Diffraction in Periodic Structures and Optimal Design of Binary Gratings. Part II: Gradient Formulas for TM Polarization

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Abstract: This paper provides the mathematical foundation of analytic formulae for derivatives of TM reflection and transmission coefficients of diffraction gratings with respect to geometric parameters of non–smooth grating profiles and interfaces. This problem arises in optimal design problems for those optical devices studied in Part I. The derivatives can be expressed by contour integrals involving the direct and adjoint solutions of TM diffraction problems.

1. Introduction

Diffractive optics is a modern technology in which optical devices are micromachined with complicated structural features on the order of the length of light waves. Exploiting diffraction effects, those devices can perform functions unattainable with conventional optics. It is widely acknowledged that geometrical optics approximations to the underlying electromagnetic field equations are not accurate for these diffractive elements, hence, their mathematical modelling has to rely on Maxwell's equations or related partial differential equations. The simplest case, the scattering of time–harmonic waves from infinite periodic structures, is a classical problem, dating back to Rayleigh and Bloch. It can be transformed to two quasiperiodic transmission problems for the Helmholtz equation in the whole plane corresponding to the TE and TM polarisation of the incoming wave, respectively. Although various numerical methods have been developed to compute the solution for a given periodic grating (among them a highly accurate integral equation code by A. Pomp, J. Creutziger and B. Kleemann, realized during their work in the group of S. Prößdorf at the Karl–Weierstrass–Institute), rigorous results on the existence and uniqueness of solutions have been obtained only during the last decade; see the references given in part I of this paper [5].

Based on a variational approach to this problem, which goes back to Bonnet-Bendhia & Starling ([1]) and Bao & Dobson (see [2]), it was also possible to develop gradient type optimization methods for finding the optimal design of diffractive gratings with desired far–field patterns. In [5] we derived analytic formulae for derivatives of certain cost functionals involving the reflection and transmission coefficients of so called binary gratings. Roughly speaking, the surface of a binary grating can be given by a periodic step–function separating different optical materials, and the derivatives have to be taken with respect to the width or height of those steps. It turned out that these derivatives can be expressed as one–dimensional integrals over the part of the surface to be varied. In the TE case one has to integrate the product of the solutions of the direct and certain adjoint problem, whereas in the TM case the integrand is the product of their gradients. Unfortunately, due to the singularities of the solutions of TM problems near corners of the grating surface, the product of gradients might be non–integrable. So the formula for the derivatives has to be modified. In [5] we have given, without proof, one of these modifications.

The topic of the present paper is to study in more detail the dependence of the solution of TM diffraction problems with respect to variations of the (non–smooth) grating profile and interfaces between different optical materials. We prove the unique solvability of these problems for quite general small variations of grating profiles and interfaces and obtain different analytic formulae for the derivatives of the reflection and transmission coefficients with respect to these variations, which can be expressed as path–independent contour integrals.

The outline of the paper is as follows. In Section 2, we briefly describe the TE and TM diffraction problems and present their variational formulations and some basic results. In Section

3, we study the perturbation of TM problems arising after sufficiently smooth (piecewise C^1) variations of interfaces. We prove the unique solvability of these perturbed problems and show that the derivative of diffraction coefficients can be expressed as a certain domain integral. This formula is simplified in Section 4 in different ways to get contour integrals or, in the case of strong singularities of solutions, contour integrals plus point functionals. In Section 5 we apply these results to the special case of binary gratings, leading in particular to a simple proof of the above mentioned modified formula.

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2. Variational formulation of TE and TM problems

Consider a diffractive grating with period d consisting of nonmagnetic materials (of permeability μ_0) with different dielectric constants ϵ. The coordinate system is chosen such that the grating is invariant in the x_3–direction and periodic in the x_1–direction. Thus the diffraction problem is determined by the function $\epsilon(x_1, x_2)$ which is d–periodic in x_1. This function is assumed to be piecewise constant and complex valued with $0 \leq \arg \epsilon < \pi$. We assume that the material above and below the grating is homogeneous with $\epsilon = \epsilon^+ > 0$ and ϵ^- respectively.

Assume that an incoming plane wave with time dependence $\exp(-i\omega t)$ is incident in the (x_1, x_2)–plane upon the grating from the top with the angle of incidence $\theta \in (-\pi/2, \pi/2)$. Then the electromagnetic field does not depend on x_3. In either case of polarization, one of the fields $\mathbf{E}$ or $\mathbf{H}$ remains parallel to the x_3–axis and is therefore determined by a single scalar quantity $v = v(x_1, x_2)$ (equal to the transverse component of $\mathbf{E}$ in the TE case and to the transverse component of $\mathbf{H}$ in the TM case). The function v satisfies two–dimensional Helmholtz equations in the regions with constant permittivity, together with some radiation condition at infinity. At the material interfaces the solutions are subjected to well known transmission conditions. For TE polarisation the solution and its normal derivative $\partial_n v$ have to cross the set of interfaces Λ between different materials continuously, whereas in TM polarisation the product $\epsilon^{-1}\partial_n v$ has to be continuous (for more details cf. the classical monograph [7]) .

For notational convenience we will change the length scale by a factor of $2\pi/d$, such that the grating becomes 2π–periodic, $\epsilon(x_1 + 2\pi, x_2) = \epsilon(x_1, x_2)$. Let us introduce the piecewise constant function

$$k = \frac{\omega d}{2\pi}(\mu_0 \epsilon)^{1/2} = \frac{d}{\lambda}\nu\,,$$

where λ is the length of the incoming plane wave and ν is the optical index of the corresponding material. The constant values of k above and below the grating are denoted by k^+ and k^-, respectively.

Then the incoming plane wave is of the form $(\mathbf{E}^i, \mathbf{H}^i) = (\mathbf{p}, \mathbf{q})\, e^{-i\omega t}\, e^{i(\alpha x_1 - \beta x_2)}$, where $\alpha = k^+ \sin\theta$, $\beta = k^+ \cos\theta$, and the total diffracted field can be obtained as superposition of solutions of the TE and TM polarisation cases.

