Shape derivatives for diffraction by non-smooth periodic interfaces

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Fakultät II - Mathematik und Naturwissenschaften

Promotionsausschuss:

Vorsitzender:	Prof. Dr. Wolfgang König
Gutachter:	Prof. Dr. Dietmar Hömberg
	Prof. Dr. Jan Sokolowski
	Dr.habil. Andreas Rathsfeld

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Zusammenfassung

In der vorliegenden Arbeit werden konische Diffraktionsprobleme bei nichtglatten Diffraktionsgittern untersucht. Ziel ist die Berechnung von Formableitungen, welche zur Rekonstruktion der streuenden Struktur genutzt werden können. Dazu werden zunächst A-priori-Abschätzungen in gewichteten Sobolevräumen vom Kondratiev-Typ bewiesen. Anschließend werden Aussagen zu Existenz und Eindeutigkeit von Lösungen in diesen Räumen getroffen. Darauf aufbauend wird dann mit Hilfe der Theorie nichtlokaler Störungen elliptischer Randwertprobleme die Existenz und Eindeutigkeit von Formableitungen gezeigt. Die Formableitungen werden anschließend charakterisiert als Lösungen von Diffraktionsproblemen mit gleichem Operator, aber modifizierten rechten Seiten. Da die Formableitungen bei Anwesenheit von Ecken im Diffraktionsgitter eine niedrige Regularität aufweisen, wird zur numerischen Berechnung ein Ansatz vorgeschlagen, der darin besteht, die Singularitäten an den Ecken mit Hilfe glatter Funktionen abzuschneiden. Dann wird eine Randintegralformulierung für das modifizierte Problem, welches die Formableitungen charakterisiert, hergeleitet. Abschließend werden für einige Beispiele numerische Resultate vorgestellt.

„Das Wissen, das Macht ist, kennt keine Schranken, weder in der Versklavung der Kreatur noch in der Willfährigkeit gegen die Herren der Welt."

THEODOR W. ADORNO, MAX HORKHEIMER
Dialektik der Aufklärung

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_3)-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, see e.g. [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 [20]. Mathematically, this can be formulated as an inverse problem for the Maxwell equations. See the books of Petit [35] and Colton/Kress [12] 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 [44] and Simon [43]. 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 standard Sobolev spaces [14] and gradient formulas for both classical TE/TM diffraction and binary gratings [16] and for conical diffraction by general non-smooth structures [15]. 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 for the inverse problem 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

$$\min \left\{ \frac{1}{2} ||F'(\Gamma_n)(\Gamma_{n+1} - \Gamma_n) - u + F(\Gamma_n)||^2 + \frac{\alpha}{2} ||\Gamma_{n+1} - \Gamma_n||^2 \right\}, \tag{1.1}$$

where F' is the shape derivative of F, α is a regularization parameter, u is a given solution for which the scattering surface has to be determined, and Γ_0 is an initial guess for the diffracting surface. In practical applications, u would be the measurement of the diffracted wave. Potthast, Chandler-Wilde and Hohage and Schormann characterized shape derivatives of solutions of Dirichlet and Neumann boundary value problems [36, 37], transmission problems for bounded, smooth domains [22] and of Dirichlet problems for unbounded rough surfaces. These are surfaces which are described by contiuous non-periodic functions with Hölder continuous gradients [11]. 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 [21] 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 [24] 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 [9] suggested a different approach for non-smooth boundaries, using non-local perturbation theory and Kondratiev's weighted Sobolev spaces [29, 25]. 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 work, 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.

This thesis is structured in the following way. The second chapter recalls the conical diffraction problem in three dimensions and its reduction to a Helmholtz problem in a two-dimensional periodic cell. Chapter 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. [14] in standard Sobolev spaces. The fourth chapter 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 terms which are concentrated on the corner points.

Although all of these results are formulated for periodic gratings, the approach is general and can be used also to show existence of shape derivatives and to provide their characterization for transmission problems e.g. for bounded obstacles with corners. As mentioned above, for Dirichlet and Neumann boundary conditions on bounded obstacles this was done in [9]. In fact, the investigation of transmission problems for bounded obstacles should be simpler than it is in the case of periodic gratings, because here the radiation condition leads to some technical difficulties, as we will see in Chapter 3.

The last chapter deals with numerical computation of shape derivatives. In order to deal with the singularities at the corner points, a cut-off ansatz is proposed which reduces the theoretical results in the Kondratiev spaces to the setting in standard Sobolev spaces. We present the idea of this ansatz and prove convergence. Then we use results obtained by Schmidt [39] to give a representation of the shape derivative as a solution of a system of boundary integral equations, which can then be discretized using e.g. a collocation method. Finally, examples for numerical computations of shape derivatives for some simple geometries are presented.

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 direction of the incoming wave lies in the (x_1, x_2) plane, we have TE diffraction, TM diffraction or a combination thereof, depending on the polarization.

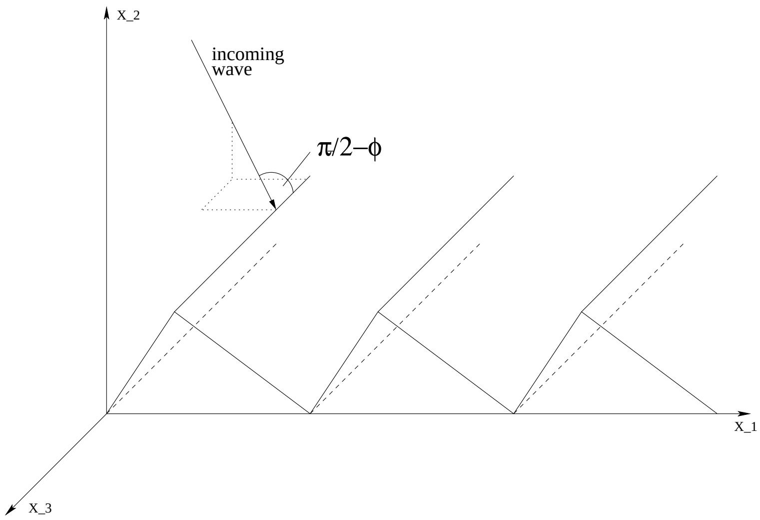

Figure 2.1: The diffraction grating

Since the incoming wave is time-harmonic, i.e. it admits the form

$$\left(\mathcal{E}^{(i)}, \mathcal{H}^{(i)}\right) = \left(\mathbf{p}e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3}e^{-i\omega t}, \mathbf{q}e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3}e^{-i\omega t}\right) = \left(\mathbf{E}^{(i)}, \mathbf{H}^{(i)}\right)e^{-i\omega t}, \qquad (2.1)$$

where $\mathbf{p}, \mathbf{q} \in \mathbb{R}^3$, $\mathbf{k} = (\alpha, -\beta, \gamma)$ is the wave vector and $\mathbf{k}/|\mathbf{k}|$ is the direction of the incoming wave, we obtain the time-harmonic Maxwell equations for the electromagnetic field $(\mathbf{E}, \mathbf{H})$, which is the sum of the incoming wave and the reflected wave above the grating, i.e. $(\mathbf{E}_1, \mathbf{H}_1) = (\mathbf{E}^{(i)}, \mathbf{H}^{(i)}) + (\mathbf{E}^{(r)}, \mathbf{H}^{(r)})$. Below the grating it is equal to the transmitted wave $(\mathbf{E}_2, \mathbf{H}_2) = (\mathbf{E}^{(t)}, \mathbf{H}^{(t)})$. The Maxwell system is

$$\begin{aligned} \nabla \times \mathbf{E} &= i\omega\mu\mathbf{H} \\ \nabla \times \mathbf{H} &= -i\omega\varepsilon\mathbf{E} \end{aligned} \tag{2.2}$$

with transmission conditions

$$\begin{aligned} \nu \times (\mathbf{E}_1 - \mathbf{E}_2) &= 0 \\ \nu \times (\mathbf{H}_1 - \mathbf{H}_2) &= 0 \end{aligned} \tag{2.3}$$

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 $\varepsilon = \varepsilon_+$ 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 (2.1), then

$$(\mathbf{E}, \mathbf{H})(x_1, x_2, x_3) = (E, H)(x_1, x_2)e^{i\gamma x_3}, \tag{2.4}$$

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), which is described in the next subsection. For details, see [14], [15], [17] and the following section.

2.2 The quasi-periodic Helmholtz problem

In this section we describe how in the given situation the Maxwell system reduces to a system of Helmholtz equations in two dimesions. The Maxwell equations give

$$\begin{aligned} E &= \frac{i}{\omega\varepsilon}\left(\frac{\partial}{\partial x_2}H_3 - i\gamma H_2, i\gamma H_1 - \frac{\partial}{\partial x_1}H_3, \frac{\partial}{\partial x_1}H_2 - \frac{\partial}{\partial x_2}H_1\right), \\ H &= \frac{1}{i\omega\mu}\left(\frac{\partial}{\partial x_2}E_3 - i\gamma E_2, i\gamma E_1 - \frac{\partial}{\partial x_1}E_3, \frac{\partial}{\partial x_1}E_2 - \frac{\partial}{\partial x_2}E_1\right), \end{aligned} \tag{2.5}$$

which immediately implies

$$E_1 = \frac{i}{\omega\varepsilon}\frac{\partial}{\partial x_2}H_3 + \frac{i\gamma}{\omega^2\varepsilon\mu}\frac{\partial}{\partial x_1}E_3 + \frac{\gamma^2}{\omega^2\varepsilon\mu}E_1.$$

This is

$$\frac{\omega^2\varepsilon\mu - \gamma^2}{\omega^2\varepsilon\mu}E_1 = \frac{i}{\omega\varepsilon}\frac{\partial}{\partial x_2}H_3 + \frac{i\gamma}{\omega^2\varepsilon\mu}\frac{\partial}{\partial x_1}E_3,$$

and likewise for E_2, H_1 and H_2. Moreover, taking the derivative with respect to x_1 of the second components in the first and in the second line of (2.5) gives

$$\frac{\partial^2}{\partial x_1^2} E_3 = i\gamma \frac{\partial}{\partial x_1} E_1 - i\omega\mu \frac{\partial}{\partial x_1} H_2,$$
$$\frac{\partial^2}{\partial x_2^2} E_3 = i\gamma \frac{\partial}{\partial x_2} E_2 + i\omega\mu \frac{\partial}{\partial x_2} H_2.$$

When ε is constant, the Maxwell equation $\nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E}$ implies

$$\operatorname{div} \mathbf{E} = 0.$$

Using this together with (2.4) and the third component of the first line of (2.5), we get

$$\begin{aligned}\left(\frac{\partial}{\partial x_1^2} + \frac{\partial}{\partial x_2^2}\right) E_3 &= i\gamma \frac{\partial}{\partial x_1} E_1 + i\gamma \frac{\partial}{\partial x_2} E_2 - i\omega\mu \left(\frac{\partial}{\partial x_1} H_2 - \frac{\partial}{\partial x_2} H_1\right) \\ &= -i\gamma \frac{\partial}{\partial x_3} E_3 - \omega^2 \mu\varepsilon E_3 \\ &= -\kappa^2 E_3.\end{aligned} \tag{2.6}$$

Analogously,

$$\left(\frac{\partial}{\partial x_1^2} + \frac{\partial}{\partial x_2^2}\right) H_3 = -\kappa^2 H_3. \tag{2.7}$$

Let $\kappa_\pm^2 := k_\pm^2 - \gamma^2$, where $k_\pm = \omega\sqrt{\mu\varepsilon_\pm}$ and $\kappa(x) := \kappa_\pm$ if $x \in \Omega^\pm$, and analogously for ε. Note that the material constants can be complex valued. Therefore, we choose the square root of $z = re^{i\phi}$ with $\phi \in [0, 2\pi)$ to be $\sqrt{z} = \sqrt{r}e^{i\phi/2}$. Then we have

$$\begin{aligned}\kappa^2 E_1 &= i\mu\omega \frac{\partial}{\partial x_2} H_3 + i\gamma \frac{\partial}{\partial x_1} E_3, \\ \kappa^2 H_1 &= -i\varepsilon\omega \frac{\partial}{\partial x_2} E_3 + i\gamma \frac{\partial}{\partial x_1} H_3, \\ \kappa^2 E_2 &= -i\mu\omega \frac{\partial}{\partial x_1} H_3 + i\gamma \frac{\partial}{\partial x_2} E_3, \\ \kappa^2 H_2 &= i\varepsilon\omega \frac{\partial}{\partial x_1} E_3 + i\gamma \frac{\partial}{\partial x_2} H_3,\end{aligned} \tag{2.8}$$

from which follows that, under the assumption $\kappa \neq 0$, the first two components of the electric and the magnetic field are determined by the third one. Writing $\nu = (\nu_1, \nu_2, 0)$, the transmission conditions (2.3) imply that the jump of

$$\nu \times E = (\nu_2 E_3, -\nu_1 E_3, \nu_1 E_2 - \nu_2 E_1),$$
$$\nu \times H = (\nu_2 H_3, -\nu_1 H_3, \nu_1 H_2 - \nu_2 H_1)$$

across the interface Γ is zero, and therefore also

$$[E_3]_\Gamma = [H_3]_\Gamma = 0,$$

where $[\cdot]_\Gamma$ denotes the jump of a function over Γ, i.e.

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

Moreover, the relations (2.8) give

$$\nu_1 E_2 - \nu_2 E_1 = \frac{1}{\kappa^2}\left(i\gamma\left(\nu_1\frac{\partial}{\partial x_2}E_3 - \nu_2\frac{\partial}{\partial x_1}E_3\right) - i\omega\mu\left(\nu_1\frac{\partial}{\partial x_1}H_3 + \nu_2\frac{\partial}{\partial x_2}H_3\right)\right),$$
$$\nu_1 H_2 - \nu_2 H_1 = \frac{1}{\kappa^2}\left(i\gamma\left(\nu_1\frac{\partial}{\partial x_2}H_3 - \nu_2\frac{\partial}{\partial x_1}H_3\right) + i\omega\varepsilon\left(\nu_1\frac{\partial}{\partial x_1}E_3 + \nu_2\frac{\partial}{\partial x_2}E_3\right)\right),$$

which implies

$$\left[\frac{\omega\varepsilon}{\kappa^2}\partial_\nu E_3 + \frac{\gamma}{\kappa^2}\partial_\tau H_3\right]_\Gamma = 0$$

and

$$\left[\frac{\omega\mu}{\kappa^2}\partial_\nu H_3 - \frac{\gamma}{\kappa^2}\partial_\tau E_3\right]_\Gamma = 0$$

with $\tau = (-\nu_2, \nu_1, 0)$. Let the period of the grating be 2π. We restrict the problem (2.2,2.3) 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 and below the grating, respectively, and with an interface Γ splitting Ω into an upper part Ω^+ and a lower part Ω^-. This is shown in Figure 2.2. Now we introduce the functions

$$u_1^+ := E_3^{(r)}|_{\Omega^\pm}, \qquad u_2^+ := H_3^{(r)}|_{\Omega^\pm}$$

and

$$u_1^- := E_3^{(t)}|_{\Omega^\pm}, \qquad u_2^- := H_3^{(t)}|_{\Omega^\pm}.$$

In view of the 2π-periodicity of the problem and the form (2.1) of the incoming wave, we look for solutions which are α-quasi-periodic in x_1, i.e.

$$u_1^\pm(x_1 + 2\pi, x_2) = e^{2\pi i\alpha}u_1^\pm(x_1, x_2), \qquad u_2^\pm(x_1 + 2\pi, x_2) = e^{2\pi i\alpha}u_2^\pm(x_1, x_2). \tag{2.9}$$

We have seen (cf. (2.6) and (2.7)) that the Maxwell equations (2.2) can then be formulated as

$$\begin{aligned}
\triangle u_1^+ + \kappa_+^2 u_1^+ &= f_1^+ \quad \text{in} \quad \Omega^+\\
\triangle u_1^- + \kappa_-^2 u_1^- &= f_1^- \quad \text{in} \quad \Omega^-\\
\triangle u_2^+ + \kappa_+^2 u_2^+ &= f_2^+ \quad \text{in} \quad \Omega^+\\
\triangle u_2^- + \kappa_-^2 u_2^- &= f_2^- \quad \text{in} \quad \Omega^-
\end{aligned} \tag{2.10}$$

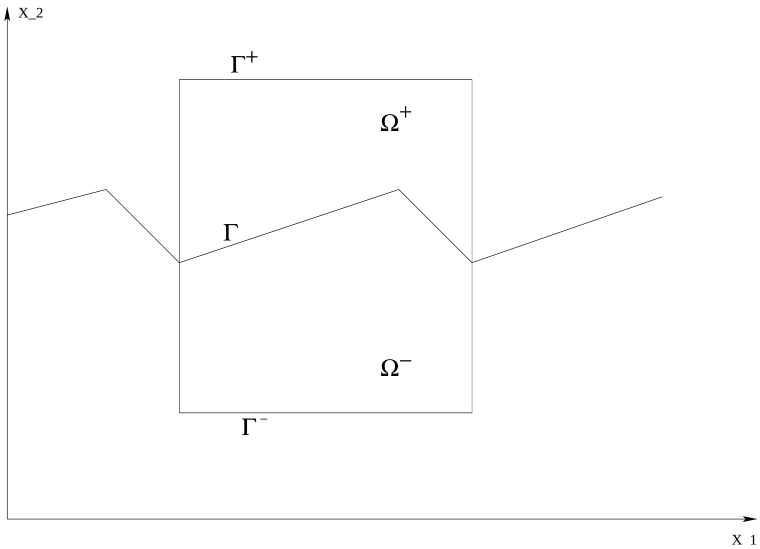

Figure 2.2: The 2D periodic cell

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

$$(u_1^{(i)}, u_2^{(i)}) = (p_3, q_3)e^{i\alpha x_1 - i\beta x_2}, \tag{2.11}$$

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. The transmission conditions (2.3) turn into

$$\begin{aligned}
\left[\frac{\gamma}{\kappa^2}\partial_\tau u_2 + \frac{\omega\varepsilon}{\kappa^2}\partial_\nu u_1\right]_\Gamma &= -\frac{\omega\varepsilon}{\kappa_+^2}\partial_\nu u_1^{(i)} - \frac{\gamma}{\kappa_+^2}\partial_\tau u_2^{(i)} =: b_1 \\
\left[\frac{\gamma}{\kappa^2}\partial_\tau u_1 - \frac{\omega\mu}{\kappa^2}\partial_\nu u_2\right]_\Gamma &= \frac{\omega\mu}{\kappa_+^2}\partial_\nu u_2^{(i)} - \frac{\gamma}{\kappa_+^2}\partial_\tau u_1^{(i)} =: b_2 \\
[u_1]_\Gamma &= -u_1^{(i)} =: b_3 \\
[u_2]_\Gamma &= -u_2^{(i)} =: b_4
\end{aligned} \tag{2.12}$$

on Γ as explained. Note that the functions u_j describe only the scattered field and not the total field. 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.

$$\mathbf{B} = \left(B^i_j(\partial_\nu, \partial_\tau) \right)^4_{i,j=1} := \begin{pmatrix} \frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu & -\frac{\omega\varepsilon_-}{\kappa_-^2}\partial_\nu & \frac{\gamma}{\kappa_+^2}\partial_\tau & -\frac{\gamma}{\kappa_-^2}\partial_\tau \\ \frac{\gamma}{\kappa_+^2}\partial_\tau & -\frac{\gamma}{\kappa_-^2}\partial_\tau & -\frac{\omega\mu}{\kappa_+^2}\partial_\nu & \frac{\omega\mu}{\kappa_-^2}\partial_\nu \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}, \tag{2.13}$$

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

Since $u_j^\pm$ is α-quasiperiodic in x_1, the functions

$$v_j^\pm(x_1, x_2) := e^{-i\alpha x_1} u_j^\pm(x_1, x_2), \qquad j = 1, 2$$

are 2π-periodic with respect to x_1. They can therefore be represented as a Fourier series

$$v_j^\pm(x_1, x_2) = \sum_{n=-\infty}^{\infty} u_{j,n}^\pm(x_2) e^{inx_1},$$

so $u_j^\pm$ can be written as

$$u_j^\pm(x_1, x_2) = \sum_{n=-\infty}^{\infty} u_{j,n}^\pm(x_2) e^{i(n+\alpha)x_1}.$$

Inserting this expansion into the Helmholtz equation leads to

$$e^{i\alpha x_1} \sum_{n=-\infty}^{\infty} \left(\frac{\partial^2}{\partial x_2^2} u_{j,n}^\pm(x_2) + (\kappa_\pm^2 - \{\alpha + n\}^2) u_{j,n}^\pm(x_2) \right) e^{inx_1} = 0.$$

Hence, every $u_{j,n}^\pm(x_2)$ has to fulfill the identity

$$\frac{\partial^2}{\partial x_2^2} u_{j,n}^\pm(x_2) + (\kappa_\pm^2 - \{\alpha + n\}^2) u_{j,n}^\pm(x_2) = 0.$$

The solutions of this equation are

$$u_{j,n}^\pm(x_2) = \tilde{A}_{j,n}^\pm e^{-i\beta_n^\pm x_2} + \tilde{B}_{j,n}^\pm e^{i\beta_n^\pm x_2}$$

with $\beta_n^\pm := \sqrt{\kappa_\pm^2 - (\alpha + n)^2}$ and integration constants $\tilde{A}_{j,n}^\pm$ and $\tilde{B}_{j,n}^\pm$. Consequently,

$$u_j^\pm(x_1, x_2) = \sum_{n=-\infty}^{\infty} \left(\tilde{A}_{j,n}^\pm e^{i(\alpha+n)x_1 - i\beta_n^\pm x_2} + \tilde{B}_{j,n}^\pm e^{i(\alpha+n)x_1 + i\beta_n^\pm x_2} \right)$$

For u_j^+, the first part of the sum constists of incoming waves, which are propagating if $\beta_n^+ \in \mathbb{R}$ or unbounded if β_n^+ is imaginary. In the same way, the second part consists of propagating and evanescent outgoing waves. Analogously, for u_j^-, the first part is a sum of downgoing waves and the second part consits of incident waves, which are also propagating if $\beta_n^- \in \mathbb{R}$ and unbounded otherwise. Note that there is only a finite number of propagating modes. In our case, we assume that there is exactly one incident wave from above (with $n = 0$) and no incidence from below. Summarizing, we have a radiation condition that demands that the scattered wave can be represented as

$$u_j^{\pm}(x_1, x_2) = \sum_{n=-\infty}^{\infty} A_{j,n}^{\pm} e^{i(\alpha+n)x_1 \pm i\beta_n^{\pm} x_2}, \tag{2.14}$$

in a neighbourhood of Γ^+ and Γ^-, respectively.

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 3.2 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 3.1. 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 $S \in \mathcal{S}$, $\chi_S \equiv 1$ in a smaller neighbourhood and $\Psi(x), \chi_S(x) \geq 0$ for all $x \in \Omega$. For $k \in \mathbb{N}$ and $\eta \in \mathbb{R}$ we define $V_\eta^k(\Omega^\pm)$ as the set of generalized functions with the finite norm

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

For $k \geq 1$, the well defined (see [33, 26]) trace space on the boundary $\partial\Omega^\pm$ is denoted by $V_\eta^{k-1/2}(\partial\Omega^\pm)$. If, as in our setting, $\Omega = \Omega^+ \cup \Omega^-$, then

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

The following lemma, which is Lemma 6.2.1 in [26], concerning embeddings of these spaces will be needed later on.

