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Analytical investigation of an integral equation method for electromagnetic scattering by biperiodic structures

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Abstract

This paper is concerned with the study of a new integral equation formulation for electromagnetic scattering by a 2π-biperiodic polyhedral Lipschitz profile. Using a combined potential ansatz, we derive a singular integral equation with Fredholm operator of index zero from time-harmonic Maxwell's equations and prove its equivalence to the electromagnetic scattering problem. Moreover, under certain assumptions on the electric permittivity and the magnetic permeability, we obtain existence and uniqueness results in the special case that the grating is smooth and, under more restrictive assumptions, in the case that the grating is of polyhedral Lipschitz regularity.

1 Introduction

We investigate the scattering of time-harmonic electromagnetic plane waves in $\mathbb{R}^3$ by a 2π-biperiodic polyhedral Lipschitz surface that separates two different materials of constant electric permittivity and magnetic permeability. The behavior of the incident and scattered waves is modeled by the system of time-harmonic Maxwell equations supplemented by transmission conditions across the interface and a suitable outgoing wave condition that ensure the tangential continuity of the electromagnetic fields as well as their boundedness at infinity. Such problems are contained in the class of diffraction problems, which have various applications in micro-optics such as the construction of holographic films, optical storage devices and antireflective coatings.

The aim of this paper is to establish new existence and uniqueness results for an equivalent integral formulation of the 2π-biperiodic electromagnetic scattering problem generalizing the results in [24], where the analogous problem for oneperiodic structures is considered. In the biperiodic case, it is however not possible to reduce the electromagnetic scattering problem to solving scalar-valued Helmholtz equations like in [24]. One has to deal with the full system of time-harmonic Maxwell equations.

Up to now, both in the one- and in the biperiodic case several integral formulations have been proposed and implemented (see, e.g., [13], [23], [24]). We derive a new formulation by adapting the approach of [12] for the problem of dielectric scattering by a bounded Lipschitz obstacle. Inspired by [19], Costabel and Le Louër choose to represent the solution in either the exterior or the interior domain by a Stratton-Chu integral ansatz and use a linear combination of an electric potential and the product of a magnetic potential with a regularizer for the solution in the other domain. The mentioned regularizer, first considered by Steinbach and Windisch in [26], takes an important role since it controls the occurrence of irregular frequencies. The existence of irregular frequencies in the biperiodic setting is still part of ongoing research (see Remark 3.18). However, we suspect that for most of the practically relevant wave numbers no irregular frequencies will occur. Therefore, we here will also work with a Stratton-Chu integral representation in one domain but only make use of a simple electric potential ansatz in the other domain. This approach yields a single singular integral equation that is shown to be equivalent to the 2π-biperiodic electromagnetic scattering problem under the assumption that the boundary integral operator C_κ^α, which is related to the electric potential, is invertible. With regard to the numerical implementation of this integral equation by the boundary element method, we need to execute less summations and multiplications with this simplified, unregularized ansatz. Since we want to extend our method to the problem of electromagnetic scattering by 2π-biperiodic multilayered structures, where a possibly large number of integral equations has to be solved, our concern with computational efficiency becomes even more meaningful. Compared to integral equation methods leading to systems of singular integral equations as presented in [13], e.g., our method has a reduced dimension posing an additional advantage concerning computations.

Despite the promising results in the treatment of diffraction problems with integral equation methods, papers providing a rigorous mathematical analysis are rare. Existing work rather focuses on the problem of biperiodic electromagnetic scattering by perfectly reflecting gratings ([2], [20], [23]) or applies variational approaches ([14], [24]), which are implemented by three-dimensional finite element methods.

The outline of this paper is as follows: Section 2 states the problem of electromagnetic scattering by a 2π-biperiodic polyhedral Lipschitz interface. We then introduce, in Section 3, all relevant tools from functional analysis that we need in order to apply a combined potential method to this problem. This approach is executed in Section 4: We derive a singular boundary integral equation and demonstrate its equivalence to the 2π-biperiodic electromagnetic scattering problem in the sense that any solution of one problem provides a solution of the other. In the main Section 5, we are concerned with the solvability of the boundary integral equation in the special case of a smooth 2π-biperiodic grating profile and in the more general case of a polyhedral Lipschitz regular 2π-biperiodic grating profile. More precisely, we deduce conditions that ensure uniqueness and existence of solutions. This involves the Fredholm properties of the operator on the left-hand side of the integral equation that are established via Gårding-type inequalities. We end with a brief conclusion and propositions on future extensions 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. The operator I refers to the identity operator.

2 The electromagnetic scattering problem

Let $\Sigma \subset \mathbb{R}^2$ be a non-self-inter- secting surface given by a piecewise C^2 parametrization

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

for $t = (t_1, t_2)^{\mathrm{T}}$, $m \in \mathbb{Z}^2$. In words, Σ corresponds to an interface that is 2π-periodic in both x_1- and in x_2-direction and may exhibit edges and corners. We will refer to this kind of regularity as polyhedral Lipschitz regularity. As it is usual in the treatment of periodic problems, we restrict the calculations in this paper to one period Γ of the surface Σ, i.e., to

$$\Gamma := \{\sigma(t) \; : \; t \in Q\}, \quad \text{where } Q := [-\pi, \pi) \times [-\pi, \pi)$$

denotes the unit-cell of the periodic lattice. The restricted profile Γ separates two regions $G_\pm \subset \mathbb{R}^3$ with materials of constant electric permittivity $\epsilon_\pm$ and constant magnetic permeability $\mu_\pm$. Its unit normal vector $\mathbf{n}$ is set to point upwards into G_+. From here on, we assume that

$$\mathrm{Im}\,(\epsilon_\pm) \geq 0 \quad \text{and} \quad \mathrm{Im}\,(\mu_\pm) \geq 0 \quad \text{in } G_\pm. \tag{2.2}$$

Let $\omega > 0$ be a fixed frequency and denote by $\kappa_\pm = \omega\sqrt{\epsilon_\pm}\sqrt{\mu_\pm}$ the wave number in $G_\pm$. 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 $0 \leq \varphi < 2\pi$. For technical purposes, we need the auxiliary polyhedral Lipschitz domain G^{H} with a fixed $\mathrm{H} \in \mathbb{R}_+$ chosen such that

$$\Gamma \subset G^{\mathrm{H}} := \left\{ x = (\tilde{x}, x_3)^{\mathrm{T}} \in Q \times \mathbb{R} \;:\; |x_3| \leq \mathrm{H} \right\}. \tag{2.3}$$

Denote by $G^{\mathrm{H}}_{\pm}$ the restrictions of G^{H} to $G_{\pm}$, i.e., $G^{\mathrm{H}}_{\pm} := G^{\mathrm{H}} \cap G_{\pm}$.

We now consider the illumination of the surface Γ from G_+ by a time-harmonic electric plane wave $\mathbf{E}^{\mathrm{i}}$ at oblique incidence. We specify $\mathbf{E}^{\mathrm{i}}$ as

$$\mathbf{E}^{\mathrm{i}} := \mathbf{p} e^{\mathrm{i}(\alpha_1 x_1 + \alpha_2 x_2 - \alpha_3 x_3)} \quad \text{with } \alpha_3 > 0 \tag{2.4}$$

and observe that it satisfies the relation

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

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 has the following properties:

$$|\alpha|^2 = \left|\kappa_+^2\right|^2 \quad \text{and} \quad \alpha \cdot \mathbf{p} = 0. \tag{2.5}$$

The total electric fields are given by $\mathbf{E}^{\mathrm{i}} + \mathbf{E}^{\mathrm{refl}}$ in G_+ and by $\mathbf{E}^{\mathrm{tran}}$ in G_-. Then the 2π-biperiodic electromagnetic scattering problem written in terms of the electric field can be formulated as follows: We look for vector fields $\mathbf{E}^{\mathrm{refl}}$ and $\mathbf{E}^{\mathrm{tran}}$ of locally finite energy, i.e.,

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

satisfying the time-harmonic Maxwell equations

$$\mathbf{curl}\,\mathbf{curl}\,\mathbf{E}^{\mathrm{refl}} - \kappa_+^2 \mathbf{E}^{\mathrm{refl}} = 0 \quad \text{in } G_+, \tag{2.6}$$

$$\mathbf{curl}\,\mathbf{curl}\,\mathbf{E}^{\mathrm{tran}} - \kappa_-^2 \mathbf{E}^{\mathrm{tran}} = 0 \quad \text{in } G_-, \tag{2.7}$$

the transmission conditions

$$\mathbf{n} \times \mathbf{E}^{\mathrm{tran}} = \mathbf{n} \times \left(\mathbf{E}^{\mathrm{refl}} + \mathbf{E}^{\mathrm{i}}\right) \qquad \text{on } \Gamma, \tag{2.8}$$

$$\mu_-^{-1}\left(\mathbf{n} \times \mathbf{curl}\,\mathbf{E}^{\mathrm{tran}}\right) = \mu_+^{-1}\left(\mathbf{n} \times \mathbf{curl}\left(\mathbf{E}^{\mathrm{refl}} + \mathbf{E}^{\mathrm{i}}\right)\right) \qquad \text{on } \Gamma \tag{2.9}$$

and the outgoing wave condition in the sense of Rayleigh series:

$$\mathbf{E}^{\mathrm{refl}}(x) = \sum_{n \in \mathbb{Z}^2} \mathbf{E}_n^{\mathrm{refl}} e^{\mathrm{i}\left(\alpha^{(n)} \cdot \tilde{x} + \beta_+^{(n)} x_3\right)}, \qquad x \in G_+ \text{ with } x_3 \geq \mathrm{H}, \tag{2.10}$$

$$\mathbf{E}^{\mathrm{tran}}(x) = \sum_{n \in \mathbb{Z}^2} \mathbf{E}_n^{\mathrm{tran}} e^{\mathrm{i}\left(\alpha^{(n)} \cdot \tilde{x} - \beta_-^{(n)} x_3\right)}, \qquad x \in G_- \text{ with } x_3 \leq -\mathrm{H}. \tag{2.11}$$

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

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

By the α-quasiperiodicity of the electric incident waves, the sought-after fields are α-quasiperiodic themselves.

3 Function spaces, traces and electromagnetic potentials

Let Ω be a polyhedral Lipschitz domain in $\mathbb{R}^3$. If Ω is bounded, we denote by $H^s(\Omega)$ the usual scalar-valued Sobolev space of order $s \in \mathbb{R}$ with the common convention that $L^2(\Omega) := H^0(\Omega)$. Otherwise, $H^s_{\mathrm{loc}}(\Omega)$ refers to the space of functions contained in $H^s(K)$ for all $K \Subset \Omega$. Their vector-valued counterparts are specified by $\mathbf{H}^s(\Omega)$ and $\mathbf{H}^s_{\mathrm{loc}}(\Omega)$. Let $\mathbf{D}$ be a differential operator. Then

$$\mathbf{H}(\mathbf{D},\Omega) := \left\{\mathbf{u} \in \mathbf{L}^2(\Omega) \ : \ \mathbf{D}\mathbf{u} \in \mathbf{L}^2(\Omega)\right\},$$
$$\mathbf{H}_{\mathrm{loc}}(\mathbf{D},\Omega) := \left\{\mathbf{u} \in \mathbf{L}^2_{\mathrm{loc}}(\Omega) \ : \ \mathbf{D}\mathbf{u} \in \mathbf{L}^2_{\mathrm{loc}}(\Omega)\right\}.$$

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

$$\mathbf{H}^s_\alpha(\Omega) := \left\{\mathbf{u} \in \mathbf{H}^s(\Omega) \ : \ \exists\, \alpha\text{-qp } \mathbf{v} \in \mathbf{H}^s_{\mathrm{loc}}(\mathbb{R}^3) \text{ such that } \mathbf{u} = \mathbf{v}|_\Omega\right\},$$
$$\mathbf{H}^s_\alpha(\mathbf{D},\Omega) := \left\{\mathbf{u} \in \mathbf{H}^s(\mathbf{D},\Omega) \ : \ \exists\, \alpha\text{-qp } \mathbf{v} \in \mathbf{H}^s_{\mathrm{loc}}(\mathbf{D},\mathbb{R}^3) \text{ such that } \mathbf{u} = \mathbf{v}|_\Omega\right\},$$
$$\mathbf{H}^s_{\alpha,\mathrm{loc}}(G_\pm) := \left\{\mathbf{u} \in \mathbf{H}^s_{\mathrm{loc}}(G_\pm) \ : \ \exists\, \alpha\text{-qp } \mathbf{v} \in \mathbf{H}^s_{\mathrm{loc}}(\mathbb{R}^3) \text{ such that } \mathbf{u} = \mathbf{v}|_{G_\pm}\right\},$$
$$\mathbf{H}^s_{\alpha,\mathrm{loc}}(\mathbf{D},G_\pm) := \left\{\mathbf{u} \in \mathbf{H}^s_{\mathrm{loc}}(\mathbf{D},G_\pm) \ : \ \exists\, \alpha\text{-qp } \mathbf{v} \in \mathbf{H}^s_{\mathrm{loc}}(\mathbf{D},\mathbb{R}^3) \text{ s.t. } \mathbf{u} = \mathbf{v}|_{G_\pm}\right\},$$

where $\Omega \subset \mathbb{R}^3$ is a bounded domain. Moreover, we define the space

$$\mathbf{H}^s_\alpha := \left\{\mathbf{u} = \sum_{n\in\mathbb{Z}^2} \mathbf{u}_n e^{\mathrm{i}\alpha^{(n)}\cdot\tilde{x}} \ : \ \|\mathbf{u}\|^2_{\alpha,s} = \sum_{n\in\mathbb{Z}^2} \left(1 + \left|\alpha^{(n)}\right|^2\right)^s |\mathbf{u}_n|^2 < \infty\right\}$$

for $s \geq 0$. The dual space of $\mathbf{H}^s_\alpha$, denoted by $\mathbf{H}^{-s}_\alpha$ for $s > 0$, arises from completing $\mathbf{L}^2_\alpha(Q)$ with respect to the norm

$$\|\mathbf{u}\|_{\alpha,-s} := \sup_{0\neq\mathbf{v}\in\mathbf{H}^s_\alpha} \frac{\left|(\mathbf{u},\mathbf{v})_{\mathbf{L}^2_\alpha(Q)}\right|}{\|\mathbf{v}\|_{\alpha,s}}.$$

Next, we specify

$$\mathbf{H}^s_\alpha(\Gamma) := \{\mathbf{u} \ : \ \mathbf{u}\circ\sigma \in \mathbf{H}^s_\alpha\} \quad \text{for } s \in [0,1].$$

Completing $\mathbf{L}^2_\alpha(\Gamma)$ with respect to the norm $\|\mathbf{u}\|_{\mathbf{H}^{-s}_\alpha(\Gamma)} := \|(\mathbf{u}\circ\sigma)(1+|\nabla\sigma|^2)^{1/2}\|_{\alpha,-s}$ yields the dual space $\mathbf{H}^{-s}_\alpha(\Gamma)$, $s \in (0,1]$, of $\mathbf{H}^s_\alpha(\Gamma)$. In the style of [6] and [7], we in particular set

$$\mathbf{V}_\alpha := \mathbf{H}^{\frac{1}{2}}_\alpha(\Gamma) \quad \text{and} \quad \mathbf{V}'_\alpha := \mathbf{H}^{-\frac{1}{2}}_\alpha(\Gamma).$$

Finally, we introduce the space $\mathbf{L}^2_{\alpha,t}(\Gamma)$, which is defined by

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

This function space is identified with the space of two-dimensional tangential vector fields - sections of the tangent bundle $T\Gamma$ of Γ for almost every $x \in \Gamma$.

Definition 3.1. *Let $\mathbf{u}$ be sufficiently smooth in $G_\pm$ and $\mathbf{u}_\pm := \mathbf{u}|_{G_\pm}$. Then we define the Dirichlet, the Neumann and the Dirichlet tangential components traces of $\mathbf{u}$ as*

$$\gamma^\pm_{\mathrm{D}}\mathbf{u} := (\mathbf{n}\times\mathbf{u}_\pm)|_\Gamma, \quad \gamma^\pm_{\mathrm{N}_\kappa}\mathbf{u} := \kappa^{-1}(\mathbf{n}\times\mathbf{curl}\,\mathbf{u}_\pm)|_\Gamma, \quad \pi^\pm_{\mathrm{D}}\mathbf{u} := ((\mathbf{n}\times\mathbf{u}_\pm)\times\mathbf{n})|_\Gamma.$$

The properties of the previously introduced traces of vector fields on Γ are deduced from those of the classical traces of vector fields with the help of suitable truncation procedures. For details on the classical traces, we refer to [4]-[8].

Remark 3.2 (Notation)**.** *Let Ω be a bounded polyhedral Lipschitz domain such that $\Gamma \subset \partial\Omega$ and let $\gamma : \mathbf{H}^1_\alpha(\Omega) \to \mathbf{V}_\alpha$ be the standard trace operator on Γ. We denote by γ^{-1} one of its right inverses. From here on, the Dirichlet trace γ_{D} and the Dirichlet tangential components trace π_{D} shall be interpreted as the composite operators $\gamma_{\mathrm{D}}\gamma^{-1}$ and $\pi_{\mathrm{D}}\gamma^{-1}$, respectively, if they act on traces lying, for instance, in the space $\mathbf{V}_\alpha$.*

We define the trace spaces $\mathbf{V}_{\alpha,\gamma}$ and $\mathbf{V}_{\alpha,\pi}$ by

$$\mathbf{V}_{\alpha,\gamma} \coloneqq \gamma_{\mathrm{D}}\left(\mathbf{V}_\alpha\right) \quad \text{and} \quad \mathbf{V}_{\alpha,\pi} \coloneqq \pi_{\mathrm{D}}\left(\mathbf{V}_\alpha\right).$$

Endowed with the norms

$$\|\mathbf{u}\|_{\mathbf{V}_{\alpha,\gamma}} \coloneqq \inf_{\mathbf{v}\in\mathbf{V}_\alpha}\left\{\|\mathbf{v}\|_{\mathbf{V}_\alpha} : \gamma_{\mathrm{D}}\mathbf{v} = \mathbf{u}\right\}, \quad \|\mathbf{u}\|_{\mathbf{V}_{\alpha,\pi}} \coloneqq \inf_{\mathbf{v}\in\mathbf{V}_\alpha}\left\{\|\mathbf{v}\|_{\mathbf{V}_\alpha} : \pi_{\mathrm{D}}\mathbf{v} = \mathbf{u}\right\},$$

the spaces $\mathbf{V}_{\alpha,\gamma}$ and $\mathbf{V}_{\alpha,\pi}$ are Hilbert spaces. These norms guarantee the continuity of the Dirichlet trace γ_{D} and the Dirichlet tangential components trace π_{D}. By construction

$$\gamma_{\mathrm{D}} : \mathbf{V}_\alpha \to \mathbf{V}_{\alpha,\gamma} \quad \text{and} \quad \pi_{\mathrm{D}} : \mathbf{V}_\alpha \to \mathbf{V}_{\alpha,\pi}$$

are isomorphisms (cf. [7, p. 683]). The density of $\mathbf{V}_\alpha$ in $\mathbf{L}^2_\alpha(\Gamma)$ yields that $\mathbf{V}_{\alpha,\gamma}$ and $\mathbf{V}_{\alpha,\pi}$ are dense subspaces of $\mathbf{L}^2_{\alpha,t}(\Gamma)$. Their dual spaces $\mathbf{V}'_{\alpha,\gamma}$ and $\mathbf{V}'_{\alpha,\pi}$ are given with respect to the pivot space $\mathbf{L}^2_{\alpha,t}(\Gamma)$. We emphasize that the spaces $\mathbf{V}_{\alpha,\gamma}$, $\mathbf{V}_{\alpha,\pi}$, $\mathbf{V}'_{\alpha,\gamma}$ and $\mathbf{V}'_{\alpha,\pi}$ are considered as spaces of tangent fields of regularity $1/2$ and $-1/2$, respectively.

In the following, we denote by $i_\gamma : \mathbf{L}^2_{\alpha,t}(\Gamma) \to \mathbf{L}^2_\alpha(\Gamma)$ and $i_\pi : \mathbf{L}^2_{\alpha,t}(\Gamma) \to \mathbf{L}^2_\alpha(\Gamma)$ the adjoint operators of γ_{D} and π_{D}. They can be extended to the following isomorphisms:

$$i_\gamma : \mathbf{V}'_{\alpha,\gamma} \to \left(\mathcal{N}(\gamma_{\mathrm{D}}) \cap \mathbf{V}_\alpha\right)^0 \subset \mathbf{V}'_\alpha \quad \text{and} \quad i_\pi : \mathbf{V}'_{\alpha,\pi} \to \left(\mathcal{N}(\pi_{\mathrm{D}}) \cap \mathbf{V}_\alpha\right)^0 \subset \mathbf{V}'_\alpha,$$

where $\cdot^0$ refers to the polar set (specified, e.g., in [27, pp. 136ff.]).

Moreover, we define an operator $r : \mathbf{L}^2_{\alpha,t}(\Gamma) \to \mathbf{L}^2_{\alpha,t}(\Gamma)$ by

$$r \coloneqq i_\pi^{-1} i_\gamma.$$

This is the rotation operator corresponding to the geometric operation $\cdot \times \mathbf{n}$. The operator r can be extended and restricted to mappings $r : \mathbf{V}_{\alpha,\pi} \to \mathbf{V}_{\alpha,\gamma}$ and $r : \mathbf{V}'_{\alpha,\pi} \to \mathbf{V}'_{\alpha,\gamma}$. For any choice of spaces r is invertible with $r^{-1} = r' = -r$, where r' denotes the adjoint operator of r with $\mathbf{L}^2_{\alpha,t}(\Gamma)$ as pivot spaces. These and further insights on the rotation operator r are deduced from its nonperiodic equivalent characterized in [6, p. 851].

Denote by ∇_Γ the tangential gradient, by $\operatorname{div}_\Gamma$ the surface divergence, by $\mathbf{curl}_\Gamma$ the tangential vector curl and by $\operatorname{curl}_\Gamma$ the surface scalar curl. The definitions of these operators on boundaries of bounded Lipschitz domains can be found in [7]. We deduce the corresponding definitions on Γ via suitable truncation procedures.

Lemma 3.3. *The surface differential operators ∇_Γ, $\mathbf{curl}_\Gamma$, $\operatorname{div}_\Gamma$ and $\operatorname{curl}_\Gamma$ give rise to bounded linear operators*

$$\nabla_\Gamma : H^{\frac{1}{2}}_\alpha(\Gamma) \to \mathbf{V}'_{\alpha,\gamma}, \qquad \mathbf{curl}_\Gamma : H^{\frac{1}{2}}_\alpha(\Gamma) \to \mathbf{V}'_{\alpha,\pi},$$

$$\operatorname{div}_\Gamma : \mathbf{V}_{\alpha,\gamma} \to H_\alpha^{-\frac{1}{2}}(\Gamma), \qquad \operatorname{curl}_\Gamma : \mathbf{V}_{\alpha,\pi} \quad \to H_\alpha^{-\frac{1}{2}}(\Gamma).$$

Moreover, the duality relations

$$\int_\Gamma \operatorname{div}_\Gamma \mathbf{u} \cdot v \, d\sigma = -\int_\Gamma \mathbf{u} \cdot \nabla_\Gamma v \, d\sigma \quad \textit{and} \quad \int_\Gamma \operatorname{curl}_\Gamma \mathbf{w} \cdot v \, d\sigma = \int_\Gamma \mathbf{w} \cdot \mathbf{curl}_\Gamma v \, d\sigma$$

hold for all $\mathbf{u} \in \mathbf{V}_{\alpha,\gamma}$, $v \in H_\alpha^{1/2}(\Gamma)$ *and* $\mathbf{w} \in \mathbf{V}_{\alpha,\pi}$.

The identities

$$\operatorname{div}_\Gamma(r(\mathbf{u})) = \operatorname{curl}_\Gamma \mathbf{u} \quad \text{and} \quad \operatorname{curl}_\Gamma(r(\mathbf{u})) = -\operatorname{div}_\Gamma \mathbf{u} \tag{3.1}$$

are used as technical tools.

