// Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 0946 – 8633

Conical diffraction by multilayer gratings: A recursive integral equations approach

Gunther Schmidt

submitted: April 5, 2011

Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: gunther.schmidt@wias-berlin.de

No. 1601
Berlin 2011

2010 *Mathematics Subject Classification.* 78A45, 78M15, 45E05, 35J05.

Key words and phrases. Diffraction, periodic structure, multilayer grating, singular integral formulation, recursive algorithm.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

In this paper we consider an integral equation algorithm to study the scattering of plane waves by multilayer diffraction gratings under oblique incidence. The scattering problem is described by a system of Helmholtz equations with piecewise constant coefficients in $\mathbb{R}^2$ coupled by special transmission conditions at the interfaces between different layers. Boundary integral methods lead to a system of singular integral equations, containing at least two equations for each interface. To deal with an arbitrary number of material layers we present the extension of a recursive procedure developed by Maystre for normal incidence, which transforms the problem to a sequence of equations with 2×2 operator matrices on each interface. Necessary and sufficient conditions for the applicability of the algorithm are derived.

1 Introduction

In this paper we study an integral equation method for the simulation of multilayer diffraction gratings. The optical devices under consideration consist of different material layers separated by non-intersecting and possibly non-smooth interfaces, which are in Cartesian coordinates periodic in x-direction and translation invariant in the z-direction. We consider the so-called *conical* or *off-plane diffraction*, i.e., the grating is illuminated by a plane wave whose direction is in general not orthogonal to the z-axis.

If a grating is modeled as an infinite periodic structure, then the electromagnetic formulation of conical diffraction can be reduced to a system of two Helmholtz equations in $\mathbb{R}^2$ with piecewise constant coefficients, which are periodic in x. Their quasiperiodic solutions have to satisfy radiation conditions and are coupled by transmission conditions at the interfaces between different grating materials. A variational formulation of this problem has been studied in [2] based on strong ellipticity estimates, which are valid under some restrictions on the permittivities ε, $0 \leq \arg \varepsilon < \pi$, of the non-magnetic grating materials, which are specified in Section 2.

Using layer potentials with the quasiperiodic fundamental solution of the Helmholtz equation the diffraction problem for multilayer gratings can be transformed to a system of integral equations over the interfaces. In [10] we proposed a combined direct and indirect integral equation approach resulting in two integral equations on each interface which contain besides the boundary integrals of the single and double layer potentials also the tangential derivative of single layer potentials, which are interpreted as singular Cauchy integrals. Besides the equivalence of the integral with the electromagnetic formulation the strong ellipticity of the integral equation system under the above condition was established.

But fortunately, the integral formulation can be analyzed under more general conditions on the coefficients. Recent progress in the design of optical metamaterials motivates to admit magnetic materials with complex permeability μ, $\arg \mu \in [0, \pi)$, and to consider also the case that ε or μ are negative, which was studied in [11] for gratings with only one interface. It was shown that the system of singular integral equations generate a Fredholm operator with index 0 in the corresponding energy spaces if $0 \leq \arg \varepsilon, \arg \mu < \pi$, and the solution of the integral equations provides a solution of the conical diffraction. This holds also in the case, when the permittivity ε or permeability μ of the grating substrate take values outside a closed interval of the negative half axis, degenerating to a point if the profile is smooth. Moreover, the solution is unique if the imaginary parts $\operatorname{Im} \varepsilon$ or $\operatorname{Im} \mu$ of the substrate parameters are positive.

The interest to integral formulations originates form the existence of efficient numerical methods for *in-plane* grating theory, where the direction of the incident wave is orthogonal to the z-axis. Integral methods were one of the first for the investigation of diffraction gratings (cf. [9]) and have been used for gratings of extremely different kind. But off-plane diffraction has not been tackled for a long time, which was one of the real deficiencies of the method. Only recently, in [4], a numerical method for one-profile gratings has been proposed, which solves the integral equations using a hybrid piecewise-trigonometric polynomial collocation method very efficiently, including certain scenarios with unfavorably large ratio period over wavelength and non-smooth profile.

For multilayer gratings with N interfaces the resulting system consists of $2N$ singular integral equations, which makes its numerical solution a very expensive computational task. For in-plane diffraction this problem was solved by D. Maystre, who developed recursive algorithms which treat in each step a discrete problem for one interface between different materials. The algorithm in [8] is based on the use of scattering matrices and applies to multilayer gratings with interfaces which can be separated by horizontal planes y = const. Its generalization to conical diffraction with applications to multilayer gratings with photonics inclusions was described in [12].

In the present paper we treat the case of general multilayer gratings following the algorithm proposed in Maystre [7]. Combining direct and indirect boundary integral approaches the conical diffraction is transformed to a sequence of equations with 2×2 operator matrices on each interface, which are closely related to the operator matrix of one-profile gratings. So the analysis of the recursive algorithm, involving the inversion of operator matrices, is performed similar to [11]. Moreover, the discretization methods from [4] can be used for the numerical realization of the algorithm. Although the inversion of discretization matrices is required, the actual demand for computer memory is comparatively small, which makes the conical diffraction problem tractable with standard PC even for a large number of layers.

The outline of the paper is as follows. In Section 2 we recall the differential formulation of the conical diffraction for multilayer gratings. Section 3 is devoted to boundary integral operators of periodic diffraction and the description of the recursive algorithm, which requires for each interface the solution of an operator equation with a 2×2 matrix of singular integral operators. The applicability of the algorithm is analyzed in Section 4. It is shown that the operator equations are solvable if and only if the corresponding matrix operator is invertible and then the algorithm provides the unique solution of the diffraction problem. Additionally we derive necessary and sufficient conditions for the invertiblity of the singular integral operator matrices.

2 Conical diffraction

We consider a multilayer periodic structure of $N+1$ homogeneous material layers $G_0 \times \mathbb{R}, \ldots, G_N \times \mathbb{R}$ of electric permittivity ε_j and magnetic permeability μ_j, which are complex-valued non-zero constants. In the following we suppose that $0 \leq \arg\varepsilon_j, \arg\mu_j \leq \pi$, such that $\arg\varepsilon_j + \arg\mu_j < 2\pi$ allowing nearly all physically interesting materials. The case of negative refraction index materials, corresponding to $\varepsilon_j, \mu_j < 0$, requires some modified integral method and will be discussed elsewhere.

The geometry of the grating is characterized by functions ε and μ, which in Cartesian coordinates (x, y, z) are piecewise constant functions not depending on z, $\varepsilon(x, y) = \varepsilon_j$, $\mu(x, y) = \mu_j$, $(x, y) \in G_j$, which are d-periodic in x, i.e., $\varepsilon(x + d, y) = \varepsilon(x, y)$ and $\mu(x + d, y) = \mu(x, y)$.

The layers are separated by d-periodic and non self-intersecting interfaces with the cross sections $\Sigma_0, \ldots, \Sigma_N$ (Fig. 1). We assume that the distance between different curves Σ_j is always positive. We refer to the semi-infinite layers G_0 and G_N as the top and bottom layer, respectively. Note that we allow the y-projections of the interfaces Σ_j to be overlapping.

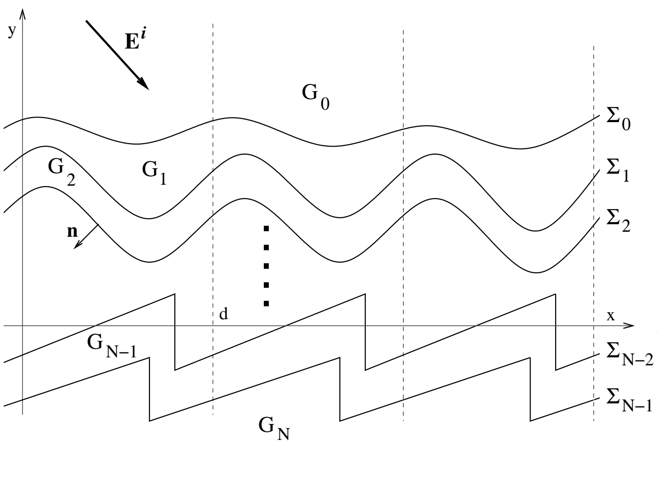

Figure 1: Cross section of a multilayer grating

The grating is illuminated by an electromagnetic plane wave with wavelength λ and given polarization from $G_0 \times \mathbb{R}$, which is filled with a lossless material, i.e., ε_0, $\mu_0 > 0$. We consider the general case of conical diffraction, i.e., we allow that the wave vector $\mathbf{k} = (\alpha, -\beta, \gamma)$ of the incident electric field

$$\mathbf{E}^i = \mathbf{p}\ \mathrm{e}^{i(\alpha x - \beta y + \gamma z)}$$

is not in the (x, y)-plane. The polarization vector $\mathbf{p}$ satisfies $\mathbf{p} \cdot \mathbf{k} = 0$ and $\mathbf{k}$ can be expressed in terms of the incidence angles ϕ (the angle between $\mathbf{k}$ and its projection on the (x, y)-plane) and θ (the angle of that projection with the y-axis):

$$\mathbf{k} = \omega(\varepsilon_0\mu_0)^{1/2}(\sin\theta\cos\phi, -\cos\theta\cos\phi, \sin\phi)\,, \quad \omega = \frac{2\pi}{\lambda}\,.$$

We look for solutions $\mathrm{e}^{\,i\omega t}(\mathbf{E}, \mathbf{H})$ of the time-harmonic Maxwell equations

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

with locally finite energy, i.e.

$$\mathbf{E}\,,\ \mathbf{H}\,,\ \boldsymbol{\nabla} \times \mathbf{E}\,,\ \boldsymbol{\nabla} \times \mathbf{H} \in \left(L^2_{loc}(\mathbb{R}^3)\right)^3. \tag{2.2}$$

Using the ansatz

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

with vector functions $E, B : \mathbb{R}^2 \to \mathbb{C}^3$ and the scaling $Z = \sqrt{\varepsilon_0/\mu_0}$, the solution of (2.1) can be reduced to a problem in $\mathbb{R}^2$. For the following we introduce the piecewise constant function taking the values

$$\kappa(x, y) = \kappa_j = \sqrt{\varepsilon_j\mu_j - \varepsilon_0\mu_0\sin^2\phi}\,, \quad (x, y) \in G_j\,,\ j = 0, \ldots, N, \tag{2.3}$$

where we choose the square root $\sqrt{z} = \sqrt{r}\, e^{\,i\varphi/2}$ for $z = r\, e^{\,i\varphi}$, $0 \le \varphi < 2\pi$. Assuming that everywhere $\kappa \ne 0$ it can be shown (cf. [2, 11]), that the finite energy condition (2.2) is satisfied only if the z–components of E and B are H^1-regular. Moreover, E_z, B_z determine the other components of the electric and magnetic fields and are solutions of the Helmholtz equations

$$(\Delta + \omega^2\kappa^2)\, E_z = (\Delta + \omega^2\kappa^2)\, B_z = 0 \tag{2.4}$$

in each of the domains G_j in which $\varepsilon(x, y)$ and $\mu(x, y)$ are constant. Furthermore, the continuity of the tangential components of $\mathbf{E}$ and $\mathbf{H}$ at the interfaces Σ_j between the domains G_j and G_{j+1} lead to transmission conditions for E_z and B_z

$$\big[E_z\big]_{\Sigma_j} = \big[B_z\big]_{\Sigma_j} = 0,\ \Big[\frac{\varepsilon\,\partial_{\mathbf{n}} E_z}{\kappa^2}\Big]_{\Sigma_j} = -\varepsilon_0\sin\phi\Big[\frac{\partial_{\mathbf{t}} B_z}{\kappa^2}\Big]_{\Sigma_j},\ \Big[\frac{\mu\,\partial_{\mathbf{n}} B_z}{\kappa^2}\Big]_{\Sigma_j} = \mu_0\sin\phi\Big[\frac{\partial_{\mathbf{t}} E_z}{\kappa^2}\Big]_{\Sigma_j}, \tag{2.5}$$

which couple the Helmholtz equations (2.4). Here $\partial_{\mathbf{n}}$ is the derivative in direction of the normal $\mathbf{n} = (n_x, n_y)$ to Σ_j pointing in G_{j+1}, $\partial_{\mathbf{t}}$ the derivative in direction of the tangential vector $\mathbf{t} = (-n_y, n_x)$, and $[\,\cdot\,]$ denotes the jump of the boundary values if crossing the interface Σ_j.

The z-components of the incoming field $E^i_z(x, y) = p_z\, \mathrm{e}^{i(\alpha x - \beta y)}$, $B^i_z(x, y) = q_z\, \mathrm{e}^{i(\alpha x - \beta y)}$ are α-quasiperiodic functions of period d, i.e., they satisfy the relation

$$u(x + d, y) = \mathrm{e}^{id\alpha}\, u(x, y)\,. \tag{2.6}$$

Therefore, E_z, B_z have to be α-quasiperiodic, too. Moreover, the scattered field has to be bounded below and above the inhomogeneous grating structure. This leads to the radiation condition, known as outgoing wave condition,

$$\begin{aligned}(E_z, B_z)(x, y) - (p_z, q_z)\,\mathrm{e}^{i(\alpha x - \beta y)} &= \sum_{n=-\infty}^{\infty} (E^{(0)}_n, B^{(0)}_n)\,\mathrm{e}^{\,i(\alpha_n x + \beta^{(0)}_n y)}, \quad y \to +\infty\,,\\ (E_z, B_z)(x, y) &= \sum_{n=-\infty}^{\infty} (E^{(N)}_n, B^{(N)}_n)\,\mathrm{e}^{\,i(\alpha_n x - \beta^{(N)}_n y)}, \quad y \to -\infty\,,\end{aligned} \tag{2.7}$$

with the so called Rayleigh coefficients $E^{(0)}_n, B^{(0)}_n, E^{(N)}_n, B^{(N)}_n \in \mathbb{C}$, and

$$\alpha_n = \alpha + \frac{2\pi n}{d}\,, \quad \beta^{(j)}_n = \sqrt{\omega^2\kappa_j^2 - \gamma^2 - \alpha_n^2} \quad \text{with } 0 \le \arg\beta^{(j)}_n < \pi\,, \quad n \in \mathbb{Z}\,. \tag{2.8}$$

Note that $\beta_n^{(0)}$ and $\beta_n^{(N)}$ are real only a for finite number of integers n, hence the diffracted far field is composed of a finite number of outgoing plane waves. The corresponding Rayleigh coefficients indicate the efficiency and the phase shift of the reflected propagating modes

$$(E_n^{(0)}, B_n^{(0)})\, \mathrm{e}^{\,i(\alpha_n x+\beta_n^{(0)} y+\gamma z)}\,, \quad y \to \infty\,,$$

and of the transmitted modes

$$(E_n^{(N)}, B_n^{(N)})\, \mathrm{e}^{\,i(\alpha_n x-\beta_n^{(N)} y+\gamma z)}\,, \quad y \to -\infty\,,$$

which exists if $\omega^2\kappa_N^2 - \gamma^2 - \alpha_n^2 \geq 0$. All other modes are exponentially decaying. 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-axis, one speaks of conical diffraction.