Lemma 3.1. *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 $V_\eta^k(\Omega)$ is continuously embedded into $V_\beta^l(\Omega)$. Moreover, $V_\eta^k(\Omega)$ is dense in $V_\beta^l(\Omega)$. If $k > l \geq 0$ and $\eta - k < \beta - l$, then this embedding is compact. Analogous statements are true for the trace spaces.*

Remark 3.1 (*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

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

□

Now we define

$$\triangle u_j^\pm = f_j^\pm - \kappa_\pm^2 u_j^\pm =: \tilde{f}_j^\pm$$

and consider only the Laplacian instead of the Helmholtz operator in the following. 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

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

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

$$\begin{aligned}
w_j^\pm(t,\theta_S^\pm) &:= v_j^\pm(e^t,\theta_S^\pm),\\
w_j &:= (w_j^+, w_j^-),\\
\varrho_j^\pm(t,\theta_S^\pm) &:= e^{2t}\sigma_j^\pm(e^t,\theta_S^\pm),\\
\varrho_j &:= (\varrho_j^+,\varrho_j^-),\\
\omega_i(t,\theta_S^\pm) &:= e^{(1-m_i)t}\phi_i(e^t,\theta_S^\pm)
\end{aligned}$$

with $m_1 = m_2 = 0$, $m_3 = m_4 = 1$ and $i = 1,\dots,4$. Using this notation, we now have the following interface problem in the ramified strip (see [33], 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 3.2. *The conical diffraction problem in the vicinity of a corner point $\mathcal{S}$ can be transformed to*

$$\begin{aligned} L^\pm(D_\theta, D_t) w_1^\pm &= \varrho_1^\pm \quad \text{in} \quad B_S^\pm \\ L^\pm(D_\theta, D_t) w_2^\pm &= \varrho_2^\pm \quad \text{in} \quad B_S^\pm \end{aligned}$$

with transmission conditions

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

where $L^\pm(D_\theta, D_t)$ is the Laplace operator transformed to polar coordinates centered at $\mathcal{S}$ and with the radial variable replaced by e^t, and $B_j^i(\partial_\theta,\partial_t)$, $i, j = 1, \ldots 4$ are the boundary operators from (2.13), also transformed to polar coordinates with center $\mathcal{S}$ and with the radial variable replaced by e^t.

Applying the Laplace transform

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

to the problem of Lemma 3.2 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 [26], Theorem 3.6.1, it can be shown that there exists a unique solution $\check{w}_j$, which satisfies

$$\sum_{j=1}^{2} ||\check{w}_j(\cdot,\lambda)||_{\mathcal{H}^{k+2}(A_S,\lambda)} \leq C_1 \left\{ \sum_{j=1}^{2} ||\check{\varrho}_j(\cdot,\lambda)||_{\mathcal{H}^{k}(A_S,\lambda)} + \sum_{j=1}^{4} (1+|\lambda|^{k+m_j+1/2})|\check{\omega}_j(\lambda)| \right\}, \tag{3.1}$$

where

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

We define

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

and

$$\mathcal{H}_\beta^k(B) := H_\beta^k(B^+) \times H_\beta^k(B^-).$$

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 $\varrho \in \mathcal{H}_{\beta_1}^k(B)$ and $\omega_j \in H_{\beta_1}^{k+m_j+1/2}(\partial B_S^+)$. Let $A(\lambda)$ be the operator of the parameter-dependent system, i.e.

$$A(\lambda)\check{w}(\cdot,\lambda) = (\check{\varrho}, \check{\omega})(\cdot,\lambda),$$

with $\check{\varrho} = (\check{\varrho}_1, \check{\varrho}_2)$, and $\check{\omega}$ analogously. Then the function

$$w_{\beta_1} := \int\limits_{\mathrm{Re}\lambda = -\beta_1} e^{\lambda t} A^{-1}(\lambda)(\check{\varrho}, \check{\omega}) d\lambda$$

is a solution in the ramified strip which belongs to the space $[\mathcal{H}_{\beta_1}^{k+2}(B_S)]^2$. If additionally $\varrho \in \mathcal{H}_{\beta_2}^k(B)$ and $\omega_j \in H_{\beta_2}^{k+m_j+1/2}(\partial B_S^+)$ with $\beta_1 > \beta_2$, then $w_{\beta_2} \in [\mathcal{H}_{\beta_1}^{k+2}(B_S)]^2$ given by

$$w_{\beta_2} := \int\limits_{\mathrm{Re}\lambda = -\beta_2} e^{\lambda t} A^{-1}(\lambda)(\check{\varrho}, \check{\omega}) d\lambda$$

is also a solution in the ramified strip. These two solutions are related by

$$w_{\beta_1} = w_{\beta_2} + \sum_{\sigma=1}^{n} \mathrm{Res}\, e^{\lambda t} A^{-1}(\lambda)(\check{\varrho}, \check{\omega})|_{\lambda=\lambda_\sigma},$$

where $\{\lambda_\sigma\}_{\sigma=1}^n$ is the set of eigenvalues of $A(\lambda)$ satisfying

$$\{\mathrm{Re}\lambda_\sigma\}_{\sigma=1}^n \subset (-\beta_1, -\beta_2),$$

cf. [26], Theorem 5.4.1. The inverse Laplace transform therefore yields a solution of the boundary value problem in the cone which depends on the choice of the line $\mathrm{Re}\lambda = -\beta$.

If

$$\tilde{f}_i \in \mathcal{V}^k_\eta(\Omega^\pm), \qquad b_j \in V^{k+m_j+1/2}_\eta(\Gamma)$$

and

$$u_j \in \mathcal{V}^{k+2}_\eta(\Omega^\pm),$$

then this solution corresponds to the original solution. In particular, Lemma 1.62 in [33] states that the mapping

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

is an isomorphism for $\beta = \eta - k + 1$. Therefore, we may choose this β and integrate equation (3.1) along the line $\mathrm{Re}\lambda = -\beta$ and use the norm equivalence

$$||u||_{H^k_\beta(B^\pm_S)} \simeq \left(\int\limits_{\mathrm{Re}\lambda=-\beta} ||\check{u}(\cdot,\lambda)||^2_{H^k(A^\pm_S,\lambda)} d\lambda \right)^{1/2}.$$

In this way we get

$$\sum_{j=1}^{2} ||w_j||_{\mathcal{H}^{k+2}_\beta(B_S)} \leq C_2 \left\{ \sum_{j=1}^{2} ||\varrho||_{\mathcal{H}^k_\beta(B_S)} + \sum_{j=1}^{4} ||\omega_j||_{H_\beta^{k+m_j+1/2}(\partial B^+_S)} \right\}. \tag{3.2}$$

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 $C \subset \mathbb{R}^2$. In terms of the Kondratiev spaces, the estimate (3.2) becomes

$$\sum_{j=1}^{2} ||v_j||_{\mathcal{V}^{k+2}_\eta(C_S)} \leq C_3 \left\{ \sum_{j=1}^{2} ||t^2\sigma_j||_{\mathcal{V}^k_{\eta-2}(C_S)} + \sum_{j=1}^{4} ||t^{1-m_j}\phi_j||_{V^{k+m_j+1/2}_{\eta+m_j-1}(\partial B^+_S)} \right\} \tag{3.3}$$

because of the isomorphism. The product rule yields

$$\sigma^\pm_j = \chi_S \triangle u^\pm_j + 2\nabla u^\pm_j \cdot \nabla \chi_S + u^\pm_j \triangle \chi_S = \chi_S \tilde{f}^\pm_j + 2\nabla u^\pm_j \nabla \chi_S + u^\pm_j \triangle \chi_S.$$

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

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

Moreover,

$$||\chi_S \tilde{f}_j||_{\mathcal{V}^k_\eta(C_S)} \leq C_5 ||\tilde{f}_j||_{\mathcal{V}^k_\eta(C_S)}$$

by Lemma 3.3 in [25]. Since

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

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

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

Analogously, we get

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

Inserting this into (3.3) yields

$$\sum_{j=1}^{2} ||v_j||_{\mathcal{V}^{k+2}_\eta(C_S)} \leq C_8 \left\{\sum_{j=1}^{2} ||\tilde{f}_j||_{\mathcal{V}^k_\eta(C_S)} + \sum_{j=1}^{4} ||b_j||_{V^{k+m_j+1/2}_\eta(\partial C_S^+)} + \sum_{j=1}^{2} ||u_j||_{\mathcal{V}^{k+1}_\eta(C_S)}\right\}. \quad (3.4)$$

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

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

Again, by the product rule, it holds that

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

and

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

Using the notation (2.13), 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

$$||g_j^\pm||_{H^k(\Omega^\pm)} \leq C_9 \left\{||\tilde{f}_j^\pm||_{V^k_\eta(\Omega^\pm)} + ||u_j^\pm||_{V^{k+1}_\eta(\Omega^\pm)}\right\}$$

and

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

Inserting this into the estimate (2.2) in [10] (originally proven by Roitberg and Sheftel [38]), namely

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

yields

$$\sum_{j=1}^{2} ||\hat{u}_j||_{\mathcal{H}^{k+2}(\Omega^\pm)} \leq C_{12} \left\{ \sum_{j=1}^{2} ||\tilde{f}_j||_{\mathcal{V}_\eta^k(\Omega^\pm)} + \sum_{j=1}^{4} ||b_j||_{V_\eta^{k+m_j+1/2}(\Gamma)} + \sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+1}(\Omega)} \right\}, \quad (3.5)$$

where $\mathcal{H}^k(\Omega) := H^k(\Omega^+) \times H^k(\Omega^-)$ as before. By adding the estimates (3.4) and (3.5) and using

$$||\tilde{f}_j||_{\mathcal{V}_\eta^k(\Omega^\pm)} \leq \tilde{C} \left\{ ||f_j||_{\mathcal{V}_\eta^k(\Omega^\pm)} + ||u_j||_{\mathcal{V}_\eta^{k+1}(\Omega^\pm)} \right\},$$

we get the desired a priori estimate.

As we have seen and as explained in [14] 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 3.2 by applying a Laplace transform. If it is assumed that $k_+^2 \neq k_-^2$, then 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. Define

$$\mathcal{A} := \bigcup_{s\in\mathcal{S}} \mathcal{A}_S.$$

We have shown the following result.

Proposition 3.1. *Assume that $k + 1 - \eta \notin \mathcal{A}$ and that the solution (u_1, u_2) of (2.9), (2.10), (2.12), (2.14) is in $[\mathcal{V}_\eta^{k+2}(\Omega)]^2$ for $k \in \mathbb{Z}, k \geq 0$. Then*

$$\sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+2}(\Omega)} \leq C \left\{ \sum_{j=1}^{2} ||f_j||_{\mathcal{V}_\eta^k(\Omega)} + \sum_{j=1}^{4} ||b_j||_{V_\eta^{k+m_j+1/2}(\Gamma)} + \sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+1}(\Omega)} \right\}. \quad (3.6)$$

Proposition 3.2. *If in addition to the assumptions of Proposition 3.1 the conical diffraction prob-*

lem (2.9), (2.10), (2.12), (2.14) is uniquely solvable, then

$$\sum_{j=1}^{2} ||u_j||_{\mathcal{V}_\eta^{k+2}(\Omega)} \leq C \left\{ \sum_{j=1}^{2} ||f_j||_{\mathcal{V}_\eta^{k}(\Omega)} + \sum_{j=1}^{4} ||b_j||_{V_\eta^{k+m_j+1/2}(\Gamma)} \right\}. \tag{3.7}$$

Proof. The proof employs the technique used in the proof of [6], 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

$$\sum_{j=1}^{2} ||u_{j,n}||_{\mathcal{V}_\eta^{k+2}(\Omega)} > n \left\{ \sum_{\substack{j=1 \\ i \in \{+,-\}}}^{2} ||L^i u_{j,n}^i||_{V_\eta^k(\Omega^i)} + \sum_{j=1}^{4} || \sum_{i=1}^{2} \left(B_j^{2i-1} u_{i,n}^+ \; + B_j^{2i} u_{i,n}^- \right) ||_{V_\eta^{k+m_j+1/2}(\Gamma)} \right\}, \tag{3.8}$$

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

$$\mathbf{L} := \begin{pmatrix} \triangle + \kappa_+^2 & 0 & 0 & 0 \\ 0 & \triangle + \kappa_+^2 & 0 & 0 \\ 0 & 0 & \triangle + \kappa_-^2 & 0 \\ 0 & 0 & 0 & \triangle + \kappa_-^2 \end{pmatrix}, \qquad \mathbf{u} := (u_1^+, u_2^+, u_1^-, u_2^-)^\top$$

and

$$\mathbf{V}_\eta^{k-1/2}(\Gamma) := \bigoplus_{j=1}^{4} V_\eta^{k-m_j-1/2}(\Gamma)$$

we can write (3.8) as

$$||\mathbf{u}_n||_{[\mathcal{V}_\eta^{k+2}(\Omega)]^2} > n \left\{ ||\mathbf{L}\mathbf{u}_n||_{[\mathcal{V}_\eta^{k}(\Omega)]^2} + ||\mathbf{B}\mathbf{u}_n||_{\mathbf{V}_\eta^{k-1/2}(\Gamma)} \right\}, \tag{3.9}$$

where the matrix operator $\mathbf{B}$ is given by (2.13). Now define

$$\mathbf{v}_n := \frac{\mathbf{u}_n}{||\mathbf{u}_n||_{[\mathcal{V}_\eta^{k+2}(\Omega)]^2}}.$$

If we insert this into (3.9) we have

$$||\mathbf{L}\mathbf{v}_n||_{[\mathcal{V}_\eta^{k}(\Omega)]^2} + ||\mathbf{B}\mathbf{v}_n||_{\mathbf{V}_\eta^{k-1/2}(\Gamma)} < \frac{2}{n}. \tag{3.10}$$

We will use the compact embeddings stated in Lemma 3.1, 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 $(\mathbf{v}_{n'})_{n'} \subseteq (\mathbf{v}_n)_n$ and functions $\Phi \in [\mathcal{V}_\eta^{k+2}(\Omega)]^2$ such that $(\mathbf{v}_{n'})_{n'} \rightharpoonup \Phi$ weakly in

$[\mathbf{V}_\eta^{k+2}(\Omega)]^2$. Because of the compact embeddings it follows that $\mathbf{v}_{n'} \to \Phi$ in the norm of $[\mathcal{V}_\eta^{k+1}(\Omega^\pm)]^2$. Proposition 3.1 implies that

$$||\mathbf{v}_{n'} - \mathbf{v}_{m'}||_{[\mathcal{V}_\eta^{k+2}(\Omega)]^2} \leq C \Big\{ ||\mathbf{L}\mathbf{v}_{n'} - \mathbf{L}\mathbf{v}_{m'}||_{[\mathcal{V}_\eta^{k}(\Omega)]^2} + ||\left(\mathbf{B}\mathbf{v}_{n'} - \mathbf{B}\mathbf{v}_{m'}\right)||_{\mathbf{V}_\eta^{k-1/2}(\Gamma)} + ||\mathbf{v}_{n'} - \mathbf{v}_{m'}||_{[\mathcal{V}_\eta^{k+1}(\Omega)]^2} \Big\},$$

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

$$||\mathbf{L}\Phi||_{0[\mathcal{V}_\eta^{k}(\Omega)]^2} = \lim_{n'\to\infty} ||\mathbf{L}\mathbf{v}_{n'}||_{[\mathcal{V}_\eta^{k}(\Omega)]^2} = 0$$

and

$$||\mathbf{B}\Phi||_{\mathbf{V}_\eta^{k-1/2}(\Gamma)} = \lim_{n'\to\infty} ||\mathbf{B}\mathbf{v}_{n'}||_{\mathbf{V}_\eta^{k-1/2}(\Gamma)} = 0$$

because of (3.10). If the kernel of the operator of the diffraction problem is trivial, then $\Phi_j^\pm = 0$. This is a contradiction and finishes the proof. □

3.2 Existence and uniqueness

3.2.1 The variational formulation

Before we prove existence and uniqueness of the solution, we recall some results on unique solvability in usual Sobolev spaces which have been obtained by Elschner et. al. [14]. In order to prove unique solvability, we need the following version of Green's formula. In the current subsection, we will need Green's formula for functions in $H^1(\Omega)$, for which it is well known.

Lemma 3.3. *Let Ω be a domain with piecewise C^m boundary, $m \geq 1$, and assume that $u \in V_\eta^2(\Omega)$ and $v \in C_0^\infty(\Omega\backslash\mathcal{S})$. Then*

$$\int_\Omega \triangle u\overline{v}dx = -\int_\Omega \nabla u\overline{\nabla v}dx + \int_{\partial\Omega} \partial_\nu u\overline{v}ds, \quad \int_\Omega \nabla u\overline{\nabla^\perp v}dx = -\int_{\partial\Omega} \partial_\tau u\overline{v}ds, \tag{3.11}$$

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

Let $u_1, u_2 \in H^1(\Omega)$ solve the conical diffraction problem (2.9), (2.10), (2.12), (2.14) with

$f_j = 0$ for all j. Applying Green's formula on the Helmholtz equations yields

$$\sum_{\sigma\in\{+,-\}} \left(\int\limits_{\Omega^\sigma} \left(\frac{\omega\varepsilon_\sigma}{\kappa_\sigma^2} \nabla u_1 \overline{\nabla\phi} - \omega\varepsilon_\sigma u_1 \overline{\phi} \right) dx - \int\limits_{\partial\Omega^\sigma} \frac{\omega\varepsilon_\sigma}{\kappa_\sigma^2} \overline{\phi} \partial_\nu u_1 ds \right) = 0,$$

$$\sum_{\sigma\in\{+,-\}} \left(\int\limits_{\Omega^\sigma} \left(\frac{\omega\mu}{\kappa_\sigma^2} \nabla u_2 \overline{\nabla\psi} - \omega\mu u_2 \overline{\psi} \right) dx - \int\limits_{\partial\Omega^\sigma} \frac{\omega\mu}{\kappa_\sigma^2} \overline{\psi} \partial_\nu u_2 ds \right) = 0$$

Let u_1 temporarily denote the total field instead of the scattered field only. Then the second equation from Lemma 3.3, (3.11) gives

$$\sum_{\sigma\in\{+,-\}} \left(\int\limits_{\Omega^\sigma} \left(\frac{\omega\varepsilon_\sigma}{\kappa_\sigma^2} \nabla u_1 \overline{\nabla\phi} - \frac{\gamma}{\kappa_\sigma^2} \nabla u_2 \overline{\nabla^\perp\phi} \;-\; \omega\varepsilon_\sigma u_1 \overline{\phi} \right) dx \right.$$
$$\left. - \int\limits_{\partial\Omega^\sigma} \left(\frac{\omega\varepsilon_\sigma}{\kappa_\sigma^2} \partial_\nu u_1 + \frac{\gamma}{\kappa_\sigma^2} \partial_\tau u_2 \right) \overline{\phi} ds \right) = 0,$$

$$\sum_{\sigma\in\{+,-\}} \left(\int\limits_{\Omega^\sigma} \left(\frac{\omega\mu}{\kappa_\sigma^2} \nabla u_2 \overline{\nabla\psi} + \frac{\gamma}{\kappa_\sigma^2} \nabla u_1 \overline{\nabla^\perp\psi} \;-\; \omega\mu u_2 \overline{\psi} \right) dx \right.$$
$$\left. - \int\limits_{\partial\Omega^\sigma} \left(\frac{\omega\mu}{\kappa_\sigma^2} \partial_\nu u_2 - \frac{\gamma}{\kappa_\sigma^2} \partial_\tau u_1 \right) \overline{\psi} ds \right) = 0.$$

Due to the transmission conditions (2.12) on the interface, the integrals over the interface vanish. On the artificial boundaries $\Gamma^\pm$, defined by

$$\Gamma^\pm = \{(x_1, \pm b) : 0 \le x_1 < 2\pi\}$$

as before, we can write for functions u_1, u_2 satisfying the radiation condition (2.14)

$$\begin{pmatrix} (\frac{\omega\varepsilon_+}{\kappa_+^2} \partial_\nu u_1^+ + \frac{\gamma}{\kappa_+^2} \partial_\tau u_2^+) \\ (\frac{\omega\mu}{\kappa_+^2} \partial_\nu u_2^+ - \frac{\gamma}{\kappa_+^2} \partial_\tau u_1^+) \end{pmatrix} (x_1, b) = - \sum_{n=-\infty}^{\infty} M_n^+ \begin{pmatrix} A_{1,n}^+ \\ A_{2,n}^+ \end{pmatrix} e^{i(n+\alpha)x_1 + i\beta_n^+ b}$$
$$- \frac{1}{\kappa_+^2} \begin{pmatrix} i\omega\epsilon_+ \beta_0^+ p_3 + i\gamma\alpha q_3 \\ i\omega\mu\beta_0^- q_3 - i\gamma\alpha p_3 \end{pmatrix} e^{i\alpha x_1 - i\beta_0^+ b}$$

and

$$\begin{pmatrix} (\frac{\omega\varepsilon_-}{\kappa_-^2} \partial_\nu u_1^- + \frac{\gamma}{\kappa_-^2} \partial_\tau u_2^-) \\ (\frac{\omega\mu}{\kappa_-^2} \partial_\nu u_2^- - \frac{\gamma}{\kappa_-^2} \partial_\tau u_1^-) \end{pmatrix} (x_1, -b) = - \sum_{n=-\infty}^{\infty} M_n^- \begin{pmatrix} A_{1,n}^- \\ A_{2,n}^- \end{pmatrix} e^{i(n+\alpha)x_1 - i\beta_n^- b}$$

with

$$M_n^{\pm} = \frac{1}{\kappa_{\pm}^2} \begin{pmatrix} -i\omega\varepsilon_{\pm}\beta_n^{\pm} & \pm i\gamma(n+\alpha) \\ \mp i\gamma(n+\alpha) & -i\omega\mu\beta_n^{\pm} \end{pmatrix} \tag{3.12}$$

and $\beta_n^{\pm} = \sqrt{\kappa_{\pm}^2 - (n+\alpha)^2}$. Now we define the operators

$$(T^{\pm}w)(x) := \sum_{n=-\infty}^{\infty} M_n^{\pm} e^{i(n+\alpha)x} \frac{1}{2\pi} \int_0^{2\pi} w(x) e^{-i(n+\alpha)x} dx, \tag{3.13}$$

which act on α-quasiperiodic vector functions $w : \mathbb{R} \to \mathbb{R}^2$. More precisely, they map

$$T^{\pm} : [H^{1/2}(\Gamma^{\pm})]^2 \to [H^{-1/2}(\Gamma^{\pm})]^2.$$

Using these operators, we can write

$$\begin{aligned} T^{+}\begin{pmatrix} u_1^+ \\ u_2^+ \end{pmatrix} &= \sum_{n=-\infty}^{\infty} M_n^{+} \begin{pmatrix} A_{1,n}^+ \\ A_{2,n}^+ \end{pmatrix} e^{i(n+\alpha)x_1 + i\beta_n^+ b} - \frac{1}{\kappa_+^2} \begin{pmatrix} i\omega\epsilon_+\beta_0^+ p_3 + i\gamma\alpha q_3 \\ i\omega\mu\beta_0^- q_3 - i\gamma\alpha p_3 \end{pmatrix} e^{i\alpha x_1 - i\beta_0^+ b}, \\ T^{-}\begin{pmatrix} u_1^- \\ u_2^- \end{pmatrix} &= \sum_{n=-\infty}^{\infty} M_n^{-} \begin{pmatrix} A_{1,n}^- \\ A_{2,n}^- \end{pmatrix} e^{i(n+\alpha)x_1 - i\beta_n^- b}. \end{aligned} \tag{3.14}$$

The variational formulation of the conical diffraction problem then reads as follows. Find α-quasiperiodic $u_1, u_2 \in H^1(\Omega^+) \times H^1(\Omega^-)$ such that

$$\begin{aligned} J(u_1, u_2; \phi, \psi) &= \int_{\Omega^\sigma} \left(\frac{\omega\varepsilon_\sigma}{\kappa_\sigma^2} \nabla u_1 \overline{\nabla\phi} - \frac{\gamma}{\kappa_\sigma^2} \nabla u_2 \overline{\nabla^{\perp}\phi} - \omega\varepsilon_\sigma u_1 \overline{\phi} + \frac{\omega\mu}{\kappa_\sigma^2} \nabla u_2 \overline{\nabla\psi} \right. \\ &\quad \left. + \frac{\gamma}{\kappa_\sigma^2} \nabla u_1 \overline{\nabla^{\perp}\psi} - \omega\mu u_2 \overline{\psi} \right) dx + \int_{\Gamma^+} T^{+} \begin{pmatrix} u_1^+ \\ u_2^+ \end{pmatrix} \cdot \begin{pmatrix} \overline{\phi} \\ \overline{\psi} \end{pmatrix} ds \\ &\quad + \int_{\Gamma^-} T^{-} \begin{pmatrix} u_1^+ \\ u_2^+ \end{pmatrix} \cdot \begin{pmatrix} \overline{\phi} \\ \overline{\psi} \end{pmatrix} ds \\ &= -\frac{2ie^{-i\beta_0^+ b}}{\kappa_+^2} \int_{\Gamma^+} \left((\omega\epsilon_+\beta_0^+ - \gamma\alpha) p_3 \overline{\phi^+} + (\omega\mu\beta_0^- + \gamma\alpha) q_3 \overline{\psi^+} \right) e^{i\alpha x_1} ds \end{aligned} \tag{3.15}$$

for all α-quasiperiodic $\phi, \psi \in H^1(\Omega^+) \times H^1(\Omega^-)$. The following result from [14] will be used later on in order to prove unique solvability in Kondratiev spaces.