The most prominent function space in this paper is the Hilbert space

$$\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma) := \left\{ \mathbf{j} \in \mathbf{V}'_{\alpha,\pi}, \operatorname{div}_\Gamma \mathbf{j} \in H_\alpha^{-\frac{1}{2}}(\Gamma) \right\}$$

endowed with the norm

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

The trace operators $\gamma_{\mathrm{D}}^\pm$ and $\gamma_{\mathrm{N}_\kappa}^\pm$ can be extended to bounded linear operators

$$\begin{aligned} \gamma_{\mathrm{D}}^\pm &: \mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl}, G_\pm) && \to \mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma), \\ \gamma_{\mathrm{N}_\kappa}^\pm &: \mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl}, G_\pm) \cap \mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl}\,\mathbf{curl}, G_\pm) && \to \mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma). \end{aligned} \tag{3.2}$$

We now define the bilinear form $\mathcal{B} : \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \times \mathbf{H}_{-\alpha}^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \to \mathbb{C}$ by

$$\mathcal{B}(\mathbf{j}, \mathbf{m}) := \int_\Gamma \mathbf{j} \cdot r(\mathbf{m}) \, d\sigma = -\int_\Gamma r(\mathbf{j}) \cdot \mathbf{m} \, d\sigma$$

and the sesquilinear form $\mathcal{B}_\mathrm{c} : \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \times \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \to \mathbb{C}$ by

$$\mathcal{B}_\mathrm{c}(\mathbf{j}, \mathbf{m}) := \int_\Gamma \mathbf{j} \cdot r(\overline{\mathbf{m}}) \, d\sigma = -\int_\Gamma r(\mathbf{j}) \cdot \overline{\mathbf{m}} \, d\sigma.$$

Lemma 3.4. *The bilinear form $\mathcal{B}$ and the sesquilinear form $\mathcal{B}_\mathrm{c}$ define nondegenerate duality products on their domains of definition in the sense that*

- *for all* $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma), \mathbf{j} \neq 0$, *there exists* $\mathbf{m} \in \mathbf{H}_{-\alpha}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ *such that* $\mathcal{B}(\mathbf{j}, \mathbf{m}) \neq 0$,
- *for all* $\mathbf{m} \in \mathbf{H}_{-\alpha}^{-1/2}(\operatorname{div}_\Gamma, \Gamma), \mathbf{m} \neq 0$, *there exists* $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ *such that* $\mathcal{B}(\mathbf{j}, \mathbf{m}) \neq 0$,

and

- *for all* $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma), \mathbf{j} \neq 0$, *there exists* $\mathbf{l} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ *such that* $\mathcal{B}_\mathrm{c}(\mathbf{j}, \mathbf{l}) \neq 0$,
- *for all* $\mathbf{l} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma), \mathbf{l} \neq 0$, *there exists* $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ *such that* $\mathcal{B}_\mathrm{c}(\mathbf{j}, \mathbf{l}) \neq 0$.

The antisymmetric relations

$$\mathcal{B}(\mathbf{j},\mathbf{m}) = -\mathcal{B}(\mathbf{m},\mathbf{j}) \quad \text{and} \quad \mathcal{B}_{\mathrm{c}}(\mathbf{j},\mathbf{l}) = -\overline{\mathcal{B}_{\mathrm{c}}(\mathbf{l},\mathbf{j})}$$

are satisfied for all densities $\mathbf{j},\mathbf{l} \in \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$ and $\mathbf{m} \in \mathbf{H}_{-\alpha}^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$.

Definition 3.5. *A sesquilinear form $S : \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma,\Gamma) \times \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma,\Gamma) \to \mathbb{C}$ is called a compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form if it can be represented as*

$$S(\cdot,\cdot) = \mathcal{B}_{\mathrm{c}}\left(K_1\cdot,\cdot\right) \quad \text{and} \quad S(\cdot,\cdot) = \mathcal{B}_{\mathrm{c}}\left(\cdot,K_2\cdot\right)$$

with compact operators $K_1, K_2 : \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma,\Gamma) \to \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$.

For technical reasons, we also consider the duality product analogous to $\mathcal{B}$ on the boundary $\partial\Omega$ of bounded Lipschitz domains Ω with an unit outer normal vector $\mathbf{n}$:

$$\mathcal{B}_{\partial\Omega} : \mathbf{H}^{-1/2}(\mathrm{div}_\Gamma,\partial\Omega) \times \mathbf{H}^{-1/2}(\mathrm{div}_\Gamma,\partial\Omega) \to \mathbb{C}, \mathcal{B}_{\partial\Omega} := \int_{\partial\Omega} \mathbf{j}\cdot r(\mathbf{m})\,d\sigma = -\int_{\partial\Omega} r(\mathbf{j})\cdot\mathbf{m}\,d\sigma,$$

which is defined in [12, § 3] together with the Hilbert space $\mathbf{H}^{-1/2}(\mathrm{div}_\Gamma,\partial\Omega)$ - the nonperiodic equivalent of the space $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$. Here, r is the nonperiodic rotation operator given in [6, p. 851]. For all $\mathbf{u},\mathbf{v} \in \mathbf{H}(\mathbf{curl},\Omega)$, we have the Green identity

$$\int_\Omega \mathbf{curl}\,\mathbf{u}\cdot\mathbf{v} - \mathbf{u}\cdot\mathbf{curl}\,\mathbf{v}\,dx = \mathcal{B}_{\partial\Omega}(\gamma_{\mathrm{D}}\mathbf{u},\gamma_{\mathrm{D}}\mathbf{v}). \tag{3.3}$$

Next, we introduce the α-quasiperiodic potential operators relevant for this work. They are based on G_κ^α, the α-quasiperiodic fundamental solution of the Helmholtz equations, specified by

$$G_\kappa^\alpha(x,y) := \frac{\mathrm{i}}{8\pi^2}\sum_{n\in\mathbb{Z}^2}\frac{e^{\mathrm{i}\left(\alpha^{(n)}\cdot(\tilde{x}-\tilde{y})+\beta^{(n)}|x_3-y_3|\right)}}{\beta^{(n)}} \quad \text{for } \mathrm{Im}\,(\kappa) > 0, \tag{3.4}$$

where

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

The Green's function G_κ^α can be analytically continued to real wave numbers on compact sets in $\mathbb{R}^3 \setminus \cup_{n\in\mathbb{Z}^2}\left(2\pi n_1, 2\pi n_2, 0\right)^{\mathrm{T}}$ if

$$(\kappa,\alpha) \notin \mathcal{R}_0 := \left\{(\kappa,\alpha) \in \mathbb{R}\times\mathbb{R}^3 \;:\; \beta^{(n)} = 0 \quad \text{for some } n \in \mathbb{Z}^2\right\}.$$

This does not include the special case that $\kappa = 0$ and $\alpha_0 := (\tilde{\alpha}, -\alpha_3)$ with $\tilde{\alpha} \in \mathbb{Z}^2$ and $\alpha_3 \in \mathbb{R}_+$, for which we introduce the alternative periodic Green's function of the Helmholtz equations $G_0^{\alpha_0}$:

$$G_0^{\alpha_0}(x,y) := \frac{1}{8\pi^2}\sum_{n\in\mathbb{Z}^2\setminus\{0\}}\frac{e^{\mathrm{i}n\cdot(\tilde{x}-\tilde{y})-|n||x_3-y_3|}}{|n|}. \tag{3.5}$$

In [9], this Green's function is studied in more detail. Amongst others, it is shown that the difference $G_0^{\alpha_0} - G_\kappa^{\alpha_0}$, $\kappa \neq 0$, is sufficiently smooth on $Q\times Q$. Therefore, $G_0^{\alpha_0}$ inherits the properties of $G_\kappa^{\alpha_0}$.

Details on the derivation of G_κ^α, $(\kappa,\alpha)\in\mathcal{R}_0$, and its analytical properties are given in the habilitation thesis [3, §3]. We will in particular resort to the fact that the difference between G_κ^α and the usual Green function in free-field conditions G_κ, defined by $G_\kappa(x,y)=\frac{1}{4\pi}\frac{e^{i\kappa|x-y|}}{|x-y|}$, is smooth, i.e.,

$$G_\kappa^\alpha(x,y)-G_\kappa(x,y)\in C^\infty(Q\times Q). \tag{3.6}$$

This goes back to [3, Theorem 3.8 and its introductory lines on p. 56].

The single layer potential is given by

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

and its trace by

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

Here as well as in the subsequent definitions, G_κ^α refers to the expression in (3.4) if $(\kappa,\alpha)\notin\mathcal{R}_0$ and to the expression in (3.5) if $\kappa=0$ and $\tilde{\alpha}\in\mathbb{Z}^2$.

Lemma 3.6. *Let $s\in(0,1)$. Then the operators S_κ^α and V_κ^α are continuous linear operators:*

$$S_\kappa^\alpha:\mathbf{H}_\alpha^{s-1}(\Gamma)\to\mathbf{H}_{\alpha,\mathrm{loc}}^{s+\frac{1}{2}}(G_+)\cup\mathbf{H}_{\alpha,\mathrm{loc}}^{s+\frac{1}{2}}(G_-), \quad V_\kappa^\alpha:\mathbf{H}_\alpha^{s-1}(\Gamma)\to\mathbf{H}_\alpha^{s}(\Gamma).$$

If Γ is smooth, the mapping properties hold for all $s\in\mathbb{R}$. Moreover, they remain valid for the corresponding scalar-valued function spaces.

For $(\kappa,\alpha)\notin\mathcal{R}_0$, these mapping properties are proven with a localization technique similar to the one used in the proof of Theorem 4.22 in [3, cf. p. 83f.]. In fact, we localize the potentials with an α-quasiperiodic partition of unity and apply the splitting $G_\kappa^\alpha=G_\kappa+(G_\kappa^\alpha-G_\kappa)$. Then the result follows from (3.6) and the known mapping properties of the single layer potential with kernel G_κ (see [11]) on artificially introduced closed interfaces. Since $G_0^{\alpha_0}-G_\kappa^{\alpha_0}$ for $\tilde{\alpha}_0\in\mathbb{Z}^2$ and $\kappa\neq 0$ is sufficiently smooth, the mapping properties of $S_0^{\alpha_0}$ and $V_0^{\alpha_0}$ are derived from those of $S_\kappa^{\alpha_0}$ and $V_\kappa^{\alpha_0}$.

By [7, Theorem 4], the two operators S_κ^α and V_κ^α act on densities $\mathbf{j}\in\mathbf{V}'_{\alpha,\pi}$ according to:

$$S_\kappa^\alpha\mathbf{j}=S_\kappa^\alpha\left(i_\pi\mathbf{j}\right) \quad \text{and} \quad V_\kappa^\alpha\mathbf{j}=\gamma\left(S_\kappa^\alpha\mathbf{j}\right). \tag{3.7}$$

Definition 3.7 (Electric potential)**.** *Let $\kappa\neq 0$. Then the electric potential $\Psi_{\mathrm{E}_\kappa}^\alpha$ is defined for a density $\mathbf{j}\in\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$ by*

$$\Psi_{\mathrm{E}_\kappa}^\alpha\mathbf{j}:=\kappa S_\kappa^\alpha\mathbf{j}+\kappa^{-1}\nabla S_\kappa^\alpha\,\mathrm{div}_\Gamma\,\mathbf{j}.$$

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

Definition 3.8 (Magnetic potential)**.** *Let $\kappa\neq 0$. Then we define the magnetic potential $\Psi_{\mathrm{M}_\kappa}^\alpha$ for a density $\mathbf{m}\in\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$ by*

$$\Psi_{\mathrm{M}_\kappa}^\alpha\mathbf{m}:=\mathbf{curl}\,S_\kappa^\alpha\mathbf{m}.$$

We in particular observe that

$$\kappa^{-1}\,\mathbf{curl}\,\Psi_{\mathrm{E}_\kappa}^\alpha=\Psi_{\mathrm{M}_\kappa}^\alpha \quad \text{and} \quad \kappa^{-1}\,\mathbf{curl}\,\Psi_{\mathrm{M}_\kappa}^\alpha=\Psi_{\mathrm{E}_\kappa}^\alpha \quad \text{for } \kappa\neq 0. \tag{3.8}$$

Lemma 3.6 and the identities (3.8) imply the following lemma.

Lemma 3.9. *For $\kappa \neq 0$, the electromagnetic potentials $\Psi^\alpha_{\mathrm{E}_\kappa}$ and $\Psi^\alpha_{\mathrm{M}_\kappa}$ map continuously from the Hilbert space $\mathbf{H}^{-1/2}_\alpha(\operatorname{div}_\Gamma, \Gamma)$ to $\mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl}, G_+) \cup \mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl}, G_-)$. For densities $\mathbf{j}, \mathbf{m}$ lying in $\mathbf{H}^{-1/2}_\alpha(\operatorname{div}_\Gamma, \Gamma)$, they satisfy the time-harmonic Maxwell equations*

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

and the outgoing wave condition (2.10)-(2.11).

Defining $[\gamma_*] \coloneqq \gamma^-_* - \gamma^+_*$ for $* \in \{\mathrm{D}, \mathrm{N}_\kappa\}$, the jump relations

$$[\gamma_\mathrm{D}]\, \Psi^\alpha_{\mathrm{E}_\kappa} = 0, \qquad [\gamma_{\mathrm{N}_\kappa}]\, \Psi^\alpha_{\mathrm{E}_\kappa} = -2\mathrm{I}, \tag{3.9}$$

$$[\gamma_\mathrm{D}]\, \Psi^\alpha_{\mathrm{M}_\kappa} = -2\mathrm{I}, \qquad [\gamma_{\mathrm{N}_\kappa}]\, \Psi^\alpha_{\mathrm{M}_\kappa} = 0. \tag{3.10}$$

hold for $\kappa \neq 0$.

Lemma 3.10 (Stratton-Chu integral representation)**.** *Assume that $\kappa \neq 0$ and let $\mathbf{E}$ satisfy time-harmonic Maxwell's equations $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa^2\mathbf{E} = 0$ as well as the outgoing wave condition in $G_+ \cup G_-$. Then $\mathbf{E}$ admits the integral representation*

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

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

The proof, which will not be presented here, is based on the classical Stratton-Chu integral representation of $\mathbf{E}$ in the bounded polyhedral Lipschitz cell G^H (see [6, Theorem 3]) and exploits (3.6).

The integral equations derived in the course of this paper are composed of the boundary integral operators

$$C^\alpha_\kappa \coloneqq \{\gamma_\mathrm{D}\}\, \Psi^\alpha_{\mathrm{E}_\kappa} = \{\gamma_{\mathrm{N}_\kappa}\}\, \Psi^\alpha_{\mathrm{M}_\kappa} \quad \text{and} \quad M^\alpha_\kappa \coloneqq \{\gamma_\mathrm{D}\}\, \Psi^\alpha_{\mathrm{M}_\kappa} = \{\gamma_{\mathrm{N}_\kappa}\}\, \Psi^\alpha_{\mathrm{E}_\kappa},$$

where $\{\gamma_*\} \coloneqq -\frac{1}{2}\left(\gamma^-_* + \gamma^+_*\right)$ for $* \in \{\mathrm{D}, \mathrm{N}_\kappa\}$. They map from $\mathbf{H}^{-1/2}_\alpha(\operatorname{div}_\Gamma, \Gamma)$ into itself, which is easily deduced from Lemma 3.9 and the mapping properties (3.2) of the trace operators. Moreover, we define, for $\mathbf{j} \in \mathbf{H}^{-1/2}_\alpha(\operatorname{div}_\Gamma, \Gamma)$ and $\kappa \neq 0$, the auxiliary operators

$$C^\alpha_{\kappa,0}\mathbf{j} \coloneqq -\kappa R^\alpha_0 \mathbf{j} + \kappa^{-1} T^\alpha_0 \mathbf{j}, \tag{3.11}$$

$$C^{\alpha,*}_0 \mathbf{j} \coloneqq R^\alpha_0 \mathbf{j} + T^\alpha_0 \mathbf{j}, \tag{3.12}$$

where

$$R^\alpha_\nu \coloneqq \gamma_\mathrm{D}\left(V^\alpha_\nu\right) \qquad T^\alpha_\nu \coloneqq \mathbf{curl}_\Gamma\, V^\alpha_\nu \operatorname{div}_\Gamma.$$

The operator $C^\alpha_{\kappa,0}$ corresponds to the principal part of the boundary integral operator C^α_κ, whereas $C^{\alpha,*}_0$ is a regularizing operator, first defined in its non-periodic version in [26]. We have the identity

$$C^{\alpha,*}_0 = \mathrm{i} C^\alpha_{\mathrm{i},0}. \tag{3.13}$$

Lemma 3.11. *The operator $\left(R^\alpha_0\right)^2$ is compact in $\mathbf{H}^{-1/2}_\alpha(\operatorname{div}_\Gamma, \Gamma)$ and $\left(T^\alpha_0\right)^2 = 0$.*

Lemma 3.12. *The operator differences $C^\alpha_\kappa - C^\alpha_{\kappa,0}$ and $M^\alpha_\kappa - M^\alpha_0$ are compact in $\mathbf{H}^{-1/2}_\alpha(\operatorname{div}_\Gamma, \Gamma)$. If Γ is smooth, the operator M^α_κ is compact in $\mathbf{H}^{-1/2}_\alpha(\operatorname{div}_\Gamma, \Gamma)$.*

Lemma 3.12 is proven similar to Lemma 3.6. It implies the compactness of the operator difference

$$M_\kappa^\alpha - M_\sigma^\alpha = (M_\kappa^\alpha - M_0^\alpha) - (M_\sigma^\alpha - M_0^\alpha) \tag{3.14}$$

in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$ for wave numbers κ, σ with $\kappa \neq \sigma$.

Lemma 3.13. *Let the material parameters in κ satisfy (2.2) and let $\sigma = \mathrm{i}\tau$ with $\tau \in \mathbb{R}_+$. Then we have the adjoint relations*

$$\mathcal{B}\left(C_\kappa^\alpha \mathbf{j}, \mathbf{m}\right) = -\mathcal{B}\left(\mathbf{j}, C_\kappa^{-\alpha}\mathbf{m}\right) \quad \textit{and} \quad \mathcal{B}\left(M_\kappa^\alpha \mathbf{j}, \mathbf{m}\right) = -\mathcal{B}\left(\mathbf{j}, M_\kappa^{-\alpha}\mathbf{m}\right), \tag{3.15}$$

$$\mathcal{B}_{\mathrm{c}}\left(C_\sigma^\alpha \mathbf{j}, \mathbf{l}\right) = \mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C_\sigma^\alpha \mathbf{l}\right) \quad \textit{and} \quad \mathcal{B}_{\mathrm{c}}\left(M_\sigma^\alpha \mathbf{j}, \mathbf{l}\right) = -\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, M_\sigma^\alpha \mathbf{l}\right) \tag{3.16}$$

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

Proof. The adjoint relations (3.15) are deduced by explicit calculations with the help of the properties of the rotation operator r, the relations

$$G_\kappa^\alpha(x, y) = G_\kappa^{-\alpha}(y, x) \quad \text{and} \quad \nabla^x G_\kappa^\alpha(x, y) = -\nabla^y G_\kappa^{-\alpha}(y, x) \quad \text{for all } x, y \in \Gamma,$$

(3.1), (3.7) and Lemma 3.3. Since $\mathcal{B}_{\mathrm{c}}(\cdot, \cdot) = \mathcal{B}(\,\cdot\,, \overline{\,\cdot\,})$, $C_\sigma^\alpha = -\overline{C_\sigma^{-\alpha}}$ and $M_\sigma^\alpha = \overline{M_\sigma^{-\alpha}}$ for $\sigma = \mathrm{i}\tau$ with $\tau \in \mathbb{R}_+$, the relations (3.16) arise from (3.15). □

The Calderon relations for the α-quasiperiodic time-harmonic Maxwell equations serve as an important tool in this paper:

$$\left(C_\kappa^\alpha\right)^2 = \mathrm{I} - \left(M_\kappa^\alpha\right)^2 \quad \text{and} \quad C_\kappa^\alpha M_\kappa^\alpha = -M_\kappa^\alpha C_\kappa^\alpha \quad \text{for } \kappa \neq 0. \tag{3.17}$$

They are deduced from the identity $P_-^\alpha P_+^\alpha = 0$ that holds for the Calderon projectors $P_\pm^\alpha := \mathrm{I} \pm A_\kappa^\alpha$, where

$$A_\kappa^\alpha := \begin{pmatrix} M_\kappa^\alpha & C_\kappa^\alpha \\ C_\kappa^\alpha & M_\kappa^\alpha \end{pmatrix}.$$

The subsequent lemma is proven with the help of the first Calderon relation and the later shown Lemma 3.19.

Lemma 3.14. *C_κ^α is a Fredholm operator of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$ for $\kappa \neq 0$.*

In fact, we can even show that C_κ^α is invertible for certain wave numbers.

Lemma 3.15. *Let $\sigma = \mathrm{i}\tau$ with $\tau \in \mathbb{R}_+$. Then the boundary integral operator C_σ^α is invertible in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$.*

Proof. We first show that C_σ^α is elliptic in the sense that

$$\mathrm{Im}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C_\sigma^\alpha \mathbf{j}\right)\right) \geq c \left\|\mathbf{j}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma)} \quad \text{for all } \mathbf{j} \in \mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma). \tag{3.18}$$

For $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$, we define the function $\mathbf{u} := \Psi_{\mathrm{E}_\sigma}^\alpha \mathbf{j}$ that solves the time-harmonic Maxwell equation

$$\mathbf{curl}\,\mathbf{curl}\,\mathbf{u} + \tau^2 \mathbf{u} = 0 \quad \text{in } G_+ \cup G_- \tag{3.19}$$

and satisfies the outgoing wave condition (2.10)-(2.11) according to Lemma 3.9. Moreover, we recall that the auxiliary domains $G^{\mathrm{H}}_{\pm}$ are defined for suitably chosen $\mathrm{H} \in \mathbb{R}_+$ such that

$$G^{\mathrm{H}}_{\pm} := G^{\mathrm{H}} \cap G_{\pm} \quad \text{with } \Gamma \subset G^{\mathrm{H}} := \{x \in Q \times \mathbb{R} \ : \ |x_3| \leq \mathrm{H}\}$$

