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Electromagnetic scattering by biperiodic multilayered gratings: A recursive integral equation approach

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Abstract

In this paper, we propose a new recursive integral equation algorithm to solve the direct problem of electromagnetic scattering by biperiodic multilayered structures with polyhedral Lipschitz regular interfaces. We work with a combined potential approach that involves one unknown density on each of the grating profiles of the multilayered scatterer. Justified by the transmission conditions of the underlying electromagnetic scattering problem, we assume that densities in adjacent layers are linearly linked by a boundary integral operator and derive a recursion for these densities. It comprehends the inversion of one boundary integral equation on each scattering interface. Our algorithm is shown to be equivalent to the biperiodic multilayered electromagnetic scattering problem. Moreover, we obtain new existence and uniqueness results for our recursive integral equation algorithm, which promises to lead to an efficient numerical implementation of the considered scattering problem. These solvability results depend on the regularity of the grating interfaces and the values of the electromagnetic material parameters of the biperiodic multilayered structure at hand.

1 Introduction

We use integral equation methods to study the scattering of time-harmonic electromagnetic plane waves by biperiodic multilayered structures. More exactly, we develop and analyze a recursive integral equation algorithm for the efficient numerical realization of the equivalent biperiodic multilayered electromagnetic scattering problem. The considered structures are modeled by vertically arranging finitely many non-self-intersecting polyhedral Lipschitz interfaces. We describe the behavior of the incident and scattered waves by the time-harmonic Maxwell equations with respect to transmission conditions across each interface of the scatterer and suitable outgoing wave conditions. In contrast to our investigation of biperiodic electromagnetic scattering by a single polyhedral Lipschitz regular grating interface from [3], the extended geometry of multilayered structures is more suitable for implementing real-world applications. The latter include various applications in micro-optics such as in the construction of holographic films, optical storage devices, antireflective coatings based on moth eyes and photonic crystals with a special band gap structure. In order to obtain an impression of the diversity of the specific research area of electromagnetic scattering by biperiodic structure, we refer the interested reader, for instance, to the articles [6], [8] and [17].

In this article, we extend an existing recursive integral equation algorithm for electromagnetic scattering by periodic multilayered structures in the case of transverse electric (TE), transverse magnetic (TM) and conical diffraction to the biperiodic setting. The first ideas in this direction were elaborated by Maystre in [16] for TE and TM diffraction. They were later refined by Schmidt in [21] for conical diffraction. The challenge faced in the extension from periodic to biperiodic structures lies in the fact that we can no longer reduce the electromagnetic scattering problem to solving scalar-valued Helmholtz equations. Instead, we have to study transmission problems for the full three-dimensional time-harmonic Maxwell equations. In the end, we obtain more complex boundary integral equations, but the general approach is similar: We assume that the field above the grating structure can be represented by the α-quasiperiodic Stratton-Chu formula and the one below by a simple electric potential ansatz with an unknown density. The potential ansatz for the fields in each of the layers of the multilayered scatterer is split into a Stratton-Chu like part and a part composed of an electric potential applied to a yet undetermined density. By this type of approach, we have one unknown density on each profile of the scattering obstacle. Under the assumption that densities in adjacent domains are linearly linked by a boundary integral operator, which is motivied by the transmission conditions of the underlying electromagnetic scattering problem, we can then derive a recursion for these densities. It includes inverting one boundary integral equation on each scattering surface.

Even though we did not actually implement the recursive integral equation algorithm, we are able to roughly predict its numerical benefit by extrapolating the numerical results from the periodic to the biperiodic setting. Our algorithm promises to be computationally very efficient in comparison with similar methods. In fact, in [19] and [4], periodic and biperiodic multilayered electromagnetic scattering problems are converted into systems of integral equations, whose size is directly proportional to the number of layers in the considered scatterer, by extending the approaches for single profile scattering from [20] and [3]. Especially in case of a large number of layers, the numerical solution of these systems of integral equations entails high computational costs. Our new recursive method, which we expect to run on a standard laptop, is estimated to easily excel the former integral formulations. Since our approach is not subjected to any additionally geometric restrictions, it moreover has a broad application radius. However, as we will observe in the course of this paper, there is quite some effort required for its implementation due to the large amount of complex matrix-matrix and matrix-vector multiplications that have to be performed. Nevertheless, it is worth to accept this issue because of the major overall numerical advantages of the recursive integral equation algorithm. We are confident that our insights are of practical significance for the treatment of the biperiodic multilayered electromagnetic scattering problem.

This article contains the outcome of Section 6.3.2 of the PhD thesis [4] on "On Integral Equation Methods for Electromagnetic Scattering by Biperiodic Structures", in which a second recursive integral equation algorithm, the recursive scattering matrix method, is presented.

After this introductory part, we formulate, in Section 2, the problem of electromagnetic scattering by biperiodic multilayered structures composed of $N \geq 2$ polyhedral Lipschitz regular grating interfaces. In the subsequent Section 3, we formally present the recursive integral equation, which also includes the introduction of biperiodic potential and boundary integral operators. The detailed derivation of the recursive integral equation algorithm is in the focus of Section 4. Moreover, we therein prove the equivalence of the electromagnetic scattering problem and our new integral equation method, provided a certain sense of applicability. Section 5 is the main part of this paper. It is concerned with the solvability of the recursive integral equation algorithm. This in particular includes proving that the occurring boundary integral equations are Fredholm of index zero depending on the regularity of the grating interfaces of the present multilayered structure. These then help to verify that solutions to the recursive integral equation algorithm exist. In addition, the uniqueness of solutions to our algorithm is rigorously studied. In particular, we state necessary and sufficient conditions on the electromagnetic material parameters to ensure the unique solvability of our recursive method. Finally, we conclude this paper in Section 6 by summarizing our insights and giving an outlook on possible continuations of our work.

Notation. For vectors $x \in \mathbb{R}^3$, we denote by $\tilde{x}$ their orthogonal projection to the (x_1, x_2)–plane. We distinguish vector-valued function spaces from scalar-valued ones by writing them in bold font.

2 The multilayered electromagnetic scattering problem

In this section, we want to formulate the 2π-biperiodic multilayered electromagnetic scattering problem treated in this article. For notational reasons, we introduce the index sets

$$K := \{1, \ldots, N-1\}, \quad K_0 := K \cup \{0\}, \quad K^N := K \cup \{N\} \quad \text{and} \quad K_0^N := K^N \cup \{0\}.$$

We consider a 2π-biperiodic multilayered structure consisting of $N \geq 2$ non-self-intersecting horizontally stacked interfaces $\Sigma_k \subset \mathbb{R}^2$, $k \in K_0$, that can be described by piecewise C^2 parametrizations

$$\sigma_k(t) := \left(t_1, t_2, x_3^{(k)}(t)\right)^{\mathrm{T}} \quad \text{such that} \quad x_3^{(k)}(t + 2\pi\, m) = x_3^{(k)}(t) \tag{2.1}$$

for $t = (t_1, t_2)^{\mathrm{T}}$, $m \in \mathbb{Z}^2$, $k \in K_0$. Speaking visually, each Σ_k is 2π-periodic in both x_1- and in x_2-direction and may exhibit edges and corners. From here on, we refer to this kind of regularity as polyhedral Lipschitz regularity. Moreover, the surfaces Σ_k are numbered in descending order from top to bottom, i.e., the top surface is Σ_0 and the bottom one Σ_N. All considerations in this paper focus only on one period of the multilayered scatterer as it is commonly seen in the treatment of periodic problems. This means that we restrict each surface Σ_k, $k \in K_0$ to one period Γ_k:

$$\Gamma_k := \{\sigma_k(t) \,:\, t \in Q\}\,, \quad \text{where } Q := [-\pi, \pi) \times [-\pi, \pi)$$

corresponds to the unit-cell of the underlying periodic lattice. The restricted profiles Γ_k, $k \in K_0$, separate $N+1$ homogeneous material layers $G_k \subset \mathbb{R}^3$, $k \in K_0^N$, of constant electric permittivity ϵ_k and constant magnetic permeability μ_k. The top domain G_0 and the bottom domain G_N are both semi-infinite, whereas all regions G_k, $k \in K$, in between are bounded polyhedral Lipschitz domains. We specify the unit normal vectors $\mathbf{n}_k := \mathbf{n}|_{\Gamma_k}$, $k \in K_0$, of Γ_k in such a way that they point upwards, i.e., into G_k. The electromagnetic material parameters ϵ_k and μ_k, $k \in K_0^N$, are assumed to be 2π-biperiodic in x_1- and in x_2- direction in G_k and to satisfy

$$\operatorname{Im}(\epsilon_k) \geq 0 \quad \text{and} \quad \operatorname{Im}(\mu_k) \geq 0 \quad \text{in } G_k, k \in K_0^N. \tag{2.2}$$

We exclude the case that $\epsilon_k = 0$ and/or $\mu_k = 0$. Moreover, we define the piecewise constant wavenumbers

$$\kappa_k := \omega\sqrt{\epsilon_k}\sqrt{\mu_k} \quad \text{in } G_k, k \in K_0^N,$$

where $\omega > 0$ is a fixed frequency. The square root of a complex number $z = re^{\mathrm{i}\varphi}$ is chosen such that $\sqrt{z} = \sqrt{r}e^{\mathrm{i}\frac{\varphi}{2}}$ for $-\pi < \varphi \leq \pi$.

In the course of this paper, we will use the auxiliary polyhedral Lipschitz regular domain G^{H} depending on a fixed $\mathrm{H} \in \mathbb{R}_+$, which is chosen such that

$$\Gamma_k \subset G^{\mathrm{H}} := \left\{x = (\tilde{x}, x_3)^{\mathrm{T}} \in Q \times \mathbb{R} \,:\, |x_3| \leq \mathrm{H}\right\} \quad \text{for all } k \in K_0. \tag{2.3}$$

Denote by G_0^{H} and G_N^{H} the restrictions of the semi-infinite domains G_0 and G_N to G^{H}, i.e.,

$$G_0^{\mathrm{H}} := G^{\mathrm{H}} \cap G_0 \quad \text{and} \quad G_N^{\mathrm{H}} := G^{\mathrm{H}} \cap G_N.$$

Moreover, we will work with the semi-infinite domains

$$G_k^+ := \{x \in Q \times \mathbb{R} \,:\, x_3 > \sigma_k(\tilde{x})\} \text{ and } G_k^- := \{x \in Q \times \mathbb{R} \,:\, x_3 < \sigma_k(\tilde{x})\}, \quad k \in K_0. \tag{2.4}$$

The interface Γ_0 is now illuminated from G_0 by a time-harmonic electric plane wave $\mathbf{E}^{\mathrm{i}}$ at oblique incidence, which is specified by

$$\mathbf{E}^{\mathrm{i}} := \mathbf{p}e^{\mathrm{i}(\alpha_1 x_1 + \alpha_2 x_2 - \alpha_3 x_3)} \quad \text{with } \alpha_3 > 0 \tag{2.5}$$

It in particular fulfills the relation

$$\mathbf{u}(\tilde{x} + 2\pi\, m, x_3) = e^{\mathrm{i}2\pi(\alpha_1 m_1 + \alpha_2 m_2)}\mathbf{u}(x) \quad \text{for all } m \in \mathbb{Z}^2.$$

This special type of periodicity up to a phase shift will be called α-quasiperiodicity (abbreviated as α-qp). The wave vector $\alpha = (\alpha_1, \alpha_2, -\alpha_3)^{\mathrm{T}}$ of the incident field exhibits the following properties:

$$|\alpha|^2 = |\kappa_0|^2 \quad \text{and} \quad \alpha \cdot \mathbf{p} = 0. \tag{2.6}$$

The total electric fields are given by $\mathbf{E}^{\mathrm{i}} + \mathbf{E}_0$ in G_0 and by $\mathbf{E}_k$ in G_k, $k \in K^N$. Then the 2π-biperiodic electromagnetic scattering problem written in terms of the electric field is expressed as follows: We look for vector fields $\mathbf{E}_k$, $k \in K_0^N$, of locally finite energy, in the sense that

$$\mathbf{E}_k, \mathbf{curl}\,\mathbf{E}_k \in \mathbf{L}^2_{\mathrm{loc}}(\mathbb{R}^3),$$

solving the time-harmonic Maxwell equations

$$\mathbf{curl}\,\mathbf{curl}\,\mathbf{E}_k - \kappa_k^2\mathbf{E}_k = 0 \quad \text{in } G_k \tag{2.7}$$

with respect to the transmission conditions

$$\gamma^-_{\mathrm{D},0}\mathbf{E}_1 = \gamma^+_{\mathrm{D},0}\mathbf{E}_0 + \gamma^+_{\mathrm{D},0}\mathbf{E}^{\mathrm{i}} \qquad \text{on } \Gamma_0, \tag{2.8}$$

$$\gamma^-_{\mathrm{N}_{\kappa_1},0}\mathbf{E}_1 = \rho_1^{-1}\left(\gamma^+_{\mathrm{N}_{\kappa_0},0}\mathbf{E}_0 + \gamma^+_{\mathrm{N}_{\kappa_0},0}\mathbf{E}^{\mathrm{i}}\right) \qquad \text{on } \Gamma_0, \tag{2.9}$$

$$\gamma^-_{\mathrm{D},k}\mathbf{E}_{k+1} = \gamma^+_{\mathrm{D},k}\mathbf{E}_k \qquad \text{on } \Gamma_k \text{ for } k \in K, \tag{2.10}$$

$$\gamma^-_{\mathrm{N}_{\kappa_{k+1}},k}\mathbf{E}_{k+1} = \rho_{k+1}^{-1}\gamma^+_{\mathrm{N}_{\kappa_k},k}\mathbf{E}_k \qquad \text{on } \Gamma_k \text{ for } k \in K. \tag{2.11}$$

Here, $\gamma^\pm_{\mathrm{D},k}$ and $\gamma^\pm_{\mathrm{N}_\kappa,k}$ refer to the Dirichlet and Neumann traces on Γ_k, $k \in K_0$:

$$\gamma^\pm_{\mathrm{D},k}\mathbf{u} := (\mathbf{n}_k \times \mathbf{u}_\pm)|_{\Gamma_k} \quad \text{and} \quad \gamma^\pm_{\mathrm{N}_\kappa,k}\mathbf{u} := \kappa^{-1}\,(\mathbf{n}_k \times \mathbf{curl}\,\mathbf{u}_\pm)|_{\Gamma_k}$$

for $\mathbf{u}$ sufficiently smooth with $\mathbf{u}_\pm := \mathbf{u}|_{G_k^\pm}$. These traces are characterized in detail, e.g., in [3]. Moreover, we impose the outgoing wave condition in the sense of Rayleigh series:

$$\mathbf{E}_0(x) = \sum_{n\in\mathbb{Z}^2} \mathbf{E}_n^0 e^{\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{x} + \beta_0^{(n)}x_3\right)}, \qquad x \in G_0 \text{ with } x_3 \geq \mathrm{H}, \tag{2.12}$$

$$\mathbf{E}_N(x) = \sum_{n\in\mathbb{Z}^2} \mathbf{E}_n^N e^{\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{x} - \beta_N^{(n)}x_3\right)}, \qquad x \in G_N \text{ with } x_3 \leq -\mathrm{H}, \tag{2.13}$$

where $n = (n_1, n_2)^{\mathrm{T}}$, $\alpha^{(n)} := (\alpha_1 + n_1, \alpha_2 + n_2)^{\mathrm{T}}$ and

$$\beta_k^{(n)} := \begin{cases} \sqrt{\kappa_k^2 - \left|\alpha^{(n)}\right|^2} & \text{with } 0 \leq \arg\left(\beta_k^{(n)}\right) < \pi \quad \text{if } \kappa_k \notin \mathbb{R}_-, \\ -\sqrt{\kappa_k^2 - \left|\alpha^{(n)}\right|^2} & \text{if } \kappa_k \in \mathbb{R}_- \text{ and } \kappa_k^2 - \left|\alpha^{(n)}\right|^2 > 0, \\ \mathrm{i}\sqrt{\left|\alpha^{(n)}\right|^2 - \kappa_k^2} & \text{if } \kappa_k \in \mathbb{R}_- \text{ and } \kappa_k^2 - \left|\alpha^{(n)}\right|^2 < 0. \end{cases}$$

Since the electric incident waves are α-quasiperiodic, the sought-after fields are also α-quasiperiodic.