In TE polarization only the x_3–component E_3 of the electric field is different from zero. It is α–quasiperiodic, $E_3(x_1 + 2\pi, x_2) = e^{2\pi i \alpha} E_3(x_1, x_2)$, and satisfies in view of the Maxwell equation the Helmholtz equation

$$\Delta E_3 + k^2 E_3 = 0 \quad \text{in } \mathbf{R}^2\,. \tag{2.1}$$

The radiation condition, that must be imposed for $|x_2| \to \infty$, states that E_3 remains bounded and that it should be representable as superposition of outgoing waves, i.e.

$$\begin{aligned} E_3 &= p_3 e^{-i\beta x_2} + \sum_{n\in\mathbf{Z}} E_n^+ e^{i(n+\alpha)x_1 + i\beta_n^+ x_2} && \text{for } x_2 \to \infty\,, \\ E_3 &= \sum_{n\in\mathbf{Z}} E_n^- e^{i(n+\alpha)x_1 - i\beta_n^- x_2} && \text{for } x_2 \to -\infty\,. \end{aligned} \tag{2.2}$$

where $E_n^\pm$ are complex numbers and

$$\beta_n^\pm = \beta_n^\pm(\alpha) := |(k^\pm)^2 - (n+\alpha)^2|^{1/2}\, e^{i\gamma_n^\pm/2}\,, \quad n \in \mathbf{Z}\,, \tag{2.3}$$

with

$$\gamma_n^\pm = \arg((k^\pm)^2 - (n+\alpha)^2)\,, \quad 0 \le \gamma_n^\pm < 2\pi\,.$$

Note that $\beta_0^+ = \beta$ and that, for real $k^\pm$,

$$\beta_n^\pm = \begin{cases} ((k^\pm)^2 - (n+\alpha)^2)^{1/2}\,, & k^\pm > |n+\alpha|\,, \\ i((n+\alpha)^2 - (k^\pm)^2)^{1/2}\,, & k^\pm < |n+\alpha|\,. \end{cases}$$

In TM polarization only the x_3–component H_3 of the electric field is different from zero. This α–quasiperiodic function satisfies the Helmholtz equation

$$\nabla \cdot \big(\frac{1}{k^2}\nabla H_3\big) + k^2 H_3 = 0 \quad \text{in } \mathbf{R^2}\,. \tag{2.4}$$

together with the radiation condition

$$\begin{aligned} H_3 &= q_3 e^{-i\beta x_2} + \sum_{n\in\mathbf{Z}} H_n^+ e^{i(n+\alpha)x_1 + i\beta_n^+ x_2} && \text{for } x_2 \to \infty\,, \\ H_3 &= \sum_{n\in\mathbf{Z}} H_n^- e^{i(n+\alpha)x_1 - i\beta_n^- x_2} && \text{for } x_2 \to -\infty\,. \end{aligned} \tag{2.5}$$

The diffraction problems admit variational formulations in a bounded periodic cell which were introduced in [1], [2]. Define for example the 2π–periodic function $u = e^{-i\alpha x_1} E_3$. It satisfies the partial differential equation

$$\Delta_\alpha u + k^2 u = 0$$

where we use the notation

$$\nabla_\alpha = \nabla + i(\alpha, 0)\,,\ \Delta_\alpha = \nabla_\alpha \cdot \nabla_\alpha = \Delta + 2i\alpha\partial_{x_1} - \alpha^2$$

The outgoing wave conditions are equivalent to nonlocal boundary conditions on some artificial boundaries $\Gamma^\pm := \{x_2 = \pm b\}$ above and below the grating, respectively, of the form

$$\partial_n u|_{\Gamma^+} = -T_\alpha^+ u - 2p_3 i\beta e^{-i\beta b}\,, \quad \partial_n u|_{\Gamma^-} = -T_\alpha^- u\,, \tag{2.6}$$

where $T_\alpha^\pm u$ is the periodic pseudodifferential operators of order 1

$$(T_\alpha^\pm v)(x) := -\sum_{n\in\mathbf{Z}} i\beta_n^\pm \hat{v}_n e^{inx}\,, \quad \hat{v}_n = (2\pi)^{-1}\int_0^{2\pi} v(x) e^{-inx}\, dx\,, \tag{2.7}$$

acting on boundary values $u|_{\Gamma^\pm} \in H_p^{s-1/2}(\Gamma^\pm)$ of functions $u \in H_p^s(\Omega)$, $s \ge 0$. Here $H_p^s(\Omega)$ denotes restriction to the rectangular domain $\Omega = [0, 2\pi] \times [-b, b]$ of all functions in the Sobolev space $H_{loc}^s(\mathbf{R}^2)$ which are 2π–periodic in x_1. Integration by parts leads to the variational formulation for the TE diffraction problem

$$\begin{aligned} B_{TE}(u,\varphi) &= \int_\Omega \nabla_\alpha u \cdot \overline{\nabla_\alpha \varphi} - \int_\Omega k^2\, u\,\bar\varphi + \int_{\Gamma^+} (T_\alpha^+ u)\,\bar\varphi + \int_{\Gamma^-} (T_\alpha^- u)\,\bar\varphi \\ &= -2ip_3\beta e^{-i\beta b} \int_{\Gamma^+} \bar\varphi\,, \quad \forall \varphi \in H_p^1(\Omega)\,. \end{aligned} \tag{2.8}$$

Analogously, the TM diffraction problem admits the variational formulation for the function $u = e^{-i\alpha x_1} H_3$:

$$\begin{aligned} B_{TM}(u,\varphi) &= \int_\Omega \frac{1}{k^2}\nabla_\alpha u \cdot \overline{\nabla_\alpha \varphi} - \int_\Omega u\,\bar\varphi + \frac{1}{(k^+)^2}\int_{\Gamma^+} (T_\alpha^+ u)\,\bar\varphi + \frac{1}{(k^-)^2}\int_{\Gamma^-} (T_\alpha^- u)\,\bar\varphi \\ &= -\frac{2iq_3\beta\, e^{-i\beta b}}{(k^+)^2}\int_{\Gamma^+} \bar\varphi\,, \quad \forall\, \varphi \in H_p^1(\Omega)\,. \end{aligned} \tag{2.9}$$

In [5], the following properties have been proved under the assumption on the optical indices of the materials, that

$$\text{Re } k(x_1, x_2) > 0 \,, \ \text{Im } k(x_1, x_2) \geq 0 \,, \ k^+ > 0 \tag{2.10}$$

which is satisfied for all practical relevant materials.

1. If Im $k > 0$ in some subdomain $\Omega_1 \subset \Omega$ then for any $\omega > 0$ there exists at most one solution $u \in H^1_p(\Omega)$.
2. For any $\theta_0 \in (0, \pi/2)$ there exists a frequency $\omega_0 > 0$ such that the variational problem (2.8) resp. (2.9) admits a unique solution $u \in H^1_p(\Omega)$ for all incidence angles θ with $|\theta| \leq \theta_0$ and all frequencies ω with $0 < \omega \leq \omega_0$.
3. The sesquilinear forms B_{TE} and B_{TM} are strongly elliptic over $H^1_p(\Omega)$, i.e., after multiplication by some complex number they satisfy a Gårding inequality.
4. (i) The diffraction problems (2.8) and (2.9) are always solvable in $H^1_p(\Omega)$. For all but a countable set of frequencies ω_j, $\omega_j \to \infty$, these solutions are unique.

   (ii) Introduce the set of Rayleigh frequencies

   $$\mathcal{R} = \left\{ (\omega, \theta) : \exists\, n \in \mathbf{Z} \text{ s. th. } (k^\pm)^2 = (n + \alpha)^2 \right\}.$$

   If for $(\omega^0, \theta^0) \notin \mathcal{R}$ the TE or TM diffraction problem is uniquely solvable, then the solution depends analytically on ω and θ in a neighbourhood of this point.