Lemma 3.4. *(i) Suppose that* $\operatorname{Im} k > 0$ *in a subdomain of* Ω *where* ε *is constant. Then the conical diffraction problem (2.9), (2.10), (2.12), (2.14), or equivalently the variational problem (3.15), has for all* $\omega > 0$ *at most one* α*-quasiperiodic solution in* $[H^1(\Omega^+) \times H^1(\Omega^-)]^2$.

(ii) Assume that $k^2 > \gamma^2$ *everywhere in* Ω *and* $(k^-)^2 > \alpha^2 + \gamma^2$*. Then the variational problem (3.15) has a unique* α*-quasiperiodic solution in* $[H^1(\Omega^+) \times H^1(\Omega^-)]^2$ *for all but a countable set of frequencies* ω_j *with* $\omega_j \to \infty$.

Proof. See sections 3.1. and 3.2. in [14], where a detailed proof of this result is given. □

We will give some additional remarks on the operators T^+ and T^- on the artificial boundaries $\Gamma^\pm$.

Definition 3.2. Let $\mathbb{T}^n := \mathbb{R}^n/2\pi\mathbb{Z}^n$ be the n-torus. Let $D(\mathbb{T}^n)$ be the space $C_0^\infty(\mathbb{T}^n)$ equipped with its usual locally convex topology. Consider the operator $A : D(\mathbb{T}^n) \to D(\mathbb{T}^n)$ defined by

$$Au(x) := \sum_{m\in\mathbb{Z}^n} a(x,m)\hat{u}(m)e^{imx},$$

with $\hat{u}(m)$ denoting the Fourier coefficients of u, and a satisfying

$$|D_x^\alpha a(x,m)| \leq C_\alpha(1+|m|)^{r-|\alpha|}, \qquad x \in \mathbb{T}^n, \quad m \in \mathbb{Z}^n$$

for some real constants C_α and r. Such functions a are said to belong to the *Hörmander class* $S_{1,0}^r(\mathbb{T}^n \times \mathbb{Z}^n)$. The operator A is called a *periodic pseudodifferential operator* of order r with *periodic symbol* a. We denote the set of such operators by $OPS^m(\mathbb{T}^n)$.

If $\Omega \subset \mathbb{R}^2$ is a bounded domain, then we can identify functions on the boundary $\partial\Omega$ with 2π-periodic functions on $\mathbb{R}$ via a 2π-periodic parametrization of $\partial\Omega$. Now consider the Dirichlet problem

$$\begin{aligned} \triangle u = 0 \qquad & \text{in} \quad \Omega \\ u = g \qquad & \text{on} \quad \partial\Omega, \end{aligned} \tag{3.16}$$

with a function $g \in H^{1/2}(\partial\Omega)$. The operator

$$\Lambda : H^{\frac{1}{2}}(\partial\Omega) \to H^{-\frac{1}{2}}(\partial\Omega) : g \mapsto \partial_\nu u$$

that assigns to a given Dirichlet data the Neumann data of the solution to the Dirichlet problem with homogeneous Laplace equation is called the *Dirichlet-to-Neumann map*. It can be seen (see eg. [18]) that the Dirichlet-to-Neumann map is a periodic pseudodifferential operator of order 1. Its principal part is

$$\Lambda_0 u(x) = \hat{u}(0) + \sum_{0\neq m\in\mathbb{Z}} |m|\hat{u}(m)e^{imx}.$$

The principal symbol of this operator is therefore

$$a_{\Lambda,0}(x,m) = |m|.$$

The condition (2.14), namely that the solution of the conical diffraction problem can be represented as a Rayleigh series in a strip around $\Gamma^\pm$, is equivalent to the nonlocal boundary conditions

$$\begin{pmatrix} (\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu u_1^+ + \frac{\gamma}{\kappa_+^2}\partial_\tau u_2^+) \\ (\frac{\omega\mu}{\kappa_+^2}\partial_\nu u_2^+ - \frac{\gamma}{\kappa_+^2}\partial_\tau u_1^+) \end{pmatrix}(x_1, b) = -\, T^+ \begin{pmatrix} u_1^+ \\ u_2^+ \end{pmatrix}(x_1, b) - \frac{1}{\kappa_+^2}\begin{pmatrix} i\omega\epsilon_+\beta_0^+ p_3 + i\gamma\alpha q_3 \\ i\omega\mu\beta_0^- q_3 - i\gamma\alpha p_3 \end{pmatrix} e^{i\alpha x_1 - i\beta_0^+ b} \tag{3.17}$$

and

$$\begin{pmatrix} (\frac{\omega\varepsilon_-}{\kappa_-^2}\partial_\nu u_1^- + \frac{\gamma}{\kappa_-^2}\partial_\tau u_2^-) \\ (\frac{\omega\mu}{\kappa_-^2}\partial_\nu u_2^- - \frac{\gamma}{\kappa_-^2}\partial_\tau u_1^-) \end{pmatrix}(x_1, -b) = -T^- \begin{pmatrix} u_1^- \\ u_2^- \end{pmatrix}(x_1, b), \tag{3.18}$$

with $T^\pm$ as defined by (3.13) and u_1^+, u_2^+ being the scattered wave above the interface. By the representation (3.13) it can be seen that $T^\pm$ can be viewed as "α-quasiperiodic" pseudodifferential operators of order 1 with symbol

$$a^\pm(x, m) = M_m^\pm.$$

Pseudodifferential operators on open subsets of $\mathbb{R}^n$ are defined analogous to Definition 3.2 as follows.

Definition 3.3. Let Ω be an open subset of $\mathbb{R}^n$. Let $E(\Omega)$ denote the space $C^\infty(\Omega)$ equipped with its usual locally convex topology. Consider the operator $A : D(\Omega) \to E(\Omega)$ defined by

$$Au(x) := \int_{\mathbb{R}^n} a(x, \xi)\hat{u}(\xi)e^{ix\xi}d\xi, \qquad x \in \Omega$$

with $\hat{u}$ denoting the Fourier transform of u, and a satisfying

$$|D_x^\alpha a(x, \xi)| \le C_\alpha(1 + |\xi|)^{r-|\alpha|}, \qquad x \in \Omega, \quad \xi \in \mathbb{R}^n$$

for some real constants C_α and r. We write $a \in S_{1,0}^r(\Omega \times \mathbb{R}^n)$. The operator A is called a *pseudodifferential operator* of order r with *symbol* a. The set of these operators is denoted by $OPS^m(\Omega)$.

3.2.2 The Fredholm property

In the following sections, we will prove an existence and uniqueness result for the solution of the conical diffraction problem. The following two Lemmas establish the Fredholm property of the problem, which is then used together with a result from [14]. The first Lemma is due to Peetre [34]. A proof can also be found in [33].

Lemma 3.5. *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) $\quad \dim\ker A < \infty$ *and* $\operatorname{ran} A$ *is closed in* $\mathcal{Y}$.

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

This Lemma, together with Proposition 3.1, 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 3.4. 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 3.6. *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. [47]. The construction of the regularizer will be carried out in four steps, combining the techniques of Wloka et al. [47], Chapter 9.3, and Kondratiev [25], as follows.

(i) First we construct regularizers for operators with constant coefficients in the plane.

(ii) Then we construct regularizers in the half space $\mathbb{R}^2_+$ for operators with 'frozen' coefficients at $x_0 \in \mathbb{R}$.

(iii) 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.

(iv) Finally we obtain a global regularizer by means of a partition of unity.

The notion 'frozen coefficients' above refers to the so-called *Freezing Lemma*, which is Lemma 7.41 from [47].

Lemma 3.7 (Freezing Lemma)**.** *Let $A \in OPS^m(\mathbb{R}^n)$. Then for every $x_0 \in \mathbb{R}^n$ and $\epsilon > 0$ we can find a neighbourhood $U(x_0)$ of x_0 and pseudodifferential operators K and T such that for $\varphi \in C_0^\infty(U(x_0))$ we have the decomposition*

$$\varphi A = \varphi\{A(x_0) + K + T\}.$$

In this sum, $A(x_0)$ is the operator A with coefficients fixed ('frozen') at x_0. Furthermore, $K \in OPS^m(\mathbb{R}^n)$ has a small norm, i.e.

$$||Ku||_{H^{l-m}(\mathbb{R}^n)} \leq \epsilon ||u||_{H^l(\mathbb{R}^n)}$$

for all $u \in H^l(\mathbb{R}^n)$ and

$$T \in \bigcap_{r \in \mathbb{R}} OPS^r(\mathbb{R}^n) =: OPS^{-\infty}(\mathbb{R}^n).$$

In order to perform step (ii) above, we 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

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

because $[\text{span}\{\nu(x)\}]^\perp$ 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 3.5. 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 3.8. *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 and that the homogeneous initial value problem*

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

has only the trivial solution for all $x \in \partial\Omega$. Then the problem

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

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

Proof. Combine Definition 9.28 and Theorem 9.29 from [47]. □

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 3.6. A pair of operators $(\mathbf{L}, \mathbf{B})$ which satisfies the assumptions of Lemma 3.8 is said to fulfill the *Shapiro-Lopatinskii condition*.

Definition 3.7. Let $(\mathbf{L}, \mathbf{B})$ be a pair of operators satisfying the Shapiro-Lopatinskii condition and fix a point $x \in \partial\Omega$. Let ϕ_j be the solution of the initial value problem

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

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 $(\mathbf{L}, \mathbf{B})$.

Lemma 3.9. *The problem (2.9), (2.10), (2.12), (2.14) satisfies the Shapiro-Lopatinskii condition if* $\varepsilon_+ \neq -\varepsilon_-$ *and* $k_\pm^2 \neq -\gamma^2$.

Proof. The system of ordinary differential equations in the sense of Definition 3.7 is

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

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 $\lim_{t\to\infty} w_{1/2}^\pm(t) = 0$, this leads to

$$w_{1/2}^\pm(t) = c_{1/2}^\pm e^{\sigma_1 t}$$

with $\sigma_1 < 0$. One of the transmission conditions in the system (2.12) 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

$$\frac{\omega\varepsilon_+}{\kappa_+^2}\frac{1}{i}\frac{d}{dt}w_1^+(t)|_{t=0} + \frac{\omega\varepsilon_-}{\kappa_-^2}\frac{1}{i}\frac{d}{dt}w_1^-(t)|_{t=0} + \frac{\gamma}{\kappa_+^2}\sigma_1 w_2^+(0) - \frac{\gamma}{\kappa_-^2}\sigma_1 w_2^-(0) = 0.$$

This is equivalent to

$$\frac{1}{i}\left(\frac{\omega\varepsilon_+}{\kappa_+^2}+\frac{\omega\varepsilon_-}{\kappa_-^2}\right)c_1\sigma_1+\left(\frac{\gamma}{\kappa_+^2}-\frac{\gamma}{\kappa_-^2}\right)c_2\sigma_1=0. \tag{3.19}$$

In the same way we get

$$-\frac{1}{i}\left(\frac{\omega\mu}{\kappa_-^2}+\frac{\omega\mu}{\kappa_+^2}\right)c_2\sigma_1+\left(\frac{\gamma}{\kappa_+^2}-\frac{\gamma}{\kappa_-^2}\right)c_1\sigma_1=0. \tag{3.20}$$

Straightforward computations show that the system (3.19)+(3.20) does not have a non-trivial solution (c_1, c_2) unless

$$\varepsilon_+ = -\varepsilon_-.$$

Now we turn to the boundary conditions on the artificial boundaries Γ^+ and Γ^-. As we have seen, the condition (2.14) is equivalent to the nonlocal boundary conditions

$$\begin{pmatrix}(\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu u_1^+ + \frac{\gamma}{\kappa_+^2}\partial_\tau u_2^+)\\(\frac{\omega\mu}{\kappa_+^2}\partial_\nu u_2^+ - \frac{\gamma}{\kappa_+^2}\partial_\tau u_1^+)\end{pmatrix}(x_1,b) = -\,T^+\begin{pmatrix}u_1^+\\u_2^+\end{pmatrix}(x_1,b)-\frac{1}{\kappa_+^2}\begin{pmatrix}i\omega\epsilon_+\beta_0^+p_3+i\gamma\alpha q_3\\ i\omega\mu\beta_0^-q_3-i\gamma\alpha p_3\end{pmatrix}e^{i\alpha x_1-i\beta_0^+b} \tag{3.21}$$

and

$$\begin{pmatrix}(\frac{\omega\varepsilon_-}{\kappa_-^2}\partial_\nu u_1^- + \frac{\gamma}{\kappa_-^2}\partial_\tau u_2^-)\\(\frac{\omega\mu}{\kappa_-^2}\partial_\nu u_2^- - \frac{\gamma}{\kappa_-^2}\partial_\tau u_1^-)\end{pmatrix}(x_1,-b) = -T^-\begin{pmatrix}u_1^-\\u_2^-\end{pmatrix}(x_1,-b), \tag{3.22}$$

The principal symbol of $T^\pm$ is

$$a_0^\pm(x,\xi) := \frac{1}{\kappa_\pm^2}\begin{pmatrix}\omega\varepsilon_\pm|\xi| & \pm i\gamma\xi\\ \mp i\gamma\xi & \omega\mu|\xi|\end{pmatrix}.$$

From the boundary condition (3.21) we get the homogeneous initial value condition

$$\begin{pmatrix}\frac{\omega\varepsilon_+}{\kappa_+^2}\frac{1}{i}\frac{d}{dt}w_1^+(t)|_{t=0}+\frac{\gamma}{\kappa_+^2}\sigma_1 w_2^+(0)\\ \frac{\omega\mu}{\kappa_+^2}\frac{1}{i}\frac{d}{dt}w_2^+(t)|_{t=0}-\frac{\gamma}{\kappa_+^2}\sigma_1 w_1^+(0)\end{pmatrix} = -\frac{1}{\kappa_+^2}\begin{pmatrix}\omega\varepsilon_+|\sigma_1| & i\gamma\sigma_1\\ -i\gamma\sigma_1 & \omega\mu|\sigma_1|\end{pmatrix}\begin{pmatrix}w_1^+(0)\\w_2^+(0)\end{pmatrix}.$$

This system has a non-trivial solution (c_1, c_2) if

$$\det\begin{pmatrix}\omega\varepsilon_+(i+1) & \gamma(i+1)\\ -\gamma(i+1) & \omega\mu(i+1)\end{pmatrix}=0,$$

which is equivalent to

$$\omega^2\varepsilon_\pm\mu+\gamma^2=0.$$

The same restriction follows from the boundary condition (3.22). □

Note that the Helmholtz equation and the transmission condition on the interface have constant coefficients, so the corresponding operators frozen at a point coincide with the operators themselves. The only point where we need Lemma 3.7 is where we have to deal with the nonlocal boundary conditions on the artificial boundaries.

We will now construct a right regularizer following the four steps explained above.

(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 [47] 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

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

where T 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.

We have shown in Lemma 3.9 that the system $(\mathbf{L}, \mathbf{B})$, with $\mathbf{B}$ being either the transmission operator on Γ or the boundary operator on $\Gamma^\pm$ with frozen coefficients at $x_0^\pm$, is Shapiro-Lopatinskii elliptic, and therefore the canonical matrix function exists in either case. For the operator on the interface we write $\mathbf{B}_\Gamma$ in the following, the boundary operators on $\Gamma^\pm$ will be denoted by $\mathbf{B}^\pm$.

First we consider the operator $(\mathbf{L}, \mathbf{B}_\Gamma)$. 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

$$\mathbf{L}_0(D_{x_1}, D_{x_2}) := \begin{pmatrix} L_0(D_{x_1}, D_{x_2}) & 0 & 0 & 0 \\ 0 & L_0(D_{x_1}, D_{x_2}) & 0 & 0 \\ 0 & 0 & L_0(D_{x_1}, D_{x_2}) & 0 \\ 0 & 0 & 0 & L_0(D_{x_1}, D_{x_2}) \end{pmatrix} \tag{3.23}$$

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

$$\mathbf{R}_1 b := \mathcal{F}_+^{-1}\Phi(\sigma', x_2)|\sigma'|^2(1+|\sigma'|^2)^{-1}\mathcal{F}_+ b, \tag{3.24}$$

where $\mathcal{F}_+$ is the partial Fourier transform and $\Phi(\sigma', x_2)$ is the canonical matrix function corresponding to the boundary value problem (cf. Definition 3.7). It is shown in [47] that this operator is also continuous from $[H^{k+2}(\mathbb{R}^2_+)]^4$ into $\bigotimes_{j=1}^4 H^{k+m_j+1/2}(\mathbb{R})$. Now we define

$$\mathbf{R}(f,b) := \mathbf{R}_0 f + \mathbf{R}_1\left(b - \mathbf{B}_\Gamma \mathbf{R}_0 f\right). \tag{3.25}$$

We show that this 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 $\mathbf{A} := (\mathbf{L}, \mathbf{B}_\Gamma)$. Denote

$$\mathbf{H}^{k+1/2}(\mathbb{R}) := \bigotimes_{j=1}^{4} H^{k+m_j+1/2}(\mathbb{R}).$$

From the boundedness of $\mathbf{B}_\Gamma, \mathbf{R}_0$ and $\mathbf{R}_1$ it follows that

$$\begin{aligned}
||\mathbf{R}_1[b - \mathbf{B}_\Gamma \mathbf{R}_0 f]||_{[H^{k+2}(\mathbb{R}^2_+)]^4} &\le C_1||b||_{\mathbf{H}^{k+1/2}(\mathbb{R})} + C_1||\mathbf{B}_\Gamma \mathbf{R}_0 f||_{\mathbf{H}^{k+1/2}(\mathbb{R})} \\
&\le C_1||b||_{\mathbf{H}^{k+1/2}(\mathbb{R})} + C_2||\mathbf{R}_0 f||_{[H^{k+2}(\mathbb{R}^2_+)]^4} \\
&\le C_1||b||_{\mathbf{H}^{k+1/2}(\mathbb{R})} + C_3||f||_{[H^{k}(\mathbb{R}^2_+)]^4},
\end{aligned}$$

so the operator $\mathbf{R}$ is bounded. Moreover, by the definitions of $\mathbf{R}_1$ and $\mathbf{R}_0$, we have

$$\mathbf{L}\mathbf{R}_0 f = f + \mathbf{V}_0 f,$$

with

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

and

$$\mathbf{B}_\Gamma \mathbf{R}_1 b = b + \mathbf{V}_1 b, \tag{3.26}$$

with

$$\mathbf{V}_1 b := -\mathcal{F}_+^{-1}(1+|\sigma'|^2)^{-1}\mathcal{F}_+ b.$$

Now we have the mapping properties

$$||\mathbf{V}_0 f||_{[H^{k+1}(\mathbb{R}^2_+)]^4} \le ||f||_{[H^{k}(\mathbb{R}^2_+)]^4}$$

and

$$||\mathbf{V}_1[b - \mathbf{B}_\Gamma \mathbf{R}_0 f]||_{\mathbf{H}^{k+3/2}(\mathbb{R})} \le C||b - \mathbf{B}_\Gamma \mathbf{R}_0 f||_{\mathbf{H}^{k+1/2}(\mathbb{R})} \le C_2(||b||_{\mathbf{H}^{k+1/2}(\mathbb{R})} + ||f||_{[H^k(\mathbb{R}_+)]^4}).$$

The operator

$$\mathbf{T}(f,b) := (\mathbf{V}_0 f, \mathbf{V}_1 b - \mathbf{V}_1 \mathbf{B}_\Gamma \mathbf{R}_0 f)$$

is therefore an operator of order -1.

Let now $\mathbf{B}^\pm$ denote the boundary operators on $\Gamma^\pm$. We fix an $x_0^+ \in \Gamma^+$ and an $x_0^- \in \Gamma^-$. The operator $\mathbf{B}^\pm$ can locally be expressed as an operator $\mathbf{B}_l^\pm \in [OPS^1(\mathbb{R})]^2$ modulo an operator $\mathbf{K}^{\pm} \in [OPS^{-1}(\mathbb{R})]^2$, i.e.

$$\mathbf{B}^{\pm} = \mathbf{B}_l^{\pm} + \mathbf{K}^{\pm}$$

in a neighbourhood $U(x_0)$, cf. [2, 18, 23, 30]. The regularizer for $\mathbf{B}_l^{\pm}$ is then constructed in the same manner as above.

(iii) Similarly, we establish local regularizing properties in the interior of $\Omega^{\pm}$ and on the interface outside the conical points. 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

$$\chi \mathbf{A} \circ \mathbf{R} \zeta = \chi \mathbf{I} \zeta + \chi \mathbf{T} \zeta, \tag{3.27}$$

where $\mathbf{T}$ is a continuous operator of order -1 and therefore, $\chi \mathbf{T} \zeta$ 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 it lies on one of the artificial boundaries $\Gamma^{\pm}$. In the latter case, we freeze the coefficients of the boundary operator at x_0, see below. We move on and suppose that x_0 lies either in the interior of $\Omega^{\pm}$ or on the interface and 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 with degree ≥ 1 on domains with Lipschitz boundaries (cf. [28]). 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

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

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.

