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Shape derivatives in Kondratiev spaces for conical diffraction

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Abstract

This paper studies conical diffraction problems with non-smooth grating structures. We prove existence, uniqueness and regularity results for solutions in weighted Sobolev spaces of Kondratiev type. An a priori estimate, which follows from these results, is then used to prove shape differentiablility of solutions. Finally, a characterization of the shape derivative as a solution of a modified transmission problem is given.

Contents

1 Introduction

We consider the scattering of a time-harmonic electromagnetic plane wave by a diffraction grating in $\mathbb{R}^3$. The simplest form of such a diffraction grating is a periodic interface between two materials with different dielectric constants. More precisely, the grating surface is a perturbation of the (x_1, x_2)-plane, which is assumed to be periodic in the x_1-direction and invariant in the x_3-direction. Scattering by such gratings occurs in the micro-optics industry, where optical devices with certain features have to be designed [1]. Additionally, it is important to solve the inverse problem of shape reconstruction, i.e. to determine the grating structure from measured data of the diffracted wave

[13]. Mathematically, this can be formulated as an inverse problem for the Maxwell equations. See the books of Petit [26] and Colton/Kress [7] for detailed explanations. Under the assumption of a periodic grating illuminated by a plane wave it is possible to reduce the 3D Maxwell transmission problem to a system of Helmholtz equations in $\mathbb{R}^2$ which are coupled by transmission conditions on the interface. The inverse problem can then be solved by an iterative Newton-type method, which makes use of certain concepts of differentiability with respect to the domain. The theory of shape calculus and shape optimization has been thoroughly investigated for example by Sokolowski and Zolesio [31] and Simon [30]. Since inverse problems of this kind are typically ill-posed, iterative methods require regularization.

In the past, different settings and approaches have been discussed. Elschner, Schmidt et al. focused on Eulerian derivatives of shape functionals. In their papers, these fuctionals depend continuously on the Rayleigh coefficients of the scattered waves. The Rayleigh coefficients themselves depend on the shape of the diffraction grating. These investigations cover existence and uniqueness results for the direct problem in usual Sobolev spaces [8] and gradient formulas for both classical TE/TM diffraction and binary gratings [10] and for conical diffraction by general non-smooth structures [9]. They also provide an existence result for material derivatives of solutions which are H^1-regular and statements about asymptotic expansions of the field components near corner points. The formulas given in these papers involve solutions of direct and adjoint problems. Therefore, two different diffraction problems have to be solved in each iteration step.

A different approach uses the shape derivative of the solution operator $F : \Gamma \mapsto u$ for a fixed incident wave, depending on the interface Γ. An iterative method is given for example by the minimization problem

$$\min \left\{ \frac{1}{2} ||F'(\Gamma_n)(\Gamma_{n+1} - \Gamma_n) - u + F(\Gamma_n)||^2 + \frac{\alpha}{2} ||\Gamma_{n+1} - \Gamma_n||^2 \right\},$$

where F' is the shape derivative of F and α is a regularization parameter. Potthast, Chandler-Wilde and Hohage and Schormann characterized shape derivatives of solutions of Dirichlet and Neumann boundary value problems [27, 28], transmission problems for bounded, smooth domains [15] and of Dirichlet problems for unbounded rough surfaces. These are surfaces which are described by contiuous non-periodic functions with Hölder continuous gradients [6]. The shape derivatives are characterized as solutions of problems with the same operator and different right-hand sides. These results were proven by representing the solution as single layer or double layer potentials and taking the shape derivative of the resulting boundary integrals. Hettlich [14] obtained the same results for Dirichlet and Neumann problems, and additionally for a transmission problem with a smooth interface, by means of weak formulations of these problems. Kirsch [16] also employed this method for a Dirichlet problem with a smooth periodic grating. This ansatz works if the shape derivative has H^1-regularity. However, if the boundaries are non-smooth, the shape derivatives, if they exist, are no longer in H^1. Bochniak and Cakoni [4] suggested a different approach for non-smooth boundaries, using non-local perturbation theory and Kondratiev's weighted Sobolev spaces [21, 17]. They showed shape differentiability of solutions for Dirichlet and Neumann problems for domains with corners with the help of an a priori estimate. In this paper, this ansatz is used to investigate shape derivatives of solutions of a system of Helmholtz equations coupled by transmission conditions on a periodic, non-smooth interface.

The paper is structured in the following way. The second section recalls the conical diffraction problem in three dimensions and its reduction to a Helmholtz problem in a two-dimensional periodic cell. Section 3 introduces Kondratiev's weighted Sobolev spaces and shows an a priori estimate for conical transmission problems in these spaces.This estimate can be sharpened if the solution is unique. In the second part of the third section a uniqueness result is shown for absorbing materials, which makes use of a former result of Elschner, Schmidt et al. [8] in standard Sobolev spaces. The last section discusses existence, uniqueness and the characterization of shape derivatives of solutions to the conical diffraction problem. Here, non-local perturbation theory and the ansatz of Bochniak and Cakoni are used. We consider perturbations which preserve the opening angles at corner points as well as perturbations which change the angles. Finally, the shape derivative is characterized as a solution of a conical diffraction problem. More precisely, the solution operator is the same as for the original problem, only the right-hand side is changed. For interfaces with corners, as opposed to smooth interfaces, the right-hand sides of the transmission conditions involve values which are concentrated on the corner points.

2 Conical diffraction

2.1 The Maxwell system

We consider a time-harmonic incoming plane wave with frequency ω illuminating a periodic diffraction grating in $\mathbb{R}^3$ dividing two materials with different dielectric coefficients. The surface structure is assumed to be infinite and periodic in x_1-direction and invariant in x_3-direction. It is then determined by a profile curve Γ being the intersection of the interface with the (x_1, x_2) plane. In the conical diffraction case the angle between the incoming wave direction and the (x_1, x_2) plane is allowed to be non zero. If the incoming wave lies in the (x_1, x_2) plane, we have TE or TM diffraction, depending on the polarization.

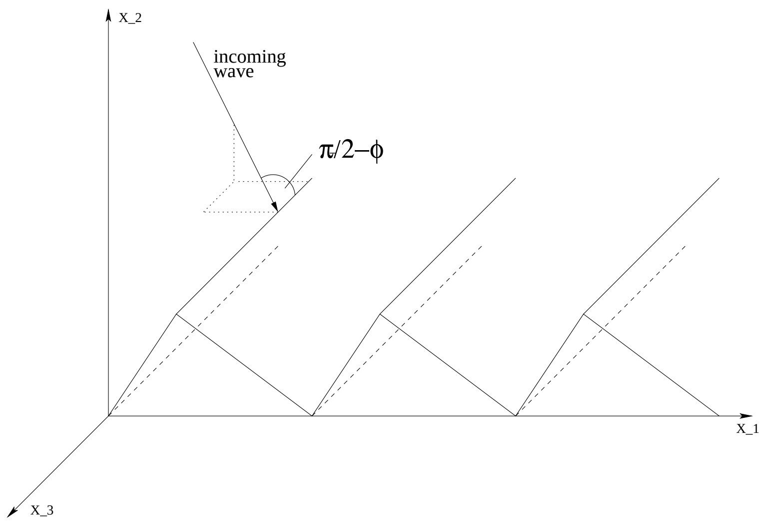

Figure 1: The diffraction grating

The electromagnetic field $(\mathcal{E}, \mathcal{H})$ is the sum $(\mathcal{E}_1, \mathcal{H}_1) = (\mathcal{E}^{(i)}, \mathcal{H}^{(i)}) + (\mathcal{E}^{(r)}, \mathcal{H}^{(r)})$ of the incoming wave and the reflected wave above and the transmitted wave $(\mathcal{E}_2, \mathcal{H}_2) = (\mathcal{E}^{(t)}, \mathcal{H}^{(t)})$ below the grating. Since the incoming wave is time-harmonic, i.e. it admits the form

$$\left(\mathcal{E}^{(i)}, \mathcal{H}^{(i)}\right) = \left(\mathbf{p}e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3}e^{-i\omega t}, \mathbf{q}e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3}e^{-i\omega t}\right) = \left(\mathbf{E}^{(i)}, \mathbf{H}^{(i)}\right)e^{-i\omega t}, \tag{1}$$

where $\mathbf{k} = (\alpha, -\beta, \gamma)$ is the wave vector and $\mathbf{k}/|\mathbf{k}|$ is the direction of the incoming wave, we obtain the time-harmonic Maxwell equations

$$\begin{aligned}\nabla \times \mathbf{E} &= i\omega\mu\mathbf{H}\\ \nabla \times \mathbf{H} &= -i\omega\epsilon\mathbf{E}\end{aligned} \tag{2}$$

with transmission conditions

$$\begin{aligned}\nu \times (\mathbf{E}_1 - \mathbf{E}_2) &= 0\\ \nu \times (\mathbf{H}_1 - \mathbf{H}_2) &= 0\end{aligned} \tag{3}$$

on the interface $\Gamma \times \mathbb{R}$, where ν is the unit normal vector to $\Gamma \times \mathbb{R}$, μ is the magnetic permeability and ϵ is the dielectric coefficient. We will assume that μ is constant, that $\epsilon = \varepsilon_+$ above the grating and $\varepsilon = \varepsilon_-$ below the grating, respectively. Here $\varepsilon_+ > 0$ and ε_- are constant. If the incoming wave is of the form (1), then

$$(\mathbf{E}, \mathbf{H})(x_1, x_2, x_3) = (E, H)(x_1, x_2)e^{i\gamma x_3},$$

and the above Maxwell system can be reduced to a system of Helmholtz equations for the third components E_3 of $E = (E_1, E_2, E_3)$ and H_3 of $H = (H_1, H_2, H_3)$ defined in the cross-section plane (x_1, x_2) described in the next subsection. For details, see [8], [9], [11] and the following section.

2.2 The quasi-periodic Helmholtz problem

We restrict the problem to a rectangular cell $\Omega := (0, 2\pi) \times (-b, b) \subset \mathbb{R}^2$ with artificial boundaries $\Gamma^\pm := \{(x_1, \pm b) : 0 < x_1 < 2\pi\}$ above resp. below the grating and with an interface Γ splitting Ω into an upper part Ω^+ and a lower part Ω^-. This is shown in Figure 2. Now we introduce the functions

$$u_1^\pm := E_3|_{\Omega^\pm} \qquad \text{and} \qquad u_2^\pm := H_3|_{\Omega^\pm}.$$

In view of the periodicity of the problem and the form of the incoming wave, we look for solutions which are α-quasi-periodic in x_1, i.e.

$$u_1^\pm(x_1 + 2\pi, x_2) = e^{2\pi i\alpha}u_1^\pm(x_1, x_2), \qquad u_2^\pm(x_1 + 2\pi, x_2) = e^{2\pi i\alpha}u_2^\pm(x_1, x_2). \tag{4}$$

The Maxwell equations (2) can then be formulated as

$$\begin{aligned}\triangle u_1^+ + \kappa_+^2 u_1^+ &= f_1^+ \quad \text{in} \quad \Omega^+\\ \triangle u_1^- + \kappa_-^2 u_1^- &= f_1^- \quad \text{in} \quad \Omega^-\\ \triangle u_2^+ + \kappa_+^2 u_2^+ &= f_2^+ \quad \text{in} \quad \Omega^+\\ \triangle u_2^- + \kappa_-^2 u_2^- &= f_2^- \quad \text{in} \quad \Omega^-\end{aligned} \tag{5}$$

Here $\kappa_\pm^2 := k_\pm^2 - \gamma^2$, where $k_\pm = \omega\sqrt{\mu\varepsilon_\pm}$ denotes the wavenumber inside $\Omega^\pm$. Let further $\kappa(x) := \kappa_\pm$ if $x \in \Omega^\pm$, and define ε in the same way. Let $[\cdot]_\Gamma$ denote the jump of a function over Γ, i.e.

$$[u]_\Gamma := u^+ - u^-$$

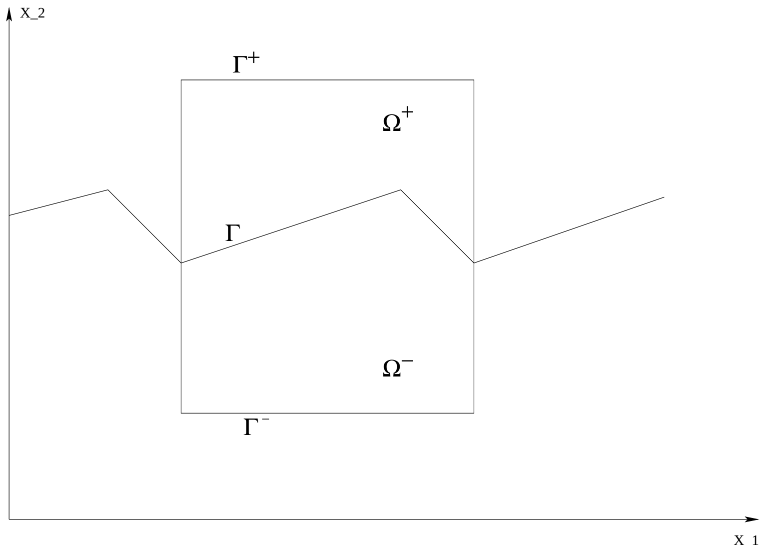

Figure 2: The 2D periodic cell

on the interface. Then the transmission conditions (3) turn into

$$\begin{aligned}
\left[\frac{\gamma}{\kappa^2}\partial_\tau u_2 + \frac{\omega\varepsilon}{\kappa^2}\partial_\nu u_1\right]_\Gamma &= -\frac{\omega\varepsilon}{\kappa_+^2}\partial_\nu u_1^{(i)} =: b_1 \\
\left[\frac{\gamma}{\kappa^2}\partial_\tau u_1 - \frac{\omega\mu}{\kappa^2}\partial_\nu u_2\right]_\Gamma &= \frac{\omega\mu}{\kappa_+^2}\partial_\nu u_2^{(i)} =: b_2 \\
[u_1]_\Gamma &= -u_1^{(i)} =: b_3 \\
[u_2]_\Gamma &= -u_2^{(i)} =: b_4
\end{aligned} \tag{6}$$

on Γ. Usually the case of $(u_1^{(i)}, u_2^{(i)})$ being a plane wave, i.e.

$$(u_1^{(i)}, u_2^{(i)}) = (p_3, q_3)e^{i(\alpha-\beta)x_2}, \tag{7}$$

and $f_j^{\pm} = 0$ for $j = 1, 2$ is of interest, but for technical reasons, we will also have to consider inhomogeneous boundary conditions and inhomogeneous right-hand sides of the Helmholtz equations. Note that the functions u_j describe only the scattered field and not the total field.
In general, the unknown functions have to satisfy a radiation condition at infinity. In the given situation this leads to the requirement that in the vicinity of Γ^+ and Γ^-, they have to be a superposition of outgoing bounded plane waves of the form

$$u_j^{\pm}(x_1, x_2) = \sum_{n=-\infty}^{\infty} A_{j,n}^{\pm} e^{i(n+\alpha)x_1 + \sqrt{\kappa_\pm^2 - (n+\alpha)^2}x_2}, \tag{8}$$

which remains bounded as $|x_2| \to \infty$. We suppose that the artificial boundaries are straight lines and that the interface is piecewise C^2 with a finite set of corner points. Moreover, we suppose that for every corner point S there exists a neighbourhood $\mathcal{U}_S$ such that $\Omega^{\pm} \cap \mathcal{U}_S = C_S^{\pm} \cap \mathcal{U}_S$, where $C_S^{\pm}$ is an infinite cone with vertex S.

In the following we will write the boundary operators as a 4×4 matrix $\mathbf{B} = (B^i_j)$, i.e.

$$\mathbf{B} = \left(B^i_j(\partial_\nu, \partial_\tau) \right)^4_{i,j=1} := \begin{pmatrix} \frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu & -\frac{\omega\varepsilon_-}{\kappa_-^2}\partial_\nu & \frac{\gamma}{\kappa_+^2}\partial_\tau & -\frac{\gamma}{\kappa_-^2}\partial_\tau \\ \frac{\gamma}{\kappa_+^2}\partial_\tau & -\frac{\gamma}{\kappa_-^2}\partial_\tau & -\frac{\omega\mu}{\kappa_+^2}\partial_\nu & \frac{\omega\mu}{\kappa_-^2}\partial_\nu \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}, \tag{9}$$

which acts on the vector $(u_1^+, u_1^-, u_2^+, u_2^-)^\top$.

3 Regularity of solutions

We are interested in shape derivatives of the solutions of the above boundary value problem. In the first subsection, we will show an a priori estimate for solutions of the conical diffraction problem. Then we give an existence and uniqueness result. This is used in Section 2.2 to show existence and uniqueness of shape derivatives.

3.1 A priori estimates

Since we deal with nonsmooth interfaces, we use weighted Sobolev spaces of the Kondratiev type, which were introduced especially for boundary value problems where the domains have corner points.