3. Variation of interfaces

Define the finite sets of indices $P^\pm = \{n \in \mathbf{Z} : \beta_n^\pm > 0\}$, where $\beta_n^\pm$ is given by (2.3). Then the Rayleigh amplitudes $E_n^\pm$ and $H_n^\pm$, $(n \in P^\pm)$, which are called the reflection resp. transmission coefficients for TE and TM polarization, correspond to the propagating modes in (2.2), (2.5) and are used to compute the so called efficiencies of the diffractive grating. Note that $P^- = \emptyset$ if Im $k^- \neq 0$.

We are interested in the solvability of the problems and the dependence of Rayleigh coefficients if parts of the interfaces Λ between different materials are varied. The variation of interfaces leads to a new piecewise constant function k_h, where we assume that meas $\Omega_h = O(h)$ with $\Omega_h = \{x \in \Omega : k(x) \neq k_h(x)\}$. Let B^h_{TE} denote the variational form of the TE problem for the perturbed geometry, then

$$\begin{aligned} \left| B^h_{TE}(u, \varphi) - B_{TE}(u, \varphi) \right| &= \left| \int_{\Omega_h} (k^2 - k_h^2)\, u\, \bar{\varphi} \right| \\ &\leq \|k^2 - k_h^2\|_{L_p(\Omega_h)} \|u\|_{L_q(\Omega_h)} \|\varphi\|_{L_r(\Omega_h)} \end{aligned}$$

for $p^{-1} + q^{-1} + r^{-1} = 1$. Hence, the variation of interfaces represents a compact and small perturbation of the form B_{TE} ensuring the unique solvability of B^h_{TE} for all sufficiently small h.

In the TM case the situation is more involved. The relation

$$\left| B^h_{TM}(u, \varphi) - B_{TM}(u, \varphi) \right| = \left| \int_{\Omega_h} \Big(\frac{1}{k^2} - \frac{1}{k_h^2} \Big) \nabla_\alpha u \, \overline{\nabla_\alpha \varphi} \right|$$

shows that the variation of interfaces is a strong perturbation of the TM diffraction problem. Therefore we consider a more regularly perturbed diffraction problem

$$B^h_{TM}(u, \varphi) = - \int_{\Gamma^+} \frac{2 i q_3 \beta\, e^{-i\beta b}}{(k^+)^2} \, \bar{\varphi} \,, \quad \forall\, \varphi \in H^1_p(\Omega) \,, \tag{3.1}$$

assuming that, for sufficiently small $|h|$, the perturbed interface Λ_h is given by

$$\Lambda_h = \Phi_h(\Lambda)\,,\ \Phi_h(x) = x + h\,\chi(x)\,. \tag{3.2}$$

Here Φ_h is a C^1 diffeomorphism of Ω onto itself, and $\chi = (\chi_1, \chi_2)$ is 2π–periodic in x_1 and has compact support in $[0, 2\pi] \times (-b, b)$.

Then we can define the isomorphism $\Psi_h : H^1_p(\Omega) \to H^1_p(\Omega)$ which maps u to $u \circ \Phi_h^{-1}$. Moreover, $k_h = \Psi_h k$ and the change of variables $y = \Phi_h(x)$ provides

$$dy = |J(x)| dx$$

with

$$J(x) = 1 + h\Big(\frac{\partial\chi_1}{\partial x_1} + \frac{\partial\chi_2}{\partial x_2}\Big) + h^2\Big(\frac{\partial\chi_1}{\partial x_1}\frac{\partial\chi_2}{\partial x_2} - \frac{\partial\chi_1}{\partial x_2}\frac{\partial\chi_2}{\partial x_1}\Big)$$

and

$$\frac{\partial}{\partial y_1} = \frac{1 + h\,\partial\chi_2/\partial x_2}{J(x)}\frac{\partial}{\partial x_1} - \frac{h\,\partial\chi_2/\partial x_1}{J(x)}\frac{\partial}{\partial x_2}$$
$$\frac{\partial}{\partial y_2} = -\frac{h\,\partial\chi_1/\partial x_2}{J(x)}\frac{\partial}{\partial x_1} + \frac{1 + h\,\partial\chi_1/\partial x_1}{J(x)}\frac{\partial}{\partial x_2}$$

Hence we obtain

$$\begin{aligned}
&\int_\Omega \Big(-\Psi_h u\overline{\Psi_h\varphi} + \frac{1}{k_h^2(y)}\nabla_\alpha\Psi_h u \cdot \overline{\nabla_\alpha\Psi_h\varphi}\Big)\,dy = -\int_\Omega u\,\overline{\varphi}\,J(x)\,dx \\
&+ \int_\Omega \frac{\big((1 + h\partial_2\chi_2)\partial_1 + i\alpha J(x) - h\partial_1\chi_2\partial_2\big)u\,\overline{\big((1 + h\partial_2\chi_2)\partial_1 - i\alpha J(x) - h\partial_1\chi_2\partial_2\big)\varphi}}{J(x)k^2(x)} \\
&+ \int_\Omega \frac{\big(-h\partial_2\chi_1\partial_1 + (1 + h\partial_1\chi_1)\partial_2\big)u\,\overline{\big(-h\partial_2\chi_1\partial_1 + (1 + h\partial_1\chi_1)\partial_2\big)\varphi}}{J(x)k^2(x)} \\
&= \int_\Omega \Big(-u\overline{\varphi} + \frac{1}{k^2}\nabla_\alpha u\overline{\nabla_\alpha\varphi}\Big)dx + hB_1(u,\varphi) + h^2B_{2,h}(u,\varphi)\,,
\end{aligned}$$

where

$$\begin{aligned}
B_1(u,\varphi) = &-\int_\Omega (\partial_1\chi_1 + \partial_2\chi_2)u\,\overline{\varphi} + \int_\Omega \frac{\partial_1\chi_1}{k^2}\big(\partial_2 u\,\overline{\partial_2\varphi} - \partial_1 u\,\overline{\partial_1\varphi} + \alpha^2 u\,\varphi\big) \\
&+ \int_\Omega \frac{\partial_2\chi_2}{k^2}\big(\partial_{1,\alpha}u\,\overline{\partial_{1,\alpha}\varphi} - \partial_2 u\,\partial_2\varphi\big) \\
&- \int_\Omega \Big(\frac{\partial_1\chi_2}{k^2}\big(\partial_{1,\alpha}u\,\overline{\partial_2\varphi} + \partial_2 u\,\overline{\partial_{1,\alpha}\varphi}\big) + \frac{\partial_2\chi_1}{k^2}\big(\partial_1 u\,\overline{\partial_2\varphi} + \partial_2 u\,\overline{\partial_1\varphi}\big)\Big)
\end{aligned} \tag{3.3}$$

and the remainder term satisfies

$$|B_{2,h}(u,\varphi)| \le c\|u\|_1\|\varphi\|_1\,,\ u,\varphi \in H^1_p(\Omega\,,\ |h| \le h_0\,.$$