If $\mathbf{B}_\Gamma$ is the operator (2.13), then the regularizer constructed in step (ii) for the half space is by the above procedure of passing to local coordinates also a local regularizer for the operator $\mathbf{A} = (\mathbf{L}, \mathbf{B}_\Gamma)$. On the artificial boundaries $\Gamma^{\pm}$, the situation is slightly more complicated. Let $\mathbf{L}^{\pm}$ be the pair of Helmholtz operators in $\Omega^{\pm}$ and denote the boundary operators on $\Gamma^{\pm}$ by $\mathbf{B}^{\pm}$. Then define $\mathbf{A} = (\mathbf{L}^{\pm}, \mathbf{B}^{\pm})$. The operator $\mathbf{B}^{\pm}$ can locally be expressed as an operator $\mathbf{B}_l^{\pm} \in [OPS^1(\mathbb{R})]^2$ modulo an operator $\mathbf{K}^{\pm} \in [OPS^{-1}(\mathbb{R})]^2$. In particular, if φ and ψ are cut-off functions such that $\varphi\psi = \varphi$, then

$$\begin{aligned}\varphi\mathbf{B}^{\pm} &= \varphi\mathbf{B}^{\pm}\psi + \varphi\mathbf{B}^{\pm}(1-\psi)\\ &= \varphi(\mathbf{B}_l^{\pm} + \mathbf{K}^{\pm})\psi + \varphi\mathbf{B}^{\pm}(1-\psi)\\ &= \varphi(\mathbf{B}_l^{\pm} + \mathbf{K}^{\pm}) - \varphi(\mathbf{B}_l^{\pm} + \mathbf{K}^{\pm} + \mathbf{B}^{\pm})(1-\psi)\\ &=: \varphi\mathbf{B}_l^{\pm} + \tilde{\mathbf{K}}^{\pm},\end{aligned}$$

with the last term on the right-hand being an element of $[OPS^{-1}]^2$ by quasi-locality, since the supports of φ and $(1-\psi)$ are disjoint. Let $\mathbf{B}_l^{\pm}(x_0)$ be the operator $\mathbf{B}_l^{\pm}$ frozen at $x_0 \in \Gamma^{\pm}$. By step (ii) we know that the operator $(\mathbf{L}^{\pm}, \mathbf{B}_l^{\pm}(x_0))$ has a right regularizer

$$\mathbf{R}(x_0) : [H^k(\mathbb{R}^2_+)]^2 \times [H^{k+1/2}(\mathbb{R})]^2 \to [H^{k+2}(\mathbb{R}^2_+)]^2.$$

By the Freezing Lemma 3.7, there exists a neighbourhood $U(x_0)$ such that for all $\chi \in C_0^{\infty}(U(x_0))$ the operator $\mathbf{A}$ can be written as

$$\chi\mathbf{A} = \chi(\mathbf{L}^{\pm}, \mathbf{B}_l^{\pm} + \tilde{\mathbf{K}}^{\pm}) = \chi\{\mathbf{L}^{\pm}, \mathbf{B}_l^{\pm}(x_0) + \mathbf{K}_{x_0} + \mathbf{T}_{x_0} + \tilde{\mathbf{K}}^{\pm}\},$$

with $\mathbf{K}_{x_0}$ having a small norm and being of the same order as $\mathbf{A}$, and $\mathbf{T}_{x_0} \in [OPS^{-\infty}]^2$. In fact, the Freezing Lemma states that by choosing χ such that its support is sufficiently small, the norm of $\mathbf{K}_{x_0}$ can be assumed to be arbitrarily small. Now we define

$$\mathbf{R}_r(x_0) := \mathbf{R}(x_0) \circ (\mathbf{I} + (0, \mathbf{K}_{x_0}) \circ \mathbf{R}(x_0))^{-1}.$$

If $\zeta \in C_0^{\infty}(U(x_0))$, then

$$\begin{aligned}\chi\mathbf{A}\mathbf{R}_r(x_0)\zeta &\equiv \chi\{\mathbf{A}(x_0) + (0, \mathbf{K}_{x_0})\}\mathbf{R}_r(x_0)\zeta\\ &\equiv \chi\{\mathbf{A}(x_0)\mathbf{R}(x_0) + (0, \mathbf{K}_{x_0})\mathbf{R}(x_0)\}(\mathbf{I} + (0, \mathbf{K}_{x_0}) \circ \mathbf{R}(x_0))^{-1}\zeta\\ &\equiv \chi\{\mathbf{I} + (0, \mathbf{K}_{x_0})\mathbf{R}(x_0)\}(\mathbf{I} + (0, \mathbf{K}_{x_0})\mathbf{R}(x_0))^{-1}\zeta\\ &= \chi\mathbf{I}\zeta,\end{aligned}$$

where $\equiv$ denotes equality modulo compact operators and $\mathbf{A}(x_0) = (\mathbf{L}^{\pm}, \mathbf{B}_l^{\pm})$. Hence $\mathbf{R}_r(x_0)$ is a local regularizer in $U(x_0)$.

(iv) 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 3.1 concerning the eigenvalues is satisfied. From Theorem 3.6.1 in [26] 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

$$\mathbf{L}_0 u_0 = \chi_S f, \qquad \mathbf{B}u_0 = \chi_S b \tag{3.28}$$

in the ramified cone C_S, with $f = (f_1^+, f_2^+, f_1^-, f_2^-)^\top$ from (2.10), $b = (b_1, \ldots, b_4)^\top$ from (2.12) and $\mathbf{B}$ from (2.13).

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, $j = 1, \ldots, n$ so that any ζ_j is equal to 1 on the support of χ_j. The partition 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

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

and

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

and set

$$\mathbf{R}(f, b) := u^*,$$

where $u_{0,j}$ satisfies the transmission problem (3.28) 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

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

in this neighbourhood for any function v. We obtain

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

where $\mathbf{T}_i$ are operators of order -1 because of the local regularizing property of $\mathbf{R}_i$, $\mathbf{D}_l$ 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 $f \mapsto u_i : [\mathcal{V}_\eta^k(\Omega)]^2 \to [\mathcal{H}^{k+2}(\Omega)]^2$ and $f \mapsto u_{j,0} : [\mathcal{V}_\eta^k(\Omega)]^2 \to [\mathcal{V}_\eta^{k+2}(\Omega)]^2$ are continuous by definition for any $k \in \mathbb{N}$, it follows that $\mathbf{K}_0 : [\mathcal{V}_\eta^k(\Omega)]^2 \to [\mathcal{V}_\eta^{k+1}(\Omega)]^2$ is continuous. Since $[\mathcal{V}_\eta^{k+1}(\Omega)]^2$ is compactly embedded into $[\mathcal{V}_\eta^k(\Omega)]^2$, the mapping is also compact from $[\mathcal{V}_\eta^k(\Omega)]^2$ into $[\mathcal{V}_\eta^k(\Omega)]^2$. The transmission conditions on the interface are treated analogously (cf. [25]). For the boundary conditions, we get

$$\begin{aligned}\mathbf{B}^{\pm}u^{*} &= \sum_{i=1}^{k}\mathbf{B}^{\pm}\zeta_i\mathbf{R_i}(\chi_i f,\chi_i b)\\ &= \sum_{i=1}^{k}\zeta_i\mathbf{B}^{\pm}\mathbf{R_i}(\chi_i f,\chi_i b) + \sum_{i=1}^{k}[\mathbf{B}^{\pm}\zeta_i - \zeta_i\mathbf{B}^{\pm}]\mathbf{R_i}(\chi_i f,\chi_i b) = b + \mathbf{T}b.\end{aligned}$$

with a compact operator $\mathbf{T}$.

The construction of the right regularizer is completed. The following Lemma is now a direct consequence of Lemma 3.5 and the existence of a right regularizer.

Lemma 3.10. *If $k+1-\eta \notin \mathcal{A}$ with $k \geq 0$, then the operator*

$$(\mathbf{L},\mathbf{B}) : [\mathcal{V}_\eta^{k+2}(\Omega)]^2 \to [\mathcal{V}_\eta^{k}(\Omega)]^2 \times \bigotimes_{j=1}^{4} V_\eta^{k+m_j+1/2}(\Gamma) \tag{3.29}$$

of problem (2.9), (2.10), (2.12), (2.14) has the Fredholm property if $\varepsilon_+ \neq -\varepsilon_-$ and $k_\pm^2 \neq -\gamma^2$.

3.2.3 Fredholm index and invertibility

Suppose that $k^2 > \gamma^2$ everywhere in Ω and $(k^-)^2 > \alpha^2+\gamma^2$. Then, due to Lemma 3.4, the operator $(\mathbf{L},\mathbf{B})$ of the diffraction problem (2.9), (2.10), (2.12), (2.14) is invertible for all but a countable set of frequencies accumulating at infinity as an operator mapping $[\mathcal{H}^1(\Omega)]^2$ into $[\mathcal{H}^{-1}(\Omega)]^2$. For the sake of brevity, let us write

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

and define $[\tilde{\mathcal{H}}^k(\Omega)]^2$ analogously. It is then easy to see that also

$$(\mathbf{L},\mathbf{B}) : [\mathcal{V}_\eta^{2}(\Omega)\cap\mathcal{H}^1(\Omega)]^2 \to [\tilde{\mathcal{V}}_\eta^{0}(\Omega)\cap\tilde{\mathcal{H}}^{-1}(\Omega)]^2$$

is invertible. Since $\mathcal{V}_\eta^2(\Omega)\cap\mathcal{H}^1(\Omega)$ is dense in $\mathcal{V}_\eta^2(\Omega)$, we know that the kernel of

$$(\mathbf{L},\mathbf{B}) : [\mathcal{V}_\eta^{2}(\Omega)]^2 \to [\tilde{\mathcal{V}}_\eta^{0}(\Omega)]^2$$

is trivial. To conclude that the operator is in fact invertible in these spaces, we show that its Fredholm index is zero.

As usual, $\Omega = \Omega^+ \cup \Omega^-$. Now we divide Ω into the two domains Ω_1^+ and Ω_1^- such that the interface Γ_1 between these domains is smooth. Let $T_t^{\pm}$ be a homotopy between $\Omega^{\pm}$ and $\Omega_1^{\pm}$ such that

$$T_t^{\pm}(0)(\Omega^{\pm}) = \Omega^{\pm}$$

and

$$T_t^{\pm}(1)(\Omega^{\pm}) = \Omega_1^{\pm}.$$

If $(\mathbf{L_t}, \mathbf{B_t})$ is the operator corresponding to the interface Γ_t and

$$(\mathbf{L_t}, \mathbf{B_t})(t) := \begin{cases} (\mathbf{L_t}, \mathbf{B_t}) \circ T_t^{+} & \text{in} \quad \Omega^{+} \\ (\mathbf{L_t}, \mathbf{B_t}) \circ T_t^{-} & \text{in} \quad \Omega^{-}, \end{cases}$$

then it is clear that $(\mathbf{L_t}, \mathbf{B_t})(t)$ has the same Fredholm index for all $t \in [0,1]$. We know by Lemma 3.4 that the index of

$$(\mathbf{L_1}, \mathbf{B_1})(1) : [\mathcal{H}^1(\Omega)]^2 \to [\tilde{\mathcal{H}}^{-1}(\Omega)]^2$$

is zero. Let χ_S be a cut-off function supported in the neighbourhood of a corner point S of Γ. As is was done previously in Chapter 3.1, we transform the interface problem for $\chi u \in [\mathcal{V}_\eta^2(\Omega)]^2$ with the operator $(\mathbf{L_1}, \mathbf{B_1})(1)$ in the cone to a parameter dependent system of ordinary differential equations

$$A_1(\lambda)\check{w}(\lambda) = \check{r}(\lambda)$$

with the operator $A_1(\lambda)$. The function $\check{w}(\lambda)$ is the Laplace transform of w, which is χu transformed to a ramified strip B_S. See Chapter 3.1. for a detailed explanation of the notation. We have seen in Chapter 3.1. that

$$\begin{aligned} \omega &= \int\limits_{\mathrm{Re}\lambda=-\beta_1} A_1^{-1}(\lambda)\check{r}(\lambda)d\lambda \\ &= \int\limits_{\mathrm{Re}\lambda=-\beta_2} A_1^{-1}(\lambda)\check{r}(\lambda)d\lambda + \sum_{\sigma=1}^{n} \mathrm{Res}\, e^{\lambda t} A_1^{-1}(\lambda)\check{r}(\lambda)|_{\lambda=\lambda_\sigma}, \end{aligned}$$

where $\{\lambda_\sigma\}_{\sigma=1}^n$ is the set of eigenvalues of $A_1(\lambda)$ satisfying

$$\{\mathrm{Re}\lambda_\sigma\}_{\sigma=1}^n \subset (-\beta_1, -\beta_2)$$

and

$$w \in [\mathcal{H}^2_{\beta_1}(\Omega)]^2.$$

The parameter β_2 can be chosen arbitrarily. Furthermore, since Γ_1 is smooth, we can see

$$\sum_{\sigma=1}^{n} \mathrm{Res}\, e^{\lambda t} A_1^{-1}(\lambda)\check{r}(\lambda)|_{\lambda=\lambda_\sigma} \in [\mathcal{H}^1(B_S)]^2.$$

Consequently,

$$\chi u \in [\mathcal{H}^1(\Omega)]^2$$

for a sufficient choice of β_2. Hence,

$$(\mathbf{L_1}, \mathbf{B_1})(1) : [\mathcal{V}^2_\eta(\Omega)]^2 \to [\tilde{\mathcal{V}}^0_\eta(\Omega)]^2$$

has Fredholm index zero. Since the index is constant if the parameter of the operator changes, we have shown the following Lemma.

Lemma 3.11. *Under the assumptions of Lemma 3.4 and Lemma 3.10, the Fredholm index of the operator*

$$(\mathbf{L}, \mathbf{B}) : [\mathcal{V}^2_\eta(\Omega)]^2 \to [\mathcal{V}^0_\eta(\Omega)]^2 \times \bigotimes_{j=1}^{4} V_\eta^{m_j+1/2}(\Gamma)$$

is zero for all but a countable set of frequencies ω_j with $\omega_j \to \infty$.

Since the operator has a trivial kernel, the following theorem follows immediately.

Theorem 3.1. *If the assumptions of Lemma 3.4 and Lemma 3.10 are true, then for all but a countable set of frequencies ω_j with $\omega_j \to \infty$ the operator*

$$(\mathbf{L}, \mathbf{B}) : [\mathcal{V}^2_\eta(\Omega)]^2 \to [\mathcal{V}^0_\eta(\Omega)]^2 \times \bigotimes_{j=1}^{4} V_\eta^{m_j+1/2}(\Gamma)$$

is invertible.

4 Material derivatives and shape derivatives

4.1 Existence and regularity of material and shape derivatives

4.1.1 Smooth perturbations of the identity

Proposition 3.2 enables us to prove the existence of shape derivatives in the same way as it is done in [9], which uses the theory of non-local perturbations of a domain, see [29]. For the moment, let Ω be just a usual bounded domain. The case of a periodic cell will be considered later. Consider a vector field $T \in [C^{k+2}(\Omega)]^2$. 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 4.1. Let Ω be a bounded domain and assume that u^ϵ is the solution of the abstract boundary value problem

$$\begin{aligned} Lu^\epsilon &= f_\epsilon \quad \text{on} \quad \Omega_\epsilon, \\ Bu^\epsilon &= g_\epsilon \quad \text{on} \quad \partial\Omega_\epsilon. \end{aligned}$$

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

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

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 4.2. 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

$$u'(T) := \dot{u}(T) - \nabla u^0 \cdot T. \tag{4.1}$$

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 4.1. As we have seen, the solution (u_1, u_2) of the conical diffraction problem (2.9), (2.10), (2.12), (2.14) is in general not in $[\mathcal{H}^2(\Omega)]^2$. In this case

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

If this is true, then the variational approach of Hettlich and Kirsch ([21],[24]) 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[9] 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 $T = 0$ near the artificial boundaries $\Gamma^\pm$. The perturbed interface will be denoted by Γ_ϵ. We investigate the transmission problem

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

with transmission conditions

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

on Γ_ϵ and the radiation condition (2.14) 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

$$\begin{aligned}
\triangle^\epsilon(u_1^{+,\epsilon} \circ T_\epsilon) + \kappa_+^2(u_1^{+,\epsilon} \circ T_\epsilon) &= 0 \circ T_\epsilon \quad \text{in} \quad \Omega^+,\\
\triangle^\epsilon(u_1^{-,\epsilon} \circ T_\epsilon) + \kappa_-^2(u_1^{-,\epsilon} \circ T_\epsilon) &= 0 \circ T_\epsilon \quad \text{in} \quad \Omega^-,\\
\triangle^\epsilon(u_2^{+,\epsilon} \circ T_\epsilon) + \kappa_+^2(u_2^{+,\epsilon} \circ T_\epsilon) &= 0 \circ T_\epsilon \quad \text{in} \quad \Omega^+,\\
\triangle^\epsilon(u_2^{-,\epsilon} \circ T_\epsilon) + \kappa_-^2(u_2^{-,\epsilon} \circ T_\epsilon) &= 0 \circ T_\epsilon \quad \text{in} \quad \Omega^-,
\end{aligned} \tag{4.2}$$

with transmission conditions

$$\begin{aligned}
\Big[\frac{\gamma}{\kappa^2}\nabla^\epsilon(u_2^\epsilon \circ T_\epsilon)\cdot(\tau_\epsilon \circ T_\epsilon) + \frac{\omega\varepsilon}{\kappa^2}\nabla^\epsilon(u_1^\epsilon \circ T_\epsilon)\cdot(\nu_\epsilon \circ T_\epsilon)\Big]_\Gamma &= -\frac{\omega\varepsilon_+}{\kappa_+^2}\nabla^\epsilon(u_1^{(i)} \circ T_\epsilon)\cdot(\nu_\epsilon \circ T_\epsilon)\\
&\quad - \frac{\gamma}{\kappa_+^2}\nabla^\epsilon(u_2^{(i)} \circ T_\epsilon)\cdot(\tau_\epsilon \circ T_\epsilon),\\
\Big[\frac{\gamma}{\kappa^2}\nabla^\epsilon(u_1^\epsilon \circ T_\epsilon)\cdot(\tau_\epsilon \circ T_\epsilon) - \frac{\omega\mu}{\kappa^2}\nabla^\epsilon(u_2^\epsilon \circ T_\epsilon)\cdot(\nu_\epsilon \circ T_\epsilon)\Big]_\Gamma &= \frac{\omega\mu}{\kappa_+^2}\nabla^\epsilon(u_2^{(i)} \circ T_\epsilon)\cdot(\nu_\epsilon \circ T_\epsilon)\\
&\quad - \frac{\gamma}{\kappa_+^2}\nabla^\epsilon(u_1^{(i)} \circ T_\epsilon)\cdot(\tau_\epsilon \circ T_\epsilon)\\
[u_1^\epsilon \circ T_\epsilon]_\Gamma &= -u_1^{(i)} \circ T_\epsilon,\\
[u_2^\epsilon \circ T_\epsilon]_\Gamma &= -u_2^{(i)} \circ T_\epsilon
\end{aligned} \tag{4.3}$$

on Γ and a radiation condition (2.14) 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 [9], 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

$$\begin{aligned}
&\tilde{\triangle}u = \operatorname{div}\Big([I \operatorname{div} T - (DT^\top + DT)]\nabla u\Big) - \operatorname{div} T\triangle u,\\
&\tilde{\nabla}u = -DT^\top\nabla u,
\end{aligned} \tag{4.4}$$

where DT denotes the Jacobian of T. Inserting the formal ansatz

$$u_j^\epsilon \circ T_\epsilon =: u_j^0 + \epsilon\dot{u}_j + \epsilon^2 v_j(\epsilon) \tag{4.5}$$

into the transformed boundary value problem on Ω and comparing the terms of order ϵ

yields

$$\begin{aligned} \triangle \dot{u}_1^+ + \kappa_+^2 \dot{u}_1^+ &= -\tilde{\triangle} u_1^{+,0} \quad \text{in} \quad \Omega^+, \\ \triangle \dot{u}_1^- + \kappa_-^2 \dot{u}_1^- &= -\tilde{\triangle} u_1^{-,0} \quad \text{in} \quad \Omega^-, \\ \triangle \dot{u}_2^+ + \kappa_+^2 \dot{u}_2^+ &= -\tilde{\triangle} u_2^{+,0} \quad \text{in} \quad \Omega^+, \\ \triangle \dot{u}_2^- + \kappa_-^2 \dot{u}_2^- &= -\tilde{\triangle} u_2^{-,0} \quad \text{in} \quad \Omega^-, \end{aligned} \tag{4.6}$$

and

$$\begin{aligned} \left[\frac{\gamma}{\kappa^2}\nabla \dot{u}_2 \cdot \tau + \frac{\omega\varepsilon}{\kappa^2}\nabla \dot{u}_1 \cdot \nu\right]_\Gamma =& -\frac{\omega\varepsilon_+}{\kappa_+^2}\nabla u_1^{(i)} \cdot \dot{\nu} - \left[\frac{\gamma}{\kappa^2}\tilde{\nabla} u_2^0 \cdot \tau + \frac{\omega\varepsilon}{\kappa^2}\tilde{\nabla} u_1^0 \cdot \nu\right]_\Gamma \\ &- \left[\frac{\gamma}{\kappa^2}\nabla u_2^0 \cdot \dot{\tau} + \frac{\omega\varepsilon}{\kappa^2}\nabla u_1^0 \cdot \dot{\nu}\right]_\Gamma - \frac{\gamma}{\kappa_+^2}\nabla u_2^{(i)} \cdot \dot{\tau}, \\ \left[\frac{\gamma}{\kappa^2}\nabla \dot{u}_1 \cdot \tau - \frac{\omega\mu}{\kappa^2}\nabla \dot{u}_2 \cdot \nu\right]_\Gamma =& \frac{\omega\mu}{\kappa_+^2}\nabla u_2^{(i)} \cdot \dot{\nu} - \left[\frac{\gamma}{\kappa^2}\tilde{\nabla} u_1^0 \cdot \tau - \frac{\omega\mu}{\kappa^2}\tilde{\nabla} u_2^0 \cdot \nu\right]_\Gamma \\ &- \left[\frac{\gamma}{\kappa^2}\nabla u_1^0 \cdot \dot{\tau} - \frac{\omega\mu}{\kappa^2}\nabla u_2^0 \cdot \dot{\nu}\right]_\Gamma - \frac{\gamma}{\kappa_+^2}\nabla u_1^{(i)} \cdot \dot{\tau}, \\ [\dot{u}_1]_\Gamma =& -\dot{u}_1^{(i)} = -\nabla u_1^{(i)} \cdot T, \\ [\dot{u}_2]_\Gamma =& -\dot{u}_2^{(i)} = -\nabla u_2^{(i)} \cdot T \end{aligned} \tag{4.7}$$

on the interface Γ. It is still to be shown that the functions $\dot{u}_j^\pm$ fulfill the same radiation condition as $u_j^\pm$, $j = 1, 2$. It is clear that $\dot{u}_j^\pm$ is α-quasiperiodic in x_1, so

$$\dot{u}_j^\pm(x_1, x_2) = e^{i\alpha x_1} \sum_{n=-\infty}^{\infty} \dot{u}_{j,n}^\pm(x_2) e^{inx_1}, \qquad j = 1, 2.$$

Since also

$$u_j^{\pm,0}(x_1, x_2) = e^{i\alpha x_1} \sum_{n=-\infty}^{\infty} u_{j,n}^{\pm,0}(x_2) e^{inx_1}$$

and

$$\left(\frac{\partial}{\partial x_2} + \kappa_\pm^2\right) u_{j,n}^{\pm,0}(x_2) = 0,$$

we have

$$0 = \left(\triangle + \epsilon\tilde{\triangle} + \epsilon^2 \triangle^R(\epsilon) + \kappa_\pm^2\right) (u_{j,n}^{\pm,\epsilon} \circ T_\epsilon) = (\triangle + \kappa_\pm^2) \left(\epsilon \dot{u}_{j,n}^\pm\right) + \epsilon\tilde{\triangle} u_{j,n}^{0,\pm} + \mathcal{O}(\epsilon^2).$$

If $T = 0$ near $\Gamma^\pm$, then also

$$\epsilon\tilde{\triangle} u_{j,n}^{0,\pm} = 0$$

near $\Gamma^\pm$. Hence,

$$\left(\frac{\partial}{\partial x_2} + \kappa_\pm^2\right) \dot{u}_{j,n}^{\pm,0}(x_2) = 0,$$

and we have shown that

$$\dot{u}_j^{\pm}(x) = \sum_{n=-\infty}^{\infty} \left(\dot{A}_{j,n}^{\pm} e^{i(n+\alpha)x_1 + i\beta_n^{\pm} x_2} + \dot{B}_{j,n}^{\pm} e^{i(n+\alpha)x_1 - i\beta_n^{\pm} x_2} \right) \tag{4.8}$$

with coefficients $\dot{A}_{j,n}^{\pm}, \dot{B}_{j,n}^{\pm} \in \mathbb{C}$. Moreover, we know that the unperturbed as well as the perturbed solution fulfill the radiation condition (2.14), i.e.

$$\begin{aligned} u_{j,n}^{\pm}(x_2) &= A_{j,n}^{\pm} e^{\pm i\beta_n^{\pm} x_2}, \\ (u_{j,n}^{\pm} \circ T_\epsilon)(x_2) &= A_{j,n}^{\pm,\epsilon} e^{\pm i\beta_n^{\pm} x_2}. \end{aligned}$$

From the ansatz (4.5) it follows that

$$(u_{j,n}^{\pm} \circ T_\epsilon)(x_2) = u_{j,n}^{\pm}(x_2) + \epsilon \dot{u}_{j,n}^{\pm}(x_2) + \epsilon^2 v_{j,n}(\epsilon, x_2). \tag{4.9}$$

Therefore, if $u_j^{\pm}$ and $(u_j^{\pm} \circ T_\epsilon)$ satisfy the radiation condition (2.14), this is also true for $\dot{u}_j^{\pm}$.