(see (2.3)). In particular, $\mathbf{u} \in \mathbf{H}_\alpha(\mathbf{curl}, G^{\mathrm{H}}_+ \cup G^{\mathrm{H}}_-) \cap \mathbf{H}_\alpha(\mathbf{curl}, G^{\mathrm{H}}_+ \cup G^{\mathrm{H}}_-)$ holds. Applying the identity

$$C^\alpha_\sigma = -\frac{1}{2}\left(\gamma^-_{\mathrm{D}} + \gamma^+_{\mathrm{D}}\right) \Psi^\alpha_{\mathrm{E}_\sigma} \overset{(3.9)_1}{=} -\gamma_{\mathrm{D}} \Psi^\alpha_{\mathrm{E}_\sigma}$$

the jump relation $(3.9)_2$ and Green's identity (3.3) in the domain $G^{\mathrm{H}}_+ \cup G^{\mathrm{H}}_-$ in terms of the unit normal vector $\mathbf{n}$ leads to

$$\begin{aligned}
\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C^\alpha_\sigma \mathbf{j}\right) &= -\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \gamma_{\mathrm{D}} \mathbf{u}\right) \overset{(3.9)_2}{=} \frac{1}{2}\left(\mathcal{B}_{\mathrm{c},\Gamma}\left(\gamma^-_{\mathrm{N}_\sigma}\mathbf{u}, \gamma^-_{\mathrm{D}}\mathbf{u}\right) - \mathcal{B}_{\mathrm{c},\Gamma}\left(\gamma^+_{\mathrm{N}_\sigma}\mathbf{u}, \gamma^+_{\mathrm{D}}\mathbf{u}\right)\right) \\
&= \frac{\mathrm{i}}{2\tau}\left(\mathcal{B}_{\mathrm{c},\Gamma}\left(\gamma^+_{\mathrm{D}}\,\mathbf{curl}\,\mathbf{u}, \gamma^+_{\mathrm{D}}\mathbf{u}\right) - \mathcal{B}_{\mathrm{c},\Gamma}\left(\gamma^-_{\mathrm{D}}\,\mathbf{curl}\,\mathbf{u}, \gamma^-_{\mathrm{D}}\mathbf{u}\right)\right) \\
&= \frac{\mathrm{i}}{2\tau}\Bigg[\int_{G^{\mathrm{H}}_+ \cup G^{\mathrm{H}}_-} |\mathbf{curl}\,\mathbf{u}|^2 - \mathbf{curl}\,\mathbf{curl}\,\mathbf{u} \cdot \overline{\mathbf{u}}\, dx \\
&\qquad + \mathcal{B}_{\mathrm{c},\Gamma^{\mathrm{H}}_+}\left(\gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_+}\mathbf{curl}\,\mathbf{u},\, \gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_+}\mathbf{u}\right) \\
&\qquad + \mathcal{B}_{\mathrm{c},\Gamma^{\mathrm{H}}_-}\left(\gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_-}\mathbf{curl}\,\mathbf{u},\, \gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_-}\mathbf{u}\right)\Bigg] \\
&\overset{(3.19)}{\geq} \frac{\mathrm{i}c_1}{2}\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl}, G^{\mathrm{H}}_+ \cup G^{\mathrm{H}}_-)} \\
&\qquad + \frac{\mathrm{i}}{2\tau}\Bigg(\mathcal{B}_{\mathrm{c},\Gamma^{\mathrm{H}}_+}\left(\gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_+}\mathbf{curl}\,\mathbf{u},\, \gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_+}\mathbf{u}\right) \\
&\qquad + \mathcal{B}_{\mathrm{c},\Gamma^{\mathrm{H}}_-}\left(\gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_-}\mathbf{curl}\,\mathbf{u},\, \gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_-}\mathbf{u}\right)\Bigg),
\end{aligned}$$

where we have $\Gamma^{\mathrm{H}}_{\pm} := \{x \in Q \times \mathbb{R} \ : \ x_3 = \pm\mathrm{H}\}$ with unit normal vectors $\mathbf{n}^{\mathrm{H}}_{\pm} := (0, 0, \pm 1)^{\mathrm{T}}$ and $c_1 := \min\{\tau, \tau^{-1}\}$. Above, we exploited $\mathcal{B}_{\mathrm{c}}(\cdot,\cdot) = \mathcal{B}(\,\cdot\,, \overline{\,\cdot\,})$. The last two terms on the right-hand side above can be explicitly computed since $\mathbf{u}$ and $\overline{\mathbf{u}}$ satisfy the outgoing wave condition with $\beta^{(n)}_{\mathrm{i}} = \mathrm{i}(\tau^2 + \left|\alpha^{(n)}\right|^2)^{\frac{1}{2}}$:

$$\mathbf{u}^{\pm}(x) = \sum_{n \in \mathbb{Z}^2} \mathbf{u}^{\pm}_n e^{\mathrm{i}\alpha^{(n)}\cdot\tilde{x} \mp \sqrt{\tau^2 + \left|\alpha^{(n)}\right|^2} x_3} \qquad \text{on } \Gamma^{\mathrm{H}}_{\pm}, \tag{3.20}$$

$$\overline{\mathbf{u}^{\pm}}(x) = \sum_{n \in \mathbb{Z}^2} \overline{\mathbf{u}^{\pm}_n} e^{-\mathrm{i}\alpha^{(n)}\cdot\tilde{x} \mp \sqrt{\tau^2 + \left|\alpha^{(n)}\right|^2} x_3} \qquad \text{on } \Gamma^{\mathrm{H}}_{\pm}, \tag{3.21}$$

where $\mathbf{u}^{\pm} := \mathbf{u}|_{\Gamma^{\mathrm{H}}_{\pm}}$. With this, the orthogonality of the trigonometric polynomials and the identity

$$\left(\alpha^{(n)}\right)_1\left(\overline{\mathbf{u}^{\pm}_n}\right)_1 + \left(\alpha^{(n)}\right)_2\left(\overline{\mathbf{u}^{\pm}_n}\right)_2 \pm \mathrm{i}\sqrt{\tau^2 + |\alpha^{(n)}|^2}\left(\overline{\mathbf{u}^{\pm}_n}\right)_3 = 0 \quad \text{on } \Gamma^{\mathrm{H}}_{\pm},$$

which goes back to inserting $\overline{\mathbf{u}}$ represented as in (3.21) into $\operatorname{div}\overline{\mathbf{u}} = 0$, we arrive at

$$\begin{aligned}
&\mathcal{B}_{\mathrm{c},\Gamma^{\mathrm{H}}_{\pm}}\left(\gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_{\pm}}\mathbf{curl}\,\mathbf{u},\, \gamma_{\mathrm{D}}|_{\Gamma^{\mathrm{H}}_{\pm}}\mathbf{u}\right) \\
&\qquad = \pm 4\pi^2 \sum_{n \in \mathbb{Z}^2}\left[\pm\sqrt{\tau^2 + |\alpha^{(n)}|^2}\left(\left|\left(\mathbf{u}^{\pm}_n\right)_1\right|^2 + \left|\left(\mathbf{u}^{\pm}_n\right)_2\right|^2\right)\right.
\end{aligned}$$

$$
\begin{aligned}
&+\mathrm{i}\left(\mathbf{u}_n^{\pm}\right)_3\left(\left(\alpha^{(n)}\right)_1\left(\overline{\mathbf{u}_n^{\pm}}\right)_1+\left(\alpha^{(n)}\right)_2\left(\overline{\mathbf{u}_n^{\pm}}\right)_2\right)\Big]\\
&\times e^{-2\sqrt{\tau^2+\left|\alpha^{(n)}\right|^2}\mathrm{H}}\\
=&\pm 4\pi^2\sum_{n\in\mathbb{Z}^2}\left[\pm\sqrt{\tau^2+|\alpha^{(n)}|^2}\left(\left|\left(\mathbf{u}_n^{\pm}\right)_1\right|^2+\left|\left(\mathbf{u}_n^{\pm}\right)_2\right|^2\right)\right.\\
&\left.\pm\sqrt{\tau^2+|\alpha^{(n)}|^2}\left|\left(\mathbf{u}_n^{\pm}\right)_3\right|^2\right]e^{-2\sqrt{\tau^2+\left|\alpha^{(n)}\right|^2}\mathrm{H}}\\
=&\,4\pi^2\sum_{n\in\mathbb{Z}^2}\sqrt{\tau^2+|\alpha^{(n)}|^2}\left|\mathbf{u}_n^{\pm}\right|^2 e^{-2\sqrt{\tau^2+\left|\alpha^{(n)}\right|^2}\mathrm{H}}.
\end{aligned}
$$

Altogether, we have

$$
\begin{aligned}
\operatorname{Im}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j},C_\sigma^\alpha\mathbf{j}\right)\right)\geq&\,\frac{c_1}{2}\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl},G_+^{\mathrm{H}}\cup G_-^{\mathrm{H}})}\\
&+\frac{2\pi^2}{\tau}\sum_{n\in\mathbb{Z}^2}\sqrt{\tau^2+|\alpha^{(n)}|^2}\left(\left|\mathbf{u}_n^{+}\right|^2+\left|\mathbf{u}_n^{-}\right|^2\right)e^{-2\sqrt{\tau^2+\left|\alpha^{(n)}\right|^2}\mathrm{H}}\\
\geq&\,\frac{c_1}{2}\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl},G_+^{\mathrm{H}}\cup G_-^{\mathrm{H}})}=\frac{c_1}{2}\left(\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl},G_+^{\mathrm{H}})}+\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl},G_-^{\mathrm{H}})}\right),
\end{aligned}
$$

where we in particular used that $\tau>0$. The Neumann jump of the electric potential $\Psi^\alpha_{\mathrm{E}_\sigma}$ implies that

$$
\begin{aligned}
\|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}&=\left\|\frac{1}{2}\left(\gamma^+_{\mathrm{N}_\sigma}\mathbf{u}-\gamma^-_{\mathrm{N}_\sigma}\mathbf{u}\right)\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}\\
&\leq\left(\left\|\gamma^+_{\mathrm{N}_\sigma}\mathbf{u}\right\|_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}+\left\|\gamma^-_{\mathrm{N}_\sigma}\mathbf{u}\right\|_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}\right)^2 \qquad (3.22)\\
&\leq 2\left(\left\|\gamma^+_{\mathrm{N}_\sigma}\mathbf{u}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}+\left\|\gamma^-_{\mathrm{N}_\sigma}\mathbf{u}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}\right).
\end{aligned}
$$

Moreover, the time-harmonic Maxwell equations (3.19) give rise to

$$
\begin{aligned}
&\|\mathbf{u}\|^2_{\mathbf{L}^2_\alpha(G_\pm^{\mathrm{H}})}=\tau^2\|\mathbf{curl}\,\mathbf{curl}\,\mathbf{u}\|^2_{\mathbf{L}^2_\alpha(G_\pm^{\mathrm{H}})}\\
\Longrightarrow\;&\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl},G_\pm^{\mathrm{H}})}=\frac{1}{2}\left(\|\mathbf{u}\|^2_{\mathbf{L}^2_\alpha(G_\pm^{\mathrm{H}})}+\tau^2\|\mathbf{curl}\,\mathbf{curl}\,\mathbf{u}\|^2_{\mathbf{L}^2_\alpha(G_\pm^{\mathrm{H}})}\right)+\|\mathbf{curl}\,\mathbf{u}\|^2_{\mathbf{L}^2_\alpha(G_\pm^{\mathrm{H}})}\\
&\qquad\geq\frac{c_2}{2}\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl}\,\mathbf{curl},G_\pm^{\mathrm{H}})}
\end{aligned}
$$

with $c_2:=\min\{1,\tau^2\}$. Since, by (3.2), the Neumann trace operators are bounded operators from $\mathbf{H}_\alpha(\mathbf{curl}\,\mathbf{curl},G_\pm^{\mathrm{H}})$ to $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma,\Gamma)$, we all in all have

$$
\begin{aligned}
\operatorname{Im}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j},C_\sigma^\alpha\mathbf{j}\right)\right)\;\geq&\;\frac{c_1c_2}{4}\left(\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl}\,\mathbf{curl},G_+^{\mathrm{H}})}+\|\mathbf{u}\|^2_{\mathbf{H}_\alpha(\mathbf{curl}\,\mathbf{curl},G_-^{\mathrm{H}})}\right)\\
\geq&\;\frac{c_1c_2c_3}{4}\left(\left\|\gamma^+_{\mathrm{N}_\sigma}\mathbf{u}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}+\left\|\gamma^+_{\mathrm{N}_\sigma}\mathbf{u}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\partial G_+^{\mathrm{H}}\setminus\Gamma)}\right)\\
&+\frac{c_1c_2c_4}{4}\left(\left\|\gamma^-_{\mathrm{N}_\sigma}\mathbf{u}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}+\left\|\gamma^-_{\mathrm{N}_\sigma}\mathbf{u}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\partial G_-^{\mathrm{H}}\setminus\Gamma)}\right)\\
\geq&\;\frac{c_1c_2}{4}\min\{c_3,c_4\}\left(\left\|\gamma^+_{\mathrm{N}_\sigma}\mathbf{u}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}+\left\|\gamma^-_{\mathrm{N}_\sigma}\mathbf{u}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)}\right)\\
\overset{(3.22)}{\geq}&\;c\,\|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma,\Gamma)},
\end{aligned}
$$

where $c := \frac{c_1 c_2}{8} \min\{c_3, c_4\}$.

In order to deduce the invertibility of C_σ^α in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ from its previously shown ellipticity, we define, for fixed $\mathbf{m} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$, the bounded linear functional $\mathbf{B}_\mathrm{c}\mathbf{m}$ by

$$(\mathbf{B}_\mathrm{c}\mathbf{m})(\mathbf{j}) := \mathcal{B}_\mathrm{c}(\mathbf{j}, \mathbf{m}) \quad \text{for all } \mathbf{j} \in \mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma). \tag{3.23}$$

This generates the bounded linear operator $\mathbf{B}_\mathrm{c} : \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \to (\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma))'$. From the Riesz representation theorem ([16, Theorem 5.2.2]), we conclude that

$$(\mathbf{j}, j\mathbf{B}_\mathrm{c} C_\sigma^\alpha \mathbf{m})_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma)} = \mathcal{B}_\mathrm{c}(\mathbf{j}, C_\sigma^\alpha \mathbf{m}),$$

where j is the Riesz isomorphism mapping from the space $(\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma))'$ into $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$. Since $\mathcal{B}_\mathrm{c}(\cdot, C_\sigma^\alpha \cdot)$ is a continuous and $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$-elliptic sesquilinear form, we in particular infer from the Lax-Milgram theorem in the version of [16, Theorem 5.2.3] that

$$j\mathbf{B}_\mathrm{c} C_\sigma^\alpha : \mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma) \to \mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma)$$

is an isomorphism with $\mathcal{R}(j\mathbf{B}_\mathrm{c} C_\sigma^\alpha) = \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$. Therefore, $\mathcal{R}(j\mathbf{B}_\mathrm{c}) = \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$. Together with the injectivity of the linear operator $\mathbf{B}_\mathrm{c}$, which arises from the nondegeneracy of the duality product $\mathcal{B}_\mathrm{c}$ given by Lemma 3.4, we derive the invertibility of $j\mathbf{B}_\mathrm{c}$ in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$. Therefore, also the boundary integral operator $C_\sigma^\alpha : \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \to \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ is invertible. □

Corollary 3.16. *The operators* $\mathrm{I} \pm M_\sigma^\alpha : \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \to \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ *are invertible for wave numbers* $\sigma = \mathrm{i}\tau$ *with* $\tau \in \mathbb{R}_+$ *and in particular satisfy the inequalities*

$$\|(\mathrm{I} \pm M_\sigma^\alpha)\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma)} \geq c_\pm \|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma)}. \tag{3.24}$$

Proof. The invertibility of $\mathrm{I} \pm M_\sigma^\alpha$ is easily deduced from

$$(C_\sigma^\alpha)^2 \overset{(3.17)_1}{=} \mathrm{I} - (M_\sigma^\alpha)^2 = (\mathrm{I} - M_\sigma^\alpha)(\mathrm{I} + M_\sigma^\alpha) = (\mathrm{I} + M_\sigma^\alpha)(\mathrm{I} - M_\sigma^\alpha)$$

since $(C_\sigma^\alpha)^2$ is invertible by Lemma 3.15. Based on the fact that $\mathrm{I} \pm M_\sigma^\alpha$ are linear and continuous in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ in addition to their invertibility, the inequalities (3.24) are a simple implication of Theorems 2.9-4 and 5.6-2 from [10]. □

We can also make a statement on the invertibility of the operator C_κ^α for wave numbers κ that can not be represented as $\mathrm{i}\tau$ with $\tau \in \mathbb{R}_+$: C_κ^α is invertible in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ if and only if κ is not a resonant frequency of a particular Dirichlet problem. This is proven by contradiction with the help of Lemma 3.10.

Lemma 3.17. *The integral operator* $C_\kappa^\alpha : \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \to \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ *is invertible if and only if the homogeneous Dirichlet problem,*

$$\begin{gathered} \mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa^2 \mathbf{E} = 0,\ \operatorname{div} \mathbf{E} = 0,\ \gamma_\mathrm{D} \mathbf{E} = 0 \\ \textit{and } \mathbf{E} \textit{ satisfies the outgoing wave condition} \end{gathered} \tag{3.25}$$

in both of the domains G_+ *and* G_-*, only has the trivial solution.*

Remark 3.18. *In the analysis of the boundary integral equation later on, we will often assume that the nullspace of C_κ^α is trivial, which is equivalent to the invertibility of C_κ^α since this is a Fredholm operator of index zero by Lemma 3.14. If $\sigma = \mathrm{i}\tau$ with $\tau \in \mathbb{R}_+$, then $C_\sigma^\alpha : \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma) \to \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$ is invertible due to Lemma 3.15. For other wave numbers, Lemma 3.17 gives a necessary and sufficient condition to ensure such a condition: the unique solvability of the Dirichlet problem (3.25) in both G_+ and G_-. Up to now, the unique or nonunique solvability of (3.25) has not yet been fully understood for all wave numbers. To the best of our knowledge, there do not exist any counterexamples to the uniqueness of (3.25) 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. However, there exist several counterexamples for grating profiles, which are invariant in x_1 or x_2 and may even be smooth (see, e.g., [17], [18]). Other typical counterexamples in the 2π-periodic framework, from which counterexamples for 2π-biperiodic geometries can be derived, involve overhanging profiles that can no longer be represented as the graph of a function (see, e.g., [15]).*

Lemma 3.19. *For $\kappa \neq 0$, the operators $\mathrm{I} \pm M_\kappa^\alpha$ are Fredholm of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$.*

Proof. If Γ is smooth, it is clear that $\mathrm{I} \pm M_\kappa^\alpha$ are Fredholm operators of index zero by the invertibility of I and the compactness of M_κ^α according to Lemma 3.12. If Γ only has polyhedral Lipschitz regularity, we reformulate $\mathrm{I} \pm M_\kappa^\alpha$ as

$$\mathrm{I} \pm M_\kappa^\alpha = (\mathrm{I} \pm M_\mathrm{i}^\alpha) \pm (M_\kappa^\alpha - M_\mathrm{i}^\alpha)\,.$$

Lemmata 3.15 and 3.12 imply that $\mathrm{I} \pm M_\mathrm{i}^\alpha$ are invertible and $M_\kappa^\alpha - M_\mathrm{i}^\alpha$ is compact in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$. Thus, in this case, the boundary integral operators $\mathrm{I} \pm M_\kappa^\alpha$ are again Fredholm of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$. □

Lemma 3.20. *The operator V_0^α is self-adjoint with respect to the complex L^2- and the complex $\mathbf{L}^2$-scalar product. Moreover, if $\tilde{\alpha} \notin \mathbb{Z}^2$, the operator V_0^α is elliptic in the sense that there exist positive constants c and $\mathbf{c}$ such that*

$$\int_\Gamma V_0^\alpha j\,\overline{j}\,d\sigma \geq c\,\|j\|^2_{H_\alpha^{-\frac{1}{2}}(\Gamma)} \quad \text{and} \quad \int_\Gamma V_0^\alpha \mathbf{j} \cdot \overline{\mathbf{j}}\,d\sigma \geq \mathbf{c}\,\|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\Gamma)} \tag{3.26}$$

for $j \in H_\alpha^{-1/2}(\Gamma)$ and $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\Gamma)$.

Proof. The self-adjointness of V_0^α with respect to the complex L^2-($\mathbf{L}^2$-)scalar product goes back to the identities $G_0^\alpha(x,y) = G_0^{-\alpha}(y,x) = \overline{G_0^\alpha}(y,x)$ for all $x, y \in \Gamma$.

For $\tilde{\alpha} \notin \mathbb{Z}^2$, we now verify the ellipticity property in $H_\alpha^{-1/2}(\Gamma)$ with a similar technique of proof as applied in the proof of Lemma 3.15. For $j \in H_\alpha^{-1/2}(\Gamma)$, we define the function $u = S_0^\alpha j$ that solves the Laplace equation in $G_\pm$. The jump relations of the scalar-valued single layer potential ([3, Theorem 4.2]) and the second Green identity in the domains $G_+^\mathrm{H} \cup G_-^\mathrm{H}$ defined in (2.3) yield

$$\begin{aligned}\int_\Gamma V_0^\alpha j\,\overline{j}\,d\sigma &= \int_\Gamma u\left(\gamma_\mathbf{n}^- \overline{u} - \gamma_\mathbf{n}^+ \overline{u}\right)\,d\sigma \\ &= \int_{G_+^\mathrm{H} \cup G_-^\mathrm{H}} |\nabla u|^2\,dx - \int_{\Gamma_-^\mathrm{H}} u \frac{\partial \overline{u}}{\partial \mathbf{n}_-^\mathrm{H}}\,d\sigma - \int_{\Gamma_+^\mathrm{H}} u \frac{\partial \overline{u}}{\partial \mathbf{n}_+^\mathrm{H}}\,d\sigma,\end{aligned} \tag{3.27}$$

where $\gamma_\mathbf{n}^\pm := \frac{\partial}{\partial \mathbf{n}}\big|_\Gamma$ denotes the normal trace and $\Gamma_\pm^\mathrm{H} := \{x \in Q \times \mathbb{R} \ : \ x_3 = \pm\mathrm{H}\}$ with $\mathbf{n}_\pm^\mathrm{H} = (0,0,\pm 1)^\mathrm{T}$. Since, for $\kappa_\pm = 0$, we have $\beta_+^{(n)} = \beta_-^{(n)} = \mathrm{i}\left|\alpha^{(n)}\right|$, the outgoing wave condition of the form

$$u(x) = \sum_{n\in\mathbb{Z}^2} u_n^+ e^{\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{x}+\beta_+^{(n)}x_3\right)}, \qquad x \in G_+ \text{ with } x_3 \geq \mathrm{H},$$

$$u(x) = \sum_{n\in\mathbb{Z}^2} u_n^- e^{\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{x}-\beta_-^{(n)}x_3\right)}, \qquad x \in G_- \text{ with } x_3 \leq -\mathrm{H},$$

with scalar-valued coefficients $u_n^{\pm}$, $n \in \mathbb{Z}^2$, implies that

$$\begin{aligned}\int_\Gamma V_0^\alpha j\,\overline{j}\,dx = &\int_{G_+^{\mathrm{H}}\cup G_-^{\mathrm{H}}} |\nabla u|^2\,dx \\ &+ 4\pi^2 \sum_{n\in\mathbb{Z}^2} \left|\alpha^{(n)}\right| \left(\left|u_n^+\right|^2 + \left|u_n^-\right|^2\right) e^{-2\left|\alpha^{(n)}\right|\mathrm{H}}.\end{aligned} \tag{3.28}$$

We define the operator $\mathcal{A} : H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}}) \times H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}}) \to \mathbb{R}$ by

$$\mathcal{A}(u,v) := \int_{G_+^{\mathrm{H}}\cup G_-^{\mathrm{H}}} \nabla u \cdot \overline{\nabla v}\,dx - \int_{\Gamma_-^{\mathrm{H}}} u \frac{\partial \overline{v}}{\partial \mathbf{n}_-^{\mathrm{H}}}\,d\sigma - \int_{\Gamma_+^{\mathrm{H}}} u \frac{\partial \overline{v}}{\partial \mathbf{n}_+^{\mathrm{H}}}\,d\sigma.$$

We observe that $\mathcal{A}(u,u)$ is exactly the right-hand side of (3.28). It can be shown to be coercive in the space $H_\alpha^1\left(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}}\right)$. Indeed, suppose $\mathcal{A}$ were not coercive, i.e., suppose (with abuse of notation) that there exists a sequence $\{u_m\}_{m\in\mathbb{N}}$ in $H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$ with $\|u_m\|_{H_\alpha^1(G_+^{\mathrm{H}}\cup G_-^{\mathrm{H}})} = 1$ such that

$$\mathcal{A}(u_m,u_m) \to 0 \quad \text{as } m \to \infty. \tag{3.29}$$

Since the sequence $\{u_m\}_{m\in\mathbb{N}}$ is bounded in $H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$, there exists a weakly convergent subsequence $\{u_{m_k}\}_{k\in\mathbb{N}}$ with weak limit $u \in H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$. We notice that the Hilbert space $H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$ is a closed subspace of $H^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$ and that $L_\alpha^2(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}}) = L^2(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$. With this and the Sobolev imbedding theorem from [1, Theorem 5.4 Case A (4)], we obtain the imbedding

$$H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}}) \hookrightarrow L_\alpha^2(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}}).$$

We deduce that $u_{m_k} \xrightarrow{k\to\infty} u$ in norm in $L_\alpha^2(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$. Moreover, we have $\nabla u_{m_k} \xrightarrow{k\to\infty} 0$ in norm in $L_\alpha^2(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$ by (3.29) and

$$4\pi^2 \sum_{n\in\mathbb{Z}^2} \left|\alpha^{(n)}\right| \left(\left|u_n^+\right|^2 + \left|u_n^-\right|^2\right) e^{-2\left|\alpha^{(n)}\right|\mathrm{H}} > 0 \tag{3.30}$$

implying that $u_{m_k} \xrightarrow{k\to\infty} u$ in norm in $H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$. Together with the weak convergence of $\{u_{m_k}\}_{k\in\mathbb{N}}$, this shows the strong convergence of $\{u_m\}_{m\in\mathbb{N}}$ to u in $H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$. From

$$\|\nabla u_m\|_{L_\alpha^2(G_+^{\mathrm{H}}\cup G_-^{\mathrm{H}})} \xrightarrow{m\to\infty} 0,$$

we deduce that $u \equiv$ constant. Equations (3.29)-(3.30) then already lead to $u \equiv 0$. Clearly, this contradicts the assumption $\|u_m\|_{H_\alpha^1(G_+^{\mathrm{H}}\cup G_-^{\mathrm{H}})} = 1$. Thus, $\mathcal{A}$ is coercive in $H_\alpha^1(G_+^{\mathrm{H}} \cup G_-^{\mathrm{H}})$.