Here we have used the notations $\partial_j = \partial/\partial x_j$, $\partial_{1,\alpha} = \partial_1 + i\alpha$ and the relation

$$J(x)^{-1} = 1 - h(\partial_1\chi_1 + \partial_2\chi_2) + O(h^2)\,,\ |h| \le h_0\,,$$

which holds uniformly in $x \in \Omega$. Since the boundary terms in the TM sesquilinear form remain unchanged, we have for $|h| \le h_0$

$$B^h_{TM}(\Psi_h u, \Psi_h\varphi) = B_{TM}(u,\varphi) + hB_1(u,\varphi) + h^2B_{2,h}(u,\varphi)\,. \tag{3.4}$$

Theorem 3.1. *If the TM diffraction problem* (2.9) *has a unique solution and the perturbation of the grating geometry is given by the regular mapping* (3.2)*, then for all sufficiently small* h *the* *perturbed problem* (3.1) *is also uniquely solvable. Moreover, the solution of this problem takes the form*

$$\Psi_h^{-1} u_h = u_0 + h u_1 + h^2 u_{2,h}\,, \tag{3.5}$$

where u_0 *is the solution of the original problem* (2.9), $u_1 \in H_p^1(\Omega)$ *solves the equation*

$$B_{TM}(u_1,\varphi) = -B_1(u,\varphi)\,, \quad \forall\, \varphi \in H_p^1(\Omega)\,, \tag{3.6}$$

and the remainder satisfies $\|u_{2,h}\|_1 \le c$ *for* $|h| \le h_0$.

Proof: Replacing u, φ with $\Psi_h^{-1}u, \Psi_h^{-1}\varphi$ in (3.4) and using the equivalence of norms $\|u\|_1 \sim \|\Psi_h u\|_1$ (uniformly in h), we obtain

$$\begin{aligned} B_{TM}^h(u,\varphi) &= B_{TM}(\Psi_h^{-1}u, \Psi_h^{-1}\varphi) + O(h)\|\Psi_h^{-1}u\|_1\|\Psi_h^{-1}\varphi\|_1 \\ &= B_{TM}(u,\varphi) + O(h)\|u\|_1\|\varphi\|_1\,. \end{aligned}$$

Hence B_{TM}^h is a small perturbation of B_{TM}, which proves the unique solvability of (3.1).

Inserting the ansatz (3.5) for the solution u_h of (3.1) into (3.4) yields the following equation for $u_{2,h}$:

$$\begin{aligned} &B_{TM}(u_{2,h},\varphi) + hB_1(u_{2,h},\varphi) + h^2 B_{2,h}(u_{2,h},\varphi) \\ &\quad = -B_1(u_1,\varphi) - B_{2,h}(u_0,\varphi) - hB_{2,h}(u_1,\varphi)\,, \quad \forall\, \varphi \in H_p^1(\Omega)\,. \end{aligned} \tag{3.7}$$

Recall that

$$\int_{\Gamma^+} \Psi_h \overline{\varphi} = \int_{\Gamma^+} \overline{\varphi}\,,$$

which implies $B_{TM}^h(u_h, \Psi_h\varphi) = B_{TM}(u_0,\varphi)$. Since the left–hand side of (3.7) takes the form $B_{TM}(u_{2,h},\varphi) + O(h)\|u_{2,h}\|_1\|\varphi\|_1$ and the right–hand side defines a (uniformly) bounded linear functional on $H_p^1(\Omega)$, we obtain a uniformly bounded solution $u_{2,h}$. ∎

Remark 3.2. Assume that Φ_h is a C^∞ isomorphism. Then it is not difficult to prove recursively that for any $N \ge 2$ the solution of (3.1) admits the expansion

$$\Psi_h^{-1}u_h = \sum_{j=0}^{N} h^j u_j + h^{N+1}u_{N+1,h}\,, \quad \|u_{N+1,h}\|_1 \le c_N\,,$$

with u_0, u_1 as above and certain functions $u_j \in H_p^1(\Omega)$, $j \ge 2$.

Now we are in the position to obtain a formula for the derivative of the Rayleigh coefficients $H_n^\pm$ with respect to the regular variations (3.2) of the interfaces Λ. These reflection and transmission coefficients are determined by the traces of the solution u of the problem (2.9) on the artificial boundaries $\Gamma^\pm$,

$$\begin{aligned} H_n^+ &= -q_3\,\delta_{0n}e^{-2i\beta b} + \frac{e^{-i\beta_n^+ b}}{2\pi}\int_{\Gamma^+} u\, e^{-inx_1}\,dx_1\,, \qquad && n \in P^+\,, \\ H_n^- &= \frac{e^{-i\beta_n^- b}}{2\pi}\int_{\Gamma^-} u\, e^{-inx_1}\,dx_1\,, && n \in P^-\,. \end{aligned} \tag{3.8}$$

Thus the derivative of $H_n^\pm$ is given by

$$DH_n^\pm(\chi) = \lim_{h\to 0}\frac{e^{-i\beta_n^\pm b}}{2\pi h}\int_{\Gamma^\pm}(u_h - u)\,e^{-inx_1}\,dx_1\,, \tag{3.9}$$

where u_h is the solution of the perturbed problem (3.1), (3.2). Let w denote the solution of the adjoint problem

$$B_{TM}(\varphi, w) = \frac{e^{-i\beta_n^\pm b}}{2\pi}\int_{\Gamma^\pm}\varphi\, e^{-inx_1}\,dx_1\,, \quad \forall \varphi \in H_p^1(\Omega)\,. \tag{3.10}$$

Then

$$\frac{e^{-i\beta_n^\pm b}}{2\pi h} \int_{\Gamma^\pm} (u_h - u)\, e^{-inx_1}\, dx_1 = \frac{1}{h} B_{TM}(u_h - u, w)\,.$$

Since the right–hand side of equation (3.10) is a functional supported at the artificial boundary $\Gamma^\pm$ one has $B_{TM}(u_h, w) = B_{TM}(\Psi_h^{-1} u_h, w)$, and (3.5) then gives

$$\begin{aligned} h^{-1} B_{TM}(u_h - u, w) &= h^{-1} B_{TM}(\Psi_h^{-1} u_h - u, w) = B_{TM}(u_1, w) + h B_{TM}(u_{2,h}, w) \\ &= -B_1(u, w) + h B_{TM}(u_{2,h}, w) \end{aligned}$$

Thus we have proved the following

Theorem 3.3. *The derivative of the reflection and transmission coefficients $H_n^\pm$ with respect to the variations* (3.2) *of the interface Λ is given by the formula*

$$DH_n^\pm(\chi) = -B_1(u, w) \tag{3.11}$$

where the sesquilinear form B_1 is defined by (3.3), *and u and w denote the solution of the direct and adjoint diffraction problems* (2.9), (3.10), *respectively.*

4. Derivative of diffraction coefficients as contour integral

Theorem 3.3 states that the derivative of the diffraction coefficients can be obtained from certain integrals with $\operatorname{supp}\nabla\chi$ as domain of integration. In the following formula (3.11) will be simplified by transforming these domain integrals to certain contour integrals. For the sake of simplicity we will consider in the following only the variation of interfaces between two different materials. This means the support of the function χ is divided by a certain part of the interface Λ into two subdomains, which will be denoted by Ω^+ and Ω^-. In each subdomain the function k takes constant values, denoted by k_+ and k_-, respectively.