To derive a integral formulation we rewrite the conical diffraction problem (2.4), (2.5), (2.7) using the notation

$$E_z(x,y) = \begin{cases} u_0 + u^i \\ u_j \end{cases}, \quad B_z(x,y) = \begin{cases} v_0 + v^i & \text{in} \quad G_0, \\ v_j & \text{in} \quad G_j\,,\ j = 1,\dots,G_N\,, \end{cases}$$

with $u^i = p_z\, \mathrm{e}^{i(\alpha x-\beta y)}$, $v^i = q_z\, \mathrm{e}^{i(\alpha x-\beta y)}$. We seek α-quasiperiodic functions $\{u_j, v_j\}_{j=0}^N$ such that

$$\text{in } G_j \qquad \Delta u_j + \omega^2\kappa_j^2 u_j = \Delta v_j + \omega^2\kappa_j^2 v_j = 0\,, \tag{2.9}$$

subject to the transmission conditions

$$\text{on } \Sigma_0 \quad \begin{cases} u_1 = u_0 + u^i\,, \ \dfrac{\varepsilon_1\,\partial_{\mathbf{n}} u_1}{\kappa_1^2} - \dfrac{\varepsilon_0 \partial_{\mathbf{n}}(u_0+u^i)}{\kappa_0^2} = \dfrac{\varepsilon_0 \sin\phi\,(\kappa_1^2-\kappa_0^2)}{\kappa_1^2\kappa_0^2}\,\partial_{\mathbf{t}} v_1\,, \\ v_1 = v_0 + v^i\,, \ \dfrac{\mu_1 \partial_{\mathbf{n}} v_1}{\kappa_1^2} - \dfrac{\mu_0 \partial_{\mathbf{n}}(v_0+v^i)}{\kappa_0^2} = -\dfrac{\mu_0 \sin\phi\,(\kappa_1^2-\kappa_0^2)}{\kappa_1^2\kappa_0^2}\,\partial_{\mathbf{t}} u_1\,, \end{cases} \tag{2.10}$$

and, for $j = 1,\dots,N-1$,

$$\text{on } \Sigma_j \quad \begin{cases} u_{j+1} = u_j\,, \ \dfrac{\varepsilon_{j+1}\partial_{\mathbf{n}} u_{j+1}}{\kappa_{j+1}^2} - \dfrac{\varepsilon_j\,\partial_{\mathbf{n}} u_j}{\kappa_j^2} = \dfrac{\varepsilon_0 \sin\phi\,(\kappa_{j+1}^2-\kappa_j^2)}{\kappa_j^2\kappa_{j+1}^2}\,\partial_{\mathbf{t}} v_{j+1}\,, \\ v_{j+1} = v_j\,, \ \dfrac{\mu_{j+1}\partial_{\mathbf{n}} v_{j+1}}{\kappa_{j+1}^2} - \dfrac{\mu_j \partial_{\mathbf{n}} v_j}{\kappa_j^2} = -\dfrac{\mu_0 \sin\phi\,(\kappa_{j+1}^2-\kappa_j^2)}{\kappa_j^2\kappa_{j+1}^2}\,\partial_{\mathbf{t}} u_{j+1}\,, \end{cases} \tag{2.11}$$

which satisfy the outgoing wave condition

$$\begin{aligned} (u_0, v_0)(x,y) &= \sum_{n=-\infty}^{\infty} (E_n^{(0)}, B_n^{(0)})\, \mathrm{e}^{\,i(\alpha_n x+\beta_n^{(0)} y)} && \text{for } y > \max_{(x,t)\in\Sigma_0} t\,, \\ (u_N, v_N)(x,y) &= \sum_{n=-\infty}^{\infty} (E_n^{(N)}, B_n^{(N)})\, \mathrm{e}^{\,i(\alpha_n x-\beta_n^{(N)} y)} && \text{for } y < \min_{(x,t)\in\Sigma_N} t\,. \end{aligned} \tag{2.12}$$

It was proved in [2] that for non-magnetic materials ($\mu_j = \mu_0$) satisfying $0 \leq \arg\,\kappa_j^2 < \pi$ the problem (2.9 - 2.12) has a H^1 regular solution $\{u_j, v_j\}$. The solution is unique

- if $\operatorname{Im}\kappa_j^2 > 0$ for some j
- for all but a countable set of frequencies ω_ℓ, $\omega_\ell \to \infty$, if κ_j^2 are positive constants.

3 Integral equation method

The integral formulation is derived from potential representations of u_j, v_j in G_j. In the following we suppose that the interfaces Σ_j are given by piecewise C^2 parametrizations

$$\sigma_j(t) = (X_j(t), Y_j(t)), \quad X_j(t+1) = X_j(t) + d, \quad Y_j(t+1) = Y_j(t)\,, \quad t \in \mathbb{R}\,, \tag{3.1}$$

i.e., the functions X_j, Y_j are piecewise C^2 with

$$|\sigma_j'(t)| = \sqrt{(X_j'(t))^2 + (Y_j'(t))^2} > 0\,.$$

Moreover, the interfaces do not intersect, i.e. $\sigma_j(t_1) = \sigma_k(t_2)$ only if $j = k$ and $t_1 - t_2 = dn$. Additionally we suppose that, if a curve Σ_j has corners, then the angles between adjacent tangents at the corners are strictly between 0 and 2π.

3.1 Potentials and boundary integrals

The single and double layer potentials on one period $\Gamma_j = \{\sigma_j(t) : t \in [t_0, t_0 + 1]\}$ of the interface Σ_j corresponding to κ_m are denoted by

$$\mathcal{S}_{\Gamma_j,m}\varphi(P) = 2\int\limits_{\Gamma_j} \Psi_{m,\alpha}(P-Q)\,\varphi(Q)\,d\sigma_Q\,, \quad \mathcal{D}_{\Gamma_j,m}\varphi(P) = 2\int\limits_{\Gamma_j} \varphi(Q)\partial_{\mathbf{n}(Q)}\Psi_{m,\alpha}(P-Q)\,d\sigma_Q\,. \tag{3.2}$$

Here $\Psi_{m,\alpha}$ is the α-quasiperiodic fundamental solution

$$\Psi_{m,\alpha}(P) = \frac{i}{4}\sum_{n\in\mathbb{Z}} H_0^{(1)}\Big(\omega\kappa_m\sqrt{(X-dn)^2+Y^2}\Big)\,\mathrm{e}^{idn\alpha}\,, \quad P = (X,Y)\,. \tag{3.3}$$

of the Helmholtz operator $-(\Delta + \omega^2\kappa_m^2)$ with the Hankel function of the first kind $H_0^{(1)}$, $d\sigma_Q$ is the integration with respect to the arc length and $\partial_{\mathbf{n}(Q)}$ denotes the normal derivative with respect the normal $\mathbf{n}$ at $Q \in \Sigma_j$.

The series (3.3) converges uniformly over compact sets in $\mathbb{R}^2 \setminus \bigcup\limits_{n\in\mathbb{Z}}\{(dn,0)\}$ if the condition

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

is satisfied. Moreover, with $\beta_n^{(m)} = \sqrt{\omega^2\kappa_m^2 - \alpha_n^2}$, $\operatorname{Im}\beta_n^{(m)} \geq 0$, Poisson's summation formula leads to the representation

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

Therefore, in the following we assume that condition (3.4) holds for all κ_j, $j = 0,\dots,N$. Note that $\Psi_{0,\alpha}$ and $\Psi_{N,\alpha}$ satisfy the radiation conditions (2.12).

In the following we use properties of the potentials and their restrictions to a surfaces Σ_k. Define the function spaces

$$H_\alpha^s(\Gamma_j) = \Big\{\mathrm{e}^{i\alpha X_j}\,\varphi :\ \varphi\circ\sigma_j \in H_p^s(0,1)\Big\}\,, \tag{3.6}$$

where $H_p^s(0,1)$, $s \in \mathbb{R}$, denotes the Sobolev space of 1-periodic functions.

Under (3.4), the potentials $u = \mathcal{S}_{\Gamma_j,m}\varphi$, $\varphi \in H_\alpha^{-1/2}(\Gamma_j)$, and $u = \mathcal{D}_{\Gamma_j,m}\psi$, $\psi \in H_\alpha^{1/2}(\Gamma)$, are outside Σ_j locally H^1 and α-quasiperiodic solutions of the Helmholtz equation

$$(\Delta + \omega^2\kappa_m^2)u = 0\,, \tag{3.7}$$

which satisfy the radiation condition

$$u(x,y) = \sum_{n=-\infty}^{\infty} u_n\,\mathrm{e}^{i\alpha_n x + i\beta_n^{(m)}|y|}\,, \quad |y| \to \infty\,. \tag{3.8}$$

The interface Σ_j divides the plane into an upper and lower part denoted by G_j^+ and G_j^-. If the α-quasiperiodic function u belongs locally to $H^1(G_j^\pm)$ with $\Delta u \in L^2_{loc}(G_j^\pm)$, satisfies the Helmholtz equation (3.7) almost everywhere and the radiation condition (3.8), then

$$\pm\frac{1}{2}\big(\mathcal{S}_{\Gamma_j,m}\partial_{\mathbf{n}}u - \mathcal{D}_{\Gamma_j,m}u\big) = \begin{cases} u & \text{in } G_j^\pm\,, \\ 0 & \text{in } G_j^\mp\,. \end{cases} \tag{3.9}$$

In particular, for an α-quasiperiodic solution u of (2.9)

$$\frac{1}{2}\big(\mathcal{S}_{\Gamma_j,j}\partial_{\mathbf{n}}u-\mathcal{D}_{\Gamma_j,j}u\big)-\frac{1}{2}\big(\mathcal{S}_{\Gamma_{j-1},j}\partial_{\mathbf{n}}u-\mathcal{D}_{\Gamma_{j-1},j}u\big)=\begin{cases} u\,, & P\in G_j\,,\\ 0\,, & P\notin\overline{G_j}. \end{cases} \tag{3.10}$$

To treat the tangential derivatives in the transmission conditions (2.10), (2.11) also operators of the form

$$\mathcal{S}_{\Gamma_j,m}\big(\partial_{\mathbf{t}}\varphi\big)(P)=2\int\limits_{\Gamma_j}\Psi_{m,\alpha}(P-Q)\,\partial_{\mathbf{t}}\varphi(Q)\,d\sigma_Q=-2\int\limits_{\Gamma_j}\varphi(Q)\,\partial_{\mathbf{t}(Q)}\Psi_{m,\alpha}(P-Q)\,d\sigma_Q\,, \tag{3.11}$$

with $\varphi\in H^{1/2}_\alpha(\Gamma_j)$ will occur. If $P\notin\Sigma$, then the right hand side of (3.11) follows from integration by parts and the quasi-periodicity of $\Psi_{m,\alpha}$ and φ, and we may introduce the potential

$$\mathcal{T}_{\Gamma_j,m}\varphi(P)=2\int\limits_{\Gamma_j}\varphi(Q)\,\partial_{\mathbf{t}(Q)}\Psi_{m,\alpha}(P-Q)\,d\sigma_Q=-\mathcal{S}_{\Gamma_j,m}\big(\partial_{\mathbf{t}}\varphi\big)(P)\,,\quad P\notin\Sigma\,. \tag{3.12}$$

For $P\in\Gamma_j$ we define the boundary integral operators

$$\begin{aligned} V^{(m)}_{jk}\varphi(P)&=2\int\limits_{\Gamma_k}\Psi_{m,\alpha}(P-Q)\,\varphi(Q)\,d\sigma_Q\,, & K^{(m)}_{jk}\varphi(P)&=2\int\limits_{\Gamma_k}\varphi(Q)\,\partial_{\mathbf{n}(Q)}\Psi_{m,\alpha}(P-Q)\,d\sigma_Q\,,\\ L^{(m)}_{jk}\varphi(P)&=2\int\limits_{\Gamma_k}\varphi(Q)\,\partial_{\mathbf{n}(P)}\Psi_{m,\alpha}(P-Q)\,d\sigma_Q\,, & H^{(m)}_{jk}\varphi(P)&=2\int\limits_{\Gamma_k}\varphi(Q)\,\partial_{\mathbf{t}(Q)}\Psi_{m,\alpha}(P-Q)\,d\sigma_Q\,. \end{aligned} \tag{3.13}$$

If $j=k$, then the last integral is interpreted as the singular integral

$$2\int\limits_{\Gamma_j}\varphi(Q)\,\partial_{\mathbf{t}(Q)}\Psi_{m,\alpha}(P-Q)\,d\sigma_Q=2\lim_{\delta\to0}\int\limits_{\Gamma_j\setminus\Gamma_j(P,\delta)}\varphi(Q)\,\partial_{\mathbf{t}(Q)}\Psi_{m,\alpha}(P-Q)\,d\sigma_Q\,,$$

where $\Gamma_j(P,\delta)$ denotes the subarc of Γ_j with the mid point P and the arc length 2δ. In view of (3.11) the singular integral is connected with the single layer potential by the relation

$$H^{(m)}_{jj}\varphi(P)=-V^{(m)}_{jj}\big(\partial_{\mathbf{t}}\varphi\big)(P)\,. \tag{3.14}$$

The operators $V^{(m)}_{jj}$, $K^{(m)}_{jj}$, $H^{(m)}_{jj}$ and $L^{(m)}_{jj}$ have properties, which are quite similar to those of the well-studied integral operators over closed curves corresponding to boundary value problems for the Helmholtz equation, in particular

$$V^{(m)}_{jj}:H^{s-1}_\alpha(\Gamma_j)\to H^s_\alpha(\Gamma_j)\,,\ H^{(m)}_{jj},\,K^{(m)}_{jj}:H^t_\alpha(\Gamma_j)\to H^t_\alpha(\Gamma_j)\,,\ L^{(m)}_{jj}:H^{-t}_\alpha(\Gamma_j)\to H^{-t}_\alpha(\Gamma_j)$$

are bounded for $s\in(0,1)$, $t\in[0,1)$. In the case $s=t=1/2$ the operators $V^{(m)}_{jj}$ and $H^{(m)}_{jj}$ are Fredholm with $\operatorname{ind}V^{(m)}_{jj}=\operatorname{ind}H^{(m)}_{jj}=0$.

