\infty$,

– Σ is a piecewise C^2 curve with corners such that the angle between adjacent tangents is strictly between 0 and 2π.

As in classical potential theory one tries to represent quasiperiodic solutions of the Helmholtz equation $\Delta u + k^2 u = 0$ outside Σ for constant k with $\arg k \in [0, \pi)$ by the single and double layer potentials

$$\frac{i}{2} \int_\Sigma H_0^{(1)}\big(k|P-Q|\big)\, \varphi(Q)\, d\sigma_Q$$

and

$$\frac{i}{2} \int_\Sigma \varphi(Q)\, \partial_{\nu(Q)} H_0^{(1)}\big(k|P-Q|\big)\, d\sigma_Q, \quad P \notin \Sigma,$$

respectively, with an α-quasiperiodic density φ on Σ, i.e., $\varphi(x+2\pi, y) = \mathbf{e}^{2\pi i \alpha} \varphi(x, y)$ for $(x, y) \in \Sigma$. Here $H_0^{(1)}$ is the Hankel function of the first kind, $d\sigma_Q$ denotes the integration with respect to the arc length and $\nu(Q)$, $Q \in \Sigma$, indicates the normal to Σ pointing downward. Using the quasiperiodicity of φ the above potentials are transformed to integrals over one period Γ of the interface Σ, i.e., all points of Σ connecting a given left boundary point $\sigma(t_0) = (X(t_0), Y(t_0))$ with the right boundary $\sigma(t_0 + 1) = (X(t_0) + 2\pi, Y(t_0))$. In the following we suppose $X(0) = 0$ and take $\sigma(0) = (0, Y(0))$ as the left boundary of Γ. The single and double layer potentials are defined by

$$
\begin{aligned}
V_\Gamma \varphi(P) &:= 2 \int_\Gamma \Psi_{k,\alpha}(P - Q)\, \varphi(Q)\, d\sigma_Q, \\
K_\Gamma \varphi(P) &:= 2 \int_\Gamma \varphi(Q)\, \partial_{\nu(Q)} \Psi_{k,\alpha}(P - Q)\, d\sigma_Q,
\end{aligned} \tag{3.2}
$$

with the fundamental solution

$$
\Psi_{k,\alpha}(P) = \frac{i}{4} \sum_{n \in \mathbf{Z}} H_0^{(1)}\Big(k\sqrt{(X - 2\pi n)^2 + Y^2}\Big) \mathbf{e}^{2\pi i n \alpha}, \quad P = (X, Y), \tag{3.3}
$$

which converges uniformly to a smooth function over compact sets in $\mathbf{R}^2 \setminus \cup_n \{(2\pi n, 0)\}$ if $k^2 \neq \alpha_n^2$ for all $n \in \mathbf{Z}$. Moreover, setting $\beta_n = \sqrt{k^2 - \alpha_n^2}$ with $\operatorname{Im} \beta_n \geq 0$ Poisson's summation formula leads to the representation

$$
\Psi_{k,\alpha}(P) = \frac{i}{4\pi} \sum_{n \in \mathbf{Z}} \frac{1}{\beta_n} \mathbf{e}^{\,i\alpha_n X + i\beta_n |Y|}. \tag{3.4}
$$

For the deviation of (3.3), (3.4), convergence properties and fast summation methods, see e.g., [**2, 9, 10**].

The function $\Psi_{k,\alpha}$ is α-quasiperiodic and satisfies the radiation condition (3.8) below. Note that

$$
\Psi_{k,m+\alpha}(P) = \Psi_{k,\alpha}(P) \quad \text{for all } m \in \mathbf{Z}, \tag{3.5}
$$

$$
\Psi_{k,-\alpha}(P) = \Psi_{k,\alpha}(-P) \quad \text{for all } P \in \mathbf{R}^2. \tag{3.6}
$$

Since α-quasiperiodic functions are also $(\alpha + m)$-quasiperiodic in view of (3.5) we restrict the range of α. In the following we will always assume that $|\alpha| \leq 1/2$ and that all $\beta_n \neq 0$.

The potentials (3.2) provide α-quasiperiodic solutions of the Helmholtz equation

$$
\Delta u + k^2 u = 0 \tag{3.7}
$$

outside the profile curve Σ which satisfy the radiation condition (3.8). And conversely, any solution admits an integral representation using the potentials (3.2). To give a precise formulation we denote by $G_+, G_- \subset \mathbf{R}^2$ the domains above and below Σ, respectively.

Lemma 3.1. *Suppose that in one of the domains G_+ or G_- the α-quasiperiodic function u has the following properties*:

(i) *u is locally a H^1-function with Δu belonging locally to L_2*;

(ii) *u satisfies the Helmholtz equation* (3.7) *almost everywhere and the radiation condition*

$$u(x,y) = \sum_{n=-\infty}^{\infty} u_n \mathbf{e}^{\,i(\alpha_n x \pm \beta_n y)}, \quad \pm y \geq H, \tag{3.8}$$

where H is such that $\Sigma \subset \{|y| < H\}$ and the $+$ and $-$ signs correspond to the cases G_+, respectively G_-.

Then u can be represented in the given domain $G_\pm$ by

$$u = \pm\frac{1}{2}\big(V_\Gamma \partial_\nu u - K_\Gamma u\big), \tag{3.9}$$

with the normal ν pointing into G_-.

Proof. Consider a bounded domain Ω with piecewise C^2 boundary such that

$$\Psi_{k,\alpha}(P-Q) - H_0^{(1)}\big(k|P-Q|\big), \quad P, Q \in \Omega,$$

is smooth. It follows from the corresponding result for the potentials with the kernel $H_0^{(1)}$ and Green's formula, cf. e.g., [**4**], that any α-quasiperiodic function u satisfying (i) and (3.7) admits the representation

$$u(P) = \int_{\partial\Omega} \Big(\Psi_{k,\alpha}(P-Q)\partial_\nu u(Q) - u(Q)\,\partial_{\nu(Q)}\Psi_{k,\alpha}(P-Q)\Big)\,d\sigma_Q, \; P \in \Omega, \tag{3.10}$$

where ν is the outward normal to Ω. To apply (3.10) we choose H and a smooth function $g(y)$, $y \in \mathbf{R}$, satisfying $g(0) = 0$ and $g(y) = 0$ for $|y| \geq H$ such that

$$\Gamma \subset D_H = \{(x,y) : g(y) \leq x \leq g(y) + 2\pi, |y| < H\}.$$

The curve Γ divides D_H into the subdomains $D_H^\pm = D_H \cap G_\pm$. The boundary $\partial D_H^\pm$ is piecewise C^2 and consists of Γ, $(0, 2\pi) \times \{\pm H\}$ and $(g(y), y)$, $(g(y) + 2\pi, y)$, $y \in (0, \pm H)$. Applying (3.10) in $D_H^\pm$ we see that for quasiperiodic u the integrals over the boundary parts $(g(y), y)$ and $(g(y) + 2\pi, y)$ cancel. Moreover, formula (3.4) allows to calculate explicitly the boundary integrals over the straight lines $(0, 2\pi) \times \pm H$ for u satisfying (3.8). In a neighborhood of the line $y = \pm H$ we have

$$u(Q) = \sum_{n \in \mathbf{Z}} u_n^\pm \mathbf{e}^{i(\alpha_n x \pm \beta_n y)}, \quad Q = (x, y),$$

and, if $Q = (x, \pm H)$ and $P = (X, Y) \in D_H^\pm$, then by (3.4)

$$\partial_{\nu(Q)} \Psi_{k,\alpha}(P - Q) = -\frac{1}{4\pi} \sum_{n \in \mathbf{Z}} \varepsilon^{i\alpha_n (X - x) + i\beta_n (H \mp Y)}.$$

It can be checked easily that for $P \in D_H^\pm$

$$\int_{(0,2\pi)\times \pm H} \Big(\Psi_{k,\alpha}(P - Q) \partial_\nu u(Q) - u(Q)\, \partial_{\nu(Q)} \Psi_{k,\alpha}(P - Q) \Big)\, d\sigma_Q = 0. \qquad \square$$

3.2. Boundary integral operators. In the following we transfer results for integral operators of the Helmholtz equation on closed curves (cf. e.g., [**5, 17**]) to our slightly different situation. First we note that the fundamental solution $\Psi_{k,\alpha}$ can be decomposed as

$$\Psi_{k,\alpha}(P) = \frac{\mathbf{e}^{i\alpha(X - \sin X)}}{2\pi} \log \frac{1}{\rho(P)} + f(P), \tag{3.11}$$

where ρ is a distance function which is periodic in X,

$$\rho^2(P) = 4 \left(\sin^2 \frac{X}{2} + \sinh^2 \frac{Y}{2} \right), \tag{3.12}$$

and $f(P)$ is C^∞ if $\rho(P) \neq 0$ with second derivatives, bounded by constant times $\big|\log \rho(P)\big|$ if $\rho(P) \to 0$. This follows from the main singularity of the 2π-periodic function

$$\mathbf{e}^{-i\alpha X} \Psi_{k,\alpha}(P) = \frac{i}{4} \sum_{n \in \mathbf{Z}} H_0^{(1)}\Big(k \sqrt{(X - 2\pi n)^2 + Y^2} \Big) \mathbf{e}^{-i\alpha(X - 2\pi n)}$$

at the points $(2\pi n, 0)$, $n \in \mathbf{Z}$, and the series expansion of the Hankel function $H_0^{(1)} = J_0 + iY_0$ (see e.g., [**17**]), which gives

$$H_0^{(1)}(z) = \frac{2i}{\pi}\left(1 - \frac{z^2}{4}F_0(z^2)\right)\log\frac{z}{2} + \left(1 + \frac{2i}{\pi}C\right) + z^2F_1(z^2),$$
$$z \in \mathbf{C} \setminus (-\infty, 0],$$

where $C = 0.5772\ldots$ is the Euler-Mascheroni constant and the functions F_j are analytic with $F_j(0) \neq 0$. Moreover, from (3.11)

$$\nabla\Psi_{k,\alpha}(P) = -\frac{\mathbf{e}^{i\alpha(X-\sin X)}}{2\pi}\frac{(\sin X, \sinh Y)}{\rho^2(P)} + g(P), \tag{3.13}$$

and the first order derivatives of g are bounded by constant times $\left|\log\rho(P)\right|$ if $\rho(P) \to 0$. Hence the kernels of the single and double layer potentials can be expanded as

(3.14)
$$\Psi_{k,\alpha}(P - Q) = \frac{\mathbf{e}^{i\alpha(X-x-\sin(X-x))}}{2\pi}\log\frac{1}{\rho(P-Q)} + f(P-Q),$$
$$\partial_{\nu(Q)}\Psi_{k,\alpha}(P - Q) = \frac{\mathbf{e}^{i\alpha(X-x-\sin(X-x))}}{2\pi} \times \frac{\nu(Q)\cdot(\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} + \nu(Q)\cdot g(P-Q), \tag{3.15}$$

where $P = (X, Y) \in \mathbf{R}^2$, $Q = (x, y) \in \Gamma$. Recall that the functions $f(P)$ and $g(P)$ are α-quasiperiodic in X and C^∞ if $\rho(P) \neq 0$ with $|\nabla_2 f(P)| \leq c|\log\rho(P)|$ and $|\nabla g(P)| \leq c|\log\rho(P)|$ for small $\rho(P)$. Here ∇_j denotes the vector of partial derivatives of order j.

Let us define the Sobolev spaces

$$H_\alpha^{\pm 1/2}(\Gamma) = \left\{\mathbf{e}^{i\alpha X(t)}\varphi(\sigma(t)),\ \varphi(\sigma(\cdot)) \in H_p^{\pm 1/2}(0,1)\right\}, \tag{3.16}$$

where $H_p^s(0,1)$, $s \in \mathbf{R}$, denotes the Sobolev space of 1-periodic functions on the real line. Clearly, $H_\alpha^{1/2}(\Gamma)$ is the trace space of α-quasiperiodic functions $u \in H^1_{\mathrm{loc}}(G_\pm)$. Using the expansions (3.14) and (3.15) it can be shown similarly to [**5**] that for $\varphi \in H_\alpha^{-1/2}(\Gamma)$,

$\psi \in H_\alpha^{1/2}(\Gamma)$ and $P \notin \Sigma$ the potentials $V_\Gamma\varphi(P)$ and $K_\Gamma\psi(P)$ satisfy the assumptions of Lemma 3.1. Moreover, the limits of the potentials for $P \in G_\pm$ tending in non-tangential direction to a point at Γ, which we indicate by the upper sign $+$, respectively $-$, are determined by the limits of the classical single and double layer potentials of the Laplacian plus the contribution of integral operators with continuous kernels. Therefore the single layer potential is continuous across Γ

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

To indicate that this operator maps into the set of α-quasiperiodic functions on Γ we introduce the notation

$$\mathcal{V}_\Gamma^{(\alpha)}\varphi(P) := 2\int_\Gamma \Psi_{k,\alpha}(P-Q)\,\varphi(Q)\,d\sigma_Q, \quad P \in \Gamma.$$

The double layer potential has a jump if crossing Γ:

(3.17)
$$\big(K_\Gamma\psi\big)^+(P) = \mathcal{K}_\Gamma^{(\alpha)}\psi(P) - \psi(P), \quad \big(K_\Gamma\psi\big)^-(P) = \mathcal{K}_\Gamma^{(\alpha)}\psi(P) + \psi(P)$$

with the boundary double layer potential

$$\begin{aligned}\mathcal{K}_\Gamma^{(\alpha)}\psi(P) := 2\int_\Gamma &\psi(Q)\,\partial_{\nu(Q)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q \\ &+ (\delta(P)-1)\psi(P), \quad P \in \Gamma.\end{aligned} \tag{3.18}$$