Definition 1. Let $\mathcal{S}$ be the set of corner points of the boundary, let r_S be the distance from $x \in \Omega^\pm$ to $S \in \mathcal{S}$ and fix a partition of unity

$$1 = \sum_{S \in \mathcal{S}} \chi_S + \Psi,$$

where χ_S and Ψ are smooth, the χ_S have compact support in the neighbourhood of $S \in \mathcal{S}$, $\chi \equiv 1$ in a smaller neighbourhood and $\Psi(x), \chi(x) \geq 0$ for all $x \in \Omega$. For $k \in \mathbb{N}$ and $\eta \in \mathbb{R}$ we define $V^k_\eta(\Omega^\pm)$ as the set of generalized functions with the finite norm

$$||u||_{V^k_\eta(\Omega^\pm)} := ||\Psi u||_{H^k(\Omega^\pm)} + \sum_{S \in \mathcal{S}} \sum_{|\beta| \leq k} ||r_S^{\eta-k+|\beta|} D^\beta(\chi_S u)||_{L^2(\Omega^\pm)}.$$

For $k \geq 1$, the well defined (see [24],[18]) trace space on the boundary $\partial\Omega^\pm$ is denoted by $V^{k-1/2}_\eta(\partial\Omega^\pm)$. If, as in our setting, $\Omega = \Omega^+ \cup \Omega^-$, then

$$\mathcal{V}^k_\eta(\Omega) := V^k_\eta(\Omega^+) \times V^k_\eta(\Omega^-).$$

The following lemma, which is Lemma 6.2.1 in [18], concerning embeddings of these spaces will be needed later on.

Lemma 1. *Let Ω be a bounded domain and $\eta, \beta \in \mathbb{R}$. If $k \geq l \geq 0$ and $\eta - k \leq \beta - l$, then $V^k_\eta(\Omega)$ is continuously embedded into $V^l_\beta(\Omega)$. Moreover, $V^k_\eta(\Omega)$ is dense in $V^l_\beta(\Omega)$. If $k > l \geq 0$ and $\eta - k < \beta - l$, then this embedding is compact. Analogous statements are true for the trace spaces.*

Remark 1 (*Dual spaces*)**.** Let Ω be a bounded domain and let k be a nonnegative integer. The dual space of $V_\eta^k(\Omega)$ is denoted by $V_\eta^k(\Omega)^*$. It is equipped with the norm

$$||u||_{V_\eta^k(\Omega)^*} = \sup\left\{|(u,v)| : ||v||_{V_\eta^k(\Omega)} = 1\right\},$$

where $(\cdot,\cdot)$ is the extension of the scalar product in $L^2(\Omega)$ to $V_\eta^k(\Omega)^* \times V_\eta^k(\Omega)$. Obviously, $V_\eta^0(\Omega)^* = V_{-\eta}^0(\Omega)$, because the weight functions cancel out in the scalar product. We define

$$V_{-\eta}^{-k}(\Omega) := V_\eta^k(\Omega)^*.$$

For every $S \in \mathcal{S}$, we set

$$v_j^\pm := \chi_S u_j^\pm$$

and extend v_j by zero outside the support of χ_S. Additionally, we define

$$\begin{aligned}
\sigma_j^\pm &:= (\triangle + \kappa_\pm^2) v_j^\pm \qquad \text{for} \qquad j = 1,2,\\
\phi_1 &:= B_1^1(\partial_\nu,\partial_\tau)v_1^+ + B_1^2(\partial_\nu,\partial_\tau)v_1^- + B_1^3(\partial_\nu,\partial_\tau)v_2^+ + B_1^4(\partial_\nu,\partial_\tau)v_2^-,\\
\phi_2 &:= B_2^1(\partial_\nu,\partial_\tau)v_1^+ + B_2^2(\partial_\nu,\partial_\tau)v_1^- + B_2^3(\partial_\nu,\partial_\tau)v_2^+ + B_2^4(\partial_\nu,\partial_\tau)v_2^-,\\
\phi_3 &:= B_3^1(\partial_\nu,\partial_\tau)v_1^+ + B_3^2(\partial_\nu,\partial_\tau)v_1^- + B_3^3(\partial_\nu,\partial_\tau)v_2^+ + B_3^4(\partial_\nu,\partial_\tau)v_2^-,\\
\phi_4 &:= B_4^1(\partial_\nu,\partial_\tau)v_1^+ + B_4^2(\partial_\nu,\partial_\tau)v_1^- + B_4^3(\partial_\nu,\partial_\tau)v_2^+ + B_4^4(\partial_\nu,\partial_\tau)v_2^-.
\end{aligned}$$

Now we switch to polar coordinates $(r,\theta_S^\pm)$ in the cone $C_S^\pm \subset \Omega^\pm$ with origin S and apply the coordinate transform $t \mapsto e^t$. We define

$$\begin{aligned}
w_j^\pm(t,\theta_S^\pm) &:= v_j^\pm(e^t,\theta_S^\pm),\\
w_j &:= (w_j^+, w_j^-),\\
\varrho_j^\pm(t,\theta_S^\pm) &:= e^{2t}\sigma_j^\pm(e^t,\theta_S^\pm),\\
\varrho_j &:= (\varrho_j^+,\varrho_j^-),\\
\omega_i(t,\theta_S^\pm) &:= e^{(3/2-m_i)t}\phi_i(e^t,\theta_S^\pm)
\end{aligned}$$

with $m_1 = m_2 = 0$, $m_3 = m_4 = 1$ and $i = 1,\ldots,4$. Using this notation, we now have the following interface problem in the ramified strip (see [24], Chapter 1.6.3)

$$B_S = B_S^+ \cup B_S^-$$

with

$$\begin{aligned}
B_S^+ &:= \{(t,\theta_S^+) : t \in \mathbb{R}, 0 < \theta_S^+ < \delta_S^+\},\\
B_S^- &:= \{(t,\theta_S^-) : t \in \mathbb{R}, \delta_S^+ < \theta_S^- < 2\pi\},
\end{aligned}$$

Lemma 2. *With the notation introduced above and $L^\pm := \triangle + \kappa_\pm^2$, the inhomogeneous conical diffraction problem in the vicinity of a corner point can be transformed to*

$$L^\pm(D_\theta,D_t)w_1^\pm \quad = \quad \varrho_1^\pm \quad \text{in} \quad B_S^\pm$$

$$L^{\pm}(D_\theta, D_t) w_2^{\pm} \quad = \quad \varrho_2^{\pm} \quad \text{in} \quad B_S^{\pm}$$

with transmission conditions

$$\begin{aligned}
B_1^1(\partial_\theta,\partial_t)w_1^+ + B_1^2(\partial_\theta,\partial_t)w_1^- + B_1^3(\partial_\theta,\partial_t)w_2^+ + B_1^4(\partial_\theta,\partial_t)w_2^- &= \omega_1,\\
B_2^1(\partial_\theta,\partial_t)w_1^+ + B_2^2(\partial_\theta,\partial_t)w_1^- + B_2^3(\partial_\theta,\partial_t)w_2^+ + B_2^4(\partial_\theta,\partial_t)w_2^- &= \omega_2,\\
B_3^1(\partial_\theta,\partial_t)w_1^+ + B_3^2(\partial_\theta,\partial_t)w_1^- + B_3^3(\partial_\theta,\partial_t)w_2^+ + B_3^4(\partial_\theta,\partial_t)w_2^- &= \omega_3,\\
B_4^1(\partial_\theta,\partial_t)w_1^+ + B_4^2(\partial_\theta,\partial_t)w_1^- + B_4^3(\partial_\theta,\partial_t)w_2^+ + B_4^4(\partial_\theta,\partial_t)w_2^- &= \omega_4.
\end{aligned}$$

Proof. See [24], Theorem 2.10. □

Applying the Laplace transform

$$\check{u}(\cdot,\lambda) := \int_{-\infty}^{\infty} e^{-\lambda t} u(\cdot,t)dt$$

to the problem of Lemma 2 leads to an "interface" problem on

$$A_S^+ \cup A_S^- := \{\theta_S^+ : 0 < \theta_S^+ < \delta_S^+\} \cup \{\theta_S^- : \delta_S^+ < \theta_S^- < 2\pi\}$$

for $\check{w}_j^{\pm}$ with inhomogeneities $\check{\varrho}_j^{\pm}$ and $\check{\omega}_j^{\pm}$. This problem depends on the parameter λ. We introduce the norms

$$||u||_{H^k(A_S^{\pm},\lambda)} := ||u||_{H^k(A_S^{\pm})} + |\lambda|^k ||u||_{L^2(A_S^{\pm})}$$

and

$$\mathcal{H}^k(A_S,\lambda) := H^k(A_S^+,\lambda) \times H^k(A_S^-,\lambda).$$

Then, as in [18], Theorem 3.6.1, where it is necessary to assume that Reλ does not coincide with the real part of one of the eigenvalues of the parameter dependent system, it can be shown that there exists a unique solution $\check{w}_j$, which satisfies

$$\sum_{j=1}^{2} ||\check{w}_j(\cdot,\lambda)||_{\mathcal{H}^{k+2}(A_S,\lambda)} \le C_1 \left\{ \sum_{j=1}^{2} ||\check{\varrho}_j(\cdot,\lambda)||_{\mathcal{H}^k(A_S,\lambda)} + \sum_{j=1}^{4} (1+|\lambda|^{k+m_j+1/2}) |\check{\omega}_j(\lambda)| \right\}, \tag{10}$$

where

$$\check{w}_j := (\check{w}_j^+, \check{w}_j^-) \qquad \text{and} \qquad \check{\varrho}_j := (\check{\varrho}_j^+, \check{\varrho}_j^-).$$

We integrate this equation along the line Re$\lambda = -\beta$ and use the norm equivalence

$$||u||_{H^k_\beta(B_S^{\pm})} \simeq \left(\int_{\mathrm{Re}\lambda=-\beta} ||\check{u}(\cdot,\lambda)||^2_{H^k(A_S^{\pm},\lambda)} d\lambda \right)^{1/2},$$

where

$$H^k_\beta(B^{\pm}) := \left\{ u \in \mathcal{D}'(B^{\pm}) : (t,\theta) \mapsto e^{\beta t} u(t,\theta) \in H^k(B^{\pm}) \right\}.$$

Furthermore,

$$\mathcal{H}^k_\beta(B) := H^k_\beta(B^+) \times H^k_\beta(B^-)$$

as usual. In this way we get

$$\sum_{j=1}^{2} ||w_j||_{\mathcal{H}_\beta^{k+2}(B_S)} \leq C_2 \left\{ \sum_{j=1}^{2} ||\varrho||_{\mathcal{H}_\beta^k(B_S)} + \sum_{j=1}^{4} ||\omega_j||_{H_\beta^{k+m_j+1/2}(\partial B_S^+)} \right\}. \tag{11}$$

The trace spaces $H_\beta^{k+m_j+1/2}(\partial B_S^\pm)$ consist of all functions u on $\partial B_S^\pm$ which satisfy

$$e^{\beta t} u \in H^{k+m_j+1/2}(\partial B_S^\pm).$$

Let Θ be the coordinate transform $(t, \theta) \mapsto (\log t, \theta)$ mapping a ramified strip $B \subset \mathbb{R}^2$ onto a ramified cone $C \subset \mathbb{R}^2$. Lemma 1.62 in [24] states that the mapping

$$\mathcal{V}_\eta^k(C) \to \mathcal{H}_\beta^k(B) : u \mapsto u \circ \Theta^{-1},$$

is an isomorphism for $\beta = \eta - k + 1$ with η and k from Definition 1. We will omit the dependence of β on k and η in the notation. In terms of these spaces the estimate (11) becomes

$$\sum_{j=1}^{2} ||v_j||_{\mathcal{V}_\eta^{k+2}(C_S)} \leq C_3 \left\{ \sum_{j=1}^{2} ||t^2 \sigma_j||_{\mathcal{V}_{\eta-2}^k(C_S)} + \sum_{j=1}^{4} ||t^{3/2-m_j} \phi_j^i||_{V_{\eta-m_j}^{k+m_j+1/2}(\partial B_S^+)} \right\} \tag{12}$$

because of the isomorphism. The product rule yields

$$\sigma_j^\pm = \chi_S(\triangle + \kappa_\pm^2) u_j^\pm + 2\nabla u_j^\pm \cdot \nabla \chi_S + u_j^\pm \triangle \chi_S = \chi_S f_j^\pm + 2\nabla u_j^\pm \nabla \chi_S + u_j^\pm \triangle \chi_S.$$

The operator $L^* u_j^\pm := 2\nabla u_j^\pm \nabla \chi_S + u_j^\pm \triangle \chi_S$ is continuous and of first order, i.e.

$$||L^* u_j||_{\mathcal{V}_\eta^k(C_S)} \leq C_4 ||u||_{\mathcal{V}_\eta^{k+1}(C_S)}$$

Moreover,

$$||\chi_S f_j||_{\mathcal{V}_\eta^k(C_S)} \leq C_5 ||f_j||_{\mathcal{V}_\eta^k(C_S)}$$

by Lemma 3.3 in [17]. Since

$$V_\eta^k(C_S) \to V_{\eta-\alpha}^k(C_S) : u \mapsto t^\alpha u$$

realizes isomorphisms, it follows by switching back to Cartesian coordinates that

$$||t^2 \sigma_j||_{\mathcal{V}_{\eta-2}^k(C_S)} \leq C_6 \left\{ ||f_j||_{\mathcal{V}_\eta^k(C_S)} + ||u_j||_{\mathcal{V}_\eta^{k+1}(C_S)} \right\}.$$

Analogously, we get

$$||t^{3/2-m_j} \phi_j||_{V_{\eta-m_j}^{k+m_j+1/2}(\{(t,\delta_s^+):t\geq 0\})} \leq C_7 \left\{ ||b_j||_{V_\eta^{k+m_j+1/2}(\partial C_S^+)} + \sum_l ||u_l||_{\mathcal{V}_\eta^{k+1}(C_S)} \right\}.$$

Inserting this into (12) yields

$$\sum_{j=1}^{2} ||v_j||_{\mathcal{V}_\eta^{k+2}(C_S)} \leq C_8 \left\{ \sum_{j=1}^{2} ||f_j||_{\mathcal{V}_\eta^k(C_S)} + \sum_{j=1}^{4} ||b_j||_{V_\eta^{k+m_j+1/2}(\partial C_S^+)} + \sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+1}(C_S)} \right\}. \tag{13}$$

Now we consider the smooth part Ψu_j. From now on we use the notation $\hat{u}_j^{\pm} := \Psi u_j^{\pm}$ and $\hat{u}_j^{\pm} := (\hat{u}_j^{+}, \hat{u}_j^{-})$ and define

$$g_j^{\pm} := (\triangle + \kappa_{\pm}^2)(\hat{u}_j^{\pm})$$

Again, by the product rule, it holds that

$$(\triangle + \kappa_{\pm}^2)(\hat{u}_j^{\pm}) = \Psi(\triangle + \kappa_{\pm}^2)u_j^{\pm} + 2\nabla u_j^{\pm} \cdot \nabla\Psi + u_j^{\pm}\triangle\Psi = \Psi f_j^{\pm} + 2\nabla u_j^{\pm} \cdot \nabla\Psi + u_j^{\pm}\triangle\Psi$$

and

$$\frac{\partial \hat{u}_j^{\pm}}{\partial \nu} = \Psi\frac{\partial u_j^{\pm}}{\partial \nu} + u_j^{\pm}\frac{\partial \Psi}{\partial \nu}, \quad \frac{\partial \Psi u_j^{\pm}}{\partial \tau} = \Psi\frac{\partial u_j^{\pm}}{\partial \tau} + u_j^{\pm}\frac{\partial \Psi}{\partial \tau}.$$

Using the notation (9), we define

$$\begin{aligned}
B_1^1(\partial_\nu,\partial_\tau)\hat{u}_1^+ + B_1^2(\partial_\nu,\partial_\tau)\hat{u}_1^- + B_1^3(\partial_\nu,\partial_\tau)\hat{u}_2^+ + B_1^4(\partial_\nu,\partial_\tau)\hat{u}_2^- &=: \Phi_1,\\
B_2^1(\partial_\nu,\partial_\tau)\hat{u}_1^+ + B_2^2(\partial_\nu,\partial_\tau)\hat{u}_1^- + B_2^3(\partial_\nu,\partial_\tau)\hat{u}_2^+ + B_2^4(\partial_\nu,\partial_\tau)\hat{u}_2^- &=: \Phi_2,\\
B_3^1(\partial_\nu,\partial_\tau)\hat{u}_1^+ + B_3^2(\partial_\nu,\partial_\tau)\hat{u}_1^- + B_3^3(\partial_\nu,\partial_\tau)\hat{u}_2^+ + B_3^4(\partial_\nu,\partial_\tau)\hat{u}_2^- &=: \Phi_3,\\
B_4^1(\partial_\nu,\partial_\tau)\hat{u}_1^+ + B_4^2(\partial_\nu,\partial_\tau)\hat{u}_1^- + B_4^3(\partial_\nu,\partial_\tau)\hat{u}_2^+ + B_4^4(\partial_\nu,\partial_\tau)\hat{u}_2^- &=: \Phi_4.
\end{aligned}$$

Note that

$$B_j^i(\partial_\nu,\partial_\tau)[\hat{u}_k^{\pm}] = \Psi B_j^i(\partial_\nu,\partial_\tau)u_k^{\pm} + u_k^{\pm} B_j^i(\partial_\nu,\partial_\tau)\Psi.$$

Analogous to the considerations above, it follows that

$$||g_j^{\pm}||_{H^k(\Omega^{\pm})} \le C_9 \left\{ ||f_j^{\pm}||_{V_\eta^k(\Omega^{\pm})} + ||u_j^{\pm}||_{V_\eta^{k+1}(\Omega^{\pm})} \right\}$$

and

$$||\Phi_j||_{H^{k-\frac{1}{2}}(\Gamma)} \le C_{10} \left\{ ||b_j||_{V_\eta^{k+m_j+1/2}(\Gamma)} + \sum_{\substack{l=1\\ i\in\{+,-\}}}^{2} ||u_l^i||_{V_\eta^{k+1}(\Omega^i)} \right\},$$

where $\mathcal{H}^k(\Omega) := H^k(\Omega) \times H^k(\Omega)$ as before. Inserting this into the estimate (2.2) in [5] (originally proven by Roitberg and Seftel [29]), namely

$$\sum_{j=1}^{2} ||\hat{u}_j||_{\mathcal{H}^{k+2}(\Omega)} \le C_{11} \left\{ \sum_{j=1}^{2} ||g_j||_{\mathcal{H}^k(\Omega)} + \sum_{j=1}^{4} ||\Phi_j||_{H^{k+m_j+1/2}(\Gamma)} \right\},$$

yields

$$\sum_{j=1}^{2} ||\hat{u}_j||_{\mathcal{H}^{k+2}(\Omega^i)} \le C_{12} \left\{ \sum_{j=1}^{2} ||f_j||_{\mathcal{V}_\eta^k(\Omega^i)} + \sum_{j=1}^{4} ||b_j||_{V_\eta^{k+m_j+1/2}(\Gamma)} + \sum_{j=1}^{2} ||u_j^i||_{\mathcal{V}_\eta^{k+1}(\Omega)} \right\}. \tag{14}$$

By adding the estimates (13) and (14) we get the desired a priori estimate.