It is a quite rare case that the single layer potential operator $V^{(m)}_{jj}$ is not invertible. This is equivalent to the existence of nontrivial solutions in one of the domains $G^\pm_j$ of the homogeneous Dirichlet problem

$$\Delta u+\omega^2\kappa_m^2u=0\,,\quad u|_{\Sigma_j}=0\,,\quad u(x,y)=\mathrm{e}^{i\alpha d}\,u(x+d,y) \tag{3.15}$$

with the radiation condition (3.8). For boundaries of rather special form such solutions were constructed in [6]. On the other hand, the nonexistence of nontrivial solutions is known if $\operatorname{Im}\kappa_m^2>0$ or if the y-component $\mathbf{n}_y$ of the normal to the profile curve Σ_j satisfies $\mathbf{n}_y(Q)\le0$ for all $Q\in\Sigma_j$, for example if Σ_j is given by a d-periodic function $y=f_j(x)$, cf. [9, Section 2.4], [3].

If $j\ne k$, then the operators (3.13) have bounded continuous kernel functions and map therefore compactly into $H^s_\alpha(\Gamma_j)$, $s\le1$. If the profile curve Σ_j is smooth, then

$$V^{(m)}_{jj}:H^{s-1}_\alpha(\Gamma_j)\to H^s_\alpha(\Gamma_j)\,,\ K^{(m)}_{jj},\,L^{(m)}_{jj}:H^s_\alpha(\Gamma_j)\to H^{s+2}_\alpha(\Gamma_j)\,,H^{(m)}_{jj}:H^s_\alpha(\Gamma_j)\to H^s_\alpha(\Gamma_j)$$

are bounded and for $j \neq k$ the operators (3.13) are compact mappings into $H^s_\alpha(\Gamma_j)$ all $s \in \mathbb{R}$.

Let us note the jump relations

$$\begin{aligned}
&\big(\mathcal{S}_{\Gamma_j,m}\varphi\big)^{\pm}(P) = V^{(m)}_{jj}\varphi(P)\,, \qquad \big(\mathcal{T}_{\Gamma_j,m}\varphi\big)^{\pm}(P) = H^{(m)}_{jj}\varphi(P)\,,\\
&\big(\mathcal{D}_{\Gamma_j,m}\psi\big)^{\pm}(P) = (K^{(m)}_{jj} \mp I)\psi(P)\,, \quad \big(\partial_{\mathbf{n}}\mathcal{S}_{\Gamma_j,m}\varphi\big)^{\pm}(P) = (L^{(m)}_{jj} \pm I)\varphi(P)\,,
\end{aligned} \tag{3.16}$$

where the upper sign $+$ resp. $-$ denotes the limits of the potentials for points in $G_j^{\pm}$ tending in non-tangential direction to $P \in \Sigma_j$.

3.2 Integral equation algorithms

The jump relations and other layer representations can be used to derive various integral formulations of the transmission problem (2.9 - 2.12) by direct or indirect boundary integral methods or combinations of them. In [10] we considered the case of two profiles and derived a 4×4 system of singular integral equations, which can be extended to the general case of N profiles using the ansatz

$$\begin{aligned}
&u_0 = \frac{1}{2}\big(\mathcal{S}_{\Gamma_0,0}\partial_{\mathbf{n}}u_0 - \mathcal{D}_{\Gamma_0,0}u_0\big)\,, \quad v_0 = \frac{1}{2}\big(\mathcal{S}_{\Gamma_0,0}\partial_{\mathbf{n}}v_0 - \mathcal{D}_{\Gamma_0,0}v_0\big)\,, \quad \text{in } G_0\,,\\
&u_1 = \mathcal{S}_{\Gamma_0,1}\varphi_0 + \mathcal{S}_{\Gamma_1,1}\varphi_1\,, \qquad v_1 = \mathcal{S}_{\Gamma_0,1}\psi_0 + \mathcal{S}_{\Gamma_1,1}\psi_1\,, \qquad \text{in } G_1\,,\\
&\left.\begin{aligned}
u_2 &= \frac{1}{2}\big(\mathcal{S}_{\Gamma_2,2}\partial_{\mathbf{n}}u_2 - \mathcal{D}_{\Gamma_2,2}u_2\big) - \frac{1}{2}\big(\mathcal{S}_{\Gamma_1,2}\partial_{\mathbf{n}}u_2 - \mathcal{D}_{\Gamma_1,2}u_2\big)\,,\\
v_2 &= \frac{1}{2}\big(\mathcal{S}_{\Gamma_2,2}\partial_{\mathbf{n}}v_2 - \mathcal{D}_{\Gamma_2,2}v_2\big) - \frac{1}{2}\big(\mathcal{S}_{\Gamma_1,2}\partial_{\mathbf{n}}v_2 - \mathcal{D}_{\Gamma_1,2}v_2\big)\,,
\end{aligned}\right\} \quad \text{in } G_2\,,\\
&\text{and so on}
\end{aligned} \tag{3.17}$$

with unknown densities $\varphi_j, \psi_j \in H_\alpha^{-1/2}(\Gamma_j)$, $j = 0, \ldots, N-1$. In the bottom layer G_N we use the representation

$$u_N = \begin{cases} \mathcal{S}_{\Gamma_{N-1},N}\varphi_{N-1} \\ \frac{1}{2}\big(\mathcal{D}_{\Gamma_{N-1},N}u_N - \mathcal{S}_{\Gamma_{N-1},N}\partial_{\mathbf{n}}u_N\big) \end{cases}, \quad v_N = \begin{cases} \mathcal{S}_{\Gamma_{N-1},N}\psi_{N-1}\,, & N \text{ odd}\\ \frac{1}{2}\big(\mathcal{D}_{\Gamma_{N-1},N}v_N - \mathcal{S}_{\Gamma_{N-1},N}\partial_{\mathbf{n}}v_N\big), & N \text{ even} \end{cases}$$

In view of (3.9) and (3.10) the Helmholtz equations (2.9) and the outgoing wave condition (2.12) are satisfied. As shown in [10] for the special case $N = 2$, the transmission conditions (2.10) and (2.11) lead to a $2N \times 2N$ system of integral equations on the profiles Γ_j. The diagonal 2×2 blocks of the system, which correspond to singular integral equations for the densities φ_j, ψ_j on the profile Γ_j, have been analyzed in [11]. Analytical properties of the $2N \times 2N$ system follow immediately from these results, some of them will be mentioned in the following. Also from the numerical point of view the approach (3.17) is not of interest, since the discretization and solution of this system in order to simulate grating structures with dozens of different material layers is beyond the possibilities of modern workstations.

Instead, we present a recursive algorithm for solving (2.9 - 2.12), which in each step treats a problem for one of the interfaces and therefore allows to solve conical diffraction problems for gratings with an arbitrary number of layers on standard PCs. The algorithm extends a method for in-plane diffraction, i.e., $\gamma = 0$, which was proposed by Maystre in [7] and described in detail in [5].

The starting point is to seek the solutions $\{u_j, v_j\}_{j=0}^N$ of (2.9 - 2.12) in the form

$$u_0 = \frac{1}{2}\big(\mathcal{S}_{\Gamma_0,0}\partial_{\mathbf{n}}u_0 - \mathcal{D}_{\Gamma_0,0}u_0\big)\,, \quad v_0 = \frac{1}{2}\big(\mathcal{S}_{\Gamma_0,0}\partial_{\mathbf{n}}v_0 - \mathcal{D}_{\Gamma_0,0}v_0\big)\,, \quad \text{in } G_0\,, \tag{3.18}$$

$$\left.\begin{aligned}
u_j &= \frac{1}{2}\big(\mathcal{S}_{\Gamma_j,j}\partial_{\mathbf{n}}u_j - \mathcal{D}_{\Gamma_j,j}u_j\big) + \mathcal{S}_{\Gamma_{j-1},j}\varphi_{j-1}\,,\\
v_j &= \frac{1}{2}\big(\mathcal{S}_{\Gamma_j,j}\partial_{\mathbf{n}}v_j - \mathcal{D}_{\Gamma_j,j}v_j\big) + \mathcal{S}_{\Gamma_{j-1},j}\psi_{j-1}\,,
\end{aligned}\right\} \quad \text{in } G_j\,,\ j = 1, \ldots, N-1 \tag{3.19}$$

$$u_N = \mathcal{S}_{\Gamma_{N-1},N}\varphi_{N-1}\,, \quad v_N = \mathcal{S}_{\Gamma_{N-1},N}\psi_{N-1}\,, \qquad \text{in } G_N\,, \tag{3.20}$$

with certain densities $\varphi_j, \psi_j \in H_\alpha^{-1/2}(\Gamma_j)$, $j = 0, \dots, N-1$. Again, the Helmholtz equations (2.9) and the outgoing wave condition (2.12) are satisfied. Note that the representations (3.19 - 3.20) are unique provided that the single layer potential operators $V^{(j)}_{j-1j-1}$ are invertible for $j = 1, \dots, N$, which will be assumed throughout.

The algorithm determines recursive relations

$$\begin{pmatrix}\varphi_j\\ \psi_j\end{pmatrix} = \mathcal{Q}_{j-1}\begin{pmatrix}\varphi_{j-1}\\ \psi_{j-1}\end{pmatrix}, \quad j = 1, \dots, N-1, \tag{3.21}$$

such that the functions $\{u_j, v_j\}_{j=0}^N$ fulfill the remaining transmission conditions (2.10) and (2.11). The initial densities (φ_0, ψ_0) and the 2×2 operator matrices $\{\mathcal{Q}_{j-1}\}$ are obtained by the following scheme:

Introduce the coefficients

$$a_j = \frac{\varepsilon_{j+1}\kappa_j^2}{\varepsilon_j \kappa_{j+1}^2}\,,\ b_j = \frac{\mu_{j+1}\kappa_j^2}{\mu_j \kappa_{j+1}^2}\,,\ c_j = \frac{\varepsilon_0}{\varepsilon_j}\Big(1 - \frac{\kappa_j^2}{\kappa_{j+1}^2}\Big)\sin\phi\,,\ d_j = \frac{\mu_0}{\mu_j}\Big(1 - \frac{\kappa_j^2}{\kappa_{j+1}^2}\Big)\sin\phi\,, \tag{3.22}$$

and determine $\mathcal{Q}_{j-1}$ by a backward recurrence for $j = N-1, \dots, 1$ as a solution of the operator equation

$$\left(\begin{pmatrix} I + K^{(j)}_{jj} & -c_j H^{(j)}_{jj} \\ d_j H^{(j)}_{jj} & I + K^{(j)}_{jj}\end{pmatrix} \mathcal{A}_j - \begin{pmatrix} a_j V^{(j)}_{jj} & 0 \\ 0 & b_j V^{(j)}_{jj}\end{pmatrix} \mathcal{B}_j\right) \mathcal{Q}_{j-1} = 2 \begin{pmatrix} V^{(j)}_{jj-1} & 0 \\ 0 & V^{(j)}_{jj-1}\end{pmatrix}. \tag{3.23}$$

The initial values are

$$\mathcal{A}_{N-1} = \begin{pmatrix} V^{(N)}_{N-1N-1} & 0 \\ 0 & V^{(N)}_{N-1N-1}\end{pmatrix}, \quad \mathcal{B}_{N-1} = \begin{pmatrix} L^{(N)}_{N-1N-1} - I & 0 \\ 0 & L^{(N)}_{N-1N-1} - I\end{pmatrix}, \tag{3.24}$$

and the subsequent terms in (3.23) are derived by

$$\begin{aligned}\mathcal{A}_{j-1} = &\begin{pmatrix} V^{(j)}_{j-1j-1} & 0 \\ 0 & V^{(j)}_{j-1j-1}\end{pmatrix} \\ &- \frac{1}{2}\left(\begin{pmatrix} K^{(j)}_{j-1j} & -c_j H^{(j)}_{j-1j} \\ d_j H^{(j)}_{j-1j} & K^{(j)}_{j-1j}\end{pmatrix} \mathcal{A}_j - \begin{pmatrix} a_j V^{(j)}_{j-1j} & 0 \\ 0 & b_j V^{(j)}_{j-1j}\end{pmatrix} \mathcal{B}_j\right) \mathcal{Q}_{j-1}\,,\end{aligned} \tag{3.25}$$

$$\mathcal{B}_{j-1} = \begin{pmatrix} V^{(j)}_{j-1j-1} & 0 \\ 0 & V^{(j)}_{j-1j-1}\end{pmatrix}^{-1} \begin{pmatrix} I + K^{(j)}_{j-1j-1} & 0 \\ 0 & I + K^{(j)}_{j-1j-1}\end{pmatrix} \mathcal{A}_{j-1} - 2\begin{pmatrix} I & 0 \\ 0 & I\end{pmatrix}. \tag{3.26}$$

Having found $\mathcal{A}_0$ and $\mathcal{B}_0$, the initial value (φ_0, ψ_0) of (3.21) is a solution of the linear equation

$$\left(\begin{pmatrix} I + K^{(0)}_{00} & -c_0 H^{(0)}_{00} \\ d_0 H^{(0)}_{00} & I + K^{(0)}_{00}\end{pmatrix} \mathcal{A}_0 - \begin{pmatrix} a_0 V^{(0)}_{00} & 0 \\ 0 & b_0 V^{(0)}_{00}\end{pmatrix} \mathcal{B}_0\right) \begin{pmatrix}\varphi_0\\ \psi_0\end{pmatrix} = 2\begin{pmatrix}u^i\\ v^i\end{pmatrix}. \tag{3.27}$$

3.3 Derivation of the recursive algorithm

The scheme is based on the ansatz

$$\begin{pmatrix}u_{j+1}|_{\Gamma_j}\\ v_{j+1}|_{\Gamma_j}\end{pmatrix} = \mathcal{A}_j \begin{pmatrix}\varphi_j\\ \psi_j\end{pmatrix}, \quad \begin{pmatrix}\partial_{\mathbf{n}} u_{j+1}|_{\Gamma_j}\\ \partial_{\mathbf{n}} v_{j+1}|_{\Gamma_j}\end{pmatrix} = \mathcal{B}_j \begin{pmatrix}\varphi_j\\ \psi_j\end{pmatrix} \quad j = 0, \dots, N-1\,, \tag{3.28}$$

with certain 2×2 linear operator matrices $\mathcal{A}_j$ and $\mathcal{B}_j$. Note first that the initial values (3.24) follow from (3.20) and the jump relation (3.16) for $\partial_{\mathbf{n}} \mathcal{S}_{\Gamma_{N-1},N}$.