Here $\delta(P) \in (0,2)$ denotes the quotient of the angle in G_+ at $P \in \Gamma$ and π, i.e., $\delta(P) = 1$ outside corner points of Γ. The normal derivative of the single layer potential exists outside corners and has the limits

(3.19)
$$\big(\partial_\nu V_\Gamma\varphi\big)^+(P) = \mathcal{L}_\Gamma^{(\alpha)}\varphi(P) + \varphi(P), \quad \big(\partial_\nu V_\Gamma\varphi\big)^-(P) = \mathcal{L}_\Gamma^{(\alpha)}\varphi(P) - \varphi(P),$$

where we denote

$$\mathcal{L}_\Gamma^{(\alpha)}\varphi(P) := 2\int_\Gamma \varphi(Q)\,\partial_{\nu(P)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q, \quad P \in \Gamma.$$

From (3.19) we derive

Corollary 3.1. *Suppose that the function u given in G_+ (G_-) satisfies the conditions of Lemma* 3.1. *Then $V_\Gamma \partial_\nu u(P) - K_\Gamma u(P) = 0$ in the opposite domain $P \in G_-$ ($P \in G_+$).*

The integral formulation of conical diffraction will contain also operators of the form

$$\mathcal{V}_\Gamma^{(\alpha)}\big(\partial_\tau \varphi\big)(P) = 2\int_\Gamma \Psi_{k,\alpha}(P-Q)\,\partial_\tau\varphi(Q)\,d\sigma_Q, \quad P \in \Gamma, \tag{3.20}$$

where φ is the restriction of an α-quasiperiodic function to Γ. Formal integration by parts gives

$$\int_\Gamma \Psi_{k,\alpha}(P-Q)\,\partial_\tau\varphi(Q)\,d\sigma_Q = -\int_\Gamma \varphi(Q)\,\partial_{\tau(Q)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q,$$

where we use the quasiperiodicity

$$\varphi(\sigma(1)) = e^{2\pi i\alpha}\varphi(\sigma(0)),\ \Psi_{k,\alpha}(P-\sigma(1)) = e^{-2\pi i\alpha}\Psi_{k,\alpha}(P-\sigma(0))$$

at the end points $\sigma(0)$ and $\sigma(1)$ of Γ. The integral on the right is defined as the principal value integral

$$\begin{aligned}\int_\Gamma &\partial_{\tau(Q)}\Psi_{k,\alpha}(P-Q)\,\varphi(Q)\,d\sigma_Q \\ &= \lim_{\delta\to 0}\int_{\Gamma\setminus\Gamma(P,\delta)} \partial_{\tau(Q)}\Psi_{k,\alpha}(P-Q)\,\varphi(Q)\,d\sigma_Q,\end{aligned} \tag{3.21}$$

where $\Gamma(P,\delta)$ denotes the subarc of Γ with the mid point P and the arc length 2δ. The existence of the limit follows from (3.13) which yields

$$\begin{aligned}\partial_{\tau(Q)}\Psi_{k,\alpha}(P-Q) = &\frac{\mathbf{e}^{i\alpha(X-x-\sin(X-x))}}{2\pi} \\ &\times \frac{\tau(Q)\cdot(\sin(X-x),\sinh(Y-y))}{\rho^2(P-Q)} \\ &+ \tau(Q)\cdot g(P-Q).\end{aligned}$$

Thus for small $\rho(P-Q)$ the non-integrable term behaves like

$$\partial_{\tau(Q)}\log\frac{1}{|P-Q|},$$

and the integral operators with the tangential and normal derivative of the logarithmic kernel are connected with the Cauchy singular integral by the formula

$$\frac{1}{\pi i}\int_\Gamma \frac{\varphi(t)dt}{t-z} = \frac{i}{\pi}\int_\Gamma \varphi(Q)\partial_{\tau(Q)} \log\frac{1}{|P-Q|}\,d\sigma_Q - \frac{1}{\pi}\int_\Gamma \varphi(Q)\partial_{\nu(Q)} \log\frac{1}{|P-Q|}\,d\sigma_Q, \tag{3.22}$$

where $t = x + iy$ and $z = X + iY \in \Gamma$. This formula holds for any piecewise Ljapunov curve Γ, cf., e.g., [**11**, Section 64]. Hence, introducing the singular integral

$$\mathcal{H}_\Gamma^{(\alpha)}\varphi(P) := 2\int_\Gamma \varphi(Q)\,\partial_{\tau(Q)}\Psi_{k,\alpha}(P-Q)\,d\sigma_Q,$$

the single layer potential of the tangential derivative (3.20) can be expressed as

$$\mathcal{V}_\Gamma^{(\alpha)}\big(\partial_\tau\varphi\big)(P) = -\mathcal{H}_\Gamma^{(\alpha)}\varphi(P). \tag{3.23}$$

3.3. Mapping properties. Recall that Γ as one period of the interface Σ is given by $\Gamma = \{\sigma(t) : t \in [0,1)\}$, cf. (3.1). We study the properties of the boundary operators in Sobolev spaces of α-quasiperiodic functions on Γ defined by

$$H_\alpha^s(\Gamma) = \big\{\mathbf{e}^{i\alpha X(t)}\varphi(\sigma(t)),\ \varphi(\sigma(\cdot)) \in H_p^s(0,1)\big\},$$

cf. (3.16), where $s \in [-1,1]$ if the profile curve Σ has corners, or $s \in \mathbf{R}$ for smooth Σ.

Performing the conformal mapping $\mathbf{e}^{iz}$, $z \in \mathbf{C}$, the open curve Γ is transformed to the closed curve

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

which has the same smoothness as Γ. Moreover, if Σ has corners, then the angles in G_+ at corner points of Σ and interior angles at the corresponding corner points of $\widetilde{\Gamma}$ coincide. Obviously, the mapping

$$\vartheta^*\varphi(P) := \mathbf{e}^{i\alpha X}\varphi(\vartheta(P))$$

with

$$\vartheta : \Gamma \ni P = (X,Y) \longrightarrow \mathbf{e}^{-Y}(\cos X, \sin X) \in \widetilde{\Gamma} \tag{3.24}$$

generates an isomorphism $\vartheta^* : H^s(\widetilde{\Gamma}) \to H^s_\alpha(\Gamma)$.

The mapping properties of $\mathcal{V}_\Gamma^{(\alpha)}$, $\mathcal{H}_\Gamma^{(\alpha)}$, $\mathcal{K}_\Gamma^{(\alpha)}$ and $\mathcal{L}_\Gamma^{(\alpha)}$ are easily obtained from those of the boundary integral operators for the Laplacian on the simple closed curve $\widetilde{\Gamma}$

$$\begin{aligned} V\varphi(P) &= \frac{1}{\pi}\int_{\widetilde{\Gamma}} \varphi(Q)\left(\log\frac{1}{|P-Q|} + c\right) d\sigma_Q,\\ H\varphi(P) &= \frac{1}{\pi}\int_{\widetilde{\Gamma}} \varphi(Q)\,\partial_{\tau(Q)}\log\frac{1}{|P-Q|}\, d\sigma_Q,\\ K\varphi(P) &= \frac{1}{\pi}\int_{\widetilde{\Gamma}} \varphi(Q)\,\partial_{\nu(Q)}\log\frac{1}{|P-Q|}\, d\sigma_Q,\\ L\varphi(P) &= \frac{1}{\pi}\int_{\widetilde{\Gamma}} \varphi(Q)\,\partial_{\nu(P)}\log\frac{1}{|P-Q|}\, d\sigma_Q. \end{aligned}$$

The parameter c in the kernel of V is chosen such that $V : H^{-1/2}(\widetilde{\Gamma}) \to H^{1/2}(\widetilde{\Gamma})$ is positive definite and therefore invertible. Here ν is the exterior normal to $\widetilde{\Gamma}$. The operator L is the adjoint of the double layer potential K with respect to the L_2 duality form on $\widetilde{\Gamma}$

$$\langle\varphi,\psi\rangle = \int_{\widetilde{\Gamma}} \varphi\,\overline{\psi}\, d\sigma, \tag{3.25}$$

therefore we write $L = K'$. The adjoint of H is obviously given by the singular integral

(3.26)

$$H'\varphi(P) = \frac{1}{\pi}\int_{\widetilde{\Gamma}} \varphi(Q)\,\partial_{\tau(P)}\log\frac{1}{|P-Q|}\, d\sigma_Q = \partial_\tau V\varphi(P), \quad P \in \widetilde{\Gamma}.$$

We list some properties of these operators needed for the following.

Lemma 3.2. *For* $0 < s < 1$ *and* $0 \le t < 1$ *the operators*

$$\begin{aligned} V : H^{s-1}(\widetilde{\Gamma}) &\longrightarrow H^s(\widetilde{\Gamma}),\\ K,\, H : H^t(\widetilde{\Gamma}) &\longrightarrow H^t(\widetilde{\Gamma}),\\ K',\, H' : H^{-t}(\widetilde{\Gamma}) &\longrightarrow H^{-t}(\widetilde{\Gamma}) \end{aligned}$$

are bounded. If $\widetilde{\Gamma}$ *is smooth, then* $V : H^{s-1}(\widetilde{\Gamma}) \to H^s(\widetilde{\Gamma})$ *is invertible,* $H, H' : H^s(\widetilde{\Gamma}) \to H^s(\widetilde{\Gamma})$ *are Fredholm with index* 0 *for all* $s \in \mathbf{R}$*, and* $K, K' : H^s(\widetilde{\Gamma}) \to H^t(\widetilde{\Gamma})$ *are bounded for all* $s, t \in \mathbf{R}$*. Moreover, the following relations hold:*

(i) $KV = VK'$, $HV = -VH'$;

(ii) $HK = -KH$, $K^2 - H^2 = I$.

Proof. The mapping properties of V and K are well known even for closed Lipschitz curves, see for example [**3**]. Since $H = -V\partial_\tau$ the boundedness of $\partial_\tau : H^s(\widetilde{\Gamma}) \to H^{s-1}(\widetilde{\Gamma})$, $0 \le s \le 1$, imply the mapping properties of H and H'. The first of the commutator relations (i) is well known, see e.g., [**5**], whereas the second follows from the definition of H and (3.26). Finally, (ii) is a consequence of

$$S = -K + iH, \quad \text{where } S\phi(z) = \frac{1}{2\pi i} \int_{\widetilde{\Gamma}} \frac{\varphi(\xi)d\xi}{\xi - z}, \quad z \in \widetilde{\Gamma}, \tag{3.27}$$

see (3.22), and the equality $S^2 = I$, which holds almost everywhere on any closed piecewise Ljapunov curve (cf. e.g., [**11**]). □

Lemma 3.3. *The boundary integral operators for the quasiperiodic Helmholtz equation on a piecewise* C^2 *curve* Γ *map boundedly*

$$\begin{aligned} \mathcal{V}_\Gamma^{(\alpha)} &: H_\alpha^{s-1}(\Gamma) \longrightarrow H_\alpha^s(\Gamma), \\ \mathcal{H}_\Gamma^{(\alpha)},\ \mathcal{K}_\Gamma^{(\alpha)} &: H_\alpha^t(\Gamma) \longrightarrow H_\alpha^t(\Gamma), \\ \mathcal{L}_\Gamma^{(\alpha)} &: H_\alpha^{-t}(\Gamma) \longrightarrow H_\alpha^{-t}(\Gamma), \end{aligned}$$

for $s \in (0,1)$*,* $t \in [0,1)$*. In the case* $s = t = 1/2$ *the operators* $\mathcal{V}_\Gamma^{(\alpha)}$ *and* $\mathcal{H}_\Gamma^{(\alpha)}$ *are Fredholm with* $\operatorname{ind} \mathcal{V}_\Gamma^{(\alpha)} = \operatorname{ind} \mathcal{H}_\Gamma^{(\alpha)} = 0$*. If the profile curve* Σ *is smooth, then*

$$\mathcal{V}_\Gamma^{(\alpha)} : H_\alpha^{s-1}(\Gamma) \longrightarrow H_\alpha^s(\Gamma),$$
$$\mathcal{K}_\Gamma^{(\alpha)},\ \mathcal{L}_\Gamma^{(\alpha)} : H_\alpha^s(\Gamma) \longrightarrow H_\alpha^{s+2}(\Gamma)$$

and

$$\mathcal{H}_\Gamma^{(\alpha)} : H_\alpha^s(\Gamma) \longrightarrow H_\alpha^s(\Gamma),$$

are bounded for all $s \in \mathbf{R}$.