3 The Recursive Integral Equation Algorithm

In this section, we present a sophisticated recursive integral equation algorithm in order to solve the 2π-biperiodic electromagnetic scattering problem. It generalizes the integral equation algorithm that was initially suggested by Maystre in [16] for TE and TM diffraction, and later extended to conical diffraction by Schmidt in [21], from 2π-periodic to 2π-biperiodic multilayered scatterers. Hereafter, we first introduce the particular biperiodic potential and boundary integral operators that occur in formulation of our algorithm. The latter is then highlighted in Section 3.2.

3.1 Biperiodic Potential and Boundary Integral Operators

The α-quasiperiodic potential operators relevant for this article are based on G_κ^α, the α-quasiperiodic fundamental solution of the time-harmonic Helmholtz equations, specified by

$$G_\kappa^\alpha(x, y) := \frac{\mathrm{i}}{8\pi^2} \sum_{n\in\mathbb{Z}^2} \frac{e^{\mathrm{i}\left(\alpha^{(n)}\cdot(\tilde{x}-\tilde{y}) + \beta^{(n)}|x_3 - y_3|\right)}}{\beta^{(n)}}, \tag{3.1}$$

where

$$\beta^{(n)} := \begin{cases} \sqrt{\kappa^2 - \left|\alpha^{(n)}\right|^2} & \text{with } 0 \leq \arg\left(\beta^{(n)}\right) < \pi \quad \text{if } \kappa \notin \mathbb{R}_-, \\ -\sqrt{\kappa^2 - \left|\alpha^{(n)}\right|^2} & \text{if } \kappa \in \mathbb{R}_- \text{ and } \kappa^2 - \left|\alpha^{(n)}\right|^2 > 0, \\ \mathrm{i}\sqrt{\left|\alpha^{(n)}\right|^2 - \kappa^2} & \text{if } \kappa \in \mathbb{R}_- \text{ and } \kappa^2 - \left|\alpha^{(n)}\right|^2 < 0. \end{cases}$$

Assuming that $\kappa^2 \neq |\alpha^{(n)}|^2$ for all $n \in \mathbb{Z}^2$, the function G_κ^α converges uniformly on compact sets in $\mathbb{R}^3 \setminus \cup_{n\in\mathbb{Z}^2} (2\pi n_1, 2\pi n_2, 0)^{\mathrm{T}}$. Details on the derivation of G_κ^α and its analytical properties are given in the habilitation thesis [1, §3].

The single layer potential on Γ_k, $k \in K_0$, is given by

$$\left(S_k^{\alpha,\kappa}\mathbf{u}\right)(x) := 2\int_{\Gamma_k} G_\kappa^\alpha(x,y)\mathbf{u}(y)\,d\sigma(y), \quad x \in (Q\times\mathbb{R})\setminus\Gamma_k.$$

We define the related operator $V_k^{\alpha,\kappa}$, $k \in K_0$, by

$$\left(V_k^{\alpha,\kappa}\mathbf{u}\right)(x) := 2\int_{\Gamma_k} G_\kappa^\alpha(x,y)\mathbf{u}(y)\,d\sigma(y) \quad \text{for } x \in \Gamma_k.$$

It corresponds to the classical trace of the single layer potential $S_k^{\alpha,\kappa}$.

Definition 3.1 (Electric and magnetic potential)**.** *The electric potential $\Psi^\alpha_{\mathrm{E}_\kappa,k}$ on Γ_k, $k \in K_0$, is defined by*

$$\Psi^\alpha_{\mathrm{E}_\kappa,k}\mathbf{j} := \kappa S_k^{\alpha,\kappa}\mathbf{j} + \kappa^{-1}\nabla S_k^{\alpha,\kappa}\operatorname{div}_\Gamma\mathbf{j}.$$

By $\mathbf{curl}\,\mathbf{curl} = -\Delta + \nabla\operatorname{div}$, it also has a representation as $\Psi^\alpha_{\mathrm{E}_\kappa,k}\mathbf{j} = \kappa^{-1}\,\mathbf{curl}\,\mathbf{curl}\,S_k^{\alpha,\kappa}\mathbf{j}$.

Moreover, we specify the magnetic potential as $\Psi^\alpha_{\mathrm{M}_\kappa,k}$ on Γ_k, $k \in K_0$, by

$$\Psi^\alpha_{\mathrm{M}_\kappa,k}\mathbf{m} := \mathbf{curl}\,S_k^{\alpha,\kappa}\mathbf{m}.$$

Taking the Dirichlet and Neumann traces of the electric and magnetic potentials as follows generates the boundary electric and magnetic potential operators:

$$C_k^{\alpha,\kappa} := \{\gamma_{\mathrm{D},k}\}\,\Psi^\alpha_{\mathrm{E}_\kappa,k} = \{\gamma_{\mathrm{N}_\kappa,k}\}\,\Psi^\alpha_{\mathrm{M}_\kappa,k} \quad \text{and} \quad M_k^{\alpha,\kappa} := \{\gamma_{\mathrm{D},k}\}\,\Psi^\alpha_{\mathrm{M}_\kappa,k} = \{\gamma_{\mathrm{N}_\kappa,k}\}\,\Psi^\alpha_{\mathrm{E}_\kappa,k},$$

where $\{\gamma_{*,k}\} := -\frac{1}{2}\left(\gamma^-_{*,k} + \gamma^+_{*,k}\right)$ for $* \in \{\mathrm{D}, \mathrm{N}_\kappa\}$ and $k \in K_0$.

Remark 3.2 (Notation)**.** *In order to keep the notation as simple and as readable as possible, we introduce the convention to replace the superscript κ_k by (k) for $k \in K_0^N$. If κ_k occurs as a subscript, we abbreviate it by k. Thus, we for example write $C_k^{\alpha,(k)}$ instead of C_k^{α,κ_k} and $\beta_k^{(n)}$ instead of $\beta_{\kappa_k}^{(n)}$.*

With the help of the previously introduced operators, we are now able to formally write down the recursive integral equation algorithm.

3.2 Presentation of the Recursive Integral Equation Algorithm

The recursive integral equation algorithm presented here is based on the following combined potential ansatz:

$$\mathbf{E}_0 = \frac{1}{2}\left(\Psi^\alpha_{\mathrm{E}_{\kappa_0},0}\gamma^+_{\mathrm{N}_{\kappa_0},0}\mathbf{E}_0 + \Psi^\alpha_{\mathrm{M}_{\kappa_0},0}\gamma^+_{\mathrm{D},0}\mathbf{E}_0\right) \quad \text{in } G_0, \tag{3.2}$$

$$\mathbf{E}_k = \frac{1}{2}\left(\Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\gamma^+_{\mathrm{N}_{\kappa_k},k}\mathbf{E}_k + \Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\gamma^+_{\mathrm{D},k}\mathbf{E}_k\right) + \Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1} \quad \text{in } G_{k\in K}, \tag{3.3}$$

$$\mathbf{E}_N = \Psi^\alpha_{\mathrm{E}_{\kappa_N},N-1}\mathbf{j}_{N-1} \quad \text{in } G_N, \tag{3.4}$$

where the unknown densities $\mathbf{j}_k$, $k \in K_0$, shall be recovered recursively. We will later verify that this is a suitable ansatz for an electric field $\mathbf{E}$ solving the electromagnetic scattering problem (2.7)-(2.13).

Our algorithm provides a recursion of the form

$$\mathbf{j}_k = \mathcal{Q}_{k-1}\mathbf{j}_{k-1} \quad \text{for } k \in K \tag{3.5}$$

such that the functions $\mathbf{E}_k$, $k \in K_0^N$, satisfy the transmission conditions (2.12)-(2.13). The scheme yielding the initial density $\mathbf{j}_0$ and the operators $\mathcal{Q}_{k-1}$, $k \in K$, is given as follows: We obtain the operator $\mathcal{Q}_{k-1}$ by a backward recurrence for $k = N-1, \dots, 1$ as a solution of the operator equation

$$\left[\left(M_k^{\alpha,(k)} + \mathrm{I}\right)\mathcal{A}_k + \rho_{k+1} C_k^{\alpha,(k)} \mathcal{B}_k\right] \mathcal{Q}_{k-1} = 2\gamma_{\mathrm{D},k}^{+} \Psi_{\mathrm{E}_{\kappa_k},k-1}^{\alpha}, \tag{3.6}$$

where

$$\rho_{k+1} := \frac{\mu_k \kappa_{k+1}}{\mu_{k+1}\kappa_k}.$$

The initial values $\mathcal{A}_{N-1}$, $\mathcal{B}_{N-1}$ for (3.6) read as

$$\mathcal{A}_{N-1} = -C_{N-1}^{\alpha,(N)} \quad \text{and} \quad \mathcal{B}_{N-1} = -\left(M_{N-1}^{\alpha,(N)} + \mathrm{I}\right) \tag{3.7}$$

and the subsequent terms are determined by the recursive relations

$$\mathcal{A}_{k-1} = -\,C_{k-1}^{\alpha,(k)} + \frac{1}{2}\left(\rho_{k+1}\gamma_{\mathrm{D},k-1}^{-}\Psi_{\mathrm{E}_{\kappa_k},k}^{\alpha}\mathcal{B}_k + \gamma_{\mathrm{D},k-1}^{-}\Psi_{\mathrm{M}_{\kappa_k},k}^{\alpha}\mathcal{A}_k\right)\mathcal{Q}_{k-1}, \tag{3.8}$$

$$\mathcal{B}_{k-1} = -\left(M_{k-1}^{\alpha,(k)} + \mathrm{I}\right) + \frac{1}{2}\left(\rho_{k+1}\gamma_{\mathrm{N}_{\kappa_k},k-1}^{-}\Psi_{\mathrm{E}_{\kappa_k},k}^{\alpha}\mathcal{B}_k + \gamma_{\mathrm{N}_{\kappa_k},k-1}^{-}\Psi_{\mathrm{E}_{\kappa_k},k}^{\alpha}\mathcal{A}_k\right)\mathcal{Q}_{k-1}. \tag{3.9}$$

Finally, the initial value $\mathbf{j}_0$ of (3.5) is a solution of the integral equation

$$\left[\left(M_0^{\alpha,(0)} + \mathrm{I}\right)\mathcal{A}_0 + \rho_1 C_0^{\alpha,(0)}\mathcal{B}_0\right]\mathbf{j}_0 = 2\gamma_{\mathrm{D},0}^{-}\mathbf{E}^{\mathrm{i}}. \tag{3.10}$$

From a numerical point of view, the recursive integral equation algorithm (3.5)-(3.10) is very interesting since the algorithm only involves the inversion of one boundary integral equation per recursion step. This allows to solve the 2π-biperiodic electromagnetic scattering problem (2.7)-(2.13) in a numerically efficient manner on a standard laptop.

The main challenge in the implementation of the recursive integral equation algorithm lies in the discretization of the boundary integral operators $\mathcal{A}_{k-1}$ and $\mathcal{B}_{k-1}$ for $k \in K^N$, given by (3.8)-(3.9), which requires to perform a large amount of complex matrix-matrix and matrix-vector multiplications. In the worst case, the latter rapidly slow down the computational speed of our algorithm. In order to tackle this issue, we suggest to either use fast multipole methods (first introduced by Greengard and Rokhlin in [9]) or methods based on hierarchical matrices (first introduced by Hackbusch and Khoromskij in [10]-[11]). Which one to choose is basically a matter of taste and experience with the respective method. Another point to be considered in the numerical realization of the algorithm (3.5)-(3.10) is the storage effort. In addition to the boundary integral operator on the left-hand side of the operator equation (3.6), the boundary integral operators $\mathcal{A}_{k-1}$, $\mathcal{B}_{k-1}$, $k \in K^N$, and $\mathcal{Q}_{k-1}$, $k \in K$. Nevertheless, our recursive integral equation algorithm seems to have a better cost-benefit ratio than comparable methods to treat the 2π-biperiodic multilayered electromagnetic scattering problem, for instance via the solution of the $N \times N$ integral equation system considered in [4].

4 Derivation of the Recursive Integral Equation Algorithm

In the following, we will derive the recursive integral equation algorithm (3.5)-(3.10) that has already been formally introduced in the previous section. This requires a suitable mathematical framework. Therefore, all relevant preliminaries are given before the actual derivation of the algorithm.

4.1 Mathematical Prerequisites

In this article, we use the functional analytic tools that are illustrated in detail in [3] and [4]. For the sake of simplicity, we only briefly state the function spaces and results necessary for all subsequent considerations.