Using (3.28) the transmission conditions (2.11) on Γ_j for $j = 1, \dots, N-1$ can be written in the form

$$\begin{pmatrix}u_j|_{\Gamma_j}\\ v_j|_{\Gamma_j}\end{pmatrix} = \mathcal{A}_j \begin{pmatrix}\varphi_j\\ \psi_j\end{pmatrix}, \ \begin{pmatrix}\partial_{\mathbf{n}} u_j|_{\Gamma_j}\\ \partial_{\mathbf{n}} v_j|_{\Gamma_j}\end{pmatrix} = \begin{pmatrix} a_j & 0 \\ 0 & b_j\end{pmatrix} \mathcal{B}_j \begin{pmatrix}\varphi_j\\ \psi_j\end{pmatrix} + \begin{pmatrix} 0 & -c_j\,\partial_{\mathbf{t}} \\ d_j\,\partial_{\mathbf{t}} & 0\end{pmatrix} \mathcal{A}_j \begin{pmatrix}\varphi_j\\ \psi_j\end{pmatrix}. \tag{3.29}$$

The representation (3.19) and the jump relation (3.16) of the double layer potential $\mathcal{D}_{\Gamma_j,j}$ imply that

$$u_j|_{\Gamma_j} = \frac{1}{2}\big(V^{(j)}_{jj}\partial_{\mathbf{n}} u_j - (K^{(j)}_{jj} - I)u_j\big) + V^{(j)}_{jj-1}\varphi_{j-1}\,, \quad v_j|_{\Gamma_j} = \frac{1}{2}\big(V^{(j)}_{jj}\partial_{\mathbf{n}} v_j - (K^{(j)}_{jj} - I)v_j\big) + V^{(j)}_{jj-1}\psi_{j-1}\,.$$

Hence (3.29) leads, in matrix notation, to the equation

$$\begin{pmatrix} a_j V_{jj}^{(j)} & 0 \\ 0 & b_j V_{jj}^{(j)} \end{pmatrix} \mathcal{B}_j \begin{pmatrix} \varphi_j \\ \psi_j \end{pmatrix} - \begin{pmatrix} I + K_{jj}^{(j)} & c_j V_{jj}^{(j)} \partial_{\mathbf{t}} \\ -d_j V_{jj}^{(j)} \partial_{\mathbf{t}} & I + K_{jj}^{(j)} \end{pmatrix} \mathcal{A}_j \begin{pmatrix} \varphi_j \\ \psi_j \end{pmatrix} = -2 \begin{pmatrix} V_{jj-1}^{(j)} \varphi_{j-1} \\ V_{jj-1}^{(j)} \psi_{j-1} \end{pmatrix}, \tag{3.30}$$

which is equivalent to (2.11). Using the singular integral $H_{jj}^{(j)} = -V_{jj}^{(j)} \partial_{\mathbf{t}}$ (see (3.14)) we obtain the relation

$$\left(\begin{pmatrix} I + K_{jj}^{(j)} & -c_j H_{jj}^{(j)} \\ d_j H_{jj}^{(j)} & I + K_{jj}^{(j)} \end{pmatrix} \mathcal{A}_j - \begin{pmatrix} a_j V_{jj}^{(j)} & 0 \\ 0 & b_j V_{jj}^{(j)} \end{pmatrix} \mathcal{B}_j \right) \begin{pmatrix} \varphi_j \\ \psi_j \end{pmatrix} = 2 \begin{pmatrix} V_{jj-1}^{(j)} & 0 \\ 0 & V_{jj-1}^{(j)} \end{pmatrix} \begin{pmatrix} \varphi_{j-1} \\ \psi_{j-1} \end{pmatrix},$$

which is satisfied by

$$\begin{pmatrix} \varphi_j \\ \psi_j \end{pmatrix} = \mathcal{Q}_{j-1} \begin{pmatrix} \varphi_{j-1} \\ \psi_{j-1} \end{pmatrix},$$

provided that $\mathcal{Q}_{j-1}$ is a solution of the operator equation (3.23), which maps the space $\left(H_\alpha^{-1/2}(\Gamma_{j-1})\right)^2$ boundedly into $\left(H_\alpha^{-1/2}(\Gamma_j)\right)^2$. The solvability of (3.23) will be discussed in the next section.

The formulas (3.25) and (3.26) for $\mathcal{A}_{j-1}$ and $\mathcal{B}_{j-1}$ are derived from relations on the upper boundary Γ_{j-1} of G_j. The representation (3.19) and (3.29) give

$$\begin{aligned} \begin{pmatrix} u_j|_{\Gamma_{j-1}} \\ v_j|_{\Gamma_{j-1}} \end{pmatrix} &= \frac{1}{2} \left(\begin{pmatrix} V_{j-1j}^{(j)} & 0 \\ 0 & V_{j-1j}^{(j)} \end{pmatrix} \begin{pmatrix} \partial_n u_j|_{\Gamma_j} \\ \partial_n v_j|_{\Gamma_j} \end{pmatrix} - \begin{pmatrix} K_{j-1j}^{(j)} & 0 \\ 0 & K_{j-1j}^{(j)} \end{pmatrix} \begin{pmatrix} u_j|_{\Gamma_j} \\ v_j|_{\Gamma_j} \end{pmatrix} \right) + \begin{pmatrix} V_{j-1j-1}^{(j)} \varphi_{j-1} \\ V_{j-1j-1}^{(j)} \psi_{j-1} \end{pmatrix} \\ &= \frac{1}{2} \left(\begin{pmatrix} a_j V_{j-1j}^{(j)} & 0 \\ 0 & b_j V_{j-1j}^{(j)} \end{pmatrix} \mathcal{B}_j - \begin{pmatrix} K_{j-1j}^{(j)} & c_j V_{j-1j}^{(j)} \partial_{\mathbf{t}} \\ -d_j V_{j-1j}^{(j)} \partial_{\mathbf{t}} & K_{j-1j}^{(j)} \end{pmatrix} \mathcal{A}_j \right) \begin{pmatrix} \varphi_j \\ \psi_j \end{pmatrix} \\ &\quad + \begin{pmatrix} V_{j-1j-1}^{(j)} & 0 \\ 0 & V_{j-1j-1}^{(j)} \end{pmatrix} \begin{pmatrix} \varphi_{j-1} \\ \psi_{j-1} \end{pmatrix}, \end{aligned}$$

which by (3.28), (3.21) and using $H_{j-1j}^{(j)} = -V_{j-1j}^{(j)} \partial_{\mathbf{t}}$ leads to (3.25).

Now (3.26) follows from (3.10) and (3.19), since

$$\begin{aligned} V_{j-1j-1}^{(j)} \varphi_{j-1} &= -\frac{1}{2} \left(V_{j-1j-1}^{(j)} \partial_{\mathbf{n}} u_j - (I + K_{j-1j-1}^{(j)}) u_j \right), \\ V_{j-1j-1}^{(j)} \psi_{j-1} &= -\frac{1}{2} \left(V_{j-1j-1}^{(j)} \partial_{\mathbf{n}} v_j - (I + K_{j-1j-1}^{(j)}) v_j \right), \end{aligned}$$

imply that on Γ_{j-1}

$$\begin{pmatrix} \partial_{\mathbf{n}} u_j \\ \partial_{\mathbf{n}} v_j \end{pmatrix} = \begin{pmatrix} (V_{j-1j-1}^{(j)})^{-1} (I + K_{j-1j-1}^{(j)}) & 0 \\ 0 & (V_{j-1j-1}^{(j)})^{-1} (I + K_{j-1j-1}^{(j)}) \end{pmatrix} \mathcal{A}_{j-1} \begin{pmatrix} \varphi_{j-1} \\ \psi_{j-1} \end{pmatrix} - 2 \begin{pmatrix} \varphi_{j-1} \\ \psi_{j-1} \end{pmatrix}.$$

Equation (3.27) follow the relations

$$V_{00}^{(0)} \partial_n u^i - (I + K_{00}^{(0)}) u^i = -2u^i, \quad V_{00}^{(0)} \partial_n v^i - (I + K_{00}^{(0)}) v^i = -2v^i$$

on the upper profile Γ_0, which hold because u^i, v^i satisfy the Helmholtz equation $(\Delta + \omega^2 \kappa_0^2) u = 0$ and the radiation condition (3.8) in $G_0^- = \mathbb{R}^2 \setminus \overline{G_0}$. Hence the transmission conditions (2.10) are fulfilled iff

$$\begin{pmatrix} I + K_{00}^{(0)} & -c_0 H_{00}^{(0)} \\ d_0 H_{00}^{(0)} & I + K_{00}^{(0)} \end{pmatrix} \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} - \begin{pmatrix} a_0 V_{00}^{(0)} & 0 \\ 0 & b_0 V_{00}^{(0)} \end{pmatrix} \begin{pmatrix} \partial_n u_1 \\ \partial_n v_1 \end{pmatrix} = 2 \begin{pmatrix} u^i \\ v^i \end{pmatrix},$$

i.e., if φ_0, ψ_0 satisfy (3.27).

Remark 3.1. *If the material in the bottom layer G_N is a perfect conductor, then the z-components of E and B have to satisfy the boundary condition*

$$E_z = u_N = 0, \quad \partial_{\mathbf{n}} B_z = \partial_{\mathbf{n}} v_N = 0 \qquad \textit{on } \Gamma_{N-1}. \tag{3.31}$$

In this case it is easy to see that the relations (3.25) *and* (3.26) *for* $j = N-1$ *with the coefficients* $a_{N-1} = 1$, $b_{N-1} = c_{N-1} = d_{N-1} = 0$, *and the initial values*

$$\mathcal{A}_{N-1} = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \quad \textit{and} \quad \mathcal{B}_{N-1} = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}$$

lead to $\mathcal{A}_{N-2}$ *and* $\mathcal{B}_{N-2}$ *satisfying*

$$\begin{pmatrix} u_{N-1}|_{\Gamma_{N-2}} \\ v_{N-1}|_{\Gamma_{N-2}} \end{pmatrix} = \mathcal{A}_{N-2} \begin{pmatrix} \varphi_{N-2} \\ \psi_{N-2} \end{pmatrix}, \quad \begin{pmatrix} \partial_{\mathbf{n}} u_{N-1}|_{\Gamma_{N-2}} \\ \partial_{\mathbf{n}} v_{N-1}|_{\Gamma_{N-2}} \end{pmatrix} = \mathcal{B}_{N-2} \begin{pmatrix} \varphi_{N-2} \\ \psi_{N-2} \end{pmatrix}.$$

Hence, the densities $\{\varphi_j, \psi_j\}$, $j = 0, \ldots, N-2$, *are derived by the same scheme* (3.21 - 3.27).