As we have seen and as explained in [10] in more detail, to each corner point $S \in \mathcal{S}$ one can attach a parameter dependent system of ordinary differential equations, which arises from the problem in Lemma 2 by applying a Laplace transform. The eigenvalues form the sets

$$\mathcal{A}_S^{\pm} := \left\{ \lambda_S \in \mathbb{C} : \left(\frac{\sin(\pi - \delta_S^{\pm})\lambda_S}{\sin \pi\lambda_S} \right)^2 = \left(\frac{k_-^2 + k_+^2}{k_-^2 - k_+^2} \right)^2 \right\} \cup \mathbb{N}\backslash\{0\},$$

where λ_S are the eigenvalues of the system, δ_S^+ and $\delta_S^- := 2\pi - \delta_S^+$ are the opening angles of the interface at the corner point S from above and from below the interface, respectively. Let λ_S^0 be the λ_S with minimal positive real part and

$$\mu^0 := \min_{S \in \mathcal{S}} \left\{ \mathrm{Re}\lambda_S^0 \right\}. \tag{15}$$

Proposition 1. *Assume that* $k+1-\eta \in (0, \mu^0)$ *and that the solution* (u_1, u_2) *of (4) - (8) is in* $[\mathcal{V}_\eta^{k+1}(\Omega)]^2$ *for* $k \in \mathbb{Z}, k \geq 0$. *Then* $(u_1, u_2) \in [\mathcal{V}_\eta^{k+2}(\Omega)]^2$ *and*

$$\sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+2}(\Omega)} \leq C \left\{ \sum_{j=1}^{2} ||f_j||_{\mathcal{V}_\eta^{k}(\Omega)} + \sum_{j=1}^{4} ||b_j||_{V_\eta^{k+m_j+1/2}(\Gamma)} + \sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+1}(\Omega)} \right\}. \tag{16}$$

Proposition 2. *If in addition to the assumptions of Proposition 1 the conical diffraction problem (4) - (8) is uniquely solvable in* $\mathcal{V}_\eta^{k+1}(\Omega)$, *then*

$$\sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+2}(\Omega)} \leq C \left\{ \sum_{j=1}^{2} ||f_j||_{\mathcal{V}_\eta^{k}(\Omega)} + \sum_{j=1}^{4} ||b_j||_{V_\eta^{k+m_j+1/2}(\Gamma)} \right\}. \tag{17}$$

Proof. The proof follows the technique used in [3], Lemma III 3.10. Suppose that the hypothesis is not satisfied. Then it follows that there exist sequences $(u_{j,n})_n \subseteq \mathcal{V}_\eta^{k+2}(\Omega)$ for $j = 1, 2$ such that

$$\sum_{j=1}^{2} ||u_{j,n}||_{\mathcal{V}_\eta^{k+2}(\Omega)} > n \left\{ \sum_{\substack{j=1 \\ i \in \{+,-\}}}^{2} ||L^i u_{j,n}^i||_{V_\eta^k(\Omega^i)} + \sum_{j=1}^{4} || \sum_{i=1}^{2} \left(B_j^{2i-1} u_{i,n}^+ + B_j^{2i} u_{i,n}^- \right) ||_{V_\eta^{k+m_j+1/2}(\Gamma)} \right\}, \tag{18}$$

where $L^\pm := \triangle + \kappa_\pm^2$ and the B_j^i are the operators of the boundary conditions. Now define

$$v_{j,n}^\pm := \frac{u_{j,n}^\pm}{||u_{j,n}^\pm||_{V_\eta^{k+2}(\Omega^\pm)}}.$$

If we insert this into (18) we have

$$\sum_{\substack{j=1 \\ i \in \{+,-\}}}^{2} ||L^i v_{j,n}^i||_{V_\eta^k(\Omega^i)} + \sum_{j=1}^{4} || \sum_{i=1}^{2} \left(B_j^{2i-1} v_{i,n}^+ + B_j^{2i} v_{i,n}^- \right) ||_{V_\eta^{k+m_j+1/2}(\Gamma)} < \frac{2}{n}. \tag{19}$$

We will use the compact embeddings stated in Lemma 1, i.e.

$$V_\eta^{k+2}(\Omega^\pm) \hookrightarrow\hookrightarrow V_\eta^{k+1}(\Omega^\pm) \hookrightarrow\hookrightarrow V_\eta^k(\Omega^\pm).$$

Since the unit sphere is closed with respect to weak convergence we can choose a subsequence $(v_{j,n'}^\pm)_{n'} \subseteq (v_{j,n}^\pm)_n$ and functions $\Phi_j^\pm \in V_\eta^{k+2}(\Omega^\pm)$ such that $(v_{j,n'}^\pm)_{n'} \rightharpoonup \Phi_j^\pm$ weakly in $V_\eta^{k+2}(\Omega^\pm)$. Since compact embeddings are completely continuous, it follows that $v_{j,n'}^\pm \to \Phi_j^\pm$ in the norm of

$V_\eta^{k+1}(\Omega^\pm)$. Proposition 1 implies that

$$\sum_{j=1}^{2} ||v_{j,n'} - v_{j,m'}||_{\mathcal{V}_\eta^{k+2}(\Omega)} \leq C \left\{ \sum_{\substack{j=1 \\ i\in\{+,-\}}}^{2} ||L^i v^i_{j,n'} - L^i v^i_{j,m'}||_{V_\eta^k(\Omega^i)} + \right.$$

$$+ \sum_{j=1}^{4} || \sum_{i=1}^{2} \left(B_j^{2i-1} v^+_{i,n'} - B_j^{2i-1} v^+_{i,m'} + B_j^{2i} v^-_{i,n'} - B_j^{2i} v^-_{i,m'} \right) ||_{V_\eta^{k+m_j+1/2}(\Gamma)}$$

$$\left. + \sum_{j=1}^{2} ||v_{j,n'} - v_{j,m'}||_{\mathcal{V}_\eta^{k+1}(\Omega)} \right\},$$

and therefore $(v^\pm_{j,n'})_{n'}$ is a Cauchy sequence in $V_\eta^{k+2}(\Omega^\pm)$ because the right-hand side tends to zero if $m', n' \to \infty$. Hence $v^\pm_{j,n'} \to \Phi^\pm_j$ in $V_\eta^{k+2}(\Omega^\pm)$ and $||\Phi^\pm_j||_{V_\eta^{k+2}(\Omega^\pm)} = 1$. On the other hand

$$\sum_{\substack{j=1 \\ i\in\{+,-\}}}^{2} ||L^i \Phi^i_j||_{V_\eta^k(\Omega^i)} = \lim_{n'\to\infty} \sum_{\substack{j=1 \\ i\in\{+,-\}}}^{2} ||L^i v^i_{j,n'}||_{V_\eta^k(\Omega^i)} = 0$$

and

$$\sum_{j=1}^{4} || \sum_{i=1}^{2} \left(B_j^{2i-1} \Phi^+_i + B_j^{2i} \Phi^-_i \right) ||_{V_\eta^{k+m_j+1/2}(\Gamma)} =$$

$$= \lim_{n'\to\infty} \sum_{j=1}^{4} || \sum_{i=1}^{2} \left(B_j^{2i-1} v^+_{i,n'} + B_j^{2i} v^-_{i,n'} \right) ||_{V_\eta^{k+m_j+1/2}(\Gamma)} = 0$$

because of (19). If the kernel of the operator of the diffraction problem is trivial, then $\Phi^\pm_j = 0$. This is a contradiction and finishes the proof. □

3.2 Existence and uniqueness

In this section, we will prove the existence and uniqueness of the solution of the conical diffraction problem for absorbing materials. The following two Lemmas establish the Fredholm property of the problem, which is then used together with a result from [8]. The first Lemma is due to Peetre [25]. A proof can also be found in [24].

Lemma 3. *Let $\mathcal{X}, \mathcal{Y}$ and $\mathcal{Z}$ be Banach spaces such that $\mathcal{X}$ is compactly embedded into $\mathcal{Z}$, and let A be a bounded linear operator from $\mathcal{X}$ into $\mathcal{Y}$. Then the following two assertions are equivalent:*

(i) $\dim\ker A < \infty$ *and* $\operatorname{ran} A$ *is closed in* $\mathcal{Y}$.

(ii) $\exists C > 0\ \forall u \in \mathcal{X} :\ ||u||_{\mathcal{X}} \leq C\{||Au||_{\mathcal{Y}} + ||u||_{\mathcal{Z}}\}$.

This Lemma, together with Proposition 1, establishes the semi-Fredholm property. In order to show that the operator of the conical diffraction problem has a finite-dimensional cokernel, we will construct a right regularizer.

Definition 2. Let A be a linear and continuous operator from a Banach space $\mathcal{X}$ into a Banach space $\mathcal{Y}$ and let R be a linear and continuous operator from $\mathcal{Y}$ into $\mathcal{X}$. If $AR - I : \mathcal{Y} \to \mathcal{Y}$ is compact, then the operator R is called a *right regularizer* for A.

Lemma 4. *Let $\mathcal{X}$ and $\mathcal{Y}$ be Banach spaces and let $A : \mathcal{X} \to \mathcal{Y}$ be a linear and continuous operator. If a right regularizer for A exists, then the dimension of the cokernel of A is finite.*

This is a classical result, cf. [33]. We will furthermore need the notions of *proper ellipticity* and *Shapiro-Lopatinskii ellipticity.* Let Ω be a bounded domain in $\mathbb{R}^2$. The inward-pointing unit normal at a point $x \in \partial\Omega$ will be denoted by $\nu(x)$. Then the tangent space $T_x\mathbb{R}^2$ can be written as a direct sum

$$T_x\mathbb{R}^2 = T_x(\partial\Omega) \oplus \operatorname{span}\{\nu(x)\}.$$

The cotangent space $T_x^*\mathbb{R}^2$ is then

$$T_x^*\mathbb{R}^2 = [T_x(\partial\Omega)]^\perp \oplus [\operatorname{span}\{\nu(x)\}]^\perp = [T_x(\partial\Omega)]^\perp \oplus T_x^*(\partial\Omega),$$

because $[\operatorname{span}\{\nu(x)\}]^\perp$ can be identified with $T_x^*(\partial\Omega)$. For $\sigma \in T_x^*\mathbb{R}^2$, we write $\sigma := (\sigma_1, \sigma_2)$, with a *cotangent* $\sigma_1 \in T_x^*(\partial\Omega)$ and a *conormal* $\sigma_2 \in [T_x(\partial\Omega)]^\perp$. Obviously, $T_x^*\mathbb{R}^2$ is canonically isomorphic to $\mathbb{R}^2$. We may also assume $\sigma \in \mathbb{C} \otimes T_x^*\mathbb{R}^2 \subset \mathbb{C}^2$, so when we write $\sigma_1 \in \mathbb{C}$ in the following, we mean in fact the coefficient of $\sigma_1 \in T_x^*(\partial\Omega)$ in the canonical basis representation of $\sigma \in \mathbb{C} \otimes T_x^*\mathbb{R}^2$.

Definition 3. Let $\mathbf{L}(x; D_{x_1}, D_{x_2})$ be an $n \times n$-matrix of elliptic differential operators and denote its principal part by $\mathbf{L}_0(x; D_{x_1}, D_{x_2})$. The operator $\mathbf{L}(x; D_{x_1}, D_{x_2})$ is called *properly elliptic* if for every $\sigma_1 \in \mathbb{C}\backslash\{0\}$ the polynomial

$$p(\lambda) := \det \mathbf{L}_0(x; \sigma_1, \lambda), \quad \lambda \in \mathbb{C}$$

has as many roots with strictly positive imaginary part as with strictly negative imaginary part, including multiplicities.

If, for example, $\mathbf{L}(x; D_{x_1}, D_{x_2})$ is a system of two Laplacians in $\mathbb{R}^2$, then

$$p(\lambda) = \det \begin{pmatrix} \sigma_1^2 + \lambda^2 & 0 \\ 0 & \sigma_1^2 + \lambda^2 \end{pmatrix}.$$

The polynomial $p(\lambda)$ has two double roots $\lambda_{1/2} = \pm i\sigma_1$. Consequently, this system is properly elliptic.

Lemma 5. *Consider the $n \times n$-matrix operator $\mathbf{L}(x; D_{x_1}, D_{x_2})$ and the $m \times n$-matrix $\mathbf{B}(x; D_{x_1}, D_{x_2})$ for $x \in \partial\Omega$, where m is the number of roots of $p(\lambda) = \det \mathbf{L}_0(x; \sigma_1, \lambda)$ with strictly positive (or equivalently, with strictly negative) imaginary part, counting multiplicities. Let $\sigma_1 \in \mathbb{C}\backslash\{0\}$. Assume that $\mathbf{L}(x; D_{x_1}, D_{x_2})$ is properly elliptic. If the homogeneous initial value problem*

$$\mathbf{L}_0\left(x; \sigma_1, \frac{1}{i}\frac{d}{dt}\right)\phi(t) = 0, \quad t > 0,$$
$$\mathbf{B}_0\left(x; \sigma_1, \frac{1}{i}\frac{d}{dt}\right)\phi(t) = 0, \quad t = 0,$$
$$\lim_{t\to\infty} \phi(t) = 0$$

has only the trivial solution, then the problem

$$\mathbf{L}_0\left(x; \sigma_1, \frac{1}{i}\frac{d}{dt}\right)\phi(t) = 0, \quad t > 0,$$

$$\mathbf{B}_0\left(x;\sigma_1,\frac{1}{i}\frac{d}{dt}\right)\phi(t)=s,\quad t=0,$$
$$\lim_{t\to\infty}\phi(t)=0$$

is uniquely solvable for every $s\in\mathbb{C}^m$.

Proof. Combine Definition 9.28 and Theorem 9.29 from [33]. □

Note that $\mathbf{B}(x;D_{x_1},D_{x_2})$ does not need to be a differential operator. It can also be pseudodifferential in the tangential variable.

Definition 4. A pair of operators $(\mathbf{L},\mathbf{B})$ which satisfies the assumptions of Lemma 5 is said to fulfill the *Shapiro-Lopatinskii condition*.

Definition 5. Let $(\mathbf{L},\mathbf{B})$ be a pair of operators satisfying the Shapiro-Lopatinskii condition. Let ϕ_j be the solution of the initial value problem

$$\mathbf{L}_0\left(x;\sigma_1,\frac{1}{i}\frac{d}{dt}\right)\phi_j(\sigma_1,t)=0,\quad t>0,$$
$$\mathbf{B}_0\left(x;\sigma_1,\frac{1}{i}\frac{d}{dt}\right)\phi_j(\sigma_1,t)=e_j,\quad t=0,$$
$$\lim_{t\to\infty}\phi(t)=0,$$

where $e_j=(0,\ldots,0,1,0,\ldots,0)$. The matrix $\Phi(\sigma_1,t)$ with columns $\phi_j(\sigma_1,t)$ is called the *canonical matrix function* of $(\mathbf{L},\mathbf{B})$.

We will now construct a right regularizer. This will be carried out in four steps, combining the techniques of Wloka et al. [33], Chapter 9.3, and Kondratiev [17], as follows. First we will construct regularizers for operators in the plane and in the half space. Using local coordinates, it is possible to use these results to construct for every point $x_0\in\Omega$ a local regularizer in a neighbourhood $U(x_0)$. It is necessary to distinguish between the case that x_0 lies in the interior of $\Omega^\pm$ and the case that x_0 lies on the boundary or on the interface. Then we obtain a global regularizer by means of a partition of unity.