We now apply the coerciveness of $\mathcal{A}$ to (3.28) and infer that

$$\int_\Gamma V_0^\alpha j\,\overline{j}\,d\sigma = \mathcal{A}(u,u) \geq c_1 \|u\|^2_{H_\alpha^1(G_+^{\mathrm{H}}\cup G_-^{\mathrm{H}})} = c_1 \left(\|u\|^2_{H_\alpha^1(G_+^{\mathrm{H}})} + \|u\|^2_{H_\alpha^1(G_-^{\mathrm{H}})}\right)$$

for a constant $c_1 > 0$. The Neumann jump of S_0^α gives

$$\|j\|^2_{H_\alpha^{-\frac{1}{2}}(\Gamma)} = \left\|\gamma_{\mathbf{n}}^- u - \gamma_{\mathbf{n}}^+ u\right\|^2_{H_\alpha^{-\frac{1}{2}}(\Gamma)} \le 2\left(\left\|\gamma_{\mathbf{n}}^- u\right\|^2_{H_\alpha^{-\frac{1}{2}}(\Gamma)} + \left\|\gamma_{\mathbf{n}}^+ u\right\|^2_{H_\alpha^{-\frac{1}{2}}(\Gamma)}\right).$$

With the boundedness of the scalar Neumann trace operators, we conclude that

$$\begin{aligned}\int_\Gamma V_0^\alpha j\,\bar{j}\,d\sigma &\ge c_1\left(\|u\|^2_{H^1_\alpha(G_+^{\mathrm{H}})} + \|u\|^2_{H^1_\alpha(G_-^{\mathrm{H}})}\right)\\ &\ge c_1\left[c_2\left(\left\|\gamma_{\mathbf{n}}^+ u\right\|^2_{H_\alpha^{-\frac{1}{2}}(\Gamma)} + \left\|\gamma_{\mathbf{n}}^+ u\right\|^2_{H_\alpha^{-\frac{1}{2}}(\partial G_+^{\mathrm{H}}\setminus\Gamma)}\right)\right.\\ &\quad\left. + c_3\left(\left\|\gamma_{\mathbf{n}}^- u\right\|^2_{H_\alpha^{-\frac{1}{2}}(\Gamma)} + \left\|\gamma_{\mathbf{n}}^- u\right\|^2_{H_\alpha^{-\frac{1}{2}}(\partial G_-^{\mathrm{H}}\setminus\Gamma)}\right)\right]\\ &\ge c_1\min\{c_2, c_3\}\left(\left\|\gamma_{\mathbf{n}}^+ u\right\|^2_{H_\alpha^{\frac{1}{2}}(\Gamma)} + \left\|\gamma_{\mathbf{n}}^- u\right\|^2_{H_\alpha^{\frac{1}{2}}(\Gamma)}\right) \ge c\,\|j\|_{H_\alpha^{-\frac{1}{2}}(\Gamma)},\end{aligned}$$

where $c := \frac{c_1}{2}\min\{c_2, c_3\}$.

The $\mathbf{H}_\alpha^{-1/2}(\Gamma)$-ellipticity of V_0^α is a simple implication of its $H_\alpha^{-1/2}$-ellipticity. □

Lemma 3.21 (cf. [7, Theorem 4])**.** *For $\tilde{\alpha} \notin \mathbb{Z}^2$, the operator V_0^α is $\mathbf{V}'_{\alpha,\pi}$-elliptic with respect to the complex $\mathbf{L}^2_{\alpha,t}$-inner product in the sense that there exists a positive constant c_π such that*

$$\int_\Gamma V_0^\alpha \mathbf{j}\cdot\bar{\mathbf{j}}\,d\sigma \ge c_\pi\,\|\mathbf{j}\|^2_{\mathbf{V}'_{\alpha,\pi}} \quad \textit{for all } \mathbf{j}\in\mathbf{V}'_{\alpha,\pi}.$$

Lemma 3.22. *The operator $C_0^{\alpha,*} : \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma) \to \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$ is skew-adjoint with respect to the bilinear form $\mathcal{B}_c$. For $\tilde{\alpha} \notin \mathbb{Z}^2$, it is elliptic in the sense that, for $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$, we have*

$$\mathcal{B}_c\left(\mathbf{j}, C_0^{\alpha,*}\mathbf{j}\right) \ge c\,\|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}, \tag{3.31}$$

where c is a positive constant. Moreover, $C_0^{\alpha,*}$ is invertible in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$.

Since we have

$$\mathcal{B}_c\left(\mathbf{j}, C_0^{\alpha,*}\mathbf{m}\right) = \int_\Gamma \mathbf{j}\cdot\overline{V_0^\alpha\mathbf{m}}\,d\sigma + \int_\Gamma \mathrm{div}_\Gamma\,\mathbf{j}\,\overline{V_0^\alpha\,\mathrm{div}_\Gamma\,\mathbf{m}}\,d\sigma \quad \text{for } \mathbf{j},\mathbf{m}\in\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma),$$

Lemma 3.22 is proven with the help of Lemmata 3.20 and 3.21.

4 Boundary integral equation formulation

In this section, we derive, based on the ideas in [21] and [24] for the 2π-periodic framework, a boundary integral equation for the electromagnetic scattering problem involving one unknown density with a combined method: In the domain G_+ above the grating surface, we use the Stratton-Chu integral representation from Lemma 3.10, and, in the domain G_- below Γ, we work with an electric potential ansatz. This approach resembles the work of Costabel and Le Louër [12] for dielectric scattering by bounded polyhedral obstacles, however we do not utilize a regularizer in form of the operator $C_0^{\alpha,*}$ to avoid the occurrence of irregular frequencies (cf. Remark 3.18). By this, we obtain a rather simple integral expression with regard to a future numerical implementation.

4.1 Derivation of the integral equation formulation

We assume that

$$\mathbf{E}^{\mathrm{refl}} = \frac{1}{2}\left(\Psi^{\alpha}_{\mathrm{E}_{\kappa_+}}\gamma^{+}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{refl}} + \Psi^{\alpha}_{\mathrm{M}_{\kappa_+}}\gamma^{+}_{\mathrm{D}}\mathbf{E}^{\mathrm{refl}}\right) \quad \text{in } G_+, \tag{4.1}$$

$$\mathbf{E}^{\mathrm{tran}} = \Psi^{\alpha}_{\mathrm{E}_{\kappa_-}}\mathbf{j} \quad \text{in } G_-, \tag{4.2}$$

where the density $\mathbf{j} \in \mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_{\Gamma}, \Gamma)$ is yet to be determined. The direct ansatz for the reflected electric field $\mathbf{E}^{\mathrm{refl}}$ in G_+ is given by the α-quasiperiodic Stratton-Chu potential representation from Lemma 3.10, whereas the indirect ansatz for the transmitted electric field $\mathbf{E}^{\mathrm{tran}}$ in G_-, a simple α-quasiperiodic electric potential ansatz, is justified by Lemma 3.9. Moreover, we require the incident electric field $\mathbf{E}^{\mathrm{i}}$ to solve the time-harmonic Maxwell equations with respect to the wave number κ_+ in absence of the scattering surface Γ. Thus, Lemma 3.10 implies that

$$\mathbf{E}^{\mathrm{i}} = -\frac{1}{2}\left(\Psi^{\alpha}_{\mathrm{E}_{\kappa_+}}\gamma^{-}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{i}} + \Psi^{\alpha}_{\mathrm{M}_{\kappa_+}}\gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{i}}\right) \quad \text{in } G_-. \tag{4.3}$$

Applying the Dirichlet traces γ^{+}_{D} in (4.1) and γ^{-}_{D} in (4.3) leads to the expressions

$$\gamma^{+}_{\mathrm{D}}\mathbf{E}^{\mathrm{refl}} = -\frac{1}{2}\left(C^{\alpha}_{\kappa_+}\gamma^{+}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{refl}} + \left(M^{\alpha}_{\kappa_+} - \mathrm{I}\right)\gamma^{+}_{\mathrm{D}}\mathbf{E}^{\mathrm{refl}}\right) \quad \text{on } \Gamma, \tag{4.4}$$

$$\gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{i}} = \frac{1}{2}\left(C^{\alpha}_{\kappa_+}\gamma^{-}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{i}} + \left(M^{\alpha}_{\kappa_+} + \mathrm{I}\right)\gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{i}}\right) \quad \text{on } \Gamma, \tag{4.5}$$

with the help of the jump relations (3.9)-(3.10). Subtracting equation (4.4) from equation (4.5) and multiplying the result by the factor 2, gives

$$C^{\alpha}_{\kappa_+}\left(\gamma^{+}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{refl}} + \gamma^{-}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{i}}\right) + \left(M^{\alpha}_{\kappa_+} + \mathrm{I}\right)\left(\gamma^{+}_{\mathrm{D}}\mathbf{E}^{\mathrm{refl}} + \gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{i}}\right) = 2\gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{i}}. \tag{4.6}$$

With

$$\rho := \frac{\mu_+\kappa_-}{\mu_-\kappa_+},$$

the transmission conditions (2.8)-(2.9) can be reformulated as

$$\gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{tran}} = \gamma^{+}_{\mathrm{D}}\mathbf{E}^{\mathrm{refl}} + \gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{i}} \quad \text{and} \quad \gamma^{-}_{\mathrm{N}_{\kappa_-}}\mathbf{E}^{\mathrm{tran}} = \rho^{-1}\left(\gamma^{+}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{refl}} + \gamma^{-}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{i}}\right). \tag{4.7}$$

We apply them in (4.6) and then insert the potential ansatz (4.2) for $\mathbf{E}^{\mathrm{tran}}$:

$$\rho C^{\alpha}_{\kappa_+}\gamma^{-}_{\mathrm{N}_{\kappa_-}}\Psi^{\alpha}_{\mathrm{E}_{\kappa_-}}\mathbf{j} + \left(M^{\alpha}_{\kappa_+} + \mathrm{I}\right)\gamma^{-}_{\mathrm{D}}\Psi^{\alpha}_{\mathrm{E}_{\kappa_-}}\mathbf{j} = 2\gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{i}}. \tag{4.8}$$

With the jump relations (3.9)-(3.10), we finally obtain the integral equation

$$\mathbf{A}_{\alpha}\mathbf{j} = -2\gamma^{-}_{\mathrm{D}}\mathbf{E}^{\mathrm{i}} \quad \text{on } \Gamma, \tag{4.9}$$

where $\mathbf{A}_{\alpha} := \rho C^{\alpha}_{\kappa_+}\left(M^{\alpha}_{\kappa_-} + \mathrm{I}\right) + \left(M^{\alpha}_{\kappa_+} + \mathrm{I}\right)C^{\alpha}_{\kappa_-}$ maps $\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_{\Gamma}, \Gamma)$ into itself.

4.2 Equivalence

By applying the Dirichlet trace γ_{D}^{-} to the assumed electric potential ansatz (4.2), we easily deduce from the jump relation (3.9) that any solution of the electromagnetic scattering problem provides a solution of the singular integral equation (4.9) if the boundary integral operator $C_{\kappa_-}^{\alpha}$ is invertible. In the following lemma, we show that, if the nullspace of $C_{\kappa_+}^{\alpha}$ is trivial, any solution of (4.9) is a solution of the electromagnetic scattering problem. The invertibility of $C_{\kappa_\pm}^{\alpha}$ translates to $\ker(C_{\kappa_\pm}^{\alpha}) = \{0\}$ since $C_{\kappa_\pm}^{\alpha}$ are Fredholm of index zero by Lemma 3.14. By Remark 3.18, it is still unclear for which wave numbers $\kappa_\pm$ the operator $C_{\kappa_\pm}^{\alpha}$ is invertible but it seems as though the requirement $\ker(C_{\kappa_\pm}^{\alpha}) = \{0\}$, frequently encountered throughout this article, is not a strong restriction as long as Γ can be represented as the graph of a function.

Lemma 4.1 (Equivalence)**.** *Let* $\mathbf{j} \in \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$ *be a solution of (4.9). Moreover, assume that* $\ker(C_{\kappa_+}^{\alpha}) = \{0\}$*. Then the functions*

$$\mathbf{E}^{\mathrm{refl}} = -\frac{1}{2}\left[\rho \Psi_{\mathrm{E}_{\kappa_+}}^{\alpha}\left(M_{\kappa_-}^{\alpha} + \mathrm{I}\right)\mathbf{j} + \Psi_{\mathrm{M}_{\kappa_+}}^{\alpha} C_{\kappa_-}^{\alpha}\mathbf{j}\right] \qquad \text{in } G_+, \tag{4.10}$$

$$\mathbf{E}^{\mathrm{tran}} = \Psi_{\mathrm{E}_{\kappa_-}}^{\alpha}\mathbf{j} \qquad \text{in } G_- \tag{4.11}$$

solve the electromagnetic scattering problem (2.6)-(2.11).

Proof. Lemma 3.9 ensures that, for any density $\mathbf{j} \in \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$, the electric field $\mathbf{E}^{\mathrm{tran}}$ defined by (4.11) is an α-quasiperiodic solution of $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa_-^2\mathbf{E} = 0$ in G_- satisfying the outgoing wave condition (2.10)-(2.11). Moreover, since the Dirichlet and Neumann traces $\gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{tran}}, \gamma_{\mathrm{N}_{\kappa_-}}^{-}\mathbf{E}^{\mathrm{tran}}$ lie in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$, Lemma 3.9 implies that the function

$$\mathbf{E}^{\mathrm{refl}} = \frac{1}{2}\left(\rho \Psi_{\mathrm{E}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{N}_{\kappa_-}}^{-}\mathbf{E}^{\mathrm{tran}} + \Psi_{\mathrm{M}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{tran}}\right) \tag{4.12}$$

is an $\mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl}, G_+)$-regular solution of $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E} - \kappa_+^2\mathbf{E} = 0$ in G_+, for which the outgoing wave condition is fulfilled. Therefore, it remains to verify the transmission conditions (4.7).

The identities (3.9)-(3.10) yield $\gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{tran}} = -C_{\kappa_-}^{\alpha}\mathbf{j}$ and $\gamma_{\mathrm{N}_{\kappa_-}}^{-}\mathbf{E}^{\mathrm{tran}} = -\left(M_{\kappa_-}^{\alpha} + \mathrm{I}\right)\mathbf{j}$ from which

$$\mathbf{E}^{\mathrm{refl}} = -\frac{1}{2}\left[\rho \Psi_{\mathrm{E}_{\kappa_+}}^{\alpha}\left(M_{\kappa_-}^{\alpha} + \mathrm{I}\right)\mathbf{j} + \Psi_{\mathrm{M}_{\kappa_+}}^{\alpha} C_{\kappa_-}^{\alpha}\mathbf{j}\right]$$

is derived. With $\gamma_{\mathrm{D}}^{+}\Psi_{\mathrm{E}_{\kappa_+}}^{\alpha} = -C_{\kappa_+}^{\alpha}$ and $\gamma_{\mathrm{D}}^{+}\Psi_{\mathrm{M}_{\kappa_+}}^{\alpha} = \left(\mathrm{I} - M_{\kappa_+}^{\alpha}\right)$, we obtain $(4.7)_1$:

$$\begin{aligned}\gamma_{\mathrm{D}}^{+}\mathbf{E}^{\mathrm{refl}} &= \frac{1}{2}\left[\rho C_{\kappa_+}^{\alpha}\left(M_{\kappa_-}^{\alpha} + \mathrm{I}\right)\mathbf{j} + \left(M_{\kappa_+}^{\alpha} + \mathrm{I}\right)C_{\kappa_-}^{\alpha}\mathbf{j}\right] - C_{\kappa_-}^{\alpha}\mathbf{j} \\ &\overset{(4.9),(4.11)}{=} \gamma_{\mathrm{D}}^{-}\left(\mathbf{E}^{\mathrm{tran}} - \mathbf{E}^{\mathrm{i}}\right).\end{aligned}$$

For the proof of the second transmission condition $(4.7)_2$, we go back to (4.12). Using the first transmission condition $\gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{tran}} = \gamma_{\mathrm{D}}^{+}\mathbf{E}^{\mathrm{refl}} + \gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{i}}$ gives

$$\mathbf{E}^{\mathrm{refl}} = \frac{1}{2}\left(\rho \Psi_{\mathrm{E}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{N}_{\kappa_-}}^{-}\mathbf{E}^{\mathrm{tran}} + \Psi_{\mathrm{M}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{D}}^{+}\mathbf{E}^{\mathrm{refl}} + \Psi_{\mathrm{M}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{i}}\right). \tag{4.13}$$

We have the following special cases of the Stratton-Chu integral representation from Lemma 3.10 in G_+:

$$\mathbf{E}^{\mathrm{refl}} = \frac{1}{2}\left(\Psi_{\mathrm{M}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{D}}^{+}\mathbf{E}^{\mathrm{refl}} + \Psi_{\mathrm{E}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{N}_{\kappa_+}}^{+}\mathbf{E}^{\mathrm{refl}}\right) \text{ and } \Psi_{\mathrm{M}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{i}} = -\Psi_{\mathrm{E}_{\kappa_+}}^{\alpha}\gamma_{\mathrm{N}_{\kappa_+}}^{-}\mathbf{E}^{\mathrm{i}}.$$

Thus, equation (4.13) can be rewritten as

$$\frac{1}{2}\Psi^{\alpha}_{\mathrm{E}_{\kappa_+}}\left(\gamma^{+}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{refl}} + \gamma^{-}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{i}}\right) = \frac{1}{2}\Psi^{\alpha}_{\mathrm{E}_{\kappa_+}}\rho\gamma^{-}_{\mathrm{N}_{\kappa_-}}\mathbf{E}^{\mathrm{tran}}$$

$$\xRightarrow{\gamma^{+}_{\mathrm{D}},\,(3.9)} \quad C^{\alpha}_{\kappa_+}\left(\gamma^{+}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{refl}} + \gamma^{-}_{\mathrm{N}_{\kappa_+}}\mathbf{E}^{\mathrm{i}}\right) = C^{\alpha}_{\kappa_+}\rho\gamma^{-}_{\mathrm{N}_{\kappa_-}}\mathbf{E}^{\mathrm{tran}}.$$

Clearly, this verifies the second transmission condition in (4.7) if $\ker(C^{\alpha}_{\kappa_+}) = \{0\}$, since then $C^{\alpha}_{\kappa_+}$, a Fredholm operator of index zero, is invertible in $\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_{\Gamma}, \Gamma)$. □

5 Solvability of the boundary integral equation

In the following, we identify conditions for the electromagnetic material parameters and the boundary integral operators $C^{\alpha}_{\kappa_\pm}$ such that the operator

$$\mathbf{A}_{\alpha} = \rho C^{\alpha}_{\kappa_+}\left(M^{\alpha}_{\kappa_-} + \mathrm{I}\right) + \left(M^{\alpha}_{\kappa_+} + \mathrm{I}\right) C^{\alpha}_{\kappa_-}$$

from the left-hand side of the singular integral equation (4.9) is Fredholm of index zero in the Hilbert space $\mathbf{H}^{-1/2}_{\alpha}(\mathrm{div}_{\Gamma}, \Gamma)$ for smooth and - under more restrictive assumptions - for polyhedral Lipschitz regular grating surfaces Γ. This property makes it possible to prove that solutions to (4.9) exist. Additionally, we present parameter choices that even provide unique solutions.

5.1 Fredholmness

Depending on the values of the electric permittivities $\epsilon_\pm$ and the magnetic permeabilities $\mu_\pm$, we obtain two Gårding inequalities for smooth grating profiles Γ. They are featured in the subsequent theorem.

Theorem 5.1 (Gårding inequalities for smooth Γ)**.** *Let the auxiliary functions $f_{\mathrm{Re}} : \mathbb{C} \times \mathbb{C} \to \mathbb{R}$ and $f_{\mathrm{Im}} : \mathbb{C} \times \mathbb{C} \to \mathbb{R}$ be defined by*

$$f_{\mathrm{Re}}(z_1, z_2) := \frac{\mathrm{Re}(z_1)\,\mathrm{Re}(z_2)}{|z_2|^2} \quad \textit{and} \quad f_{\mathrm{Im}}(z_1, z_2) := \frac{\mathrm{Im}(z_1)\,\mathrm{Im}(z_2)}{|z_2|^2}.$$

Moreover, assume that Γ is smooth and $\epsilon_\pm$, $\mu_\pm$ fulfill the conditions (2.2). In the case that either

(i) $f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-) \geq 0$ and $f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) \geq 0$, or

(ii) $f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-) \geq 0$, $f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) < 0$ and

$$|\mathrm{Re}\,(\mu_+)| \geq |\mathrm{Re}\,(\mu_-)|$$

with $|\mathrm{Re}\,(\mu_+)| = |\mathrm{Re}\,(\mu_-)|$ only if $\mathrm{Im}(\mu_+) > 0$, or

(iii) $f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-) < 0$, $f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) \geq 0$ and

$$|\mathrm{Re}\,(\epsilon_+)| \leq |\mathrm{Re}\,(\epsilon_-)|$$

with $|\mathrm{Re}\,(\epsilon_+)| = |\mathrm{Re}\,(\epsilon_-)|$ only if $\mathrm{Im}(\epsilon_-) > 0$, or *(iv)* $f_{\mathrm{Re}}(\epsilon_+,\epsilon_-)+f_{\mathrm{Im}}(\epsilon_+,\epsilon_-)<0$, $f_{\mathrm{Re}}(\mu_-,\mu_+)+f_{\mathrm{Im}}(\mu_-,\mu_+)<0$ *and*

$$|\mathrm{Re}\,(\epsilon_+)|\leq|\mathrm{Re}\,(\epsilon_-)| \qquad \textit{with equality only if } \mathrm{Im}(\epsilon_-)>0$$

if $|f_{\mathrm{Re}}(\epsilon_+,\epsilon_-)+f_{\mathrm{Im}}(\epsilon_+,\epsilon_-)|\geq|f_{\mathrm{Re}}(\mu_-,\mu_+)+f_{\mathrm{Im}}(\mu_-,\mu_+)|$, *or*

$$|\mathrm{Re}\,(\mu_+)|\geq|\mathrm{Re}\,(\mu_-)| \qquad \textit{with equality only if } \mathrm{Im}(\mu_+)>0$$

if $|f_{\mathrm{Re}}(\epsilon_+,\epsilon_-)+f_{\mathrm{Im}}(\epsilon_+,\epsilon_-)|<|f_{\mathrm{Re}}(\mu_-,\mu_+)+f_{\mathrm{Im}}(\mu_-,\mu_+)|$

holds, we have

$$\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j},\rho^{-1}\mathbf{A}_\alpha C^\alpha_{\kappa_+}C_0^{\alpha,*}\mathbf{j}\right)+C_{\mathrm{I}}\left(\mathbf{j},\mathbf{j}\right)\right)\geq c_{\mathrm{I}}\left\|\mathbf{j}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}, \tag{5.1}$$

where C_I is a compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form and c_I a positive constant.
In the case that either

(v) $f_{\mathrm{Re}}(\epsilon_-,\epsilon_+)+f_{\mathrm{Im}}(\epsilon_-,\epsilon_+)\geq 0$ *and* $f_{\mathrm{Re}}(\mu_+,\mu_-)+f_{\mathrm{Im}}(\mu_+,\mu_-)<0$ *and*

$$|\mathrm{Re}\,(\mu_+)|\leq|\mathrm{Re}\,(\mu_-)|$$

with $|\mathrm{Re}\,(\mu_+)|=|\mathrm{Re}\,(\mu_-)|$ *only if* $\mathrm{Im}(\mu_-)>0$, *or*

(vi) $f_{\mathrm{Re}}(\epsilon_-,\epsilon_+)+f_{\mathrm{Im}}(\epsilon_-,\epsilon_+)<0$, $f_{\mathrm{Re}}(\mu_+,\mu_-)+f_{\mathrm{Im}}(\mu_+,\mu_-)\geq 0$ *and*

$$|\mathrm{Re}\,(\epsilon_+)|\geq|\mathrm{Re}\,(\epsilon_-)|$$

with $|\mathrm{Re}\,(\epsilon_+)|=|\mathrm{Re}\,(\epsilon_-)|$ *only if* $\mathrm{Im}(\epsilon_+)>0$, *or*

(vii) $f_{\mathrm{Re}}(\epsilon_-,\epsilon_+)+f_{\mathrm{Im}}(\epsilon_-,\epsilon_+)<0$, $f_{\mathrm{Re}}(\mu_+,\mu_-)+f_{\mathrm{Im}}(\mu_+,\mu_-)<0$ *and*

$$|\mathrm{Re}\,(\epsilon_+)|\geq|\mathrm{Re}\,(\epsilon_-)| \qquad \textit{with equality only if } \mathrm{Im}(\epsilon_+)>0$$

if $|f_{\mathrm{Re}}(\epsilon_-,\epsilon_+)+f_{\mathrm{Im}}(\epsilon_-,\epsilon_+)|\geq|f_{\mathrm{Re}}(\mu_+,\mu_-)+f_{\mathrm{Im}}(\mu_+,\mu_-)|$, *or*

$$|\mathrm{Re}\,(\mu_+)|\leq|\mathrm{Re}\,(\mu_-)| \qquad \textit{with equality only if } \mathrm{Im}(\mu_-)>0$$

if $|f_{\mathrm{Re}}(\epsilon_-,\epsilon_+)+f_{\mathrm{Im}}(\epsilon_-,\epsilon_+)|<|f_{\mathrm{Re}}(\mu_+,\mu_-)+f_{\mathrm{Im}}(\mu_+,\mu_-)|$

is fulfilled, we have the Gårding inequality

$$\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j},-\mathbf{A}_\alpha C^\alpha_{\kappa_-}C_0^{\alpha,*}\mathbf{j}\right)+C_{\mathrm{II}}(\mathbf{j},\mathbf{j})\right)\geq c_{\mathrm{II}}\left\|\mathbf{j}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}, \tag{5.2}$$

where C_{II} is a compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form and c_{II} a positive constant.