Proof. Obviously

$$\begin{aligned} &\vartheta^* V(\vartheta^*)^{-1}\varphi(P) \\ &\qquad = \frac{1}{\pi}\int_\Gamma \mathbf{e}^{i\alpha(X-x)}\left(\log\frac{1}{|\vartheta(P)-\vartheta(Q)|}+c\right)\varphi(Q)|\vartheta'(Q)|\,d\sigma_Q, \end{aligned}$$

where $P=(X,Y)\in\Gamma$ and $|\vartheta'(Q)| = \mathbf{e}^{-y}$ for $Q=(x,y)$. Introduce the multiplication operator

$$M\varphi(P) = \mathbf{e}^Y\varphi(P), \quad P=(X,Y)\in\Gamma, \tag{3.28}$$

which is invertible in $H_\alpha^{s-1}(\Gamma)$. Then it is evident from (3.14) that

$$\begin{aligned} &\mathcal{V}_\Gamma^{(\alpha)}\varphi(P) - \vartheta^* V(\vartheta^*)^{-1}M\varphi(P) \\ &= \int_\Gamma\left(2\Psi_{k,\alpha}(P-Q) - \frac{\mathbf{e}^{i\alpha(X-x)}}{\pi}\left(\log\frac{1}{|\vartheta(P)-\vartheta(Q)|}+c\right)\right)\varphi(Q)\,d\sigma_Q \\ &= \frac{1}{\pi}\int_\Gamma\left(\mathbf{e}^{i\alpha(X-x)}\left(\log\frac{|\vartheta(P)-\vartheta(Q)|}{\rho(P-Q)}\right.\right. \\ &\qquad\left.\left. + (1-\mathbf{e}^{i\alpha\sin(x-X)})\log\rho(P-Q) - c\right) + f(P-Q)\right)\varphi(Q)\,d\sigma_Q. \end{aligned}$$

Since the kernel is C^∞ if $\rho(P-Q)\neq 0$ one has only to study its behavior for $\rho(P-Q)\to 0$. From (3.12), the relations

$$|\vartheta(P)-\vartheta(Q)|^2 = 4\mathbf{e}^{-Y-y}\left(\sin^2\frac{X-x}{2}+\sinh^2\frac{Y-y}{2}\right) = \mathbf{e}^{-Y-y}\rho^2(P-Q) \tag{3.29}$$

and

$$|\nabla(1 - \mathbf{e}^{-i\alpha \sin X}) \log \rho(P)| \leq c|\log \rho(P)|$$

we derive that

$$\begin{aligned}\mathcal{V}_\Gamma^{(\alpha)}\varphi(P) &- \vartheta^* V(\vartheta^*)^{-1} M\varphi(P) \\ &= \frac{\mathbf{e}^{i\alpha X}}{2\pi} \int_\Gamma \Big(-Y - y + \widetilde{f}(P-Q)\Big)\, \mathbf{e}^{-i\alpha x} \varphi(Q)\, d\sigma_Q,\end{aligned}$$

where the periodic function $\widetilde{f}$ satisfies $|\nabla \widetilde{f}(P)| \leq c|\log \rho(P)|$ as $\rho(P) \to 0$. Hence $\mathcal{V}_\Gamma^{(\alpha)} - \vartheta^* V(\vartheta^*)^{-1} M$ maps the space $H_\alpha^{-1}(\Gamma)$ boundedly into $H_\alpha^1(\Gamma)$ (cf. [**17**]), which implies that

$$\mathcal{V}_\Gamma^{(\alpha)} - \vartheta^* V(\vartheta^*)^{-1} M : H_\alpha^{s-1}(\Gamma) \longrightarrow H_\alpha^s(\Gamma) \tag{3.30}$$

is compact for $s \in (0,1)$. Additionally, for smooth Γ the $\widetilde{f}(P)$ is C^∞ for $\rho(P) \neq 0$, hence the mapping (3.30) is compact for all s. Thus, the assertions for $\mathcal{V}_\Gamma^{(\alpha)}$ follow from Lemma 3.2.

The assertions concerning $\mathcal{K}_\Gamma^{(\alpha)}$, $\mathcal{H}_\Gamma^{(\alpha)}$ and $\mathcal{L}_\Gamma^{(\alpha)}$ follow from the compactness of the differences

$$\begin{gathered}\mathcal{K}_\Gamma^{(\alpha)} - \vartheta^* K(\vartheta^*)^{-1},\ \mathcal{H}_\Gamma^{(\alpha)} - \vartheta^* H(\vartheta^*)^{-1} : H_\alpha^t(\Gamma) \longrightarrow H_\alpha^t(\Gamma), \\ \mathcal{L}_\Gamma^{(\alpha)} - M^{-1}\vartheta^* K'(\vartheta^*)^{-1} M : H_\alpha^{-t}(\Gamma) \longrightarrow H_\alpha^{-t}(\Gamma), \\ 0 \leq t < 1,\end{gathered} \tag{3.31}$$

which can be shown similarly. For example, by (3.15), respectively (3.24),

$$\begin{aligned}\mathcal{K}_\Gamma^{(\alpha)}\varphi(P) = \frac{1}{\pi}\int_\Gamma \bigg(&\mathbf{e}^{i\alpha(X - x - \sin(X-x))} \frac{\nu(Q)\cdot(\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} \\ &+ \nu(Q)\cdot g(P-Q)\bigg)\varphi(Q)\, d\sigma_Q,\end{aligned}$$

$$\begin{aligned}\vartheta^* K(\vartheta^*)^{-1}&\varphi(P) \\ &= \frac{1}{\pi}\int_\Gamma \mathbf{e}^{i\alpha(X-x)} \frac{\nu(\vartheta(Q))\cdot(\vartheta(P) - \vartheta(Q))}{|\vartheta(P) - \vartheta(Q)|^2}\, \varphi(Q)\, |\vartheta'(Q)|\, d\sigma_Q.\end{aligned}$$

For $\nu(Q) = (\nu_x, \nu_y)$ the normal to $\widetilde{\Gamma}$ at $\vartheta(Q)$ is given by $\nu(\vartheta(Q)) = (-\nu_x \sin x - \nu_y \cos x, \nu_x \cos x - \nu_y \sin x)$, and consequently

$$\nu(Q) \cdot (\sin(X-x), \sinh(Y-y)) = \nu_x \sin(X-x) + \nu_y \sinh(Y-y),$$

$$\nu(\vartheta(Q)) \cdot (\vartheta(P) - \vartheta(Q)) |\vartheta'(Q)| = \mathbf{e}^{-Y-y} \Big(\nu_x \sin(X-x) + \nu_y \big(\mathbf{e}^{Y-y} - \cos(X-x) \big) \Big).$$

Hence by (3.29),

$$\frac{\nu(Q) \cdot (\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} - \frac{\nu(\vartheta(Q)) \cdot (\vartheta(P) - \vartheta(Q))}{|\vartheta(P) - \vartheta(Q)|^2} |\vartheta'(Q)| = \nu_y \frac{\sinh(Y-y) - \mathbf{e}^{Y-y} + \cos(X-x)}{\rho^2(P-Q)} = \nu_y \frac{\cos(X-x) - \cosh(Y-y)}{\rho^2(P-Q)} = -\frac{\nu_y}{2},$$

and we derive

$$\mathcal{K}_\Gamma^{(\alpha)} \varphi(P) - \vartheta^* K (\vartheta^*)^{-1} \varphi(P) = \frac{1}{\pi} \int_\Gamma \left(\nu(Q) \cdot g(P-Q) - \frac{\mathbf{e}^{i\alpha(X-x)} \nu_y}{2} \right) \varphi(Q) \, d\sigma_Q + \frac{\mathbf{e}^{i\alpha X}}{\pi} \int_\Gamma \big(\mathbf{e}^{i\alpha \sin(x-X)} - 1 \big) \frac{\nu(Q) \cdot (\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} \times \mathbf{e}^{-i\alpha x} \varphi(Q) \, d\sigma_Q.$$

Analogously,

$$\mathcal{H}_\Gamma^{(\alpha)} \varphi(P) - \vartheta^* H (\vartheta^*)^{-1} \varphi(P) = \frac{1}{\pi} \int_\Gamma \left(\tau(Q) \cdot g(P-Q) - \frac{\mathbf{e}^{i\alpha(X-x)} \tau_y}{2} \right) \varphi(Q) \, d\sigma_Q + \frac{\mathbf{e}^{i\alpha X}}{\pi} \int_\Gamma \big(\mathbf{e}^{i\alpha \sin(x-X)} - 1 \big) \times \frac{\tau(Q) \cdot (\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} \mathbf{e}^{-i\alpha x} \varphi(Q) \, d\sigma_Q$$

with $\tau(Q) = (\tau_x, \tau_y)$. The components of the vector function

$$\begin{aligned}\big(1 - \mathbf{e}^{i\alpha \sin(x-X)}\big) \frac{(\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} &= i\alpha \sin(X-x) \frac{(\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} \\ &\quad + O(\rho(P-Q))\end{aligned}$$

generate compact operators in $H^t_\alpha(\Gamma)$. This follows from the relation

$$\begin{aligned}\sin(X-x) \frac{(\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} &= (\sin(X-x), \sinh(Y-y)) \partial_X \log \rho(P-Q) \\ &= \partial_X \big(\sin(X-x), \sinh(Y-y)) \log \rho(P-Q)\big) \\ &\quad - (\cos(X-x), 0) \log \rho(P-Q),\end{aligned}$$

which shows that $(\mathcal{K}^{(\alpha)}_\Gamma - \vartheta^* K (\vartheta^*)^{-1})\varphi$, $(\mathcal{H}^{(\alpha)}_\Gamma - \vartheta^* H (\vartheta^*)^{-1})\varphi \in H^{1-\varepsilon}_\alpha(\Gamma)$ for any $\varepsilon > 0$ if $\varphi \in L_2(\Gamma)$.

Since for $\nu(P) = (\nu_X, \nu_Y)$

$$\frac{\nu(P) \cdot (\sin(X-x), Y-y)}{\rho^2(P-Q)} - \frac{\nu(\vartheta(P)) \cdot (\vartheta(P) - \vartheta(Q))}{|\vartheta(P) - \vartheta(Q)|^2} \, |\vartheta'(Q)| \mathbf{e}^{-Y+y} = \frac{\nu_Y}{2},$$

one can write

$$\begin{aligned}\mathcal{L}^{(\alpha)}_\Gamma \varphi(P) - M^{-1} \vartheta^* K' (\vartheta^*)^{-1} M \varphi(P) &= \frac{1}{\pi} \int_\Gamma \left(\nu(P) \cdot g(P-Q) + \frac{\mathbf{e}^{i\alpha(X-x)} \nu_Y}{2} \right) \varphi(Q) \, d\sigma_Q \\ &\quad - \frac{\mathbf{e}^{i\alpha X}}{\pi} \int_\Gamma \big(\mathbf{e}^{i\alpha \sin(x-X)} - 1 \big) \\ &\quad \times \frac{\nu(P) \cdot (\sin(X-x), \sinh(Y-y))}{\rho^2(P-Q)} \, \mathbf{e}^{-i\alpha x} \, \varphi(Q) \, d\sigma_Q,\end{aligned}$$

which is compact in $H^{-t}_\alpha(\Gamma)$. □

From Lemmas 3.1 and 3.2 we obtain

Corollary 3.2. *The operator* $\mathcal{V}_\Gamma^{(\alpha)} : H_\alpha^{-1/2}(\Gamma) \to H_\alpha^{1/2}(\Gamma)$ *is invertible if and only if the homogeneous Dirichlet problem in both of the domains* G_+ *and* G_-

$$\Delta u + k^2 u = 0, \qquad u|_\Sigma = 0 \text{ and } u \text{ satisfies (3.8)}, \tag{3.32}$$

have only the trivial solution.

Remark 3.1. Two well-known sufficient conditions for the unique solvability of (3.32) in G_+ (and consequently in G_-) are

• $\operatorname{Im} k^2 > 0$;

• the profile curve Σ is non-overhanging, i.e., the y-component of the normal satisfies $\nu_y(P) \le 0$ for all $P \in \Sigma$, cf. [**13**, Section 2.4], [**7**].

3.4. Transposed operators. In the following we consider also equations with adjoint operators. It is useful for a physical interpretation that the kernel functions of the adjoints satisfy the radiation condition (3.8). Note that the spaces $H_\alpha^s(\Gamma)$ and $H_{-\alpha}^{-s}(\Gamma)$ are dual with respect to the bilinear form

$$\big[\varphi, \psi\big]_\Gamma := \int_\Gamma \varphi\, \psi \, d\sigma, \tag{3.33}$$

and we will consider transposed operators with respect to (3.33). Hence, if $A : H_\alpha^s(\Gamma) \to H_\alpha^t(\Gamma)$, then the transposed $A' : H_{-\alpha}^{-t}(\Gamma) \to H_{-\alpha}^{-s}(\Gamma)$. From (3.6) we obtain the following connections between the integral operators associated with $\Psi_{k,\alpha}$ and $\Psi_{k,-\alpha}$.

Lemma 3.4. $\big(\mathcal{V}_\Gamma^{(\alpha)}\big)' = \mathcal{V}_\Gamma^{(-\alpha)}$, $\big(\mathcal{K}_\Gamma^{(\alpha)}\big)' = \mathcal{L}_\Gamma^{(-\alpha)}$, $\big(\mathcal{L}_\Gamma^{(\alpha)}\big)' = \mathcal{K}_\Gamma^{(-\alpha)}$,

$$\big(\mathcal{H}_\Gamma^{(\alpha)}\big)'\varphi(P) = \frac{1}{\pi}\int_\Gamma \partial_{\tau(P)} \Psi_{k,-\alpha}(P-Q)\, \varphi(Q)\, d\sigma_Q = \partial_\tau \mathcal{V}_\Gamma^{(-\alpha)} \varphi(P).$$

4. Integral equation formulations for coated gratings.

4.1. Geometry. Here we apply the integral representations to the solution of the conical diffraction problem (2.4)–(2.6) for the special

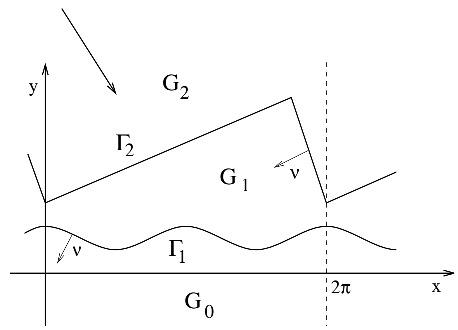

FIGURE 1. Cross section of a coated grating.

case of single-coated gratings, which consist of a substrate (the domain $\mathrm{G}_0 \times \mathbf{R}$) with a periodically corrugated surface which is overcoated with some optical material filling the domain $\mathrm{G}_1 \times \mathbf{R}$ (cf. Figure 1).