Let $\Gamma \subset \Omega$ be a simple closed piecewise smooth curve enclosing the domain G such that $k = const$ in G. Let $\nu = (\nu_1, \nu_2)$ be the exterior normal to Γ, $\tau = (-\nu_2, \nu_1)$ the tangential vector, and introduce the weighted normal and tangential derivatives

$$\partial_{\nu,\alpha} = \nu_1 \partial_{1,\alpha} + \nu_2 \partial_2\ ,\ \ \partial_{\tau,\alpha} = -\nu_2 \partial_{1,\alpha} + \nu_1 \partial_2\ .$$

We denote by $B_1(u, w; G)$ the right–hand side of (3.3) where the integrals are taken over G instead of Ω.

Lemma 4.1. *If* $\operatorname{supp}\chi \cap \Gamma$ *does not contain a corner point of Λ, then*

$$B_1(u, w; G) = \int_\Gamma \Big((\chi, \nu)\mathcal{J} + (\chi, \tau)\mathcal{K} + \chi_1 \mathcal{L} \Big)\,, \tag{4.1}$$

where

$$\begin{aligned} \mathcal{J} &= -u\overline{w} + \frac{1}{k^2}(\partial_{\tau,\alpha} u\, \overline{\partial_{\tau,\alpha} w} - \partial_{\nu,\alpha} u\, \overline{\partial_{\nu,\alpha} w}) \\ \mathcal{K} &= -\frac{1}{k^2}(\partial_{\nu,\alpha} u\, \overline{\partial_{\tau,\alpha} w} + \partial_{\tau,\alpha} u\, \overline{\partial_{\nu,\alpha} w}) \\ \mathcal{L} &= \frac{i\alpha}{k^2}(u\, \overline{\partial_{\tau,\alpha} w} - \partial_{\nu,\alpha} u\, \overline{w})\,. \end{aligned}$$

P r o o f : We have

$$
\begin{aligned}
&B_1(u,w;G)\\
&= \int_G \frac{1}{k^2}\Big(\partial_1\chi_1\big((\alpha^2-k^2)u\,\overline{w}+\partial_2 u\,\overline{\partial_2 w}-\partial_1 u\,\overline{\partial_1 w}\big)-\partial_2\chi_1\big(\partial_1 u\,\overline{\partial_2 w}+\partial_2 u\,\overline{\partial_1 w}\big)\Big)\\
&+\int_G \frac{1}{k^2}\Big(\partial_2\chi_2(-k^2\,u\,\overline{w}+\partial_{1,\alpha}u\,\overline{\partial_{1,\alpha}w}-\partial_2 u\,\overline{\partial_2 w})-\partial_1\chi_2\big(\partial_{1,\alpha}u\,\overline{\partial_2 w}+\partial_2 u\,\overline{\partial_{1,\alpha}w}\big)\Big)\\
&=: I_1+I_2\,.
\end{aligned}
$$

Let us start with the integral I_1. Green's formula yields

$$
\begin{aligned}
&\int_G \partial_2\chi_1\big(\partial_1 u\,\overline{\partial_2 w}+\partial_2 u\,\overline{\partial_1 w}\big)=-\int_G \chi_1\Big(\partial_1 u\,\overline{\partial_2^2 w}+\partial_2^2 u\,\overline{\partial_1 w}+\partial_1(\partial_2 u\,\overline{\partial_2 w})\Big)\\
&+\int_\Gamma \chi_1\big(\partial_1 u\,\overline{\partial_2 w}+\partial_2 u\,\overline{\partial_1 w}\big)\nu_2=-\int_G \chi_1\big(\partial_1 u\,\overline{\partial_2^2 w}+\partial_2^2 u\,\overline{\partial_1 w}\big)\\
&+\int_G \partial_1\chi_1\partial_2 u\,\overline{\partial_2 w}+\int_\Gamma \chi_1\Big(\big(\partial_1 u\,\overline{\partial_2 w}+\partial_2 u\,\overline{\partial_1 w}\big)\nu_2-\partial_2 u\,\overline{\partial_2 w}\,\nu_1\Big)\,,
\end{aligned}
$$

$$
\begin{aligned}
&\int_G \partial_1\chi_1\,\partial_1 u\,\overline{\partial_1 w}=-\int_G \chi_1\big(\partial_1^2 u\,\overline{\partial_1 w}+\partial_1 u\,\overline{\partial_1^2 w}\big)+\int_\Gamma \chi_1\partial_1 u\,\overline{\partial_1 w}\,\nu_1\\
&-\int_G \chi_1\big((\partial_1^2 u+2i\alpha\partial_1 u)\overline{\partial_1 w}+\partial_1 u(\overline{\partial_1^2 w+2i\alpha\partial_1 w})\big)+\int_\Gamma \chi_1\partial_1 u\,\overline{\partial_1 w}\,\nu_1\,,
\end{aligned}
$$

$$
\int_G \partial_1\chi_1\,u\,\overline{w}=-\int_G \chi_1\big(\partial_1 u\,\overline{w}+u\,\overline{\partial_1 w}\big)+\int_\Gamma \chi_1\,u\,\overline{w}\,\nu_1\,,
$$

which implies

$$
\begin{aligned}
I_1=&\frac{1}{k^2}\int_G \chi_1\partial_1 u\,(\partial_1^2\overline{w}+\partial_2^2\overline{w}-2i\alpha\partial_1\overline{w}+(k^2-\alpha^2)\overline{w})\\
&+\frac{1}{k^2}\int_G \chi_1(\partial_1^2 u+\partial_2^2 u+2i\alpha\partial_1 u+(k^2-\alpha^2)u)\,\partial_1\overline{w}\\
&-\frac{1}{k^2}\int_\Gamma \chi_1\Big(\big(\partial_1 u\,\partial_2\overline{w}+\partial_2 u\,\partial_1\overline{w}\big)\nu_2+\big(\partial_1 u\,\partial_1\overline{w}-\partial_2 u\,\partial_2\overline{w}\big)\,\nu_1\Big)\\
&-\frac{k^2-\alpha^2}{k^2}\int_\Gamma \chi_1\,u\,\overline{w}\,\nu_1\,.
\end{aligned}
$$