In order to prove Theorem 5.1 in a structured manner, we specify two auxiliary results for its proof after its main implication, which states that the operator $\mathbf{A}_\alpha$ is Fredholm of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$ under certain assumptions on the electromagnetic material parameters.

Corollary 5.2 (Fredholmness for smooth Γ)**.** *Let the assumptions of Theorem 5.1 hold. Moreover, assume that the electromagnetic material parameters satisfy*

$$\epsilon_+ \neq -\epsilon_- \quad \textit{and} \quad \mu_+ \neq -\mu_-. \tag{5.3}$$

Then $\mathbf{A}_\alpha$ is a Fredholm operator of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$.

Proof. The Fredholmness of the operator $\mathbf{A}_\alpha$ is deduced from the Gårding inequalities given by Theorem 5.1 following the argumentation of the proof of Lemma 3.15. The condition (5.3) unifies the conditions (i)-(vii) from the previous theorem. For a fixed density $\mathbf{m} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$, let $\mathbf{B}_\mathrm{c}\mathbf{m}$ be the bounded linear functional from (3.23) and $\mathbf{B}_\mathrm{c}$ the thereby generated bounded linear operator. Furthermore, denote by K_I, K_{II} the compact operators corresponding to the compact $\mathcal{B}_\mathrm{c}$-related bilinear forms C_I and C_{II}. Depending on the values of $\epsilon_\pm$ and $\mu_\pm$, we can then show with the help of (5.1) or (5.2) that

$$\rho^{-1} j \mathbf{B}_\mathrm{c} \mathbf{A}_\alpha C_{\kappa_+}^\alpha C_0^{\alpha,*} + jK_1 \quad \text{or} \quad -j\mathbf{B}_\mathrm{c}\mathbf{A}_\alpha C_{\kappa_-}^\alpha C_0^{\alpha,*} + jK_2,$$

are invertible by the Lax-Milgram theorem from [16, Theorem 5.2.3]. We recall that j is the Riesz isomorphism. Since $C_0^{\alpha,*}$ is invertible by Lemma 3.22, and the operators $C_{\kappa_\pm}^\alpha$ and $M_\mathrm{i}^\alpha \pm \mathrm{I}$ are Fredholm operators of index zero by Lemmata 3.14 and 3.19, we conclude, arguing as in the proof of Lemma 3.15, that also $\mathbf{A}_\alpha$ is a Fredholm operator of index zero in $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$. □

Auxiliary results

We define the auxiliary operators

$$I_1^\pm := -(C_{\kappa_\pm}^\alpha)^2 C_0^{\alpha,*} \quad \text{and} \quad I_2^\pm := -C_{\kappa_\pm,0}^\alpha C_{\kappa_\mp,0}^\alpha C_0^{\alpha,*}. \tag{5.4}$$

Technically relevant representations of $I_1^\pm$ and $I_2^\pm$ are given below.

Lemma 5.3. *Each of the operators I_1^+ and I_1^- have the two representations*

$$I_1^\pm = -\left(\mathrm{I} + M_\mathrm{i}^\alpha\right) C_0^{\alpha,*} \left(\mathrm{I} + M_\mathrm{i}^\alpha\right) + C_{1,+}^\pm \quad \textit{or} \tag{5.5}$$

$$I_1^\pm = -\left(\mathrm{I} - M_\mathrm{i}^\alpha\right) C_0^{\alpha,*} \left(\mathrm{I} - M_\mathrm{i}^\alpha\right) + C_{1,-}^\pm, \tag{5.6}$$

where $C_{1,+}^\pm$ and $C_{1,-}^\pm$ are compact operators. If Γ is smooth, we even have

$$I_1^\pm = -C_0^{\alpha,*} + C_1^\pm \tag{5.7}$$

with a compact operator $C_1^\pm$. The operator $I_2^\pm$ can be represented as

$$I_2^\pm = \left(\kappa_\pm \kappa_\mp^{-1} R_0^\alpha T_0^\alpha + \kappa_\pm^{-1}\kappa_\mp T_0^\alpha R_0^\alpha\right) C_0^{\alpha,*} + C_2^\pm, \tag{5.8}$$

where $C_2^\pm$ is a compact operator.

Moreover, we have

$$-\mathcal{B}_\mathrm{c}\left(\mathbf{j}, R_0^\alpha T_0^\alpha R_0^\alpha \mathbf{j}\right) = \int_\Gamma \left(\mathrm{div}_\Gamma(\gamma_\mathrm{D}(V_0^\alpha \mathbf{j}))\right) \overline{V_0^\alpha\, \mathrm{div}_\Gamma(\gamma_\mathrm{D}(V_0^\alpha \mathbf{j}))}\, d\sigma \geq 0, \tag{5.9}$$

$$-\mathcal{B}_\mathrm{c}\left(\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \mathbf{j}\right) = \int_\Gamma \left(i_\pi\, \mathbf{curl}_\Gamma\, V_0^\alpha\, \mathrm{div}_\Gamma\, \mathbf{j}\right) \cdot \overline{V_0^\alpha\left(i_\pi\, \mathbf{curl}_\Gamma\, V_0^\alpha\, \mathrm{div}_\Gamma\, \mathbf{j}\right)}\, d\sigma \geq 0 \tag{5.10}$$

for $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$.

Proof. We first derive the two representations (5.5) and (5.6) of $I_1^+ = -(C^\alpha_{\kappa_+})^2 C_0^{\alpha,*}$. The first Calderon relation $(3.17)_1$ yields

$$\left(C^\alpha_{\kappa_+}\right)^2 = \mathrm{I} - \left(M^\alpha_{\kappa_+}\right)^2 = \left(\mathrm{I} \pm M^\alpha_{\kappa_+}\right)\left(\mathrm{I} \mp M^\alpha_{\kappa_+}\right) = \left(\mathrm{I} \pm M^\alpha_{\mathrm{i}}\right)\left(\mathrm{I} \mp M^\alpha_{\mathrm{i}}\right)$$
$$\underbrace{\pm\left(M^\alpha_{\kappa_+} - M^\alpha_{\mathrm{i}}\right)\left(\mathrm{I} \mp M^\alpha_{\kappa_+}\right) \mp \left(\mathrm{I} \pm M^\alpha_{\mathrm{i}}\right)\left(M^\alpha_{\kappa_+} - M^\alpha_{\mathrm{i}}\right)}_{=: C^+_{11,\pm}},$$

where $C^+_{11,\pm}$ is compact due to (3.14). Next, we use the representation (3.13) of $C_0^{\alpha,*}$, the second Calderon relation $(3.17)_2$ and Lemma 3.12 to arrive at

$$\begin{aligned}
\left(\mathrm{I} \mp M^\alpha_{\mathrm{i}}\right) C_0^{\alpha,*} &= C_0^{\alpha,*} \mp \mathrm{i} M^\alpha_{\mathrm{i}} C^\alpha_{\mathrm{i}} \underbrace{\mp \mathrm{i} M^\alpha_{\mathrm{i}}\left(C^\alpha_{\mathrm{i},0} - C^\alpha_{\mathrm{i}}\right)}_{=: C^+_{12,\pm} \text{ (compact)}} \\
&= C_0^{\alpha,*} \pm \mathrm{i} C^\alpha_{\mathrm{i}} M^\alpha_{\mathrm{i}} + C^+_{12,\pm} \\
&= C_0^{\alpha,*}\left(\mathrm{I} \pm M^\alpha_{\mathrm{i}}\right) \underbrace{\pm \mathrm{i}\left(C^\alpha_{\mathrm{i}} - C^\alpha_{\mathrm{i},0}\right) M^\alpha_{\mathrm{i}}}_{=: C^+_{13,\pm} \text{ (compact)}} + C^+_{12,\pm}.
\end{aligned}$$

Collecting the results above, we have verified the representations (5.5) and (5.6) for I_1^+ with the compact operator $C^+_{1,\pm} := -C^+_{11,\pm} C_0^{\alpha,*} - \left(\mathrm{I} \pm M^\alpha_{\mathrm{i}}\right)\left(C^+_{12,\pm} + C^+_{13,\pm}\right)$. Analogously, we obtain (5.5) and (5.6) for I_1^-. For smooth Γ, the representation (5.7) easily arises from the representation (5.5) recalling that M^α_{i} is a compact operator according to Lemma 3.12 in this case.

Next, we derive an alternative representation of the operator $I_2^\pm$. The definitions (3.11)-(3.12) and Lemma 3.11 yield

$$\begin{aligned}
I_2^\pm &= -C^\alpha_{\kappa_\pm,0} C^\alpha_{\kappa_\mp,0} C_0^{\alpha,*} = -\left(-\kappa_\pm R_0^\alpha + \kappa_\pm^{-1} T_0^\alpha\right)\left(-\kappa_\mp R_0^\alpha + \kappa_\mp^{-1} T_0^\alpha\right) C_0^{\alpha,*} \\
&= \left(\kappa_\pm \kappa_\mp^{-1} R_0^\alpha T_0^\alpha + \kappa_\pm^{-1} \kappa_\mp T_0^\alpha R_0^\alpha\right) C_0^{\alpha,*} \underbrace{- \kappa_\pm \kappa_\mp \left(R_0^\alpha\right)^2 C_0^{\alpha,*}}_{=: C_2^\pm \text{ (compact)}},
\end{aligned}$$

which proves (5.8).

Together with the properties of the rotation operator r and Lemma 3.3, (3.1), (3.7) as well as the self-adjointness and the ellipticity of V_0^α in the sense of Lemma 3.20, we finally verify (5.9) and (5.10) by rigorous calculations. ☐

Lemma 5.4. *For* $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$*, we have*

$$\mathcal{B}_\mathrm{c}(\mathbf{j}, R_0^\alpha T_0^\alpha C_0^{\alpha,*}\mathbf{j}) = \mathcal{B}_\mathrm{c}\left(\mathbf{j}, R_0^\alpha T_0^\alpha R_0^\alpha \mathbf{j}\right), \tag{5.11}$$
$$\mathcal{B}_\mathrm{c}(\mathbf{j}, T_0^\alpha R_0^\alpha C_0^{\alpha,*}\mathbf{j}) = \mathcal{B}_\mathrm{c}\left(\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \mathbf{j}\right) + C_1(\mathbf{j}, \mathbf{j}), \tag{5.12}$$

where C_1 is a compact $\mathcal{B}_\mathrm{c}$-related sesquilinear form.

If Γ is smooth, we moreover have

$$-\mathcal{B}_\mathrm{c}(\mathbf{j}, R_0^\alpha T_0^\alpha R_0^\alpha \mathbf{j}) - \mathcal{B}_\mathrm{c}(\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \mathbf{j}) = \mathcal{B}_\mathrm{c}\left(\mathbf{j}, C_0^{\alpha,*}\mathbf{j}\right) + \mathrm{Re}\left(C_2(\mathbf{j}, \mathbf{j})\right) \tag{5.13}$$

with a compact $\mathcal{B}_\mathrm{c}$-related sesquilinear form C_2.

Proof. With the identity $\left(T_0^\alpha\right)^2 = 0$ from Lemma 3.11, we easily obtain

$$\mathcal{B}_\mathrm{c}(\mathbf{j}, R_0^\alpha T_0^\alpha C_0^{\alpha,*}\mathbf{j}) = \mathcal{B}_\mathrm{c}(\mathbf{j}, R_0^\alpha T_0^\alpha R_0^\alpha \mathbf{j}),$$

which coincides with (5.11). In a similar way, we observe that

$$\mathcal{B}_{\mathrm{c}}(\mathbf{j}, T_0^\alpha R_0^\alpha C_0^{\alpha,*}\mathbf{j}) \overset{(5.10)}{=} \mathcal{B}_{\mathrm{c}}(\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \mathbf{j}) + C_1(\mathbf{j},\mathbf{j}),$$

where $C_1(\cdot,\cdot) := \mathcal{B}_{\mathrm{c}}(\cdot, C_{11}\cdot)$ with the compact operator $C_{11} := T_0^\alpha (R_0^\alpha)^2$ is a compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form. This gives (5.12).

Now, assume that Γ is smooth. It remains to prove the representation (5.13). Lemma 3.11 as well as the previously proven identities (5.11) and (5.12) yield that

$$\begin{aligned} -\mathcal{B}_{\mathrm{c}}(\mathbf{j}, R_0^\alpha T_0^\alpha R_0^\alpha \mathbf{j}) - \mathcal{B}_{\mathrm{c}}(\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \mathbf{j}) &= -\mathcal{B}_{\mathrm{c}}(\mathbf{j}, (C_0^{\alpha,*})^3\mathbf{j}) - \mathcal{B}_{\mathrm{c}}(\mathbf{j}, (R_0^\alpha)^2 C_0^{\alpha,*}\mathbf{j}) \\ &\quad + C_1(\mathbf{j},\mathbf{j}) \\ &\overset{(3.13)}{=} \mathcal{B}_{\mathrm{c}}(\mathbf{j}, (C_{\mathrm{i}}^\alpha)^2 C_0^{\alpha,*}\mathbf{j}) + C(\mathbf{j},\mathbf{j}), \end{aligned}$$

where

$$\begin{aligned} C(\cdot,\cdot) := &-\mathcal{B}_{\mathrm{c}}(\cdot, (R_0^\alpha)^2 C_0^{\alpha,*}\cdot) + C_1(\cdot,\cdot) + \mathcal{B}_{\mathrm{c}}(\cdot, (C_{\mathrm{i},0}^\alpha - C_{\mathrm{i}}^\alpha)^2 C_0^{\alpha,*}\cdot) \\ &+ \mathcal{B}_{\mathrm{c}}(\cdot, C_{\mathrm{i}}^\alpha (C_{\mathrm{i},0}^\alpha - C_{\mathrm{i}}^\alpha) C_0^{\alpha,*}\cdot) + \mathcal{B}_{\mathrm{c}}(\cdot, (C_{\mathrm{i},0}^\alpha - C_{\mathrm{i}}^\alpha) C_{\mathrm{i}}^\alpha C_0^{\alpha,*}\cdot) \end{aligned}$$

is a compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form by Lemmata 3.11 and 3.12. With the help of the first Calderon relation $(3.17)_1$ for C_{i}^α, we then deduce that

$$\begin{aligned} -\mathcal{B}_{\mathrm{c}}(\mathbf{j}, R_0^\alpha T_0^\alpha R_0^\alpha \mathbf{j}) - \mathcal{B}_{\mathrm{c}}(\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \mathbf{j}) = \mathcal{B}_{\mathrm{c}}(\mathbf{j}, C_0^{\alpha,*}\mathbf{j}) - \mathcal{B}_{\mathrm{c}}(\mathbf{j}, (M_{\mathrm{i}}^\alpha)^2 C_0^{\alpha,*}\mathbf{j}) \\ + C(\mathbf{j},\mathbf{j}). \end{aligned}$$

By Lemma 3.12, the operator M_{i}^α and thus the sesquilinear form $\mathcal{B}_{\mathrm{c}}(\cdot, (M_{\mathrm{i}}^\alpha)^2 C_0^{\alpha,*}\cdot)$ are compact. Therefore, (5.13) holds for the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form

$$C_2(\cdot,\cdot) := C(\cdot,\cdot) - \mathcal{B}_{\mathrm{c}}(\cdot, (M_{\mathrm{i}}^\alpha)^2 C_0^{\alpha,*}\cdot).$$

□

With the help of the above auxiliary lemmata, we now deduce the existence of Gårding inequalities for the operator $\mathbf{A}_\alpha$ as stated in Theorem 5.1.

Proof of Theorem 5.1. We only consider the proof of the Gårding inequality (5.1), the inequality (5.2) is shown analogously. We first assume that $\tilde{\alpha} \notin \mathbb{Z}^2$. With the second Calderon relation $(3.17)_2$, we rewrite $\mathbf{A}_\alpha$ as

$$\mathbf{A}_\alpha = \rho C_{\kappa_+}^\alpha + C_{\kappa_-,0}^\alpha + C_{11},$$

where the operator C_{11} defined by $C_{11} := \rho C_{\kappa_+}^\alpha M_{\kappa_-}^\alpha + M_{\kappa_+}^\alpha C_{\kappa_-}^\alpha + (C_{\kappa_-}^\alpha - C_{\kappa_-,0}^\alpha)$ is compact according to Lemma 3.12. In other words: $\mathbf{A}_\alpha$ is a compact perturbation of

$$\mathbf{A}_\alpha^{\mathrm{I}} := \rho C_{\kappa_+}^\alpha + C_{\kappa_-,0}^\alpha$$

and it remains to prove a Gårding inequality of the form (5.1) for the operator

$$I_\alpha^{\mathrm{I}} := \rho^{-1} \mathbf{A}_\alpha^{\mathrm{I}} C_{\kappa_+}^\alpha C_0^{\alpha,*}$$

instead of for $\rho^{-1}\mathbf{A}_\alpha C_{\kappa_+}^\alpha C_0^{\alpha,*}$. The operator I_α^{I} can be expressed as

$$I_\alpha^{\mathrm{I}} \overset{(5.4)}{=} -I_1^+ - \rho^{-1} I_2^- + C_{12} \tag{5.14}$$

with the operator $C_{12} := \rho^{-1} C^{\alpha}_{\kappa_-,0}(C^{\alpha}_{\kappa_+,0} - C^{\alpha}_{\kappa_+})C^{\alpha,*}_0$ that is compact by Lemma 3.12. Next, we separately study the first two operators on the right-hand side of (5.14). By (5.7) from Lemma 5.3, there exists a compact $\mathcal{B}_{\rm c}$-related sesquilinear form $C^{\rm I}_1$ such that

$$-\operatorname{Re}\left(\mathcal{B}_{\rm c}\left(\mathbf{j}, I_1^+\mathbf{j}\right)\right) + \operatorname{Re}\left(C^{\rm I}_1(\mathbf{j},\mathbf{j})\right) = \mathcal{B}_{\rm c}\left(\mathbf{j}, C^{\alpha,*}_0\mathbf{j}\right). \tag{5.15}$$

We now use the representation (5.8) of I_2^- from Lemma 5.3 with a compact operator C_{13} and the fact that the identities (5.9) and (5.10) imply that $\mathcal{B}_{\rm c}\left(\mathbf{j}, R^{\alpha}_0 T^{\alpha}_0 R^{\alpha}_0\mathbf{j}\right) \in \mathbb{R}$ and $\mathcal{B}_{\rm c}\left(\mathbf{j}, T^{\alpha}_0 R^{\alpha}_0 T^{\alpha}_0\mathbf{j}\right) \in \mathbb{R}$ for $\mathbf{j} \in \mathbf{H}^{-1/2}_{\alpha}(\operatorname{div}_\Gamma, \Gamma)$ to obtain

$$\begin{aligned}
-\operatorname{Re}\left(\mathcal{B}_{\rm c}\left(\mathbf{j}, \rho^{-1} I_2^-\mathbf{j}\right)\right) \overset{(5.8)}{=}\; & -\operatorname{Re}\left(\frac{\overline{\mu}_-}{\overline{\mu}_+}\mathcal{B}_{\rm c}\left(\mathbf{j}, R^{\alpha}_0 T^{\alpha}_0 C^{\alpha,*}_0\mathbf{j}\right)\right) \\
& -\operatorname{Re}\left(\frac{\overline{\epsilon}_+}{\overline{\epsilon}_-}\mathcal{B}_{\rm c}\left(\mathbf{j}, T^{\alpha}_0 R^{\alpha}_0 C^{\alpha,*}_0\mathbf{j}\right)\right) \\
& -\operatorname{Re}\left(\overline{\rho}^{-1}\mathcal{B}_{\rm c}\left(\mathbf{j}, C_{13}\mathbf{j}\right)\right) \\
\overset{(5.11),(5.12)}{=}\; & -\operatorname{Re}\left(\frac{\overline{\mu}_-}{\overline{\mu}_+}\mathcal{B}_{\rm c}\left(\mathbf{j}, R^{\alpha}_0 T^{\alpha}_0 R^{\alpha}_0\mathbf{j}\right)\right) \\
& -\operatorname{Re}\left(\frac{\overline{\epsilon}_+}{\overline{\epsilon}_-}\mathcal{B}_{\rm c}\left(\mathbf{j}, T^{\alpha}_0 R^{\alpha}_0 T^{\alpha}_0\mathbf{j}\right)\right) \\
& +\operatorname{Re}\left(\frac{\overline{\epsilon}_+}{\overline{\epsilon}_-}C_1(\mathbf{j},\mathbf{j})\right) - \operatorname{Re}\left(\overline{\rho}^{-1}\mathcal{B}_{\rm c}\left(\mathbf{j}, C_{13}\mathbf{j}\right)\right) \\
\overset{(5.9),(5.10)}{=}\; & -\operatorname{Re}\left(\frac{\overline{\mu}_-}{\overline{\mu}_+}\right)\mathcal{B}_{\rm c}\left(\mathbf{j}, R^{\alpha}_0 T^{\alpha}_0 R^{\alpha}_0\mathbf{j}\right) \\
& -\operatorname{Re}\left(\frac{\overline{\epsilon}_+}{\overline{\epsilon}_-}\right)\mathcal{B}_{\rm c}\left(\mathbf{j}, T^{\alpha}_0 R^{\alpha}_0 T^{\alpha}_0\mathbf{j}\right) + \operatorname{Re}\left(C^{\rm I}_2(\mathbf{j},\mathbf{j})\right),
\end{aligned} \tag{5.16}$$

where the compact $\mathcal{B}_{\rm c}$-related sesquilinear form $C^{\rm I}_2$ is given by

$$C^{\rm I}_2(\cdot,\cdot) := -\frac{\overline{\epsilon}_+}{\overline{\epsilon}_-}C_1(\cdot,\cdot) - \overline{\rho}^{-1}\mathcal{B}_{\rm c}\left(\cdot, C_{13}\cdot\right)$$

with the compact $\mathcal{B}_{\rm c}$-related sesquilinear form C_1 from (5.12). The two quotients of material parameters occurring in (5.16) can be reformulated as

$$\operatorname{Re}\left(\frac{\overline{\mu}_-}{\overline{\mu}_+}\right) = f_{\rm Re}(\mu_-,\mu_+) + f_{\rm Im}(\mu_-,\mu_+)$$

and

$$\operatorname{Re}\left(\frac{\overline{\epsilon}_+}{\overline{\epsilon}_-}\right) = f_{\rm Re}(\epsilon_+,\epsilon_-) + f_{\rm Im}(\epsilon_+,\epsilon_-).$$

Therefore, (5.16) reads as

$$\begin{aligned}
&-\operatorname{Re}\left(\mathcal{B}_{\rm c}\left(\mathbf{j}, \rho^{-1} I_2^-\mathbf{j}\right)\right) \\
&\qquad\geq -\left(f_{\rm Re}(\mu_-,\mu_+) + f_{\rm Im}(\mu_-,\mu_+)\right)\mathcal{B}_{\rm c}\left(\mathbf{j}, R^{\alpha}_0 T^{\alpha}_0 R^{\alpha}_0\mathbf{j}\right) \\
&\qquad\quad -\left(f_{\rm Re}(\epsilon_+,\epsilon_-) + f_{\rm Im}(\epsilon_+,\epsilon_-)\right)\mathcal{B}_{\rm c}\left(\mathbf{j}, T^{\alpha}_0 R^{\alpha}_0 T^{\alpha}_0\mathbf{j}\right) + \operatorname{Re}\left(C^{\rm I}_2(\mathbf{j},\mathbf{j})\right).
\end{aligned}$$

Summarizing the considerations up to now gives

$$\begin{aligned}\operatorname{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathrm{j}, \rho^{-1}\mathbf{A}_\alpha C^\alpha_{\kappa_+} C^{\alpha,*}_0 \mathbf{j}\right) + C_{\mathrm{I},1}(\mathbf{j},\mathbf{j})\right) \\ \geq \mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C^{\alpha,*}_0\mathbf{j}\right) - (f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+))\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, R^\alpha_0 T^\alpha_0 R^\alpha_0 \mathbf{j}\right) \\ - (f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-))\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, T^\alpha_0 R^\alpha_0 T^\alpha_0 \mathbf{j}\right)\end{aligned} \tag{5.17}$$

with the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form $C_{\mathrm{I},1}$:

$$C_{\mathrm{I},1}(\cdot,\cdot) \coloneqq -\mathcal{B}_{\mathrm{c}}(\cdot, \rho^{-1}C_{11}C^\alpha_{\kappa_+}C^{\alpha,*}_0\cdot) - \mathcal{B}_{\mathrm{c}}\left(\cdot, C_{12}\cdot\right) + C^{\mathrm{I}}_1(\cdot,\cdot) - C^{\mathrm{I}}_2(\cdot,\cdot).$$

From here on, equation (5.17) serves as the basis for each of the four cases depending on the signs of $f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-)$ and $f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+)$ for which we want to prove (5.1).