It remains to show that the solution $\dot{u}$ of the transmission problem (4.6)+(4.7)+(4.8) is indeed the material derivative of u_j for $j = 1, 2$, i.e. we have to show that

$$\sum_{j=1}^{2} ||u_j^\epsilon \circ T_\epsilon - u_j^0 - \epsilon \dot{u}_j||_{\mathcal{V}_\eta^l(\Omega)} \leq C\epsilon^2 \tag{4.10}$$

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

$$\triangle^\epsilon v_j^{\pm} + \kappa_{\pm}^2 v_j^{\pm} = -\epsilon^2 \left(\triangle^R u_j^{\pm,0} + \tilde{\triangle} \dot{u}_j^{\pm} \right) - \epsilon^3 \triangle^R \dot{u}_j^{\pm} \quad \text{in} \quad \Omega^{\pm} \tag{4.11}$$

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

$$\begin{aligned} &\left[\frac{\gamma}{\kappa^2} \nabla^\epsilon v_2 \cdot (\tau_\epsilon \circ T_\epsilon) + \frac{\omega\varepsilon}{\kappa^2} \nabla^\epsilon v_1 \cdot (\nu_\epsilon \circ T_\epsilon) \right]_\Gamma = \\ &= \epsilon^2 \Bigg\{ -\frac{\omega\varepsilon_+}{\kappa_+^2} \tilde{\nabla} u_1^{(i)} \cdot \dot{\nu} - \Bigg[\frac{\gamma}{\kappa^2} \left(\nabla \dot{u}_2 \cdot \dot{\tau} + \nabla u_2^0 \cdot \tau_R + \tilde{\nabla} u_2^0 \cdot \dot{\tau} + \tilde{\nabla} \dot{u}_2 \cdot \tau + \nabla^R u_2^0 \cdot \tau \right) + \\ &+ \frac{\omega\varepsilon}{\kappa^2} \left(\nabla \dot{u}_1 \cdot \dot{\nu} + \nabla u_1^0 \cdot \nu_R + \tilde{\nabla} u_1^0 \cdot \dot{\nu} + \tilde{\nabla} \dot{u}_1 \cdot \nu + \nabla^R u_1 \cdot \nu \right) \Bigg]_\Gamma - \frac{\gamma}{\kappa_+^2} \tilde{\nabla} u_2^{(i)} \cdot \dot{\tau} \Bigg\} \\ &+ \mathcal{P}_1(\epsilon^3, \epsilon^4, \epsilon^5) \end{aligned} \tag{4.12}$$

and

$$\left[\frac{\gamma}{\kappa^2} \nabla^\epsilon v_1 \cdot (\tau_\epsilon \circ T_\epsilon) - \frac{\omega\mu}{\kappa^2} \nabla^\epsilon v_2 \cdot (\nu_\epsilon \circ T_\epsilon) \right]_\Gamma =$$

$$
\begin{aligned}
&= \epsilon^2 \left\{ \frac{\omega\mu}{\kappa_+^2} \tilde{\nabla} u_2^{(i)} \cdot \dot{\nu} - \left[\frac{\gamma}{\kappa^2} \left(\nabla \dot{u}_1 \cdot \dot{\tau} + \nabla u_1^0 \cdot \tau_R + \tilde{\nabla} u_1^0 \cdot \dot{\tau} + \tilde{\nabla} \dot{u}_1 \cdot \tau + \nabla^R u_1^0 \cdot \tau \right) + \right. \right. \\
&+ \left. \left. \frac{\omega\mu}{\kappa^2} \left(\nabla \dot{u}_2 \cdot \dot{\nu} + \nabla u_2^0 \cdot \nu_R + \tilde{\nabla} u_2^0 \cdot \dot{\nu} + \tilde{\nabla} \dot{u}_2 \cdot \nu + \nabla^R u_2 \cdot \nu \right) \right]_\Gamma - \frac{\gamma}{\kappa_+^2} \tilde{\nabla} u_1^{(i)} \cdot \dot{\tau} \right\} \\
&+ \mathcal{P}_1(\epsilon^3, \epsilon^4, \epsilon^5), \qquad (4.13) \\
&[v_1]_\Gamma = 0, \\
&[v_2]_\Gamma = 0.
\end{aligned}
$$

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 (4.11) - (4.13), 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 3.2 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 $-\tilde{\triangle} u_j^{\pm,0} \in V_\eta^k(\Omega^\pm)$ on the right-hand sides of the Helmholtz equations and the right-hand sides of the boundary conditions are in $V_\eta^{k+1/2}(\Gamma)$ and in $V_\eta^{k+3/2}(\Gamma)$, respectively. Therefore $\dot{u}_j^\pm \in V_\eta^{k+2}(\Omega^\pm)$ also by Proposition 3.2 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 3.2 to the perturbed problem above and immediately obtain (4.10). Summarizing we can state the following theorem.

Theorem 4.1. *Suppose that the operator (3.29) is invertible. Then the material derivative $(\dot{u}_1, \dot{u}_2)$ of the solution to the conical diffraction problem 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 Perturbations which change angles at corner points

Regular perturbations of the identity that were considered in the previous section leave the angles at corner points unchanged. If we want to change those angles, we have to allow continuous piecewise smooth perturbations. In this case, a Dirac delta occurs in the first equation of (4.4). Consequently, we need a different representation of the perturbed boundary for the coordinate transform $x \mapsto x_\epsilon$, that leads to the perturbed problem (4.2) + (4.3).

The following statements can be found with more detailed explanations in [29], Chapter 5.5.2. Let $\{V_j\}_{j=1}^J$ be open sets in $\mathbb{R}^2$ that cover the interface Γ, i.e.

$$\Gamma \subset \bigcup_{j=1}^{J} V_j.$$

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 $\Gamma \cap V_j$, $\chi_j \equiv 1$ on $\Gamma \cap V_j$ and $\Gamma_\epsilon \subseteq \{\chi_j = 1\}$. In this way, we generate a mapping

$$(\xi_1^j, \xi_2^j) \mapsto (\zeta_1^j, \zeta_2^j) : \Gamma_\epsilon \cap V_j \to \Gamma \cap V_j \tag{4.14}$$

for the smooth parts of the boundary. In each cone

$$C_S = \{x = x(r,\theta) \in \mathbb{R}^2 : r > 0, \theta \in (-\theta_0, \theta_0)\} \tag{4.15}$$

with origin S, we proceed in the following way. Assume that 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

$$H(t) = at^\xi + \mathcal{O}(t^{\xi+1}), \quad \xi \geq 1. \tag{4.16}$$

An illustration is given in Figure 4. In this setting, we do not move the corner point, and the perturbation is symmetric. Non-smooth perturbations which move the corner can be considered as a composition of a smooth perturbation moving the corner with a non-smooth perturbation which leaves the corner invariant. Remarks on non-symmetric perturbations will be given later on. Then the domain $C_S(\epsilon)$ is given by

$$\{(r,\theta) : -\theta_0 - \epsilon r^{\xi-1} b(r,\epsilon) \leq \theta \leq \theta_0 + \epsilon r^{\xi-1} b(r,\epsilon)\} \tag{4.17}$$

with a smooth function b. Then one can construct a mapping of $C_S(\epsilon)$ onto C_S by introducing a mapping $(r,\theta) \mapsto (R,\Theta)$ with

$$R = r, \quad \Theta = \theta_0 \left(\theta_0 + \epsilon r^{\xi-1} b(r,\epsilon)\right)^{-1} \theta. \tag{4.18}$$

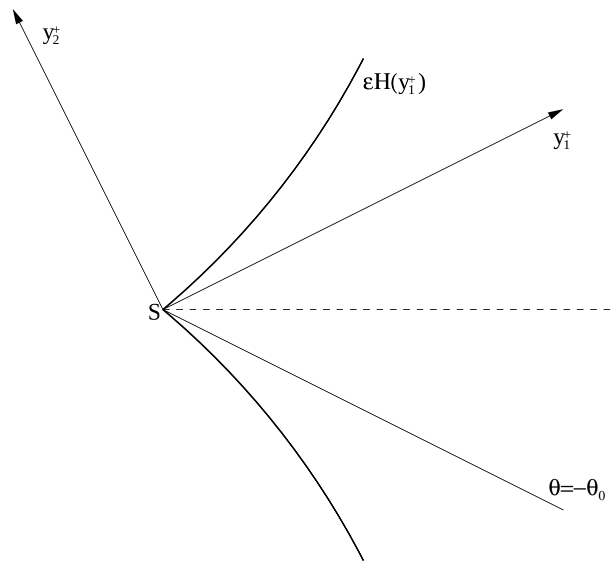

Figure 4.1: Boundary perturbation near a corner point

With the local mappings (4.14) and (4.18) we can assemble a diffeomorphism (cf. [29])

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

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

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

and

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

Remark 4.2. The symmetric structure of (4.17) 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 (4.17) 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 (4.18) and allows essentially the same considerations, only with more long-winded notation. □

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 in the following way. Since T_ϵ is smooth with respect to ϵ, we can write

$$T_\epsilon(x) = T_0(x) + \epsilon\left\{\frac{d}{d\epsilon}\, T_\epsilon(x)|_{\epsilon=0}\right\} + \mathcal{O}(\epsilon^2)$$

and replace T in the definition of the shape derivative, i.e.

$$u' := \dot{u} - \nabla u^0 \cdot \left\{\frac{d}{d\epsilon}\, T_\epsilon(x)|_{\epsilon=0}\right\}.$$

Theorem 4.2. *By the above considerations, Theorem 4.1 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 (4.16). Let us for simplicity return to the case of a symmetric perturbation.

According to [29], 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

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

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

$$\frac{1}{r}\frac{\partial}{\partial\theta} \sim \frac{1}{R}\left(1 + \sum_{k=1}^{\infty}\epsilon^k \sum_{j=1}^{k} R^{j(\xi-1)} \frac{\theta_0^{-j}}{(k-j)!}\left(\frac{\partial}{\partial\epsilon}(-1)^j\right)^{k-j} b^j(R,0)\right)\frac{\partial}{\partial\Theta},$$
$$\frac{\partial}{\partial r} \sim \frac{\partial}{\partial R} - \frac{1}{R}\sum_{k=1}^{\infty}\epsilon^k \sum_{j=1}^{k} R^{j(\xi-1)} \frac{\theta_0^{-j}}{(k-j)!}\left(\xi - 1 + \frac{R}{j}\frac{\partial}{\partial R}\right)\left(\frac{\partial}{\partial\epsilon}\right)^{k-j}(-1)^j b^j(R,0)\Theta\frac{\partial}{\partial\Theta}. \tag{4.19}$$

4.2 Characterization of the shape derivative

The goal of this section is the characterization of shape derivatives as solutions to a modified transmission problem. In order to do this, we state the following Lemma.

Lemma 4.1. *Suppose that Ω is a domain with piecewise C^n boundary Γ, $n \geq 1$, and that the function $v(\Omega)$ is shape differentiable in direction T on Ω. Then the shape derivative of the domain integral*

$$F(\Omega)(v) = \int_\Omega v dx$$

in direction T is

$$F'(\Omega; T)(v) = \int_\Omega v'(T) dx + \int_\Gamma v(T \cdot \nu) ds. \tag{4.20}$$

Let $\tilde{\kappa}$ be the curvature of Γ and let $\{S_j\}_{j=1}^m$ be the set of corner points of Γ. The indices are chosen such that the corner S_{j+1} follows the corner S_j in positive direction, and set $S_{m+1} := S_1$. Let $u(\Gamma)$ also be shape differentiable in direction T, and let $v'(T) = 0$ if T is constant. Assume that there *exists a family of smooth vector field T_ϵ, $\epsilon > 0$, vanishing near the corner points, such that*

$$\lim_{\epsilon\to 0} \int_\Gamma u'(T_\epsilon)ds = \int_\Gamma u'(T)ds. \tag{4.21}$$

(We will see later on that this is satisfied in the situation which is relevant for our particular situation). Then the shape derivative of the boundary integral

$$G(\Omega)(u) = \int_\Gamma uds$$

in direction T is given by

$$G'(\Omega;T)(u) = \int_\Gamma u'(T)ds + \int_\Gamma u\tilde{\kappa}(T\cdot\nu)ds + \sum_{j=1}^m \zeta_j. \tag{4.22}$$

where

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

with and $\tau^\pm$ denoting the left, resp. the right limit of the unit tangent vector. If $u(\Gamma) = v(\Omega)|_\Gamma$, then

$$G'(\Omega;T)(v) = \int_\Gamma v'(T)ds + \int_\Gamma \{\partial_\nu v + v\tilde{\kappa}\}(T\cdot\nu)ds + \sum_{j=1}^m \zeta_j, \tag{4.23}$$

Proof. The proof follows essentially [44] and [48, 45]. Formula (4.20) is shown in section 2.31 of [44]. Also in [44], section 2.33 it is shown that for the Eulerian derivative of the functional

$$G(\Omega)(u) = \int_\Gamma uds$$

is given by

$$\begin{aligned} G'(\Omega;T)(u) &= \int_\Gamma u'(T)ds + \int_\Gamma \{\nabla_\Gamma u\cdot T + u\mathrm{div}_\Gamma(T)\}ds \\ &= \int_\Gamma u'(T)ds + \int_\Gamma \mathrm{div}_\Gamma(uT)ds. \end{aligned} \tag{4.24}$$

Observe that

$$\mathrm{div}_\Gamma([T\cdot\nu]\nu) = [T\cdot\nu]\mathrm{div}_\Gamma(\nu),$$

since

$$\mathrm{div}_\Gamma([T\cdot\nu]\nu) = (\nabla_\Gamma[T\cdot\nu])\cdot\nu + [T\cdot\nu]\mathrm{div}_\Gamma\nu = [T\cdot\nu]\mathrm{div}_\Gamma\nu,$$

because $\nabla_\Gamma[T\cdot\nu]$ is a tangent vector. Also,

$$\mathrm{div}_\Gamma(uT) = u[T\cdot\nu]\mathrm{div}_\Gamma\nu.$$

Moreover, $\tilde{\kappa} = \mathrm{div}_\Gamma(\nu)$ on a C^2 manifold. So if Γ is at least C^2, then

$$G'(\Omega;T) = \int_\Gamma u'(T)ds + \int_\Gamma u\tilde{\kappa}(T\cdot\nu)ds.$$

Now let $\{\psi_j\}_{j=1}^n$ be a smooth partition of unity, i.e.

$$\psi_j \in C^\infty(\mathbb{R}^2), \quad j = 1\ldots n, \quad \sum_{j=1}^n \psi_j = 1 \quad \text{in} \quad \overline{\Omega},$$

such that each each ψ_j has a compact support that contains exactly one corner point. Without loss of generality, we assume that $\psi_j(S_i) = \delta_{ij}$ and that supp $\psi_j \subset U(S_j)$, where $U(S_j)$ is a neighbourhood of S_j. Define

$$\begin{aligned} T_j &:= \psi_j T, \\ u_j &:= \psi_j u, \\ \Gamma_j &:= \Gamma \cap U(S_j), \\ \Gamma_{i,j} &:= \Gamma_i \cap \Gamma_j \quad \text{for} \quad i \neq j. \end{aligned}$$

With

$$A_{i,j}(T_j) := \int_{\Gamma_{i,j}} u_i'(T_j)ds + \int_{\Gamma_{i,j}} \left\{\nabla_\Gamma u_i \cdot T_j + u_i \mathrm{div}_\Gamma(T_j)\right\} ds \tag{4.25}$$

and

$$B_j(T_j) := \int_{\Gamma_j} u_j'(T_j)ds + \int_{\Gamma_j} \left\{\nabla_\Gamma u_j \cdot T_j + u_j \mathrm{div}_\Gamma(T_j)\right\} ds, \tag{4.26}$$

we can write

$$\begin{aligned} G'(\Omega;T)(u) &= \int_\Gamma u'(T)ds + \int_\Gamma \left\{\nabla_\Gamma u \cdot T + u\mathrm{div}_\Gamma(T)\right\} ds \\ &= \sum_{i\neq j} A_{i,j} + \sum_j B_j. \end{aligned} \tag{4.27}$$

Define furthermore

$$W_j := T_j - T_j(S_j).$$

Now we choose another set of cut-off functions $\theta_j^\epsilon \in C^\infty(\Gamma_j)$ vanishing near S_j and converging pointwise to 1 for $\epsilon \to 0$ for every point near S_j except for S_j itself. Then define

$W_j^\epsilon := \theta_j^\epsilon W_j$. Together with (4.24), this implies

$$\lim_{\epsilon\to 0} B_j(W_j^\epsilon) = \lim_{\epsilon\to 0}\left(\int_{\Gamma_j} u'(W_j^\epsilon)ds + \int_{\Gamma_j} \mathrm{div}_\Gamma(uW_j^\epsilon)ds\right)$$
$$= \lim_{\epsilon\to 0}\left(\int_{\Gamma_j} u'(W_j^\epsilon)ds + \int_{\Gamma_j} u\tilde{\kappa}[W_j^\epsilon\cdot\nu]ds\right)$$

If we assume that

$$\lim_{\epsilon\to 0}\int_\Gamma v'(W_j^\epsilon)ds = \int_\Gamma v'(W_j)ds,$$

we get

$$\lim_{\epsilon\to 0} B_j(W_j^\epsilon) = \int_{\Gamma_j} u'(W_j)ds + \int_{\Gamma_j} u\tilde{\kappa}(W_j\cdot\nu)ds,$$

since W_j^ϵ is bounded pointwise by W_j. Because of the definition of W_j,

$$B_j(T_j) = B_j(W_j) + B_j(T_j(S_j)).$$

Since $T_j(S_j) = T(S_j)$ is constant, we have by assumption $u'(T_j(S_j)) = 0$, and therefore, by using the definition (4.26) and the fact that $\mathrm{div}_\Gamma(T(S_j)) = 0$,

$$B_j(T_j) = \int_{\Gamma_j} u'(T_j)ds + \int_{\Gamma_j}\tilde{\kappa}u(\{T_j - T(S_j)\}\cdot\nu)ds + \int_{\Gamma_j}\{\nabla_\Gamma u\cdot T(S_j)\}ds.$$

Hence,

$$B_j(T_j) = \int_{\Gamma_j} u'(T_j)ds + \int_{\Gamma_j}\tilde{\kappa}u(T_j\cdot\nu)ds + \int_{\Gamma_j}\{(\nabla_\Gamma u - \tilde{\kappa}u_j\nu)\cdot T(S_j)\}ds. \tag{4.28}$$

Let $\gamma_j : [0,1] \to \Gamma_j$ be the arc-length parametrization of Γ_j with $\gamma_j(1) = S_j$. Due to $\nabla_\Gamma u = \partial_\tau u\tau$, we have

$$\int_{\Gamma_j}\nabla_\Gamma u ds = \int_0^1 \frac{du(\gamma_j(t))}{dt}\tau(\gamma_j(t))dt = u(S_j)\tau^-(S_j) - u(\gamma_j(0))\tau(\gamma_j(0))$$
$$- \int_0^1 u(\gamma_j(t))\frac{d\tau(\gamma_j(t))}{dt}dt,$$

where $\tau^-(S_j) := \lim_{t\nearrow 1}\tau(\gamma_j(t))$. Since ν is outward pointing and the parametrization is with respect to the arc length, we have

$$\frac{d\tau}{dt} = -\tilde{\kappa}\nu,$$

and therefore

$$\int_{\Gamma_j} \{\nabla_\Gamma u - \tilde{\kappa} u \nu\} ds = u(S_j)\tau^-(S_j) - u(\gamma_j(0))\tau(\gamma_j(0)). \tag{4.29}$$

If we take the sum of (4.29) over all j, we get formula (4.22), recalling (4.27),(4.25) and (4.28). If u is the restriction of a function z which is defined on the whole domain, i.e. $u = z|_\Gamma$, then (see formula (2.174) in [44])

$$u'(T) = z'(T)|_\Gamma + [T \cdot \nu]\partial_\nu z,$$

which implies (4.23). □

Remark 4.3. We need to show that assumption (4.21) is fulfilled for the situation that is interesting for our context. The lemma will be needed to compute the shape derivative of the integral

$$G(\Omega) = \int_\Gamma \partial_\nu u^{(i)} ds,$$

where $u^{(i)}$ is an incoming plane wave above the interface Γ. Let S_j be a corner point of Γ and let $W_j^\epsilon = \theta_j^\epsilon W_j$ be as in the proof of Lemma 4.1, with θ_j^ϵ defined such that $\partial_\tau \theta_j^\epsilon$ is with respect to ϵ uniformly bounded by an integrable function. For the shape derivative of $\partial_\nu u^{(i)}$ we have

$$\left(\partial_\nu u^{(i)}\right)'(W_j^\epsilon) = \nu' \cdot \nabla u^{(i)} + \nu \cdot \partial_\nu(\nabla u^{(i)})[W_j^\epsilon \cdot \nu]. \tag{4.30}$$

Furthermore, the shape derivative of the unit normal can be expressed as (cf. [42])

$$\nu'(W_j^\epsilon) = -(D_\Gamma W_j^\epsilon)^\top \nu,$$

where $D_\Gamma W_j^\epsilon$ is the tangential Jacobian of W_j^ϵ. The tangential Jacobian of a vector field T is defined by

$$(D_\Gamma T)_{i,j} := [\nabla_\Gamma T_i]_j^\top,$$

i.e. the rows of the matrix are given by the tangential gradient of the component functions. By straigtforward computaions,

$$D_\Gamma(\theta_j^\epsilon W_j) = \theta_j^\epsilon D_\Gamma W_j + \begin{pmatrix} (W_j)_1[\nabla_\Gamma \theta_j^\epsilon]^\top \\ (W_j)_2[\nabla_\Gamma \theta_j^\epsilon]^\top \end{pmatrix}.$$

Using (**??**) and (4.30), we conclude that $(\partial_\nu u^{(i)})'(W_j^\epsilon)$ is bounded pointwise by an integrable function and Lebesgue's theorem implies

$$\lim_{\epsilon\to\infty} \int\limits_{\Gamma\cap U(S_j)} \left(\partial_\nu u^{(i)}\right)' (W_j^\epsilon) ds = \int\limits_{\Gamma\cap U(S_j)} \left(\partial_\nu u^{(i)}\right)' (W_j) ds,$$

i.e. assumption (4.21) is satisfied. □

Lemma 4.1 can now be used for the characterization of shape derivatives. We apply a technique from [44]. We discuss a simple model problem first and then use the results to characterize shape derivatives of solutions of the more complicated problem (2.9), (2.10), (2.12), (2.14). 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 assume that u_1 and u_2 satisfy radiation conditions of the form (2.14) on Γ^+, and Γ^-, respectively, with Ω, Γ and $\Gamma^\pm$ as described in Section 2.2. 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 $\eta < 1$. Choose test functions $v_1 \in C_0^\infty(\Omega^+)$ and $v_2 \in C_0^\infty(\Omega^-)$. Then the Helmholtz equation and Green's formula give

$$\int\limits_{\Omega^\pm} \left\{\nabla u_j \nabla v_j + \kappa_\pm^2 u_j v_j\right\} dx = 0.$$

Applying Lemma 4.1 then gives, using the fact that the test functions vanish near the boundary of $\Omega^\pm$ and that $v_j' = 0$,

$$\int\limits_{\Omega^\pm} \left\{\nabla u_j' \nabla v_j + \kappa_\pm^2 u_j' v_j\right\} dx = 0.$$

Therefore, u_1' and u_2' satisfy the Helmholtz equation in the interior of Ω^+ and Ω^-, respectively.