4 Analysis of the algorithm

We call the algorithm (3.21 – 3.27) *applicable*, if for $j = N-1, \ldots, 1$ in descending order there exist solutions $\mathcal{Q}_{j-1} : \big(H_\alpha^{-1/2}(\Gamma_{j-1})\big)^2 \to \big(H_\alpha^{-1/2}(\Gamma_j)\big)^2$ of the operator equations (3.23), which we write as

$$\mathcal{C}_j \mathcal{Q}_{j-1} = 2\, \mathcal{V}_{j-1}\,, \tag{4.1}$$

with the 2×2 operator matrices

$$\mathcal{C}_j = \begin{pmatrix} I + K_{jj}^{(j)} & -c_j H_{jj}^{(j)} \\ d_j H_{jj}^{(j)} & I + K_{jj}^{(j)} \end{pmatrix} \mathcal{A}_j - \begin{pmatrix} a_j V_{jj}^{(j)} & 0 \\ 0 & b_j V_{jj}^{(j)} \end{pmatrix} \mathcal{B}_j\,, \quad \mathcal{V}_{j-1} = \begin{pmatrix} V_{jj-1}^{(j)} & 0 \\ 0 & V_{jj-1}^{(j)} \end{pmatrix}. \tag{4.2}$$

Then the formulas (3.25), (3.26), (4.2) lead to the bounded mappings

$$\mathcal{B}_{j-1} : \big(H_\alpha^{-1/2}(\Gamma_{j-1})\big)^2 \to \big(H_\alpha^{-1/2}(\Gamma_{j-1})\big)^2, \quad \mathcal{A}_{j-1}, \mathcal{C}_{j-1} : \big(H_\alpha^{-1/2}(\Gamma_{j-1})\big)^2 \to \big(H_\alpha^{1/2}(\Gamma_{j-1})\big)^2,$$

and in the successive step one has to solve the equation (4.1) for $\mathcal{Q}_{j-2}$ or, if $j = 1$, the equation (3.27), which can be written as

$$\mathcal{C}_0 \begin{pmatrix} \varphi_0 \\ \psi_0 \end{pmatrix} = 2 \begin{pmatrix} u^i \\ v^i \end{pmatrix}. \tag{4.3}$$

If there exists a solution $\varphi_0, \psi_0 \in H_\alpha^{-1/2}(\Gamma_0)$, then the scheme (3.21) leads by construction to a H^1-regular solution of the conical diffraction (2.4, 2.5, 2.7) for the multilayer grating

$$\begin{pmatrix} E_z \\ B_z \end{pmatrix} = \begin{cases} \begin{pmatrix} u^i \\ v^i \end{pmatrix} + \dfrac{1}{2} \left(\begin{pmatrix} a_0 \mathcal{S}_{\Gamma_0,0} & 0 \\ 0 & b_0 \mathcal{S}_{\Gamma_0,0} \end{pmatrix} \mathcal{B}_0 - \begin{pmatrix} \mathcal{D}_{\Gamma_0,0} & -c_0 \mathcal{T}_{\Gamma_0,0} \\ d_0 \mathcal{T}_{\Gamma_0,0} & \mathcal{D}_{\Gamma_0,0} \end{pmatrix} \mathcal{A}_0 \right) \begin{pmatrix} \varphi_0 \\ \psi_0 \end{pmatrix} & \text{in } G_0\,, \\[2ex] \dfrac{1}{2} \left(\begin{pmatrix} a_j \mathcal{S}_{\Gamma_j,j} & 0 \\ 0 & b_j \mathcal{S}_{\Gamma_j,j} \end{pmatrix} \mathcal{B}_j - \begin{pmatrix} \mathcal{D}_{\Gamma_j,j} & -c_j \mathcal{T}_{\Gamma_j,j} \\ d_j \mathcal{T}_{\Gamma_j,j} & \mathcal{D}_{\Gamma_j,j} \end{pmatrix} \mathcal{A}_j \right) \begin{pmatrix} \varphi_j \\ \psi_j \end{pmatrix} & \\ \quad + \begin{pmatrix} \mathcal{S}_{\Gamma_{j-1},j} & 0 \\ 0 & \mathcal{S}_{\Gamma_{j-1},j} \end{pmatrix} \begin{pmatrix} \varphi_{j-1} \\ \psi_{j-1} \end{pmatrix} & \text{in } G_j\,, \quad j = 1, \ldots, N-1\,, \\[2ex] \begin{pmatrix} \mathcal{S}_{\Gamma_N,N+1} & 0 \\ 0 & \mathcal{S}_{\Gamma_N,N+1} \end{pmatrix} \begin{pmatrix} \varphi_N \\ \psi_N \end{pmatrix} & \text{in } G_N\,, \end{cases} \tag{4.4}$$

with the layer potentials defined in (3.2) and (3.12).

Hence, if the operators $V_{jj}^{(j+1)}$ are invertible, then the recursive algorithm is applicable if and only if the equations (4.1) and (4.3) are solvable. In this section we derive conditions for the solvability of these equations, which follow from Fredholm properties of the operator matrices $\mathcal{C}_j$. Recall that a linear operator $A : X \to Y$ is Fredholm, if its range $\mathrm{R}(A) \subset Y$ is closed, and its nullspace $\mathrm{N}(A)$ and the factor space $Y/\,\mathrm{R}(A)$ are finite dimensional. The index of A is defined as $\operatorname{ind} A = \dim \mathrm{N}(A) - \dim(Y/\,\mathrm{R}(A))$. We denote by $\Phi_0(X, Y)$ the set of bounded Fredholm operators of index 0 mapping the space X into Y, and set $\Phi_0(X) = \Phi_0(X, Y)$.

The Fredholm properties of $\mathcal{C}_j$ will be studied similar to the 2×2 system of singular integral equations for one-profile gratings in [10, 11], using associated boundary integral operators of the Laplacian over a closed curve. We introduce the system of non-intersecting closed curves

$$\widetilde{\Gamma}_j = \left\{ \mathrm{e}^{-Y_j(t)} \left(\cos X_j(t), \sin X_j(t) \right) : t \in [0,1] \right\},$$

which is the image of the grating interfaces $\{\Sigma_j\}$ under the conformal mapping e^{iz}, $z \in \mathbb{C}$. Obviously, $\widetilde{\Gamma}_j$ has the same smoothness as Σ_j and the angles in G_j^+ at corner points of Σ_j and interior angles at the corresponding corner points of $\widetilde{\Gamma}_j$ coincide. We introduce the double and layer potentials of the Laplacian over $\widetilde{\Gamma}_j$

$$\widetilde{\mathcal{S}}_j \varphi(P) = \int_{\widetilde{\Gamma}_j} \Psi(P-Q)\, \varphi(Q)\, d\sigma_Q\,, \quad \widetilde{\mathcal{D}}_j \varphi(P) = \int_{\widetilde{\Gamma}_j} \varphi(Q) \partial_{\mathbf{n}(Q)} \Psi(P-Q)\, d\sigma_Q\,, \tag{4.5}$$

with the fundamental solution $\Psi(P) = -\log|P|/2\pi$ and similar to (3.13) the corresponding integral operators $\widetilde{V}_{jk}$, $\widetilde{K}_{jk}$, $\widetilde{L}_{jk}$, and $\widetilde{H}_{jk} = -\widetilde{V}_{jk}\partial_{\mathbf{t}}$, which map functions on $\widetilde{\Gamma}_k$ to functions on $\widetilde{\Gamma}_j$.

For completeness we give some well known properties of these operators. If $j \neq k$, then the mappings are compact from $H^s(\widetilde{\Gamma}_k)$ into $H^1(\widetilde{\Gamma}_j)$, since their kernels are bounded and continuous. For $j = k$ one has in the energy spaces $H^{\pm 1/2}(\widetilde{\Gamma}_j)$ that $\widetilde{V}_{jj} : H^{-1/2}(\widetilde{\Gamma}_j) \to H^{1/2}(\widetilde{\Gamma}_j)$, and $\widetilde{K}_{jj}, \widetilde{H}_{jj} : H^{1/2}(\widetilde{\Gamma}_j) \to H^{1/2}(\widetilde{\Gamma})$ are bounded. With respect to the L_2-duality $\widetilde{L}_{jj}$ is the adjoint of $\widetilde{K}_{jj}$, whereas $\widetilde{V}_{jj}$ is symmetric. Furthermore, $\mathrm{N}(I + \widetilde{K}_{jj}) = \mathrm{N}(H_{jj}) = \mathbf{P}_0$, where $\mathbf{P}_0$ denotes the set of constant functions, and the operators $\widetilde{V}_{jj}, \widetilde{H}_{jj}$ are Fredholm with index 0, $\widetilde{V}_{jj} \in \Phi_0(H^{-1/2}(\widetilde{\Gamma}_j), H^{1/2}(\widetilde{\Gamma}_j))$, $\widetilde{H}_{jj} \in \Phi_0(H^{1/2}(\widetilde{\Gamma}_j))$. In the following the relations between the integral operators

$$\widetilde{V}_{jj}\widetilde{L}_{jj} = \widetilde{K}_{jj}\widetilde{V}_{jj}\,, \quad \widetilde{H}_{jj}\widetilde{K}_{jj} = -\widetilde{K}_{jj}\widetilde{H}_{jj}\,, \quad \widetilde{K}_{jj}^2 - \widetilde{H}_{jj}^2 = I\,, \tag{4.6}$$

will be used, the second and third identity can be found in [11].

Using the double layer potential operators $\widetilde{K}_{jj}$ over $\widetilde{\Gamma}_j$ the main result can be formulated as follows:

Theorem 4.1. *Let the grating parameters ε_j, μ_j with $\arg\varepsilon_j, \arg\mu_j \in [0,\pi]$, $\arg\varepsilon_j + \arg\mu_j < 2\pi$, be such that the operators $V_{jj}^{(j+1)}$ are invertible and that*

$$(\varepsilon_{j+1} + \varepsilon_j)I + (\varepsilon_{j+1} - \varepsilon_j)\widetilde{K}_{jj}\,,\ (\mu_{j+1} + \mu_j)I + (\mu_{j+1} - \mu_j)\widetilde{K}jj \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma}_j)\big) \tag{4.7}$$

for all $j = 0, \ldots, N-1$. The algorithm (3.21 – 3.27) *is applicable if and only if $\mathrm{N}(\mathcal{C}_j) = \{0\}$, $j \geq 1$. Then the equation* (3.27) *is solvable and any solution (φ_0, ψ_0) provides via* (3.21), (4.4) *a solution of the conical diffraction problem* (2.4, 2.5, 2.7).

Since for a closed Lipschitz curve $\widetilde{\Gamma}_j$ the operator $\lambda I + \widetilde{K}_{jj} \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma}_j)\big)$ if $\lambda \notin (-1,1)$, see [11, Lemma 5.1], conditions (4.7) are satisfied if the ratios

$$\frac{\varepsilon_j}{\varepsilon_{j+1}}, \frac{\mu_j}{\mu_{j+1}} \notin (-\infty, 0) \qquad \text{for all } j\,. \tag{4.8}$$

Noting that for a closed, sufficiently smooth curve $\widetilde{\Gamma}_j$ and all $\lambda \neq 0$ we have $\lambda I + \widetilde{K}_{jj} \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma}_j)\big)$ and that the single layer potentials are invertible on function profiles, Theorem 4.1 admits to formulate

Corollary 4.1. *Suppose that the profile curves Σ_j are given by d-periodic C^2-functions and let $\varepsilon_{j+1} \neq -\varepsilon_j$ and $\mu_{j+1} \neq -\mu_j$. If $\mathrm{N}(\mathcal{C}_j) = \{0\}$, $j = N-1, \ldots, 1$, then the algorithm* (3.21 – 3.27) *provides a solution of the conical diffraction problem* (2.4, 2.5, 2.7).

Remark 4.1. *For a piecewise C^2-curve one can expect the existence of $\rho < 1$ depending on the angles of $\widetilde{\Gamma}_j$, such that for $\lambda \notin (-\rho, \rho)$ the operator $\lambda I + \widetilde{K}_{jj}$ is Fredholm with index 0. For example, in the space $C(\widetilde{\Gamma}_j)$ the parameter ρ is equal to $\max|\pi - \alpha_s|/\pi$, where the maximum is taken over all interior angles α_s of $\widetilde{\Gamma}_j$, see* [1]. *However, the precise bounds for the Sobolev space $H^{1/2}(\widetilde{\Gamma}_j)$ are unknown.*

The proof of Theorem 4.1 consists of two parts. First we show in Proposition 4.1 that (4.7) is necessary and sufficient in order that the operators $\mathcal{C}_j$ are Fredholm with index 0, provided of course that Q_j exist for $j < N-2$. Then Proposition 4.2 states that the equations (4.1) are solvable only if $\mathrm{R}(\mathcal{C}_j) = \big(\big(H_\alpha^{1/2}(\Gamma_j)\big)\big)^2$ and that the right hand side of (4.3) (u^i, v^i) belongs to the range of $\mathcal{C}_0$ also if $\mathrm{N}(\mathcal{C}_0) \neq \{0\}$. Finally, in Subsection 4.3 we consider the case that $\mathrm{N}(\mathcal{C}_j) \neq \{0\}$ and discuss conditions ensuring that the nullspaces $\mathrm{N}(\mathcal{C}_j)$ are trivial.