Case (i): $f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-) \geq 0$ and $f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+) \geq 0.$

In this case, the positive definiteness of $-\mathcal{B}_{\mathrm{c}}(\cdot, R^\alpha_0 T^\alpha_0 R^\alpha_0\cdot)$ and $-\mathcal{B}_{\mathrm{c}}(\cdot, T^\alpha_0 R^\alpha_0 T^\alpha_0\cdot)$ ensured by (5.9) and (5.10), and the ellipticity of the operator $C^{\alpha,*}_0$ with respect to $\mathcal{B}_{\mathrm{c}}$ in the sense of Lemma 3.22 immediately imply the Gårding inequality

$$\operatorname{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \rho^{-1}\mathbf{A}_\alpha C^\alpha_{\kappa_+} C^{\alpha,*}_0 \mathbf{j}\right) + C_{\mathrm{I},1}(\mathbf{j},\mathbf{j})\right) \geq \mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C^{\alpha,*}_0\mathbf{j}\right) \overset{(3.31)}{\geq} c_{\mathrm{I},1}\left\|\mathbf{j}\right\|^2_{\mathbf{H}^{-\frac{1}{2}}_\alpha(\operatorname{div}_\Gamma,\Gamma)},$$

where $c_{\mathrm{I},1}$ is the positive constant from Lemma 3.22.

Case (ii): $f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-) \geq 0$, $f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+) < 0$ and

$$|\operatorname{Re}(\mu_+)| > |\operatorname{Re}(\mu_-)| \quad \text{with equality only if } \operatorname{Im}(\mu_+) > 0.$$

We apply the identity (5.13) from Lemma 5.4 in (5.17) and arrive at

$$\begin{aligned}&\operatorname{Re}\left[\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \rho^{-1}\mathbf{A}_\alpha C^\alpha_{\kappa_+} C^{\alpha,*}_0 \mathbf{j}\right) + C_{\mathrm{I},1}(\mathbf{j},\mathbf{j})\right] \\ &\overset{(5.13)}{\geq} \left(1 + f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+)\right)\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C^{\alpha,*}_0\mathbf{j}\right) \\ &\quad - \left[f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-) - (f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+))\right]\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, R^\alpha_0 T^\alpha_0 R^\alpha_0\mathbf{j}\right) \\ &\quad + \operatorname{Re}\left(C^{\mathrm{I}}_3(\mathbf{j},\mathbf{j})\right) \\ &\overset{(5.10)}{\geq} \left(1 + f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+)\right)\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C^{\alpha,*}_0\mathbf{j}\right) + \operatorname{Re}\left(C^{\mathrm{I}}_3(\mathbf{j},\mathbf{j})\right)\end{aligned}$$

with the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form C^{I}_3 given by

$$C^{\mathrm{I}}_3(\cdot,\cdot) \coloneqq (f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+))\mathcal{B}_{\mathrm{c}}\left(\cdot, C_2\cdot\right),$$

where C_2 is the compact operator corresponding to the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form from (5.13). Since here we have $f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+) < 0$ and $|\operatorname{Re}(\mu_+)| > |\operatorname{Re}(\mu_-)|$) with equality only if $\operatorname{Im}(\mu_+) > 0$, and

$$f_{\mathrm{Im}}(\mu_-,\mu_+) = \frac{\operatorname{Im}(\mu_-)\operatorname{Im}(\mu_+)}{|\mu_+|^2} \geq 0$$

due to (2.2), we observe that if $\operatorname{Im}(\mu_+) = 0$, then

$$1 + f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+) > 1 - \frac{|\operatorname{Re}(\mu_+)|^2}{|\mu_+|^2} = 0$$

and if $\mathrm{Im}(\mu_+) > 0$, then

$$1 + f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) \geq 1 - \frac{|\mathrm{Re}(\mu_+)|^2}{|\mu_+|^2} + f_{\mathrm{Im}}(\mu_-, \mu_+) > 0.$$

That means, we altogether have $1 + f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) > 0$. Together with the ellipticity property (3.31) of the operator $C_0^{\alpha,*}$, we can show that

$$\begin{aligned} &\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \rho^{-1}\mathbf{A}_\alpha C_{\kappa_+}^\alpha C_0^{\alpha,*}\mathbf{j}\right) + C_{\mathrm{I},2}(\mathbf{j},\mathbf{j})\right) \\ &\qquad \geq \left(1 + f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+)\right) \mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C_0^{\alpha,*}\mathbf{j}\right) \overset{(3.31)}{\geq} c_{\mathrm{I},2} \left\|\mathbf{j}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}, \end{aligned}$$

where $c_{\mathrm{I},2} \coloneqq \left(1 + f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+)\right) c_{\mathrm{I},1}$ is a positive constant and $C_{\mathrm{I},2}$ the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form given by $C_{\mathrm{I},2} \coloneqq C_{\mathrm{I},1} - C_3^{\mathrm{I}}$.

Case (iii): $f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-) < 0$, $f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) \geq 0$ and

$$|\mathrm{Re}(\epsilon_+)| \leq |\mathrm{Re}(\epsilon_-)| \quad \text{with equality only if } \mathrm{Im}(\epsilon_-) > 0.$$

We advance similar as in case (ii) and obtain

$$\begin{aligned} &\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \rho^{-1}\mathbf{A}_\alpha C_{\kappa_+}^\alpha C_0^{\alpha,*}\mathbf{j}\right) + C_{\mathrm{I},3}(\mathbf{j},\mathbf{j})\right) \\ &\qquad \geq \left(1 + f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-)\right) \mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C_0^{\alpha,*}\mathbf{j}\right) \overset{(3.31)}{\geq} c_{\mathrm{I},3} \left\|\mathbf{j}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}, \end{aligned}$$

where $c_{\mathrm{I},3} \coloneqq \left(1 + f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-)\right) c_{\mathrm{I},1}$ is a positive constant and $C_{\mathrm{I},3}$ a compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form.

Case (iv): $f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-) < 0$, $f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) < 0$ and

$$|\mathrm{Re}\left(\epsilon_+\right)| \leq |\mathrm{Re}\left(\epsilon_-\right)| \qquad \textit{with equality only if } \mathrm{Im}(\epsilon_-) > 0$$

if $|f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-)| \geq |f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+)|$, or

$$|\mathrm{Re}\left(\mu_+\right)| \geq |\mathrm{Re}\left(\mu_-\right)| \qquad \textit{with equality only if } \mathrm{Im}(\mu_+) > 0$$

if $|f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-)| < |f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+)|$.

Without loss of generality, we assume that

$$|f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-)| \geq |f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+)|$$

and apply the identity (5.13) from Lemma 5.4 in (5.17). This leads to

$$\begin{aligned} &\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \rho^{-1}\mathbf{A}_\alpha C_{\kappa_+}^\alpha C_0^{\alpha,*}\mathbf{j}\right) + C_{\mathrm{I},1}(\mathbf{j},\mathbf{j})\right) \\ &\overset{(5.13)}{\geq} \left(1 + f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-)\right) \mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C_0^{\alpha,*}\mathbf{j}\right) \\ &\qquad - \underbrace{\left[f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) - \left(f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-)\right)\right]}_{\geq 0} \mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \mathbf{j}\right) \\ &\qquad + \mathrm{Re}\left(C_4^{\mathrm{I}}\left(\mathbf{j},\mathbf{j}\right)\right) \\ &\overset{(5.9)}{\geq} \left(1 + f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-)\right) \mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C_0^{\alpha,*}\mathbf{j}\right) + \mathrm{Re}\left(C_4^{\mathrm{I}}\left(\mathbf{j},\mathbf{j}\right)\right) \end{aligned}$$

with the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form C_4^{I} given by

$$C_4^{\mathrm{I}}(\cdot,\cdot) := (f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-))\mathcal{B}_{\mathrm{c}}(\cdot, C_2\cdot)\,,$$

where C_2 is the compact operator corresponding to the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form from (5.13). In the considered case, we have $f_{\mathrm{Im}}(\epsilon_+,\epsilon_-) > 0$ by assumption (2.2) as well as the inequality $f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-) < 0$ and $|\mathrm{Re}(\epsilon_+)| \leq |\mathrm{Re}(\epsilon_-)|$ with equality only if $\mathrm{Im}(\epsilon_-) > 0$. Therefore, we deduce in the same manner as in case (ii) that

$$1 + f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-) > 0.$$

The ellipticity property (3.31) of the operator $C_0^{\alpha,*}$ finally implies that

$$\begin{aligned}&\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \rho^{-1}\mathbf{A}_\alpha C_{\kappa_+}^\alpha C_0^{\alpha,*}\mathbf{j}\right) + C_{\mathrm{I},4}(\mathbf{j},\mathbf{j})\right)\\ &\qquad \geq (1 + f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-))\,\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, C_0^{\alpha,*}\mathbf{j}\right) \overset{(3.31)}{\geq} c_{\mathrm{I},4}\,\|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}\,,\end{aligned}$$

where $c_{\mathrm{I},4} := (1 + f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-))\,c_{\mathrm{I},1}$ is a positive constant and $C_{\mathrm{I},4}$ the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form given by $C_{\mathrm{I},4} := C_{\mathrm{I},1} - C_4^{\mathrm{I}}$.

All in all, we have thus shown the validity of the Gårding inequality (5.1) for $\tilde{\alpha} \notin \mathbb{Z}^2$. In this case, the second Gårding inequality (5.2) is proven in a similar manner based on the compact perturbation $\mathbf{A}_\alpha^{\mathrm{II}} = \rho C_{\kappa_+,0}^\alpha + C_{\kappa_-}^\alpha$ of the operator $\mathbf{A}_\alpha$.

For $\tilde{\alpha} \in \mathbb{Z}^2$, the operator $C_0^{\alpha,*}$ is no longer elliptic in the sense of Lemma 3.22. However, $C_0^{\alpha,*}$ is a compact perturbation of the invertible operator $\mathrm{i}C_{\mathrm{i}}^\alpha$, which satisfies the ellipticity property

$$\mathrm{Re}(-\mathrm{i}\mathcal{B}_{\mathrm{c}}(\mathbf{j}, C_{\mathrm{i}}^\alpha\mathbf{j})) \overset{(3.18)}{\geq} \|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}\,.$$

Hence, up to an additional compact perturbation, the proof of this theorem can be carried out analogously for $\tilde{\alpha} \in \mathbb{Z}^2$. □

In the above proof, we implicitly used that the boundary integral operator M_κ^α is compact in the Hilbert space $\mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$. If Γ only exhibits polyhedral Lipschitz regularity, this is no longer true. Nevertheless, we are able to derive a Gårding inequality for nonsmooth Γ with a similar technique of proof, however under more restrictive assumptions.

Theorem 5.5 (Gårding inequalities for polyhedral Lipschitz Γ)**.** *Assume that Γ is of polyhedral Lipschitz regularity and that $\epsilon_\pm$, $\mu_\pm$ fulfill the conditions (2.2). If*

$$f_{\mathrm{Re}}(\epsilon_+,\epsilon_-) + f_{\mathrm{Im}}(\epsilon_+,\epsilon_-) \geq 0 \quad \textit{and} \quad f_{\mathrm{Re}}(\mu_-,\mu_+) + f_{\mathrm{Im}}(\mu_-,\mu_+) \geq 0,$$

then the Gårding inequality

$$\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, -\rho^{-1}\mathbf{A}_\alpha C_{\kappa_+}^\alpha C_0^{\alpha,*}\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}\right) + C(\mathbf{j},\mathbf{j})\right) \geq c\,\|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)} \tag{5.18}$$

holds with a compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form C and a positive constant c.

Proof. Since the ideas behind the proofs of Theorems 5.1 and 5.5 are the same, we only sketch how to prove the Gårding inequality (5.18) in the following.

We start by assuming that $\tilde{\alpha} \notin \mathbb{Z}^2$. With the second Calderon relation $(3.17)_2$, the operator $\mathbf{A}_\alpha$ can be reformulated as

$$\mathbf{A}_\alpha = -\rho \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right) C_{\kappa_+}^\alpha + \left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right) C_{\kappa_-,0}^\alpha + C_{11},$$

where the operator C_{12} defined by

$$\begin{aligned} C_{11} \coloneqq \rho \left[\left(M_{\mathrm{i}}^\alpha - M_{\kappa_+}^\alpha\right) C_{\kappa_+}^\alpha + C_{\kappa_+}^\alpha \left(M_{\kappa_-}^\alpha - M_{\kappa_+}^\alpha\right)\right] + \left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right)\left(C_{\kappa_-}^\alpha - C_{\kappa_-,0}^\alpha\right) \\ + \left(M_{\kappa_+}^\alpha - M_{\mathrm{i}}^\alpha\right) C_{\kappa_-}^\alpha \end{aligned}$$

is compact due to Lemma 3.12 and observation (3.14). Hence, $\mathbf{A}_\alpha$ is a compact perturbation of

$$\mathbf{A}_\alpha^{\mathrm{I}} \coloneqq -\rho \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right) C_{\kappa_+}^\alpha + \left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right) C_{\kappa_-,0}^\alpha$$

and it remains to prove a Gårding inequality of the form (5.1) for the operator

$$\begin{aligned} I_\alpha^{\mathrm{I}} &\coloneqq -\rho^{-1} \mathbf{A}_\alpha^{\mathrm{I}} C_{\kappa_+}^\alpha C_0^{\alpha,*} \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right) \\ &\overset{(5.4)}{=} -\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right) I_1^+ \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right) + \rho^{-1}\left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right) I_2^- \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right) + C_{12} \end{aligned}$$

with the operator $C_{12} \coloneqq \rho^{-1}\left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right) C_{\kappa_-,0}^\alpha \left(C_{\kappa_+,0}^\alpha - C_{\kappa_+}^\alpha\right) C_0^{\alpha,*}\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)$. The latter is compact by Lemma 3.12. The identity (5.5) from Lemma 5.3 implies the existence of a compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form C_1^{I} such that

$$\begin{aligned} &\mathrm{Re}\left(-\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right) I_1^+ \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}\right)\right) + \mathrm{Re}\left(C_1^{\mathrm{I}}(\mathbf{j},\mathbf{j})\right) \\ &\quad= \mathcal{B}_{\mathrm{c}}\left(\left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right)\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}, C_0^{\alpha,*}\left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right)\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}\right) \\ &\quad\overset{(3.31)}{\geq} c_1^{\mathrm{I}} \left\|\left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right)\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}\right\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)} \overset{(3.24)}{\geq} c_1^{\mathrm{I}} c_2^{\mathrm{I}} c_3^{\mathrm{I}} \|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}, \end{aligned} \tag{5.19}$$

where we in particular applied the skew-adjointness of M_{i}^α ensured by Lemma 3.13. Exploiting that $\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, R_0^\alpha T_0^\alpha R_0^\alpha \mathbf{j}\right) \in \mathbb{R}$ and $\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \mathbf{j}\right) \in \mathbb{R}$ for all densities $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\mathrm{div}_\Gamma, \Gamma)$ by (5.9) and (5.10), we observe that the representation (5.8) of I_2^- from Lemma 5.3 with a compact operator C_{13}, Lemma 3.11 and Lemma 3.13 lead to

$$\begin{aligned} &\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathbf{j}, \left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right)\rho^{-1} I_2^- \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}\right)\right) \\ &\overset{(5.11),(5.12)}{=} -\left(f_{\mathrm{Re}}\left(\mu_-, \mu_+\right) + f_{\mathrm{Im}}\left(\mu_-, \mu_+\right)\right)\mathcal{B}_{\mathrm{c}}\left(\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}, R_0^\alpha T_0^\alpha R_0^\alpha \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}\right) \\ &\quad - \left(f_{\mathrm{Re}}\left(\epsilon_+, \epsilon_-\right) + f_{\mathrm{Im}}\left(\epsilon_+, \epsilon_-\right)\right)\mathcal{B}_{\mathrm{c}}\left(\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}, T_0^\alpha R_0^\alpha T_0^\alpha \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}\right) \\ &\quad + \mathrm{Re}\left(C_2^{\mathrm{I}}(\mathbf{j},\mathbf{j})\right) \overset{(5.9),(5.10)}{\geq} \mathrm{Re}\left(C_2^{\mathrm{I}}(\mathbf{j},\mathbf{j})\right), \end{aligned} \tag{5.20}$$

where the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form C_2^{I} is defined by

$$\begin{aligned} C_2^{\mathrm{I}}(\cdot,\cdot) \coloneqq \frac{\overline{\epsilon}_+}{\overline{\epsilon}_-}\mathcal{B}_{\mathrm{c}}\left(\cdot, \left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right) C_{14} \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\cdot\right) \\ + \overline{\rho}^{-1}\mathcal{B}_{\mathrm{c}}\left(\cdot, \left(M_{\mathrm{i}}^\alpha + \mathrm{I}\right) C_{13} \left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\cdot\right) \end{aligned}$$

with the compact operator C_{14} corresponding to the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form C_1 from (5.12). From (5.19) and (5.20), we altogether conclude that

$$\mathrm{Re}\left(\mathcal{B}_{\mathrm{c}}\left(\mathrm{j}, -\rho^{-1}\mathbf{A}_\alpha C_{\kappa_+}^\alpha C_0^{\alpha,*}\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\mathbf{j}\right) + C(\mathbf{j},\mathbf{j})\right) \geq c\,\|\mathbf{j}\|^2_{\mathbf{H}_\alpha^{-\frac{1}{2}}(\mathrm{div}_\Gamma,\Gamma)}$$

with the compact $\mathcal{B}_{\mathrm{c}}$-related sesquilinear form C,

$$C(\cdot,\cdot) \coloneqq \mathcal{B}_{\mathrm{c}}\left(\cdot, \rho^{-1} C_{11} C_{\kappa_+}^\alpha C_0^{\alpha,*}\left(M_{\mathrm{i}}^\alpha - \mathrm{I}\right)\cdot\right) - \mathcal{B}_{\mathrm{c}}\left(\cdot, C_{12}\cdot\right) + C_1^{\mathrm{I}}(\cdot,\cdot) - C_2^{\mathrm{I}}(\cdot,\cdot),$$

and the positive constant $c := c_1^{\mathrm{I}} c_2^{\mathrm{I}} c_3^{\mathrm{I}}$. This proves our theorem for $\tilde{\alpha} \notin \mathbb{Z}^2$.

For $\tilde{\alpha} \in \mathbb{Z}^2$, the operator $C_0^{\alpha,*}$ does not feature the ellipticity property from Lemma 3.22. However, $C_0^{\alpha,*}$ is a compact perturbation of the invertible operator $\mathrm{i}C_{\mathrm{i}}^{\alpha}$, which is elliptic in the sense that

$$\mathrm{Re}(-\mathrm{i}\mathcal{B}_{\mathrm{c}}(\mathbf{j}, C_{\mathrm{i}}^{\alpha}\mathbf{j})) \overset{(3.18)}{\geq} \|\mathbf{j}\|^2_{\mathbf{H}_{\alpha}^{-\frac{1}{2}}(\mathrm{div}_{\Gamma},\Gamma)} . \tag{5.21}$$

Hence, up to an additional compact perturbation in (5.19), the proof of this theorem remains the same for $\tilde{\alpha} \in \mathbb{Z}^2$. □

Remark 5.6. *By Lemma 3.12, $C_0^{\alpha,*} \overset{(3.13)}{=} \mathrm{i}C_{\mathrm{i},0}^{\alpha}$ is a compact perturbation of the invertible operator $\mathrm{i}C_{\mathrm{i}}^{\alpha}$, for which the ellipticity property (5.21) holds. This has already been exploited in the proofs of Theorems 5.1 and 5.5 for the case of a wave vector α such that $\tilde{\alpha} \in \mathbb{Z}^2$. Due to this ellipticity property, it is also possible to replace the boundary integral operator $C_0^{\alpha,*}$ directly in the formulation of both Theorems 5.1 and 5.5 directly by the boundary integral operator $\mathrm{i}C_{\mathrm{i}}^{\alpha}$ without any obvious pros and cons. We choose to use $C_0^{\alpha,*}$ in this article since, from our point of view, it simplifies the notation (by (3.12), $C_0^{\alpha,*}$ has the nice representation as $C_0^{\alpha,*} = R_0^{\alpha} + T_0^{\alpha}$, which in particular does not involve an additional i).*

Corollary 5.7 (Fredholmness for polyhedral Lipschitz Γ)**.** *Let the assumptions of Theorem 5.5 hold. Moreover, assume that the electromagnetic material parameters satisfy*

$$\mathrm{Re}(\epsilon_+)\,\mathrm{Re}(\epsilon_-) \geq -\,\mathrm{Im}(\epsilon_+)\,\mathrm{Im}(\epsilon_-) \text{ and } \mathrm{Re}(\mu_+)\,\mathrm{Re}(\mu_-) \geq -\,\mathrm{Im}(\mu_+)\,\mathrm{Im}(\mu_-). \tag{5.22}$$

Then $\mathbf{A}_{\alpha}$ is a Fredholm operator of index zero in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma)$.

This corollary is proven in the same manner as Corollary 5.2.

Remark 5.8. *The assumption (5.22) on the electric permittivities $\epsilon_{\pm}$ and the magnetic permeabilities $\mu_{\pm}$ is a direct implication of the assumption*

$$f_{\mathrm{Re}}(\epsilon_+, \epsilon_-) + f_{\mathrm{Im}}(\epsilon_+, \epsilon_-) \geq 0 \quad \text{and} \quad f_{\mathrm{Re}}(\mu_-, \mu_+) + f_{\mathrm{Im}}(\mu_-, \mu_+) \geq 0$$

from Theorem 5.5. It should hold for most materials found in nature as well as for some materials with a negative refraction index. We aim to present even more parameter constellations that yield the Fredholmness of index zero of the boundary integral operator $\mathbf{A}_{\alpha}$ in our future work. This should be possible in comparison with the results in the 2π-periodic setting.

5.2 Uniqueness

Under certain assumptions on the electromagnetic parameters and the boundary integral operators $C_{\kappa_{\pm}}^{\alpha}$, we can prove uniqueness of solutions to the singular integral equation (4.9).

Theorem 5.9 (Uniqueness)**.** *Let condition (2.2) be satisfied and assume that one of the following situations holds for the electromagnetic material parameters:*

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

$$\mathrm{Im}\,(\epsilon_-) \geq 0 \quad \text{and} \quad \mathrm{Im}\,(\mu_-) \geq 0 \quad \text{with} \quad \mathrm{Im}\,(\epsilon_- + \mu_-) > 0;$$

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

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

(iii) $\operatorname{Im}(\epsilon_\pm) \geq 0$ *and* $\operatorname{Im}(\mu_\pm) \geq 0$ *with* $\operatorname{Im}(\epsilon_\pm + \mu_\pm) > 0$*;*

(iv) $\epsilon_\pm, \mu_\pm \in \mathbb{R}$ *such that*

$$\operatorname{sgn}(\epsilon_\pm \mu_\pm) < 0 \quad \textit{and} \quad \operatorname{sgn}(\epsilon_+ \epsilon_-), \operatorname{sgn}(\mu_+ \mu_-) > 0.$$

Then the singular integral equation (4.9) has at most one solution $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ *if we have* $\ker(C^\alpha_{\kappa_\pm}) = \{0\}$.

We need the following two auxiliary results for the proof of Theorem 5.9. They are easily verified by simple calculations.