(i) Assume that $L_0(D_{x_1},D_{x_2}):H^{k+2}(\mathbb{R}^2)\to H^k(\mathbb{R}^2)$ is the principal part of an elliptic differential operator. Let $\mathcal{F}$ denote the Fourier transform on $\mathbb{R}^2$ and $\sigma=(\sigma_1,\sigma_2)$. It is shown in [33] that the operator $R:H^k(\mathbb{R}^2)\to H^{k+2}(\mathbb{R}^2)$ defined by

$$Rf:=\mathcal{F}^{-1}|\sigma|^2(1+|\sigma|^2)^{-1}L_0^{-1}(\sigma_1,\sigma_2)\mathcal{F}f,$$

is a right regularizer for $L_0(D_{x_1},D_{x_2})$ and

$$L_0\circ R=I+K,$$

where K is an operator of order -1. In our case, $L_0(D_{x_1},D_{x_2})$ is the Laplacian and $L_0(\sigma_1,\sigma_2)=\sigma_1^2+\sigma_2^2$.

(ii) Let u_1^+ and u_2^+ be functions defined on the upper half plane $\mathbb{R}^2_+$. Analogously, assume that u_1^- and u_2^- are functions on the lower half plane $\mathbb{R}^2_-$. Assume further that these functions fulfill a Helmholtz system coupled via transmission conditions on the x_1-axis. Then the functions

$u^-_{1/2}(x_1, -x_2)$ are defined on $\mathbb{R}^2_+$ and the transmission problem becomes a boundary value problem with boundary values on the x_1-axis. Let $r : H^k(\mathbb{R}^2) \to H^k(\mathbb{R}^2_+)$ denote the restriction of a function on $\mathbb{R}^2$ to $\mathbb{R}^2_+$ and let $\vartheta : H^k(\mathbb{R}^2_+) \to H^k(\mathbb{R}^2)$ be a linear and continuous extension operator. Now define

$$\mathbf{L}_0(D_{x_1}, D_{x_2}) := \begin{pmatrix} L_0(D_{x_1}, D_{x_2}) & 0 & 0 & 0 \\ 0 & L_0(D_{x_1}, D_{x_2}) & 0 & 0 \\ 0 & 0 & L_0(D_{x_1}, D_{x_2}) & 0 \\ 0 & 0 & 0 & L_0(D_{x_1}, D_{x_2}) \end{pmatrix} \tag{20}$$

with $L_0(D_{x_1}, D_{x_2})$ from step (i). Then the operator $\mathbf{R}_0$ defined by

$$\mathbf{R}_0 f := r\mathcal{F}^{-1}|\sigma|^2(1+|\sigma|^2)^{-1}\mathbf{L}_0^{-1}(\sigma_1, \sigma_2)\mathcal{F}\vartheta f$$

is a continuous operator from $[H^k(\mathbb{R}^2)]^4$ into $[H^{k+2}(\mathbb{R}^2)]^4$. Additionally we define

$$\mathbf{R}_1 b := \mathcal{F}_+^{-1}\Phi(\sigma', x_2)|\sigma'|^2(1+|\sigma'|^2)^{-1}\mathcal{F}_+ b, \tag{21}$$

with $b = (b_1, \ldots, b_4)^\top$ from (6), $\mathcal{F}_+$ is the truncated Fourier transform on $\mathbb{R}^2_+$ and $\Phi(\sigma', x_2)$ is the canonical matrix function corresponding to the boundary value problem (cf. Definition 5). The system of ordinary differential equations in the sense of Definition 5 is

$$\mathbf{L}_0\left(\sigma_1, \mp\frac{1}{i}\frac{d}{dt}\right) w^\pm_{1/2}(t) = \left(\sigma_1^2 - \frac{d^2}{dt^2}\right) w^\pm_{1/2}(t) = 0, \quad t > 0.$$

The sign of d/dt alternates because the "inward" direction changes depending on whether the original Helmholtz equation of the interface problem applies to the region above or below the interface. With $\lim_{t\to\infty} w^\pm_{1/2}(t) = 0$, this leads to $w^\pm_{1/2}(t) = c^\pm_{1/2}e^{\sigma_1 t}$. One of the transmission conditions in the system (6) is $u_1^- - u_1^+ = u_1^{(i)}$. The homogeneous initial value condition following from this is $0 = w_1^-(0) - w_1^+(0) = c_1^- - c_1^+$, so $c_1^- = c_1^+ =: c_1$. Analogously, $c_2^- = c_2^+ =: c_2$. From

$$\left[\frac{\gamma}{\kappa^2}\partial_\tau u_2 + \frac{\omega\varepsilon}{\kappa^2}\partial_\nu u_1\right]_\Gamma = -\frac{\omega\varepsilon}{\kappa_+^2}\partial_\nu u_1^{(i)}$$

we have the homogeneous initial value condition

$$\frac{\omega\varepsilon_+}{\kappa_+^2}\frac{d}{dt}w_1^+(t)|_{t=0} - \frac{\omega\varepsilon_-}{\kappa_-^2}\frac{d}{dt}w_1^-(t)|_{t=0} + \frac{\gamma}{\kappa_+^2}\sigma_1 w_2^+(0) - \frac{\gamma}{\kappa_-^2}\sigma_1 w_2^-(0) = 0.$$

This is equivalent to

$$\left(\frac{\omega\varepsilon_+}{\kappa_+^2} - \frac{\omega\varepsilon_-}{\kappa_-^2}\right)c_1\sigma_1 + \left(\frac{\gamma}{\kappa_+^2} - \frac{\gamma}{\kappa_-^2}\right)c_2\sigma_1 = 0.$$

In the same way we get

$$\left(\frac{\omega\mu}{\kappa_-^2} - \frac{\omega\mu}{\kappa_+^2}\right)c_2\sigma_1 + \left(\frac{\gamma}{\kappa_+^2} - \frac{\gamma}{\kappa_-^2}\right)c_1\sigma_1 = 0.$$

This system has a non-trivial solution if and only if

$$\varepsilon_+ = \varepsilon_-,$$

which would only be satisfied if there was no interface. It follows that $c_1 = c_2 = 0$. The system $(\mathbf{L}, \mathbf{B})$, with $\mathbf{B}$ from (9), is therefore Shapiro-Lopatinskii elliptic, and the canonical matrix function exists. Then it is shown in [33] that the operator

$$\mathbf{R}(f, b) := \mathbf{R}_0 f + \mathbf{R}_1 (b - \mathbf{B} \circ \mathbf{R}_0 f), \tag{22}$$

is bounded from $[H^k(\mathbb{R}^2_+)]^4 \times \bigotimes_{j=1}^4 H^{k+m_j+1/2}(\mathbb{R})$ into $[H^{k+2}(\mathbb{R}^2_+)]^4$ and that it is a right regularizer for the operator $\mathbf{A} := (\mathbf{L}, \mathbf{B})$.

As explained in detail in [8], the radiation condition (8) for the original problem induces boundary conditions on the artificial boundaries Γ^+ and Γ^-. These boundary conditions involve the Dirichlet-to-Neumann map. In general, it maps the Dirichlet data of an exterior solution to the Neumann data. In our case, we must distinguish between the upper and the lower artificial boundary and the Dirichlet-to-Neumann map consists of two parts. More precisely, from [8] we take the periodic pseudodifferential operators of order 1

$$(T_j^{\pm})\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}(x) := \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} e^{i(n+\alpha)x} \begin{pmatrix} M_{n,j}^{\pm,1} \\ M_{n,j}^{\pm,2} \end{pmatrix} \cdot \int_0^{2\pi} \begin{pmatrix} u_1(x) \\ u_2(x) \end{pmatrix} e^{-i(n+\alpha)x} dx, \qquad j = 1, 2,$$

acting on α-quasi-periodic functions. The exact definition of the coefficients $M_{n,j}^{\pm,k}$ is given in [8]. Then we have the nonlocal boundary conditions

$$\begin{aligned} \frac{\omega\varepsilon_+}{\kappa_+^2} \partial_\nu u_1^+ + \frac{\gamma}{\kappa_+^2} \partial_\tau u_2^+ + T_1^+ \begin{pmatrix} u_1^+ \\ u_2^+ \end{pmatrix} &= 0, \\ -\frac{\omega\mu}{\kappa_+^2} \partial_\nu u_2^+ + \frac{\gamma}{\kappa_+^2} \partial_\tau u_1^+ + T_2^+ \begin{pmatrix} u_1^+ \\ u_2^+ \end{pmatrix} &= 0 \end{aligned} \tag{23}$$

on Γ^+ and

$$\begin{aligned} -\frac{\omega\varepsilon_-}{\kappa_-^2} \partial_\nu u_1^1 - \frac{\gamma}{\kappa_-^2} \partial_\tau u_2^- + T_1^- \begin{pmatrix} u_1^- \\ u_2^- \end{pmatrix} &= 0, \\ \frac{\omega\mu}{\kappa_-^2} \partial_\nu u_2^- - \frac{\gamma}{\kappa_-^2} \partial_\tau u_1^- + T_2^+ \begin{pmatrix} u_1^- \\ u_2^- \end{pmatrix} &= 0 \end{aligned} \tag{24}$$

on Γ^-. Now let $T_j^{\pm}$ denote the respective Dirichlet-to-Neumann maps on the half space, with $\Gamma^{\pm}$ replaced by the x_1-axis. Let $\mathbf{T}^+$ denote the boundary operator for the boundary conditions (23) and $\mathbf{T}^-$ shall denote the boundary operator of the boundary conditions (24), respectively.

Let $\mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$ denote the one-dimensional torus. Define the periodization operator

$$(\mathcal{P}u)(x) := \sum_{k=-\infty}^{\infty} u(x + 2\pi k),$$

which is a linear and continuous map from $H^s(\mathbb{R})$ into $H^s(\mathbb{T})$. If $\chi \in C_0^\infty(\mathbb{R})$, then

$$\mathcal{P}(\chi u) = (\mathcal{P}\chi) u$$

for any periodic function u.

Fix a point x_0 on the real line and a neighbourhood $U(x_0)$. Suppose that ζ and ξ are smooth cut-off functions such that

$$U(x_0) \subset \operatorname{supp} \zeta \subset \operatorname{supp} \xi \subset (a, b)$$

and assume that the length of the interval (a, b) is smaller than the period 2π. Let T_p be a periodic pseudodifferential operator of order r, i.e. T_p maps $H^s(\mathbb{T})$ into $H^{s-r}(\mathbb{T})$. Assume that T is a pseudodifferential operator on $H^s(\mathbb{R})$ satisfying

$$\xi T_p([\mathcal{P}\zeta]u) = \xi T(\zeta u) \tag{25}$$

for any 2π-periodic function u. Wloka's construction ([33]) applies to non-local pseudodifferential operators on the real line. The regularizer for the operators $(\mathbf{A}, \xi \mathbf{T}^{\pm} \mathcal{P} \zeta)$ is constructed as in (21) and (22) with $b = 0$, because both (23) and (24) have homogeneous right-hand sides. The existence of a canonical matrix function is assured in the same way as it was done earlier for the transmission conditions. Because of (25), the results can be carried over to periodic operators as well. Since in the following we will construct regularizers in small neighbourhoods, we only need to consider one type of boundary conditions at once.

(iii) We establish local regularizing properties. Suppose that $x_0 \in \Omega$ and that the neighbourhood $U(x_0)$ lies in the interior of $\Omega^+ \cup \Omega^-$. Let χ and ζ be two smooth functions with compact support in $U(x_0)$. Then

$$\chi \mathbf{A} \circ \mathbf{R} \zeta = \chi \mathbf{I} \zeta + \chi \mathbf{K} \zeta, \tag{26}$$

where $\mathbf{K}$ is a continuous operator of order -1 and therefore, $\chi \mathbf{K} \zeta$ is compact from $[H^k(U(x_0))]^4$ into $[H^k(U(x_0))]^4$. We call the operator $\mathbf{R}$ a *local regularizer*.

Now surround any corner point on the interface Γ with an ϵ-neighbourhood and assume that x_0 either lies on the interface Γ so that a neighbourhood $U(x_0)$ does not intersect with any of these ϵ-neighbourhoods, or that that is lies on one of the artificial boundaries $\Gamma^{\pm}$. We introduce local coordinates

$$\kappa : U(x_0) \to V \subseteq \mathbb{R}^2.$$

To simplify the notation, consider two linear spaces $X(\Omega)$ and $Y(\Omega)$ of functions defined on Ω. Let $A : X(\Omega) \to Y(\Omega)$ be a linear operator. Let further $r : Y(\Omega) \to Y(U(x_0))$ be the restriction operator, and assume that there exists a continuous extension operator $i : X(U(x_0)) \to X(\Omega)$. The existence of such an extension operator is assured for Sobolev spaces on sufficiently smooth domains. This holds true in particular for Sobolev spaces on domains with Lipschitz boundaries (cf. [20]). Now we define

$$A_r := r \circ A \circ i : X(U(x_0)) \to Y(U(x_0)).$$

Then we have the commutative diagram

$$\begin{array}{ccc} X(U(x_0)) & \xrightarrow{A_r} & Y(U(x_0)) \\ \uparrow {\scriptstyle \kappa^*} & & \downarrow {\scriptstyle (\kappa^*)^{-1}} \\ X(V) & \xrightarrow{A_\kappa} & Y(V). \end{array}$$

Here, κ^* is the pull-back map, $(\kappa^*)^{-1}$ is the push-forward map and $A_\kappa := (\kappa^*)^{-1} \circ A_r \circ \kappa^*$ is the push-forward of A_r. By this construction and by step (ii) we have a local regularizer and an equation like (26) also for neighbourhoods which contain smooth parts of the interface or parts of the smooth artificial boundaries.

Let χ_S be a cut-off function with support inside the ϵ-neighbourhood of the corner point S. Suppose that the assumption of Proposition 1 concerning the eigenvalues is satisfied. From Theorem 3.6.1 in [18] and the considerations made in the previous subsection, it follows that there exists a solution $u_0 = (u^+_{1,0}, u^+_{2,0}, u^-_{1,0}, u^-_{2,0})^\top$ of the problem

$$\mathbf{L}_0 u_0 = \chi_S f, \qquad \mathbf{B} u_0 = \chi_S b \tag{27}$$

in the ramified cone C_S, with $f = (f_1^+, f_2^+, f_1^-, f_2^-)^\top$ from (5), $b = (b_1, \dots, b_4)^\top$ from (6) and $\mathbf{B}$ from (9).

(iv) We cover $\overline{\Omega}$ with a finite number of open sets $U(x_j)$, take a partition of unity $\{\chi_j\}_{j=1}^n$ and functions ζ_j, $j = 1, \dots, n$ so that any ζ_j is equal to 1 on the support of χ_j. The indexing of this set should be chosen such that no $\chi_j \in \{\chi_i\}_{i=1}^k$ has a support containing a corner point of the interface. According to step (iii), here we have local regularizers $\{\mathbf{R}_i\}_{i=1}^k$. We define

$$u_i := \mathbf{R}_i(\chi_i f, \chi_i b), \qquad i = 1, \dots, k$$

and

$$u^* := \sum_{i=1}^k \zeta_i u_i + \sum_{j=k+1}^n \zeta_j u_{0,j},$$

where $u_{0,j}$ satisfies the transmission problem (27) in the cone corresponding to the corner point x_j that lies in the support of χ_j. Since $\zeta_j = 1$ in a neighbourhood of the respective corner point, we have

$$\triangle(\zeta_j v) = \zeta_j \triangle v + 2\nabla\zeta_j \cdot \nabla v + v\triangle\zeta_j = \zeta_j \triangle v$$

in this neighbourhood for any function v. We obtain

$$\begin{aligned}
\mathbf{L}u^* &= \sum_{i=1}^k \zeta_i \mathbf{L}_0 u_i + \sum_{j=k+1}^n \zeta_j \mathbf{L} u_{0,j} + \sum_{i=1}^k \mathbf{D}_i u_i + \sum_{j=k+1}^n \mathbf{D}_j u_{0,j} \\
&= \sum_{i=1}^k \zeta_i \chi_i f + \sum_{i=1}^k \zeta_i \mathbf{K}_i(f, b) + \sum_{j=k+1}^n \zeta_j \chi_j f + \sum_{i=1}^k \mathbf{D}_i u_i + \sum_{j=k+1}^n \mathbf{D}_j u_{0,j} \\
&= f + \sum_{i=1}^k \zeta_i \mathbf{K}_i(f, b) + \mathbf{K}_0 f,
\end{aligned}$$

where $\mathbf{K}_i$ are local regularizers, $\mathbf{D}_l$ denotes first order differential operators with coefficients vanishing near the corner points and

$$\mathbf{K}_0 f := \sum_{i=1}^k \mathbf{D}_i u_i + \sum_{j=k+1}^n \mathbf{D}_j u_{j,0}.$$

Since the mappings $f \mapsto u_i : [\mathcal{V}^k_\eta(\Omega)]^2 \to [\mathcal{H}^{k+2}(\Omega)]^2$ and $f \mapsto u_{j,0} : [\mathcal{V}^k_\eta(\Omega)]^2 \to [\mathcal{V}^{k+2}_\eta(\Omega)]^2$ are continuous by definition for any $k \in \mathbb{N}$, it follows that $\mathbf{K}_0 : [\mathcal{V}^k_\eta(\Omega)]^2 \to [\mathcal{V}^{k+1}_\eta(\Omega)]^2$ is continuous. Since $[\mathcal{V}^{k+1}_\eta(\Omega)]^2$ is compactly embedded into $[\mathcal{V}^k_\eta(\Omega)]^2$, the mapping is also compact from $[\mathcal{V}^k_\eta(\Omega)]^2$ into $[\mathcal{V}^k_\eta(\Omega)]^2$. The transmission conditions on the interface are treated analogously (cf. [17]). For the boundary conditions, Wloka's construction can be applied without changes because the artificial boundaries are smooth. The construction of the right regularizer is completed. The following Lemma is now a direct consequence of Lemma 3 and the existence of a right regularizer.