Note that $u,w\in H^2(G\cap\mathrm{supp}\chi)$, and since

$$
\Delta_\alpha u+k^2 u=\Delta_\alpha w+\overline{k}^2 w=0\quad\text{ in } G\,,
$$

we obtain

$$
\begin{aligned}
I_1=&-\frac{1}{k^2}\int_\Gamma \chi_1\Big(\big(\partial_1 u\,\partial_2\overline{w}+\partial_2 u\,\partial_1\overline{w}\big)\nu_2+\big(\partial_1 u\,\partial_1\overline{w}-\partial_2 u\,\partial_2\overline{w}\big)\,\nu_1\Big)\\
&-\frac{k^2-\alpha^2}{k^2}\int_\Gamma \chi_1\,u\,\overline{w}\,\nu_1\,.
\end{aligned}
$$

Simple calculations show that

$$
\begin{aligned}
&\big(\partial_1 u\,\partial_2\overline{w}+\partial_2 u\,\partial_1\overline{w}\big)\nu_2+\big(\partial_1 u\,\partial_1\overline{w}-\partial_2 u\,\partial_2\overline{w}\big)\,\nu_1-\alpha^2\,u\,\overline{w}\,\nu_1\\
&=\big(\partial_{\nu,\alpha}u\,\overline{\partial_{\nu,\alpha}w}-\partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}w}\big)\nu_1-\big(\partial_{\nu,\alpha}u\,\overline{\partial_{\tau,\alpha}w}+\partial_{\tau,\alpha}u\,\overline{\partial_{\nu,\alpha}w}\big)\nu_2\\
&\quad+i\,\alpha\big(\partial_{\nu,\alpha}u\,\overline{w}-u\,\overline{\partial_{\nu,\alpha}w}\big)\,.
\end{aligned}
$$

Therefore we have

$$I_1 = I_1(\chi_1) = \int_\Gamma \Big(\chi_1 \nu_1 \mathcal{J} - \chi_1 \nu_2 \mathcal{K} + \chi_1 \mathcal{L}\Big) .$$

Similarly one verifies that

$$I_2 = I_2(\chi_2) = \int_\Gamma \Big(\chi_2 \nu_2 \mathcal{J} + \chi_2 \nu_1 \mathcal{K}\Big) ,$$

which finishes the proof of (4.1). ∎

Remark 4.2. An inspection of the above proof shows that $I_1 = I_1(\chi_1) = 0$ if $\chi_1 \equiv 1$ in G. Moreover, since

$$\int_\Gamma (u \, \overline{\partial_{\nu,\alpha} w} - \partial_{\nu,\alpha} u \, \overline{w}) = 0$$

by the second Green formula, the third integral in (4.1) vanishes if χ_1 is constant. Thus, for $\chi_1 \equiv 1$ the integral $I_1(\chi_1)$ takes the form

$$\int_\Gamma \big(\nu_1 \mathcal{J} - \nu_2 \mathcal{K}\big)$$

and is zero as long as $\Gamma \subset \overline{\Omega^+}$ (or $\Gamma \subset \overline{\Omega^-}$) does not contain a corner of the interface Λ. Analogously, $I_2 = I_2(\chi_2)$ with $\chi_2 \equiv 1$ always vanishes in that case.

Corollary 4.3. *If Λ has no corner points, then*

$$DH_n^{\pm}(\chi) = -B_1(u,w) = \int_\Lambda (\chi, \nu) \left[\frac{1}{k^2}\big(\partial_{\nu,\alpha} u \, \overline{\partial_{\nu,\alpha} w} - \partial_{\tau,\alpha} u \, \overline{\partial_{\tau,\alpha} w}\big)\right]_\Lambda . \tag{4.2}$$

Here ν denotes the normal to Λ pointing from Ω^+ into Ω^- and $[v]_\Lambda$ stands for the jump $v|_\Lambda^+ - v|_\Lambda^-$ across Λ, where $v|_\Lambda^\pm$ represents the limit as the interface is approached from the region $\Omega^\pm$.

Proof: Applying Lemma 4.1 with $G = \Omega^\pm$, we obtain

$$\begin{aligned} B_1(u,w) &= B_1(u,w;\Omega^+) + B_1(u,w;\Omega^-) \\ &= \int_\Lambda \Big((\chi,\nu)\mathcal{J}|_\Lambda^+ + (\chi,\tau)\mathcal{K}|_\Lambda^+ + \chi_1 \mathcal{L}|_\Lambda^+\Big) - \int_\Lambda \Big((\chi,\nu)\mathcal{J}|_\Lambda^- + (\chi,\tau)\mathcal{K}|_\Lambda^- + \chi_1 \mathcal{L}|_\Lambda^-\Big). \end{aligned}$$

Recall that $\operatorname{supp}\chi \cap \Gamma = \emptyset$ and the integrands are 2π–periodic in x_1. Using the transmission conditions for u and w then gives

$$[u\,\overline{w}]_\Lambda = [\mathcal{K}]_\Lambda = [\mathcal{L}]_\Lambda = 0 ,$$

hence

$$B_1(u,w) = \int_\Lambda (\chi, \nu) \left[\frac{1}{k^2}\big(\partial_{\tau,\alpha} u \, \overline{\partial_{\tau,\alpha} w} - \partial_{\nu,\alpha} u \, \overline{\partial_{\nu,\alpha} w}\big)\right]_\Lambda . \quad ∎$$

We now extend formula (4.2) to the case of corner points. Assume first that Λ has exactly one corner point at O, and denote by δ the angle at O seen from Ω^+. Without loss of generality we may assume that Ω^+ locally coincides with the sector $\{(r,\varphi) : 0 < r < \infty, |\varphi| < \delta/2\}$, where (r,φ) denote polar coordinates centered at O.

To describe the singularities of solutions to problem (2.9) near O, consider the transcendental equation

$$\frac{\sin(\pi-\delta)\lambda}{\sin\pi\lambda} = \sigma\,\frac{k_-^2+k_+^2}{k_-^2-k_+^2}\,, \qquad \sigma=\pm 1\,. \tag{4.3}$$

Denote by λ_0 the unique zero of (4.3) in the strip $0<\mathrm{Re}\,\lambda<1$ if it exists. It was proved in [6, Lemma 4.2] that (4.3) has exactly one simple root in that strip if $|k_-|\neq k_+$ and no root there if $|k_-|=k_+$. Moreover (see [6, Thm. 4.1]), the solution $u\in H^1_p(\Omega)$ of the TM diffraction problem (2.9) satisfies

$$\xi u|_{\Omega^\pm} = C + C^\pm r^{\lambda_0} u_0^\pm + u_1^\pm\,, \tag{4.4}$$

where ξ is a smooth cut–off function near O, C and $C^\pm$ are certain complex constants, the remainder terms $u_1^\pm$ satisfy

$$u_1^\pm \in H^{2-\epsilon}(\Omega^\pm) \quad \text{for all} \quad \epsilon>0\,,$$

and the functions $u_0^\pm$ take the form

$$u_0^+(\varphi)=\cos\lambda_0\varphi\,,\ u_0^-(\varphi)=\cos\lambda_0(\varphi-\pi) \tag{4.5}$$

or

$$u_0^+(\varphi)=\sin\lambda_0\varphi\,,\ u_0^-(\varphi)=\sin\lambda_0(\varphi-\pi) \tag{4.6}$$

corresponding to the case $\sigma=+1$ or $\sigma=-1$ in (4.3). For fixed $\varepsilon>0$, let $O_{\pm\varepsilon}$ be the two points on Λ satisfying $\mathrm{dist}(O,O_{\pm\varepsilon})=\varepsilon$ and set $\Lambda_\varepsilon=\Lambda\setminus(\overline{OO_{-\varepsilon}}\cup\overline{OO_\varepsilon})$.