The structure is illuminated in $\mathrm{G}_2 \times \mathbf{R}$ by a plane wave which is reflected and, possibly, transmitted in a finite number of outgoing plane waves. We assume that in the (x, y)-plane the interfaces are given by two simple, nonintersecting curves Σ_1 and Σ_2, either C^∞ or piecewise C^2, the open arcs Γ_j, $j = 1, 2$, denote one period of the corresponding profile curve. The wavenumber of the material inside $G_j \times \mathbf{R}$ is denoted by k_j and the z-components of the illuminating field are $u^{(i)}(x, y)\mathbf{e}^{i\gamma z}$, $v^{(i)}(x, y)\mathbf{e}^{i\gamma z}$ with

$$u^{(i)}(x, y) = p_z \mathbf{e}^{i(\alpha+m)x - i\beta y}, \;\; v^{(i)}(x, y) = q_z \mathbf{e}^{i(\alpha+m)x - i\beta y},$$

where $\alpha + m = k_2 \sin\theta \cos\phi$ with $|\alpha| < 1/2$ and $m \in \mathbf{Z}$, $\beta = k_2 \cos\theta \cos\phi$, $\gamma = k_2 \sin\phi$, $|\theta|, |\phi| < \pi/2$.

Assuming $\kappa_j^2 = k_j^2 - \gamma^2 \neq 0$ we look for solutions (E_z, B_z) of the conical diffraction problem (2.4), (2.6) with the transmission conditions (2.5) imposed on the curves Γ_1 and Γ_2. We formulate this as

Problem $\mathbf{D}^{(\alpha)}$: Denote

$$E_z(x,y) = \begin{cases} u_2 + u^{(i)} & \text{in } G_2, \\ u_1 & \text{in } G_1, \\ u_0 & \text{in } G_0, \end{cases} \tag{4.1}$$
$$B_z(x,y) = \begin{cases} v_2 + v^{(i)} & \text{in } G_2, \\ v_1 & \text{in } G_1, \\ v_0 & \text{in } G_0, \end{cases}$$

we seek α-quasiperiodic functions $u_j, v_j \in H^1_{\mathrm{loc}}(G_j)$ such that

(4.2)
$$\text{in } G_j \qquad \Delta u_j + \kappa_j^2 u_j = \Delta v_j + \kappa_j^2 v_j = 0$$

(4.3)
$$\text{on } \Gamma_1 \begin{cases} u_0 = u_1, \ \frac{k_0^2\,\partial_\nu u_0}{\kappa_0^2} - \frac{k_1^2\,\partial_\nu u_1}{\kappa_1^2} = \frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{\kappa_0^2\kappa_1^2}\,\partial_\tau v_1, \\ v_0 = v_1, \ \frac{\partial_\nu v_0}{\kappa_0^2} - \frac{\partial_\nu v_1}{\kappa_1^2} = -\frac{\gamma\,(\kappa_0^2-\kappa_1^2)}{k_2\kappa_0^2\kappa_1^2}\,\partial_\tau u_1, \end{cases}$$

(4.4)
$$\text{on } \Gamma_2 \begin{cases} u_1 = u_2 + u^{(i)}, \ \frac{k_1^2\,\partial_\nu u_1}{\kappa_1^2} - \frac{k_2^2\,\partial_\nu (u_2+u^{(i)})}{\kappa_2^2} = \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\partial_\tau v_1, \\ v_1 = v_2 + v^{(i)}, \ \frac{\partial_\nu v_1}{\kappa_1^2} - \frac{\partial_\nu (v_2+v^{(i)})}{\kappa_2^2} = -\frac{\gamma(\kappa_1^2-\kappa_2^2)}{k_2\kappa_1^2\kappa_2^2}\,\partial_\tau u_1, \end{cases}$$

$$(u_2,v_2)(x,y) = \sum_{n=-\infty}^{\infty} (\widehat{u}_{2n}, \widehat{v}_{2n}) \mathbf{e}^{i(\alpha_n x - \beta_n^{(2)} y)} \quad \text{for } y > H, \tag{4.5}$$
$$(u_0,v_0)(x,y) = \sum_{n=-\infty}^{\infty} (\widehat{u}_{0n}, \widehat{v}_{0n}) \mathbf{e}^{i(\alpha_n x - \beta_n^{(0)} y)} \quad \text{for } y < -H.$$

Here we assume that $\beta_n^{(j)} = \sqrt{\kappa_j^2 - \alpha_n^2} \neq 0$ for all n.

4.2. Integral equations. As proposed in [**14**] we represent the unknown functions using single-layer potentials and Green's formula alternately in consecutive subdomains G_j. Then the transmission conditions lead to integral equations over Γ_j for the densities of the single-layer potentials.

To start with we use Lemma 3.1 to represent

$$u_0 = \frac{1}{2}\big(- V_{\Gamma_1,0}\partial_\nu u_0 + K_{\Gamma_1,0} u_0\big) \quad \text{in } G_0,$$
$$u_2 = \frac{1}{2}\big(V_{\Gamma_2,2}\partial_\nu u_2 - K_{\Gamma_2,2} u_2\big) \quad \text{in } G_2.$$

By $V_{\Gamma_m,j}$ we denote the single layer potential defined on Γ_m with the fundamental solution $\Psi_{\kappa_j,\alpha}$ where $\arg\kappa_j \in [0,\pi)$. Correspondingly $K_{\Gamma_m,j}$ is the double layer potential over Γ_m with the normal derivative of $\Psi_{\kappa_j,\alpha}$ as kernel function. The solution in G_1 is sought by single-layer potentials

$$u_1 = V_{\Gamma_1,1} w_1 + V_{\Gamma_2,1} w_2 \tag{4.6}$$

with certain auxiliary densities $w_j \in H_\alpha^{-1/2}(\Gamma_j)$, $j = 1,2$. Taking the limits on the curves Γ_j the jump relations (3.17) and (3.19) lead to

(4.7)
$$2u_0|_{\Gamma_1} = -\mathcal{V}_{11,0}\partial_\nu u_0 + (I + \mathcal{K}_{11,0})\, u_0,$$
(4.8)
$$u_1|_{\Gamma_1} = \mathcal{V}_{11,1} w_1 + \mathcal{V}_{12,1} w_2, \quad \partial_\nu u_1|_{\Gamma_1} = (I + \mathcal{L}_{11,1}) w_1 + \mathcal{L}_{12,1} w_2,$$
(4.9)
$$u_1|_{\Gamma_2} = \mathcal{V}_{21,1} w_1 + \mathcal{V}_{22,1} w_2, \quad \partial_\nu u_1|_{\Gamma_2} = \mathcal{L}_{21,1} w_1 - (I - \mathcal{L}_{22,1}) w_2,$$
(4.10)
$$2u_2|_{\Gamma_2} = \mathcal{V}_{22,2}\partial_\nu u_2 + (I - \mathcal{K}_{22,2})\, u_2.$$

Here we use the notation

$$\mathcal{V}_{\ell m,j}\varphi(P) = \mathcal{V}_{\ell m,j}^{(\alpha)}\varphi(P) = 2\int_{\Gamma_m} \Psi_{\kappa_j,\alpha}(P-Q)\,\varphi(Q)\,d\sigma_Q, \quad P \in \Gamma_\ell, \tag{4.11}$$

the operators $\mathcal{K}_{\ell m,j} = \mathcal{K}_{\ell m,j}^{(\alpha)}$ and $\mathcal{L}_{\ell m,j} = \mathcal{L}_{\ell m,j}^{(\alpha)}$ are defined analogously. To simplify the notation of the integral operators we will omit the upper index (α) in this section.

Analogously we represent v_j as

$$\begin{aligned} v_0 &= \frac{1}{2}\big(- V_{\Gamma_1,0}\partial_\nu v_0 + K_{\Gamma_1,0} v_0\big),\\ v_2 &= \frac{1}{2}\big(V_{\Gamma_2,2}\partial_\nu v_2 - K_{\Gamma_2,2} v_2\big),\\ v_1 &= V_{\Gamma_1,1}\tau_1 + V_{\Gamma_2,1}\tau_2 \end{aligned} \tag{4.12}$$

with $\tau_j \in H_\alpha^{-1/2}(\Gamma_j)$, which imply the equations (4.7)–(4.10) with u replaced by v and w replaced by τ.

By substituting (4.8) into (4.7) and taking into account the interface conditions (4.3) for u_j and $\partial_\nu u_j$, one obtains

$$\frac{k_1^2}{\kappa_1^2}\mathcal{V}_{11,0}\big((I+\mathcal{L}_{11,1})w_1+\mathcal{L}_{12,1}w_2\big) + \frac{k_0^2}{\kappa_0^2}\big(I-\mathcal{K}_{11,0}\big)\big(\mathcal{V}_{11,1}w_1+\mathcal{V}_{12,1}w_2\big) + \frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{\kappa_0^2\kappa_1^2}\mathcal{V}_{11,0}\,\partial_\tau v_1 = 0.$$

Now we use (3.23) to introduce the singular integral

(4.13)
$$\mathcal{H}_{1,0}v_1(P) = -\mathcal{V}_{11,0}\,\partial_\tau v_1(P) = 2\int_{\Gamma_1} v_1(Q)\,\partial_{\tau_Q}\Psi_{\kappa_0,\alpha}(P-Q)\,d\sigma_Q,\ P\in\Gamma_1.$$

Hence, by relation (4.8) specified for $v_1|_{\Gamma_1}$ the last equation transforms to

$$\frac{k_1^2}{\kappa_1^2}\mathcal{V}_{11,0}\big((I+\mathcal{L}_{11,1})w_1+\mathcal{L}_{12,1}w_2\big) + \frac{k_0^2}{\kappa_0^2}\big(I-\mathcal{K}_{11,0}\big)\big(\mathcal{V}_{11,1}w_1+\mathcal{V}_{12,1}w_2\big) - \frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{\kappa_0^2\kappa_1^2}\,\mathcal{H}_{1,0}\big(\mathcal{V}_{11,1}\tau_1+\mathcal{V}_{12,1}\tau_2\big) = 0. \tag{4.14}$$

Based on relation (4.7) for v_0 and using (4.3) for v_j and $\partial_\nu v_j$ we get a second equation on Γ_1

$$\frac{1}{\kappa_1^2}\mathcal{V}_{11,0}\big((I+\mathcal{L}_{11,1})\tau_1+\mathcal{L}_{12,1}\tau_2\big) + \frac{1}{\kappa_0^2}\big(I-\mathcal{K}_{11,0}\big)\big(\mathcal{V}_{11,1}\tau_1+\mathcal{V}_{12,1}\tau_2\big) + \frac{\gamma(\kappa_0^2-\kappa_1^2)}{k_2\kappa_0^2\kappa_1^2}\,\mathcal{H}_{1,0}(\mathcal{V}_{11,1}w_1+\mathcal{V}_{12,1}w_2) = 0. \tag{4.15}$$

Concerning the equations on the upper profile Γ_2 we note that Lemma 3.1 gives

$$u^{(i)} = \frac{1}{2}\big(K_{\Gamma_2,2}u^{(i)} - V_{\Gamma_2,2}\partial_\nu u^{(i)}\big) \quad \text{in } G_0 \cup \Sigma_1 \cup G_1,$$

and therefore (4.10) implies

$$\mathcal{V}_{22,2}\,\partial_\nu(u_2 + u^{(i)}) - (I + \mathcal{K}_{22,2})(u_2 + u^{(i)}) = -2u^{(i)}.$$

By using (4.9) and the transmission condition (4.4) this equation is transformed to

$$\begin{aligned}\text{(4.16)}\quad \frac{k_1^2}{\kappa_1^2}\mathcal{V}_{22,2}\,(\mathcal{L}_{21,1}w_1 - (I - \mathcal{L}_{22,1})w_2)& \\ - \frac{k_2^2}{\kappa_2^2}\,(I + \mathcal{K}_{22,2})\,(\mathcal{V}_{21,1}w_1 + \mathcal{V}_{22,1}w_2)& \\ + \frac{\gamma k_2(\kappa_1^2 - \kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{H}_{2,2}\,(\mathcal{V}_{21,1}\tau_1 + \mathcal{V}_{22,1}\tau_2)& \\ = -\frac{2k_2^2}{\kappa_2^2}\,u^{(i)},&\end{aligned}$$

where the last term on the left follows from (4.9) for $v_1|_{\Gamma_2}$ and from the definition
(4.17)

$$\mathcal{H}_{2,2}v_1(P) = -\mathcal{V}_{22,2}\partial_\tau v_1(P) = 2\int_{\Gamma_2} v_1(Q)\,\partial_{\tau_Q}\Psi_{\kappa_2,\alpha}(P-Q)\,d\sigma_Q.$$

The equation corresponding to the remaining jump condition on Γ_2 reads as

$$\begin{aligned}\text{(4.18)}\quad \frac{1}{\kappa_1^2}\mathcal{V}_{22,2}\,(\mathcal{L}_{21,1}\tau_1 - (I - \mathcal{L}_{22,1})\tau_2)& \\ - \frac{1}{\kappa_2^2}\,(I + \mathcal{K}_{22,2})\,(\mathcal{V}_{21,1}\tau_1 + \mathcal{V}_{22,1}\tau_2)& \\ - \frac{\gamma(\kappa_1^2 - \kappa_2^2)}{k_2\kappa_1^2\kappa_2^2}\,\mathcal{H}_{2,2}(\mathcal{V}_{21,1}w_1 + \mathcal{V}_{22,1}w_2)& \\ = -\frac{2}{\kappa_2^2}\,v^{(i)}.&\end{aligned}$$

The equations (4.14), (4.15), (4.16) and (4.18) form a system of singular integral equations for the unknowns w_j and τ_j. The first two equations are given on Γ_1, whereas the last two are imposed on Γ_2.