Lemma 6. *If $k+1-\eta \in (0,\mu^0)$ with μ^0 from equation (15), then the operator*

$$(\mathbf{L},\mathbf{B}) : [\mathcal{V}_\eta^{k+2}(\Omega)]^2 \to [\mathcal{V}_\eta^{k}(\Omega)]^2 \times \bigotimes_{j=1}^{4} V_\eta^{k+m_j+1/2}(\Gamma)$$

of problem (4) - (8) has the Fredholm property.

In order to investigate the regularity of solutions, let us recall some results about asymptotic expansions which have been obtained in [10] for classical TM diffraction and are true for conical diffraction as well, see [8]. Choose $s > 1$ with $s-1 \neq \operatorname{Re}\lambda$ for all $\lambda \in \bigcup_{S\in\mathcal{S}}(\mathcal{A}_S^+ \cup \mathcal{A}_S^-)$. Again we switch to polar coordinates (r_S,θ_S) centered at $S \in \mathcal{S}$. According to the theory of asymptotic analysis (see e.g. [17], [18], [23], [8], [10]), any solution $\{u_j\}, j=1,\dots,4$, admits an expansion of the form

$$u_j(x) = \sum_{S\in\mathcal{S}} \sum_{l=1}^{L_S} \sum_{p=0}^{p_S^l} C_{S,j}\chi_S(x) d_{S,j,l,p}(\theta_S(x)) r_S(x)^{\lambda_S} \log^p(r_S(x)) + w_j(x), \tag{28}$$

where χ_S are cut-off functions, $\{\{d_{S,j,l,p}\}_p\}_l$ is a system of Jordan chains for the eigenvalue $\lambda_S \in \mathcal{A}_S^\pm$, which consists of smooth functions in θ_S, and p_S^l depends on the geometric multiplicity of λ_S and on the length of the lth Jordan chain. Furthermore $w_j \in H^s(\Omega^\pm)$.

Since $r_S(x)^{\lambda_S} \in H^{1+\operatorname{Re}\lambda_S-\epsilon}(\Omega^\pm)$ for any $\epsilon > 0$, we have $\nabla r_S(x)^{\lambda_S} \in H^{\operatorname{Re}\lambda_S-\epsilon}(\Omega^\pm)$. On the other hand, $\nabla r_S(x)^{\lambda_S} \notin H^{\operatorname{Re}\lambda_S}(\Omega^\pm)$. Thus we can remark the following.

Remark 2. Let (u_1,u_2) be a solution of the conical diffraction problem (4) - (8). If $\mu^0 < 1$ for the μ^0 defined in (15) and the coefficients $C_{S,j}$ in the asymptotic expansion (28) do not vanish, then

$$u_j \notin H^2(\Omega^+) \times H^2(\Omega^-)$$

for $j=1,2$. This is also reflected by the fact that

$$\mathcal{V}_\eta^k(\Omega) \hookrightarrow H^k(\Omega^+) \times H^k(\Omega^-)$$

if and only if $\eta \le 0$. The condition $1-\eta \in (0,\mu^0)$ means in particular that $1-\mu^0 < \eta$, so $\eta > 0$ if $\mu^0 < 1$.

Remark 3. Let b be a function defined on Ω^+ which satisfies $b = \mathcal{O}(r_S^a)$ for some $a \in \mathbb{R}$ and $c > 0$ in the neighbourhood of a corner point S. If b is in $V_\eta^{3/2}(\Gamma)$, then $a > 1-\eta$. In particular, $b(x) \to 0$ as $r \to 0$, which is not true if the right-hand sides of (6) are restrictions of incoming plane waves (7) or of their normal derivatives to Γ. To overcome this difficulty, we define

$$u_{1/2}^+ =: u_{1/2}^{(s)} + u_{1/2}^{(i)},$$

where $u_{1/2}^{(s)}$ is the scattered wave, which leads to homogeneous boundary conditions on the non-smooth interface and accordingly modified radiation conditions

$$u_j^+(x_1,x_2) = \sum_{n=-\infty}^{\infty} A_{j,n}^\pm e^{i(n+\alpha)x_1 + \sqrt{\kappa_\pm^2-(n+\alpha)^2}x_2} + u_{1/2}^{(i)} \tag{29}$$

in a vicinity of Γ^+. The estimate (17) from Proposition 2 then needs to be replaced with

$$\sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+2}(\Omega)} \le C \left\{ \sum_{j=1}^{2} ||f_j||_{\mathcal{V}_\eta^{k}(\Omega)} + \sum_{j=1}^{4} ||b_j||_{V_\eta^{k+m_j+1/2}(\Gamma)} + \sum_{j=1}^{2} ||u_j^{(i)}||_{\mathcal{V}_\eta^{k+1}(\Omega)} \right\}. \tag{30}$$

In order to prove unique solvability, we need the following version of Green's formula. For simplicity only real valued functions are considered.

Lemma 7. *Let Ω be a domain with piecewise C^m boundary, $m \geq 1$, and assume that $\eta < 1$ and $u, v \in V^2_\eta(\Omega)$. Then*

$$\int_\Omega \triangle u v dx = -\int_\Omega \nabla u \nabla v dx + \int_{\partial\Omega} \partial_\nu u v ds, \quad \int_\Omega \nabla u \nabla^\perp v dx = -\int_{\partial\Omega} \partial_\tau u v ds, \tag{31}$$

where $\nabla^\perp = (-\partial_2, \partial_1)$.

Proof. The Lemma follows by a density argument from Lemma 3.4. in [19] and formula (2.21) in [8]. See also [2] and [12] for a detailed discussion of Green's formula. □

Proposition 3. *Consider a diffraction problem of the form (4) - (8) with homogeneous boundary conditions and homogeneous Helmholtz equations, i.e. $f_i^\pm = 0$ for $i = 1, 2$ and $b_j = 0$ for $j = 1, \dots, 4$, and radiation conditions (29) near Γ^+. Assume that the incoming wave admits a representation*

$$u_1^{(i)}(x_1, x_2) = p_3 e^{i\alpha x_1 - i\beta x_2}, \quad u_2^{(i)}(x_1, x_2) = q_3 e^{i\alpha x_1 - i\beta x_2} \tag{32}$$

near Γ^+, which includes incoming plane waves with real α and β. Assume that $\operatorname{Im} k > 0$ in a subdomain $\Omega_1 \subseteq \Omega$ and that ϵ is constant in Ω_1. Then for every η with $1 - \eta \in (0, \mu^0)$, the conical diffraction problem (4) - (8) has a unique solution in $\mathcal{V}^2_\eta(\Omega)$.

Proof. We are looking for α-quasiperiodic solutions. If u is an α-quasiperiodic function in x_1, then $v := e^{-i\alpha x_1} u$ is 2π-periodic in x_1. Let $P(v_1, v_2; \phi, \psi)$ be the sesquilinear form corresponding to the conical diffraction problem for the modulated solution v, which is given in [8]. Then the problem can be formulated as follows: Find 2π-periodic functions $v_1, v_2 \in \mathcal{H}^1(\Omega)$ so that

$$J(v_1, v_2; \phi, \psi) = -\frac{2ie^{-i\beta b}}{\kappa_+^2} \int_{\Gamma^+} \left(\omega\epsilon p_3 \overline{\phi^+} + \omega\mu q_3 \overline{\psi^+} \right) ds \tag{33}$$

for all 2π-periodic $\phi, \psi \in \mathcal{H}^1(\Omega)$, $\phi = (\phi^+, \phi^-)$, $\psi = (\psi^+, \psi^-)$, where $\Gamma^+ = \{(x_1, b) : 0 \geq x_1 \geq 2\pi\}$. According to [8], setting

$$J(v_1, v_2; \phi, \psi) = \left(\mathcal{J} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \begin{pmatrix} \phi \\ \psi \end{pmatrix} \right) \tag{34}$$

generates a bounded linear operator

$$\mathcal{J} : [\mathcal{H}^1(\Omega)]^2 \to [\mathcal{H}^{-1}(\Omega)]^2.$$

Due to Theorem 3.1 in [8], the variational equation (33), and equivalently (4) - (8), has at most one solution in $[\mathcal{H}^1(\Omega)]^2$. By Lemma 1, $\mathcal{V}^2_\eta(\Omega) \hookrightarrow \mathcal{V}^1_0(\Omega)$ for $\eta < 1$, and $\mathcal{V}^1_0(\Omega) \hookrightarrow \mathcal{H}^1(\Omega)$. Theorem 3.1 from [8] provides uniqueness of solutions in $\mathcal{H}^1(\Omega)$ for conical diffraction problems with absorbing materials. Therefore, there is also at most one solution in $\mathcal{V}^2_\eta(\Omega)$ for $\eta < 1$.

If we restrict the operator to $[\mathcal{V}^2_\eta(\Omega)]^2$, we have

$$\mathcal{J} : [\mathcal{V}^2_\eta(\Omega)]^2 \to [\mathcal{V}^0_\eta(\Omega)]^2.$$

Chapter 8.3.3. from [18] tells us that $\mathcal{J}$ is Fredholm if and only if the operator of the strong problem is Fredholm. By Lemma 6, $\mathcal{J}$ is indeed a Fredholm operator.

The adjoint operator $\mathcal{J}^*$ is given by

$$\left(\mathcal{J}^*\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \begin{pmatrix} \phi \\ \psi \end{pmatrix}\right) = \overline{J(\phi,\psi;v_1,v_2)}.$$

It maps $[\mathcal{V}^0_{-\eta}(\Omega)]^2$ into $[\mathcal{V}^{-2}_{-\eta}(\Omega)]^2$. Moreover, we have

$$\mathrm{Re}(iJ(v_1,v_2;v_1,v_2)) \geq \frac{\omega\beta}{2\pi}\left(\epsilon^+\left|\int_0^{2\pi} v_1^+(x_1,b)dx_1\right|^2 + \mu\left|\int_0^{2\pi} v_2^+(x_1,b)dx_1\right|^2\right) \tag{35}$$

for every $v_1, v_2 \in \mathcal{V}^2_\eta(\Omega)$ (cf. the proof of Corollary 3.2 in [8]). Since $\mathcal{V}^2_\eta(\Omega)$ is dense in $\mathcal{V}^0_{-\eta}(\Omega)$ for $\eta \leq 1$, we have

$$\left(\ker\mathcal{J}^* \cap \mathcal{V}^2_\eta(\Omega)\right)^\perp = (\ker\mathcal{J}^*)^\perp.$$

Therefore, the right-hand side of (33) vanishes for every $(\phi,\psi) \in \ker\mathcal{J}^*$, and every (f_1, f_2) which satisfies

$$\left(\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \begin{pmatrix} \phi \\ \psi \end{pmatrix}\right) = -\frac{2ie^{-i\beta b}}{\kappa_+^2}\int_{\Gamma^+}\left(\omega\epsilon p_3\overline{\phi^+} + \omega\mu q_3\overline{\psi^+}\right)ds,$$

is orthogonal to the kernel of the adjoint operator. Since $\mathcal{J}$ is a Fredholm operator, we have

$$\mathrm{ran}\,\mathcal{J} = (\ker\mathcal{J}^*)^\perp.$$

Thus, there is a unique solution in $[\mathcal{V}^2_\eta(\Omega)]^2$ for every right-hand side that satisfies (32). □

4 Shape derivatives

4.1 Existence and regularity of shape derivatives

4.1.1 Smooth perturbations of the domains

Proposition 2 enables us to prove the existence of shape derivatives in the same way as it is done in [4], which uses the theory of non-local perturbations of a domain, see [21]. Consider a vector field $T \in [C(\Omega)]^2$ which is C^{k+2}. This vector field generates a diffeomorphism

$$T_\epsilon(v) := v + \epsilon T(v)$$

and perturbed domains

$$\Omega_\epsilon := T_\epsilon(\Omega).$$

We can now define material and shape derivatives.

Definition 6. Let Ω be a bounded domain and assume that u^ϵ is the solution of the boundary value problem

$$Lu^\epsilon = f_\epsilon \quad \text{on} \quad \Omega_\epsilon,$$

$$Bu^\epsilon = g_\epsilon \quad \text{on} \quad \partial\Omega_\epsilon$$

in a function space $X(\Omega_\epsilon)$, with Ω_ϵ as above. The *material derivative* of $u := u^0$ in direction T is defined as

$$\dot{u}(T) := \frac{d(u^\epsilon \circ T_\epsilon)}{d\epsilon}\bigg|_{\epsilon=0}$$

with convergence in $X(\Omega)$.

We could also define a derivative

$$\lim_{\epsilon \searrow 0} \frac{u^\epsilon(x) - u^0(x)}{\epsilon} =: u'(x).$$

This limit is defined only pointwise, since the domains on which the functions u^ϵ are defined change with ϵ. We can formally write

$$\frac{1}{\epsilon}\left\{(u^\epsilon \circ T_\epsilon)(x) - u^0(x)\right\} = \frac{1}{\epsilon}\left\{u^\epsilon(x) - u^0(x)\right\} + \nabla u^\epsilon(x) \cdot T(x) + \mathcal{O}(\epsilon).$$

This motivates the following definition.

Definition 7. Suppose that the material derivative of a function u exists in a function space $X(\Omega)$ and that $\nabla u^0 \cdot T \in Y \subseteq X(\Omega)$. Then the *shape derivative* of u is globally defined as

$$u'(T) := \dot{u}(T) - \nabla u^0 \cdot T. \tag{36}$$

If we are interested in functions on the boundary $\partial\Omega$, we have to replace the gradient in the above formula with its tangential component. We say that u is *shape differentiable* in direction T in a function space Y, if its shape derivative $u'(T)$ exists in Y.

Remark 4. Remark 2 stated that for $\mu^0 < 1$ solution $(u_1.u_2)$ of the conical diffraction problem (4) - (8) is likely not in $[\mathcal{H}^2(\Omega)]^2$. Then

$$(u_1, u_2)' \notin [\mathcal{H}^1(\Omega)]^2.$$

If this is the case, then the variational approach of Hettlich and Kirsch ([14],[16]) cannot immediately be applied to problems in domains with corners in general, because for this technique H^1-regularity of the shape derivative is a crucial requirement. For this reason we use a different approach suggested by Bochniak and Cakoni[4] for mixed boundary value problems.

We return to our transmission problem. Let T_ϵ be a smooth perturbation as above. Since we are only interested in perturbations of the interface Γ, we assume that for every ϵ we have $\partial\Omega^\epsilon = \partial\Omega$. The perturbed interface will be denoted by Γ_ϵ. If we are interested in functions on the boundary $\partial\Omega$, we have to replace the gradient in the above formula with its tangential component. We investigate the transmission problem

$$\begin{aligned}
\triangle u_1^{+,\epsilon} + \kappa_+^2 u_1^{+,\epsilon} &= f_1^+ \quad \text{in} \quad \Omega_\epsilon^+, \\
\triangle u_1^{-,\epsilon} + \kappa_-^2 u_1^{-,\epsilon} &= f_-^1 \quad \text{in} \quad \Omega_\epsilon^-, \\
\triangle u_2^{+,\epsilon} + \kappa_+^2 u_2^{+,\epsilon} &= f_+^2 \quad \text{in} \quad \Omega_\epsilon^+, \\
\triangle u_2^{-,\epsilon} + \kappa_-^2 u_2^{-,\epsilon} &= f_-^2 \quad \text{in} \quad \Omega_\epsilon^-,
\end{aligned}$$

with transmission conditions

$$\begin{aligned}
\Big[\frac{\gamma}{\kappa^2}\nabla u_2^\epsilon\cdot\tau_\epsilon+\frac{\omega\varepsilon}{\kappa^2}\nabla u_1^\epsilon\cdot\nu_\epsilon\Big]_\Gamma &= -\frac{\omega\epsilon_+}{\kappa_+^2}\nabla u_1^{(i)}\cdot\nu_\epsilon,\\
\Big[\frac{\gamma}{\kappa^2}\nabla u_1^\epsilon\cdot\tau_\epsilon-\frac{\omega\mu}{\kappa^2}\nabla u_2^\epsilon\cdot\nu_\epsilon\Big]_\Gamma &= \frac{\omega\mu}{\kappa_+^2}\nabla u_2^{(i)}\cdot\nu_\epsilon,\\
[u_1^\epsilon]_\Gamma &= -u_1^{(i)},\\
[u_2^\epsilon]_\Gamma &= -u_2^{(i)}
\end{aligned}$$

on Γ_ϵ and a radiation condition (8) with $u_j^\pm$ replaced by $u_j^{\pm,\epsilon}$. Here, ν_ϵ is the unit normal to the perturbed interface Γ_ϵ and τ_ϵ is the unit tangential vector to Γ_ϵ. By the coordinate transform $x\mapsto x_\epsilon:=T_\epsilon(x)$ we get