Let Ω be a polyhedral Lipschitz domain in $\mathbb{R}^3$. Then

$$\mathbf{H}\left(\mathbf{curl},\Omega\right) := \left\{\mathbf{u}\in\mathbf{L}^2(\Omega)\ :\ \mathbf{curl}\,\mathbf{u}\in\mathbf{L}^2(\Omega)\right\} \qquad \text{for a bounded domain } \Omega,$$
$$\mathbf{H}_{\mathrm{loc}}\left(\mathbf{curl},\Omega\right) := \left\{\mathbf{u}\in\mathbf{L}^2_{\mathrm{loc}}(\Omega)\ :\ \mathbf{curl}\,\mathbf{u}\in\mathbf{L}^2_{\mathrm{loc}}(\Omega)\right\} \qquad \text{for an unbounded domain } \Omega.$$

Both spaces are endowed with their natural graph norm. We consider the following α-quasiperiodic Sobolev spaces for $s\in\mathbb{R}$:

$$\mathbf{H}^s_\alpha(\mathbf{curl},G_k) := \left\{\mathbf{u}\in\mathbf{H}^s(\mathbf{curl},G_k)\ :\ \exists\ \alpha\text{-qp}\ \mathbf{v}\in\mathbf{H}^s(\mathbf{curl},\mathbb{R}^3)\text{ such that }\mathbf{u}=\mathbf{v}|_{G_k}\right\},\ k\in K,$$
$$\mathbf{H}^s_{\alpha,\mathrm{loc}}(\mathbf{curl},G_k) := \left\{\mathbf{u}\in\mathbf{H}^s_{\mathrm{loc}}(\mathbf{curl},G_k)\ :\ \exists\ \alpha\text{-qp}\ \mathbf{v}\in\mathbf{H}^s_{\mathrm{loc}}(\mathbf{curl},\mathbb{R}^3)\text{ s. t. }\mathbf{u}=\mathbf{v}|_{G_k}\right\},\ k\in\{0,N\}.$$

For $k\in K_0$, we denote by $H^{-1/2}_\alpha(\Gamma_k)$ and $\mathbf{H}^{-1/2}_\alpha(\Gamma_k)$ the α-quasiperiodic versions of the common scalar- and vector-valued fractional Sobolev spaces $H^{-1/2}(\Gamma_k)$ and $\mathbf{H}^{-1/2}(\Gamma_k)$ on polyhedral Lipschitz interfaces. The trace space $\mathbf{V}^k_{\alpha,\pi}$, $k\in K_0$, is given by

$$\mathbf{V}^k_{\alpha,\pi} := \pi_{\mathrm{D},k}\left(\mathbf{H}^{\frac{1}{2}}_\alpha(\Gamma_k)\right),$$

where $\pi_{\mathrm{D},k}$ refers to the Dirichlet tangential components trace (see [3, Definition 3.1]). This is a Hilbert space with respect to the natural graph norm

$$\|\mathbf{u}\|_{\mathbf{V}^k_{\alpha,\pi}} := \inf_{\mathbf{v}\in\mathbf{H}^{1/2}_\alpha(\Gamma_k)}\left\{\|\mathbf{v}\|_{\mathbf{H}^{\frac{1}{2}}_\alpha(\Gamma_k)}\ :\ \pi_{\mathrm{D},k}\mathbf{v}=\mathbf{u}\right\}.$$

The dual space of $\mathbf{V}^k_{\alpha,\pi}$, $k\in K_0$, denoted by $(\mathbf{V}^k_{\alpha,\pi})'$, is specified with respect to the pivot space

$$\mathbf{L}^2_{\alpha,t}(\Gamma_k) := \left\{\mathbf{u}\in\mathbf{L}^2_\alpha(\Gamma_k)\ :\ \mathbf{u}\cdot\mathbf{n}_k=0\right\}.$$

We identify the latter space with the space of two-dimensional tangential vector fields - sections of the tangent bundle $T\Gamma_k$ of Γ_k for almost every $x\in\Gamma_k$. The previously introduced spaces now enable us to define the most prominent space in this article:

$$\mathbf{H}^{-\frac{1}{2}}_\alpha(\mathrm{div}_\Gamma,\Gamma_k) := \left\{\mathbf{j}\in\left(\mathbf{V}^k_{\alpha,\pi}\right)',\mathrm{div}_\Gamma\,\mathbf{j}\in H^{-\frac{1}{2}}_\alpha(\Gamma_k)\right\} \quad \text{for } k\in K_0.$$

Endowed with the norm

$$\|\mathbf{j}\|_{\mathbf{H}^{-\frac{1}{2}}_\alpha(\mathrm{div}_\Gamma,\Gamma_k)} := \|\mathbf{j}\|_{(\mathbf{V}^k_{\alpha,\pi})'} + \|\mathbf{j}\|_{H^{-\frac{1}{2}}_\alpha(\Gamma_k)}$$

$\mathbf{H}^{-1/2}_\alpha(\mathrm{div}_\Gamma,\Gamma_k)$ is a Hilbert space. Herein, the operator div_Γ denotes the surface divergence (see, e.g., [2, Section 3]).

We now turn to the mapping properties of the electric and magnetic potential operators $\Psi^\alpha_{\mathrm{E}_\kappa,k}$ and $\Psi^\alpha_{\mathrm{M}_\kappa,k}$, $k\in K_0$, as well as the boundary electric and magnetic potential operators $C^{\alpha,\kappa}_k$ and $M^{\alpha,\kappa}_k$, $k\in K_0$.

Lemma 4.1. *The electromagnetic potentials $\Psi^\alpha_{\mathrm{E}_\kappa,k}$ and $\Psi^\alpha_{\mathrm{M}_\kappa,k}$ are continuous operators with the following mapping properties:*

$$\Psi^\alpha_{*,k}:\begin{cases}\mathbf{H}^{-\frac{1}{2}}_\alpha(\mathrm{div}_\Gamma,\Gamma_k)\to\mathbf{H}_\alpha(\mathbf{curl},G_k)\cup\mathbf{H}_\alpha(\mathbf{curl},G_{k+1}) & \textit{for } k\in K\setminus\{N-1\},\\ \mathbf{H}^{-\frac{1}{2}}_\alpha(\mathrm{div}_\Gamma,\Gamma_k)\to\mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl},G_k)\cup\mathbf{H}_\alpha(\mathbf{curl},G_{k+1}) & \textit{for } k=0,\\ \mathbf{H}^{-\frac{1}{2}}_\alpha(\mathrm{div}_\Gamma,\Gamma_k)\to\mathbf{H}_\alpha(\mathbf{curl},G_k)\cup\mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl},G_{k+1}) & \textit{for } k=N-1,\\ \mathbf{H}^{-\frac{1}{2}}_\alpha(\mathrm{div}_\Gamma,\Gamma_k)\to\mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl},G_k^+)\cup\mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl},G_k^-) & \textit{for } k\in K_0,\end{cases}$$

where $* \in \{\mathrm{E}_\kappa, \mathrm{M}_\kappa\}$ and $G_k^\pm$ are the semi-infinite domains from (2.4). For $\mathbf{j}, \mathbf{m} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$, these potentials satisfy the time-harmonic Maxwell equations

$$\left(\mathbf{curl}\,\mathbf{curl} - \kappa^2\right) \Psi^\alpha_{\mathrm{E}_\kappa,k}\mathbf{j} = 0 \quad \text{and} \quad \left(\mathbf{curl}\,\mathbf{curl} - \kappa^2\right) \Psi^\alpha_{\mathrm{M}_\kappa,k}\mathbf{m} = 0$$

in G_k. Moreover, for $k \in \{0, N\}$, the outgoing wave condition (2.12)-(2.13) is fullfilled.

Lemma 4.2. *For $k \in K_0$, the boundary integral operators $C_k^{\alpha,\kappa}$ and $M_k^{\alpha,\kappa}$ give rise to bounded linear operators, $C_k^{\alpha,\kappa}, M_k^{\alpha,\kappa} : \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k) \to \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$.*

Lemma 4.3 ([3, Lemma 3.13 and Corollary 3.15 for $\Gamma := \Gamma_k$]). *The boundary integral operator $C_k^{\alpha,\kappa}$ is a Fredholm operator of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$ for $k \in K_0$.*

Defining $[\gamma_{*,k}] := \gamma_{*,k}^- - \gamma_{*,k}^+$ for $* \in \{\mathrm{D}, \mathrm{N}_\kappa\}$ and $k \in K_0$, the jump relations

$$[\gamma_{\mathrm{D},k}]\, \Psi^\alpha_{\mathrm{E}_\kappa,k} = 0, \qquad [\gamma_{\mathrm{N}_\kappa,k}]\, \Psi^\alpha_{\mathrm{E}_\kappa,k} = -2\mathrm{I}, \tag{4.1}$$

$$[\gamma_{\mathrm{D},k}]\, \Psi^\alpha_{\mathrm{M}_\kappa,k} = -2\mathrm{I}, \qquad [\gamma_{\mathrm{N}_\kappa,k}]\, \Psi^\alpha_{\mathrm{M}_\kappa,k} = 0 \tag{4.2}$$

hold. With their help, we are able to deduce the identities

$$\gamma^\pm_{\mathrm{D},k}\Psi^\alpha_{\mathrm{E}_\kappa,k} = \gamma^\pm_{\mathrm{N}_\kappa,k}\Psi^\alpha_{\mathrm{M}_\kappa,k} = -C_k^{\alpha,\kappa}, \tag{4.3}$$

$$\gamma^\pm_{\mathrm{N}_\kappa,k}\Psi^\alpha_{\mathrm{E}_\kappa,k} = \gamma^\pm_{\mathrm{D},k}\Psi^\alpha_{\mathrm{M}_\kappa,k} = -M_k^{\alpha,\kappa} \pm \mathrm{I}. \tag{4.4}$$

The subsequent two integral representations take an important role in the hereafter demonstrated derivation of the recursive integral equation algorithm (3.5)-(3.10).

Lemma 4.4 (α-quasiperiodic Stratton-Chu integral representation, [5, Theorem 4.21]). *Let $\mathbf{E}$ satisfy the α-quasiperiodic time-harmonic Maxwell equations $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa^2\mathbf{E} = 0$ as well as the outgoing wave condition in $G_k^+ \cup G_k^-$ (see (2.4)). Then $\mathbf{E}$ admits the integral representation*

$$\mathbf{E}(x) = -\frac{1}{2}\left(\Psi^\alpha_{\mathrm{E}_\kappa,k}\mathbf{j}(x) + \Psi^\alpha_{\mathrm{M}_\kappa,k}\mathbf{m}(x)\right) \quad \text{for } x \in G_k^+ \cup G_-^k,$$

where $\mathbf{j} := [\gamma_{\mathrm{N}_\kappa,k}]\,\mathbf{E}$ and $\mathbf{m} := [\gamma_{\mathrm{D},k}]\,\mathbf{E}$.

Lemma 4.5 (combined Stratton-Chu type integral representation, [5, Lemma 6.15]). *Let the electric field $\mathbf{E}$ a solution of time-harmonic Maxwell's equations $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa^2\mathbf{E} = 0$ in the bounded domain G_k, $k \in K$. Then $\mathbf{E}$ has the unique representation*

$$\mathbf{E} = \frac{1}{2}\left(\Psi^\alpha_{\mathrm{E}_\kappa,k}\gamma^+_{\mathrm{N}_\kappa,k}\mathbf{E} + \Psi^\alpha_{\mathrm{M}_\kappa,k}\gamma^+_{\mathrm{D},k}\mathbf{E}\right) + \Psi^\alpha_{\mathrm{E}_\kappa,k-1}\mathbf{j} \quad \text{in } G_k \tag{4.5}$$

with the density $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_{k-1})$ if $\mathcal{N}(C_{k-1}^{\alpha,\kappa}) = \{0\}$.

We call such a representation a combined α-quasiperiodic Stratton-Chu type integral representation.

4.2 Detailed Derivation

Let $\mathbf{E} := \mathbf{E}_k$ in G_k, $k \in K_0^N$, be given by the potential ansatz (3.2)-(3.4) that includes the unknown densities $\mathbf{j}_k \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$, $k \in K_0$. Then $\mathbf{E}$ is a solution of time-harmonic Maxwell equations (2.7) and additionally satisfies the outgoing wave condition (2.12)-(2.13) for $k \in \{0, N\}$ according to Lemma 4.1. By Lemma 4.5 and by the definition of the boundary electric potential operator $C_{k-1}^{\alpha,(k)}$, the representations (3.3) and (3.4) are unique if

$$\mathcal{N}\left(C_{k-1}^{\alpha,(k)}\right) = \{0\} \quad \text{for } k \in K^N. \tag{4.6}$$

We will therefore assume (4.6) from here on.

Since there is exactly one density $\mathbf{j}_k$ per material layer G_k for $k \in K_0$, the basis of a recursion in terms of $\mathbf{j}_k$ lies in somehow connecting the densities in adjacent domains. It will become clear in the course of the following considerations that the transmission conditions (2.8)-(2.11) provide such a connection.

We now make the ansatz

$$\gamma^-_{\mathrm{D},k}\mathbf{E}_{k+1} = \mathcal{A}_k\mathbf{j}_k, \quad \gamma^-_{\mathrm{N}_{\kappa_{k+1}},k}\mathbf{E}_{k+1} = \mathcal{B}_k\mathbf{j}_k, \quad k \in K_0, \tag{4.7}$$

where $\mathcal{A}_k$, $\mathcal{B}_k$ are bounded linear operators

$$\mathcal{A}_k, \mathcal{B}_k : \mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma_k) \to \mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma_k). \tag{4.8}$$

This seems plausible and reasonable if the electric fields $\mathbf{E}_{k+1}$, $k \in K_0$, are represented as in (3.3)-(3.4). Indeed, with the help of the identities (4.3)-(4.4), it then can be easily shown that the left-hand sides of (4.7) are bounded linear operators mapping the Hilbert space $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$ into itself.

With the ansatz (4.7), the initial values (3.7) for $\mathcal{A}_{N-1}$, $\mathcal{B}_{N-1}$ arise from the jump relations (4.1) after separately applying the Dirichlet trace $\gamma^-_{\mathrm{D},N-1}$ and the Neumann trace $\gamma^-_{\mathrm{N}_{\kappa_N},N-1}$ to the electric field $\mathbf{E}_N$ represented by the electric potential ansatz (3.4).

By (4.7), we can moreover express the transmission conditions (2.8)-(2.11) across Γ_k in terms of $\mathcal{A}_k$, $\mathcal{B}_k$ as

$$\gamma^+_{\mathrm{D},k}\mathbf{E}_k = \mathcal{A}_k\mathbf{j}_k, \quad \gamma^+_{\mathrm{N}_{\kappa_k},k}\mathbf{E}_k = \rho_{k+1}\mathcal{B}_k\mathbf{j}_k \quad \text{for } k \in K. \tag{4.9}$$

This turns out to be the essential ingredient for the derivation of the recursion (3.5) for the densities j_k, $k \in K$. In fact, first mapping the electric field $\mathbf{E}_k$ written in its representation (3.3) to Γ_k by the Dirichlet trace $\gamma^+_{\mathrm{D},k}$ for $k \in K$ and then exploiting (4.9) leads to

$$\begin{aligned}
\gamma^+_{\mathrm{D},k}\mathbf{E}_k &\overset{(4.3),(4.4)}{=} -\frac{1}{2}\left[C_k^{\alpha,(k)}\gamma^+_{\mathrm{N}_{\kappa_k},k}\mathbf{E}_k + \left(M_k^{\alpha,(k)} - \mathrm{I}\right)\gamma^+_{\mathrm{D},k}\mathbf{E}_k\right] + \gamma^+_{\mathrm{D},k}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1} \\
&\overset{(4.9)}{\Longrightarrow} \boxed{\left[\left(M_k^{\alpha,(k)} + \mathrm{I}\right)\mathcal{A}_k + \rho_{k+1}C_k^{\alpha,(k)}\mathcal{B}_k\right]\mathbf{j}_k = 2\gamma^+_{\mathrm{D},k}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1},}
\end{aligned}$$

which is satisfied by

$$\mathbf{j}_k = \mathcal{Q}_{k-1}\mathbf{j}_{k-1}$$

provided that $\mathcal{Q}_{k-1}$ is a solution of the operator equation (3.6). The operator $\mathcal{Q}_{k-1}$ maps $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_{k-1})$ boundedly into $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$ due to Lemma 4.2 and the mapping properties of $\mathcal{A}_k$ and $\mathcal{B}_k$ specified by (4.8).

It remains to derive the formulas (3.8) and (3.9) for $\mathcal{A}_{k-1}$ and $\mathcal{B}_{k-1}$, $k \in K$. Using the potential ansatz (3.3), we observe that

$$\begin{aligned}
\gamma^-_{\mathrm{D},k-1}\mathbf{E}_k &\overset{(4.3)}{=} \frac{1}{2}\left[\gamma^-_{\mathrm{D},k-1}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\gamma^+_{\mathrm{N}_{\kappa_k},k}\mathbf{E}_k + \gamma^-_{\mathrm{D},k-1}\Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\gamma^+_{\mathrm{D},k}\mathbf{E}_k\right] - C_{k-1}^{\alpha,(k)}\mathbf{j}_{k-1} \\
&\overset{(3.5),(4.9)}{=} \frac{1}{2}\left[\left(\rho_{k+1}\gamma^-_{\mathrm{D},k-1}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\mathcal{B}_k + \gamma^-_{\mathrm{D},k-1}\Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\mathcal{A}_k\right)\mathcal{Q}_{k-1} + 2C_{k-1}^{\alpha,(k)}\right]\mathbf{j}_{k-1}.
\end{aligned}$$

Inserting the ansatz (4.7) then finally yields (3.8).