Remark 4.1. In the case $\gamma = 0$, i.e., incidence parallel to the (x, y)-plane, the two equations (4.14), (4.16) describe the TE polarization and (4.15), (4.18) the TM polarization case. These equations have been introduced in [**14**]. It is shown that they are optimal with respect to the numerical expense compared with other integral equation formulations. Some issues of the implementation and fast solution of the integral equations with $\gamma = 0$ using spline and polynomial collocation methods are discussed in [**16**].

4.3. Structure of the system. After multiplying (4.15), (4.18) with k_2^2 and suitable ordering of the unknowns we write (4.14), (4.15), (4.16) and (4.18) as an equation with a 4×4 operator matrix

$$\mathbf{A}^{(\alpha)} W = \mathbf{a}^{(\alpha)}, \tag{4.19}$$

where we denote

$$\mathbf{A}^{(\alpha)} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{pmatrix},$$

$$W = \begin{pmatrix} w_1 \\ \tau_1 \\ w_2 \\ \tau_2 \end{pmatrix}, \quad \mathbf{a}^{(\alpha)} = \frac{2k_2^2}{\kappa_2^2} \begin{pmatrix} 0 \\ 0 \\ u^{(i)} \\ v^{(i)} \end{pmatrix}.$$

Here the sign (α) indicates that all integral operators appearing in $\mathbf{A}^{(\alpha)}$ are connected with the fundamental solutions $\Psi_{\kappa_j,\alpha}$, and $u^{(i)} = p_z \mathbf{e}^{i(\alpha+m)x - i\beta y}$, $v^{(i)} = q_z \mathbf{e}^{i(\alpha+m)x - i\beta y}$. We remark that as long as $(\alpha+n)^2 < \kappa_2^2$ the system (4.19) with $u^{(i)} = p_z \mathbf{e}^{i(\alpha+n)x - i\beta_n^{(2)} y}$, $v^{(i)} = q_z \mathbf{e}^{i(\alpha+n)x - i\beta_n^{(2)} y}$ has the physical interpretation of the diffraction of a plane wave with the wave vector $(\alpha+n, -\beta_n^{(2)}, \gamma)$, since $\beta_n^{(2)} = \sqrt{\kappa_2^2 - (\alpha+n)^2} > 0$.

The 2×2 diagonal blocks $\mathcal{A}_{11}$ and $\mathcal{A}_{22}$ of $\mathbf{A}^{(\alpha)}$ have the elements

$$
(4.20)\qquad
\begin{aligned}
&\mathcal{A}_{11}: \begin{cases} A_{11} = \frac{k_1^2}{\kappa_1^2}\mathcal{V}_{11,0}(I+\mathcal{L}_{11,1}) + \frac{k_0^2}{\kappa_0^2}\big(I-\mathcal{K}_{11,0}\big)\mathcal{V}_{11,1}, \\ A_{12} = -A_{21} = -\frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{\kappa_0^2\kappa_1^2}\,\mathcal{H}_{1,0}\mathcal{V}_{11,1}, \\ A_{22} = \frac{k_2^2}{\kappa_1^2}\mathcal{V}_{11,0}(I+\mathcal{L}_{11,1}) + \frac{k_2^2}{\kappa_0^2}(I-\mathcal{K}_{11,0})\mathcal{V}_{11,1}, \end{cases} \\
&\mathcal{A}_{22}: \begin{cases} A_{33} = \frac{k_2^2}{\kappa_2^2}(I+\mathcal{K}_{22,2})\mathcal{V}_{22,1} + \frac{k_1^2}{\kappa_1^2}\mathcal{V}_{22,2}(I-\mathcal{L}_{22,1}), \\ A_{34} = -A_{43} = -\frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{H}_{2,2}\mathcal{V}_{22,1}, \\ A_{44} = \frac{k_2^2}{\kappa_2^2}(I+\mathcal{K}_{22,2})\mathcal{V}_{22,1} + \frac{k_2^2}{\kappa_1^2}\mathcal{V}_{22,2}(I-\mathcal{L}_{22,1}), \end{cases}
\end{aligned}
$$

and we conclude from Lemma 3.3 that

$$
(4.21)\qquad \mathcal{A}_{jj} : \big(H_\alpha^{s-1}(\Gamma_j)\big)^2 \to \big(H_\alpha^{s}(\Gamma_j)\big)^2, \quad s \in (0,1),
$$

are bounded operators. Here $\big(H_\alpha^{s}(\Gamma_j)\big)^2$ denotes the space of vector functions (w,τ) with components from $H_\alpha^s(\Gamma_j)$. The two off-diagonal blocks of $\mathbf{A}^{(\alpha)}$ are given by

$$
\begin{aligned}
&\mathcal{A}_{12}: \begin{cases} A_{13} = \frac{k_1^2}{\kappa_1^2}\mathcal{V}_{11,0}\mathcal{L}_{12,1} + \frac{k_0^2}{\kappa_0^2}(I-\mathcal{K}_{11,0})\mathcal{V}_{12,1}, \\ A_{14} = -A_{23} = -\frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{\kappa_0^2\kappa_1^2}\,\mathcal{H}_{1,0}\mathcal{V}_{12,1}, \\ A_{24} = \frac{k_2^2}{\kappa_1^2}\mathcal{V}_{11,0}\mathcal{L}_{12,1} + \frac{k_2^2}{\kappa_0^2}(I-\mathcal{K}_{11,0})\mathcal{V}_{12,1}, \end{cases} \\
&\mathcal{A}_{21}: \begin{cases} A_{31} = -\frac{k_1^2}{\kappa_1^2}\mathcal{V}_{22,2}\mathcal{L}_{21,1} + \frac{k_2^2}{\kappa_2^2}(I+\mathcal{K}_{22,2})\mathcal{V}_{21,1}, \\ A_{32} = -A_{41} = -\frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{H}_{2,2}\mathcal{V}_{21,1}, \\ A_{42} = -\frac{k_2^2}{\kappa_1^2}\mathcal{V}_{22,2}\mathcal{L}_{21,1} + \frac{k_2^2}{\kappa_2^2}(I+\mathcal{K}_{22,2})\mathcal{V}_{21,1}, \end{cases}
\end{aligned}
$$

and obviously

$$
(4.22)\qquad
\begin{aligned}
&\mathcal{A}_{12} : \big(H_\alpha^{s-1}(\Gamma_2)\big)^2 \longrightarrow \big(H_\alpha^{s}(\Gamma_1)\big)^2, \\
&\mathcal{A}_{21} : \big(H_\alpha^{s-1}(\Gamma_1)\big)^2 \longrightarrow \big(H_\alpha^{s}(\Gamma_2)\big)^2, \quad s \in (0,1),
\end{aligned}
$$

are bounded. Hence the system (4.19) generates a bounded operator

$$\mathbf{A}^{(\alpha)} : \big(H^{s-1}_\alpha(\Gamma_1)\big)^2 \times \big(H^{s-1}_\alpha(\Gamma_2)\big)^2 \to \big(H^{s}_\alpha(\Gamma_1)\big)^2 \times \big(H^{s}_\alpha(\Gamma_2)\big)^2,$$

where $s \in (0,1)$ for the curves Γ_j with corners, and $s \in \mathbf{R}$ in the case of smooth Γ_j.

4.4. Transposed system. Similarly, the use of the single layer ansatz outside, i.e.,

$$u_0 = V_{\Gamma_1,0} w_1,\ v_0 = V_{\Gamma_1,0}\tau_1,\ u_2 = V_{\Gamma_2,2} w_2,\ v_2 = V_{\Gamma_2,2}\tau_2 \tag{4.23}$$

in G_0, respectively G_2, with w_j, $\tau_j \in H^{-1/2}_\alpha(\Gamma_j)$, and Green's formula representation in G_1 (see (3.10))

$$\begin{aligned} u_1 &= \frac{1}{2}\big(V_{\Gamma_1,1}\,\partial_\nu u_1 - K_{\Gamma_1,1} u_1 - V_{\Gamma_2,1}\,\partial_\nu u_1 + K_{\Gamma_2,1} u_1\big),\\ v_1 &= \frac{1}{2}\big(V_{\Gamma_1,1}\,\partial_\nu v_1 - K_{\Gamma_1,1} v_1 - V_{\Gamma_2,1}\,\partial_\nu v_1 + K_{\Gamma_2,1} v_1\big), \end{aligned} \tag{4.24}$$

lead to a system of integral equations

$$\mathbf{B}^{(\alpha)} W = \begin{pmatrix} B_{11} & B_{12} & B_{13} & B_{14}\\ B_{21} & B_{22} & B_{23} & B_{24}\\ B_{31} & B_{32} & B_{33} & B_{34}\\ B_{41} & B_{42} & B_{43} & B_{44} \end{pmatrix} \begin{pmatrix} w_1\\ \tau_1\\ w_2\\ \tau_2 \end{pmatrix} = \mathbf{b}^{(\alpha)}, \tag{4.25}$$

where the elements of $\mathbf{B}^{(\alpha)}$ are given by

$$\begin{aligned} B_{11} &= \frac{k_1^2}{\kappa_1^2}\,(I + \mathcal{K}_{11,1})\mathcal{V}_{11,0} + \frac{k_0^2}{\kappa_0^2}\,\mathcal{V}_{11,1}(I - \mathcal{L}_{11,0}),\\ B_{12} &= -B_{21} = \frac{\gamma k_2(\kappa_0^2 - \kappa_1^2)}{\kappa_0^2\kappa_1^2}\,\mathcal{V}_{11,1}\partial_\tau \mathcal{V}_{11,0},\\ B_{13} &= \frac{k_2^2}{\kappa_2^2}\,\mathcal{V}_{12,1}(I + \mathcal{L}_{22,2}) - \frac{k_1^2}{\kappa_1^2}\,\mathcal{K}_{12,1}\mathcal{V}_{22,2},\\ B_{14} &= -B_{23} = \frac{\gamma k_2(\kappa_1^2 - \kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{V}_{12,1}\partial_\tau \mathcal{V}_{22,2},\\ B_{22} &= \frac{k_2^2}{\kappa_1^2}\,(I + \mathcal{K}_{11,1})\mathcal{V}_{11,0} + \frac{k_2^2}{\kappa_0^2}\,\mathcal{V}_{11,1}(I - \mathcal{L}_{11,0}), \end{aligned}$$

$$
\begin{aligned}
B_{24} &= \frac{k_2^2}{\kappa_2^2}\,\mathcal{V}_{12,1}(I+\mathcal{L}_{22,2}) - \frac{k_2^2}{\kappa_1^2}\,\mathcal{K}_{12,1}\mathcal{V}_{22,2},\\
B_{31} &= \frac{k_1^2}{\kappa_1^2}\,\mathcal{K}_{21,1}\mathcal{V}_{11,0} + \frac{k_0^2}{\kappa_0^2}\,\mathcal{V}_{21,1}(I-\mathcal{L}_{11,0}),\\
B_{32} &= -B_{41} = \frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{\kappa_0^2\kappa_1^2}\,\mathcal{V}_{21,1}\partial_\tau\mathcal{V}_{11,0},\\
B_{33} &= \frac{k_2^2}{\kappa_2^2}\,\mathcal{V}_{22,1}(I+\mathcal{L}_{22,2}) + \frac{k_1^2}{\kappa_1^2}\,(I-\mathcal{K}_{22,1})\mathcal{V}_{22,2},\\
B_{34} &= -B_{43} = \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{V}_{22,1}\partial_\tau\mathcal{V}_{22,2},\\
B_{42} &= \frac{k_2^2}{\kappa_1^2}\,\mathcal{K}_{21,1}\mathcal{V}_{11,0} + \frac{k_2^2}{\kappa_0^2}\,\mathcal{V}_{21,1}(I-\mathcal{L}_{11,0}),\\
B_{44} &= \frac{k_2^2}{\kappa_2^2}\,\mathcal{V}_{22,1}(I+\mathcal{L}_{22,2}) + \frac{k_2^2}{\kappa_1^2}\,(I-\mathcal{K}_{22,1})\mathcal{V}_{22,2}.
\end{aligned}
$$

The right-hand side $\mathbf{b}^{(\alpha)} \in \left(H_\alpha^{1/2}(\Gamma_1)\right)^2 \times \left(H_\alpha^{1/2}(\Gamma_2)\right)^2$ of (4.25) has the components

(4.26)

$$
\begin{aligned}
b_1^{(\alpha)} &= \frac{k_1^2}{\kappa_1^2}\,\mathcal{K}_{12,1}u^{(i)} - \frac{k_2^2}{\kappa_2^2}\,\mathcal{V}_{12,1}\partial_\nu u^{(i)} - \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{V}_{12,1}\partial_\tau v^{(i)},\\
b_2^{(\alpha)} &= \frac{k_2^2}{\kappa_1^2}\,\mathcal{K}_{12,1}v^{(i)} - \frac{k_2^2}{\kappa_2^2}\,\mathcal{V}_{12,1}\partial_\nu v^{(i)} + \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{V}_{12,1}\partial_\tau u^{(i)},\\
b_3^{(\alpha)} &= \frac{k_1^2}{\kappa_1^2}\,(\mathcal{K}_{22,1}-I)u^{(i)} - \frac{k_2^2}{\kappa_2^2}\,\mathcal{V}_{22,1}\partial_\nu u^{(i)} - \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{V}_{22,1}\partial_\tau v^{(i)},\\
b_4^{(\alpha)} &= \frac{k_2^2}{\kappa_1^2}\,(\mathcal{K}_{22,1}-I)v^{(i)} - \frac{k_2^2}{\kappa_2^2}\,\mathcal{V}_{22,1}\partial_\nu v^{(i)} + \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{V}_{22,1}\partial_\tau u^{(i)}.
\end{aligned}
$$

Recall that $u^{(i)} = p_z \mathbf{e}^{i(\alpha+m)x-i\beta y}$, $v^{(i)} = q_z \mathbf{e}^{i(\alpha+m)x-i\beta y}$ and that the integral operators are connected with the fundamental solutions $\Psi_{\kappa_j,\alpha}$.