$$\begin{aligned}
&\triangle^\epsilon(u_1^{+,\epsilon}\circ T_\epsilon)+\kappa_+^2(u_1^{+,\epsilon}\circ T_\epsilon)=f_1^+\circ T_\epsilon \quad\text{in}\quad \Omega^+,\\
&\triangle^\epsilon(u_1^{-,\epsilon}\circ T_\epsilon)+\kappa_-^2(u_1^{-,\epsilon}\circ T_\epsilon)=f_1^-\circ T_\epsilon \quad\text{in}\quad \Omega^-,\\
&\triangle^\epsilon(u_2^{+,\epsilon}\circ T_\epsilon)+\kappa_+^2(u_2^{+,\epsilon}\circ T_\epsilon)=f_2^+\circ T_\epsilon \quad\text{in}\quad \Omega^+,\\
&\triangle^\epsilon(u_2^{-,\epsilon}\circ T_\epsilon)+\kappa_-^2(u_2^{-,\epsilon}\circ T_\epsilon)=f_2^-\circ T_\epsilon \quad\text{in}\quad \Omega^-,
\end{aligned}\tag{37}$$

with transmission conditions

$$\begin{aligned}
\Big[\frac{\gamma}{\kappa^2}\nabla^\epsilon(u_2^\epsilon\circ T_\epsilon)\cdot(\tau_\epsilon\circ T_\epsilon)+\frac{\omega\varepsilon}{\kappa^2}\nabla^\epsilon(u_1^\epsilon\circ T_\epsilon)\cdot(\nu_\epsilon\circ T_\epsilon)\Big]_\Gamma &= -\frac{\omega\varepsilon_+}{\kappa_+^2}\nabla^\epsilon(u_1^{(i)}\circ T_\epsilon)\cdot(\nu_\epsilon\circ T_\epsilon),\\
\Big[\frac{\gamma}{\kappa^2}\nabla^\epsilon(u_1^\epsilon\circ T_\epsilon)\cdot(\tau_\epsilon\circ T_\epsilon)-\frac{\omega\mu}{\kappa^2}\nabla^\epsilon(u_2^\epsilon\circ T_\epsilon)\cdot(\nu_\epsilon\circ T_\epsilon)\Big]_\Gamma &= \frac{\omega\mu}{\kappa_+^2}\nabla^\epsilon(u_2^{(i)}\circ T_\epsilon)\cdot(\nu_\epsilon\circ T_\epsilon),\\
[u_1^\epsilon\circ T_\epsilon]_\Gamma &= -u_1^{(i)}\circ T_\epsilon,\\
[u_2^\epsilon\circ T_\epsilon]_\Gamma &= -u_2^{(i)}\circ T_\epsilon
\end{aligned}\tag{38}$$

on Γ and a radiation condition (8) with $u_j^\pm$ replaced by $u_j^{\pm,\epsilon}\circ T_\epsilon$ and $A_{j,n}^\pm$ replaced by $A_{j,n}^{\pm,\epsilon}$. Here $\triangle^\epsilon=\partial^2_{x_{1,\epsilon}}+\partial^2_{x_{2,\epsilon}}$ is the Laplacian and $\nabla^\epsilon=(\partial_{x_{1,\epsilon}},\partial_{x_{2,\epsilon}})^\top$ is the gradient with respect to x_ϵ. As it is shown in [4], the operators $\triangle^\epsilon$ and ∇^ϵ depend smoothly on ϵ and admit the Taylor expansion

$$\begin{aligned}
\triangle^\epsilon &= \triangle+\epsilon\tilde\triangle+\epsilon^2\triangle^R(\epsilon),\\
\nabla^\epsilon &= \nabla+\epsilon\tilde\nabla+\epsilon^2\nabla^R(\epsilon),
\end{aligned}$$

with

$$\begin{aligned}
&\tilde\triangle u=\operatorname{div}\Big([I\operatorname{div}T-(DT^\top+DT)]\nabla u\Big)-\operatorname{div}T\triangle u,\\
&\tilde\nabla u=-DT^\top\cdot\nabla u,
\end{aligned}\tag{39}$$

where DT denotes the Jacobian of T. We return to the investigation of the transmission problem. Inserting the formal ansatz

$$u_j^\epsilon\circ T_\epsilon=:u_j^0+\epsilon\dot u_j+\epsilon^2 v_j(x)\tag{40}$$

into the transformed boundary value problem on Ω, taking into account that $\dot f_j^\pm=0$ for $j=1,2$, and comparing the terms of order ϵ, yields

$$\begin{aligned}
\triangle \dot{u}_1^+ + \kappa_+^2 \dot{u}_1^+ &= -\tilde{\triangle} u_1^{+,0} \quad \text{in} \quad \Omega^+,\\
\triangle \dot{u}_1^- + \kappa_-^2 \dot{u}_1^- &= -\tilde{\triangle} u_1^{-,0} \quad \text{in} \quad \Omega^-,\\
\triangle \dot{u}_2^+ + \kappa_+^2 \dot{u}_2^+ &= -\tilde{\triangle} u_2^{+,0} \quad \text{in} \quad \Omega^+,\\
\triangle \dot{u}_2^- + \kappa_-^2 \dot{u}_2^- &= -\tilde{\triangle} u_2^{-,0} \quad \text{in} \quad \Omega^-,
\end{aligned} \tag{41}$$

and

$$\begin{aligned}
\left[\frac{\gamma}{\kappa^2}\nabla \dot{u}_2 \cdot \tau + \frac{\omega\varepsilon}{\kappa^2}\nabla \dot{u}_1 \cdot \nu\right]_\Gamma &= -\frac{\omega\varepsilon_+}{\kappa_+^2}\nabla u_1^{(i)} \cdot \dot{\nu} - \left[\frac{\gamma}{\kappa^2}\tilde{\nabla} u_2^0 \cdot \tau + \frac{\omega\varepsilon}{\kappa^2}\tilde{\nabla} u_1^0 \cdot \nu\right]_\Gamma\\
&\quad - \left[\frac{\gamma}{\kappa^2}\nabla u_2^0 \cdot \dot{\tau} + \frac{\omega\varepsilon}{\kappa^2}\nabla u_1^0 \cdot \dot{\nu}\right]_\Gamma,\\
\left[\frac{\gamma}{\kappa^2}\nabla \dot{u}_1 \cdot \tau - \frac{\omega\mu}{\kappa^2}\nabla \dot{u}_2 \cdot \nu\right]_\Gamma &= \frac{\omega\mu}{\kappa_+^2}\nabla u_2^{(i)} \cdot \dot{\nu} - \left[\frac{\gamma}{\kappa^2}\tilde{\nabla} u_1^0 \cdot \tau - \frac{\omega\mu}{\kappa^2}\tilde{\nabla} u_2^0 \cdot \nu\right]_\Gamma\\
&\quad - \left[\frac{\gamma}{\kappa^2}\nabla u_1^0 \cdot \dot{\tau} - \frac{\omega\mu}{\kappa^2}\nabla u_2^0 \cdot \dot{\nu}\right]_\Gamma,\\
[\dot{u}_1]_\Gamma &= -\dot{u}_1^{(i)} = 0,\\
[\dot{u}_2]_\Gamma &= -\dot{u}_2^{(i)} = 0
\end{aligned} \tag{42}$$

on the interface Γ. Near Γ^+ and Γ^-, we use the ansatz

$$A_{j,n}^{\pm,\epsilon} =: A_{j,n}^{\pm,0} + \epsilon \dot{A}_{j,n}^{\pm} + \epsilon^2 R_{j,n}^{\pm}(\epsilon). \tag{43}$$

Expanding $u_j^\epsilon \circ T_\epsilon$ into a Taylor series at $\epsilon = 0$, and using (43) together with (40), yields

$$\dot{u}_j^{\pm}(x) = \sum_{n=-\infty}^{\infty} \left\{ \dot{A}_{j,n}^{\pm} + A_{j,n}^{\pm,0} \begin{pmatrix} i(n+\alpha) \\ \left(\kappa_\pm^2 - (n+\alpha)^2\right)^{1/2} \end{pmatrix} \cdot T \right\} e^{i(n+\alpha)x_1 + \sqrt{\kappa_\pm^2 - (n+\alpha)^2} x_2} \tag{44}$$

near the artificial boundaries. It remains to show that the solution $\dot{u}$ of the transmission problem (41)+(42)+(44) is indeed the material derivative of u_j for $j = 1, 2$, i.e. we have to show that

$$\sum_{j=1}^{2} ||u_j^\epsilon \circ T_\epsilon - u_j^0 - \epsilon \dot{u}_j||_{\mathcal{V}_\eta^l(\Omega)} \leq C\epsilon^2 \tag{45}$$

for some suitable l and η. In fact we will prove this for $l = k+2$, $k \geq 0$. By straightforward calculations we see that the functions $v_j^\pm = u_j^{\pm,\epsilon} \circ T_\epsilon - u_j^{\pm,0} - \epsilon \dot{u}_j^\pm$ satisfy the equation

$$\triangle^\epsilon v_j^\pm + \kappa_\pm^2 v_j^\pm = -\epsilon^2 \left(\triangle^R u_j^{\pm,0} + \tilde{\triangle} \dot{u}_j^\pm\right) - \epsilon^3 \triangle^R \dot{u}_j^\pm \quad \text{in} \quad \Omega^\pm \tag{46}$$

for $j = 1, 2$. With $\nu_\epsilon = \nu_0 + \epsilon\dot{\nu} + \epsilon^2 \nu_R$ and $\tau_\epsilon = \tau_0 + \epsilon\dot{\tau} + \epsilon^2 \tau_R$ the transmission conditions on Γ become

$$\begin{aligned}
&\left[\frac{\gamma}{\kappa^2}\nabla^\epsilon v_2 \cdot (\tau_\epsilon \circ T_\epsilon) + \frac{\omega\varepsilon}{\kappa^2}\nabla^\epsilon v_1 \cdot (\nu_\epsilon \circ T_\epsilon)\right]_\Gamma =\\
&= \epsilon^2 \left\{ -\frac{\omega\varepsilon_+}{\kappa_+^2}\tilde{\nabla} u_1^{(i)} \cdot \dot{\nu} - \left[\frac{\gamma}{\kappa^2}\left(\nabla \dot{u}_2 \cdot \dot{\tau} + \nabla u_2^0 \cdot \tau_R + \tilde{\nabla} u_2^0 \cdot \dot{\tau} + \tilde{\nabla} \dot{u}_2 \cdot \tau + \nabla^R u_2^0 \cdot \tau\right) + \right.\right.
\end{aligned} \tag{47}$$

$$+ \frac{\omega\varepsilon}{\kappa^2}\left(\nabla\dot u_1\cdot\dot\nu + \nabla u_1^0\cdot\nu_R + \tilde\nabla u_1^0\cdot\dot\nu + \tilde\nabla\dot u_1\cdot\nu + \nabla^R u_1\cdot\nu\right)\Big]_\Gamma\Big\} + \mathcal{P}_1(\epsilon^3,\epsilon^4,\epsilon^5)$$

and

$$\Big[\frac{\gamma}{\kappa^2}\nabla^\epsilon v_1\cdot(\tau_\epsilon\circ T_\epsilon) - \frac{\omega\mu}{\kappa^2}\nabla^\epsilon v_2\cdot(\nu_\epsilon\circ T_\epsilon)\Big]_\Gamma =$$
$$= \epsilon^2\Big\{\frac{\omega\mu}{\kappa_+^2}\tilde\nabla u_2^{(i)}\cdot\dot\nu - \Big[\frac{\gamma}{\kappa^2}\left(\nabla\dot u_1\cdot\dot\tau + \nabla u_1^0\cdot\tau_R + \tilde\nabla u_1^0\cdot\dot\tau + \tilde\nabla\dot u_1\cdot\tau + \nabla^R u_1^0\cdot\tau\right) +$$
$$+ \frac{\omega\mu}{\kappa^2}\left(\nabla\dot u_2\cdot\dot\nu + \nabla u_2^0\cdot\nu_R + \tilde\nabla u_2^0\cdot\dot\nu + \tilde\nabla\dot u_2\cdot\nu + \nabla^R u_2\cdot\nu\right)\Big]_\Gamma\Big\} + \mathcal{P}_1(\epsilon^3,\epsilon^4,\epsilon^5), \qquad (48)$$
$$[v_1]_\Gamma = 0,$$
$$[v_2]_\Gamma = 0.$$

Here, $\mathcal{P}_{1/2}(\epsilon^3,\epsilon^4,\epsilon^5)$ are polynomials in ϵ involving the powers $\epsilon^3,\epsilon^4,\epsilon^5$ with coefficients $\tilde\nabla\dot u_j^\pm\cdot\dot\nu, \tilde\nabla u_j^{\pm,0}\cdot\nu_R, \nabla^R u_j^{\pm,0}\cdot\dot\nu, \nabla^R\dot u_j^\pm\cdot\nu, \nabla\dot u_j^\pm\cdot\nu_R, \tilde\nabla\dot u_j^\pm\cdot\nu_R, \nabla^R u_j^{\pm,0}\cdot\nu_R, \nabla^R\dot u_j^\pm\cdot\dot\nu, \nabla^R\dot u_j^\pm\cdot\nu_R$. Since $u_j^{\pm,\epsilon}\cdot T_\epsilon$, $u_j^{\pm,0}$ and $\dot u_j^\pm$ all satisfy a radiation condition, this also applies to $v_j^\pm$.

Non-local perturbation theory tells us that the operator S_ϵ of the transmission problem (46) - (48), which maps a solution (v_1,v_2) to the corresponding right-hand side, is a small perturbation of the operator S of the original problem. Therefore, if S is invertible, this is also true for S_ϵ by a Neumann series argument. Moreover, since $(u_j^{\pm,0})_{j=1,\dots,4}$ is a solution of the conical diffraction problem with homogeneous Helmholtz equations and smooth incoming waves or their normal derivatives as right-hand sides of the boundary conditions we see by Proposition 2 that $u_j^{\pm,0}\in V_\eta^{k+2}(\Omega^\pm)$. Hence, $\nabla u_j^{\pm,0}|_\Gamma\in V_\eta^{k+1/2}(\Gamma)$ and $\triangle^R u_j^{\pm,0}\in V_\eta^k(\Omega^\pm)$ because $\triangle^R$ is an operator of second order.

Now $(\dot u_j^\pm)_{j=1,\dots,4}$ is a solution of an inhomogeneous conical diffraction problem with $-\tilde\triangle u_j^{\pm,0}$ on the right-hand sides of the Helmholtz equations and the right-hand sides of the boundary conditions are $\nabla u_j^{\pm,0}\cdot\nu$ and $\nabla u_j^{\pm,0}\cdot\tau$ respectively. Therefore $\dot u_j^\pm\in V_\eta^{k+2}(\Omega^\pm)$ also by Proposition 2 and $\tilde\triangle\dot u_j^\pm, \triangle^R\dot u_j^\pm\in V_\eta^k(\Omega^\pm)$, $\nabla\dot u_j^\pm|_\Gamma, \tilde\nabla\dot u_j^\pm|_\Gamma\in V_\eta^{k+1/2}(\Gamma)$.
Additionally $\tilde\nabla u_j^{\pm,0}|_\Gamma, \nabla^R u_j^{\pm,0}|_\Gamma\in V_\eta^{k+1/2}(\Gamma)$ and all coefficients of the ϵ-powers in $\mathcal{P}_i(\epsilon^3,\epsilon^4,\epsilon^5)$, $i=1,2$ belong to $V_\eta^{k+1/2}(\Gamma)$. The incoming wave is smooth and therefore fulfills all necessary smoothness assumptions as well. In the norm of this space, $\mathcal{P}_i(\epsilon^3,\epsilon^4,\epsilon^5)=\mathcal{O}(\epsilon^3)$ for $i=1,2$.

By these considerations, we can apply Proposition 2 to the perturbed problem above and immediately obtain (45). Summarizing we can state the following theorem.

Theorem 1. *Suppose that the conical diffraction problem has a unique solution (u_1,u_2) belonging to $[\mathcal{V}_\eta^{k+1}(\Omega)]^2$ and that the assumptions of Proposition 1 are satisfied. Then, according to Proposition 1, $(u_1,u_2)\in[\mathcal{V}_\eta^{k+2}(\Omega)]^2$. Furthermore, the material derivative $(\dot u_1,\dot u_2)$ exists and belongs to $[\mathcal{V}_\eta^{k+2}(\Omega)]^2$ and the shape derivative (u_1',u_2') lies in $[\mathcal{V}_\eta^{k+1}(\Omega)]^2$.*

4.1.2 Piecewise smooth perturbations

Regular perturbations of the identity that were considered in the previous section leave the the angles at corner points unchanged. If we want to change those angles, we have to allow piecewise smooth perturbations. In this case, a Dirac delta occurs in the first equation of (39). Consequently,

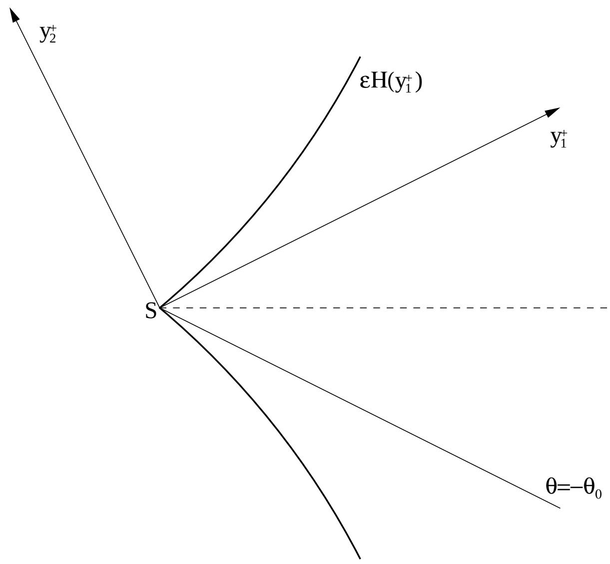

Figure 3: Boundary perturbation near a corner point

we need a different representation of the perturbed boundary for the coordinate transform $x \mapsto x_\epsilon$, that leads to the perturbed problem (37) + (38).