It was shown earlier in this chapter that if the direct solution satisfies the radiation condition (2.14), as it is assumed here, then this radiation condition is also satisfied by the material derivatives. Since furthermore

$$u_j' = \dot{u}_j - \nabla u_j \cdot T,$$

the radiation condition is also satisfied by the shape derivatives if we assume further that $T = 0$ near Γ^+ and Γ^-. The shape derivatives can be therefore be represented by a

Rayleigh series

$$\left(u_j^{\pm}\right)'(x_1, x_2) = \sum_{j=-\infty}^{\infty} \left(A_j^{\pm}\right)' e^{i(n+\alpha)x_1 \pm i\beta_n x_2}. \tag{4.31}$$

with $\left(A_j^{\pm}\right)' \in \mathbb{C}$ if x_2 is close to $\pm b$.

Assume now that $v \in C^\infty(\overline{\Omega})$, that $e^{-i\alpha x_1}v(x_1, x_2)$ is again 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

$$\begin{aligned}\int_{\Omega^+} \left\{\nabla u_1 \nabla v - \kappa_+^2 u_1 v\right\} dx - \int_{\Omega^-} \nabla u_2 \nabla^\perp v dx - \int_{\Gamma} \left\{\partial_\nu u_1 - \partial_\tau u_2\right\} v ds = \\ = \int_{\Omega^+} \left\{\nabla u_1 \nabla v - \kappa_+^2 u_1 v\right\} dx - \int_{\Omega^-} \nabla u_2 \nabla^\perp v dx - \int_{\Gamma} \partial_\nu u^{(i)} v ds = 0.\end{aligned} \tag{4.32}$$

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 4.1 and using the fact that $\nabla u_j' \nabla v \in L^1(\Omega)$ for u_j and v as above, 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

$$\zeta_j = \nu^- \cdot \nabla u^{(i)}(S_{j+1}) v(S_{j+1}) [T(S_{j+1}) \cdot \tau^-(S_{j+1})] - \nu^+ \cdot \nabla u^{(i)}(S_j) v(S_j) [T(S_j) \cdot \tau^+(S_j)]. \tag{4.33}$$

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

$$\begin{aligned}\int_{\Gamma} \left\{\partial_\nu u_1' - \partial_\tau u_2'\right\} v ds = \int_{\Gamma} \left\{-\nabla u_2 \nabla^\perp v - \nabla u_1 \nabla v + \kappa_+^2 u_1 v\right\} (T \cdot \nu) ds \\ + \int_{\Gamma} \left(\partial_\nu u_1^{(i)}\right)' v ds + \int_{\Gamma} \partial_\nu u_1^{(i)} v \tilde{\kappa} (T \cdot \nu) ds + \sum_{j=1}^{m} \zeta_j.\end{aligned} \tag{4.34}$$

Let

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

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 [44], it follows that

$$\begin{aligned}\int_\Gamma \nabla u_1\nabla v(T\cdot\nu)ds &= -\int_\Gamma v\,\mathrm{div}_\Gamma((T\cdot\nu)\nabla u_1)ds + \int_\Gamma \tilde{\kappa}(T\cdot\nu)[\nabla u_1\cdot\nu]v ds\\ &= -\int_\Gamma v\,\mathrm{div}_\Gamma\left((T\cdot\nu)\nabla u_1|_\tau\right)ds.\end{aligned}\tag{4.35}$$

The last equality is Proposition 2.57 in [44]. 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 (4.34) 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 $u_1' - u_2'$. Because of the boundary condition $u_1 - u_2 = u^{(i)}$ on Γ, we have

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

Taking the shape derivative on both sides and choosing $\partial_\nu v = 0$ yields

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

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

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

We get

$$\int_\Gamma \{u_1' - u_2'\} v ds = \int_\Gamma (u^{(i)})' v ds - \sum_{l=1}^{m} \xi_l + \sum_{l=1}^{m} \rho_l = \int_\Gamma (u^{(i)})' v ds$$

because the two sums cancel out. Thus, it follows that

$$u_1' - u_2' = \left(u^{(i)}\right)'.$$

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

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

with ζ_j from (4.33), on Γ. We see that the differential equation and the boundary operators on Γ of the problem that characterizes the shape derivative are the same as the differential equation and the boundary operators of the original model problem. Only the right-hand side changes. These results can be carried over to our original problem

(2.9), (2.10), (2.12), (2.14). We have furthermore shown that the shape derivatives satisfy the radiation condition (4.31). We obtain the following theorem on the characterization of shape derivatives.

Theorem 4.3. *Assume that $(u_1^0, u_2^0) \in [\mathcal{V}_\eta^{k+2}(\Omega)]^2$ is the unique solution of the problem (2.9), (2.10), (2.12), (2.14). Define*

$$\begin{aligned}\zeta_{1,j} :=& \nu^- \cdot \frac{\omega\varepsilon_+}{\kappa_+^2} \nabla u_1^{(i)}(S_{j+1}) v(S_{j+1})[T(S_{j+1}) \cdot \tau^-(S_{j+1})] \\ &- \nu^+ \cdot \frac{\omega\varepsilon_+}{\kappa_+^2} \nabla u_1^{(i)}(S_j) v(S_j)[T(S_j) \cdot \tau^+(S_j)] \\ &+ \tau^- \cdot \frac{\gamma}{\kappa_+^2} \nabla u_2^{(i)}(S_{j+1}) v(S_{j+1})[T(S_{j+1}) \cdot \tau^-(S_{j+1})] \\ &- \tau^+ \cdot \frac{\gamma}{\kappa_+^2} \nabla u_2^{(i)}(S_j) v(S_j)[T(S_j) \cdot \tau^+(S_j)]\end{aligned}$$

and

$$\begin{aligned}\zeta_{2,j} :=& \nu^- \cdot \frac{\omega\mu}{\kappa_+^2} \nabla u_2^{(i)}(S_{j+1}) v(S_{j+1})[T(S_{j+1}) \cdot \tau^-(S_{j+1})] \\ &- \nu^+ \cdot \frac{\omega\mu}{\kappa_+^2} \nabla u_2^{(i)}(S_j) v(S_j)[T(S_j) \cdot \tau^+(S_j)] \\ &- \tau^- \cdot \frac{\gamma}{\kappa_+^2} \nabla u_1^{(i)}(S_{j+1}) v(S_{j+1})[T(S_{j+1}) \cdot \tau^-(S_{j+1})] \\ &+ \tau^+ \cdot \frac{\gamma}{\kappa_+^2} \nabla u_1^{(i)}(S_j) v(S_j)[T(S_j) \cdot \tau^+(S_j)]\end{aligned}$$

with $\nu^\pm$, $\tau^\pm$ and $\{S_j\}_{j=1}^m$ from Lemma 4.1. 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

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

with the transmission conditions

$$\begin{aligned}\int_\Gamma \left[\frac{\gamma}{\kappa^2}\partial_\tau u_2' + \frac{\omega\varepsilon}{\kappa^2}\partial_\nu u_1'\right]_\Gamma v ds =& \int_\Gamma \mathrm{div}_\Gamma \left((T\cdot\nu)\left[\frac{\gamma}{\kappa^2}\nabla u_2^0|_\tau + \frac{\omega\varepsilon}{\kappa^2}\nabla^\perp u_1^0|_\tau\right]_\Gamma\right) v ds \\ &- \int_\Gamma \left\{\tilde{\kappa}(T\cdot\nu)\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu u_1^{(i)} + \frac{\omega\varepsilon_+}{\kappa_+^2}\nu' \cdot \nabla u_1^{(i)}\right\} v ds \\ &- \int_\Gamma \left\{\tilde{\kappa}(T\cdot\nu)\frac{\gamma}{\kappa_+^2}\partial_\tau u_2^{(i)} + \frac{\gamma}{\kappa_+^2}\tau' \cdot \nabla u_2^{(i)}\right\} v ds\end{aligned}$$

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

for all $v \in C^\infty(\overline{\Omega})$ and

$$
\begin{aligned}
\left[u_1'\right]_\Gamma &= \left(u_1^{(i)}\right)',\\
\left[u_2'\right]_\Gamma &= \left(u_2^{(i)}\right)'
\end{aligned}
$$

on the interface Γ and a radiation condition of the form (4.31).

Remark 4.4. (i) The weak formulation of the transmission condition in Theorem 4.3 can formally be written in the following form involving Dirac deltas:

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

with

$$\begin{aligned}\zeta_{1,j} :=& \nu^- \cdot \frac{\omega\varepsilon_+}{\kappa_+^2} \nabla u_1^{(i)} (T\cdot\tau^-)\delta_{S_{j+1}} - \nu^+ \cdot \frac{\omega\varepsilon_+}{\kappa_+^2} \nabla u_1^{(i)} (T\cdot\tau^+)\delta_{S_j} \\ &+ \tau^- \cdot \frac{\gamma}{\kappa_+^2} \nabla u_2^{(i)} (T\cdot\tau^-)\delta_{S_{j+1}} - \tau^+ \cdot \frac{\gamma}{\kappa_+^2} \nabla u_2^{(i)} (T\cdot\tau^+)\delta_{S_j}\end{aligned} \tag{4.36}$$

and

$$\begin{aligned}\zeta_{2,j} :=& \nu^- \cdot \frac{\omega\mu}{\kappa_+^2} \nabla u_2^{(i)} (T\cdot\tau^-)\delta_{S_{j+1}} - \nu^+ \cdot \frac{\omega\mu}{\kappa_+^2} \nabla u_2^{(i)} (T\cdot\tau^+)\delta_{S_j} \\ &- \tau^- \cdot \frac{\gamma}{\kappa_+^2} \nabla u_1^{(i)} (T\cdot\tau^-)\delta_{S_{j+1}} - \tau^+ \cdot \frac{\gamma}{\kappa_+^2} \nabla u_1^{(i)} (T\cdot\tau^+)\delta_{S_j}\end{aligned}$$

(ii) The incoming waves satisfy the homogeneous Helmholtz equation, i.e.

$$\triangle u_j^{(i)} + \kappa_+^2 u_j^{(i)} = 0$$

in Ω^+. Green's formula gives e.g.

$$-\int\limits_{\Omega^+} \nabla u_1^{(i)} \nabla v dx + \int\limits_{\Gamma} \partial_\nu u_1^{(i)} v ds + \int\limits_{\Omega^+} \kappa_+^2 u_1^{(i)} v + \int\limits_{\Omega^+} \nabla u_2^{(i)} \nabla^\perp v dx + \int\limits_{\Gamma} \partial_\tau u_2^{(i)} v ds = 0$$

with a suitable test function v as described above. Also as before, taking the shape derivative gives

$$\begin{aligned}&-\int\limits_{\Omega^+} \nabla (u_1^{(i)})' \nabla v dx + \int\limits_{\Omega^+} \kappa_+^2 (u_1^{(i)})' v dx - \int\limits_{\Gamma} \nabla u_1^{(i)} \nabla v (T\cdot\nu) ds + \int\limits_{\Gamma} \kappa_+^2 u_1^{(i)} v (T\cdot\nu) ds \\ &+ \int\limits_{\Omega^+} \nabla (u_2^{(i)})' \nabla^\perp v dx + \int\limits_{\Gamma} \nabla u_2^{(i)} \nabla^\perp v (T\cdot\nu) ds = -\int\limits_{\Gamma} \left(\partial_\nu u_1^{(i)}\right)' v ds - \int\limits_{\Gamma} \tilde{\kappa} \partial_\nu u_1^{(i)} v (T\cdot\nu) ds \\ &- \int\limits_{\Gamma} \left(\partial_\tau u_2^{(i)}\right)' v ds - \int\limits_{\Gamma} \tilde{\kappa} \partial_\tau u_2^{(i)} v (T\cdot\nu) ds - \sum_{k=1}^{m} \zeta_{1,k}.\end{aligned}$$

Since the incoming waves do not depend on the geometry, their shape derivatives vanish, so do their traces on the interface Γ. Therefore

$$-\int\limits_{\Omega^+} \nabla (u_1^{(i)})' \nabla v dx + \int\limits_{\Omega^+} \kappa_+^2 (u_1^{(i)})' v dx + \int\limits_{\Gamma} \partial_\nu \left(u_1^{(i)}\right)' v ds = 0$$

and

$$\int\limits_{\Omega^+} \nabla (u_2^{(i)})' \nabla^\perp v dx + \int\limits_{\Gamma} \partial_\tau \left(u_2^{(i)}\right)' v ds = 0,$$

so

$$-\int_\Gamma \nabla u_1^{(i)} \nabla v (T\cdot\nu) ds + \int_\Gamma \kappa_+^2 u_1^{(i)} v(T\cdot\nu) ds + \int_\Gamma \nabla u_2^{(i)} \nabla^\perp v(T\cdot\nu) ds =$$
$$-\int_\Gamma \left(\partial_\nu u_1^{(i)}\right)' v ds - \int_\Gamma \tilde{\kappa}\partial_\nu u_1^{(i)} v(T\cdot\nu) ds - \int_\Gamma \left(\partial_\tau u_2^{(i)}\right)' v ds - \int_\Gamma \tilde{\kappa}\partial_\tau u_2^{(i)} v(T\cdot\nu) ds - \sum_{k=1}^m \zeta_{1,k}.$$

On the other hand, we have seen (cf. (4.35)) that

$$\int_\Gamma \nabla u_j^{(i)} \nabla v[T\cdot\nu] ds = -\int_\Gamma v \mathrm{div}_\Gamma\{(T\cdot\nu)\nabla u_j^{(i)}|_\Gamma\} ds$$

and that

$$\int_\Gamma \nabla u_j^{(i)} \nabla^\perp v[T\cdot\nu] ds = \int_\Gamma v \mathrm{div}_\Gamma\{(T\cdot\nu)\nabla^\perp u_j^{(i)}|_\Gamma\} ds.$$

It follows that if we set

$$u_j^+ =: u_j^{(s)} + u_j^{(i)},$$

for $j = 1, 2$, i.e. if u_j^+ denotes the total field instead of the scattered field only, then Theorem 4.3 can be formulated without the terms involving $u_{1/2}^{(i)}$. □

5 Computation of shape derivatives

We have seen in the last chapters that the shape derivatives of solutions to the conical diffraction problem fail to be of H^1 regularity in the presence of a non-smooth interface. In this chapter, we will give an ansatz for computing shape derivatives that consists in formulating the conical diffraction problem as a system of integral equations and then using a collocation method to discretize and solve the system. We make use of results by Gunther Schmidt [39, 40, 41]. However, in these papers, only the direct problem is considered, whose solutions are more regular than their shape derivatives, as we have seen before, and the regularity assumptions that are made there are not true for the situation we are considering. Therefore, the following strategy will be followed in order to cope with this difficulty.

We will first show that there exists a sequence of cut-off functions supported near the corner points, such that the sequence of cut-off operators converges pointwise to the identity in the Kondratiev spaces V_η^k for all $\eta \in \mathbb{R}$. If $u \in \mathcal{H}^1(\Omega)$ is a shape differentiable solution of the original conical diffraction problem, then its shape derivative u' belongs to $\mathcal{V}_\eta^1(\Omega)$ with a suitable η and satisfies a transmission problem in accordance with Theorem 4.3. Now u' can be approximated by a sequence of functions $\tilde{u}_j$ which satisfy the transmission problem with right-hand sides smoothened by a multiplication with a cut-off function. Since these smoothened right-hand sides are in $\mathcal{H}^1(\Omega)$, this is also true for the approximating functions. This process is described in the following section of this chapter.

In the second section we then describe the formulation of the characterization of the shape derivative as a system of boundary integral equations. It will be assumed that, due to the above cut-off process, all necessary regularity assumptions are fulfilled.

5.1 Regularization of corner singularities

5.1.1 Construction of a smooth cut-off function and convergence of the cut-off process

The following construction of a smooth cut-off function is well known. However, we include it for convenience. Define the function

$$p(x) := \begin{cases} e^{-1/x} & x > 0 \\ 0 & x \leq 0. \end{cases}$$

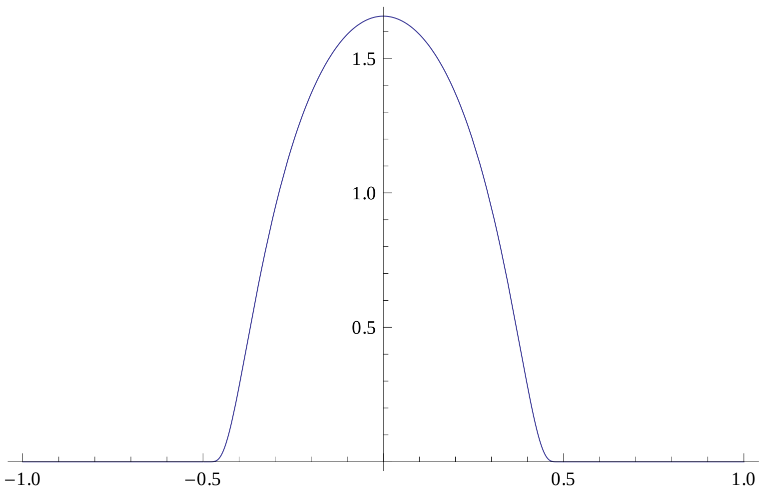

Figure 5.1: Friedrichs' mollifier

Define further

$$q(x) := s \left(\int_{-1}^{1} \frac{1}{1-y^2} dy \right)^{-1} p\left(1 - s^2 x^2\right).$$

We choose $s > 2$. Then q is a C^∞-function with support in $(-\frac{1}{2}, \frac{1}{2})$. It is called *Friedrichs' mollifier* in the literature. The integral

$$\psi(x) := \int_{-\infty}^{x} q(y) dy$$

leads to a smooth monotone function which is equal to 1 for $x > 1/2$ and vanishes for $x < -1/2$.

Let Ω be a domain which is smooth except for a corner point S. In the neighbourhood of S, we switch to polar coordinates (r, φ) centered at S. We introduce cut-off functions

$$\chi_j(r, \varphi) := \psi \left(\frac{r - 2^{-(j+1)}}{2^{-j}} \right) \tag{5.1}$$

which vanish for small r and are equal to 1 for $r \geq 2^{-j}$. Note that

$$|| \frac{\partial^n}{\partial r^n} \chi_j ||_{L^\infty} \leq 2^{nj} C, \tag{5.2}$$

with a constant C which does not depend on j. Now we are in the position to prove the following Lemma.

Lemma 5.1. *Let u be a function in $V^k_\eta(\Omega)$ with $\eta > 0$ and $k \geq 0$. Then*

$$||u - \chi_j u||_{V^k_\eta(\Omega)} \to 0$$

for $j \to \infty$.

Proof. Let ξ be a cut-off function with support near the corner point S and define Ψ so that $\xi + \Psi = 1$ in Ω. Then

$$||\chi_j u||_{V^k_\eta(\Omega)} = ||\Psi \chi_j u||_{H^k(\Omega)} + \sum_{|\alpha| \leq k} ||r^{\eta - k + |\alpha|} D^\alpha \left(\xi \chi_j u\right)||_{L^2(\Omega)}.$$

The last sum on the right-hand side can be estimated as

$$\begin{aligned}
\sum_{|\alpha| \leq k} ||r^{\eta-k+|\alpha|} D^\alpha (\xi \chi_j u)||_{L^2(\Omega)} \leq \\
&\leq \sum_{|\alpha| \leq k} \sum_{\beta : |\beta| \leq |\alpha|} C_{\alpha,\beta} ||r^{\eta-k+|\alpha|} \left(D^\beta \chi_j\right) \left(D^{\alpha-\beta} \xi u\right) ||_{L^2(\Omega)} \\
&\leq \sum_{|\alpha| \leq k} \sum_{\beta : |\beta| \leq |\alpha|} C_{\alpha,\beta} ||r^{|\beta|} D^\beta \chi_j||_{L^\infty(\Omega)} ||r^{\eta-k-|\beta|+|\alpha|} \left(D^{\alpha-\beta} \xi u\right) ||_{L^2(\Omega)}.
\end{aligned}$$

Since

$$\frac{\partial}{\partial r} \chi_j(r, \varphi) = 0$$

for $r > 2^{-j}$, we only need to consider $r < 2^{-j}$, and therefore

$$||r^n \frac{\partial^n}{\partial r^n} \chi_j||_{L^\infty(\Omega)} < C$$

with C not depending on j, i.e. we have

$$\begin{aligned}
\sum_{|\alpha| \leq k} ||r^{\eta-k+|\alpha|} D^\alpha (\xi \chi_j u)||_{L^2(\Omega)} &\leq \tilde{C} \sum_{|\alpha| \leq k} \sum_{|\beta| \leq |\alpha|} ||r^{\eta-k-|\beta|+|\alpha|} \left(D^{\alpha-\beta} \xi u\right) ||_{L^2(\Omega)} \\
&\leq C \sum_{|\alpha| \leq k} ||r^{\eta-k+|\alpha|} D^\alpha (\xi u)||_{L^2(\Omega)}.
\end{aligned}$$

The sequence of cut-off operators is therefore uniformly bounded in $V^k_\eta(\Omega)$, i.e.

$$||\chi_j u||_{V^k_\eta(\Omega)} \leq C ||u||_{V^k_\eta(\Omega)}.$$

By Lebesgue's dominated convergence theorem it follows that

$$\lim_{j \to \infty} ||u - \chi_j u||_{V^k_\eta(\Omega)} = || \lim_{j \to \infty} (u - \chi_j u)||_{V^k_\eta(\Omega)} = 0.$$

□

5.1.2 Application to boundary value problems

Let Ω be a bounded domain in $\mathbb{R}^2$ with boundary Γ. Assume that Γ has a finite number of corner points. As usual, the set of corner points is denoted by $\mathcal{S}$. We consider the boundary value problem

$$\begin{aligned} \mathbf{L}u &= f \quad \text{in} \quad \Omega, \\ \mathbf{B}u &= g \quad \text{on} \quad \Gamma \end{aligned} \tag{5.3}$$

with an elliptic $n \times n$-matrix operator $\mathbf{L}$ of order 2 and an $m \times n$-matrix $\mathbf{B}$ of boundary operators. Assume that

$$f \in [V_\eta^{k-2}(\Omega)]^n \qquad \text{and} \qquad g \in \bigoplus_{j=1}^{m} V_\eta^{k-m_j-1/2}(\Gamma) =: \mathbf{V}_\eta^{k-1/2}(\Gamma),$$

with an integer $k \geq 2$, $m_j \in \{0,1\}$ and $\eta \geq 0$. Assume furthermore that $u \in [V_\eta^k(\Omega)]^n$ is the unique solution of the boundary value problem (5.3) satisfying the a priori estimate

$$||u||_{[V_\eta^k(\Omega)]^n} \leq C\left\{||f||_{[V_\eta^{k-2}(\Omega)]^n} + ||g||_{\mathbf{V}_\eta^{k-1/2}(\Gamma)}\right\}, \tag{5.4}$$

with a constant C independent of u. Now define the sequences

$$f_j := \chi_j f$$

and

$$g_j := \chi_j g$$

with χ_j introduced in the previous subsection. We have shown that

$$\tilde{f}_j \to f$$

in $[V_\eta^{k-2}(\Omega)]^n$ and

$$\tilde{g}_j \to g$$

in $\mathbf{V}_\eta^{k-1/2}(\Gamma)$.