Due to the following observation we call (4.25) a transposed system. Suppose that the field illuminating the given grating has the wave vector $(-\alpha-m,-\beta,\gamma)$. Then the ansatz (4.23), (4.24) with w_j, $\tau_j \in H_{-\alpha}^{-1/2}(\Gamma_j)$ leads to the equations (4.25), but the integral operators are associated with the fundamental solutions $\Psi_{\kappa_j,-\alpha}$ and the right-hand side is determined by $u^{(i)} = p_z \mathbf{e}^{-i(\alpha+m)x-i\beta y}$, $v^{(i)} = q_z \mathbf{e}^{-i(\alpha+m)x-i\beta y}$.

By using (3.6) and Lemma (3.4) it is easy to see that the elements B_{jk} of the corresponding 4×4 operator matrix which we denote by $\mathbf{B}^{(-\alpha)}$ are the transpose of the elements A_{kj} of $\mathbf{A}^{(\alpha)}$. Moreover, if we define for $W = (w_1, \tau_1, w_2, \tau_2)$, $\Phi = (\varphi_1, \psi_1, \varphi_2, \psi_2)$ the bilinear form

$$[W, \Phi] = \sum_{j=1}^{2} [w_j, \varphi_j]_{\Gamma_j} + [\tau_j, \psi_j]_{\Gamma_j}, \tag{4.27}$$

cf. (3.33), where $W \in (H^s_\alpha(\Gamma_1))^2 \times (H^s_\alpha(\Gamma_2))^2$, $\Phi \in (H^{-s}_{-\alpha}(\Gamma_1))^2 \times (H^{-s}_{-\alpha}(\Gamma_2))^2$, then we obtain

Lemma 4.1. *For any α the operator $\mathbf{B}^{(-\alpha)}$ is the transpose of $\mathbf{A}^{(\alpha)}$ with respect to* (4.27)*, i.e.,*

$$[\mathbf{A}^{(\alpha)} W, \Phi] = [W, \mathbf{B}^{(-\alpha)} \Phi]$$

for all $W \in (H^{-1/2}_\alpha(\Gamma_1))^2 \times (H^{-1/2}_\alpha(\Gamma_2))^2$ and $\Phi \in (H^{-1/2}_{-\alpha}(\Gamma_1))^2 \times (H^{-1/2}_{-\alpha}(\Gamma_2))^2$.

Remark 4.2. Obviously, the structure of the 2×2 diagonal blocks of $\mathbf{A}^{(\alpha)}$ and $\mathbf{B}^{(\alpha)}$ is determined only by the chosen representation of the solutions on both sides of the interface Σ_j. So the Green's formula representation below and the single layer representation above Σ_j lead to a 2×2 matrix block for the densities w_j, τ_j which is structured as $\mathcal{A}_{11}$ or the matrix $\mathcal{B}_{22} = (B_{ik})^4_{i,k=3}$, whereas in the opposite case the matrix structure is analog to $\mathcal{A}_{22}$ or $\mathcal{B}_{11} = (B_{ik})^2_{i,k=1}$.

Consider, in particular, the conical diffraction on noncoated gratings, for example the grating depicted in Figure 1 with $k_0 = k_1$. Then the single layer potential ansatz $u_1 = V_{\Gamma_2,1} w_2$, $v_1 = V_{\Gamma_2,1} \tau_2$ in $\overline{G_0 \cap G_1}$ and

$$u_2 = \frac{1}{2}\big(V_{\Gamma_2,2} \partial_\nu u_2 - K_{\Gamma_2,2} u_2\big), \qquad v_2 = \frac{1}{2}\big(V_{\Gamma_2,2} \partial_\nu v_2 - K_{\Gamma_2,2} v_2\big) \quad \text{in } G_2$$

lead to the system

$$\mathcal{A}_{22} \begin{pmatrix} w_2 \\ \tau_2 \end{pmatrix} = \frac{2k_2^2}{\kappa_2^2} \begin{pmatrix} u^{(i)} \\ v^{(i)} \end{pmatrix}.$$

The representations $u_2 = V_{\Gamma_2,2}w_2$, $v_1 = V_{\Gamma_2,2}\tau_2$ in the upper domain G_2 and the representation formula

$$u_1 = \frac{1}{2}\big(K_{\Gamma_2,1}u_1 - V_{\Gamma_2,1}\partial_\nu u_1\big),$$
$$v_1 = \frac{1}{2}\big(K_{\Gamma_2,1}v_1 - V_{\Gamma_2,1}\partial_\nu v_1\big) \quad \text{in } G_0 \cap \Sigma_1 \cap G_1$$

imply the integral equation system

$$\mathcal{B}_{22}\begin{pmatrix} w_2 \\ \tau_2 \end{pmatrix} = \begin{pmatrix} b_3^{(\alpha)} \\ b_4^{(\alpha)} \end{pmatrix}.$$

5. Solvability of the integral equations. Here we show that the systems (4.19) with the operator matrix $\mathbf{A}^{(\alpha)}$ and (4.25) with $\mathbf{B}^{(\alpha)}$ are equivalent to the diffraction problem $\mathbf{D}^{(\alpha)}$ if the two conditions

(A) the operators $\mathcal{V}_{11,0}^{(\alpha)}$ and $\mathcal{V}_{22,2}^{(\alpha)}$ are invertible,

(B) the operators $\mathcal{V}_{11,1}^{(\alpha)}$ and $\mathcal{V}_{22,1}^{(\alpha)}$ are invertible,

are satisfied. Recall the definition of the single layer potentials

$$\mathcal{V}_{\ell\ell,j}^{(\alpha)}\varphi(P) = \mathcal{V}_{\ell\ell,j}\varphi(P) = 2\int_{\Gamma_\ell} \Psi_{\kappa_j,\alpha}(P-Q)\,\varphi(Q)\,d\sigma_Q, \quad P \in \Gamma_\ell.$$

Furthermore, the operators $\mathbf{A}^{(\alpha)}$ and $\mathbf{B}^{(\alpha)}$ are Fredholm with index 0 and satisfy a Gårding inequality, if the condition (2.7) is satisfied. This will be shown in subsection 5.2.

From Remark 4.2 and the proofs given below it follows easily that the results apply to the integral equation systems which are obtained for multiple-coated gratings by using the alternate single-layer potential and Green's formula representations.

5.1. Equivalence. The conditions which ensure that a solution of the system (4.19) or (4.25) provides a solution of the diffraction problem $\mathbf{D}^{(\alpha)}$ and vice versa are formulated in the following

Proposition 5.1. (i) *Under condition* (A) *any solution of* (4.19) *provides a solution of* $\mathbf{D}^{(\alpha)}$.

(ii) *Under condition* (B) *any solution of* $\mathbf{D}^{(\alpha)}$ *provides a solution of* (4.19).

Proposition 5.2. (i) *If condition* (B) *holds, then any solution of* (4.25) *provides a solution of* $\mathbf{D}^{(\alpha)}$.

(ii) *Let* $u_j, v_j \in H^1_{\mathrm{loc}}(G_j)$ *be a solution of* $\mathbf{D}^{(\alpha)}$ *and assume condition* (A). *Then*

$$w_1 = \mathcal{V}_{11,0}^{-1} u_0, \ \tau_1 = \mathcal{V}_{11,0}^{-1} v_0, \ w_2 = \mathcal{V}_{22,2}^{-1} u_2, \ \tau_1 = \mathcal{V}_{22,2}^{-1} v_2.$$

is a solution of (4.25).

For the proof we need some properties of the single layer potentials in the domain G_1.

Lemma 5.1. (i) *If* $V_{\Gamma_1,1}\varphi_1 = V_{\Gamma_2,1}\varphi_2$ *in* G_1, $\varphi_j \in H_\alpha^{-1/2}(\Gamma_j)$, *then* $V_{\Gamma_1,1}\varphi_1 = V_{\Gamma_2,1}\varphi_2 = 0$.

(ii) *Under condition* (B) *any* α*-quasiperiodic solution of* $\Delta u + \kappa_1^2 u = 0$ *in* G_1 *admits the unique representation*

$$u = V_{\Gamma_1,1}\varphi_1 + V_{\Gamma_2,1}\varphi_2, \quad \varphi_j \in H_\alpha^{-1/2}(\Gamma_j).$$

Proof. (i) The function w which coincides with

$$w_1(P) = V_{\Gamma_1,1}\varphi_1(P), \ P \in G_1 \cup \Sigma_2 \cup G_2,$$

and

$$w_2(P) = V_{\Gamma_2,1}\varphi_2(P), \ P \in G_0 \cup \Sigma_1 \cup G_1,$$

is smooth, solves the Helmholtz equation $\Delta u + \kappa_j^2 u = 0$ in $\mathbf{R}^2$ and satisfies the outgoing wave condition for $|y| \to \infty$. Thus $w_1 = 0$ in $\overline{G_1 \cup G_2}$ and $w_2 = 0$ in $\overline{G_0 \cup G_1}$.

(ii) Since by (3.10)

$$u = \frac{1}{2}\big(V_{\Gamma_1,1}\,\partial_\nu u - K_{\Gamma_1,1}u - V_{\Gamma_2,1}\,\partial_\nu u + K_{\Gamma_2,1}u\big),$$

and $\mathcal{V}_{jj,1}$ are invertible, there exist uniquely defined $\varphi_j \in H_\alpha^{-1/2}(\Gamma_j)$ such that

$$V_{\Gamma_1,1}\varphi_1 = \frac{1}{2}\big(V_{\Gamma_1,1}\,\partial_\nu u - K_{\Gamma_1,1}u\big) \quad \text{in } G_1 \cup \Sigma_2 \cup G_2,$$
$$V_{\Gamma_2,1}\varphi_2 = \frac{1}{2}\big(K_{\Gamma_2,1}u - V_{\Gamma_2,1}\,\partial_\nu u\big) \quad \text{in } G_0 \cup \Sigma_1 \cup G_1. \qquad \square$$

Proof of Proposition 5.1. For arbitrary $w_j, \tau_j \in H_\alpha^{-1/2}(\Gamma_j)$, $j = 1, 2$, the functions

$$u_1 = V_{\Gamma_1,1}w_1 + V_{\Gamma_2,1}w_2, \qquad v_1 = V_{\Gamma_1,1}\tau_1 + V_{\Gamma_2,1}\tau_2, \tag{5.1}$$

are solutions of the Helmholtz equation $\Delta u + \kappa_1^2 u = 0$ in G_1 with $u_1|_{\Gamma_2}, v_1|_{\Gamma_2} \in H_\alpha^{1/2}(\Gamma_2)$, $\partial_\nu u_1|_{\Gamma_2}, \partial_\nu v_1|_{\Gamma_2} \in H_\alpha^{-1/2}(\Gamma_2)$. Therefore,

(5.2)
$$u_2 = \frac{\kappa_2^2}{2k_2^2}\left(V_{\Gamma_2,2}\left(\frac{k_1^2}{\kappa_1^2}\,\partial_\nu u_1 - \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\partial_\tau v_1\right) - \frac{k_2^2}{\kappa_2^2}\,K_{\Gamma_2,2}u_1\right),$$
$$v_2 = \frac{\kappa_2^2}{2}\left(V_{\Gamma_2,2}\left(\frac{1}{\kappa_1^2}\,\partial_\nu v_1 + \frac{\gamma(\kappa_1^2-\kappa_2^2)}{k_2\kappa_1^2\kappa_2^2}\,\partial_\tau u_1\right) - \frac{1}{\kappa_2^2}\,K_{\Gamma_2,2}v_1\right),$$

solve $\Delta u + \kappa_2^2 u = 0$ in G_2, satisfy the outgoing wave condition (4.5) and have the boundary values

$$u_2|_{\Gamma_2} = \frac{\kappa_2^2}{2k_2^2}\left(\mathcal{V}_{22,2}\left(\frac{k_1^2}{\kappa_1^2}\,\partial_\nu u_1 - \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\partial_\tau v_1\right) + \frac{k_2^2}{\kappa_2^2}\,(I-\mathcal{K}_{22,2})u_1\right),$$
$$v_2|_{\Gamma_2} = \frac{\kappa_2^2}{2}\left(\mathcal{V}_{22,2}\left(\frac{1}{\kappa_1^2}\,\partial_\nu v_1 + \frac{\gamma(\kappa_1^2-\kappa_2^2)}{k_2\kappa_1^2\kappa_2^2}\,\partial_\tau u_1\right) + \frac{1}{\kappa_2^2}(I-\mathcal{K}_{22,2})v_1\right).$$