Theorem 4.4. *With* $\mathcal{G} := (\chi,\nu)\left[\frac{1}{k^2}\left(\partial_{\nu,\alpha}u\,\overline{\partial_{\nu,\alpha}w} - \partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}w}\right)\right]_\Lambda$ *we have*

$$DH_n^\pm(\chi) = \lim_{\varepsilon\to 0}\left(\int_{\Lambda_\varepsilon}\mathcal{G} + \frac{\varepsilon}{2\lambda_0-1}\big(\mathcal{G}(O_{-\varepsilon})+\mathcal{G}(O_\varepsilon)\big)\right). \tag{4.7}$$

Remark 4.5. Since the function $\overline{w}$ also admits the representation (4.4)–(4.6) (with other constants C, $C^\pm$ and remainder terms), one obtains that $\mathcal{G}(x)=O(r^{2\lambda_0-2})$ as $r\to 0$. Thus (4.7) coincides with formula (4.2) if $\mathrm{Re}\,\lambda_0>1/2$. This is always true if k_- is real; cf. [3]. Note that the case $\lambda_0=1/2$ is excluded by our assumptions (2.10) if k_- is complex.

Proof of Theorem 4.4: Let $\Omega_\varepsilon^\pm=\Omega^\pm\setminus\{r\le\varepsilon\}$ and denote by $S_\varepsilon^\pm$ the (clockwise oriented) circular arcs $\Omega_\varepsilon^\pm\cap\{r=\varepsilon\}$ with endpoints $O_{-\varepsilon}$, O_ε. Applying Lemma 4.1 with $G=\Omega_\varepsilon^\pm$ gives

$$B_1(u,w)=\lim_{\varepsilon\to 0}\Big(B_1(u,w;\Omega_\varepsilon^+)+B_1(u,w;\Omega_\varepsilon^-)\Big)=\lim_{\varepsilon\to 0}\Big(-\int_{\Lambda_\varepsilon}\mathcal{G}+\int_{S_\varepsilon^+}\mathcal{H}+\int_{S_\varepsilon^-}\mathcal{H}\Big)\,,$$

where $\mathcal{H}:=(\chi,\nu)\mathcal{J}+(\chi,\tau)\mathcal{K}+\chi_1\mathcal{L}$; cp. (4.1). It remains to show that, for $\mathrm{Re}\,\lambda_0\le 1/2$ and $\lambda_0\neq 1/2$

$$\int_{S_\varepsilon^\pm}\mathcal{H} = \mp\frac{\varepsilon}{2\lambda_0-1}\Big((\mathcal{H}|_\Lambda^\pm)(O_\varepsilon)+(\mathcal{H}|_\Lambda^\pm)(O_{-\varepsilon})\Big)+o(\varepsilon) \tag{4.8}$$

as $\varepsilon\to 0$. To prove this, it is enough to replace $\mathcal{H}$ by

$$\frac{(\chi(O),\nu)}{k^2}\left(\partial_\tau u\,\partial_\tau\overline{w}-\partial_\nu u\,\partial_\nu\overline{w}\right)-\frac{(\chi(O),\tau)}{k^2}\left(\partial_\nu u\,\partial_\tau\overline{w}+\partial_\tau u\,\partial_\nu\overline{w}\right)$$

and to insert the principal asymptotic term

$$u^0(r,\varphi)=\begin{cases} r^{\lambda_0}u_0^+(\varphi)\,, & \varphi\in(-\delta/2,\delta/2),\\ r^{\lambda_0}u_0^-(\varphi)\,, & \varphi\in(\delta/2,2\pi-\delta/2),\end{cases}$$

for u and $\overline{w}$, with $u_0^\pm$ defined in (4.5) or (4.6).

Thus (4.8) is proved provided we have shown that

$$\int_{S_\varepsilon^\pm} \mathcal{H}_0 = \mp \frac{\varepsilon}{2\lambda_0 - 1}\Big((\mathcal{H}_0|_\Lambda^\pm)(O_\varepsilon) + (\mathcal{H}_0|_\Lambda^\pm)(O_{-\varepsilon})\Big), \tag{4.9}$$

where

$$\mathcal{H}_0 = (\chi(O), \nu)\big((\partial_\tau u^0)^2 - (\partial_\nu u^0)^2\big) - 2(\chi(O), \tau)\partial_\nu u^0\, \partial_\tau u^0 \ .$$

Consider, for example, (4.9) with the plus sign and $u_0^+ = \cos\lambda_0\varphi$. Since $\nu = -(\cos\varphi, \sin\varphi)$, $\tau = (\sin\varphi, -\cos\varphi)$, $\partial_\nu = -\partial_r$, $\partial_\tau = r^{-1}\partial_\varphi$ on S_ε^+, we then have

$$\begin{aligned}
\int_{S_\varepsilon^+} \mathcal{H}_0 &= \int_{S_\varepsilon^+} \lambda_0^2 r^{2\lambda_0 - 2}\big(\chi_1(O)\cos\varphi + \chi_2(O)\sin\varphi\big)\big(\cos^2\lambda_0\varphi - \sin^2\lambda_0\varphi\big) \\
&\quad + \int_{S_\varepsilon^+} 2\lambda_0^2 r^{2\lambda_0 - 2}\big(\chi_1(O)\sin\varphi - \chi_2(O)\cos\varphi\big)\sin\lambda_0\varphi\,\cos\lambda_0\varphi \\
&= \lambda_0^2\,\varepsilon^{2\lambda_0 - 1}\Big(\chi_1(O)\int_{-\delta/2}^{\delta/2}(\cos\varphi\,\cos 2\lambda_0\varphi + \sin\varphi\,\sin 2\lambda_0\varphi)\,d\varphi \\
&\qquad - \chi_2(O)\int_{-\delta/2}^{\delta/2}(\cos\varphi\,\sin 2\lambda_0\varphi - \sin\varphi\,\cos 2\lambda_0\varphi)\,d\varphi\Big) \\
&= \lambda_0^2\,\varepsilon^{2\lambda_0 - 1}\Big(\chi_1(O)\int_{-\delta/2}^{\delta/2}\cos(2\lambda_0 - 1)\varphi\,d\varphi - \chi_2(O)\int_{-\delta/2}^{\delta/2}\sin(2\lambda_0 - 1)\varphi\,d\varphi\Big) \\
&= \frac{2\chi_1(O)\lambda_0^2\,\varepsilon^{2\lambda_0 - 1}}{2\lambda_0 - 1}\,\sin(2\lambda_0 - 1)\delta/2\ .
\end{aligned}$$