Let now $\tilde{u}_j$ be the solution of the boundary value problem

$$\begin{aligned} \mathbf{L}\tilde{u}_j &= \tilde{f}_j \quad \text{in} \quad \Omega \\ \mathbf{B}\tilde{u}_j &= \tilde{g}_j \quad \text{on} \quad \Gamma \end{aligned} \tag{5.5}$$

and $\tilde{u}_j \in [V_\eta^k(\Omega)]^n$ for any $k \in \mathbb{N}$ and $\eta \in \mathbb{R}$. If the system (5.5) satisfies the estimate (5.4), then it follows that

$$||\tilde{u}_j - u||_{[V_\eta^k(\Omega)]^n} \leq C\left\{||\tilde{f}_j - f||_{[V_\eta^{k-2}(\Omega)]^n} + ||\tilde{g}_j - g||_{\mathbf{V}_\eta^{k-1/2}(\Gamma)}\right\},$$

and therefore $\tilde{u}_j \to u$ in $V_\eta^k(\Omega)$ as $j \to \infty$.

Let now Ω be again the bounded periodic cell as in the previous chapters. We apply the above results to the characterization of the shape derivative $(u_1', u_2') \in [\mathcal{V}_\eta^1(\Omega)]^2$, $\eta \in (0,1)$, in Theorem 4.3 in the following way. Assume that the interface has (for simplicity) one corner point S. Let χ_j be a sequence of cut-off functions vanishing near S as constructed above. Then we multiply the right-hand sides of the boundary conditions by the cut-off function χ_j, which gives an approximated solution $(\tilde{u}_1, \tilde{u}_2)$. This is an element of $[\mathcal{V}_{\tilde{\eta}}^1(\Omega)]^2$ for any $\tilde{\eta} \in \mathbb{R}$.

5.2 Formulation with boundary integral equations

5.2.1 Potentials

Our goal is to represent the shape derivatives using single-layer and double layer potentials using the α-quasiperiodic fundamental solutions

$$\Psi_{k,\alpha}(p) = \frac{i}{4} \sum_{n=-\infty}^{\infty} H_0^{(1)} \left(k\sqrt{(x_1 - 2\pi n)^2 + x_2^2} \right) e^{2\pi i n \alpha}, \qquad p = (x_1, x_2),$$

of the Helmholtz equation. Here, $H_0^{(1)}$ is the Hankel function of the first kind of order 0. From now on, we remove the artificial boundaries of the rectangular cell and consider domains $\Omega^\pm$ which are unbounded in the y-direction.

Definition 5.1. The *single-layer potential* is defined as

$$V_\Gamma \phi(p) := 2 \int_\Gamma \Psi_{k,\alpha}(p-q)\phi(q) ds_q, \qquad p \notin \Gamma$$

and the *double layer potential* is

$$K_\Gamma \phi(p) := 2 \int_\Gamma \phi(q) \partial_{\nu(q)} \Psi_{k,\alpha}(p-q) ds_q, \qquad p \notin \Gamma,$$

with ν pointing into Ω^-.

These potentials provide α-quasiperiodic solutions of the Helmholtz equation

$$\triangle u + k^2 u = 0$$

outside the interface Γ. These solutions satisfy the outgoing-wave condition, i.e. there exist $u_n \in \mathbb{C}$ depending on u such that

$$u(x,y) = \sum_{n=-\infty}^{\infty} u_n e^{i(n+\alpha)x_1 \pm i\beta_n x_2} \tag{5.6}$$

if $|x_2|$ is greater than the maximal or minimal x_2 coordinate of the interface. We will make use of the following lemma. It can be found with a complete proof as Lemma 3.1 in [39].

Lemma 5.2 (Representation formula). *Assume that in Ω^+ or in Ω^- the function u satisfies the Helmholtz equation almost everywhere and the radiation condition (5.6), that u is locally in H^1 and that $\triangle u$ belongs locally to L^2. Then u can be represented by*

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

in $\Omega^\pm$.

The definitions of the potentials are not valid for points on the interface Γ. As in classical potential theory, it can be shown that the potentials satisfy the following jump relations (see e.g. [12]). The single-layer potential is continuous across Γ, i.e. we have

$$V_\Gamma^+ \phi(p) = V_\Gamma^- \phi(p) = 2\int_\Gamma \Psi_{k,\alpha}(p-q)\phi(q)ds_q, \qquad p \in \Gamma,$$

with the upper signs $+$ and $-$ denoting the limit of V_Γ from above or below the interface, respectively. We introduce the boundary single-layer potential

$$\mathcal{V}_\Gamma \phi(p) := 2\int_\Gamma \Psi_{k,\alpha}(p-q)\phi(q)ds_q, \qquad p \in \Gamma.$$

The double layer potential has a jump across Γ. More precisely, if we denote the boundary double layer potential by

$$\mathcal{K}_\Gamma \phi(p) := 2\int_\Gamma \phi(q)\partial_{\nu(q)}\Psi_{k,\alpha}(p-q)ds_q + (\beta(p)-1)\phi(p), \qquad p \in \Gamma,$$

where $\beta(p)$ is the quotient of the angle in Ω^+ at p and π, we have

$$K_\Gamma^+ \phi(p) = \mathcal{K}_\Gamma \phi(p) - \phi(p)$$

and

$$K_\Gamma^- \phi(p) = \mathcal{K}_\Gamma \phi(p) + \phi(p).$$

The normal derivative of the single-layer potential exists outside corners and has the jumps

$$(\partial_\nu V_\Gamma)^+ \phi(p) = \mathcal{L}_\Gamma \phi(p) + \phi(p)$$

and

$$(\partial_\nu V_\Gamma)^- \phi(p) = \mathcal{L}_\Gamma \phi(p) - \phi(p),$$

with

$$\mathcal{L}_\Gamma \phi(p) := 2\int_\Gamma \phi(q)\partial_{\nu(p)}\Psi_{k,\alpha}(p-q)ds_q, \qquad p \in \Gamma \backslash \mathcal{S},$$

where $\mathcal{S}$ denotes the set of corners. Because of the tangential derivatives that occur in the transmission condition of the conical diffraction problem, we also need the operator

$$\mathcal{J}_\Gamma\phi(p) := \partial_\tau \mathcal{V}_\Gamma\phi(p) = 2\int_\Gamma \phi(q)\partial_{\tau(p)}\Psi_{k,\alpha}(p-q)ds_q, \qquad p \in \Gamma\backslash\mathcal{S}. \tag{5.7}$$

Note that this is a sigular integral, which has to be understood in the Cauchy principal value sense. Due to [39], the boundary integral operators have the following mapping properties.

Lemma 5.3. *Let Γ be a piecewise C^2 curve. Then the boundary integral operators for the Helmholtz equation map boundedly*

$$\mathcal{V}_\Gamma : H^{s-1}(\Gamma) \to H^s(\Gamma), \qquad \mathcal{K}_\Gamma : H^t(\Gamma) \to H^t(\Gamma), \qquad \mathcal{L}_\Gamma, \mathcal{J}_\Gamma : H^{-t}(\Gamma) \to H^{-t}(\Gamma)$$

for $s \in (0,1)$ and $t \in [0,1)$.

5.2.2 Boundary integral equations for the shape derivative

Now we give an integral equation formulation for the transmission problem describing the shape derivatives. Making use of the cut-off ansatz explained at the beginning of this chapter, we can assume that all direct solutions and shape derivatives considered from now on are sufficiently smooth. However, they are only approximations of the original direct solutions and their shape derivatives. We will start with the original problem (2.9), (2.10), (2.12), (2.14). Inserting the boundary conditions $[u_1]_\Gamma = -u_1^{(i)}$ and $[u_2]_\Gamma = -u_2^{(i)}$ into the first two equations of (2.12), we get

$$\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu\left(u_1^+ + u_1^{(i)}\right) - \frac{\omega\varepsilon_-}{\kappa_-^2}\partial_\nu u_1^- - \frac{\gamma(\kappa_-^2-\kappa_+^2)}{\kappa_-^2\kappa_+^2}\partial_\tau u_2^- = 0$$

and

$$-\frac{\omega\mu}{\kappa_+^2}\partial_\nu\left(u_2^+ + u_2^{(i)}\right) + \frac{\omega\mu}{\kappa_-^2}\partial_\nu u_2^- - \frac{\gamma(\kappa_-^2-\kappa_+^2)}{\kappa_-^2\kappa_+^2}\partial_\tau u_1^- = 0.$$

Using the same methods as in the previous section, we can take the shape derivatives and get

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

$$
\begin{aligned}
-\frac{\omega\mu}{\kappa_+^2}\partial_\nu(u_2^+)' + \frac{\omega\mu}{\kappa_-^2}\partial_\nu(u_2^-)' - \frac{\gamma(\kappa_-^2-\kappa_+^2)}{\kappa_-^2\kappa_+^2}\partial_\tau(u_1^-)'& \\
= \operatorname{div}_\Gamma\left((T\cdot\nu)\left\{\frac{\omega\mu}{\kappa_-^2}\nabla u_2^{-,0}|_\tau - \frac{\omega\mu}{\kappa_+^2}\nabla u_2^{+,0}|_\tau - \frac{\gamma(\kappa_-^2-\kappa_+^2)}{\kappa_-^2\kappa_+^2}\nabla^\perp u_1^{-,0}|_\tau\right\}\right)& \\
- \tilde\kappa(T\cdot\nu)\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu u_2^{(i)} + \frac{\omega\varepsilon_+}{\kappa_+^2}\left(\nu\cdot\nabla u_2^{(i)}\right)' + (T\cdot\nu)\left[\omega\mu u_2^0\right]_\Gamma - \sum_{j=1}^m \zeta_{2,j}.& \qquad (5.8)
\end{aligned}
$$

To simplify the notation, we define

$$
\begin{aligned}
h_1 :=& \operatorname{div}_\Gamma\left((T\cdot\nu)\left\{\frac{\omega\varepsilon_+}{\kappa_+^2}\nabla u_1^{+,0}|_\tau - \frac{\omega\varepsilon_-}{\kappa_-^2}\nabla u_1^{-,0}|_\tau - \frac{\gamma(\kappa_-^2-\kappa_+^2)}{\kappa_-^2\kappa_+^2}\nabla^\perp u_2^{-,0}|_\tau\right\}\right) \\
&- \tilde\kappa(T\cdot\nu)\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu u_1^{(i)} + \frac{\omega\varepsilon_+}{\kappa^2}\left(\nu\cdot\nabla u_1^{(i)}\right)' + (T\cdot\nu)\left[\omega\varepsilon u_1^0\right]_\Gamma - \sum_{j=1}^m \zeta_j, \\
h_2 :=& \operatorname{div}_\Gamma\left((T\cdot\nu)\left\{\frac{\omega\mu}{\kappa_-^2}\nabla u_2^{-,0}|_\tau - \frac{\omega\mu}{\kappa_+^2}\nabla u_2^{+,0}|_\tau - \frac{\gamma(\kappa_-^2-\kappa_+^2)}{\kappa_-^2\kappa_+^2}\nabla^\perp u_1^{-,0}|_\tau\right\}\right) \\
&- \tilde\kappa(T\cdot\nu)\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu u_2^{(i)} + \frac{\omega\varepsilon_+}{\kappa_+^2}\left(\nu\cdot\nabla u_2^{(i)}\right)' + (T\cdot\nu)\left[\omega\mu u_2^0\right]_\Gamma - \sum_{j=1}^m \zeta_j.
\end{aligned}
$$

Furthermore, we have

$$
\begin{aligned}
\left[u_1'\right]_\Gamma =& g_1, \\
\left[u_2'\right]_\Gamma =& g_2.
\end{aligned} \qquad (5.9)
$$

with

$$
g_1 := \left(u_1^{(i)}\right)', \qquad g_2 := \left(u_2^{(i)}\right)'.
$$

Due to Lemma 5.2, we can represent $(u_1^+)'$ as

$$
2(u_1^+)' = V_{\Gamma,+}\partial_\nu(u_1^+)' - K_{\Gamma,+}(u_1^+)'. \qquad (5.10)
$$

By $V_{\Gamma,+}$ and $K_{\Gamma,+}$ we denote the potentials with respect to the fundamental solution in Ω^+. The jump relations on Γ yield

$$
2(u_1^+)' = \mathcal{V}_\Gamma^+\partial_\nu(u_1^+)' + (I-\mathcal{K}_\Gamma^+)(u_1^+)'. \qquad (5.11)
$$

on Γ. We seek $(u_1^-)'$ as a single-layer potential

$$
(u_1^-)' = V_{\Gamma,-}\rho \qquad (5.12)
$$

in Ω^- with a density function $\rho \in H^{-1/2}(\Gamma)$. Here, the jump relations give

$$
(u_1^-)' = \mathcal{V}_\Gamma^-\rho, \qquad \partial_\nu(u_1^-)' = (\mathcal{L}_\Gamma^- - I)\rho \qquad (5.13)
$$

on Γ. Analogously, we can write

$$2(u_2^+)' = V_{\Gamma,+}\partial_\nu(u_2^+)' - K_{\Gamma,+}(u_2^+)'. \tag{5.14}$$

and use the ansatz

$$(u_2^-)' = V_{\Gamma,-}\sigma \tag{5.15}$$

with a second density function $\sigma \in H^{-1/2}(\Gamma)$. Again, the jump relations give

$$2(u_2^+)' = \mathcal{V}_\Gamma^+\partial_\nu(u_2^+)' + (I - \mathcal{K}_\Gamma^+)(u_2^+)' \tag{5.16}$$

and

$$(u_2^-)' = \mathcal{V}_\Gamma^-\sigma, \qquad \partial_\nu(u_2^-)' = (\mathcal{L}_\Gamma^- - I)\sigma. \tag{5.17}$$

From equation (5.11) it follows that

$$0 = \mathcal{V}_\Gamma^+\frac{\omega\varepsilon_+}{\kappa_+^2}\partial_\nu(u_1^+)' - (I + \mathcal{K}_\Gamma^+)\frac{\omega\varepsilon_+}{\kappa_+^2}(u_1^+)'.$$

Inserting the transmission conditions (5.8) and (5.9) into this equation yields

$$\mathcal{V}_\Gamma^+\left\{\frac{\omega\varepsilon_-}{\kappa_-^2}\partial_\nu(u_1^-)' + \frac{\gamma(\kappa_-^2 - \kappa_+^2)}{\kappa_-^2\kappa_+^2}\partial_\tau(u_2^-)' + h_1\right\} - (I + \mathcal{K}_\Gamma^+)\frac{\omega\varepsilon_+}{\kappa_+^2}\left\{(u_1^-)' + g_1\right\} = 0.$$

Together with (5.13) and (5.7) we get

$$\begin{aligned}\frac{\omega\varepsilon_-}{\kappa_-^2}\mathcal{V}_\Gamma^+(\mathcal{L}_\Gamma^- - I)\rho - \frac{\omega\varepsilon_+}{\kappa_+^2}(I + \mathcal{K}_\Gamma^+)\mathcal{V}_\Gamma^-\rho + \frac{\gamma(\kappa_-^2 - \kappa_+^2)}{\kappa_-^2\kappa_+^2}\mathcal{V}_\Gamma^+\mathcal{J}_\Gamma^-\sigma& \\ = -\mathcal{V}_\Gamma^+h_1 + \frac{\omega\varepsilon_+}{\kappa_+^2}(I + \mathcal{K}_\Gamma^+)g_1& \\ =: r_1.&\end{aligned} \tag{5.18}$$

In the same way it follows that

$$\begin{aligned}\frac{\omega\mu}{\kappa_-^2}\mathcal{V}_\Gamma^+(\mathcal{L}_\Gamma^- - I)\sigma - \frac{\omega\mu}{\kappa_+^2}(I + \mathcal{K}_\Gamma^+)\mathcal{V}_\Gamma^-\sigma - \frac{\gamma(\kappa_-^2 - \kappa_+^2)}{\kappa_-^2\kappa_+^2}\mathcal{V}_\Gamma^+\mathcal{J}_\Gamma^-\rho& \\ = -\mathcal{V}_\Gamma^+h_2 + \frac{\omega\mu}{\kappa_+^2}(I + \mathcal{K}_\Gamma^+)g_2& \\ =: r_2.&\end{aligned} \tag{5.19}$$

All in all, we have a system

$$\mathbf{A}\begin{pmatrix}\rho\\ \sigma\end{pmatrix} = \begin{pmatrix}r_1\\ r_2\end{pmatrix} \tag{5.20}$$

with

$$\mathbf{A} = \begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix}$$

and

$$A_{11} = \frac{\omega\varepsilon_-}{\kappa_-^2}\mathcal{V}_\Gamma^+(\mathcal{L}_\Gamma^- - I) - \frac{\omega\varepsilon_+}{\kappa_+^2}(I + \mathcal{K}_\Gamma^+)\mathcal{V}_\Gamma^-$$
$$A_{12} = \frac{\gamma(\kappa_-^2 - \kappa_+^2)}{\kappa_-^2\kappa_+^2}\mathcal{V}_\Gamma^+\mathcal{J}_\Gamma^-$$
$$A_{21} = -\frac{\gamma(\kappa_-^2 - \kappa_+^2)}{\kappa_-^2\kappa_+^2}\mathcal{V}_\Gamma^+\mathcal{J}_\Gamma^-$$
$$A_{22} = \frac{\omega\mu}{\kappa_-^2}\mathcal{V}_\Gamma^+(\mathcal{L}_\Gamma^- - I) - \frac{\omega\mu}{\kappa_+^2}(I + \mathcal{K}_\Gamma^+)\mathcal{V}_\Gamma^-.$$

The matrix operator $\mathbf{A}$ is a bounded operator

$$\mathbf{A} : [H^{s-1}(\Gamma)]^2 \to [H^s(\Gamma)]^2$$

for $s \in (0,1)$, cf. Chapter 4.1. in [40].

5.2.3 Equivalence and solvability of the integral equations

We recall here some results from [40] and investigate properties of the system (5.20) of integral equations. Because of the ansatz we made in (5.12) and (5.15), it is clear that if u_1' and u_2' solve the diffraction problem given in Theorem 4.3, then ρ and σ solve the system (5.20) if $\mathcal{V}_\Gamma^+$ is invertible. The following result is similar to Lemma 4.1. in [40].

Proposition 5.1. *Let $\rho, \sigma \in H^{-1/2}(\Gamma)$ solve (5.20). If the kernel of the single-layer potential $\mathcal{V}_\Gamma^+$ is trivial, then the functions*

$$(u_1^+)' = \frac{1}{2}\left(aV_{\Gamma,+}(\mathcal{L}_\Gamma^- - I)\rho + V_{\Gamma,+}\frac{\kappa_+^2}{\omega\varepsilon_+}h_1 - K_{\Gamma,+}\mathcal{V}_\Gamma^-\rho - K_{\Gamma,+}g_1 + c_1V_{\Gamma,+}\mathcal{J}_\Gamma^-\sigma\right)$$
$$(u_2^+)' = \frac{1}{2}\left(bV_{\Gamma,+}(\mathcal{L}_\Gamma^- - I)\sigma - V_{\Gamma,+}\frac{\kappa_+^2}{\omega\mu}h_2 - K_{\Gamma,+}\mathcal{V}_\Gamma^-\sigma - K_{\Gamma,+}g_2 - c_2V_{\Gamma,+}\mathcal{J}_\Gamma^-\rho\right)$$

with

$$a = \frac{\varepsilon_-\kappa_+^2}{\varepsilon_+\kappa_-^2}, \qquad b = \frac{\kappa_+^2}{\kappa_-^2}, \qquad c_1 = \frac{\gamma(\kappa_-^2 - \kappa_+^2)}{\omega\varepsilon_+\kappa_-^2}, \qquad c_2 = \frac{\gamma(\kappa_-^2 - \kappa_+^2)}{\omega\mu\kappa_-^2}$$

and

$$(u_1^-)' = V_{\Gamma,-}\rho, \qquad (u_2^-)' = V_{\Gamma,-}\sigma \tag{5.21}$$

solve the homogeneous Helmholtz equation in Ω^+ and in Ω^-, respectively. Additionally, they satisfy the radiation condition (5.6) and the transmission conditions (5.8) and (5.9).