Let w_j, τ_j be a solution of (4.19). Because of

$$\partial_\nu u_1|_{\Gamma_2} = \mathcal{L}_{21,1}w_1 - (I-\mathcal{L}_{22,1})w_2,$$
$$\partial_\nu v_1|_{\Gamma_2} = \mathcal{L}_{21,1}\tau_1 - (I-\mathcal{L}_{22,1})\tau_2,$$

$$\mathcal{H}_{2,2}\,(\mathcal{V}_{21,1}w_1 + \mathcal{V}_{22,1}w_2) = -\mathcal{V}_{22,2}\,\partial_\tau u_1,$$
$$\mathcal{H}_{2,2}\,(\mathcal{V}_{21,1}\tau_1 + \mathcal{V}_{22,1}\tau_2) = -\mathcal{V}_{22,2}\,\partial_\tau v_1,$$

the last two equations of (4.19) imply that

$$\frac{k_1^2}{\kappa_1^2}\,\mathcal{V}_{22,2}\,\partial_\nu u_1 + \frac{k_2^2}{\kappa_2^2}(I-\mathcal{K}_{22,2})u_1 - \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\mathcal{V}_{22,2}\,\partial_\tau v_1 = \frac{2k_2^2}{\kappa_2^2}(u_1-u^{(i)})|_{\Gamma_2},$$

$$\frac{1}{\kappa_1^2}\,\mathcal{V}_{22,2}\,\partial_\nu v_1 + \frac{1}{\kappa_2^2}(I-\mathcal{K}_{22,2})v_1 + \frac{\gamma(\kappa_1^2-\kappa_2^2)}{k_2\kappa_1^2\kappa_2^2}\,\mathcal{V}_{22,2}\,\partial_\tau u_1 = \frac{2}{\kappa_2^2}(v_1-v^{(i)})|_{\Gamma_2},$$

which gives $u_2+u^{(i)}=u_1$, $v_2+v^{(i)}=v_1$ on Γ_2. Since by Corollary 3.1

$$K_{\Gamma_2,2}u^{(i)} = V_{\Gamma_2,2}\partial_\nu u^{(i)}, \quad K_{\Gamma_2,2}v^{(i)} = V_{\Gamma_2,2}\partial_\nu v^{(i)}$$

in G_2, formulas (5.2) transform to

$$\begin{aligned} u_2 &= \frac{1}{2}\Big(V_{\Gamma_2,2}\frac{\kappa_2^2}{k_2^2}\Big(\frac{k_1^2}{\kappa_1^2}\,\partial_\nu u_1 - \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\partial_\tau v_1\Big) \\ &\qquad - K_{\Gamma_2,2}u_2 - V_{\Gamma_2,2}\,\partial_\nu u^{(i)}\Big), \\ v_2 &= \frac{1}{2}\Big(V_{\Gamma_2,2}\,\kappa_2^2\Big(\frac{1}{\kappa_1^2}\,\partial_\nu v_1 + \frac{\gamma(\kappa_1^2-\kappa_2^2)}{k_2\kappa_1^2\kappa_2^2}\,\partial_\tau u_1\Big) \\ &\qquad - K_{\Gamma_2,2}v_2 - V_{\Gamma_2,2}\,\partial_\nu v^{(i)}\Big), \end{aligned}$$

which are valid in G_2. Hence Lemma 3.1 implies

$$\begin{aligned} V_{\Gamma_2,2}\frac{k_2^2}{\kappa_2^2}\big(\partial_\nu u_2 + \partial_\nu u^{(i)}\big) &= V_{\Gamma_2,2}\Big(\frac{k_1^2}{\kappa_1^2}\partial_\nu u_1 - \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\,\partial_\tau v_1\Big), \\ V_{\Gamma_2,2}\frac{1}{\kappa_2^2}\big(\partial_\nu v_2 + \partial_\nu v^{(i)}\big) &= V_{\Gamma_2,2}\Big(\frac{1}{\kappa_1^2}\partial_\nu v_1 + \frac{\gamma(\kappa_1^2-\kappa_2^2)}{k_2\kappa_1^2\kappa_2^2}\,\partial_\tau u_1\Big), \end{aligned}$$

which shows that u_2, v_2 satisfy the transmission conditions (4.4) if $\ker\mathcal{V}_{22,2}=\{0\}$.

Analogously one shows that the functions

(5.3)

$$u_0 = \frac{\kappa_0^2}{2k_0^2}\left(\frac{k_0^2}{\kappa_0^2}K_{\Gamma_1,0}u_1 - V_{\Gamma_1,0}\left(\frac{k_1^2}{\kappa_1^2}\,\partial_\nu u_1 - \frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{\kappa_0^2\kappa_1^2}\,\partial_\tau v_1\right)\right),$$
$$v_0 = \frac{\kappa_0^2}{2}\left(\frac{1}{\kappa_0^2}K_{\Gamma_1,0}v_1 - V_{\Gamma_1,0}\left(\frac{1}{\kappa_1^2}\,\partial_\nu v_1 + \frac{\gamma(\kappa_0^2-\kappa_1^2)}{k_2\kappa_0^2\kappa_1^2}\,\partial_\tau u_1\right)\right),$$

which satisfy (4.2) and (4.5), are subjected to the jump conditions (4.3) if $\dim\ker\mathcal{V}_{11,0}=0$.

Assertion (ii) is a simple consequence of Lemma 5.1 (ii), since

$$w_1 = \frac{1}{2}\big(\partial_\nu u_1|_{\Gamma_1} - \mathcal{V}_{11,1}^{-1}(\mathcal{K}_{11,1}-I)u_1\big),$$
$$w_2 = \frac{1}{2}\big(\partial_\nu u_1|_{\Gamma_2} - \mathcal{V}_{22,1}^{-1}(\mathcal{K}_{22,1}+I)u_1\big),$$
$$\tau_1 = \frac{1}{2}\big(\partial_\nu v_1|_{\Gamma_1} - \mathcal{V}_{11,1}^{-1}(\mathcal{K}_{11,1}-I)v_1\big),$$
$$\tau_2 = \frac{1}{2}\big(\partial_\nu v_1|_{\Gamma_2} - \mathcal{V}_{22,1}^{-1}(\mathcal{K}_{22,1}+I)v_1\big),$$

are uniquely determined. □

Proof of Proposition 5.2. (i) Defining the functions

(5.4) $u_0 = V_{\Gamma_1,0}w_1,\ v_0 = V_{\Gamma_1,0}\tau_1$ and $u_2 = V_{\Gamma_2,2}w_2,\ v_2 = V_{\Gamma_2,2}\tau_2$

in G_0, respectively G_2, and

(5.5)

$$\begin{aligned} u_1 = {} & V_{\Gamma_1,1}\left(\frac{k_0^2\kappa_1^2}{2\kappa_0^2k_1^2}\,\partial_\nu u_0 - \frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{2\kappa_0^2k_1^2}\,\partial_\tau v_0\right) \\ & - \frac{1}{2}K_{\Gamma_1,1}u_0 \\ & - V_{\Gamma_2,1}\left(\frac{\kappa_1^2k_2^2}{2k_1^2\kappa_2^2}\,\partial_\nu(u_2+u^{(i)}) + \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{2k_1^2\kappa_2^2}\partial_\tau(v_2+v^{(i)})\right) \\ & + \frac{1}{2}K_{\Gamma_2,1}(u_2+u^{(i)}), \end{aligned}$$
$$v_1 = V_{\Gamma_1,1}\left(\frac{\kappa_1^2}{2\kappa_0^2}\,\partial_\nu v_0 + \frac{\gamma(\kappa_0^2-\kappa_1^2)}{2k_2\kappa_0^2}\,\partial_\tau u_0\right) - \frac{1}{2}K_{\Gamma_1,1}v_0$$

$$- V_{\Gamma_2,1}\left(\frac{\kappa_1^2}{2\kappa_2^2}\,\partial_\nu(v_2+v^{(i)}) - \frac{\gamma(\kappa_1^2-\kappa_2^2)}{2k_2\kappa_2^2}\,\partial_\tau(u_2+u^{(i)})\right)$$
$$+ \frac{1}{2}K_{\Gamma_2,1}(v_2+v^{(i)}),$$

in G_1, it can be shown similarly to the proof of Proposition 5.1 that the equations (4.25) imply

$$u_1|_{\Gamma_1} = u_0|_{\Gamma_1},\ v_1|_{\Gamma_1} = v_0|_{\Gamma_1},\ u_1|_{\Gamma_2} = (u_2+u^{(i)})|_{\Gamma_2},\ v_1|_{\Gamma_2} = (v_2+v^{(i)})|_{\Gamma_2}.$$

Comparing then (5.5) with the representations (4.24) we obtain that in G_1

$$V_{\Gamma_1,1}\left(\frac{k_0^2}{\kappa_0^2}\partial_\nu u_0 - \frac{\gamma k_2(\kappa_0^2-\kappa_1^2)}{\kappa_0^2\kappa_1^2}\,\partial_\tau v_1 - \frac{k_1^2}{\kappa_1^2}\partial_\nu u_1\right)$$
$$= V_{\Gamma_2,1}\left(\frac{k_2^2}{\kappa_2^2}\,\partial_\nu(u_2+u^{(i)}) + \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)}{\kappa_1^2\kappa_2^2}\partial_\tau v_1 - \frac{k_1^2}{\kappa_1^2}\partial_\nu u_1\right),$$

$$V_{\Gamma_1,1}\left(\frac{1}{\kappa_0^2}\partial_\nu v_0 + \frac{\gamma(\kappa_0^2-\kappa_1^2)}{k_2\kappa_0^2\kappa_1^2}\,\partial_\tau u_1 - \frac{1}{\kappa_1^2}\partial_\nu v_1\right)$$
$$= V_{\Gamma_2,1}\left(\frac{1}{\kappa_2^2}\,\partial_\nu(v_2+v^{(i)}) - \frac{\gamma(\kappa_1^2-\kappa_2^2)}{k_2\kappa_1^2\kappa_2^2}\,\partial_\tau u_1 - \frac{1}{\kappa_1^2}\,\partial_\nu v_1\right),$$

which implies by Lemma 5.1 that

$$\frac{k_0^2\partial_\nu u_0}{\kappa_0^2} - \frac{k_1^2\partial_\nu u_1}{\kappa_1^2} - \frac{\gamma k_2(\kappa_0^2-\kappa_1^2)\,\partial_\tau v_1}{\kappa_0^2\kappa_1^2},$$
$$\frac{\partial_\nu v_0}{\kappa_0^2} - \frac{\partial_\nu v_1}{\kappa_1^2} + \frac{\gamma(\kappa_0^2-\kappa_1^2)\,\partial_\tau u_1}{k_2\kappa_0^2\kappa_1^2} \in \ker \mathcal{V}_{11,1},$$

$$\frac{k_2^2\partial_\nu(u_2+u^{(i)})}{\kappa_2^2} - \frac{k_1^2\partial_\nu u_1}{\kappa_1^2} + \frac{\gamma k_2(\kappa_1^2-\kappa_2^2)\,\partial_\tau v_1}{\kappa_1^2\kappa_2^2},$$
$$\frac{\partial_\nu(v_2+v^{(i)})}{\kappa_2^2} - \frac{\partial_\nu v_1}{\kappa_1^2} - \frac{\gamma(\kappa_1^2-\kappa_2^2)\,\partial_\tau u_1}{k_2\kappa_1^2\kappa_2^2} \in \ker \mathcal{V}_{22,1}.$$

Assertion (ii) follows immediately from the ansatz (4.23), (4.24). ◻

5.2. Strong ellipticity.

Theorem 5.1. *Let* $\kappa_2^2 = k_2^2 - \gamma^2 > 0$ *and* $\kappa_j^2 = k_j^2 - \gamma^2 \neq 0$ *satisfy* $\arg \kappa_j^2 \in [0, \pi)$, $j = 0, 1$. *Then* $\mathbf{A}^{(\alpha)}$ *and* $\mathbf{B}^{(\alpha)}$ *are Fredholm mappings* $\left(H_\alpha^{-1/2}(\Gamma_1)\right)^2 \times \left(H_\alpha^{-1/2}(\Gamma_2)\right)^2 \to \left(H_\alpha^{1/2}(\Gamma_1)\right)^2 \times \left(H_\alpha^{1/2}(\Gamma_2)\right)^2$ *of index* 0 *for all* α, $(\alpha + n)^2 \neq \kappa_j^2$ *and* $n \in \mathbf{Z}$. *In particular,* $\dim \ker \mathbf{A}^{(\alpha)} = \dim \ker \mathbf{B}^{(-\alpha)}$.