4.1 Fredholm properties of $\mathcal{C}_j$

Proposition 4.1. *Let $j = N-1,\dots,0$ and assume the existence of $\mathcal{Q}_j : \big(H^{1/2}_\alpha(\Gamma_j)\big)^2 \to \big(H^{1/2}_\alpha(\Gamma_{j+1})\big)^2$ for $j < N-1$. The operator matrix $\mathcal{C}_j \in \Phi_0\big((H^{-1/2}_\alpha(\Gamma_j))^2, (H^{1/2}_\alpha(\Gamma_j))^2\big)$ if and only if (4.7) holds.*

To connect diffraction boundary integrals over Γ_j with boundary integrals of the Laplacian over $\widetilde{\Gamma}_j$ we use the mappings

$$\vartheta_j^*\varphi(P) := \mathrm{e}^{i\alpha X_j}\,\varphi(\vartheta_j(P)) \quad \text{with} \quad \vartheta_j : \Gamma_j \ni P = (X_j, Y_j) \to \mathrm{e}^{-Y_j}(\cos X_j, \sin X_j) \in \widetilde{\Gamma}_j\,, \tag{4.9}$$

which generate isomorphisms $\vartheta_j^* : H^s(\widetilde{\Gamma}_j) \to H^s_\alpha(\Gamma_j)$, and the multiplication operators

$$M_j\varphi(P) = \mathrm{e}^{Y_j}\varphi(P)\,, \quad P = (X_j, Y_j) \in \Gamma_j\,, \tag{4.10}$$

which are invertible in $H^s_\alpha(\Gamma_j)$. The asymptotics of the fundamental solution $\Psi_{m,\alpha}$ implies that

$$\begin{aligned}
&V^{(m)}_{jj} - \vartheta_j^*\widetilde{V}_{jj}(\vartheta_j^*)^{-1}M_j :\ H^{s-1}_\alpha(\Gamma_j) \to H^s_\alpha(\Gamma_j)\,,\\
&K^{(m)}_{jj} - \vartheta_j^*\widetilde{K}_{jj}(\vartheta_j^*)^{-1},\ H^{(m)}_{jj} - \vartheta_j^*\widetilde{H}_{jj}(\vartheta_j^*)^{-1} :\ \ H^t_\alpha(\Gamma_j) \to H^t_\alpha(\Gamma_j)\,,\\
&L^{(m)}_{jj} - M_j^{-1}\vartheta_j^*\widetilde{L}_{jj}(\vartheta_j^*)^{-1}M_j :\ H^{-t}_\alpha(\Gamma_j) \to H^{-t}_\alpha(\Gamma_j)\,,
\end{aligned} \tag{4.11}$$

are compact mappings for $0 < s < 1$ and $0 \le t < 1$ if Γ_j has corners, and for all s, t for smooth Γ_j (cf. [10]). Hence, we derive from (3.25), (3.26) together with (4.6)

Lemma 4.1. *Suppose that $\mathcal{Q}_j : \big(H^{1/2}_\alpha(\Gamma_j)\big)^2 \to \big(H^{1/2}_\alpha(\Gamma_{j+1})\big)^2$ exists. The differences*

$$\begin{aligned}
&\mathcal{A}_j - \begin{pmatrix} \vartheta_j^* & 0\\ 0 & \vartheta_j^*\end{pmatrix}\begin{pmatrix} \widetilde{V}_{jj} & 0\\ 0 & \widetilde{V}_{jj}\end{pmatrix}\begin{pmatrix} (\vartheta_j^*)^{-1}M_j & 0\\ 0 & (\vartheta_j^*)^{-1}M_j\end{pmatrix},\\
&\mathcal{B}_j - \begin{pmatrix} \vartheta_j^* & 0\\ 0 & \vartheta_j^*\end{pmatrix}\begin{pmatrix} \widetilde{L}_{jj} - I & 0\\ 0 & \widetilde{L}_{jj} - I\end{pmatrix}\begin{pmatrix} (\vartheta_j^*)^{-1}M_j & 0\\ 0 & (\vartheta_j^*)^{-1}M_j\end{pmatrix},
\end{aligned}$$

map $\big(H^{-1/2}_\alpha(\Gamma_j)\big)^2$ compactly into $\big(H^{1/2}_\alpha(\Gamma_j)\big)^2$ and into $\big(H^{-1/2}_\alpha(\Gamma_j)\big)^2$, respectively.

Define the matrix

$$\widetilde{\mathcal{C}}_j = \begin{pmatrix} (1+a_j)I + (1-a_j)\widetilde{K}_{jj} & -c_j\,\widetilde{H}_{jj}\\ d_j\,\widetilde{H}_{jj} & (1+b_j)I + (1-b_j)\widetilde{K}_{jj}\end{pmatrix}\begin{pmatrix} \widetilde{V}_{jj} & 0\\ 0 & \widetilde{V}_{jj}\end{pmatrix},$$

and apply once more (4.6):

Lemma 4.2. *The difference*

$$\mathcal{C}_j - \begin{pmatrix} \vartheta_j^* & 0\\ 0 & \vartheta_j^*\end{pmatrix}\widetilde{\mathcal{C}}_j\begin{pmatrix} (\vartheta_j^*)^{-1}M_j & 0\\ 0 & (\vartheta_j^*)^{-1}M_j\end{pmatrix} : \big(H^{-1/2}_\alpha(\Gamma_j)\big)^2 \to \big(H^{1/2}_\alpha(\Gamma_j)\big)^2$$

is compact provided that $\mathcal{Q}_j : \big(H^{1/2}_\alpha(\Gamma_j)\big)^2 \to \big(H^{1/2}_\alpha(\Gamma_{j+1})\big)^2$ exists for $j < N-1$.

Now the proof of Proposition 4.1 follows from

Lemma 4.3. *Under (4.7) the operator matrix $\widetilde{\mathcal{C}}_j \in \Phi_0\big((H^{-1/2}(\widetilde{\Gamma}_j))^2, (H^{1/2}(\widetilde{\Gamma}_j))^2\big)$.*

Proof. Since $\widetilde{V}_{jj} \in \Phi_0(H^{-1/2}(\widetilde{\Gamma}_j), H^{1/2}(\widetilde{\Gamma}_j))$ it remains to show that (4.7) implies

$$\widetilde{\mathcal{F}}_j = \begin{pmatrix} (1+a_j)I + (1-a_j)\widetilde{K}_{jj} & -c_j\,\widetilde{H}_{jj}\\ d_j\,\widetilde{H}_{jj} & (1+b_j)I + (1-b_j)\widetilde{K}_{jj}\end{pmatrix} \in \Phi_0\big((H^{1/2}(\widetilde{\Gamma}_j))^2\big).$$

In the case $c_j = d_j = 0$ this is obvious for both possibilities $\phi = 0$ or $\kappa^2_{j+1} = \kappa^2_j$, since $aI + b\widetilde{K}_{jj} \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma}_j)\big)$ is equivalent to $aI - b\widetilde{K}_{jj} \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma}_j)\big)$.

Otherwise we show that $\widetilde{\mathcal{F}}_j + \widetilde{\mathcal{T}}$ is invertible for some compact operator $\widetilde{\mathcal{T}}$ iff (4.7) holds. We perturb the off-diagonal elements with a rank 1 operator e such that $\widetilde{H}_1 = \widetilde{H}_{jj} + \mathrm{e}$ is invertible and consider the operator matrix

$$\widetilde{\mathcal{F}}_j + \widetilde{\mathcal{T}} = \begin{pmatrix} (1+a_j)I + (1-a_j)\widetilde{K}_{jj} & -c_j\,\widetilde{H}_1 \\ d_j\,\widetilde{H}_1 & (1+b_j)I + (1-b_j)\widetilde{K}_{jj} \end{pmatrix}.$$

Using the abbreviation

$$A_\pm = (1+a_j)I \pm (1-a_j)\widetilde{K}_{jj}\,, \quad B_\pm = (1+b_j)I \pm (1-b_j)\widetilde{K}_{jj}\,,$$

and the relation

$$\begin{pmatrix} -(d_j\widetilde{H}_1)^{-1}B_+ & I \\ I & 0 \end{pmatrix} = \begin{pmatrix} 0 & I \\ I & (d_j\widetilde{H}_1)^{-1}B_+ \end{pmatrix}^{-1}$$

we transform

$$\widetilde{\mathcal{F}}_j + \widetilde{\mathcal{T}} = \begin{pmatrix} -A_+(d_j\widetilde{H}_1)^{-1}B_+ - c_j\widetilde{H}_1 & A_+ \\ 0 & d_j\widetilde{H}_1 \end{pmatrix}\begin{pmatrix} 0 & I \\ I & (d_j\widetilde{H}_1)^{-1}B_+ \end{pmatrix}.$$

Thus $\widetilde{\mathcal{F}}_j \in \Phi_0\big((H^{1/2}(\widetilde{\Gamma}_j))^2\big)$ iff $A_+(d_j\widetilde{H}_1)^{-1}B_+ + c_j\widetilde{H}_1 \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma}_j)\big)$. Since by (4.6)

$$A_+(\widetilde{H}_1)^{-1} = (\widetilde{H}_1)^{-1}A_- + (1-a_j)(\widetilde{H}_1)^{-1}(\mathrm{e}\,\widetilde{K}_{jj} + \widetilde{K}_{jj}\,\mathrm{e})(\widetilde{H}_1)^{-1}\,,$$

this is true if and only if $(d_j\widetilde{H}_1)^{-1}(A_-B_+ + c_jd_j\widetilde{H}_1^2) \in \Phi_0\big(H^{1/2}(\widetilde{\Gamma}_j)\big)$. Using $\widetilde{H}_{jj} = \widetilde{H}_1 - \mathrm{e}$ and $\widetilde{H}_{jj}^2 = \widetilde{K}_{jj}^2 - I$ from (4.6) we conclude, that $\widetilde{\mathcal{F}}_j \in \Phi_0\big((H^{1/2}(\widetilde{\Gamma}_j))^2\big)$ if and only if

$$A_-B_+ + c_jd_j\widetilde{H}_{jj}^2 = ((1+a_j)(1+b_j) - c_jd_j)I + 2(a_j - b_j)\widetilde{K}_{jj} - ((1-a_j)(1-b_j) - c_jd_j)\widetilde{K}_{jj}^2$$

is Fredholm with index 0. The definition of the coefficients (3.22) and the relation $\kappa_j^2 = \varepsilon_j\mu_j - \delta^2$ with $\delta^2 = \varepsilon_0\mu_0\sin^2\phi$ give after some algebra

$$A_-B_+ + c_jd_j\widetilde{H}_{jj}^2 = \frac{\kappa_j^2}{\varepsilon_j\mu_j\kappa_{j+1}^2}\big((\varepsilon_{j+1}+\varepsilon_j)I + (\varepsilon_{j+1}-\varepsilon_j)\widetilde{K}_{jj}\big)\big((\mu_{j+1}+\mu_j)I - (\mu_{j+1}-\mu_j)\widetilde{K}_{jj}\big),$$

which shows that (4.7) is equivalent to $\widetilde{\mathcal{F}}_j \in \Phi_0\big((H^{1/2}(\widetilde{\Gamma}_j))^2\big)$. □

Remark 4.2. *It is shown in* [10] *that the* $2N \times 2N$ *integral equation system, arising from the ansatz* (3.17)*, has diagonal* 2×2 *blocks of the form*

$$\begin{pmatrix} I + K_{jj}^{(j)} & -c_jH_{jj}^{(j)} \\ d_jH_{jj}^{(j)} & I + K_{jj}^{(j)} \end{pmatrix}\begin{pmatrix} V_{jj}^{(j+1)} & 0 \\ 0 & V_{jj}^{(j+1)} \end{pmatrix} - \begin{pmatrix} a_jV_{jj}^{(j)} & 0 \\ 0 & b_jV_{jj}^{(j)} \end{pmatrix}\begin{pmatrix} L_{jj}^{(j+1)} - I & 0 \\ 0 & L_{jj}^{(j+1)} - I \end{pmatrix}$$

or its transposed with respect to the duality (4.12)*. This matrix is by Lemma* 4.1 *a compact perturbation of* $\mathcal{C}_j$*, hence the* $2N \times 2N$ *integral equation system generates a Fredholm operator with index* 0 *iff the conditions* (4.7) *are satisfied. Then the integral equation system is solvable even if the nullspace is non-trivial, which can be proved as in* [11] *by characterizing the kernel of the transposed operator. Hence, the transmission problem* (2.9 - 2.12) *is solvable and admits also resonant solutions.*

4.2 Range of $\mathcal{C}_j$

Lemma 4.4. *If* $V_{j-1j-1}^{(j)}$ *is invertible, then* $\mathrm{R}(\mathcal{V}_{j-1})$ *is dense in* $\big(H_\alpha^{1/2}(\Gamma_j)\big)^2$.

Proof. The bilinear form

$$[\varphi,\psi]_{\Gamma_j} = \int_{\Gamma_j} \varphi\,\psi\,d\sigma \tag{4.12}$$

extends to a duality between the spaces $H^s_\alpha(\Gamma_j)$ and $H^{-s}_{-\alpha}(\Gamma_j)$, see (3.6). Because of $\Psi_{m,-\alpha}(P) = \Psi_{m,\alpha}(-P)$ for all $P \in \mathbb{R}^2$, we obtain

$$\big[V^{(j)}_{jj-1}\varphi, \psi\big]_{\Gamma_j} = 2 \int\limits_{\Gamma_{j-1}} \varphi(Q)\, d\sigma_Q \int\limits_{\Gamma_j} \Psi_{j,-\alpha}(Q-P)\, \psi(P)\, d\sigma_P = \big[\varphi, \widehat{\mathcal{S}}_{\Gamma_j,j}\psi\big]_{\Gamma_{j-1}} ,$$

where $\widehat{\mathcal{S}}_{\Gamma_j,j}$ denotes the single layer diffraction potential on Γ_j with the fundamental solution $\Psi_{j,-\alpha}$. If $\mathrm{R}(V^{(j)}_{jj-1})$ is not dense in $H^{1/2}_\alpha(\Gamma_j)$, then there exists $\psi \in H^{-1/2}_{-\alpha}(\Gamma_j)$ such that

$$\big[V^{(j)}_{jj-1}\varphi, \psi\big]_{\Gamma_j} = \big[\varphi, \widehat{\mathcal{S}}_{\Gamma_j,j}\psi\big]_{\Gamma_{j-1}} = 0 \qquad \text{for all } \ \varphi \in H^{-1/2}_\alpha(\Gamma_{j-1})\,.$$

Hence for all $P \in \Gamma_{j-1}$ the function $\widehat{\mathcal{S}}_{\Gamma_j,j}\psi(P) = 0$, i.e., the quasiperiodic Dirichlet problem

$$\Delta u + \omega^2\kappa_j^2 u = 0\,, \quad u|_{\Sigma_{j-1}} = 0\,, \quad u(x,y) = \mathrm{e}^{-i\alpha d}\, u(x+d,y) \tag{4.13}$$

has a nontrivial solution in G^+_{j-1}. Therefore the single layer potential $\widehat{\mathcal{S}}_{\Gamma_{j-1},j}\psi|_{\Gamma_{j-1}}$ with the fundamental solution $\Psi_{j,-\alpha}$ on Γ_{j-1}, which is the transpose of $V^{(j)}_{j-1j-1}$ with respect to (4.12), is not invertible. $\square$

Proposition 4.2. *Under the assumptions of Theorem* 4.1 *the equations* (4.1) *are solvable iff* $\mathrm{N}(\mathcal{C}_j) = \{0\}$, $j = N-1, \dots, 1$. *In this case* $(u^i, v^i)^T \in \mathrm{R}(\mathcal{C}_0)$.