In a similar way, we arrive at

$$\begin{aligned}
&\gamma^-_{\mathrm{N}_{\kappa_k},k-1}\mathbf{E}_k \\
&\quad\overset{(4.4)}{=} \frac{1}{2}\left[\gamma^-_{\mathrm{N}_{\kappa_k},k-1}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\gamma^+_{\mathrm{N}_{\kappa_k},k}\mathbf{E}_k + \gamma^-_{\mathrm{N}_{\kappa_k},k-1}\Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\gamma^+_{\mathrm{D},k}\mathbf{E}_k\right] - \left(M_{k-1}^{\alpha,(k)} + \mathrm{I}\right)\mathbf{j}_{k-1}
\end{aligned}$$

$$\overset{(3.5),(4.9)}{=} \frac{1}{2}\left[\left(\rho_{k+1}\gamma^-_{\mathrm{N}_{\kappa_k},k-1}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\mathcal{B}_k + \gamma^-_{\mathrm{N}_{\kappa_k},k-1}\Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\mathcal{A}_k\right)\mathcal{Q}_{k-1} + 2\left(M^{\alpha,(k)}_{k-1} + \mathrm{I}\right)\right]\mathbf{j}_{k-1},$$

which ensures (3.9) with the help of the ansatz (4.7).

The subsequent lemma shows that an initial density $\mathbf{j}_0 \in \mathbf{H}^{-1/2}_\alpha(\mathrm{div}_\Gamma, \Gamma_0)$ for the recursive relations (3.5), i.e., a solution of the integral equation (3.10), exists if and only if the transmission conditions (2.8) and (2.9) across Γ_0 are satisfied.

Lemma 4.6. *The transmission conditions (2.8) and (2.9) across Γ_0,*

$$\gamma^-_{\mathrm{D},0}\mathbf{E}_1 = \gamma^+_{\mathrm{D},0}\mathbf{E}_0 + \gamma^-_{\mathrm{D},0}\mathbf{E}^{\mathrm{i}} \quad \text{and} \quad \rho_1\gamma^-_{\mathrm{N}_{\kappa_1},0}\mathbf{E}_1 = \gamma^+_{\mathrm{N}_{\kappa_0},0}\mathbf{E}_0 + \gamma^-_{\mathrm{N}_{\kappa_1},0}\mathbf{E}^{\mathrm{i}}, \tag{4.10}$$

hold if and only if

$$\left(M^{\alpha,(0)}_0 + \mathrm{I}\right)\gamma^-_{\mathrm{D},0}\mathbf{E}_1 + \rho_1 C^{\alpha,(0)}_0\gamma^-_{\mathrm{N}_{\kappa_1},0}\mathbf{E}_1 = 2\gamma^-_{\mathrm{D},0}\mathbf{E}^{\mathrm{i}} \quad \text{on } \Gamma_0, \tag{4.11}$$

i.e., if and only if there exists a solution $\mathbf{j}_0 \in \mathbf{H}^{-1/2}_\alpha(\mathrm{div}_\Gamma, \Gamma_0)$ of (3.10).

Remark 4.7. *Assume that the material in the bottom layer G_N is a perfect electric conductor, i.e., the boundary conditions*

$$\gamma^-_{\mathrm{D},N-1}\mathbf{E}_N = \gamma^-_{\mathrm{N}_{\kappa_N},N-1}\mathbf{E}_N = 0 \quad \text{on } \Gamma_{N-1}$$

hold and therefore $\mathbf{E}_N = 0$ by its α-quasiperiodic Stratton-Chu integral representation. Then the densities $\mathbf{j}_k \in \mathbf{H}^{-1/2}_\alpha(\mathrm{div}_\Gamma, \Gamma_k)$, $k \in K \setminus \{N-1\}$, can also be derived by the scheme (3.5)-(3.10). Indeed, the relations (3.8) and (3.9) for $k = N-1$ and the initial values $\mathcal{A}_{N-1} = 0$ and $\mathcal{B}_{N-1} = 0$ yield the operators

$$\mathcal{A}_{N-2} = -C^{\alpha,(N-1)}_{N-2} \quad \text{and} \quad \mathcal{B}_{N-2} = -\left(M^{\alpha,(N-1)}_{N-2} + \mathrm{I}\right)$$

satisfying

$$\gamma^-_{\mathrm{D},N-2}\mathbf{E}_{N-1} = \mathcal{A}_{N-2}\mathbf{j}_{N-2} \quad \text{and} \quad \gamma^-_{\mathcal{N}_{\kappa_{N-1}},N-2}\mathbf{E}_{N-1} = \mathcal{B}_{N-2}\mathbf{j}_{N-2}.$$

Thus, we can interpret the scatterer as if it were a 2π-biperiodic multilayered scatterer consisting only of $N-1$ interfaces and apply the scheme (3.5)-(3.10) for the indices $k \in K \setminus \{N-1\}$.

4.3 Equivalence

The aim of this section is to show the equivalence of the recursive algorithm (3.5)-(3.10) and the electromagnetic scattering problem (2.7)-(2.13) in the sense that solutions to one problem yield solutions of the other and vice versa. We start by specifying the situations in which the integral equation algorithm (3.5)-(3.10) is mathematically meaningful.

Definition 4.8 (Applicability of algorithm (3.5)-(3.10))**.** *We call the recursive algorithm (3.5)-(3.10) applicable if, for $k = N-1, \ldots, 1$, there exist in descending order solutions*

$$\mathcal{Q}_{k-1} : \mathbf{H}^{-\frac{1}{2}}_\alpha(\mathrm{div}_\Gamma, \Gamma_{k-1}) \to \mathbf{H}^{-\frac{1}{2}}_\alpha(\mathrm{div}_\Gamma, \Gamma_k)$$

to the operator equations (3.6), which we rewrite as

$$\mathcal{C}_k\mathcal{Q}_{k-1} = 2\gamma^+_{\mathrm{D},k}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1} \tag{4.12}$$

with the operator $\mathcal{C}_k : \mathbf{H}^{-1/2}_\alpha(\mathrm{div}_\Gamma, \Gamma_k) \to \mathbf{H}^{-1/2}_\alpha(\mathrm{div}_\Gamma, \Gamma_k)$ defined by

$$\mathcal{C}_k := \left(M^{\alpha,(k)}_k + \mathrm{I}\right)\mathcal{A}_k + \rho_{k+1}C^{\alpha,(k)}_k\mathcal{B}_k. \tag{4.13}$$

We easily observe that Definition 4.8 is reasonable: Assume that, for $k = N-1, \ldots, 1$, there exist solutions $\mathcal{Q}_{k-1}$ to the operator equations (4.12). Then, based on the initial values $\mathcal{A}_{N-1}$ and $\mathcal{B}_{N-1}$ from (3.7), the formula (4.13) first gives rise to the bounded operater $\mathcal{C}_{N-1}$ mapping from $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_{N-1})$ into itself with which we can solve the operator equation (4.12) for $k = N-1$. From its solution $\mathcal{Q}_{N-2}$, the operators $\mathcal{A}_{N-2}, \mathcal{B}_{N-2}, \mathcal{C}_{N-2}$ - mapping from $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_{N-2})$ into itself - can be constructed by (3.8), (3.9) and (4.13). We continue this process iteratively until $k = 1$ and then solve the integral equation (3.10) that can be represented as

$$\mathcal{C}_0 \mathbf{j}_0 = 2\gamma_{\mathrm{D},0}^{-} \mathbf{E}^{\mathrm{i}}. \tag{4.14}$$

The density $\mathbf{j}_0 \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_0)$ is the initial value for the recursion (3.5) that uses the operators $\mathcal{Q}_{k-1}$ for $k \in K$.

Definition 4.8 does not require the operator $\mathcal{C}_0$ to be invertible. This leaves space for resonant solutions of the recursive algorithm (3.5)-(3.10) to occur. We will study this situation in detail in Section 5.4.

Lemma 4.9 (Equivalence)**.** *Assume that the algorithm (3.5)-(3.10) is applicable in the sense of Definition 4.8 and that we have $\mathcal{N}(C_k^{\alpha,(k)}) = \{0\}$ for $k \in K_0$. Then, if there exists a solution $\mathbf{j}_0$ of (4.14) lying in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_0)$, the functions*

$$\mathbf{E}_0 = \frac{1}{2}\left[\rho_1 \Psi^\alpha_{\mathrm{E}_{\kappa_0},0}\mathcal{B}_0 + \Psi^\alpha_{\mathrm{M}_{\kappa_0},0}\mathcal{A}_0\right]\mathbf{j}_0 \qquad \text{in } G_0, \tag{4.15}$$

$$\mathbf{E}_k = \frac{1}{2}\left[\rho_{k+1} \Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\mathcal{B}_k + \Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\mathcal{A}_k\right]\mathbf{j}_k + \Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1} \qquad \text{in } G_k, k \in K, \tag{4.16}$$

$$\mathbf{E}_N = \Psi^\alpha_{\mathrm{E}_{\kappa_N},N-1}\mathbf{j}_{N-1} \qquad \text{in } G_N \tag{4.17}$$

solve the electromagnetic scattering problem (2.7)-(2.13).

If, on the other hand, there exists a solution of the electromagnetic scattering problem (2.7)-(2.13) and the assumption (4.6), i.e.,

$$\mathcal{N}\left(C_{k-1}^{\alpha,(k)}\right) = \{0\}, \quad k \in K^N,$$

holds, then there exist solutions $\mathbf{j}_k \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$, $k \in K_0$, of the algorithm (3.5)-(4.14).

Proof. We first show that a given initial density $\mathbf{j}_0 \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_0)$ solving (4.14) provides a solution of the 2π-biperiodic multilayered electromagnetic scattering problem (2.7)-(2.13) under the assumption that the recursive integral equation algorithm (3.5)-(3.10) is applicable. In this case, we are able to derive the densities $\mathbf{j}_k \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$ for $k \in K$ by the recurrence relation (3.5) using the initial density $\mathbf{j}_0$. Lemma 4.1 ensures that, for any density $\mathbf{j}_{N-1} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_{N-1})$, the electric field $\mathbf{E}_N = \Psi^\alpha_{\mathrm{E}_{\kappa_N},N-1}\mathbf{j}_{N-1}$, given by the ansatz (4.17), is an α-quasiperiodic solution of $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa_N^2\mathbf{E} = 0$ in G_N satisfying the outgoing wave condition (2.13). Moreover, the electric fields $\mathbf{E}_k$, $k \in K$, given by

$$\mathbf{E}_k = \frac{1}{2}\left(\rho_{k+1}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\gamma^{-}_{\mathrm{N}_{\kappa_{k+1}},k}\mathbf{E}_{k+1} + \Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\gamma^{-}_{\mathrm{D},k}\mathbf{E}_{k+1}\right) + \Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1} \tag{4.18}$$

lie in $\mathbf{H}_\alpha(\mathbf{curl}, G_k)$ and solve the equations $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa_k^2\mathbf{E} = 0$ by Lemma 4.1 as

$$\gamma^{-}_{\mathrm{D},k}\mathbf{E}_{k+1}, \gamma^{-}_{\mathrm{N}_{\kappa_{k+1}},k}\mathbf{E}_{k+1} \in \mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma_k) \quad \text{for } k \in K \tag{4.19}$$

due to the mapping properties of the Dirichlet and the Neumann trace. The mapping properties (4.19) are still valid for $k = 0$. Hence, the function

$$\mathbf{E}_0 = \frac{1}{2}\left(\rho_1\Psi^\alpha_{\mathrm{E}_{\kappa_0},0}\gamma^{-}_{\mathrm{N}_{\kappa_1},0}\mathbf{E}_1 + \Psi^\alpha_{\mathrm{M}_{\kappa_0},0}\gamma^{-}_{\mathrm{D},0}\mathbf{E}_1\right) \tag{4.20}$$

is an $\mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl}, G_0)$-regular solution of $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa_0^2\mathbf{E} = 0$ in G_0 for which additionally the outgoing wave condition (2.12) is fulfilled, according to (4.19) and Lemma 4.1. It therefore remains to verify the transmission conditions (2.8)-(2.11). Throughout this proof, we will consider the fields with index k or $k+1$ in descending order $k = N-1, \dots, 0$.

For $k = N-1, \dots, 1$, we separately apply the Dirichlet trace $\gamma_{\mathrm{D},k}^-$ and the Neumann trace $\gamma_{\mathrm{N}_{\kappa_{k+1}},k}^-$ to the electric fields $\mathbf{E}_{k+1}$ represented as in (4.18). Together with the ansatz (4.7) of the recursive algorithm (3.5)-(3.10) for $\mathbf{E}_{k+2}$, this leads to

$$\begin{aligned}
\gamma_{\mathrm{D},k}^-\mathbf{E}_{k+1} &\overset{(4.3)}{=} \frac{1}{2}\left[\rho_{k+2}\gamma_{\mathrm{D},k}^-\Psi^\alpha_{\mathrm{E}_{\kappa_{k+1}},k+1}\mathcal{B}_{k+1} + \gamma_{\mathrm{D},k}^-\Psi^\alpha_{\mathrm{M}_{\kappa_{k+1}},k+1}\mathcal{A}_{k+1}\right]\mathbf{j}_{k+1} - C_k^{\alpha,(k+1)}\mathbf{j}_k,\\
\gamma_{\mathrm{N}_{\kappa_{k+1}},k}^-\mathbf{E}_{k+1} &\overset{(4.4)}{=} \frac{1}{2}\left[\rho_{k+2}\gamma_{\mathrm{N}_{\kappa_{k+1}},k}^-\Psi^\alpha_{\mathrm{E}_{\kappa_{k+1}},k+1}\mathcal{B}_{k+1} + \gamma_{\mathrm{N}_{\kappa_{k+1}},k}^-\Psi^\alpha_{\mathrm{M}_{\kappa_{k+1}},k+1}\mathcal{A}_{k+1}\right]\mathbf{j}_{k+1}\\
&\quad - \left(M_k^{\alpha,(k+1)} + \mathrm{I}\right)\mathbf{j}_k.
\end{aligned}$$

Inserted into the representation (4.18) of the electric field $\mathbf{E}_k$, this implies that

$$\begin{aligned}
\mathbf{E}_k = \frac{1}{2}\Bigg\{&\rho_{k+1}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\left[\frac{1}{2}\left(\rho_{k+2}\gamma_{\mathrm{N}_{\kappa_{k+1}},k}^-\Psi^\alpha_{\mathrm{E}_{\kappa_{k+1}},k+1}\mathcal{B}_{k+1} + \gamma_{\mathrm{N}_{\kappa_{k+1}},k}^-\Psi^\alpha_{\mathrm{M}_{\kappa_{k+1}},k+1}\mathcal{A}_{k+1}\right)\mathbf{j}_{k+1}\right.\\
&\left.- \left(M_k^{\alpha,(k+1)} + \mathrm{I}\right)\mathbf{j}_k\right]\\
&+ \Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\left[\frac{1}{2}\left(\rho_{k+2}\gamma_{\mathrm{D},k}^-\Psi^\alpha_{\mathrm{E}_{\kappa_{k+1}},k+1}\mathcal{B}_{k+1} + \gamma_{\mathrm{D},k}^-\Psi^\alpha_{\mathrm{M}_{\kappa_{k+1}},k+1}\mathcal{A}_{k+1}\right)\mathbf{j}_{k+1} - C_k^{\alpha,(k+1)}\mathbf{j}_k\right]\Bigg\}\\
&+ \Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1}.
\end{aligned}$$

In the next step, in which we apply the Dirichlet trace $\gamma_{\mathrm{D},k}^+$ to $\mathbf{E}_k$ represented as above, we exploit the applicability of the algorithm (3.5)-(3.10), in the sense that $\mathbf{j}_{k-1}$ solves the operator equation (3.6), and the recursive relation (3.5) to arrive at

$$\begin{aligned}
\gamma_{\mathrm{D},k}^+\mathbf{E}_k &\overset{(3.8),(3.9)}{=} -\frac{1}{2}\left[\rho_{k+1}C_k^{\alpha,(k)}\mathcal{B}_k + \left(M_k^{\alpha,(k)} - \mathrm{I}\right)\mathcal{A}_k\right]\mathcal{Q}_{k-1}\mathbf{j}_{k-1} + \gamma_{\mathrm{D},k}^+\Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1}\\
&\overset{(3.6)}{=} \mathcal{A}_k\mathcal{Q}_{k-1}\mathbf{j}_{k-1} \overset{(3.5)}{=} \mathcal{A}_k\mathbf{j}_k \overset{(4.7)_1}{=} \gamma_{\mathrm{D},k}^-\mathbf{E}_{k+1}
\end{aligned}$$

with the help of (4.3) and (4.4). This proves the transmission condition (2.10). In a similar way, we can verify the transmission condition (2.8).