The following statements can be found with more detailed explanations in [21], Chapter 5.5.2. Let $\{V_j : j = 1, \ldots, J\}$ be an open covering of the interface Γ. In each set which does not include a corner point, we introduce local coordinates (ξ_1^j, ξ_2^j) with the ξ_2^j-axis pointing in the normal direction at Γ. Then the perturbed interface Γ_ϵ can be given in each V_j by $\xi_2^j = \epsilon T_j(\xi_1^j)$ with a smooth function T_j and small positive ϵ. Now we introduce new coordinates (ζ_1^j, ζ_2^j) given by $\zeta_1^j = \xi_1^j$ and $\zeta_2^j = \xi_2^j - \epsilon T_j(\xi_1^j)\chi_j(\xi_2^j)$, where χ_j is a cut-off function with a support containing V_j and $\chi_j \equiv 1$ on V_j. In this way, we generate a coordinate transform

$$(\xi_1^j, \xi_2^j) \mapsto (\zeta_1^j, \zeta_2^j) : \Gamma_\epsilon \cap V_j \to \Gamma \cap V_j \tag{49}$$

for the smooth parts of the boundary. In each cone $C_S = \{x = x(r, \theta) \in \mathbb{R}^2 : r > 0, \theta \in (-\theta_0, \theta_0)\}$ with origin S, we proceed in the following way. The perturbed boundary $\partial C_S(\epsilon)$ of the cone can be given by

$$y_2^\pm = \epsilon H(y_1^\pm), \quad y_1^\pm \geq 0$$

with $(y_1^\pm, y_2^\pm)$ denoting cartesian coordinates with origin S. The $y_1^\pm$-axis is given by $\{x : \theta = \pm\theta_0\}$ and the $y_2^\pm$-axis by $\{x : \theta = \pm\theta_0 \pm \pi/2\}$. Furthermore, H is a smooth function with

$$H(t) = at^\xi + \mathcal{O}(t^{\xi+1}), \quad \xi \geq 1. \tag{50}$$

An illustration is given in Figure 4. Then the domain $C_S(\epsilon)$ is given by

$$\theta_0 - \epsilon r^{\xi-1} b(r, \epsilon) \leq \theta \leq \theta_0 + \epsilon r^{\xi-1} b(r, \epsilon) \tag{51}$$

with a smooth function b. Then one can construct a mapping of $C_S(\epsilon)$ onto C_S by introducing new polar coordinates (R, Θ) with

$$R = r, \quad \Theta = \theta_0 \left(\theta_0 + \epsilon r^{\xi-1} b(r,\epsilon)\right)^{-1} \theta. \tag{52}$$

With the local coordinate transforms (49) and (52) we can assemble a diffeomorphism

$$T_\epsilon : \Omega_\epsilon \mapsto \Omega,$$

where Ω_ϵ is the perturbed domain.

For simplicity, we consider only functions H which are linear, i.e. the perturbation of a cone is again a cone. If $H(t) = at$ with $a > 0$, then $b(r,\epsilon) = \epsilon^{-1} \arctan(a\epsilon)$ and the perturbed cone $C_S(\epsilon)$ is given by angles θ which satisfy

$$-\theta_0 - \arctan(a\epsilon) \leq \theta \leq \theta_0 + \arctan(a\epsilon).$$

In the polar coordinates (R, Θ) we have

$$R = r, \quad \Theta = \theta_0 \left(\theta_0 + \arctan(a\epsilon)\right)^{-1} \theta.$$

The Laplace operator in these coordinates is

$$\triangle^\epsilon u = \frac{\partial^2}{\partial R^2} u + \frac{1}{R}\frac{\partial}{\partial R} u + \left(1 + \theta_0^{-1} \arctan(a\epsilon)\right)^{-2} \frac{1}{R^2} \frac{\partial^2}{\partial \Theta^2} u$$

and the gradient is

$$\nabla^\epsilon u = \left\{ \frac{\partial}{\partial R} u \right\} \vec{R} + \left\{ \left(1 + \theta_0^{-1} \arctan(a\epsilon)\right)^{-1} \frac{1}{R}\frac{\partial}{\partial \Theta} u \right\} \vec{\Theta},$$

where $\vec{R}$ and $\vec{\Theta}$ are the unit vectors in the polar coordinate system. As before, we can expand these operators into Taylor series and obtain

$$\triangle^\epsilon u = \frac{\partial^2}{\partial R^2} u + \frac{1}{R}\frac{\partial}{\partial R} u + \frac{1}{R^2}\frac{\partial^2}{\partial \Theta^2} u \left(1 - 2\epsilon a \theta_0 + \mathcal{O}(\epsilon^2)\right)$$

and

$$\nabla^\epsilon u = \left\{ \frac{\partial}{\partial R} u \right\} \vec{R} + \left\{ \frac{1}{R}\frac{\partial}{\partial \Theta} u \right\} \vec{\Theta} \left(1 - \epsilon a \theta_0 + \mathcal{O}(\epsilon^2)\right).$$

Now we can proceed in the same way as in the previous section. We only have to replace the perturbation of the identity, that has been considered there, with the diffeomorphism T_ϵ constructed in this section.

Theorem 2. *By the above considerations, Theorem 1 is also true for perturbations which change the angle at corner points.*

Theoretically, this theorem could also be stated for the more general case that $\xi > 1$ in equation (50). According to [21], we obtain the following. In polar coordinates with respect to r and θ we have

$$\frac{\partial}{\partial x_1} = \cos\theta \frac{\partial}{\partial r} - \frac{1}{r}\sin\theta \frac{\partial}{\partial \theta},$$

$$\frac{\partial}{\partial x_2} = \sin\theta \frac{\partial}{\partial r} + \frac{1}{r}\cos\theta \frac{\partial}{\partial \theta}$$

and

$$\begin{aligned}
\frac{1}{r}\frac{\partial}{\partial \theta} &= \frac{1}{R}\left(1 + \frac{1}{\theta_0}\epsilon R^{\xi-1} b(R,\epsilon)\right)^{-1} \frac{\partial}{\partial \Theta}, \\
\frac{\partial}{\partial r} &= \frac{\partial}{\partial R} - \left(1 + \frac{1}{\theta_0}\epsilon R^{\xi-1} b(R,\epsilon)\right)^{-1} \left[\frac{\partial}{\partial r}\left(1 + \frac{1}{\theta_0}\epsilon r^{\xi-1} b(r,\epsilon)\right)\right]_{r=R} \Theta \frac{\partial}{\partial \Theta}.
\end{aligned}$$

Expanding this in a Taylor series at $\epsilon = 0$ yields

$$\begin{aligned}
\frac{1}{r}\frac{\partial}{\partial \theta} &\asymp \frac{1}{R}\left(1 + \sum_{k=1}^{\infty} \epsilon^k \sum_{j=1}^{k} R^{j(\xi-1)} \frac{\theta_0^{-j}}{(k-j)!}\left(\frac{\partial}{\partial \epsilon}\right)^{k-j} b^j(R,0)\right) \frac{\partial}{\partial \Theta}, \\
\frac{\partial}{\partial r} &\asymp \frac{\partial}{\partial R} - \frac{1}{R}\sum_{k=1}^{\infty} \epsilon^k \sum_{j=1}^{k} R^{j(\xi-1)} \frac{\theta_0^{-j}}{(k-j)!}\left(\xi - 1 + \frac{R}{j}\frac{\partial}{\partial R}\right)\left(\frac{\partial}{\partial \epsilon}\right)^{k-j} b^j(R,0)\Theta \frac{\partial}{\partial \Theta}
\end{aligned} \tag{53}$$

The differential operators of the perturbed transmission problem (45) - (48) can be represented by series of so-called admissible operators if $\xi \geq 1$. These are defined as follows (see also [18]).

Definition 8. The operator

$$P(x, D_x) = \sum_{\alpha \leq k} p_\alpha(x) D_x^\alpha$$

is called *admissible* of order k in the vicinity of a corner point S if the coefficients p_α have the form

$$p_\alpha(x) = r^{|\alpha|-k} p_\alpha^{(0)}(r,\theta)$$

in this neighbourhood, where $p_\alpha^{(0)} \in C^\infty((0,\infty) \times \overline{C_S^\pm}) \cap C([0,\infty) \times \overline{C_S^\pm})$ and

$$(rD_r)^j D_\theta^\gamma \left(p_\alpha^{(0)}(r,\theta) - p_\alpha^{(0)}(0,\theta)\right) \to 0$$

for every $j = 0, 1, \ldots$ as $r \to 0$ uniformly with respect to $\theta \in \overline{C_S^\pm}$. As usual, (r,θ) are polar coordinates in the cone $C_S^\pm$ with origin S. P is said to be a *model operator* if it has the form

$$P(x, D_x) = r^{-k} \sum_{j=0}^{k} p_j(\theta, D_\theta)(rD_r)^j$$

with $p_j(\theta, D_\theta)$ being differential operators of order $\leq k - j$ with smooth coefficients on $\overline{C_S^\pm}$. If P is a boundary operator, then additionally $P(x, D_x)u|_{\partial C_S^\pm}$ has to depend only on $u|_{\partial C_S^\pm}$ for every smooth function u in the vicinity of $\partial C_S^\pm$.

To apply the theory used in Chapter 1, we need admissibility of the occurring differential operators. According to [18], every model operator is admissible. It is easy to show that the differential operators in (4) - (8) are model operators. If $\xi < 1$, then the perturbed transmission problem is not admissible any more because the coefficients in (53) do not behave in the way that was required in Definition 8, and Proposition 1 is no longer true.

The concept of admissibility does not apply to the boundary conditions (23) and (24) because of the occurring pseudodifferential operators and because the artificial boundaries do not have corners. The theory of the first section also includes this kind of operators, see Chapter 9 of Wloka's book [33], where pseudodifferential boundary operators are treated explicitely for smooth boundaries.

Remark 5. The symmetric structure of (51) is not necessary for the above considerations. We could also represent the perturbed boundary by two functions H_1 and H_2 with

$$H_1(t) = a_1 t^{\xi_1} + \mathcal{O}(t^{\xi_1+1}), \quad H_2(t) = a_2 t^{\xi_2} + \mathcal{O}(t^{\xi_2+1}), \quad \xi_1, \xi_2 \geq 1.$$

The inequality (51) would then change to

$$-\theta_0 - \epsilon r^{\xi_1 - 1} b_1(r,\epsilon) \leq \theta \leq \theta_0 + \epsilon r^{\xi_2 - 1} b_2(r,\epsilon)$$

with smooth functions b_1 and b_2. Define

$$\begin{aligned} \theta_1 &:= -\theta_0 - \epsilon r^{\xi_1 - 1} b_1(r,\epsilon), \\ \theta_2 &:= \theta_0 + \epsilon r^{\xi_2 - 1} b_2(r,\epsilon). \end{aligned}$$

The new polar coordinates

$$R = r, \quad \Theta = \theta_0 \theta_1^{-1} \left(\frac{\theta_1}{\theta_1 - \theta_2} \theta - \frac{\theta_1 \theta_2}{\theta_1 - \theta_2} \right) + \theta_0 \theta_2^{-1} \left(\frac{\theta_2}{\theta_2 - \theta_1} \theta - \frac{\theta_2 \theta_1}{\theta_2 - \theta_1} \right)$$

induce a mapping of $C_S(\epsilon)$ onto C_S. This is similar to (52) and allows essentially the same considerations, only with more long-winded notation.

4.2 Characterization of the shape derivative

Once the shape differentiability of the solution of the conical diffraction problem has been proved, the diffraction problem for the $\dot{u}_j$ is no longer merely formal. Indeed it is a valid characterization of the material derivative. We could now establish a similar characterization for the shape derivative by inserting its definition (7).

Let us assume that the shape derivative u'_j of the solution of (4) - (8) exists in $\mathcal{V}^l_\eta(\Omega)$ for some $l \in \mathbb{Z}, l \geq 0, \eta \in \mathbb{R}$. Inserting (7) into

$$\triangle \dot{u}_j^{\pm} + \kappa_{\pm}^2 \dot{u}_j^{\pm} = -\tilde{\triangle} u_j^{\pm},$$

we get

$$\triangle \left(u_j^{\pm}\right)' + \kappa_{\pm}^2 \left(u_j^{\pm}\right)' + \triangle \left(\nabla u_j^{\pm} \cdot T\right) + \kappa_{\pm}^2 \left(\nabla u_j^{\pm} \cdot T\right) = -\tilde{\triangle} u_j^{\pm}.$$

If T is only piecewise smooth, then this equation has to be understood in the sense of distributions. Straightforward calculations and the Helmholtz equation yield

$$\triangle \left(\nabla u_j^{\pm} \cdot T\right) + \tilde{\triangle} u_j^{\pm} = T \cdot \nabla \left(\triangle u_j^{\pm}\right) = -\kappa_{\pm}^2 \left(\nabla u_j^{\pm} \cdot T\right).$$

Thus $\left(u_j^{\pm}\right)'$ also satisfies the homogeneous Helmholtz equation in Ω. Let us now investigate the radiation condition. Let Γ be a part of the boundary $\partial\Omega$ and let

$$u_j^{\pm}(x) = r_j^{\pm}(x)$$

for every x in a neighbourhood of $\Gamma^{\pm}$. The perturbed boundary condition is

$$u_{j,\epsilon}^{\pm}(x + \epsilon T(x)) = r_{j,\epsilon}^{\pm}(x + \epsilon T(x)).$$

We expand this into a Taylor series and get $r^{\pm}_{j,0} \neq r^{\pm}_{j,\epsilon}$ if $\epsilon \neq 0$. We have $u^{\pm}_{j,0} = r^{\pm}_{j,0}$ in a neighbourhood of Γ, not only on Γ itself. Hence, $\nabla r^{\pm}_{j,0} = \nabla u^{\pm}_{j,0}$, and it follows that

$$\left(u_j^{\pm}\right)' = \left(r_j^{\pm}\right)' + \nabla r^{\pm}_{j,0} \cdot T - \nabla u_0 \cdot T = \left(r_j^{\pm}\right)'.$$

In our case, $r_j^{\pm}$ is of the form

$$r_j^{\pm}(x_1, x_2) = \sum_{n=-\infty}^{\infty} A^{\pm}_{j,n} e^{i(n+\alpha)x_1 + \sqrt{\kappa_{\pm}^2 - (n+\alpha)^2}x_2}.$$

Hence, its shape derivative has the form

$$\left(r_j^{\pm}\right)'(T)(x_1, x_2) = \sum_{n=-\infty}^{\infty} \left(A^{\pm}_{j,n}\right)'(T) e^{i(n+\alpha)x_1 + \sqrt{\kappa_{\pm}^2 - (n+\alpha)^2}x_2}.$$

In order to formulate transmission conditions for shape derivatives for transmission problems, we state the following Lemma.