Proof. The operator equations (4.1) are solvable only if $\mathrm{R}(\mathcal{C}_j) \supset \mathrm{R}(\mathcal{V}_{j-1})$. Since $\mathcal{C}_j$ is Fredholm with index 0, Lemma 4.4 implies $\mathrm{R}(\mathcal{C}_j) = \big(H^{1/2}_\alpha(\Gamma_j)\big)^2$ and therefore $\mathrm{N}(\mathcal{C}_j) = \{0\}$.

To establish the second assertion we take a solution u, v of the transmission problem (2.9 - 2.12), which exists due to Remark 4.2. We set $u_j = u|_{G_j}$, $v_j = v|_{G_j}$, $j = 1, \dots, N-1$ and define, since the operators $V^{(j)}_{j-1j-1}$ are invertible, the $H^{-1/2}_\alpha$ densities

$$\begin{aligned}
\varphi_{j-1} &= \frac{1}{2}\big((V^{(j)}_{j-1j-1})^{-1}(I + K^{(j)}_{j-1j-1})u_j - \partial_{\mathbf{n}} u_j|_{\Gamma_{j-1}}\big)\,, \\
\psi_{j-1} &= \frac{1}{2}\big((V^{(j)}_{j-1j-1})^{-1}(I + K^{(j)}_{j-1j-1})v_j - \partial_{\mathbf{n}} v_j|_{\Gamma_{j-1}}\big)\,,
\end{aligned}$$

for $j = 1, \dots, N-1$ and

$$\varphi_{N-1} = (V^{(N)}_{N-1N-1})^{-1} u_N\,, \ \psi_{N-1} = (V^{(N)}_{N-1N-1})^{-1} v_N\,.$$

Since the operators $\mathcal{C}_j$ are invertible for $j \geq 1$, it is easy to see that the densities φ_j, ψ_j satisfy all relations obtained in Subsection 3.3. In particular, φ_0, ψ_0 satisfy the equation (3.27). $\square$

4.3 Uniqueness

Let us consider the case that $\mathrm{N}(\mathcal{C}_k) \neq \{0\}$. If $k > 0$, then the algorithm fails by Theorem 4.1. Otherwise the homogeneous equation (4.3) has a non-zero solution, giving rise to resonant solutions of conical diffraction. After a more detailed description of this situation, the technique is applied in Proposition 4.3 to find conditions under which all operator matrices $\mathcal{C}_j$ have a trivial nullspace.

Lemma 4.5. *If* $\mathrm{N}(\mathcal{C}_j) = \{0\}$, $j = N-1, \dots, k+1$, *and* $\mathrm{N}(\mathcal{C}_k) \neq \{0\}$, *then there exist nontrivial solutions of the transmission problem in the reduced grating structure with the profiles* $\Sigma_k, \dots, \Sigma_{N-1}$ *and the upper semi-infinite layer* G^+_k, *i.e. quasiperiodic solutions of the corresponding Helmholtz equations* (2.9) *in* G^+_k *and* G_j, *satisfying the transmission conditions* (2.11) *for* $j = k, \dots, N-1$, *and the outgoing wave condition*

$$\begin{aligned}
(u,v)(x,y) &= \sum_{n=-\infty}^{\infty} (\hat{u}^+_n, \hat{v}^+_n)\, \mathrm{e}^{i(\alpha_n x + \beta^{(k)}_n y)} \qquad \textit{for } y > \max_{(x,t)\in\Sigma_k} t\,, \\
(u,v)(x,y) &= \sum_{n=-\infty}^{\infty} (\hat{u}^-_n, \hat{v}^-_n)\, \mathrm{e}^{i(\alpha_n x - \beta^{(N)}_n y)} \qquad \textit{for } y < \min_{(x,t)\in\Sigma_N} t\,.
\end{aligned} \tag{4.14}$$

Moreover, the coefficients $\hat{u}^\pm_n, \hat{v}^\pm_n$ *in* (4.14) *vanish if* $\beta^{(k)}_n > 0$ *or* $\beta^{(N)}_n > 0$, *correspondingly.*

Proof. Let $\varphi_k, \psi_k \in \mathrm{N}(\mathcal{C}_k)$ and set

$$\begin{pmatrix}\varphi_j\\ \psi_j\end{pmatrix} = \mathcal{Q}_{j-1}\begin{pmatrix}\varphi_{j-1}\\ \psi_{j-1}\end{pmatrix}, \quad j = k+1,\dots,N-1\,.$$

We introduce the function pair (u,v) given by (4.4) in G_j, $j = k+1,\dots,N$, and in G_k^+ by

$$\begin{pmatrix}u\\ v\end{pmatrix} = \frac{1}{2}\left(\begin{pmatrix} a_k\mathcal{S}_{\Gamma_k,k} & 0\\ 0 & b_k c\mathcal{S}_{\Gamma_k,k}\end{pmatrix}\mathcal{B}_k - \begin{pmatrix}\mathcal{D}_{\Gamma_k,k} & -c_k\mathcal{T}_{\Gamma_k,k}\\ d_k\mathcal{T}_{\Gamma_k,k} & \mathcal{D}_{\Gamma_k,k}\end{pmatrix}\mathcal{A}_k\right)\begin{pmatrix}\varphi_k\\ \psi_k\end{pmatrix}.$$

It is evident, that these functions are a non-trivial solution of the homogeneous problem for the reduced geometry.

To prove that the Rayleigh coefficients $\hat{u}_n^\pm, \hat{v}_n^\pm$ vanish for arbitrary non-trivial solutions (u,v) we proceed as in [2, 11]. Choose 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_j, $j = k,\dots,N-1$. Multiplying the Helmholtz equations (2.9) with

$$\frac{\varepsilon}{\varepsilon_0\kappa^2}\,\overline{u} \quad\text{and}\quad \frac{\mu}{\mu_0\kappa^2}\,\overline{v}$$

respectively, and applying Green's formula in the subdomains $\Omega_H\cap G_j$ and $\Omega_H\cap G_k^+$, the quasi-periodicity of u and v and the transmission conditions (2.11) lead to the equations

$$\int\limits_{\Omega_H}\frac{\varepsilon}{\varepsilon_0}\Big(\frac{1}{\kappa^2}|\nabla u|^2 - \omega^2\,|u|^2\Big) + \sum_{j=k}^{N-1}\sin\phi\int\limits_{\Gamma_j}\Big[\frac{1}{\kappa^2}\Big]\partial_{\mathbf{t}}v\,\overline{u} = \frac{\varepsilon_k}{\varepsilon_0\kappa_k^2}\int\limits_{\Gamma(H)}\partial_{\mathbf{n}}u\,\overline{u} + \frac{\varepsilon_N}{\varepsilon_0\kappa_N^2}\int\limits_{\Gamma(-H)}\partial_{\mathbf{n}}u\,\overline{u}\,, \tag{4.15}$$

$$\int\limits_{\Omega_H}\frac{\mu}{\mu_0}\Big(\frac{1}{\kappa^2}|\nabla v|^2 - \omega^2\,|v|^2\Big) - \sum_{j=k}^{N-1}\sin\phi\int\limits_{\Gamma_j}\Big[\frac{1}{\kappa^2}\Big]\partial_{\mathbf{t}}u\,\overline{v} = \frac{\mu_k}{\mu_0\kappa_k^2}\int\limits_{\Gamma(H)}\partial_{\mathbf{n}}v\,\overline{v} + \frac{\mu_N}{\mu_0\kappa_N^2}\int\limits_{\Gamma(-H)}\partial_{\mathbf{n}}v\,\overline{v}\,, \tag{4.16}$$

where $[1/\kappa^2] = 1/\kappa_j^2 - 1/\kappa_{j+1}^2$ on Γ_j, and $\Gamma(\pm H)$ denotes the upper resp. lower straight boundary of Ω_H. Using the identity

$$\int\limits_{\Omega}\nabla g\,\overline{\nabla^\perp f} = -\int\limits_{\partial\Omega}\partial_{\mathbf{t}}g\,\overline{f} \quad\text{ with } \nabla^\perp = (\partial_y, -\partial_x)\,,$$

which holds for closed Lipschitz domains Ω and $f,g\in H_p^1(\Omega)$, the integrals over Γ_j are transformed to domain integrals such that

$$\begin{aligned}
&\int\limits_{\Omega_H}\frac{\varepsilon}{\varepsilon_0}\Big(\frac{1}{\kappa^2}|\nabla u|^2 - \omega^2\,|u|^2\Big) + \sum_{j=k}^{N-1}\sin\phi\int\limits_{\Gamma_j}\Big[\frac{1}{\kappa^2}\Big]\partial_{\mathbf{t}}v\,\overline{u}\\
&= \int\limits_{\Omega_H}\Big(\frac{\varepsilon}{\varepsilon_0\kappa^2}|\nabla u|^2 - \frac{\sin\phi}{\kappa^2}\nabla v\cdot\nabla^\perp\overline{u} - \frac{\omega^2\varepsilon}{\varepsilon_0}\,|u|^2\Big) + \frac{\sin\phi}{\kappa_k^2}\int\limits_{\Gamma(H)}\partial_x v\,\overline{u} - \frac{\sin\phi}{\kappa_N^2}\int\limits_{\Gamma(-H)}\partial_x v\,\overline{u}\,,\\
&\int\limits_{\Omega_H}\frac{\mu}{\mu_0}\Big(\frac{1}{\kappa^2}|\nabla v|^2 - \omega^2\,|v|^2\Big) - \sum_{j=k}^{N-1}\sin\phi\int\limits_{\Gamma_j}\Big[\frac{1}{\kappa^2}\Big]\partial_{\mathbf{t}}u\,\overline{v}\\
&= \int\limits_{\Omega_H}\Big(\frac{\mu}{\mu_0\kappa^2}|\nabla v|^2 + \frac{\sin\phi}{\kappa^2}\nabla u\cdot\nabla^\perp\overline{v} - \frac{\omega^2\mu}{\mu_0}\,|v|^2\Big) - \frac{\sin\phi}{\kappa_k^2}\int\limits_{\Gamma(H)}\partial_x u\,\overline{v} + \frac{\sin\phi}{\kappa_N^2}\int\limits_{\Gamma(-H)}\partial_x u\,\overline{v}\,.
\end{aligned}$$

Note that (4.14) leads to

$$\begin{aligned}
&\int\limits_{\Gamma(H)}\partial_{\mathbf{n}}u\,\overline{u} = i\sum_{n\in\mathbb{Z}}\beta_n^{(k)}|\hat{u}_n^+|^2\;\mathrm{e}^{-2H\,\mathrm{Im}\,\beta_n^{(k)}}, \quad \int\limits_{\Gamma(H)}\partial_x v\,\overline{u} = i\sum_{n\in\mathbb{Z}}\alpha_n\hat{v}_n^+\;\overline{\hat{u}_n^+}\;\mathrm{e}^{-2H\,\mathrm{Im}\,\beta_n^{(k)}},\\
&\int\limits_{\Gamma(-H)}\partial_{\mathbf{n}}u\,\overline{u} = i\sum_{n\in\mathbb{Z}}\beta_n^{(N)}|\hat{u}_n^-|^2\;\mathrm{e}^{-2H\,\mathrm{Im}\,\beta_n^{(N)}}, \quad \int\limits_{\Gamma(-H)}\partial_x v\,\overline{u} = i\sum_{n\in\mathbb{Z}}\alpha_n\hat{v}_n^-\;\overline{\hat{u}_n^-}\;\mathrm{e}^{-2H\,\mathrm{Im}\,\beta_n^{(N)}}\,.
\end{aligned}$$

Hence (4.15) and (4.16) take the form

$$\int\limits_{\Omega_H}\Big(\frac{\varepsilon}{\varepsilon_0\kappa^2}|\nabla u|^2 - \frac{\sin\phi}{\kappa^2}\nabla v\cdot\nabla^\perp\overline{u} - \frac{\omega^2\varepsilon}{\varepsilon_0}\,|u|^2\Big) = \frac{i}{\kappa_k^2}\sum_{n\in\mathbb{Z}}\Big(\frac{\varepsilon_k\beta_n^{(k)}}{\varepsilon_0}\hat{u}_n^+ - \alpha_n\sin\phi\,\hat{v}_n^+\Big)\overline{\hat{u}_n^+}\ \mathrm{e}^{-2H\,\mathrm{Im}\,\beta_n^{(k)}}$$

$$+\frac{i}{\kappa_N^2}\sum_{n\in\mathbb{Z}}\Big(\frac{\varepsilon_N\beta_n^{(N)}}{\varepsilon_0}\,\hat{u}_n^- - \alpha_n\sin\phi\,\hat{v}_n^-\Big)\overline{\hat{u}_n^-}\ \mathrm{e}^{-2H\,\mathrm{Im}\,\beta_n^{(N)}}\,, \tag{4.17}$$

$$\int\limits_{\Omega_H}\Big(\frac{\mu}{\mu_0\kappa^2}|\nabla v|^2 + \frac{\sin\phi}{\kappa^2}\nabla u\cdot\nabla^\perp\overline{v} - \frac{\omega^2\mu}{\mu_0}\,|v|^2\Big) = \frac{i}{\kappa_k^2}\sum_{n\in\mathbb{Z}}\Big(\frac{\mu_k\beta_n^{(k)}}{\mu_0}\hat{v}_n^+ + \alpha_n\sin\phi\,\hat{u}_n^+\Big)\overline{\hat{v}_n^+}\ \mathrm{e}^{-2H\,\mathrm{Im}\,\beta_n^{(k)}}$$

$$+\frac{i}{\kappa_N^2}\sum_{n\in\mathbb{Z}}\Big(\frac{\mu_N\beta_n^{(N)}}{\mu_0}\hat{v}_n^- + \alpha_n\sin\phi\,\hat{u}_n^-\Big)\overline{\hat{v}_n^-}\ \mathrm{e}^{-2H\,\mathrm{Im}\,\beta_n^{(N)}}\,. \tag{4.18}$$