For the proof of the transmission condition (2.11), we go back to the representation (4.18) of $\mathbf{E}_k$ and insert the transmission condition (2.10) that we already derived above. This gives

$$\mathbf{E}_k = \frac{1}{2}\left(\rho_{k+1}\Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\gamma_{\mathrm{N}_{\kappa_{k+1}},k}^-\mathbf{E}_{k+1} + \Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\gamma_{\mathrm{D},k}^+\mathbf{E}_k\right) + \Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1}. \tag{4.21}$$

Alternatively, the electric field $\mathbf{E}_k$ can be expressed in G_k in terms of the potential ansatz (3.3) ensured by Lemma 4.5:

$$\mathbf{E}_k = \frac{1}{2}\left(\Psi^\alpha_{\mathrm{M}_{\kappa_k},k}\gamma_{\mathrm{D},k}^+\mathbf{E}_k + \Psi^\alpha_{\mathrm{E}_{\kappa_k},k}\gamma_{\mathrm{N}_{\kappa_k},k}^+\mathbf{E}_k\right) + \Psi^\alpha_{\mathrm{E}_{\kappa_k},k-1}\mathbf{j}_{k-1}$$

with the same density $\mathbf{j}_{k-1} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_{k-1})$ as in (4.21). With this, equation (4.21) can be rewritten as

$$C_k^{\alpha,(k)}\gamma_{\mathrm{N}_{\kappa_k},k}^+\mathbf{E}_k = C_k^{\alpha,(k)}\left(\rho_{k+1}\gamma_{\mathrm{N}_{\kappa_{k+1}},k}^-\mathbf{E}_{k+1}\right)$$

after applying the Dirichlet trace $\gamma_{\mathrm{D},k}^+$. Since the nullspace of $C_k^{\alpha,(k)}$ is trivial by assumption, we deduce that the transmission condition (2.11) holds. We prove the transmission condition (2.9) analogously.

Now, we consider an electromagnetic scattering problem (2.7)-(2.13) for which the electromagnetic material parameters ϵ_k, μ_k, $k \in K_0^N$, are chosen in such a way that the recursive integral equation algorithm (3.5)-(3.10) is applicable. The potential ansatz used in the derivation of the algorithm is well-defined due to the assumption $\mathcal{N}(C_{k-1}^{\alpha,(k)}) = \{0\}$ for $k \in K^N$. In particular, the transmission conditions (2.8) and (2.9) hold for the electric fields $\mathbf{E}_0$ in G_0 and $\mathbf{E}_1$ in G_1. By Lemma 4.6, there exists a density $\mathbf{j}_0 \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_0)$ that solves the integral equation (3.10) and thus serves as an initial value for the recursive relations (3.5). Due to the applicability of the recursive integral equation algorithm (3.5)-(3.10), we altogether obtain, for $k \in K_0$, densities $\mathbf{j}_k \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$ solving the recursive algorithm. □

5 Solvability of the Recursive Integral Equation Algorithm

Below we want to analyze the recursive integral equation algorithm (3.5)-(3.10). From Definition 4.8, we know that this algorithm is applicable if and only if the operator equations (4.12), i.e.,

$$\mathcal{C}_k \mathcal{Q}_{k-1} = 2\gamma_{\mathrm{D},k}^+ \Psi_{\mathrm{E}_{\kappa_k},k-1}^\alpha \quad \text{for } k \in K^{N-1},$$

are solvable. If there additionally exists at least one solution of the integral equation (4.14), i.e., of

$$\mathcal{C}_0 \mathbf{j}_0 = 2\gamma_{\mathrm{D},0}^- \mathbf{E}^{\mathrm{i}},$$

we obtain solutions of the corresponding electromagnetic scattering problem (2.7)-(2.13). Thus, the analysis of the integral equation algorithm (3.5)-(4.14) consists in investigating the solvability of the operator equations (4.12) and the integral equation (4.14), which is closely linked to the Fredholm properties of the integral operators $\mathcal{C}_k$. Under certain assumptions on the electromagnetic material parameters, they are shown to be Fredholm operators of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$ for smooth surfaces Γ_k and under more restrictive assumptions also for polyhedral Lipschitz regular surfaces Γ_k. With this, we can show that there are material parameter combinations for which there exist (possibly nonunique) solutions of the algorithm (3.5)-(3.10). Further assumptions on the electromagnetic material parameters then even guarantee the existence of unique solutions.

5.1 Preliminaries

To understand the technical results obtained in the course of this section, we need further auxiliary tools and results. These are presented in the following. In particular, we deepen our understanding of the boundary electric potential operator $C_k^{\alpha,\kappa}$, $k \in K_0$.

We begin with the definition of the bilinear form $\mathcal{B}_k : \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k) \times \mathbf{H}_{-\alpha}^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k) \to \mathbb{C}$:

$$\mathcal{B}_k(\mathbf{j}, \mathbf{m}) := \int_{\Gamma_k} \mathbf{j} \cdot r_k(\mathbf{m}) \, d\sigma \quad \text{for } k \in K_0,$$

where $r_k : \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k) \to (\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k))'$ is the rotation operator corresponding to the geometric operation $\cdot \times \mathbf{n}_k$ (see, e.g., [4]). It is non-degenerate in the sense of [18, Definition 1.2.1], which is proven in [5, Lemma 2.57].

The subsequent lemma provides an expression for the adjoint operator of the boundary integral operator $\gamma_{\mathrm{D},k}^+ \Psi_{\mathrm{E}_\kappa,m}^\alpha$, $k, m \in K_0$, with respect to the dual systems (see [18, Definition 1.2.3])

$$\mathcal{B}_m \left(\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma_m), \mathbf{H}_{-\alpha}^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma_m) \right) \text{ and } \mathcal{B}_k \left(\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma_k), \mathbf{H}_{-\alpha}^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma_k) \right).$$

Lemma 5.1 ([5, Lemma 6.9]). *Let $k, m \in K_0$. The adjoint operator $(\gamma_{\mathrm{D},k}^+ \Psi_{\mathrm{E}_\kappa,m}^\alpha)'$ of $\gamma_{\mathrm{D},k}^+ \Psi_{\mathrm{E}_\kappa,m}^\alpha$ with respect to the dual systems $\mathcal{B}_m(\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_m), \mathbf{H}_{-\alpha}^{-1/2}(\mathrm{div}_\Gamma, \Gamma_m)$ and $\mathcal{B}_k(\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k), \mathbf{H}_{-\alpha}^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k))$*

is $(\gamma^{+}_{\mathrm{D},k}\Psi^{\alpha}_{\mathrm{E}_\kappa,m})' = -\gamma^{-}_{\mathrm{D},m}\Psi^{-\alpha}_{\mathrm{E}_\kappa,k}$. *Thus, we have*

$$\mathcal{B}_k\left(\gamma^{+}_{\mathrm{D},k}\Psi^{\alpha}_{\mathrm{E}_\kappa,m}\mathbf{m},\mathbf{j}\right) = -\mathcal{B}_m\left(\mathbf{m},\gamma^{-}_{\mathrm{D},m}\Psi^{-\alpha}_{\mathrm{E}_\kappa,k}\mathbf{j}\right) \tag{5.1}$$

for all $\mathbf{m}\in\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_m)$ *and all* $\mathbf{j}\in\mathbf{H}^{-1/2}_{-\alpha}(\mathrm{div}_\Gamma,\Gamma_k)$.

The subsequent result is concerned with the invertibility of $C^{\alpha,\kappa}_k$.

Lemma 5.2 ([3, Lemma 3.16 for $\Gamma := \Gamma_k$])**.** *The boundary integral operator $C^{\alpha,\kappa}_k$ is invertible in the Hilbert space $\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_k)$ if and only if the homogeneous Dirichlet problem,*

$$\begin{cases}\mathbf{curl}\,\mathbf{curl}\,\mathbf{E}-\kappa^2\mathbf{E}=0,\ \mathrm{div}\,\mathbf{E}=0,\ \gamma_{\mathrm{D},k}\mathbf{E}=0\\ \text{and } \mathbf{E} \text{ satisfies the outgoing wave condition}\end{cases} \tag{5.2}$$

only has the trivial solution in both of the domains G^{+}_k and G^{-}_k.

Remark 5.3. *For several results in this article, we require the invertibility of the boundary integral operator $C^{\alpha,\kappa}_k$ in $\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_k)$, which is equivalent to the uniqueness of (5.2) by Lemma 5.2. To the best of our knowledge, there do not exist any counterexamples to the uniqueness of (5.2) in the special situation encountered in this article that the grating profiles are representable as the graphs of "real" 2π-biperiodic functions - meaning that the scattering interfaces are not allowed to be invariant in x_1- or x_2-direction. However, there exist several counterexamples for grating profiles, which are invariant in x_1- or x_2-direction and may even be smooth (see, e.g., [14], [15]). Nevertheless, we assess the assumption that $C^{\alpha,\kappa}_k$ is invertible not to be very restrictive. For details, we refer, for instance, to [5, Remark 4.43].*

5.2 Fredholmness

This section is devoted to studying the Fredholm properties of the operator $\mathcal{C}_k$, $k\in K_0$, as the left-hand side of the operator equations (4.12) and the integral equation (4.14). We recall the exact representations of $\mathcal{C}_k$ as

$$\mathcal{C}_k = \left(M^{\alpha,(k)}_k+\mathrm{I}\right)\mathcal{A}_k+\rho_{k+1}C^{\alpha,(k)}_k\mathcal{B}_k.$$

We now separately investigate the operators $\mathcal{C}_{N-1}$ and $\mathcal{C}_k$, $k\in K_0\setminus\{N-1\}$, starting with the latter. Inserting the recursive relations (3.8) and (3.9) for the operators $\mathcal{A}_k$ and $\mathcal{B}_k$, a reordering of terms leads to

$$\mathcal{C}_k = -\rho_{k+1}C^{\alpha,(k)}_k\left(M^{\alpha,(k+1)}_k+\mathrm{I}\right)-\left(M^{\alpha,(k)}_k+\mathrm{I}\right)C^{\alpha,(k+1)}_k+C^k_\alpha \tag{5.3}$$

for $k\in K_0\setminus\{N-1\}$, where the operator $C^k_\alpha:\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_k)\to\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_k)$ is defined by

$$\begin{aligned}C^k_\alpha :=\ & \frac{1}{2}\left(M^{\alpha,(k)}_k+\mathrm{I}\right)\left(\rho_{k+2}\gamma^{-}_{\mathrm{D},k}\Psi^{\alpha}_{\mathrm{E}_{\kappa_{k+1}},k+1}\mathcal{B}_{k+1}+\gamma^{-}_{\mathrm{D},k}\Psi^{\alpha}_{\mathrm{M}_{\kappa_{k+1}},k+1}\mathcal{A}_{k+1}\right)\mathcal{Q}_k\\ &+\frac{\rho_{k+1}}{2}C^{\alpha,(k)}_k\left(\rho_{k+2}\gamma^{-}_{\mathrm{N}_{\kappa_{k+1}},k}\Psi^{\alpha}_{\mathrm{E}_{\kappa_{k+1}},k+1}\mathcal{B}_{k+1}+\gamma^{-}_{\mathrm{N}_{\kappa_{k+1}},k}\Psi^{\alpha}_{\mathrm{M}_{\kappa_{k+1}},k+1}\mathcal{A}_{k+1}\right)\mathcal{Q}_k.\end{aligned}$$

Under the assumption that the recursive integral equation algorithm (3.5)-(3.10) is applicable in terms of Definition 4.8, i.e., $\mathcal{Q}_k:\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_k)\to\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_{k+1})$ exists for $k\in K_0\setminus\{N-1\}$, the operator C^k_α is compact for $k\in K_0\setminus\{N-1\}$. In fact, since the kernels of the operators

$$\gamma^{-}_{\mathrm{D},k}\Psi^{\alpha}_{\mathrm{E}_{\kappa_{k+1}},k+1}=\gamma^{-}_{\mathrm{N}_{\kappa_{k+1}},k}\Psi^{\alpha}_{\mathrm{M}_{\kappa_{k+1}},k+1}\quad\text{and}\quad\gamma^{-}_{\mathrm{D},k}\Psi^{\alpha}_{\mathrm{M}_{\kappa_{k+1}},k+1}=\gamma^{-}_{\mathrm{N}_{\kappa_{k+1}},k}\Psi^{\alpha}_{\mathrm{E}_{\kappa_{k+1}},k+1},$$

which map from $\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_{k+1})$ to $\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_\Gamma,\Gamma_k)$, are sufficiently smooth on $\Gamma_k\times\Gamma_{k+1}$, these operators are compact. All other operators occurring in C^k_α are bounded in each of their domains of definition. This easily entails the compactness of C^k_α. Next, we turn to the remaining part of the operator $\mathcal{C}_k$ represented as in

(5.3). We recall the operator $\mathbf{A}_\alpha$ given as the left-hand side of the singular integral equation (4.9) from [3], in which we studied one profile scattering across an interface Γ. For $\Gamma := \Gamma_k$, we denote the operator $\mathbf{A}_\alpha$ by $\mathbf{A}_\alpha^k$. With this, we can express $\mathcal{C}_k$ as

$$\mathcal{C}_k = -\mathbf{A}_\alpha^k + C_\alpha^k \quad \text{for } k \in K_0 \setminus \{N-1\}.$$

Assuming that

$$\epsilon_{k+1} \neq -\epsilon_k \quad \text{and} \quad \mu_{k+1} \neq -\mu_k \tag{5.4}$$

if Γ_k is smooth, or

$$\operatorname{Re}(\epsilon_k)\operatorname{Re}(\epsilon_{k+1}) + \operatorname{Im}(\epsilon_k)\operatorname{Im}(\epsilon_{k+1}) \geq 0 \quad \text{and} \quad \operatorname{Re}(\mu_k)\operatorname{Re}(\mu_{k+1}) + \operatorname{Im}(\mu_k)\operatorname{Im}(\mu_{k+1}) \geq 0 \tag{5.5}$$

if Γ_k is of polyhedral Lipschitz regularity, the operator $\mathbf{A}_\alpha^k : \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k) \to \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k)$ is a Fredholm of index zero. This is verified by [3, Corollaries 5.2 and 5.7]. From the compactness of C_α^k, we then conclude that $\mathcal{C}_k$ is a Fredholm operator of index zero in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k)$ for $k \in K_0 \setminus \{N-1\}$.