Lemma 5.10. *Let the electromagnetic material parameters* $\epsilon_\pm$ *and* $\mu_\pm$ *satisfy (2.2). Then if* $\kappa_\pm \in \mathbb{R}$, *we have*

$$\operatorname{Im}\left(\beta_\pm^{(n)}\right) > 0 \quad \textit{for all except of a finite number } N_\pm \textit{ of } n \in \mathbb{Z}^2.$$

For the excluded $n \in N_\pm$, *the identity* $\operatorname{Im}\left(\beta_\pm^{(n)}\right) = 0$ *holds. For all other values of* $\kappa_\pm$, *we have*

$$\operatorname{Im}\left(\beta_\pm^{(n)}\right) > 0 \quad \textit{for all } n \in \mathbb{Z}^2.$$

Lemma 5.11. *Let the electromagnetic material parameters* $\epsilon_\pm$ *and* $\mu_\pm$ *satisfy (2.2). Then we have*

$$\operatorname{Im}\left(\frac{\epsilon_\pm}{\kappa_\pm^2}\right) \leq 0. \tag{5.23}$$

Proof of Theorem 5.9. This theorem is proven by contradiction. We assume that there exists a non-trivial solution $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ of the homogeneous singular integral equation (4.9), i.e., we have $\mathbf{E}^{\mathrm{i}} = \gamma_{\mathrm{D}}^- \mathbf{E}^{\mathrm{i}} = \gamma_{\mathrm{N}_{\kappa_+}}^- \mathbf{E}^{\mathrm{i}} = 0$. Lemma 4.1 provides solutions $\mathbf{E}^{\mathrm{refl}}$ in G_+ and $\mathbf{E}^{\mathrm{tran}}$ in G_- of the electromagnetic scattering problem (2.6)-(2.11) expressed in terms of $\mathbf{j}$ as

$$\mathbf{E}^{\mathrm{refl}} = -\frac{1}{2}\left[\rho \Psi^\alpha_{\mathrm{E}_{\kappa_+}}\left(M^\alpha_{\kappa_-} + \mathrm{I}\right)\mathbf{j} + \Psi^\alpha_{\mathrm{M}_{\kappa_+}} C^\alpha_{\kappa_-}\mathbf{j}\right] \quad \text{in } G_+, \tag{5.24}$$

$$\mathbf{E}^{\mathrm{tran}} = \Psi^\alpha_{\mathrm{E}_{\kappa_-}}\mathbf{j} \quad \text{in } G_-. \tag{5.25}$$

Here, the transmission conditions across Γ read as

$$\gamma_{\mathrm{D}}^- \mathbf{E}^{\mathrm{tran}} = \gamma_{\mathrm{D}}^+ \mathbf{E}^{\mathrm{refl}} \quad \text{and} \quad \mu_+ \gamma_{\mathrm{D}}^- \left(\mathbf{curl}\, \mathbf{E}^{\mathrm{tran}}\right) = \mu_- \gamma_{\mathrm{D}}^+ \left(\mathbf{curl}\, \mathbf{E}^{\mathrm{refl}}\right). \tag{5.26}$$

We aim to find a variational formulation for the electric field $\mathbf{E}$ specified by

$$\mathbf{E} := \begin{cases} \mathbf{E}^{\mathrm{refl}} & \text{in } G_+, \\ \mathbf{E}^{\mathrm{tran}} & \text{in } G_-. \end{cases}$$

For this, we first multiply the equation $\mathbf{curl}\,\mathbf{curl}\,\mathbf{E}-\kappa^2\mathbf{E}=0$ by $\frac{\epsilon}{\kappa^2}\overline{\mathbf{E}}$. Then we integrate the resulting expression over the domain $\Omega := \left(G^{\mathrm{H}}\cap G_+\right)\cup\left(G^{\mathrm{H}}\cap G_-\right)$, where G^{H} is given by (2.3) and finally apply Green's identity (3.3). This is possible since $\mathbf{E}\in\mathbf{H}(\mathbf{curl},\Omega)$. We obtain

$$\begin{aligned}
0 &= \int_\Omega \left(\mathbf{curl}\,\mathbf{curl}\,\mathbf{E}-\kappa^2\mathbf{E}\right)\cdot\frac{\epsilon}{\kappa^2}\overline{\mathbf{E}}\,dx \\
&= \int_{G^{\mathrm{H}}} \frac{\epsilon}{\kappa^2}\left|\mathbf{curl}\,\mathbf{E}\right|^2-\epsilon\left|\mathbf{E}\right|^2\,dx \\
&\quad + \mathcal{B}_{\partial G_+^{\mathrm{H}}}\left(\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\frac{\epsilon_+}{\kappa_+^2}\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right)+\mathcal{B}_{\partial G_-^{\mathrm{H}}}\left(\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\frac{\epsilon_-}{\kappa_-^2}\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right).
\end{aligned}$$

The α-quasiperiodicity of the integrands implies, for $j\in\{1,2\}$, that

$$\begin{aligned}
&\mathcal{B}_{\{x\in\partial G_\pm^{\mathrm{H}}\,:\,x_j=-\pi\}}\left(\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\frac{\epsilon}{\kappa^2}\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right)\\
&\qquad\qquad + \mathcal{B}_{\{x\in\partial G_\pm^{\mathrm{H}}\,:\,x_j=\pi\}}\left(\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\frac{\epsilon}{\kappa^2}\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right)=0.
\end{aligned}$$

We denote by $\mathbf{n}_\pm^{\mathrm{H}}$ the outer unit normals on $\Gamma_\pm^{\mathrm{H}}$ that take the values $\mathbf{n}_\pm^{\mathrm{H}}=(0,0,\pm1)^{\mathrm{T}}$. Using this and the periodicity relations from above leads to

$$\begin{aligned}
0 \;&=\; \int_{G^{\mathrm{H}}} \frac{\epsilon}{\kappa^2}\left|\mathbf{curl}\,\mathbf{E}\right|^2-\epsilon\left|\mathbf{E}\right|^2\,dx \\
&\quad + \mathcal{B}_{\partial G_+^{\mathrm{H}}}\left(\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\frac{\epsilon_+}{\kappa_+^2}\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right)+\mathcal{B}_{\partial G_-^{\mathrm{H}}}\left(\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\frac{\epsilon_-}{\kappa_-^2}\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right) \\
&\quad - \int_{\Gamma_+^{\mathrm{H}}}\frac{\epsilon_+}{\kappa_+^2}\left(r|_{\Gamma_+^{\mathrm{H}}}\left(\gamma_{\mathrm{D}}|_{\Gamma_+^{\mathrm{H}}}\,\mathbf{curl}\,\mathbf{E}^{\mathrm{refl}}\right)\right)\gamma_{\mathrm{D}}|_{\Gamma_+^{\mathrm{H}}}\,\overline{\mathbf{E}}^{\mathrm{refl}}\,d\sigma \\
&\quad - \int_{\Gamma_-^{\mathrm{H}}}\frac{\epsilon_-}{\kappa_-^2}\left(r|_{\Gamma_-^{\mathrm{H}}}\left(\gamma_{\mathrm{D}}|_{\Gamma_-^{\mathrm{H}}}\,\mathbf{curl}\,\mathbf{E}^{\mathrm{tran}}\right)\right)\gamma_{\mathrm{D}}|_{\Gamma_-^{\mathrm{H}}}\,\overline{\mathbf{E}}^{\mathrm{tran}}\,d\sigma \\
&\overset{(5.26)_1}{=} \int_{G^{\mathrm{H}}} \frac{\epsilon}{\kappa^2}\left|\mathbf{curl}\,\mathbf{E}\right|^2-\epsilon\left|\mathbf{E}\right|^2\,dx-\mathcal{B}_\Gamma\left(\frac{\epsilon_+}{\kappa_+^2}\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right) \\
&\quad + \mathcal{B}_\Gamma\left(\frac{\epsilon_-}{\kappa_-^2}\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right) \\
&\quad + \int_{\Gamma_+^{\mathrm{H}}}\frac{\epsilon_+}{\kappa_+^2}\left[\left(\mathbf{curl}\,\mathbf{E}^{\mathrm{refl}}\right)_1\overline{\mathbf{E}}_2^{\mathrm{refl}}-\left(\mathbf{curl}\,\mathbf{E}^{\mathrm{refl}}\right)_2\overline{\mathbf{E}}_1^{\mathrm{refl}}\right]\,d\sigma \\
&\quad + \int_{\Gamma_-^{\mathrm{H}}}\frac{\epsilon_-}{\kappa_-^2}\left[\left(\mathbf{curl}\,\mathbf{E}^{\mathrm{tran}}\right)_2\overline{\mathbf{E}}_1^{\mathrm{tran}}-\left(\mathbf{curl}\,\mathbf{E}^{\mathrm{tran}}\right)_1\overline{\mathbf{E}}_2^{\mathrm{tran}}\right]\,d\sigma \\
&\overset{(5.26)_2}{=} \int_{G^{\mathrm{H}}} \frac{\epsilon}{\kappa^2}\left|\mathbf{curl}\,\mathbf{E}\right|^2-\epsilon\left|\mathbf{E}\right|^2\,dx+\mathcal{B}_\Gamma\left(\underbrace{\left(\frac{\mu_-\epsilon_-}{\mu_+\kappa_-^2}-\frac{\epsilon_+}{\kappa_+^2}\right)}_{=0}\gamma_{\mathrm{D}}\left(\mathbf{curl}\,\mathbf{E}\right),\gamma_{\mathrm{D}}\overline{\mathbf{E}}\right) \\
&\quad + \int_{\Gamma_+^{\mathrm{H}}}\frac{\epsilon_+}{\kappa_+^2}\left[\left(\mathbf{curl}\,\mathbf{E}^{\mathrm{refl}}\right)_1\overline{\mathbf{E}}_2^{\mathrm{refl}}-\left(\mathbf{curl}\,\mathbf{E}^{\mathrm{refl}}\right)_2\overline{\mathbf{E}}_1^{\mathrm{refl}}\right]\,d\sigma \\
&\quad + \int_{\Gamma_-^{\mathrm{H}}}\frac{\epsilon_-}{\kappa_-^2}\left[\left(\mathbf{curl}\,\mathbf{E}^{\mathrm{tran}}\right)_2\overline{\mathbf{E}}_1^{\mathrm{tran}}-\left(\mathbf{curl}\,\mathbf{E}^{\mathrm{tran}}\right)_1\overline{\mathbf{E}}_2^{\mathrm{tran}}\right]\,d\sigma.
\end{aligned}$$

In the above calculation, we exploited that the expressions $r|_{\Gamma_\pm^{\mathrm{H}}}\left(\gamma_{\mathrm{D}}|_{\Gamma_\pm^{\mathrm{H}}}\cdot\right)$ on the plane surfaces $\Gamma_\pm^{\mathrm{H}}$

can be understood as the classical cross product $(\mathbf{n}_{\pm}^{\mathrm{H}} \times \gamma_{\mathrm{D}}|_{\Gamma_{\pm}^{\mathrm{H}}} \cdot)$. The outgoing wave condition (2.10)-(2.11), which is satisfied by $\mathbf{E}^{\mathrm{refl}}$ and $\mathbf{E}^{\mathrm{tran}}$, yields that

$$\alpha_1^{(n)} \left(\overline{\mathbf{E}}_n\right)_1 + \alpha_2^{(n)} \left(\overline{\mathbf{E}}_n\right)_2 \pm \overline{\beta_{\pm}^{(n)}} \left(\overline{\mathbf{E}}_n\right)_3 = 0 \quad \text{in } G_{\pm} \text{ with } x_3 \geq \mathrm{H}$$

since $\operatorname{div} \mathbf{E} = 0$. With this and another application of the outgoing wave condition (2.10)-(2.11), we obtain

$$\int_{\Gamma_{\pm}^{\mathrm{H}}} \frac{\epsilon_{\pm}}{\kappa_{\pm}^2} \left[(\mathbf{curl}\, \mathbf{E})_1 \overline{\mathbf{E}}_2 - (\mathbf{curl}\, \mathbf{E})_2 \overline{\mathbf{E}}_1 \right] \, d\sigma = - \sum_{n \in \mathbb{Z}^2} M_n^{\alpha,\pm} \mathbf{E}_n \cdot \overline{\mathbf{E}}_n e^{-2\, \mathrm{Im}\left(\beta_{\pm}^{(n)}\right) \mathrm{H}},$$

where

$$M_n^{\alpha,\pm} := \frac{\mathrm{i} 4\pi^2 \epsilon_{\pm}}{\kappa_{\pm}^2} \begin{pmatrix} \beta_{\pm}^{(n)} & 0 & 0 \\ 0 & \beta_{\pm}^{(n)} & 0 \\ 0 & 0 & \overline{\beta_{\pm}^{(n)}} \end{pmatrix}. \tag{5.27}$$

Inserted into the variational equation for $\mathbf{E}$ from above, this yields

$$\begin{aligned} \int_{G^{\mathrm{H}}} \frac{\epsilon}{\kappa^2} |\mathbf{curl}\, \mathbf{E}|^2 - \epsilon |\mathbf{E}|^2 \, dx = \sum_{n \in \mathbb{Z}^2} \Bigg(& M_n^{\alpha,+} \mathbf{E}_n^{\mathrm{refl}} \cdot \overline{\mathbf{E}}_n^{\mathrm{refl}} e^{-2\, \mathrm{Im}\left(\beta_{+}^{(n)}\right) \mathrm{H}} \\ & + M_n^{\alpha,-} \mathbf{E}_n^{\mathrm{tran}} \cdot \overline{\mathbf{E}}_n^{\mathrm{tran}} e^{-2\, \mathrm{Im}\left(\beta_{-}^{(n)}\right) \mathrm{H}} \Bigg). \end{aligned} \tag{5.28}$$

Next, we take the imaginary part of (5.28) and let H tend to ∞. By Lemma 5.10, $\mathrm{Im}(\beta_{\pm}^{(n)}) \geq 0$ holds for all $n \in \mathbb{N}$, where $\mathrm{Im}(\beta_{\pm}^{(n)}) = 0$ only for a finite number of $n \in \mathbb{Z}^2$ if $\kappa_{\pm} \in \mathbb{R}$. Thus,

$$\begin{aligned} & \lim_{\mathrm{H} \to \infty} \int_{G_{+}^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_{+}}{\kappa_{+}^2}\right) \left|\mathbf{curl}\, \mathbf{E}^{\mathrm{refl}}\right|^2 - \mathrm{Im}\left(\epsilon_{+}\right) \left|\mathbf{E}^{\mathrm{refl}}\right|^2 \, dx \\ & \quad + \lim_{\mathrm{H} \to \infty} \int_{G_{-}^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_{-}}{\kappa_{-}^2}\right) \left|\mathbf{curl}\, \mathbf{E}^{\mathrm{tran}}\right|^2 - \mathrm{Im}\left(\epsilon_{-}\right) \left|\mathbf{E}^{\mathrm{tran}}\right|^2 \, dx \\ & = 4\pi^2 \left[\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_{+}}{\kappa_{+}^2}\right) \sum_{n \in B_{+}} \beta_{+}^{(n)} \left|\mathbf{E}_n^{\mathrm{refl}}\right|^2 + \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_{-}}{\kappa_{-}^2}\right) \sum_{n \in B_{-}} \beta_{-}^{(n)} \left|\mathbf{E}_n^{\mathrm{tran}}\right|^2 \right] \end{aligned} \tag{5.29}$$

with $B_{\pm} := \{n \in \mathbb{Z}^2 \ : \ \beta_{\pm}^{(n)} > 0\}$ as $\kappa_{\pm} \notin \mathbb{R}_{-}$. Then in particular the limit expression on the left-hand side of (5.29) exists. We will now consider situations (i)-(iii) for the electric permittivities $\epsilon_{\pm}$ and the magnetic permeabilities $\mu_{\pm}$. Situation (iv) will later be treated separately. With Lemma 5.11, we easily arrive at

$$\begin{aligned} & \lim_{\mathrm{H} \to \infty} \int_{G_{+}^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_{+}}{\kappa_{+}^2}\right) \left|\mathbf{curl}\, \mathbf{E}^{\mathrm{refl}}\right|^2 - \mathrm{Im}\left(\epsilon_{+}\right) \left|\mathbf{E}^{\mathrm{refl}}\right|^2 \, dx \\ & \quad + \lim_{\mathrm{H} \to \infty} \int_{G_{-}^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_{-}}{\kappa_{-}^2}\right) \left|\mathbf{curl}\, \mathbf{E}^{\mathrm{tran}}\right|^2 - \mathrm{Im}\left(\epsilon_{-}\right) \left|\mathbf{E}^{\mathrm{tran}}\right|^2 \, dx \leq 0. \end{aligned}$$

Moreover, we infer from Lemma 5.10 that the right-hand side of equation (5.29) is only non-vanishing in the situations (i)-(iii) if either $\epsilon_{+}, \mu_{+} \in \mathbb{R}_{+}$ or $\epsilon_{-}, \mu_{-} \in \mathbb{R}_{+}$. We then have

$$\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_{\pm}}{\kappa_{\pm}^2}\right) = \mathrm{Re}\left(\frac{\epsilon_{\pm}}{\kappa_{\pm}^2}\right) > 0.$$

Thus,

$$4\pi^2 \left[\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_+}{\kappa_+^2} \right) \sum_{n\in B_+} \beta_+^{(n)} \left| \mathbf{E}_n^{\mathrm{refl}} \right|^2 + \mathrm{Im}\left(\mathrm{i}\frac{\epsilon_-}{\kappa_-^2} \right) \sum_{n\in B_-} \beta_-^{(n)} \left| \mathbf{E}_n^{\mathrm{tran}} \right|^2 \right] \geq 0$$

is valid in the situations (i)-(iii). Inserting the previous two inequalities in (5.29) yields

$$\begin{aligned} &\lim_{\mathrm{H}\to\infty} \int_{G_+^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_+}{\kappa_+^2} \right) \left| \mathbf{curl}\, \mathbf{E}^{\mathrm{refl}} \right|^2 - \mathrm{Im}\left(\epsilon_+\right) \left| \mathbf{E}^{\mathrm{refl}} \right|^2 \, dx \\ &\qquad + \lim_{\mathrm{H}\to\infty} \int_{G_-^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_-}{\kappa_-^2} \right) \left| \mathbf{curl}\, \mathbf{E}^{\mathrm{tran}} \right|^2 - \mathrm{Im}\left(\epsilon_-\right) \left| \mathbf{E}^{\mathrm{tran}} \right|^2 \, dx = 0. \end{aligned}$$

We in particular deduce that

$$\begin{aligned} &\lim_{\mathrm{H}\to\infty} \int_{G_-^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_-}{\kappa_-^2} \right) \left| \mathbf{curl}\, \mathbf{E}^{\mathrm{tran}} \right|^2 - \mathrm{Im}\left(\epsilon_-\right) \left| \mathbf{E}^{\mathrm{tran}} \right|^2 \, dx = 0 \quad \text{in the cases (i), (iii),} \\ &\lim_{\mathrm{H}\to\infty} \int_{G_+^{\mathrm{H}}} \mathrm{Im}\left(\frac{\epsilon_+}{\kappa_+^2} \right) \left| \mathbf{curl}\, \mathbf{E}^{\mathrm{refl}} \right|^2 - \mathrm{Im}\left(\epsilon_+\right) \left| \mathbf{E}^{\mathrm{refl}} \right|^2 \, dx = 0 \quad \text{in case (ii).} \end{aligned}$$

The assumption $\mathrm{Im}(\epsilon_-), \mathrm{Im}(\mu_-) \geq 0$ with $\mathrm{Im}(\epsilon_- + \mu_-) > 0$ in cases (i) and (iii) as well as the assumption $\mathrm{Im}(\epsilon_+), \mathrm{Im}(\mu_+) \geq 0$ with $\mathrm{Im}(\epsilon_+ + \mu_+) > 0$ in case (ii) then imply that we at least have

$$\lim_{\mathrm{H}\to\infty} \int_{G_-^{\mathrm{H}}} \left| \mathbf{E}^{\mathrm{tran}} \right|^2 \, dx = 0 \quad \text{or} \quad \lim_{\mathrm{H}\to\infty} \int_{G_-^{\mathrm{H}}} \left| \mathbf{curl}\, \mathbf{E}^{\mathrm{tran}} \right|^2 \, dx = 0 \tag{5.30}$$

in the cases (i) and (iii), and

$$\lim_{\mathrm{H}\to\infty} \int_{G_+^{\mathrm{H}}} \left| \mathbf{E}^{\mathrm{refl}} \right|^2 \, dx = 0 \quad \text{or} \quad \lim_{\mathrm{H}\to\infty} \int_{G_+^{\mathrm{H}}} \left| \mathbf{curl}\, \mathbf{E}^{\mathrm{refl}} \right|^2 \, dx = 0 \tag{5.31}$$

in case (ii). Due to the non-negative integrand and the definition of the domain G^{H}, we conclude that

$$\mathbf{E}^{\mathrm{tran}} = 0 \quad \text{a.e. in } G_-$$

in cases (i) and (iii), and

$$\mathbf{E}^{\mathrm{refl}} = 0 \quad \text{a.e. in } G_+$$

in case (ii) if the first identities in (5.30) and (5.31) are given. If the second identities in (5.30) and in (5.31) are given, we obtain that

$$\mathbf{curl}\, \mathbf{E}^{\mathrm{tran}} = 0 \quad \text{a.e. in } G_-$$

in cases (i) and (iii), and

$$\mathbf{curl}\, \mathbf{E}^{\mathrm{refl}} = 0 \quad \text{a.e. in } G_+$$

in case (ii). From the time-harmonic Maxwell equations $\mathbf{curl}\,\mathbf{curl}\, \mathbf{E}^{\mathrm{tran}} - \kappa_-^2 \mathbf{E}^{\mathrm{tran}} = 0$ in G_- and $\mathbf{curl}\,\mathbf{curl}\, \mathbf{E}^{\mathrm{refl}} - \kappa_+^2 \mathbf{E}^{\mathrm{refl}} = 0$ in G_+, respectively, we then again arrive at

$$\begin{cases} \mathbf{E}^{\mathrm{tran}} = 0 \quad \text{a.e. in } G_-, & \text{in situations (i) and (iii),} \\ \mathbf{E}^{\mathrm{refl}} = 0 \quad \text{a.e. in } G_+, & \text{in situation (ii).} \end{cases}$$

In situation (ii), we conclude that $\gamma_{\mathrm{D}}^{+}\mathbf{E}^{\mathrm{refl}} = \gamma_{\mathrm{N}_{\kappa_+}}^{+}\mathbf{E}^{\mathrm{refl}} = 0$. Hence, the transmission conditions (5.26) entail that $\gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{tran}} = \gamma_{\mathrm{N}_{\kappa_-}}^{-}\mathbf{E}^{\mathrm{tran}} = 0$ a.e. in G_- and thus $\mathbf{E}^{\mathrm{tran}} = 0$ a.e. in G_- by Lemma 3.10.

Now, let the electromagnetic material parameters satisfy condition (iv) of this theorem. We go back to equation (5.28) and multiply it by the imaginary factor i. Taking its imaginary part and applying the limit of $\mathrm{H} \to \infty$ then in particular gives

$$\lim_{\mathrm{H}\to\infty} \int_{G_-^{\mathrm{H}}} \operatorname{Im}\left(\mathrm{i}\frac{\epsilon_-}{\kappa_-^2}\right) \left|\mathbf{curl}\,\mathbf{E}^{\mathrm{tran}}\right|^2 - \operatorname{Im}(\mathrm{i}\epsilon_-)\left|\mathbf{E}^{\mathrm{tran}}\right|^2 \, dx = 0.$$

The arguments that have been applied in situations (i)-(iii) now analogously yield $\mathbf{E}^{\mathrm{tran}} = 0$ a.e. in G_-.

In this theorem, we assume that the nullspace of the boundary integral operator $C_{\kappa_-}^{\alpha}$ is trivial. Then $C_{\kappa_-}^{\alpha}$, a Fredholm operator of index zero, is invertible in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma)$. This and the electric potential ansatz for $\mathbf{E}^{\mathrm{tran}}$ finally yield that

$$\Psi_{\mathrm{E}_{\kappa_-}}^{\alpha}\mathbf{j} \overset{(5.25)}{=} \mathbf{E}^{\mathrm{tran}} = 0 \implies \gamma_{\mathrm{D}}^{-}\Psi_{\mathrm{E}_{\kappa_-}}^{\alpha}\mathbf{j} = -C_{\kappa_-}^{\alpha}\mathbf{j} = 0 \implies \mathbf{j} = -\left(C_{\kappa_-}^{\alpha}\right)^{-1} 0 = 0$$

in all of the situations (i)-(iv). This contradicts the assumption that $\mathbf{j}$ is nontrivial, i.e., under the assumptions of this theorem, the singular integral equation (4.9) is uniquely solvable. □

5.3 Existence

This section is concerned with the existence of solutions to (4.9). We distinguish between situations, in which the operator $\mathbf{A}_{\alpha}$ definitely has a trivial nullspace, and situations, in which $\mathbf{A}_{\alpha}$ may possess a nontrivial nullspace. Expressed in other words, the operator $\mathbf{A}_{\alpha}$ is not invertible in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma)$ in the latter situations, provided that $\mathbf{A}_{\alpha}$ fulfills the requirements of Corollaries 5.2 or 5.7 and thus is a Fredholm operator of index zero.

Theorem 5.12 (Existence I)**.** *Let $\epsilon_{\pm}$, $\mu_{\pm}$ satisfy the assumptions of Theorem 5.9 such that*

$$\epsilon_+ \neq -\epsilon_- \text{ and } \mu_+ \neq -\mu_- \tag{5.32}$$

if Γ is smooth, or

$$\operatorname{Re}(\epsilon_+)\operatorname{Re}(\epsilon_-) \geq -\operatorname{Im}(\epsilon_+)\operatorname{Im}(\epsilon_-) \text{ and } \operatorname{Re}(\mu_+)\operatorname{Re}(\mu_-) \geq -\operatorname{Im}(\mu_+)\operatorname{Im}(\mu_-) \tag{5.33}$$

if Γ is only of polyhedral Lipschitz regularity. Then there exists a unique solution $\mathbf{j}$ in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma)$ of the singular integral equation (4.9).