Proof. Analogous to the proof of Lemma 4.1 in [39], we see that the single-layer potentials (5.21) solve the homogeneous Helmholtz equation in Ω^- and satisfy the outgoing-wave condition (5.6). By using (5.21) and the jump relations (cf. equations (5.13) and (5.17)), we get

$$
\begin{aligned}
(u_1^+)' &= \frac{1}{2}\left(V_{\Gamma,+}\left(a\partial_\nu(u_1^-)' + c_1\partial_\tau(u_2^-)' + \frac{\kappa_+^2}{\omega\varepsilon_+}h_1\right) - K_{\Gamma,+}\left((u_1^-)' + g_1\right)\right),\\
(u_2^+)' &= \frac{1}{2}\left(V_{\Gamma,+}\left(b\partial_\nu(u_2^-)' - c_2\partial_\tau(u_1^-)' - \frac{\kappa_+^2}{\omega\mu}h_2\right) - K_{\Gamma,+}\left((u_2^-)' + g_2\right)\right),
\end{aligned}
\tag{5.22}
$$

which are locally in H^1 in the interior of Ω^+ and satisfy $\triangle(u_j^+)' + \kappa_+^2(u_j^+)' = 0$ for $j = 1, 2$. The boundary values of these functions are

$$
\begin{aligned}
(u_1^+)'|_\Gamma &= \frac{1}{2}\left(\mathcal{V}_\Gamma^+\left(a\partial_\nu(u_1^-)' + c_1\partial_\tau(u_2^-)' + \frac{\kappa_+^2}{\omega\varepsilon_+}h_1\right) + (I - \mathcal{K}_\Gamma^+)\left((u_1^-)' + g_1\right)\right),\\
(u_2^+)'|_\Gamma &= \frac{1}{2}\left(\mathcal{V}_\Gamma^+\left(b\partial_\nu(u_2^-)' - c_2\partial_\tau(u_1^-)' - \frac{\kappa_+^2}{\omega\mu}h_2\right) + (I - \mathcal{K}_\Gamma^+)((u_2^-)' + g_2)\right)
\end{aligned}
\tag{5.23}
$$

A direct consequence of (5.20) and $\partial_\nu(u_1^-)'|_\Gamma = (\mathcal{L}_\Gamma^- - I)\rho$ is

$$
\begin{aligned}
a\mathcal{V}_\Gamma^+\partial_\nu(u_1^-)' + (I - \mathcal{K}_\Gamma^+)(u_1^-)' + c_1\mathcal{V}_\Gamma^+\partial_\tau(u_2^-)' &= \left(2(u_1^-)' + \frac{\kappa_+^2}{\omega\varepsilon^+}r_1\right)|_\Gamma,\\
b\mathcal{V}_\Gamma^+\partial_\nu(u_2^-)' + (I - \mathcal{K}_\Gamma^+)(u_2^-)' - c_2\mathcal{V}_\Gamma^+\partial_\tau(u_1^-)' &= \left(2(u_2^-)' + \frac{\kappa_+^2}{\omega\mu}r_2\right)|_\Gamma,
\end{aligned}
$$

with r_1 and r_2 from (5.18) and (5.19). Plugging this into (5.23), we get

$$
(u_1^+)' - (u_1^-)' = g_1, \qquad (u_2^+)' - (u_2^-)' = g_2.
$$

on Γ. Using this and (5.11) and (5.16) in (5.22) implies

$$
\mathcal{V}_\Gamma^+\left(a\partial_\nu(u_1^-)' + c_1\partial_\tau(u_2^-)' + \frac{\kappa_+^2}{\omega\varepsilon_+}h_1\right) = (I + \mathcal{K}_\Gamma^+)(u_1^+)' = \mathcal{V}_\Gamma^+\partial_\nu(u_1^+)'
$$

and

$$
\mathcal{V}_\Gamma^+\left(b\partial_\nu(u_2^-)' - c_2\partial_\tau(u_1^-)' - \frac{\kappa_+^2}{\omega\mu}h_2\right) = (I + \mathcal{K}_\Gamma^+)(u_2^+)' = \mathcal{V}_\Gamma^+\partial_\nu(u_2^+)'.
$$

Therefore, the boundary conditions (5.8) are satisfied if $\mathcal{V}_\Gamma^+$ has a trivial kernel. □

The question of invertibility of $\mathcal{V}_\Gamma^\pm$ in answered by Corollary 3.2. in [39]. It is cited in the following proposition.

Proposition 5.2. *The operator $\mathcal{V}_\Gamma^\pm : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ has a trivial kernel if and only if the homogeneous Dirichlet problems*

$$
\begin{aligned}
\triangle u + \kappa_\pm^2 &= 0 \quad \text{in} \quad \Omega^\pm\\
u &= 0 \quad \text{on} \quad \Gamma
\end{aligned}
$$

with radiation conditions (5.6) have only the trivial solution.

Now let $\gamma(t) = (\gamma_1(t), \gamma_2(t))$ ba a piecewise C^2 parametrization of the interface Γ such that

$$\gamma_1(t+1) = \gamma_1(t) + 2\pi, \qquad \gamma_2(t+1) = \gamma_2(t)$$

and

$$|\gamma'(t)| = \sqrt{[\gamma_1'(t)]^2 + [\gamma_2'(t)]^2} > 0$$

for $t \in \mathbb{R}$. Moreover, let $\gamma(t_1) \neq \gamma(t_2)$ if $t_1 \neq t_2$. Then we define the closed curve

$$\tilde{\Gamma} := \{e^{-\gamma_2(t)}(\cos\gamma_1(t), \sin\gamma_1(t)) : t \in [0,1]\}.$$

The curve Γ has the same smoothness properties as Γ and every corner of $\tilde{\Gamma}$ has the same opening angle as the corresponding corner on Γ. Let

$$\Phi(x) := -\frac{1}{2\pi} \log|x|$$

be the fundamental solution of the Laplacian in $\mathbb{R}^2$. Now we define the boundary integral operators $\mathcal{V}_{\tilde{\Gamma}}$, $\mathcal{K}_{\tilde{\Gamma}}$, $\mathcal{L}_{\tilde{\Gamma}}$ and $\mathcal{J}_{\tilde{\Gamma}}$ in the same way as the operators $\mathcal{V}_\Gamma$, $\mathcal{K}_\Gamma$, $\mathcal{L}_\Gamma$ and $\mathcal{J}_\Gamma$ in Chapter 5.2.1 by replacing Γ with $\tilde{\Gamma}$ and Ψ with Φ.

Remark 5.1. We cite the following result from [39]. Let $H_p^s(\Gamma)$ be the space of functions which are α-quasiperiodic in x_1 and belong to $H^s(\Gamma)$ and let $\Phi_0(X)$ be the set of bounded Fredholm operators with index 0 in the space X. If

$$(\varepsilon_+ + \varepsilon_-)I_{\tilde{\Gamma}} + (\varepsilon_+ - \varepsilon_-)\mathcal{K}_{\tilde{\Gamma}} \in \Phi_0\left(H_p^{1/2}(\tilde{\Gamma})\right), \tag{5.24}$$

then the matrix $\mathbf{A} : [H^{-1/2}(\Gamma)]^2 \to [H^{1/2}(\Gamma)]^2$ is a Fredholm operator with index 0. If $\tilde{\Gamma}$ is sufficienty smooth, then (5.24) is satisfied if $\varepsilon_+ \neq -\varepsilon_-$. □

5.3 Computed Rayleigh coefficients

In this section we give a few examples for derivatives of Rayleigh coefficients of transmitted fields with respect to perturbations of the interface Γ. We consider only classical TE and TM diffraction. In all examples, we assume that Γ is illuminated from above by an incoming plane wave

$$(u_1^{(i)}, u_2^{(i)})(x,y) = (p,q)e^{i\alpha x_1 - i\beta x_2}. \tag{5.25}$$

The material constants are chosen to have the values

$$\mu = 1, \qquad \varepsilon_+ = 1, \qquad \varepsilon_- = 2$$

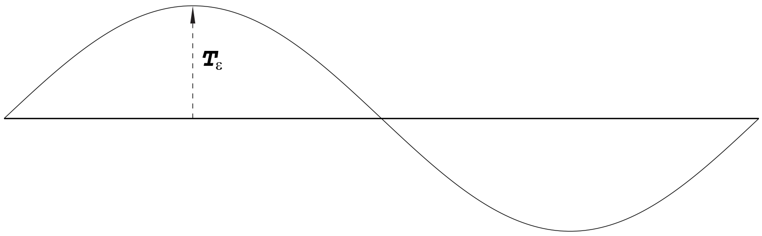

Figure 5.2: Sinusoidal perturbation of a flat grating

and the wavelength λ of the incoming wave is chosen such that

$$\frac{d}{\lambda} = 2,$$

where d is the grating period, and the incident angle is set to be $\pi/4$. In this case, the sum

$$u_j^-(x_1, x_2) = \sum_{n=-\infty}^{\infty} A_{j,n}^- e^{i(\alpha+n)x_1 - i\beta_n^- x_2},$$

contains at most six outgoing modes, because $\beta_{-4}^-, \ldots, \beta_1^- \in \mathbb{R}$ and all other β_n^- have a non-zero imaginary part. We compute the shape derivative in direction T_ϵ of the transmitted modes and compare these with a forward difference. More precisely, if $u_j^{-,\epsilon}$ is the solution for the perturbed interface and

$$u_j^{-,\epsilon}(x_1, x_2) = \sum_{n=-\infty}^{\infty} A_{j,n}^{-,\epsilon} e^{i(\alpha+n)x_1 - i\beta_n^- x_2},$$

then

$$A_{j,n}^{-,\epsilon} - A_{j,n}^- \approx (A_{j,n}^-)'(T_\epsilon)$$

should hold. First we consider a smooth perturbation T_ϵ of a flat grating $\Gamma = \{(x_1, 0) : x_1 \in [0, 2\pi)\}$ such that the perturbed interface Γ_ϵ is represented by

$$\Gamma_\epsilon = \{(x_1, T_\epsilon(x_1))\} = \{(x_1, \epsilon \sin x_1) : x_1 \in [0, 2\pi)\},$$

where $\epsilon = 0.01\pi$. The results are in Table 5.1, which shows the TE modes, and in Table 5.2 for TM polarization. The first two columns contain the orders of the outgoing modes and the angle of their direction. The next columns show the Rayleigh coefficients of the unperturbed solution, the Rayleigh coefficients of the solution with respect to the perturbed interface, the difference of those two quantities, and finally the computed shape derivative in direction T_ϵ. All coefficients are given as multiples of the coefficients p and q in (5.25). The biggest difference between $A_{j,n}^{-,\epsilon} - A_{j,n}^-$ and $(A_{j,n}^-)'(T_\epsilon)$ is in the TE mode of first order, where

$$|A_{1,1}^{-,\epsilon} - A_{1,1}^- - (A_{1,1}^-)'(T_\epsilon)| \approx 6.3 \cdot 10^{-4}$$

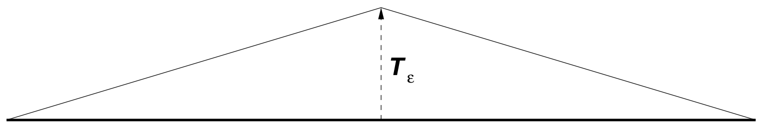

Figure 5.3: Triangular perturbation of a flat grating

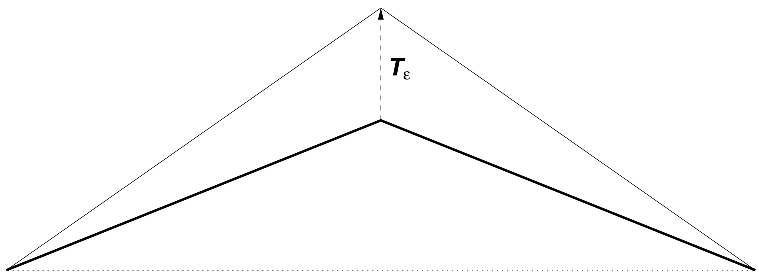

Figure 5.4: Triangular perturbation of a flat grating

The next case we consider is a triangular perturbation of a flat grating, which is illustrated in Figure 5.3. The results are in Table 5.3 and 5.4. The biggest error here occurs also in the TE mode of first oder, where now

$$|A_{1,1}^{-,\epsilon} - A_{1,1}^{-} - (A_{1,1}^{-})'(T_\epsilon)| \approx 6.4 \cdot 10^{-4}.$$

Finally we show the TE case for a triangular perturbation of a triangular grating, as illustrated in Figure 5.4. The largest error here occurs also in the mode of first order, where

$$|A_{1,1}^{-,\epsilon} - A_{1,1}^{-} - (A_{1,1}^{-})'(T_\epsilon)| \approx 10.6 \cdot 10^{-4}.$$

The average error over all modes is

$$\frac{1}{6}\sum_{n=-4}^{1}\left|A_{1,n}^{-,\epsilon} - A_{1,n}^{-} - (A_{1,n}^{-})'(T_\epsilon)\right| \approx 5.5 \cdot 10^{-4}.$$

Consider again the cut-off function

$$\chi_j(r,\varphi) := \psi\left(\frac{r - 2^{-(j+1)}}{2^{-j}}\right) \tag{5.26}$$

defined in Section 5.1.1. The optimal choice of the cut-off function clearly depends at the same time on the singularities at the corners and on the discretization. If the discretization is coarse and the singularities are mild, then it might be the best choice to forego the cut-off completely. Also for the example of a triangular perturbation of a triangular grating given here, no cut off was necessary, even though 600 collocation points were used. In general, if the singulatities are mild, then j in the definition of χ_j can be chosen to be large, and if the singularities are severe, then j needs to be smaller. It would be interesting to find a general strategy how to choose the cut-off function and the discetization simultaneously. This was not possible the course of this work.

mode	angle	$A^{-}_{1,n} \cdot 10$	$A^{-,\epsilon}_{1,n} \cdot 10$	$(A^{-,\epsilon}_{1,n} - A^{-}_{1,n}) \cdot 10$	$(A^{-}_{1,n})' \cdot 10$
-4	-66.09	0	0	0	0
-3	-34.10	0	0	0	0
-2	-11.95	0	(0.001, 0.000)	(0.001, 0.000)	0
-1	8.42	0	(-0.095, 0.000)	(-0.095, 0.000)	(-0.097, 0.003)
0	30.00	(7.320, 0.000)	(7.318, 0.003)	(0.002, 0.003)	0
1	58.60	0	(0.169, -0.155)	(0.169, -0.155)	(0.166, -0.149)

Table 5.1: flat grating, sinus perturbation, TE polarisation

mode	angle	$A^{-}_{1,n} \cdot 10$	$A^{-,\epsilon}_{1,n} \cdot 10$	$(A^{-,\epsilon}_{1,n} - A^{-}_{1,n}) \cdot 10$	$(A^{-}_{1,n})' \cdot 10$
-4	-66.09	0	0	0	0
-3	-34.10	0	0	0	(0, 0.001)
-2	-11.95	0	(-0.001, 0.000)	(-0.001, 0.000)	0
-1	8.42	0	(-0.095, 0.000)	(-0.095, 0.000)	(-0.095, 0.001)
0	30.00	(7.579, 0)	(7.577, 0.001)	(-0.002, 0.001)	0
1	58.60	0	(0.176, -0.055)	(0.176, -0.055)	(0.174, -0.055)

Table 5.2: flat grating, sinus perturbation, TM polarisation

mode	angle	$A^{-}_{1,n} \cdot 10$	$A^{-,\epsilon}_{1,n} \cdot 10$	$(A^{-,\epsilon}_{1,n} - A^{-}_{1,n}) \cdot 10$	$(A^{-}_{1,n})' \cdot 10$
-4	-66.09	0	0	0	0
-3	-34.10	0	(0.000, 0.012)	(0.000, 0.012)	(0.000, 0.012)
-2	-11.95	0	(0.001, 0.000)	(0.001, (0.000)	0
-1	8.42	0	(0.004, -0.078)	(0.004, -0.078)	(0.003, -0.078)
0	30.00	(7.320, 0)	(7.315, 0.240)	(-0.005, 0.240)	(-0.007, 0.238)
1	58.60	0	(-0.126 -0.138)	(-0.126, -0.138)	(-0.122, -0.133)

Table 5.3: flat grating, triangular perturbation, TE polarisation

mode	angle	$A^-_{1,n} \cdot 10$	$A^{-,\epsilon}_{1,n} \cdot 10$	$(A^{-,\epsilon}_{1,n} - A^-_{1,n}) \cdot 10$	$(A^-_{1,n})' \cdot 10$
-4	-66.09	0	0	0	0
-3	-34.10	0	(0.000, 0.002)	(0.000, 0.002)	(0.000, 0.002)
-2	-11.95	0	0	0	0
-1	8.42	0	(0.003, -0.077)	(0.003, -0.077)	(0.004, -0.077)
0	30.00	(7.579, 0.000)	(7.573, 0.247)	(-0.006, 0.247)	(-0.003, 0.247)
1	58.60	0	(-0.044, -0.143)	(-0.044, -0.143)	(-0.042, -0.141)

Table 5.4: flat grating, triangular perturbation, TM polarisation

mode	angle	$A^-_{1,n} \cdot 10$	$A^{-,\epsilon}_{1,n} \cdot 10$	$(A^{-,\epsilon}_{1,n} - A^-_{1,n}) \cdot 10$	$(A^-_{1,n})' \cdot 10$
-4	-66.09	(-0.029, 0.265)	(-0.040, 0.271)	(-0.011, 0.006)	(-0.009, 0.006)
-3	-34.10	(-0.301, 0.062)	(-0.308, 0.050)	(-0.007, -0.012)	(-0.006, -0.013)
-2	-11.95	(-0.320, 0.891)	(-0.391, 0.906)	(-0.071, 0.015)	(-0.069, 0.020)
-1	8.42	(2.013, 1.255)	(1.972, 1.393)	(-0.041, 0.137)	(-0.035, 0.140)
0	30.00	(0.112, 5.983)	(-0.131, 5.950)	(-0.243, -0.032)	(-0.239, -0.032)
1	58.60	(-2.439, -3.864)	(-2.420, -3.892)	(0.020, -0.028)	(0.027, -0.022)

Table 5.5: triangular grating, triangular perturbation, TE polarisation

5.4 Another possible numerical approach

The cut-off ansatz seems to be relatively crude. Another method to deal with low regularity of solutions is the so-called dual singular function method. We give only a short overview without any proofs. Details can be found in [7], from which the following results are taken.

For the Dirichlet problem for the Laplace equation

$$\begin{aligned} -\triangle u &= f \qquad \text{in} \qquad \Omega \subset \mathbb{R}^2 \\ u &= 0 \qquad \text{on} \qquad \partial\Omega \end{aligned} \tag{5.27}$$

with Ω being a bounded domain with a corner S, the solution u admits an expansion

$$u = \sum_{j=1}^{n} k_j s_j + w$$

with

$$s_j(r,\theta) = \chi_S(r) r^{\frac{j\pi}{\omega}} \sin \frac{j\pi\theta}{\omega}$$

for $j \in \mathbb{N}$ with polar coordinates (r, θ) centered at the corner, χ_S is a smooth cut-off function near the corner S, ω is the interior angle at S and w is a function with a higher regularity than u. The singular functions for the adjoint operator are

$$s_{-j}(r,\theta) = \chi_S(r) r^{-\frac{j\pi}{\omega}} \sin \frac{j\pi\theta}{\omega}.$$

The constants k_j are given by (see [7], Theorem 2.1)

$$k_j = \frac{1}{i\pi} \left\{ (f, s_{-j}) + (u, \triangle s_{-j}) \right\}.$$

The dual singular function method then consists in the following iterative procedure. First set $k_j^0 = 0$ for $j = 1, \ldots, n$. Then determine the approximate functions u_h^j, w_h^j from a finite-element space F_h by

$$J(w_h^i, v_h) = \left(f + \sum_{j=1}^{n} k_j^{i-1} \triangle s_j, v_h \right)_{L^2(\Omega)} \qquad \text{for all} \qquad v_h \in F_h,$$

$$u_h^i = w_h^i + \sum_{j=1}^{n} k_j^{i-1} s_j,$$

$$k_j^i = \frac{1}{i\pi} \int_\Omega (f s_{-j} + u_h^i \triangle s_{-j}), \qquad j = 1, \ldots, n,$$

where J is the bilinear form of the variational formulation of the problem (5.27). Let u_h be the projection of u on the finite-element space F_h. For the first iterate of the above iterative procedure we have $u_h^1 = u_h$. The limit for $i \to \infty$ is denoted by $\tilde{u}_h$, analogously for the limit of $\tilde{k}_j^i$. Then it can be shown that if $||\cdot||$ is the norm of a Sobolev space in which $s_{j,h}$ converges to s_j for $h \to 0$, then

$$||u - \tilde{u}_h|| + \sum_{j=1}^{n} |k_j - \tilde{k}_j^h| \leq C||w - w_h||,$$

i.e. $\tilde{u}_h$ converges to u as fast as the finite-element approximation of the regular part w_h converges to w.

A similar method has been proposed by Bochniak [8] for boundary element methods for more general boundary value problems. One of the crucial difficulties in this method is the exact computation of the singularities. This is not possible for our diffraction problems, as explained in Chapter 3. One could ask, however, whether this method could also be employed with only approximated singularities.

6 Summary and perspective

In this thesis, the theory about regularity of solutions to elliptic boundary value problems in non-smooth domains in Kondratiev's weighted Sobolev spaces has been used to prove an a priori estimate for solutions of conical diffraction problems. By a standard result, this a priori estimate is equivalent to the semi-Fredholm property, i.e. the property that the operator of the problem has a finite-dimensional kernel and that its rank is closed. By constructing a right regularizer, it was then shown that the dimension of the cokernel is also finite and that the operator therefore has the Fredholm property. Subsequently, the Fredholm property was used to extend a result from [14] about uniqueness of solutions in standard Sobolev spaces to Kondratiev spaces V^2_η with $\eta > 0$, which are not embedded in H^2. With the help of non-local perturbation theory, the a priori estimate and the uniqueness result, it was then possible to prove existence of shape derivatives of solutions to conical diffraction problems. Additionally, a characterization of these shape derivatives has been obtained. In particular, it was shown that the shape derivative solves a diffraction problem which has the same operator, but different right-hand sides than the original problem. Moreover, the right-hand sides of the transmission conditions involve terms which are concentrated on the corner points. Since the direct solutions are not in H^2, the shape derivatives do not have H^1 regularity due to the singularities at the corner points. Finally, a boundary integral equation approach has been suggested as an ansatz for the numerical computation of shape derivatives. To overcome the difficulties arising from the corner singularities of the solutions, an ansatz that consists in cutting off the singularities has been proposed. The actual numerical computations, however, definitely need improvement because only TE and TM diffraction and no actual conical diffraction could be treated so far. The relatively large errors also need to be studied, although the reasons probably lie in the implementation and not in the analysis of the problem. Finally, it would be desirable to implement an optimization algorithm that can be used for shape reconstruction.

One of the next steps could be to extend the theory for interfaces that are invariant in one direction to biperiodic interfaces. The structure of this problem is different in this case, since a reduction to a system of Helmholtz equations is not possible any more and the full time-harmonic Maxwell system needs to be investigated. It might be possible to use results obtained by Bao, Dobson and Schmidt [5, 41] concerning existence, uniqueness and regularity of solutions in standard Sobolev spaces. These papers are in some sense equivalent to [14], which has been used for the one-dimensional setting. Moreover, there is a theory on Kondratiev spaces on three-dimansional non-smooth domains [31] which extends the original 2D theory developed by Kondratiev. Since three-dimensional domains can have corners and edges, these spaces include two weights, one with respect to the distance to the corners and an additional one with respect to the distance to the edges. It would be interesting to investigate whether and under which additional assumptions a result like Proposition 3.1 can be obtained for the Maxwell interface problem.

Moreover, as already mentioned in the introduction, there are results by Chandler-Wilde and Potthast on scattering by rough surfaces [11]. The surface is in this case not assumed to be periodic, i.e. it can be represented by

$$\Gamma = \{(x_1, x_2) : x_2 = f(x_1), x_1 \in \mathbb{R}\}$$

with a function $f \in C^2(\mathbb{R})$ that has no periodicity. The domain can therefore not be restricted to a bounded cell as in our case. The method used in this work to show shape differentiability of the solutions is the boundary integral equation ansatz also used in [36, 37]. More precisely, the solution of a boundary value problem is represented as a potential, and then the shape derivative of the boundary integral is computed. In [11], only Dirichlet problems are considered. A task could be to find out whether shape derivatives for rough unbounded surfaces can also be treated for interface problems, where in addition the interface is only piecewise smooth.

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List of Figures

List of Tables