Next, consider the boundary integral operator $\mathcal{C}_{N-1}$, which can be expressed as

$$\mathcal{C}_{N-1} \overset{(3.7)}{=} -\left(M_{N-1}^{\alpha,(N-1)} + \mathrm{I}\right) C_{N-1}^{\alpha,(N)} - \rho_N C_{N-1}^{\alpha,(N-1)} \left(M_{N-1}^{\alpha,(N)} + \mathrm{I}\right) = -A_\alpha^{N-1}.$$

With similar considerations as before, we then immediately deduce its Fredholmness of index zero in the Hilbert space $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_{N-1})$ provided that (5.4) holds for $k = N-1$ if Γ_{N-1} is smooth or that (5.5) holds for $k = N-1$ if Γ_{N-1} is polyhedral Lipschitz regular.

We summarize our insights in the following theorem.

Theorem 5.4 (Fredholmness of $\mathcal{C}_k$). *Let Γ_k, $k \in K_0$, be one interface of the considered 2π-biperiodic multilayered structure. Moreover, let the electromagnetic material parameters be chosen in accordance with assumption (2.2) such that*

$$\epsilon_{k+1} \neq -\epsilon_k \quad \textit{and} \quad \mu_{k+1} \neq -\mu_k$$

if Γ_k is smooth, or

$$\operatorname{Re}(\epsilon_k)\operatorname{Re}(\epsilon_{k+1}) + \operatorname{Im}(\epsilon_k)\operatorname{Im}(\epsilon_{k+1}) \geq 0 \quad \textit{and} \quad \operatorname{Re}(\mu_k)\operatorname{Re}(\mu_{k+1}) + \operatorname{Im}(\mu_k)\operatorname{Im}(\mu_{k+1}) \geq 0$$

if Γ_k is polyhedral Lipschitz regular. Then the operator $\mathcal{C}_k$ given by

$$\mathcal{C}_k = \left(M_k^{\alpha,(k)} + \mathrm{I}\right)\mathcal{A}_k + \rho_{k+1} C_k^{\alpha,(k)} \mathcal{B}_k,$$

where $\mathcal{A}_k$ and $\mathcal{B}_k$ arise from from (3.8) and (3.9), is a Fredholm operator of index zero in the Hilbert space $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k)$.

5.3 Existence

With the help of Theorem 5.4 on the Fredholmness of the integral operators $\mathcal{C}_k$, $k \in K_0$, it is possible to prove the main result in the analysis of the recursive integral equation algorithm (3.5)-(3.10). For its formulation, we introduce two assumptions on the electromagnetic material parameters. Their use will become clear in the course of this section.

Assumption 5.5. *Let the electromagnetic material parameters $\epsilon_k, \mu_k \in \mathbb{R}$, $k \in K_0^N$, satisfy (2.2) such that $\operatorname{sgn}(\epsilon_0\mu_0) > 0$ and $\operatorname{sgn}(\mu_0\mu_N) > 0$ if $\operatorname{sgn}(\epsilon_N\mu_N) > 0$.*

Assumption 5.6. *Let the electric permittivities and magnetic permeabilities ϵ_k, μ_k, $k \in K_0^N$, satisfy (2.2) such that $\epsilon_0, \mu_0 \notin \mathbb{R}_-$ and $\epsilon_N, \mu_N \in \mathbb{R}_-$. Moreover, assume that one of the following situations holds for ϵ_j, ϵ_{j+1}, μ_j and μ_{j+1} for some $j \in K_0$:*

(i) $\epsilon_j, \mu_j \in \mathbb{R}$ *such that at least one of them is positive and*

$$\operatorname{Im}(\epsilon_{j+1}) \geq 0 \quad \textit{and} \quad \operatorname{Im}(\mu_{j+1}) \geq 0 \quad \textit{with} \quad \operatorname{Im}(\epsilon_{j+1} + \mu_{j+1}) > 0;$$

(ii) $\epsilon_{j+1}, \mu_{j+1} \in \mathbb{R}$ *such that at least one of them is positive and*

$$\operatorname{Im}(\epsilon_j) \geq 0 \quad \textit{and} \quad \operatorname{Im}(\mu_j) \geq 0 \quad \textit{with} \quad \operatorname{Im}(\epsilon_j + \mu_j) > 0;$$

(iii) $\operatorname{Im}(\epsilon_j), \operatorname{Im}(\epsilon_{j+1}), \operatorname{Im}(\mu_j), \operatorname{Im}(\mu_{j+1}) \geq 0$ *with*

$$\operatorname{Im}(\epsilon_j + \mu_j) > 0 \quad \textit{and} \quad \operatorname{Im}(\epsilon_{j+1} + \mu_{j+1}) > 0.$$

Theorem 5.7 (Existence)**.** *Let the electromagnetic material parameters ϵ_k and μ_k satisfying (2.2) be chosen such that the nullspaces of the operators $C_{k-1}^{\alpha,(k)}$ are trivial for all $k \in K^N$ and such that*

$$\epsilon_{k+1} \neq -\epsilon_k \quad \textit{and} \quad \mu_{k+1} \neq -\mu_k \tag{5.6}$$

if Γ_k is smooth, or

$$\operatorname{Re}(\epsilon_k)\operatorname{Re}(\epsilon_{k+1}) + \operatorname{Im}(\epsilon_k)\operatorname{Im}(\epsilon_{k+1}) \geq 0 \quad \textit{and} \quad \operatorname{Re}(\mu_k)\operatorname{Re}(\mu_{k+1}) + \operatorname{Im}(\mu_k)\operatorname{Im}(\mu_{k+1}) \geq 0 \tag{5.7}$$

if Γ_k is only of polyhedral Lipschitz regularity. Moreover, suppose that Assumptions 5.5 or 5.6 are satisfied. Then the recursive integral equation algorithm (3.5)-(3.10) is applicable if and only if $\mathcal{N}(\mathcal{C}_k) = \{0\}$ for $k \in K$. In this case, equation (3.10) is solvable and any solution $\mathbf{j}_0 \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_0)$ provides a solution of the electromagnetic scattering problem (2.7)-(2.13).

The proof of Theorem 5.7 relies on the two subsequent auxiliary results.

Lemma 5.8. *If $C_{k-1}^{\alpha,(k)}$ is invertible, then $\mathcal{R}(\gamma_{\mathrm{D},k}^+ \Psi_{\mathrm{E}_{\kappa_k},k-1}^\alpha)$ is dense in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k)$.*

Proof. Let $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_{k-1})$ and $\mathbf{m} \in \mathbf{H}_{-\alpha}^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k)$. Assume that $C_{k-1}^{\alpha,(k)}$ is invertible and that $\mathcal{R}(\gamma_{\mathrm{D},k}^+ \Psi_{\mathrm{E}_{\kappa_k},k-1}^\alpha)$ is not dense in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k)$. Then there exists a density $\mathbf{m} \neq 0$ in $\mathbf{H}_{-\alpha}^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k)$ such that

$$\mathcal{B}_k\left(\gamma_{\mathrm{D},k}^+ \Psi_{\mathrm{E}_{\kappa_k},k-1}^\alpha \mathbf{j}, \mathbf{m}\right) \overset{(5.1)}{=} -\mathcal{B}_{k-1}\left(\mathbf{j}, \gamma_{\mathrm{D},k-1}^- \Psi_{\mathrm{E}_{\kappa_k},k}^{-\alpha} \mathbf{m}\right) = 0 \quad \text{for all } \mathbf{j} \in \mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma_{k-1}),$$

where we exploited Lemma 5.1. Hence, for all $x \in \Gamma_{k-1}$, the function $\gamma_{\mathrm{D},k-1}^- \Psi_{\mathrm{E}_{\kappa_k},k}^{-\alpha} \mathbf{m}(x) = 0$ since $\mathcal{B}_k$ and $\mathcal{B}_{k-1}$ are nondegenerate in the sense of [18, Definition 1.2.1]. Together with Lemma 4.1, we moreover deduce that the $(-\alpha)$-quasiperiodic vector-valued Dirichlet problem (5.2) has at least the nontrivial solution $\mathbf{E} := \Psi_{\mathrm{E}_{\kappa_k},k}^{-\alpha} \mathbf{m}$ in G_{k-1}^+. Then Lemma 5.2 yields that $C_{k-1}^{-\alpha,(k)}$ is not invertible in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_{k-1})$. Hence, the Fredholm operator $(-C_{k-1}^{\alpha,(k)})$ is also not invertible in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_{k-1})$ despite our assumption of the contrary. We therefore conclude that $\mathcal{R}(\gamma_{\mathrm{D},k}^+ \Psi_{\mathrm{E}_{\kappa_k},k-1}^\alpha)$ is dense in the Hilbert space $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma_k)$ by contraposition. □

Lemma 5.9. *Under the assumptions of Theorem 5.7, the operator equations (4.12) are solvable if and only if $\mathcal{N}(\mathcal{C}_k) = \{0\}$ for all $k \in K$. Then $2\gamma_{\mathrm{D},0}^- \mathbf{E}^{\mathrm{i}} \in \mathcal{R}(\mathcal{C}_0)$.*

Proof. We first assume that the operator equations (4.12), i.e.,

$$\mathcal{C}_k \mathcal{Q}_{k-1} = 2\gamma_{\mathrm{D},k}^{-} \Psi_{\mathrm{E}_{\kappa_k},k-1}^{\alpha}, \quad k = N-1,\dots,1,$$

are solvable. This is the case only if

$$\mathcal{R}(\mathcal{C}_k) \supset \mathcal{R}(\gamma_{\mathrm{D},k}^{-} \Psi_{\mathrm{E}_{\kappa_k},k-1}^{\alpha}) \quad \text{for } k \in K. \tag{5.8}$$

Under the assumptions of Theorem 5.7, Theorem 5.4 implies that $\mathcal{C}_k$ are Fredholm operators of index zero in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma_k)$ for $k \in K$. Since moreover the boundary integral operators $C_{k-1}^{\alpha,(k)}$ are Fredholm operators of index zero for $k \in K$ by Lemma 4.3, the assumption of Theorem 5.7 that these operators all have a trivial nullspace yields that they are in particular invertible in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma_{k-1})$. Taking all considerations so far into account, an application of Lemma 5.8 gives that

$$\mathcal{R}(\mathcal{C}_k) = \mathcal{R}(\gamma_{\mathrm{D},k}^{-} \Psi_{\mathrm{E}_{\kappa_k},k-1}^{\alpha}) = \mathbf{H}_{\alpha}^{-\frac{1}{2}}(\mathrm{div}_{\Gamma}, \Gamma_k), \quad k = N-1,\dots,1,$$

and therefore $\mathcal{N}(\mathcal{C}_k) = 0$ for $k \in K$ due to the Fredholm properties of $\mathcal{C}_k$.

Next, assume that $\mathcal{N}(\mathcal{C}_k) = 0$ for $k \in K$. From Theorem 5.4, we infer that $\mathcal{C}_k$ are Fredholm operators of index zero in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma_k)$ for $k \in K$. Then we can already deduce the invertibility of $\mathcal{C}_k$, $k \in K$, and conclude that the recursive integral equation algorithm (3.5)-(3.10) is applicable in the sense of Definition 4.8, i.e., the operator equations (4.12) are solvable.

Under the assumptions of Theorem 5.7, it is possible to apply either [4, Theorem 5.8] or [4, Theorem 5.9], which state that depending on the parity of the number of grating interfaces N of the 2π-biperiodic multilayered structure the systems of linear integral equations [4, (4.13)] or [4, (4.14)] are solvable. By [4, Lemma 4.4], the mentioned systems are equivalent to the 2π-biperiodic electromagnetic scattering problem (2.7)-(2.13), meaning that there exists a solution $\mathbf{E}_k$ in G_k of (2.7)-(2.13) for $k \in K_0^N$. This in turn verifies that there exist solutions of the recursive integral equation algorithm (3.5)-(3.10) by Lemma 4.9, which is applicable since $\mathcal{N}(C_{k-1}^{\alpha,(k)}) = \{0\}$ for $k \in K^N$. In particular, we therefore have $2\gamma_{\mathrm{D},0}^{-}\mathbf{E}^{\mathrm{i}} \in \mathcal{R}(\mathcal{C}_0)$. □

Proof of Theorem 5.7. Theorem 5.7 is easily shown with the help of Lemma 5.9, from which we immediately deduce that the recursive integral equation is applicable in the sense of Definition 4.8 and that moreover $2\gamma_{\mathrm{D},0}^{-}\mathbf{E}^{\mathrm{i}} \in \mathcal{R}(\mathcal{C}_0)$. This means that there exists a solution to the integral equation (3.10) yielding an initial value $\mathbf{j}_0 \in \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma_0)$ for the recursive relations (3.5). This density provides a solution of the recursive integral equation algorithm (3.5)-(3.10), which on the other hand gives rise to a solution of the electromagnetic scattering problem (2.7)-(2.13) by Lemma 4.9. The integral equation algorithm can be applied due to the assumption $\mathcal{N}(\mathcal{C}_k) = \{0\}$ for $k \in K$, Lemma 4.9 due to the assumption $\mathcal{N}(C_{k-1}^{\alpha,(k)}) = \{0\}$ for $k \in K^N$. □

5.4 Uniqueness

Assume that $\mathcal{N}(\mathcal{C}_l) \neq \{0\}$. If $l > 0$, then the algorithm (3.5)-(3.10) fails by Theorem 5.7. If $l = 0$, then the homogeneous equation (4.14),

$$\mathcal{C}_0 \mathbf{j}_0 = 0,$$

has a nontrivial solution. This generates resonant solutions of the 2π-biperiodic multilayered electromagnetic scattering problem (2.7)-(2.13). Below, we will first study in detail the case that

$$\mathcal{N}(\mathcal{C}_k) = \{0\} \quad \text{for } k = N-1,\dots,l+1, \quad \text{and} \quad \mathcal{N}(\mathcal{C}_l) \neq \{0\}.$$

Second, we state conditions on the electromagnetic material parameters in Theorem 5.14 ensuring that all operators $\mathcal{C}_k$, $k \in K_0$, have a trivial nullspace meaning that

$$\mathcal{R}(\mathcal{C}_k) = \mathbf{H}_{\alpha}^{-\frac{1}{2}}(\mathrm{div}_{\Gamma}, \Gamma_k) \quad \text{for } k \in K_0$$

if the operators $\mathcal{C}_k$ fulfill the requirements of Theorem 5.4. Together with Theorem 5.7, this implies the unique solvability of the equations (4.12).