Proof. Theorem 5.9 implies that the solutions to the singular integral equation (4.9) are unique if they exist. This translates to $\ker(\mathbf{A}_{\alpha}) = \{0\}$ since $\mathbf{A}_{\alpha}$ is a linear operator. Moreover, depending on whether Γ is smooth or polyhedral Lipschitz regular, $\mathbf{A}_{\alpha}$ is a Fredholm operator of index zero in $\mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma)$ by Corollary 5.2 or Corollary 5.7, which are applicable due to the assumptions (5.32)-(5.33). Hence, $\mathbf{A}_{\alpha}$ is invertible with $\operatorname{range}(\mathbf{A}_{\alpha}) = \mathbf{H}_{\alpha}^{-1/2}(\mathrm{div}_{\Gamma}, \Gamma)$ and we altogether obtain that

$$-2\gamma_{\mathrm{D}}^{-}\mathbf{E}^{\mathrm{i}} \in \mathbf{H}_{\alpha}^{-\frac{1}{2}}(\mathrm{div}_{\Gamma}, \Gamma) = \operatorname{range}(\mathbf{A}_{\alpha})$$

for all incident fields $\mathbf{E}^{\mathrm{i}} \in \mathbf{H}_{\alpha,\mathrm{loc}}(\mathbf{curl}, G_- \cup G_+)$. □

Theorem 5.9 does not hold for material parameters satisfying (2.2) such that $\epsilon_\pm, \mu_\pm \in \mathbb{R}$ (except for case (iv) from Theorem 5.9). In these cases, $\mathbf{A}_\alpha$ may possess a nontrivial nullspace and, therefore, the existence of (possibly nonunique) solutions to (4.9) is not guaranteed. The subsequent theorem states conditions on the electromagnetic material parameters such that the integral equation (4.9) is solvable.

Theorem 5.13 (Existence II). *Let $\epsilon_\pm, \mu_\pm \in \mathbb{R}$ such that $\operatorname{sgn}(\epsilon_+\mu_+) > 0$ and*

$$\operatorname{sgn}(\mu_+\mu_-) > 0 \quad \text{if } \operatorname{sgn}(\epsilon_-\mu_-) > 0.$$

Additionally, assume that

$$\epsilon_+ \neq -\epsilon_- \text{ and } \mu_+ \neq -\mu_- \tag{5.34}$$

if Γ is smooth, or

$$\operatorname{Re}(\epsilon_+)\operatorname{Re}(\epsilon_-) \geq -\operatorname{Im}(\epsilon_+)\operatorname{Im}(\epsilon_-) \text{ and } \operatorname{Re}(\mu_+)\operatorname{Re}(\mu_-) \geq -\operatorname{Im}(\mu_+)\operatorname{Im}(\mu_-) \tag{5.35}$$

if Γ is only polyhedral Lipschitz regular. Then there exists a solution density $\mathbf{j}$ in $\mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ of the singular integral equation $\mathbf{A}_\alpha \mathbf{j} = -2\gamma_{\mathrm{D}}^- \mathbf{E}^{\mathrm{i}}$ if the boundary integral operator $C_{\kappa_-}^\alpha$ has a trivial nullspace.

We now present the basic idea of the proof of Theorem 5.13. Let the assumptions of Theorem 5.13 be satisfied. We denote by $\mathbf{A}'_\alpha$ the adjoint operator of $\mathbf{A}_\alpha$ with respect to the duality product $\mathcal{B}$. By Lemma 3.13, it reads as

$$\mathbf{A}'_\alpha = \rho\left(M_{\kappa_-}^{-\alpha} - \mathrm{I}\right) C_{\kappa_+}^{-\alpha} + C_{\kappa_-}^{-\alpha}\left(M_{\kappa_+}^{-\alpha} - \mathrm{I}\right) \tag{5.36}$$

with $\rho = \frac{\mu_+\kappa_-}{\mu_-\kappa_+}$. For $\mathbf{j} \in \mathbf{H}_\alpha^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$, we observe that

$$\mathcal{B}\left(\mathbf{A}_\alpha \mathbf{j}, \mathbf{m}\right) = \mathcal{B}\left(\mathbf{j}, \mathbf{A}'_\alpha \mathbf{m}\right) = 0 \quad \text{for all } \mathbf{m} \in \mathbf{H}_{-\alpha}^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma), \mathbf{m} \in \ker\left(\mathbf{A}'_\alpha\right). \tag{5.37}$$

In words, this means that the range of $\mathbf{A}_\alpha$ is orthogonal to the nullspace of $\mathbf{A}'_\alpha$ with respect to the bilinear form $\mathcal{B}$. Moreover, the assumptions (5.34) and (5.35) justify the application of Corollary 5.2 if Γ is smooth or of Corollary 5.7 if Γ only is polyhedral Lipschitz regular. This implies that the operator $\mathbf{A}_\alpha$ is a Fredholm operator of index zero for the chosen material parameter constellations and thus of closed range. All in all, we can therefore reduce the proof of Theorem 5.13 to showing that

$$\mathcal{B}\left(-2\gamma_{\mathrm{D}}^- \mathbf{E}^{\mathrm{i}}, \mathbf{m}\right) = 0 \quad \text{for all } \mathbf{m} \in \mathbf{H}_{-\alpha}^{-\frac{1}{2}}(\operatorname{div}_\Gamma, \Gamma) \text{ with } \mathbf{A}'_\alpha \mathbf{m} = 0. \tag{5.38}$$

Proof of Theorem 5.13. The functions

$$\mathbf{E}^{\mathrm{refl}} = \Psi_{\mathrm{E}_{\kappa_+}}^{-\alpha} \mathbf{m} \qquad \text{in } G_+ \text{ and} \tag{5.39}$$

$$\mathbf{E}^{\mathrm{tran}} = \frac{1}{2}\left[\rho^{-1}\Psi_{\mathrm{E}_{\kappa_-}}^{-\alpha}\left(M_{\kappa_+}^{-\alpha} - \mathrm{I}\right)\mathbf{m} + \Psi_{M_{\kappa_-}}^{-\alpha} C_{\kappa_+}^{-\alpha}\mathbf{m}\right] \qquad \text{in } G_- \tag{5.40}$$

are $(-\alpha)$-quasiperiodic, satisfy the time-harmonic Maxwell equations in G_+ and in G_-, respectively, and the outgoing wave condition (2.10)-(2.11) with α replaced by $(-\alpha)$:

$$\mathbf{E}^{\mathrm{refl}}(x) = \sum_{n\in\mathbb{Z}^2} \mathbf{E}_n^{\mathrm{refl}} e^{\mathrm{i}\left(-\alpha^{(n)}\cdot\tilde{x} + \beta_+^{(n)} x_3\right)} \qquad \text{for } x \in G_+ \text{ with } x_3 \geq \mathrm{H},$$

$$\mathbf{E}^{\mathrm{tran}}(x) = \sum_{n\in\mathbb{Z}^2} \mathbf{E}_n^{\mathrm{tran}} e^{-\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{x}+\beta_-^{(n)}x_3\right)} \qquad \text{for } x \in G_- \text{ with } x_3 \le -\mathrm{H}.$$

Taking the Dirichlet trace of the fields $\mathbf{E}^{\mathrm{refl}}$ in G_+ and $\mathbf{E}^{\mathrm{tran}}$ in G_- given in (5.39) and (5.40) implies that

$$\begin{aligned}\gamma_{\mathrm{D}}^+\mathbf{E}^{\mathrm{refl}} &\overset{(3.9)}{=} -C_{\kappa_+}^{-\alpha}\mathbf{m},\\ \gamma_{\mathrm{D}}^-\mathbf{E}^{\mathrm{tran}} &\overset{(3.9),(3.10)}{=} -\frac{1}{2}\left[\rho^{-1}C_{\kappa_-}^{-\alpha}\left(M_{\kappa_+}^{-\alpha}-\mathrm{I}\right)\mathbf{m}+\left(M_{\kappa_-}^{\alpha}+\mathrm{I}\right)C_{\kappa_+}^{-\alpha}\mathbf{m}\right].\end{aligned}$$

Since $\mathbf{A}'_\alpha\mathbf{m}=0$, i.e., $\left[\rho\left(M_{\kappa_-}^{-\alpha}-\mathrm{I}\right)C_{\kappa_+}^{-\alpha}+C_{\kappa_-}^{-\alpha}\left(M_{\kappa_+}^{-\alpha}-\mathrm{I}\right)\right]\mathbf{m}=0$, we obtain

$$\gamma_{\mathrm{D}}^-\mathbf{E}^{\mathrm{tran}} = -C_{\kappa_+}^{-\alpha}\mathbf{m} = \gamma_{\mathrm{D}}^+\mathbf{E}^{\mathrm{refl}} \quad \text{on } \Gamma. \tag{5.41}$$

This gives a first transmission condition.

We go back to the representation of the transmitted field $\mathbf{E}^{\mathrm{tran}}$ as in (5.40). The use of the identity

$$\Psi_{\mathrm{E}_{\kappa_-}}^{-\alpha}\left(M_{\kappa_+}^{-\alpha}-\mathrm{I}\right)\mathbf{m} \overset{(3.10)_1}{=} -\Psi_{\mathrm{E}_{\kappa_-}}^{-\alpha}\gamma_{\mathrm{N}_{\kappa_+}}^+\mathbf{E}^{\mathrm{refl}}$$

and the transmission condition (5.41) leads to

$$\mathbf{E}^{\mathrm{tran}} = -\frac{1}{2}\left(\rho^{-1}\Psi_{\mathrm{E}_{\kappa_-}}^{-\alpha}\gamma_{\mathrm{N}_{\kappa_+}}^+\mathbf{E}^{\mathrm{refl}}+\Psi_{\mathrm{M}_{\kappa_-}}^{-\alpha}\gamma_{\mathrm{D}}^-\mathbf{E}^{\mathrm{tran}}\right). \tag{5.42}$$

We then insert the Stratton-Chu integral representation of $\mathbf{E}^{\mathrm{tran}}$ given by Lemma 3.10 into (5.42) and arrive at

$$\rho^{-1}\Psi_{\mathrm{E}_{\kappa_-}}^{-\alpha}\gamma_{\mathrm{N}_{\kappa_+}}^+\mathbf{E}^{\mathrm{refl}} = \Psi_{\mathrm{E}_{\kappa_-}}^{-\alpha}\gamma_{\mathrm{N}_{\kappa_-}}^-\mathbf{E}^{\mathrm{tran}}.$$

Since we assumed that $\ker(C_{\kappa_-}^{\alpha})=\{0\}$, it is clear that the boundary integral operators $C_{\kappa_-}^{\alpha}$ and $C_{\kappa_-}^{-\alpha}=-(C_{\kappa_-}^{\alpha})'$ are invertible. With this, a second transmission condition arises:

$$\gamma_{\mathrm{N}_{\kappa_-}}^-\mathbf{E}^{\mathrm{tran}} = \rho^{-1}\gamma_{\mathrm{N}_{\kappa_+}}^+\mathbf{E}^{\mathrm{refl}}.$$

Hence, $\mathbf{E}$ given by (5.39) and (5.40) is a $(-\alpha)$-quasiperiodic solution of the homogeneous electromagnetic scattering problem (2.6)-(2.11).

In particular, the constructed $(-\alpha)$-quasiperiodic function $\mathbf{E}$ satisfies a variational equation similar to (5.29) after exchanging α by $(-\alpha)$:

$$\begin{aligned}&\lim_{\mathrm{H}\to\infty}\int_{G_+^{\mathrm{H}}}\mathrm{Im}\left(\frac{\epsilon_+}{\kappa_+^2}\right)\left|\mathbf{curl}\,\mathbf{E}^{\mathrm{refl}}\right|^2-\mathrm{Im}\left(\epsilon_+\right)\left|\mathbf{E}^{\mathrm{refl}}\right|^2\,dx\\ &\qquad+\lim_{\mathrm{H}\to\infty}\int_{G_-^{\mathrm{H}}}\mathrm{Im}\left(\frac{\epsilon_-}{\kappa_-^2}\right)\left|\mathbf{curl}\,\mathbf{E}^{\mathrm{tran}}\right|^2-\mathrm{Im}\left(\epsilon_-\right)\left|\mathbf{E}^{\mathrm{tran}}\right|^2\,dx\\ &=4\pi^2\left[\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_+}{\kappa_+^2}\right)\sum_{n\in B_+}\beta_+^{(n)}\left|\mathbf{E}_n^{\mathrm{refl}}\right|^2+\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_-}{\kappa_-^2}\right)\sum_{n\in B_-}\beta_-^{(n)}\left|\mathbf{E}_n^{\mathrm{tran}}\right|^2\right],\end{aligned}$$

where $B_\pm := \{n\in\mathbb{Z}^2 \;:\; \beta_\pm^{(n)}\in\mathbb{R}\setminus\{0\}\}$. Since all occurring material parameters are real, the left-hand side of the above equation vanishes. Therefore, we have

$$\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_+}{\kappa_+^2}\right)\sum_{n\in B_+}\beta_+^{(n)}\left|\mathbf{E}_n^{\mathrm{refl}}\right|^2+\mathrm{Im}\left(\mathrm{i}\frac{\epsilon_-}{\kappa_-^2}\right)\sum_{n\in B_-}\beta_-^{(n)}\left|\mathbf{E}_n^{\mathrm{tran}}\right|^2=0. \tag{5.43}$$

Moreover, the assumptions imposed on the electric permittivities $\epsilon_\pm$ and the magnetic permeabilities $\mu_\pm$ in this theorem ensure that

$$\operatorname{sgn}\left(\operatorname{Im}\left(\mathrm{i}\frac{\epsilon_+}{\kappa_+^2}\right)\operatorname{Im}\left(\mathrm{i}\frac{\epsilon_-}{\kappa_-^2}\right)\right) = \operatorname{sgn}\left(\frac{1}{\omega^4\mu_+\mu_-}\right) > 0$$

if $\operatorname{sgn}(\epsilon_-\mu_-) > 0$. The case $\operatorname{sgn}(\epsilon_-\mu_-) < 0$ corresponds to the situation in which ϵ_- and μ_- have different signs. This implies that $\operatorname{Re}(\kappa_-) = 0$ and thus $\operatorname{Re}(\beta_-^{(n)}) = 0$. Then the second sum on the left-hand side of (5.43) vanishes. Altogether, we deduce from (5.43) that

$$\mathbf{E}_n^{\text{refl}} = 0 \quad \text{for those } n \in \mathbb{Z}^2 \text{ such that } \beta_+^{(n)} \in \mathbb{R}\setminus\{0\}. \tag{5.44}$$

We observe that

$$\beta_+^{(0)} = \sqrt{\kappa_+^2 - |-\alpha^{(0)}|^2} = \sqrt{\kappa_+^2 - |-\tilde{\alpha}|^2} \overset{(2.4)}{=} \alpha_3 > 0. \tag{5.45}$$

Therefore,

$$\mathbf{E}_0^{\text{refl}} = 0 \tag{5.46}$$

arises from (5.44). In the following, we derive, from (5.46), that

$$\mathbf{f} = 0 \quad \text{or} \quad \alpha \parallel \mathbf{f} \tag{5.47}$$

for all $\mathbf{m} \in \mathbf{H}_{-\alpha}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ such that $\mathbf{m} \in \ker(\mathbf{A}'_\alpha)$, where $\mathbf{f} = (f_1, f_2, f_3)^{\mathrm{T}}$ with

$$f_j := \int_\Gamma (i_\pi \mathbf{m}_j)(y) e^{\mathrm{i}(\tilde{\alpha}\cdot\tilde{y} - \alpha_3 y_3)}\, d\sigma(y) \quad \text{for } j \in \{1,2,3\}.$$

For this, let $x \in G_+$ such that x lies above Γ. Then the Rayleigh coefficients $\mathbf{E}_n^{\text{refl}}$ can be computed via the representation of $\mathbf{E}^{\text{refl}}(x) = \Psi_{\mathrm{E}_{\kappa_+}}^{-\alpha}\mathbf{m}(x)$, by Definition 3.7, as

$$\mathbf{E}^{\text{refl}}(x) = \kappa_+ S_{\kappa_+}^{-\alpha}\mathbf{m}(x) + \kappa_+^{-1}\nabla S_{\kappa_+}^{-\alpha}\operatorname{div}_\Gamma \mathbf{m}(x),$$

by

$$\begin{aligned}
\mathbf{E}_n^{\text{refl}} &= \frac{1}{|Q|}\int_Q \mathbf{E}^{\text{refl}}(x)\, e^{\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{x} - \beta_+^{(n)}x_3\right)}\, d\tilde{x} \\
&\overset{(3.7)}{=} \frac{2}{|Q|}\int_Q \Bigg[\kappa_+ \int_\Gamma G_{\kappa_+}^{-\alpha}(x,y)\, i_\pi\mathbf{m}(y)\, d\sigma(y) \\
&\quad + \kappa_+^{-1}\int_\Gamma \left(\nabla^x G_{\kappa_+}^{-\alpha}(x,y)\right)\operatorname{div}_\Gamma \mathbf{m}(y)\, d\sigma(y)\Bigg] e^{\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{x} - \beta_+^{(n)}x_3\right)}\, d\tilde{x}.
\end{aligned}$$

The representation of $G_{\kappa_+}^{-\alpha}(x,y)$ given by (3.4) for $y \in \Gamma$, i.e., for $x_3 > y_3$, then yields

$$\begin{aligned}
\mathbf{E}_n^{\text{refl}} &= \frac{\mathrm{i}\kappa_+}{\beta_+^{(n)}}\int_\Gamma e^{\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{y} - \beta_+^{(n)}y_3\right)} i_\pi\mathbf{m}(y)\, d\sigma(y) \\
&\quad + \frac{1}{\kappa_+\beta_+^{(n)}}\int_\Gamma \begin{pmatrix}\alpha_1^{(n)} \\ \alpha_2^{(n)} \\ -\beta_+^{(n)}\end{pmatrix} e^{\mathrm{i}\left(\alpha^{(n)}\cdot\tilde{y} - \beta_+^{(n)}y_3\right)}\operatorname{div}_\Gamma \mathbf{m}(y)\, d\sigma(y).
\end{aligned} \tag{5.48}$$

Above, we exploited the orthogonality of the trigonometric polynomials. By (5.48), the vanishing of the Rayleigh coefficient $\mathbf{E}_0^{\text{refl}}$ leads to

$$\mathbf{E}_0^{\text{refl}} = 0 \quad \Leftrightarrow \quad \mathbf{Mf} \overset{(5.46)}{=} \mathbf{g} \tag{5.49}$$

with

$$\mathbf{M} := \frac{\mathrm{i}\kappa_+}{\alpha_3}\mathrm{I}_3 \quad \text{and} \quad \mathbf{g} := \frac{1}{\kappa_+\alpha_3}\begin{pmatrix}-\alpha_1\\-\alpha_2\\\alpha_3\end{pmatrix}\int_\Gamma e^{\mathrm{i}(\tilde{\alpha}\cdot\tilde{y}-\alpha_3 y_3)}\,\mathrm{div}_\Gamma\,\mathbf{m}(y)\,d\sigma(y),$$

where we used (5.45) and I_3 denotes the identity in $\mathbb{R}^{3\times3}$. Since $\mathbf{M}$ is invertible, we obtain

$$\mathbf{f} = \frac{\mathrm{i}}{\kappa_+^2}\begin{pmatrix}\alpha_1\\\alpha_2\\-\alpha_3\end{pmatrix}\int_\Gamma e^{\mathrm{i}(\tilde{\alpha}\cdot\tilde{y}-\alpha_3 y_3)}\,\mathrm{div}_\Gamma\,\mathbf{m}(y)\,d\sigma(y) \tag{5.50}$$

from (5.49). We now take a closer look at the integral on the right-hand side. With the help the duality relation between div_Γ and ∇_Γ from Lemma 3.3 and the identity $\nabla_\Gamma u = \pi_{\mathrm{D}}(\nabla u)$ (cf. [7, Proposition 3.4]), we observe that

$$\begin{aligned}
\int_\Gamma e^{\mathrm{i}(\tilde{\alpha}\cdot\tilde{y}-\alpha_3 y_3)}\,\mathrm{div}_\Gamma\,\mathbf{m}(y)\,d\sigma(y) &= -\int_\Gamma \nabla_\Gamma e^{\mathrm{i}(\tilde{\alpha}\cdot\tilde{y}-\alpha_3 y_3)}\cdot\mathbf{m}(y)\,d\sigma(y)\\
&= -\int_\Gamma \pi_{\mathrm{D}}\left(\nabla^y e^{\mathrm{i}(\tilde{\alpha}\cdot\tilde{y}-\alpha_3 y_3)}\right)\cdot\mathbf{m}(y)\,d\sigma\\
&= -\int_\Gamma \nabla^y e^{\mathrm{i}(\tilde{\alpha}\cdot\tilde{y}-\alpha_3 y_3)}\cdot i_\pi\mathbf{m}(y)\,d\sigma\\
&= -\mathrm{i}\begin{pmatrix}\alpha_1\\\alpha_2\\-\alpha_3\end{pmatrix}\cdot\int_\Gamma e^{\mathrm{i}(\tilde{\alpha}\cdot\tilde{y}-\alpha_3 y_3)} i_\pi\mathbf{m}(y)\,d\sigma\\
&= -\alpha_1 f_1 - \alpha_2 f_2 + \alpha_3 f_3.
\end{aligned}$$

Inserting this into (5.50) and exploiting the identity $\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = \mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{c}(\mathbf{a}\cdot\mathbf{b})$ for $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}\in\mathbb{C}^3$, we arrive at

$$\begin{aligned}
\mathbf{f} = \frac{1}{\kappa_+^2}(\alpha_1 f_1 + \alpha_2 f_2 - \alpha_3 f_3)\begin{pmatrix}\alpha_1\\\alpha_2\\-\alpha_3\end{pmatrix} \quad &\Longleftrightarrow \quad \frac{1}{\kappa_+^2}\left[\alpha\times(\alpha\times\mathbf{f})\right] = 0\\
&\Longleftrightarrow \quad \mathbf{f} = 0 \quad \text{or} \quad \alpha \parallel \mathbf{f}
\end{aligned}$$

for all wave vectors $\alpha = (\alpha_1, \alpha_2, -\alpha_3)^{\mathrm{T}}$ satisfying (2.5), i.e., $|\alpha|^2 = \kappa_+^2$ since $\kappa_+^2 \in \mathbb{R}$. This verifies (5.47).

By simple manipulations involving the identity $r(\gamma_{\mathrm{D}}\,\cdot\,) = \pi_{\mathrm{D}}(\,\cdot\,)$ (cf. [7, (17)]), we observe that

$$\mathcal{B}\left(-2\gamma_{\mathrm{D}}^-\mathbf{E}^{\mathrm{i}}, \mathbf{m}\right) = 2\int_\Gamma \mathbf{E}^{\mathrm{i}}(y)\cdot i_\pi\mathbf{m}(y)\,d\sigma(y).$$

Inserting the representation of the incident plane wave $\mathbf{E}^{\mathrm{i}}$ as $\mathbf{E}^{\mathrm{i}} = \mathbf{p}e^{\mathrm{i}(\alpha\cdot\tilde{y}-\alpha_3 y_3)}$ in the equation above, we finally conclude that

$$\mathcal{B}\left(-2\gamma_{\mathrm{D}}^-\mathbf{E}^{\mathrm{i}}, \mathbf{m}\right) = 2\mathbf{p}\cdot\mathbf{f} \overset{(5.47)}{=} 0 \quad \text{for all } \mathbf{m}\in\mathbf{H}_{-\alpha}^{-\frac{1}{2}}(\mathrm{div}_\Gamma, \Gamma) \text{ with } \mathbf{A}_\alpha'\mathbf{m} = 0.$$

This completes the proof. □

6 Conclusion

In this paper, we have derived a singular boundary integral equation for the scattering of time-harmonic plane waves by a 2π-biperiodic polyhedral Lipschitz surface that separates two different materials. This extends the approach of [24], in which 2π-periodic scatterers are treated. In the domain above the interface we have chosen a potential ansatz via the Stratton-Chu integral representation and in the domain below the interface a simple electric potential ansatz. This ansatz is related to the one in [12] for dielectric scattering by a bounded object. The resulting integral equation is obtained via potential methods and it has been proven to be equivalent to the electromagnetic scattering problem. The main part of this paper was devoted to the Fredholm properties of the boundary integral equation that were established with the help of the two Gårding inequalities from Theorem 5.1 in the special case of a smooth grating interface and with the help of the Gårding inequality from Theorem 5.5 in the presence of a polyhedral Lipschitz regular grating interface. In particular, we used this property to prove the existence of solutions of the integral equation. With an appropriate variational formulation, we also ensured the uniqueness of solutions under certain assumptions on the electromagnetic material parameters.

The next step consists in the further extension of this work to multilayered gratings. In this context, we propose, based on the ideas in [21] and [25], a recursive integral equation algorithm with which only one integral equation has to be evaluated at one time instead of a whole system of equations.

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