Lemma 8. *Suppose that Ω is a domain with piecewise C^m boundary, $m \geq 1$, that the function u is shape differentiable in direction T on Ω and that $u|_{\partial\Omega}$ is also shape differentiable in direction T. Then the shape derivative of the domain integral*

$$F(\Omega)(u) = \int_{\Omega} u dx$$

in direction T is

$$F'(\Omega; T)(u) = \int_{\Omega} u'(T) dx + \int_{\partial\Omega} u(T \cdot \nu) ds.$$

Let $\tilde{\kappa}$ be the curvature of $\partial\Omega$ and let $\{S_j\}_{j=1}^m$ be the set of corner points of $\partial\Omega$. The shape derivative of the boundary integral

$$G(\Omega)(u) = \int_{\partial\Omega} u ds$$

in direction T is given by

$$G'(\Omega; T)(u) = \int_{\partial\Omega} u'(T) ds + \int_{\partial\Omega} \left\{\partial_\nu u + u\tilde{\kappa}(T \cdot \nu)\right\} ds + \sum_{j=1}^{m} \zeta_j,$$

where

$$\zeta_j = u(S_j)[T(S_{j+1}) \cdot \tau^-(S_{j+1})] - u(S_j)[T(S_j) \cdot \tau^+(S_j)],$$

with $\nu^{\pm}$ and $\tau^{\pm}$ denoting the left, resp. the right limit of the unit normal and the unit tangent vector. If u is only defined on $\partial\Omega$, then

$$G'(\Omega; T)(u) = \int_{\partial\Omega} u'(T) ds + \int_{\partial\Omega} u\tilde{\kappa}(T \cdot \nu) ds + \sum_{j=1}^{m} \zeta_j.$$

Proof. See [31], Chapters 2.31, 2.33 and 3.8. □

This Lemma can now be used for the characterization of transmission conditions over the interface. We apply a technique from [31]. Again, we discuss a simple model problem first and then use the results to characterize shape derivatives of solutions of the more complicated problem (4) - (8). Let (u_1, u_2) be a shape differentiable solution of the transmission problem

$$\begin{aligned} \triangle u_1 + \kappa_+^2 u_1 &= 0 \quad \text{in} \quad \Omega^+ \\ \triangle u_2 + \kappa_-^2 u_2 &= 0 \quad \text{in} \quad \Omega^- \\ \partial_\nu u_1 - \partial_\tau u_2 &= \partial_\nu u^{(i)} \quad \text{on} \quad \Gamma \\ u_1 - u_2 &= u^{(i)} \quad \text{on} \quad \Gamma \end{aligned}$$

and suitable boundary conditions on $\Gamma^\pm$, with Ω, Γ and $\Gamma^\pm$ as described in Section 1.2. The exact form of the boundary conditions is not important because we are only interested in the transmission conditions. Let u_j be an α-quasiperiodic functions satisfying $u_j \in V_\eta^k(\Omega^\pm), j = 1, 2$ with $k \geq 2$ and $\eta < 1$. Assume further that v is a test function which satisfies the same regularity requirements as u_1 and u_2, that $e^{i\alpha x_1} v(x_1, x_2)$ is periodic in x_1, $\partial_\nu v = 0$ on $\Gamma^+ \cup \Gamma^- \cup \Gamma$ and $v = 0$ on $\Gamma^+ \cup \Gamma^-$. Then Green's formula yields

$$\int_{\Omega^+} \left\{ \nabla u_1 \nabla v - \kappa_+^2 u_1 v \right\} dx - \int_{\Omega^-} \nabla u_2 \nabla^\perp v dx - \int_\Gamma \{ \partial_\nu u_1 - \partial_\tau u_2 \} v ds = 0.$$

Note that, because of the periodicity, the contributions of the boundary integrals over the parts of the boundary parallel to the x_2-axis cancel out. By Lemma 8 and by the chain rule for Fréchet derivatives, taking the shape derivative in direction T gives

$$\begin{aligned} \int_{\Omega^+} \nabla u_1' \nabla v dx - \int_{\Omega^-} \nabla u_2' \nabla^\perp v dx - \int_{\Omega^+} \kappa_+^2 u_1' v dx + \int_\Gamma \nabla u_1 \nabla v [T \cdot \nu] ds + \int_\Gamma \nabla u_2 \nabla^\perp v (T \cdot \nu) ds \\ - \int_\Gamma \kappa_+^2 u_1 v (T \cdot \nu) ds = \int_\Gamma \left(\partial_\nu u_1^{(i)} \right)' v ds + \int_\Gamma \tilde{\kappa} \partial_\nu u_1^{(i)} v (T \cdot \nu) ds + \sum_{j=1}^m \zeta_j, \end{aligned}$$

where $\tilde{\kappa}$ denotes the curvature of Γ and

$$\zeta_j = \nu^- \cdot \nabla u^{(i)}(S_{j+1}) v(S_{j+1}) [T(S_{j+1}) \cdot \tau^-(S_{j+1})] - \nu^+ \cdot \nabla u^{(i)}(S_j) v(S_j) [T(S_j) \cdot \tau^+(S_j)]. \tag{54}$$

Since

$$\int_{\Omega^+} \left\{ \nabla u_1' \nabla v - \kappa_+^2 u_1' v \right\} dx - \int_\Gamma \partial_\nu u_1' v ds = 0$$

and

$$\int_{\Omega^-} \nabla u_2' \nabla^\perp v dx + \int_\Gamma \partial_\tau u_2' v ds = 0,$$

it follows that

$$\begin{aligned} \int_\Gamma \{ \partial_\nu u_1' - \partial_\tau u_2' \} v ds = \int_\Gamma \left\{ -\nabla u_2 \nabla^\perp v - \nabla u_1 \nabla v + \kappa_+^2 u_1 v \right\} (T \cdot \nu) ds \\ + \int_\Gamma \left(\partial_\nu u_1^{(i)} \right)' v ds + \int_\Gamma \partial_\nu u_1^{(i)} v \tilde{\kappa} (T \cdot \nu) ds + \sum_{j=1}^m \zeta_j. \end{aligned} \tag{55}$$

Let

$$\mathrm{div}_\Gamma V := \left(\mathrm{div} V - (DV \cdot \nu) \cdot \nu \right)|_\Gamma$$

denote the tangential divergence of a vector field V. As usual, DV is the Jacobian of the vector field V. Additionally, let

$$\nabla u|_\tau := \nabla u - (\nu \cdot \nabla u)\nu = (\tau \cdot \nabla u)\tau$$

be the tangential gradient of u. Then by

$$\int_\Gamma (\nabla u \cdot V + u\mathrm{div}_\Gamma V)\, ds = \int_\Gamma (\partial_\nu u + \tilde{\kappa} u)(V \cdot \nu) ds,$$

which is formula (2.145) from [31], it follows that

$$\begin{aligned}\int_\Gamma \nabla u_1 \nabla v (T\cdot\nu) ds &= -\int_\Gamma v\mathrm{div}_\Gamma((T\cdot\nu)\nabla u_1) ds + \int_\Gamma \tilde{\kappa}(T\cdot\nu)[\nabla u_1 \cdot \nu] v ds \\ &= -\int_\Gamma v\mathrm{div}_\Gamma\left((T\cdot\nu)\nabla u_1|_\tau\right) ds.\end{aligned}$$

The last equality is Proposition 2.57 in [31]. In the same way we obtain

$$\begin{aligned}\int_\Gamma \nabla u_2 \nabla^\perp v (T\cdot\nu) ds &= -\int_\Gamma \nabla^\perp u_2 \nabla v (T\cdot\nu) ds \\ &= \int_\Gamma v\mathrm{div}_\Gamma \left((T\cdot\nu)\nabla^\perp u_2\right) ds - \int_\Gamma \tilde{\kappa}(T\cdot\nu)[\nabla^\perp u_2 \cdot \nu] v ds \\ &= \int_\Gamma v\mathrm{div}_\Gamma \left((T\cdot\nu)\nabla^\perp u_2|_\tau\right) ds.\end{aligned}$$

Inserting this into (55) yields

$$\begin{aligned}\int_\Gamma \left\{\partial_\nu u_1' - \partial_\tau u_2'\right\} v ds = \int_\Gamma \mathrm{div}_\Gamma \left((T\cdot\nu)\left\{\nabla u_1|_\tau - \nabla^\perp u_2|_\tau\right\}\right) v ds + \int_\Gamma \kappa_+^2 u_1 (T\cdot\nu) v ds + \\ + \int_\Gamma \left(\partial_\nu u^{(i)}\right)' v ds + \int_\Gamma \tilde{\kappa}\partial_\nu u^{(i)} (T\cdot\nu) v ds + \sum_{j=1}^m \zeta_j.\end{aligned}$$

Now consider the jumps $u_1' - u_2'$. We have

$$\int_\Gamma \{u_1 - u_2\} v ds = \int_\Gamma u^{(i)} v ds.$$

Taking the shape derivative on both sides yields

$$\begin{aligned}\int_\Gamma (\{u_1 - u_2\} v)' ds + \int_\Gamma \left\{\partial_\nu(u_1 - u_2) + \tilde{\kappa} u^{(i)}\right\}(T\cdot\nu) v ds + \sum_{l=1}^m \xi_l = \\ = \int_\Gamma (u^{(i)})' v ds + \int_\Gamma \tilde{\kappa} u^{(i)} (T\cdot\nu) v ds + \sum_{l=1}^m \rho_l,\end{aligned}$$

where

$$\xi_j = \{u_1 - u_2\}(S_{j+1}) v(S_{j+1})[T(S_{j+1}) \cdot \tau^-(S_{j+1})] - \{u_1 - u_2\}(S_j) v(S_j)[T(S_j) \cdot \tau^+(S_j)]$$

and

$$\rho_j = u^{(i)}(S_{j+1})v(S_{j+1})[T(S_{j+1}) \cdot \tau^-(S_{j+1})] - u^{(i)}(S_j)v(S_j)[T(S_j) \cdot \tau^+(S_j)].$$

The incoming wave does not depend on the geometry, consequently $(u^{(i)})' = 0$. Furthermore, we have

$$v' = \partial_\nu v(T \cdot \nu).$$

If we assume that the jump of the normal derivative of v across the interface is zero, we get

$$\int_\Gamma \{u_1' - u_2'\} v ds = -\int_\Gamma \partial_\nu(u_1 - u_2)(T \cdot \nu) v ds - \sum_{l=1}^m \xi_l + \sum_{l=1}^m \rho_l = -\int_\Gamma \partial_\nu(u_1 - u_2)(T \cdot \nu) v ds,$$

because the two sums cancel out and the incoming wave does not depend on Γ. Thus, it follows that

$$u_1' - u_2' = -\partial_\nu(u_1 - u_2)(T \cdot \nu).$$

Summarizing everything, we have obtained that the shape derivative of the solution of the model problem satisfies Helmholtz system

$$\begin{aligned} \triangle u_1' + \kappa_+^2 u_1' &= 0 \quad \text{in} \quad \Omega^+ \\ \triangle u_2' + \kappa_-^2 u_2' &= 0 \quad \text{in} \quad \Omega^- \end{aligned}$$

with transmission conditions

$$\begin{aligned} \int_\Gamma \left\{\partial_\nu u_1' - \partial_\tau u_2'\right\} v ds &= \int_\Gamma \operatorname{div}_\Gamma \left((T \cdot \nu) \left\{ \nabla u_1|_\tau - \nabla^\perp u_2|_\tau \right\} \right) v ds + \int_\Gamma \kappa_+^2 u_1 (T \cdot \nu) v ds + \\ &+ \int_\Gamma \left(\partial_\nu u^{(i)}\right)' v ds + \int_\Gamma \tilde{\kappa} \partial_\nu u^{(i)} (T \cdot \nu) v ds + \sum_{j=1}^m \zeta_j, \\ u_1' - u_2' &= -\partial_\nu(u_1 - u_2)(T \cdot \nu), \end{aligned}$$

with ζ_j from (54), on Γ. We assumed a suitable boundary condition for the model problem, but we did not investigate this in general. Nevertheless, if this suitable boundary condition is a radiation condition of the form (8), then the shape derivatives u_j' also satisfies this radiation condition. We see that the operator of the problem that characterizes the shape derivative is the same as the operator of the original model problem. Only the right-hand side changes. These results can be carried over to our original problem (4) - (8). We obtain the following theorem on the characterization of shape derivatives.

Theorem 3. *Assume that $(u_1^0, u_2^0) \in [\mathcal{V}_\eta^{k+2}(\Omega)]^2$ is the unique solution of the problem (4) - (8). Define*

$$\zeta_j := \nu^- \cdot \frac{\omega \varepsilon_+}{\kappa_+^2} \nabla u_1^{(i)}(S_{j+1}) v(S_{j+1}) [T(S_{j+1}) \cdot \tau^-(S_{j+1})] - \nu^+ \cdot \frac{\omega \varepsilon_+}{\kappa_+^2} \nabla u_1^{(i)}(S_j) v(S_j) [T(S_j) \cdot \tau^+(S_j)]$$

and

$$\xi_j := \nu^- \cdot \frac{\omega \mu}{\kappa_+^2} \nabla u_2^{(i)}(S_{j+1}) v(S_{j+1}) [T(S_{j+1}) \cdot \tau^-(S_{j+1})] - \nu^+ \cdot \frac{\omega \mu}{\kappa_+^2} \nabla u_2^{(i)}(S_j) v(S_j) [T(S_j) \cdot \tau^+(S_j)]$$

with $\nu^\pm$, $\tau^\pm$ and $\{S_j\}_{j=1}^m$ from Lemma 8. Then the shape derivative of (u_1^0, u_2^0) exists in $[\mathcal{V}_\eta^{k+1}(\Omega)]^2$. It satisfies the Helmholtz system

$$\triangle (u_1^+)' + \kappa_+^2 (u_1^+)' = 0 \quad \text{in} \quad \Omega^+$$

$$\triangle(u_1^-)' + \kappa_-^2 (u_1^-)' = 0 \quad \text{in} \quad \Omega^-$$
$$\triangle(u_2^+)' + \kappa_+^2 (u_2^+)' = 0 \quad \text{in} \quad \Omega^+$$
$$\triangle(u_2^-)' + \kappa_-^2 (u_2^-)' = 0 \quad \text{in} \quad \Omega^-$$

with the transmission conditions

$$\int_\Gamma \left[\frac{\gamma}{\kappa^2}\partial_\tau u_2' + \frac{\omega\varepsilon}{\kappa^2}\partial_\nu u_1'\right]_\Gamma v ds = \int_\Gamma \operatorname{div}_\Gamma \left((T\cdot\nu)\left[\frac{\gamma}{\kappa^2}\nabla u_2^0|_\tau + \frac{\omega\varepsilon}{\kappa^2}\nabla^\perp u_1^0|_\tau\right]_\Gamma\right) v ds$$
$$- \int_\Gamma \left\{\tilde{\kappa}(T\cdot\nu)\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu u_1^{(i)} + \frac{\omega\varepsilon_+}{\kappa^2}\nu'\cdot\nabla u_1^{(i)}\right\} v ds$$
$$+ \int_\Gamma \kappa_+^2 (T\cdot\nu)\left[u_1^0\right]_\Gamma v ds - \sum_{j=1}^m \zeta_j,$$
$$\int_\Gamma \left[\frac{\gamma}{\kappa^2}\partial_\tau u_1' - \frac{\omega\mu}{\kappa^2}\partial_\nu u_2'\right]_\Gamma v ds = \int_\Gamma \operatorname{div}_\Gamma \left((T\cdot\nu)\left[\frac{\gamma}{\kappa^2}\nabla u_1^0|_\tau - \frac{\omega\mu}{\kappa^2}\nabla^\perp u_2^0|_\tau\right]_\Gamma\right) v ds$$
$$+ \int_\Gamma \left\{\tilde{\kappa}(T\cdot\nu)\frac{\omega\mu}{\kappa_+^2}\partial_\nu u_2^{(i)} + \frac{\omega\mu}{\kappa^2}\nu'\cdot\nabla u_2^{(i)}\right\} v ds$$
$$+ \int_\Gamma \kappa_+^2 (T\cdot\nu)\left[u_2^0\right]_\Gamma v ds + \sum_{j=1}^m \xi_j$$

and

$$\left[u_1'\right]_\Gamma = -\partial_\nu \left[u_1\right]_\Gamma (T\cdot\nu),$$
$$\left[u_2'\right]_\Gamma = -\partial_\nu \left[u_2\right]_\Gamma (T\cdot\nu)$$

on the interface Γ *and a radiation condition of the form (8).*

Remark 6. (i) The weak formulation of the transmission condition in Theorem 3 can formally be written in the following form involving Dirac deltas:

$$\left[\frac{\gamma}{\kappa^2}\partial_\tau u_2' + \frac{\omega\varepsilon}{\kappa^2}\partial_\nu u_1'\right]_\Gamma = \operatorname{div}_\Gamma \left((T\cdot\nu)\left[\frac{\gamma}{\kappa^2}\nabla u_2^0|_\tau + \frac{\omega\varepsilon}{\kappa^2}\nabla^\perp u_1^0|_\tau\right]_\Gamma\right)$$
$$- \tilde{\kappa}(T\cdot\nu)\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu u_1^{(i)} + \frac{\omega\varepsilon_+}{\kappa^2}\nu'\cdot\nabla u_1^{(i)}$$
$$+ \kappa_+^2 (T\cdot\nu)\left[u_1^0\right]_\Gamma - \sum_{j=1}^m \zeta_j,$$
$$\left[\frac{\gamma}{\kappa^2}\partial_\tau u_1' - \frac{\omega\mu}{\kappa^2}\partial_\nu u_2'\right]_\Gamma = \operatorname{div}_\Gamma \left((T\cdot\nu)\left[\frac{\gamma}{\kappa^2}\nabla u_1^0|_\tau - \frac{\omega\mu}{\kappa^2}\nabla^\perp u_2^0|_\tau\right]_\Gamma\right)$$
$$+ \tilde{\kappa}(T\cdot\nu)\frac{\omega\mu}{\kappa_+^2}\partial_\nu u_2^{(i)} + \frac{\omega\mu}{\kappa^2}\nu'\cdot\nabla u_2^{(i)}$$
$$+ \kappa_+^2 (T\cdot\nu)\left[u_2^0\right]_\Gamma + \sum_{j=1}^m \xi_j$$

with

$$\zeta_j := \nu^-\cdot\frac{\omega\varepsilon_+}{\kappa_+^2}\nabla u_1^{(i)}(T\cdot\tau^-)\delta_{S_{j+1}} - \nu^+\cdot\frac{\omega\varepsilon_+}{\kappa_+^2}\nabla u_1^{(i)}(T\cdot\tau^+)\delta_{S_j}$$

and

$$\xi_j := \nu^- \cdot \frac{\omega\mu}{\kappa_+^2} \nabla u_2^{(i)} (T \cdot \tau^-) \delta_{S_{j+1}} - \nu^+ \cdot \frac{\omega\mu}{\kappa_+^2} \nabla u_2^{(i)} (T \cdot \tau^+) \delta_{S_j}.$$

(ii) In the case of incoming plane waves, according to Remark 3, we set

$$u_{1/2}^+ =: u_{1/2}^{(s)} + u_{1/2}^{(i)}.$$

Since the incoming waves do not depend on the geometry, their shape derivatives vanish. The terms in Theorem 3 involving $u_{1/2}^{(i)}$ drop as well.

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