Definition 5.10 (Reduced electromagnetic scattering problem)**.** *Let l be an arbitrary integer taken from the set $\{0, \dots, N-1\}$. Given an incident electric plane wave $\mathbf{E}^{\mathrm{i}}$ of the form (2.5), the 2π-biperiodic electromagnetic scattering problem in the reduced grating structure with the interfaces $\Gamma_l, \dots, \Gamma_{N-1}$ and the upper semi-infinite layer G_l^+, specified by*

$$G_l^+ := \{x \in Q \times \mathbb{R} \,:\, x_3 > \sigma_l(\tilde{x})\},$$

is then formulated as follows: Find an α-quasiperiodic electric field

$$\mathbf{E} := \begin{cases} \mathbf{E}_l & \text{in } G_l^+, \\ \mathbf{E}_k & \text{in } G_k, k = l+1, \dots, N, \end{cases}$$

of finite energy, in the sense that

$$\mathbf{E}_k, \mathbf{curl}\,\mathbf{E}_k \in \mathbf{L}^2(\mathbb{R}^3) \quad \text{for all } k = l, \dots, N,$$

solving the time-harmonic Maxwell equations

$$\begin{aligned} \mathbf{curl}\,\mathbf{curl}\,\mathbf{E}_l - \kappa_l^2 \mathbf{E}_l &= 0 && \text{in } G_l^+, \\ \mathbf{curl}\,\mathbf{curl}\,\mathbf{E}_k - \kappa_k^2 \mathbf{E}_l &= 0 && \text{in } G_k, k = l+1, \dots, N, \end{aligned}$$

with respect to the transmission conditions

$$\gamma_{\mathrm{D},l}^- \mathbf{E}_{l+1} = \gamma_{\mathrm{D},l}^+ \mathbf{E}_l + \gamma_{\mathrm{D},l}^+ \mathbf{E}^{\mathrm{i}} \qquad \text{on } \Gamma_l, \tag{5.9}$$

$$\gamma_{\mathrm{N}_{\kappa_{l+1}},l}^- \mathbf{E}_{l+1} = \rho_{l+1}^{-1} \left(\gamma_{\mathrm{N}_{\kappa_l},l}^+ \mathbf{E}_l + \gamma_{\mathrm{N}_{\kappa_l},l}^+ \mathbf{E}^{\mathrm{i}} \right) \qquad \text{on } \Gamma_l, \tag{5.10}$$

$$\gamma_{\mathrm{D},k}^- \mathbf{E}_{k+1} = \gamma_{\mathrm{D},k}^+ \mathbf{E}_k \qquad \text{on } \Gamma_k \text{ for } k = l+1, \dots, N-1, \tag{5.11}$$

$$\gamma_{\mathrm{N}_{\kappa_{k+1}},k}^- \mathbf{E}_{k+1} = \rho_{k+1}^{-1} \gamma_{\mathrm{N}_{\kappa_k},k}^+ \mathbf{E}_k \qquad \text{on } \Gamma_k \text{ for } k = l+1, \dots, N-1. \tag{5.12}$$

Additionally, we impose the outgoing wave condition

$$\mathbf{E}_l(x) = \sum_{n \in \mathbb{Z}^2} \mathbf{E}_n^l e^{\mathrm{i}\left(\alpha^{(n)} \cdot \tilde{x} + \beta_l^{(n)} x_3 \right)} \qquad \text{for } x \in G_{l,+}^{\mathrm{H},+}, \tag{5.13}$$

$$\mathbf{E}_N(x) = \sum_{n \in \mathbb{Z}^2} \mathbf{E}_n^N e^{\mathrm{i}\left(\alpha^{(n)} \cdot \tilde{x} - \beta_N^{(n)} x_3 \right)} \qquad \text{for } x \in G_N^{\mathrm{H},-}, \tag{5.14}$$

where

$$G_{l,+}^{\mathrm{H},+} := \big((Q \times \mathbb{R}) \setminus G^{\mathrm{H}} \big) \cap G_l^+ \quad \text{and} \quad G_N^{\mathrm{H},-} := \big((Q \times \mathbb{R}) \setminus G^{\mathrm{H}} \big) \cap G_N$$

with $\mathrm{H} \in \mathbb{R}_+$ chosen such that

$$\Gamma_k \subset G^{\mathrm{H}} := \{x \in Q \times \mathbb{R} \,:\, |x_3| \le \mathrm{H}\} \quad \text{for all } k = l, \dots, N-1. \tag{5.15}$$

Lemma 5.11. *Let $\mathcal{N}(\mathcal{C}_k) = \{0\}$ for $k = N-1, \dots, l+1$, and $\mathcal{N}(\mathcal{C}_l) \neq \{0\}$. Moreover, let assumption (2.2) be satisfied for the electric permittivities ϵ_k and the magnetic permeabilities μ_k, $k = N, \dots, l+1$, such that $\epsilon_l, \mu_l \in \mathbb{R}_-$ as well as $\epsilon_N, \mu_N \in \mathbb{R}_-$. Then there exist nontrivial solutions of the 2π-biperiodic electromagnetic scattering problem in the reduced grating structure with the interfaces $\Gamma_l, \dots, \Gamma_{N-1}$ and the upper semi-infinite layer G_l^+ in the sense of Definition 5.10.*

Moreover, the Rayleigh coefficients $\mathbf{E}_n^+$ from (5.13) vanish if

$$\beta_l^{(n)} > 0, \quad \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_l}{\kappa_l^2}\right) > 0 \quad \textit{and} \quad \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_N}{\kappa_N^2}\right) \geq 0. \tag{5.16}$$

Similarly the Rayleigh coefficients $\mathbf{E}_n^-$ from (5.14) are zero if

$$\beta_N^{(n)} > 0, \quad \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_N}{\kappa_N^2}\right) > 0 \quad \textit{and} \quad \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_l}{\kappa_l^2}\right) \geq 0. \tag{5.17}$$

For the proof of Lemma 5.11, we require two auxiliary results that are easily shown by simple manipulations.

Lemma 5.12. *Assume that (2.2) holds for the electric permittivities ϵ_k and the magnetic permeabilities μ_k, $k \in K_0^N$. Then, if $\kappa_k \in \mathbb{R}$ for some $k \in K_0^N$, we have*

$$\mathrm{Im}\left(\beta_k^{(n)}\right) > 0 \quad \textit{for all except of a finite number } N_k \textit{ of } n \in \mathbb{Z}^2.$$

The excluded $n \in N_k$ satisfy $\mathrm{Im}(\beta_k^{(n)}) = 0$. For all other values of κ_k, the imaginary part of $\beta_k^{(n)}$ is non-negative for all $n \in \mathbb{Z}^2$.

Lemma 5.13. *Let the electromagnetic material parameters ϵ_k and μ_k, $k \in K_0^N$, satisfy (2.2). Then we have*

$$\mathrm{Im}\left(\frac{\epsilon_k}{\kappa_k^2}\right) \leq 0 \quad \textit{for all } k \in K_0^N. \tag{5.18}$$

Proof of Lemma 5.11. Let $\mathbf{j}_l \in \mathcal{N}\left(\mathcal{C}_l\right) \setminus \{0\}$ and set

$$\mathbf{j}_k = \mathcal{Q}_{k-1}\mathbf{j}_{k-1}, \quad k = l+1, \dots, N-1. \tag{5.19}$$

In order to verify Lemma 5.11, we reuse the ideas of the proof of [4, Theorem 5.4]. We construct a nontrivial solution

$$\mathbf{E} := \mathbf{E}_k \quad \begin{cases} \text{in } G_l^+ & \text{for } k = l, \\ \text{in } G_k & \text{for } k = l+1, \dots, N \end{cases}$$

of the homogeneous electromagnetic scattering problem in the reduced grating structure composed of the densities $\mathbf{j}_k \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$, $k = l+1, \dots, N-1$, from (5.19). We then have access to a variational equation in terms of $\mathbf{E}$ similar to the one derived in the proof of [4, Theorem 5.4] for a complete 2π-biperiodic N-layered profile grating structure. With its help, we finally deduce the assertions on the Rayleigh coefficients of the electric fields in the domains $G_{l,+}^{\mathrm{H},+}$ and $G_N^{\mathrm{H},-}$.

Let $\mathbf{E}$ be given by (4.16)-(4.17) in G_k, $k = l+1, \dots, N$, and by

$$\mathbf{E} = \frac{1}{2}\left[\rho_{l+1}\Psi^\alpha_{\mathrm{E}_{\kappa_l},l}\mathcal{B}_l + \Psi^\alpha_{\mathrm{M}_{\kappa_l},l}\mathcal{A}_l\right]\mathbf{j}_l \quad \text{in } G_l^+. \tag{5.20}$$

Since $\mathcal{N}\left(\mathcal{C}_l\right) \neq \{0\}$, it is clear that such a function $\mathbf{E}$ is a nontrivial solution of the homogeneous electric scattering problem in the reduced geometry with respect to the transmission conditions

$$\gamma_{\mathrm{D},k}^+\mathbf{E}_k = \gamma_{\mathrm{D},k}^-\mathbf{E}_{k+1} \quad \text{and} \quad \mu_{k+1}\gamma_{\mathrm{D},k}^+\left(\mathbf{curl}\,\mathbf{E}_k\right) = \mu_k\gamma_{\mathrm{D},k}^-\left(\mathbf{curl}\,\mathbf{E}_{k+1}\right). \tag{5.21}$$

This arises from an argumentation analogous to the one from the first part of the proof of Lemma 4.9. Therefore, it remains to prove that the Rayleigh coefficients $\mathbf{E}_n^l$ in (5.13) and $\mathbf{E}_n^N$ in (5.14) vanish for arbitrary nontrivial solutions $\mathbf{E}$ if $\beta_l^{(n)} > 0$ and $\beta_N^{(n)} > 0$, respectively. For this, we exploit a variational formulation in the domain G^{H} introduced in (5.15) for a fixed $\mathrm{H} \in \mathbb{R}_+$. Speaking visually, G^{H} is a periodically extendable cell of width 2π in both x_1- and x_2-direction that is bounded by the plane surfaces

$$\Gamma_{\pm}^{\mathrm{H}} \coloneqq \{x \in Q \times \mathbb{R} \;:\; x_3 = \pm\mathrm{H}\}$$

with the outer normals $\mathbf{n}_{\pm}^{\mathrm{H}} = (0,0,\pm 1)^{\mathrm{T}}$ and contains the interfaces Γ_k, $k = l, \ldots, N-1$. The specific variational formulation that we have in mind arises from adapting the corresponding lines in the proof of [4, Theorem 5.4] to our reduced geometry setting. In order to avoid lengthy repetitions, we just present the resulting equation, which we will further manipulate in the following:

$$\begin{aligned}\int_{G^{\mathrm{H}}} \frac{\epsilon}{\kappa^2} \left|\mathbf{curl}\,\mathbf{E}\right|^2 - \epsilon \left|\mathbf{E}\right|^2 \, dx \\ = \sum_{n \in \mathbb{Z}^2} \left(M_n^{\alpha,l} \mathbf{E}_n^l \cdot \overline{\mathbf{E}}_n^l e^{-2\,\mathrm{Im}\left(\beta_l^{(n)}\right)} + M_n^{\alpha,N} \mathbf{E}_n^N \cdot \overline{\mathbf{E}}_n^N e^{-2\,\mathrm{Im}\left(\beta_N^{(n)}\right)} \right),\end{aligned} \tag{5.22}$$

where

$$M_n^{\alpha,l} \coloneqq \frac{\mathrm{i}4\pi^2\epsilon_l}{\kappa_l^2} \begin{pmatrix} \beta_l^{(n)} & 0 & 0 \\ 0 & \beta_l^{(n)} & 0 \\ 0 & 0 & \overline{\beta_l^{(n)}} \end{pmatrix}, \quad M_n^{\alpha,N} \coloneqq \frac{\mathrm{i}4\pi^2\epsilon_N}{\kappa_N^2} \begin{pmatrix} \beta_N^{(n)} & 0 & 0 \\ 0 & \beta_N^{(n)} & 0 \\ 0 & 0 & \overline{\beta_N^{(n)}} \end{pmatrix}.$$

We take the imaginary part of (5.22) and let $\mathrm{H} \to \infty$. Exploiting that, by Lemma 5.12, we have $\mathrm{Im}(\beta_l^{(n)}) \geq 0$ and $\mathrm{Im}(\beta_N^{(n)}) \geq 0$ for all $n \in \mathbb{Z}^2$ with $\mathrm{Im}(\beta_l^{(n)}) = 0$ and $\mathrm{Im}(\beta_N^{(n)}) = 0$ only for a finite number of $n \in \mathbb{Z}^2$ if $\kappa_l^2 \in \mathbb{R}$, we then obtain that

$$\begin{aligned}\lim_{\mathrm{H}\to\infty} \int_{G_{l,+}^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_l}{\kappa_l^2}\right) \left|\mathbf{curl}\,\mathbf{E}_l\right|^2 - \mathrm{Im}\left(\epsilon_l\right) \left|\mathbf{E}_l\right|^2 \, dx \\ + \sum_{k=l+1}^{N-1} \int_{G_k} \mathrm{Im}\left(\frac{\epsilon_k}{\kappa_k^2}\right) \left|\mathbf{curl}\,\mathbf{E}_k\right|^2 - \mathrm{Im}\left(\epsilon_k\right) \left|\mathbf{E}_k\right|^2 \, dx \\ + \lim_{\mathrm{H}\to\infty} \int_{G_N^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_N}{\kappa_N^2}\right) \left|\mathbf{curl}\,\mathbf{E}_N\right|^2 - \mathrm{Im}\left(\epsilon_N\right) \left|\mathbf{E}_N\right|^2 \, dx \\ = 4\pi^2 \left[\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_l}{\kappa_l^2}\right) \sum_{B_l} \beta_l^{(n)} \left|\mathbf{E}_n^l\right|^2 + \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_N}{\kappa_N^2}\right) \sum_{B_N} \beta_N^{(n)} \left|\mathbf{E}_n^N\right|^2 \right]\end{aligned} \tag{5.23}$$

with $B_l \coloneqq \{n \in \mathbb{Z}^2 \;:\; \beta_l^{(n)} > 0\}$ and $B_N \coloneqq \{n \in \mathbb{Z}^2 \;:\; \beta_N^{(n)} > 0\}$ as $\kappa_l, \kappa_N \notin \mathbb{R}_-$. This means that in particular the limit expression on the left-hand side exists. The assumptions of this theorem concerning the electromagnetic material parameters make an application of Lemma 5.13 possible. Indeed, with $\mathrm{Im}(\epsilon_k/\kappa_k^2) \leq 0$, according to (5.18), and $-\mathrm{Im}(\epsilon_k) \leq 0$ for all $k = l, \ldots, N$, we arrive at

$$\begin{aligned}\lim_{\mathrm{H}\to\infty} \int_{G_{l,+}^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_l}{\kappa_l^2}\right) \left|\mathbf{curl}\,\mathbf{E}_l\right|^2 - \mathrm{Im}\left(\epsilon_l\right) \left|\mathbf{E}_l\right|^2 \, dx \\ + \sum_{k=l+1}^{N-1} \int_{G_k} \mathrm{Im}\left(\frac{\epsilon_k}{\kappa_k^2}\right) \left|\mathbf{curl}\,\mathbf{E}_k\right|^2 - \mathrm{Im}\left(\epsilon_k\right) \left|\mathbf{E}_k\right|^2 \, dx \\ + \lim_{\mathrm{H}\to\infty} \int_{G_N^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_N}{\kappa_N^2}\right) \left|\mathbf{curl}\,\mathbf{E}_N\right|^2 - \mathrm{Im}\left(\epsilon_N\right) \left|\mathbf{E}_N\right|^2 \, dx \leq 0.\end{aligned} \tag{5.24}$$

Next, we take a look at the right-hand side of equation (5.23). Under the assumption that (5.16) and (5.17) hold, we observe that the right-hand side of equation (5.23) is non-negative. Altogether, we therefore have

$$\begin{aligned} 0 \overset{(5.24)}{\geq} & \lim_{\mathrm{H}\to\infty} \int_{G^{\mathrm{H}}_{l,+}} \mathrm{Im}\left(\frac{\epsilon_l}{\kappa_l^2}\right) |\mathbf{curl}\,\mathbf{E}_l|^2 - \mathrm{Im}\left(\epsilon_l\right) |\mathbf{E}_l|^2 \; dx \\ & + \sum_{k=l+1}^{N-1} \int_{G_k} \mathrm{Im}\left(\frac{\epsilon_k}{\kappa_k^2}\right) |\mathbf{curl}\,\mathbf{E}_k|^2 - \mathrm{Im}\left(\epsilon_k\right) |\mathbf{E}_k|^2 \; dx \\ & + \lim_{\mathrm{H}\to\infty} \int_{G^{\mathrm{H}}_{N}} \mathrm{Im}\left(\frac{\epsilon_N}{\kappa_N^2}\right) |\mathbf{curl}\,\mathbf{E}_N|^2 - \mathrm{Im}\left(\epsilon_N\right) |\mathbf{E}_N|^2 \; dx \\ = & \; 4\pi^2 \left[\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_l}{\kappa_l^2}\right) \sum_{B_l} \beta_l^{(n)} \left|\mathbf{E}_n^l\right|^2 + \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_N}{\kappa_N^2}\right) \sum_{B_N} \beta_N^{(n)} \left|\mathbf{E}_n^N\right|^2 \right] \geq 0. \end{aligned} \tag{5.25}$$

In fact, this in particular gives

$$\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_l}{\kappa_l^2}\right) \sum_{B_l} \beta_l^{(n)} \left|\mathbf{E}_n^l\right|^2 + \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_N}{\kappa_N^2}\right) \sum_{B_N} \beta_N^{(n)} \left|\mathbf{E}_n^N\right|^2 = 0,$$

from which we easily deduce that the Rayleigh coefficients $\mathbf{E}_n^l$ from (5.13) and $\mathbf{E}_n^N$ from (5.14) vanish if (5.16) and (5.17), respectively, are true. □

In the following theorem, we establish conditions on the grating parameters such that all $\mathcal{C}_k$ are invertible, which in consequence ensures the uniqueness of solutions to the recursive integral equation algorithm (3.5)-(3.10).