The assertion of Theorem 5.1 follows from Lemma 4.1 and the Lemmas 5.2–5.4 given below. Consider the off-diagonal blocks (4.22) of $\mathbf{A}^{(\alpha)}$. Since for $k \neq j$ the operators

$$\begin{aligned} \mathcal{V}_{jk,m} &: H_\alpha^{-1/2}(\Gamma_k) \longrightarrow H_\alpha^{1/2}(\Gamma_j), \\ \mathcal{K}_{jk,m} &: H_\alpha^{1/2}(\Gamma_k) \to H_\alpha^{1/2}(\Gamma_j), \\ \mathcal{L}_{jk,m} &: H_\alpha^{-1/2}(\Gamma_k) \to H_\alpha^{-1/2}(\Gamma_j), \end{aligned}$$

and therefore $\mathcal{A}_{jk} : \left(H_\alpha^{-1/2}(\Gamma_k)\right)^2 \to \left(H_\alpha^{1/2}(\Gamma_j)\right)^2$ are compact, we have

Lemma 5.2. *The operator* $\mathbf{A}^{(\alpha)}$ *is Fredholm if and only if both* $\mathcal{A}_{jj} : \left(H_\alpha^{-1/2}(\Gamma_j)\right)^2 \to \left(H_\alpha^{1/2}(\Gamma_j)\right)^2$, $j = 1, 2$, *are Fredholm. Then* $\operatorname{ind} \mathbf{A}^{(\alpha)} = \operatorname{ind} \mathcal{A}_{11} + \operatorname{ind} \mathcal{A}_{22}$.

Next we consider one of the operator matrices $\mathcal{A}_{jj}$ given by (4.20). As in subsection 3.3 we relate the elements of $\mathcal{A}_{jj}$ to boundary integral operators of the Laplacian on the closed curve $\widetilde{\Gamma}$ obtained from Γ_j by the transformation $\vartheta = \mathbf{e}^{iz}$. Then the proof of Lemma 3.3 lets us conclude that the operators

$$\begin{gathered} \mathcal{V}_{jj,m}(I \pm \mathcal{L}_{jj,1}) - \vartheta^* V (I \pm K')(\vartheta^*)^{-1} M_j : H_\alpha^{-1/2}(\Gamma_j) \to H_\alpha^{1/2}(\Gamma_j), \\ \left(I \pm \mathcal{K}_{jj,m}\right)\mathcal{V}_{jj,1} - \vartheta^* (I \pm K) V (\vartheta^*)^{-1} M_j : H_\alpha^{-1/2}(\Gamma_j) \to H_\alpha^{1/2}(\Gamma_j), \\ \mathcal{H}_{j,m}\mathcal{V}_{jj,1} - \vartheta^* H V (\vartheta^*)^{-1} M_j : H_\alpha^{-1/2}(\Gamma_j) \to H_\alpha^{1/2}(\Gamma_j), \end{gathered}$$

are compact (cf. (3.28), (3.30)–(3.31). Here M_j denotes the multiplication operator

$$M_j \varphi(P) = e^Y \varphi(P), \quad P = (X, Y) \in \Gamma_j.$$

Introducing

$$(5.6)\quad \widetilde{\mathcal{A}}_j = \begin{pmatrix} \left(\frac{k_j^2}{\kappa_j^2}+\frac{k_{j-1}^2}{\kappa_{j-1}^2}\right)V+\left(\frac{k_j^2}{\kappa_j^2}-\frac{k_{j-1}^2}{\kappa_{j-1}^2}\right)KV & -\gamma k_2\left(\frac{1}{\kappa_j^2}-\frac{1}{\kappa_{j-1}^2}\right)HV \\ \gamma k_2\left(\frac{1}{\kappa_j^2}-\frac{1}{\kappa_{j-1}^2}\right)HV & \left(\frac{k_2^2}{\kappa_j^2}+\frac{k_2^2}{\kappa_{j-1}^2}\right)V+\left(\frac{k_2^2}{\kappa_j^2}-\frac{k_2^2}{\kappa_{j-1}^2}\right)KV \end{pmatrix}$$

and using the relation $KV = VK'$ we see from (4.20) that the differences

$$\mathcal{A}_{jj} - \begin{pmatrix} \vartheta^* & 0 \\ 0 & \vartheta^* \end{pmatrix} \widetilde{\mathcal{A}}_j \begin{pmatrix} (\vartheta^*)^{-1}M_j & 0 \\ 0 & (\vartheta^*)^{-1}M_j \end{pmatrix} : \left(H_\alpha^{-1/2}(\Gamma_j)\right)^2 \longrightarrow \left(H_\alpha^{1/2}(\Gamma_j)\right)^2$$

$j = 1, 2$, are compact operators. Consequently, we derive

Lemma 5.3. *The* 2×2 *operator matrix* $\mathcal{A}_{jj} : \left(H_\alpha^{-1/2}(\Gamma_j)\right)^2 \to \left(H_\alpha^{1/2}(\Gamma_j)\right)^2$ *is Fredholm if and only if* $\widetilde{\mathcal{A}}_j : \left(H^{-1/2}(\widetilde{\Gamma})\right)^2 \to \left(H^{1/2}(\widetilde{\Gamma})\right)^2$ *is a Fredholm operator and* $\operatorname{ind}\mathcal{A}_{jj} = \operatorname{ind}\widetilde{\mathcal{A}}_j$.

Hence it remains to study $\widetilde{\mathcal{A}}_j$ given on a closed piecewise C^2 curve $\widetilde{\Gamma}$. Since by construction the symmetric operator $V : H^{-1/2}(\widetilde{\Gamma}) \to H^{1/2}(\widetilde{\Gamma})$ is positive definite we can define an inner product on $H^{-1/2}(\widetilde{\Gamma})$ by

$$(5.7)\qquad (u, v)_V = \langle Vu, v\rangle,$$

where $\langle\cdot,\cdot\rangle$ is the duality pairing (3.25) between $H^{1/2}(\widetilde{\Gamma})$ and $H^{-1/2}(\widetilde{\Gamma})$. The inner product generates an equivalent norm on $H^{-1/2}(\widetilde{\Gamma})$, which is denoted by $\|u\|_{-1/2} = \langle Vu, u\rangle^{1/2}$. For $U = (u, v) \in \left(H^{-1/2}(\widetilde{\Gamma})\right)^2$, $\Phi = (\phi, \psi) \in \left(H^{1/2}(\widetilde{\Gamma})\right)^2$ we define

$$\big\langle \Phi, U \big\rangle = \langle \phi, u\rangle + \langle \psi, v\rangle \quad \text{and} \quad \|U\|_{-1/2}^2 = \langle Vu, u\rangle + \langle Vv, v\rangle = (U, U)_V.$$

Since the kernels of K and H are real-valued we have

$$\langle K\phi, v\rangle = \langle \phi, K'v\rangle,\ \langle H\phi, v\rangle = \langle \phi, H'v\rangle,\ \phi \in H^{1/2}(\widetilde{\Gamma}),\ v \in H^{-1/2}(\widetilde{\Gamma}),$$

and therefore by Lemma 3.2 (i)

$$(K'u,v)_V = (u,K'v)_V, \qquad (H'u,v)_V = -(u,H'v)_V, \quad u,v \in H^{-1/2}(\widetilde{\Gamma}). \tag{5.8}$$

Lemma 5.4. *Under the assumptions of Theorem* 5.1 *there exist* $\theta \in \mathbf{C}$ *and* $c > 0$ *such that the operator matrix* $\widetilde{\mathcal{A}}_j$ *defined by* (5.6) *satisfies*

$$\operatorname{Re}\left\langle \theta \widetilde{\mathcal{A}}_j U, U \right\rangle \geq c\,\|U\|^2_{-1/2} \tag{5.9}$$

for all $U = (u,v) \in \left(H^{-1/2}(\widetilde{\Gamma})\right)^2$.

Proof. Consider first the case $\gamma = 0$. Then by (5.6)

$$\widetilde{\mathcal{A}}_j = \begin{pmatrix} 2V & 0 \\ 0 & \left(\frac{k_2^2}{\kappa_j^2}(I+K) + \frac{k_2^2}{\kappa_{j-1}^2}(I-K)\right)V \end{pmatrix}.$$

It follows from Lemma 3.2 (i) and (5.8) that

$$\left\langle \widetilde{\mathcal{A}}_j U, U \right\rangle = 2\|u\|^2_{-1/2} + \frac{k_2^2}{\kappa_j^2}\big(v,(I+K')v\big)_V + \frac{k_2^2}{\kappa_{j-1}^2}\big(v,(I-K')v\big)_V$$

with the selfadjoint operators $I \pm K'$. Moreover, it was shown in [**4**] (see also [**18**]) that

$$\big(v,(I+K')v\big)_V \geq 0, \quad \big(v,(I-K')v\big)_V \geq c_1\,\|v\|^2_{-1/2}, \quad c_1 > 0,$$

for all $v \in H^{-1/2}(\widetilde{\Gamma})$. By assumption the factors k_2^2/κ_ℓ^2, $\ell = 0,1,2$, lie in an open half-plane containing the positive real axis. Hence there exists a θ with $\operatorname{Re}\theta > 0$ such that $\operatorname{Re}\theta/\kappa_\ell^2 > 0$, $\ell = 0,1,2$, which leads to

$$\left\langle \theta \widetilde{\mathcal{A}}_j U, U \right\rangle \geq 2\operatorname{Re}\theta\|u\|^2_{-1/2} + c_1 k_2^2 \operatorname{Re}\frac{\theta}{\kappa_{j-1}^2}\|v\|^2_{-1/2}.$$

Let $\gamma \neq 0$ and denote

$$a = \frac{1}{\kappa_j^2} + \frac{1}{\kappa_{j-1}^2}, \qquad b = \frac{1}{\kappa_j^2} - \frac{1}{\kappa_{j-1}^2}.$$

Noting that

$$\frac{k_j^2}{\kappa_j^2} + \frac{k_{j-1}^2}{\kappa_{j-1}^2} = 2 + \gamma^2 a, \qquad \frac{k_j^2}{\kappa_j^2} - \frac{k_{j-1}^2}{\kappa_{j-1}^2} = \gamma^2 b,$$

we write $\widetilde{\mathcal{A}}_j$ in the form

$$\widetilde{\mathcal{A}}_j = \Lambda \left(\begin{pmatrix} 2\gamma^{-2} I & 0 \\ 0 & 0 \end{pmatrix} + a\mathcal{I} + b\mathcal{S} \right) \Lambda \mathcal{V}$$

with the matrices

$$\Lambda = \begin{pmatrix} \gamma & 0 \\ 0 & k_2 \end{pmatrix}, \qquad \mathcal{V} = \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix},$$
$$\mathcal{I} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \qquad \mathcal{S} = \begin{pmatrix} K & -H \\ H & K \end{pmatrix}.$$

It follows from Lemma 3.2 (ii) that $\mathcal{S}^2 = \mathcal{I}$, which allows us to define the projection operators

$$\mathcal{P}_\pm = \frac{1}{2}\big(\mathcal{I} \pm \mathcal{S}\big)$$

in $\big(H^{1/2}(\widetilde{\Gamma})\big)^2$. Moreover, by Lemma 3.2 (i)

$$\begin{pmatrix} K & -H \\ H & K \end{pmatrix} \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} = \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} K' & H' \\ -H' & K' \end{pmatrix},$$

implying that the adjoint operators $\mathcal{P}'_\pm$ acting in $\big(H^{-1/2}(\widetilde{\Gamma})\big)^2$ are selfadjoint with respect to the inner product $(\cdot,\cdot)_V$. Thus we obtain

$$\widetilde{\mathcal{A}}_j = \Lambda\mathcal{V} \left(\begin{pmatrix} 2\gamma^{-2} & 0 \\ 0 & 0 \end{pmatrix} + (a+b)\,\mathcal{P}'_+ + (a-b)\,\mathcal{P}'_- \right) \Lambda,$$

and therefore

$$\big\langle \widetilde{\mathcal{A}}_j U, U \big\rangle = 2(u,u)_V + \frac{2}{\kappa_j^2}\big(\mathcal{P}'_+ \Lambda U, \Lambda U\big)_V + \frac{2}{\kappa_{j-1}^2}\big(\mathcal{P}'_- \Lambda U, \Lambda U\big)_V.$$

As before we find θ satisfying $\operatorname{Re}\theta > 0$ and $\operatorname{Re}\theta/\kappa_\ell^2 > 0$, $\ell = 0,1,2$, and $c > 0$ such that

$$\operatorname{Re}\left\langle \theta \widetilde{\mathcal{A}}_j U, U \right\rangle \geq c\Big(\|u\|^2_{-1/2} + \|\mathcal{P}'_+ \Lambda U\|^2_{-1/2} + \|\mathcal{P}'_- \Lambda U\|^2_{-1/2} \Big). \qquad \square$$

Since the number θ can be chosen not depending on j, in fact Lemma 5.4 implies a stronger result, which, in particular, can be used to justify the convergence of numerical methods for solving (4.19 and (4.25).

Corollary 5.1. *Under the conditions of Theorem* 5.1 *the operator* $\mathbf{A}^{(\alpha)}$ (*and consequently* $\mathbf{B}^{(\alpha)}$) *is strongly elliptic in the sense that there exist* $c > 0$ *and a compact operator* $\mathbf{K} : \big(H_\alpha^{-1/2}(\Gamma_1)\big)^2 \times \big(H_\alpha^{-1/2}(\Gamma_2)\big)^2 \to \big(H_\alpha^{1/2}(\Gamma_1)\big)^2 \times \big(H_\alpha^{1/2}(\Gamma_2)\big)^2$ *such that*

$$\Big| \Big[(\mathbf{A}^{(\alpha)} + \mathbf{K}) W, \overline{W} \Big] \Big| \geq c \|W\|^2_{-1/2}$$

for all $W \in \big(H_\alpha^{-1/2}(\Gamma_1)\big)^2 \times \big(H_\alpha^{-1/2}(\Gamma_2)\big)^2$. *Here* $\overline{W}$ *is the vector of the complex conjugates of the components of* W *and the duality form is defined by* (4.27).

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