We rewrite the left hand side of the quadratic form (4.17, 4.18) for the vector $(u,v)^T$

$$\int\limits_{\Omega_H}\Big(BU\cdot\overline{U} - \frac{\omega^2\varepsilon}{\varepsilon_0}\,|u|^2 - \frac{\omega^2\mu}{\mu_0}\,|v|^2\Big)$$

by using the 4×4 matrix B and the vector U

$$B = \frac{1}{\kappa^2}\begin{pmatrix} \varepsilon/\varepsilon_0 & 0 & 0 & -\sin\phi \\ 0 & \mu/\mu_0 & \sin\phi & 0 \\ 0 & \sin\phi & \varepsilon/\varepsilon_0 & 0 \\ -\sin\phi & 0 & 0 & \mu/\mu_0 \end{pmatrix}, \quad U = \begin{pmatrix} \partial_x u \\ \partial_x v \\ \partial_y u \\ \partial_y v \end{pmatrix}.$$

Letting $H\to\infty$, we see that

$$\lim_{H\to\infty}\int\limits_{\Omega_H}\Big(BU\cdot\overline{U} - \frac{\omega^2\varepsilon}{\varepsilon_0}\,|u|^2 - \frac{\omega^2\mu}{\mu_0}\,|v|^2\Big) = \sum_{\beta_n^{(k)}>0} M_n^+\begin{pmatrix}\hat{u}_n^+\\ \hat{v}_n^+\end{pmatrix}\cdot\overline{\begin{pmatrix}\hat{u}_n^+\\ \hat{v}_n^+\end{pmatrix}} + \sum_{\beta_n^{(N)}>0} M_n^-\begin{pmatrix}\hat{u}_n^-\\ \hat{v}_n^-\end{pmatrix}\cdot\overline{\begin{pmatrix}\hat{u}_n^-\\ \hat{v}_n^-\end{pmatrix}},$$

where $M_n^\pm$ are the matrices

$$M_n^+ = \frac{i}{\kappa_k^2}\begin{pmatrix} \varepsilon_k\beta_n^{(k)}/\varepsilon_0 & -\alpha_n\sin\phi \\ \alpha_n\sin\phi & \mu_k\beta_n^{(k)}/\mu_0 \end{pmatrix}, \quad M_n^- = \frac{i}{\kappa_N^2}\begin{pmatrix} \varepsilon_N\beta_n^{(N)}/\varepsilon_0 & \alpha_n\sin\phi \\ -\alpha_n\sin\phi & \mu_N\beta_n^{(N)}/\mu_0 \end{pmatrix},$$

and the sums are finite, because of $\mathrm{Im}\,\beta_n^{(k)}>0$ and $\mathrm{Im}\,\beta_n^{(N)}>0$ for almost all n. If $\beta_n^{(k)}>0$ or $\beta_n^{(N)}>0$, then the corresponding matrix $M_n^\pm$ satisfies obviously $\mathrm{Im}(M_n^\pm)>0$, hence we get

$$\lim_{H\to\infty}\mathrm{Im}\int\limits_{\Omega_H}\Big(BU\cdot\overline{U} - \frac{\omega^2\varepsilon}{\varepsilon_0}\,|u|^2 - \frac{\omega^2\mu}{\mu_0}\,|v|^2\Big) \ge 0\,.$$

On the other hand, it will be shown in Lemma 4.6 that the assumption $\mathrm{Im}\,\varepsilon,\mathrm{Im}\,\mu\ge 0$ implies

$$\mathrm{Im}\int\limits_{\Omega_H}\Big(BU\cdot\overline{U} - \frac{\omega^2\varepsilon}{\varepsilon_0}\,|u|^2 - \frac{\omega^2\mu}{\mu_0}\,|v|^2\Big) \le 0, \tag{4.19}$$

and therefore

$$\sum_{\beta_n^{(k)}>0}\mathrm{Im}\,M_n^+\begin{pmatrix}\hat{u}_n^+\\ \hat{v}_n^+\end{pmatrix}\cdot\overline{\begin{pmatrix}\hat{u}_n^+\\ \hat{v}_n^+\end{pmatrix}} + \sum_{\beta_n^{(N)}>0}\mathrm{Im}\,M_n^-\begin{pmatrix}\hat{u}_n^-\\ \hat{v}_n^-\end{pmatrix}\cdot\overline{\begin{pmatrix}\hat{u}_n^-\\ \hat{v}_n^-\end{pmatrix}} = 0\,.$$

□

Lemma 4.6. *If* $\mathrm{Im}\,\varepsilon,\mathrm{Im}\,\mu\ge 0$*, then* (4.19) *holds.*

Proof. To show that

$$\operatorname{Im} \int_{\Omega_H} BU \cdot \overline{U} = -\operatorname{Re} \int_{\Omega_H} iBU \cdot \overline{U} \le 0\,, \tag{4.20}$$

we write as in [2, 11]

$$i\mathcal{U}^{-1} B \mathcal{U} = \begin{pmatrix} N^+ & 0 \\ 0 & N^- \end{pmatrix} \quad \text{with} \quad N^\pm = \frac{1}{\kappa^2} \begin{pmatrix} i\varepsilon/\varepsilon_0 & \pm \sin\phi \\ \mp \sin\phi & i\mu/\mu_0 \end{pmatrix},\ \mathcal{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} I & iI \\ iI & I \end{pmatrix},$$

where I is the 2×2 identity matrix and $\mathcal{U}$ is therefore unitary. Introducing the differential operators $\partial^+ = (\partial_x - i\partial_y)/\sqrt{2}$ and $\partial^- = (\partial_y - i\partial_x)/\sqrt{2}$, one can transform

$$\int_{\Omega_H} iBU \cdot \overline{U} = \int_{\Omega_H} \Big(N^+ \partial^+ \binom{u}{v} \cdot \overline{\binom{u}{v}} + N^- \partial^- \binom{u}{v} \cdot \overline{\binom{u}{v}} \Big).$$

If $\operatorname{Im}\varepsilon_j = \operatorname{Im}\mu_j = 0$, then $\operatorname{Re} N^\pm|_{G_j} = 0$. Hence (4.20) is proved if

$$\operatorname{Re} N^\pm|_{G_j} = \begin{pmatrix} -\operatorname{Im} \dfrac{\varepsilon_j}{\varepsilon_0 \kappa_j^2} & \pm i \operatorname{Im} \dfrac{\sin\phi}{\kappa_j^2} \\ \mp i \operatorname{Im} \dfrac{\sin\phi}{\kappa_j^2} & -\operatorname{Im} \dfrac{\mu_j}{\mu_0 \kappa_j^2} \end{pmatrix} \ge 0$$

for $\operatorname{Im}\varepsilon_j + \operatorname{Im}\mu_j > 0$. The last relation is equivalent to the inequalities

$$-\operatorname{Im} \frac{\varepsilon_j}{\kappa_j^2} \ge 0 \quad \text{and} \quad \operatorname{Im} \frac{\varepsilon_j}{\kappa_j^2} \operatorname{Im} \frac{\mu_j}{\kappa_j^2} - \varepsilon_0 \mu_0 \sin^2\phi \Big(\operatorname{Im} \frac{1}{\kappa_j^2} \Big)^2 \ge 0\,. \tag{4.21}$$

Denoting $\phi_\varepsilon = \arg \varepsilon_j$, $\phi_\mu = \arg \mu_j$, $\phi_\kappa = \arg \kappa_j^2$, the assumptions

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

together with $\kappa_j^2 = \varepsilon_j \mu_j - \varepsilon_0 \mu_0 \sin^2\phi$ lead to $0 < \phi_\kappa - \phi_\varepsilon, \phi_\kappa - \phi_\mu \le \pi$, and therefore

$$-\operatorname{Im} \frac{\varepsilon_j}{\kappa_j^2} = \Big| \frac{\varepsilon_j}{\kappa_j^2} \Big| \sin(\phi_\kappa - \phi_\varepsilon) \ge 0\,.$$

Finally, (4.20) follows from the observation that because of

$$\operatorname{Im} \frac{\varepsilon_0 \mu_0 \sin^2\phi}{\kappa_j^2} = \operatorname{Im} \frac{\varepsilon_j \mu_j}{\kappa_j^2}\,,$$

the second inequality in (4.21) is equivalent to

$$\sin(\phi_\varepsilon - \phi_\kappa) \sin(\phi_\mu - \phi_\kappa) + \sin(\phi_\varepsilon + \phi_\mu - \phi_\kappa) \sin\phi_\kappa = \sin\phi_\varepsilon \sin\phi_\mu \ge 0\,. \qquad \square$$

Finally, sufficient conditions for the invertibility of all $\mathcal{C}_j$ can be deduced from

Proposition 4.3. *Assume the conditions of Theorem* 4.1 *and* $\mathrm{N}(\mathcal{C}_{N-1}) = \ldots = \mathrm{N}(\mathcal{C}_{k+1}) = \{0\}$. *If for some* $j = k+1, \ldots, N$ *the imaginary part of* ε_j *or* μ_j *is positive,* $\operatorname{Im}(\varepsilon_j + \mu_j) > 0$, *then* $\mathrm{N}(\mathcal{C}_k) = \{0\}$.

Proof. Suppose that $\mathrm{N}(\mathcal{C}_k) \ne \{0\}$ and consider as in the proof of Lemma 4.5 the solution of the homogeneous transmission problem (u, v) in the reduced grating structure with the profiles $\Sigma_k, \ldots, \Sigma_{N-1}$ and the top layer G_k^+, for which we have shown

$$\operatorname{Im} \int_{\Omega_H} \Big(BU \cdot \overline{U} - \frac{\omega^2 \varepsilon}{\varepsilon_0} |u|^2 - \frac{\omega^2 \mu}{\mu_0} |v|^2 \Big) = 0\,.$$

Using the notation in the proof of Lemma 4.6 we have therefore

$$\int\limits_{\Omega_H} \left(\frac{\operatorname{Im}\varepsilon}{\varepsilon_0}\, |u|^2 + \frac{\operatorname{Im}\mu}{\mu_0}\, |v|^2 \right) = \operatorname{Re} \int\limits_{\Omega_H} \left(N^+ \partial^+ \binom{u}{v} \cdot \overline{\partial^+ \binom{u}{v}} + N^- \partial^- \binom{u}{v} \cdot \overline{\partial^- \binom{u}{v}} \right) = 0\,.$$

If $\operatorname{Im}\varepsilon_j, \operatorname{Im}\mu_j > 0$, then $u = v = 0$ in G_j. If otherwise, for example $\operatorname{Im}\varepsilon_j = 0$, then $v = 0$ and $\operatorname{Im}\kappa_j^2 \neq 0$, implying that

$$\operatorname{Re} \int\limits_{\Omega_H \cap G_j} \left(N^+ \partial^+ \binom{u}{0} \cdot \overline{\partial^+ \binom{u}{0}} + N^- \partial^- \binom{u}{0} \cdot \overline{\partial^- \binom{u}{0}} \right) = \frac{2\varepsilon_j \sin\phi_\kappa}{\varepsilon_0 |\kappa_j^2|} \int\limits_{\Omega_H \cap G_j} |\nabla u|^2 = 0\,,$$

which yields $u = 0$ in G_j because of $\Delta u + \omega^2 \kappa_j^2 u = 0$.

Hence, u, v solve in the neighboring layers Helmholtz equations with vanishing boundary values and normal derivatives at the common interfaces (due to the transmission condition (2.11)). By Holmgren's theorem the homogeneous transmission problem has therefore only the trivial solution $u = v = 0$ and the invertibility of $V_{kk}^{(k+1)}$ implies that $\varphi_k = \psi_k = 0$. □

References

[1] B. V. Bazalij, V. Yu. Shelepov, On the spectrum of the potential of a double layer on a curve of bounded rotation, in: Boundary value problems for differential equations, **239**, Naukova Dumka: Kiev, 13–30 (1980).

[2] J. Elschner, R. Hinder, F. Penzel, & G. Schmidt, Existence, uniqueness and regularity for solutions of the conical diffraction problem, Math. Models and Methods in Appl. Sci. **10** (2000), 317–341.

[3] J. Elschner & M. Yamamoto, An inverse problem in periodic diffraction optics: Reconstruction of Lipschitz grating profiles, Appl. Analysis **81** (2002), 1307–1328.

[4] L. I. Goray, G. Schmidt, Solving conical diffraction with integral equations, J. Opt. Soc. Am. A **27** (2010), 585–597.

[5] L. I. Goray, J. F. Seely, & S. Yu. Sadov, Spectral separation of the efficiencies of the inside and outside orders of soft-x-ray-extreme-ultraviolet gratings at near normal incidence, J. Appl. Physics **100** (2006), 094901

[6] V. Yu. Gotlib, On solutions of the Helmholtz equation that are concentrated near a plane periodic boundary. (Russian) Zap. Nauchn. Sem. POMI **250** (1998), 83–96; Translation in J. Math. Sci. (New York) **102** (2000), no. 4, 4188–4194.

[7] D. Maystre, A new general integral theory for dielectric coated gratings, J. Opt. Soc. Am. **68** (1978), 490–495.

[8] D. Maystre, Electromagnetic study of photonic band gaps, Pure Appl. Opt **3** (1994), 975–993.

[9] R. Petit (ed.) Electromagnetic theory of gratings. Topics in Current Physics, Vol. **22**, Springer: Berlin, 1980.

[10] G. Schmidt, Integral equations for conical diffraction by coated grating, J. Int. Equ. Appl. **23** (2011), 71–112.

[11] G. Schmidt, Boundary Integral Methods for Periodic Scattering Problems, in: A. Laptev (ed.), Around the Research of Vladimir Maz'ya II. Partial Differential Equations, IMS **12**, Springer: New York, Dordrecht, Heidelberg, London, 2010, 337–364.

[12] G. Schmidt, B. H. Kleemann, Integral equation methods from grating theory to photonics: An overview and new approaches for conical diffraction, J. mod. Opt **58** (2011), 407–423.