Theorem 5.14. *Let the grating parameters ϵ_k, μ_k be chosen according to assumption (2.2) such that, for all $k = l, \dots, N-1$,*

$$\epsilon_k \neq -\epsilon_{k+1} \quad \textit{and} \quad \mu_k \neq -\mu_{k+1} \tag{5.26}$$

if Γ_k is smooth, or

$$\begin{aligned} \mathrm{Re}(\epsilon_k)\,\mathrm{Re}(\epsilon_{k+1}) + \mathrm{Im}(\epsilon_k)\,\mathrm{Im}(\epsilon_{k+1}) \geq 0, \\ \mathrm{Re}(\mu_k)\,\mathrm{Re}(\mu_{k+1}) + \mathrm{Im}(\mu_k)\,\mathrm{Im}(\mu_{k+1}) \geq 0 \end{aligned} \tag{5.27}$$

if Γ_k is polyhedral Lipschitz regular, and such that the elements of the parameter pairs ϵ_l, μ_l as well as ϵ_N, μ_N are each not both in $\mathbb{R}_-$. Moreover, assume that $\mathcal{N}(C_k^{\alpha,(k+1)}) = \{0\}$ for $k = l, \dots, N-1$, and $\mathcal{N}(\mathcal{C}_{N-1}) = \dots = \mathcal{N}(\mathcal{C}_{l+1}) = \{0\}$. If, for some $j = l+1, \dots, N$, the imaginary part of ϵ_j or μ_j is positive, i.e.,

$$\mathrm{Im}\left(\epsilon_j + \mu_j\right) > 0 \quad \textit{for some } j = l+1, \dots, N,$$

then $\mathcal{N}\left(\mathcal{C}_l\right) = \{0\}$.

Theorem 5.14 in particular exploits a type of Holmgren's uniqueness theorem (HUT) for time-harmonic Maxwell's equations. The original version of Holmgren's theorem is found in [13].

Theorem 5.15 (HUT for time-harmonic Maxwell's equations)**.** *Let G be a connected and bounded Lipschitz polyhedral domain and $\mathbf{E} \in \mathbf{H}\left(\mathbf{curl}, G\right)$ a solution of the time-harmonic Maxwell equations*

$$\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa^2 \mathbf{E} = 0 \quad \textit{in } G.$$

If there exists an open set U such that $U \cap \partial G \neq \emptyset$ and

$$\gamma_{\mathrm{D}} \mathbf{E} = \gamma_{\mathrm{N}_\kappa} \mathbf{E} = 0 \quad \textit{on } U \cap \partial G \tag{5.28}$$

holds, then $\mathbf{E}$ already vanishes in all of G.

Theorem 5.15 can be verified by adapting the proof of Theorem 3.5 in [12], which presents the corresponding result for acoustics, to electromagnetics (see also [7, Theorem 6.5]).

Proof of Theorem 5.14. We prove this theorem by contradiction. We assume that $\mathcal{N}(\mathcal{C}_l) \neq \{0\}$. Then, by Lemma 5.11, there exist nontrivial solutions $\mathbf{j}_k \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$, $k = l, \dots, N-1$, of the recursive integral equation algorithm (3.5)-(3.10). Now, consider the solution $\mathbf{E}$ to the homogeneous electromagnetic scattering problem in the reduced grating structure with the scattering surfaces $\Gamma_l, \dots, \Gamma_{N-1}$ and the top layer G_l^+, which was defined in Definition 5.10. Let j be the characteristic index G_j for which $\mathrm{Im}(\epsilon_j + \mu_j) > 0$ holds in G_j. The inequality (5.25) from the proof of Theorem 5.11 remains valid here since the values of the electromagnetic material parameters are chosen such that $\mathrm{Im}(\mathrm{i}\epsilon_l/\kappa_l^2) \geq 0$ and $\mathrm{Im}(\mathrm{i}\epsilon_N/\kappa_N^2) \geq 0$ if $\beta_l^{(n)}, \beta_N^{(n)} \in \mathbb{R} \setminus \{0\}$. In particular, we deduce from (5.25) that at least either

$$\mathrm{Im}\left(\frac{\epsilon_j}{\kappa_j^2}\right) \int_{G^{\mathrm{H}} \cap G_j} |\mathbf{curl}\, \mathbf{E}_j|^2 \, dx = 0 \quad \text{or} \quad \mathrm{Im}\,(\epsilon_j) \int_{G^{\mathrm{H}} \cap G_j} |\mathbf{E}_j|^2 \, dx = 0. \tag{5.29}$$

This goes back to the following properties of the electric permittivity ϵ_j and the magnetic permeability μ_j: $\mathrm{Im}(\epsilon_j) \geq 0$ and $\mathrm{Im}(\epsilon_j/\kappa_j^2) = \mathrm{Im}(1/(\omega^2\mu_j)) \leq 0$, which can not simultaneously vanish under the assumptions of this theorem. If $\mathrm{Im}(\epsilon_j) > 0$, the equation $(5.29)_2$ gives $\mathbf{E}_j = 0$ a.e. in G_j. On the other hand, if $\mathrm{Im}(\epsilon_j/\kappa_j^2) < 0$, we obtain $\mathbf{curl}\,\mathbf{E}_j = 0$ a.e. in G_j from $(5.29)_1$. Since $\mathbf{E}_j$ satisfies the time-harmonic Maxwell equations $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa_j^2\mathbf{E} = 0$ in G_j, this again gives $\mathbf{E}_j = 0$ a.e. in the domain G_j. Thus, the statement

$$\mathbf{E}_j = 0 \quad \text{a.e. in } G_j \text{ for some } j = l+1, \dots, N$$

always holds. We then in particular have

$$\gamma_{\mathrm{D},j-1}^- \mathbf{E}_j = \gamma_{\mathrm{N}_{\kappa_j},j-1}^- \mathbf{E}_j = 0 \quad \text{and} \quad \gamma_{\mathrm{D},j}^+ \mathbf{E}_j = \gamma_{\mathrm{N}_{\kappa_j},j}^+ \mathbf{E}_j = 0 \quad (\text{if } j \neq N \text{ for the latter}). \tag{5.30}$$

The electric fields $\mathbf{E}_{j-1}$ and $\mathbf{E}_{j+1}$ in the neighboring domains G_{j-1} and G_{j+1} are solutions of the homogeneous electromagnetic scattering problem in these domains. They solve $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa_{j-1}^2\mathbf{E} = 0$ in G_{j-1} and $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa_{j+1}^2\mathbf{E} = 0$ in G_{j+1}, respectively, and satisfy

$$\begin{aligned} \gamma_{\mathrm{D},j-1}^+ \mathbf{E}_{j-1} &= \gamma_{\mathrm{D},j-1}^- \mathbf{E}_j = 0 \qquad \text{and} \qquad \gamma_{\mathrm{N}_{\kappa_{j-1}},j-1}^+ \mathbf{E}_{j-1} = \gamma_{\mathrm{N}_{\kappa_j},j-1}^- \mathbf{E}_j = 0, \\ \gamma_{\mathrm{D},j+1}^+ \mathbf{E}_j &= \gamma_{\mathrm{D},j+1}^- \mathbf{E}_{j+1} = 0 \qquad \text{and} \qquad \gamma_{\mathrm{N}_{\kappa_j},j+1}^+ \mathbf{E}_j = \gamma_{\mathrm{N}_{\kappa_{j+1}},j+1}^- \mathbf{E}_{j+1} = 0 \end{aligned}$$

with the help of the transmission conditions (5.21) across Γ_{j-1} and Γ_{j+1}. Thus, by Holmgren's uniqueness theorem in the version of Theorem 5.15, we conclude that $\mathbf{E}_{j-1}$ (for $j \neq l+1$) and $\mathbf{E}_{j+1}$ (for $j \neq N-1$) already vanish in G_{j-1} and in G_{j+1}. In the special cases that either $j = l+1$ or $j = N-1$, we observe that

$$\begin{aligned} \mathbf{E}_l &= \frac{1}{2}\left(\Psi_{\mathrm{E}_{\kappa_l},l}^\alpha \gamma_{\mathrm{N}_{\kappa_l},l}^+ \mathbf{E}_l + \Psi_{\mathrm{M}_{\kappa_l},l}^\alpha \gamma_{\mathrm{D},l}^+ \mathbf{E}_l\right) \overset{(5.30)}{=} 0 \qquad &&\text{in } G_l^+ \quad \text{or} \\ \mathbf{E}_N &= -\frac{1}{2}\left(\Psi_{\mathrm{E}_{\kappa_N},N-1}^\alpha \gamma_{\mathrm{N}_{\kappa_N},N-1}^- \mathbf{E}_N + \Psi_{\mathrm{M}_{\kappa_N},N-1}^\alpha \gamma_{\mathrm{D},N-1}^- \mathbf{E}_N\right) \overset{(5.30)}{=} 0 \qquad &&\text{in } G_N \end{aligned}$$

by the Stratton-Chu integral representation from Lemma 4.4. Reapplying Theorem 5.15 - and if necessary Lemma 4.4 in G_l^+ and G_N - in an iterative manner finally yields that the homogeneous electromagnetic scattering problem only possesses the trivial solution $\mathbf{E} = 0$. In G_{l+1}, the electric field $\mathbf{E}_{l+1}$ can be uniquely represented as

$$\mathbf{E}_{l+1} = \frac{1}{2}\left(\Psi_{\mathrm{E}_{\kappa_{l+1}},l+1}^\alpha \gamma_{\mathrm{N}_{\kappa_{l+1}},l+1}^+ \mathbf{E}_{l+1} + \Psi_{\mathrm{M}_{\kappa_{l+1}},l+1}^\alpha \gamma_{\mathrm{D},l+1}^+ \mathbf{E}_{l+1}\right) + \Psi_{\mathrm{E}_{\kappa_{l+1}},l}^\alpha \mathbf{j}_l$$

by Lemma 4.5. Due to $\mathbf{E}_{l+1} = 0$, we arrive at

$$\Psi_{\mathrm{E}_{\kappa_{l+1}},l}^\alpha \mathbf{j}_l = 0 \quad \xRightarrow{\gamma_{\mathrm{D},l}^-,(4.3)} \quad C_l^{\alpha,(l+1)} \mathbf{j}_l = 0.$$

Hence, $\mathbf{j}_l = 0$ since $C_l^{\alpha,(l+1)}$ is invertible as a consequence of $\mathcal{N}(C_l^{\alpha,(l+1)}) = \{0\}$ and Lemma 4.3. The assumptions (5.26) and (5.27) infer, by Theorem 5.4, that $\mathcal{C}_k$ are Fredholm operators of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$ for $k = l+1, \ldots, N-1$. Since $\mathcal{N}(\mathcal{C}_{N-1}) = \cdots = \mathcal{N}(\mathcal{C}_{l+1}) = \{0\}$, the boundary integral operators $\mathcal{C}_k$, $k = l+1, \ldots, N-1$, are invertible in the Hilbert spaces $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma_k)$. Thus, the recursive integral equation algorithm (3.5)-(3.10) is applicable. With the initial density $\mathbf{j}_l = 0$, the recursive relations (3.5) for the indices $k = l+1, \ldots, N-1$ finally imply that

$$\mathbf{j}_k = 0 \quad \text{for all } k = l, \ldots, N-1.$$

This contradicts the existence of nontrivial solutions to (3.5)-(3.10). Hence, $\mathcal{N}(\mathcal{C}_l) = \{0\}$. □

If the assumptions of Theorem 5.14 are satisfied for $l = 1$, then the recursive integral equation algorithm (3.5)-(3.10) is applicable and provides a (possibly nonunique) solution of the 2π-biperiodic multilayered electromagnetic scattering problem (2.7)-(2.13) by Theorem 5.7. Assuming that Theorem 5.14 moreover holds for $l = 0$, there even exists a unique solution of the 2π-biperiodic multilayered electromagnetic scattering problem (2.7)-(2.13) according to Theorem 5.7 and Lemma 5.11.

6 Conclusion

In this article, we considered biperiodic multilayered structures consisting of at least two vertically stacked non-self-intersecting biperiodic polyhedral Lipschitz regular grating interfaces. Illuminating such structures from above by an incident plane wave induces the biperiodic multilayered electromagnetic scattering problem. Our objective was to treat this problem with the help of a recursive integral equation algorithm suitable for the efficient numerical implementation of the scattering problem. We achieved this by extending an already existing integral equation algorithm based on the transmission conditions across the grating interfaces of the considered multilayered structure. It was developed by Maystre in [16] for the solution of the analogous oneperiodic scattering problem in the case of TE and TM diffraction and later extended by Schmidt in [21] to conical diffraction. The extension to the biperiodic setting is challenging because the electromagnetic scattering problem can then no longer be reduced to studying a set of scalar-valued Helmholtz equations equipped with suitable transmission and radiation conditions. Instead, the full three-dimensional time-harmonic Maxwell equations have to be considered. Provided that our biperiodic recursive integral equation algorithm is applicable in a certain sense, we verified its equivalence to the biperiodic multilayered electromagnetic scattering problem. Moreover, we showed new existence and uniqueness results. Just as in the single profile setting studied in [3], the existence results rely on the Fredholm properties of the the involved boundary integral equations, which can be deduced from the Fredholm properties of the integral equation of the corresponding one-profile problem. That means that it holds under quite general assumptions on the electromagnetic material parameters if the grating interface corresponding to the particular integral equation is smooth, and under more restrictive assumptions if it is of polyhedral Lipschitz regularity. The uniqueness results were proven with the help of variational methods.

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