On the other hand, since $\nu = (\sin\delta/2, \cos\delta/2)$, $\tau = (\cos\delta/2, -\sin\delta/2)$, $\partial_\nu = r^{-1}\partial_\varphi$, $\partial_\tau = \partial_r$ on $\{\varphi = -\delta/2\}$ and $\nu = (\sin\delta/2, -\cos\delta/2)$, $\tau = (-\cos\delta/2, -\sin\delta/2)$, $\partial_\nu = -r^{-1}\partial_\varphi$, $\partial_\tau = -\partial_r$ on $\{\varphi = \delta/2\}$, we obtain

$$\begin{aligned}
(\mathcal{H}_0|_\Lambda^+)(O_\varepsilon) &= \big(\chi_1(O)\sin\delta/2 + \chi_2(O)\cos\delta/2\big)\lambda_0^2\,\varepsilon^{2\lambda_0 - 2}\cos\lambda_0\delta \\
&\quad - \big(\chi_1(O)\cos\delta/2 - \chi_2(O)\sin\delta/2\big)\lambda_0^2\,\varepsilon^{2\lambda_0 - 2}\sin\lambda_0\delta\ , \\
(\mathcal{H}_0|_\Lambda^+)(O_{-\varepsilon}) &= \big(\chi_1(O)\sin\delta/2 - \chi_2(O)\cos\delta/2\big)\lambda_0^2\,\varepsilon^{2\lambda_0 - 2}\cos\lambda_0\delta \\
&\quad - \big(\chi_1(O)\cos\delta/2 + \chi_2(O)\sin\delta/2\big)\lambda_0^2\,\varepsilon^{2\lambda_0 - 2}\sin\lambda_0\delta\ ,
\end{aligned}$$

which implies

$$\begin{aligned}
&\frac{\varepsilon}{2\lambda_0 - 1}\Big((\mathcal{H}_0|_\Lambda^+)(O_\varepsilon) + (\mathcal{H}_0|_\Lambda^+)(O_{-\varepsilon})\Big) \\
&\quad = -2\chi_1(O)\frac{\lambda_0^2\,\varepsilon^{2\lambda_0 - 1}}{2\lambda_0 - 1}(\cos\delta/2\,\sin\lambda_0\delta - \sin\delta/2\,\cos\lambda_0\delta) \\
&\quad = -\frac{2\chi_1(O)\lambda_0^2\,\varepsilon^{2\lambda_0 - 1}}{2\lambda_0 - 1}\,\sin(2\lambda_0 - 1)\delta/2\ ,
\end{aligned}$$

hence (4.9) for the plus sign. In the other cases the proof of (4.9) is analogous. ∎

Remark 4.6. The extension of (4.7) to the case of finitely many corners $O_1, \ldots, O_r$ of Λ with angles $\delta_1, \ldots, \delta_r$ is straightforward. Let $O_{j,\pm\varepsilon} \in \Lambda$ be the points with $\operatorname{dist}(O_j, O_{j,\pm\varepsilon}) = \varepsilon$. Then formula (4.7) holds with $\Lambda_\varepsilon = \Lambda \setminus \bigcup_{j=1}^{r}(\overline{O_j O_{j,-\varepsilon}} \cup \overline{O_j O_{j,\varepsilon}})$ and the correction terms replaced by the sum

$$\sum_{j=1}^{r} \frac{\varepsilon}{2\lambda_j - 1}\Big(\mathcal{G}(O_{j,-\varepsilon}) + \mathcal{G}(O_{j,\varepsilon})\Big)\Big) ,$$

where λ_j denotes the root of equation (4.3) (with $\delta = \delta_j$) in the strip $0 < \operatorname{Re}\lambda < 1$.

Note that formula (4.7) requires the knowledge of the zero λ_0 of the transcendental equation (4.3). An alternative expression for $DH_n^{\pm}(\chi)$ can be given by a path–independent contour integral.

Theorem 4.7. *Assume that* Λ *has only one corner point at* O*, and let* $\Gamma = \partial G \subset \Omega$ *be an arbitrary simple closed piecewise smooth curve around* O*. Then*

$$\begin{aligned} DH_n^{\pm}(\chi) \; &= \int_\Gamma \Big((\chi(O),\nu)\mathcal{J} + (\chi(O),\tau)\mathcal{K}\Big) \\ &+ \int_{G\cap\Lambda} (\chi - \chi(O),\nu)\left[\frac{1}{k^2}\big(\partial_{\nu,\alpha}u\,\overline{\partial_{\nu,\alpha}w} - \partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}w}\big)\right]_\Lambda \\ &+ \int_{\Lambda\setminus G} (\chi,\nu)\left[\frac{1}{k^2}\big(\partial_{\nu,\alpha}u\,\overline{\partial_{\nu,\alpha}w} - \partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}w}\big)\right]_\Lambda \end{aligned} \tag{4.10}$$

To prove (4.10), we first extend Lemma 4.1 to the case where $\operatorname{supp}\chi \cap \Gamma$ contains a corner point of the interface Λ.

Lemma 4.8. *Let* $\Gamma = \partial G$ *be a simple closed piecewise smooth curve such that* $k = const$ *in* G *and that* $\operatorname{supp}\chi \cap \Gamma$ *contains exactly one corner point* O *of* Λ*. Then*

$$B_1(u,w;G) = \int_\Gamma \Big((\chi - \chi(O),\nu)\mathcal{J} + (\chi - \chi(O),\tau)\mathcal{K} + \chi_1\mathcal{L}\Big). \tag{4.11}$$

P r o o f : Let $G_\varepsilon = G \setminus \{r \le \varepsilon\}$, $r = \operatorname{dist}(x,O)$ and $\Gamma_\varepsilon = \partial G_\varepsilon$. Replacing χ by $\chi - \chi(O)$, as in the proof of Lemma 4.1 one obtains by partial integration that

$$B_1(u,w;G) = \lim_{\varepsilon\to 0} B_1(u,w;G_\varepsilon) = \lim_{\varepsilon\to 0} \int_{\Gamma_\varepsilon} \Big((\chi - \chi(O),\nu)\mathcal{J} + (\chi - \chi(O),\tau)\mathcal{K} + \chi_1\mathcal{L}\Big).$$

Recall that the integral of $\chi_1(O)\mathcal{L}$ vanishes; see Remark 4.2. Using the asymptotics (4.4) of u and $\overline{w}$, one can pass to the limit in the last expression giving formula (4.11). ∎

P r o o f of Theorem 4.7: Lemma 4.8 applied to $G = \Omega^{\pm}$ and the transmission conditions for u and w yield

$$\begin{aligned} B_1(u,w) \; &= \Big(B_1(u,w;\Omega^+) + B_1(u,w;\Omega^-)\Big) \\ &= \int_{\partial\Omega} \Big((\chi - \chi(O),\nu)\mathcal{J} + (\chi - \chi(O),\tau)\mathcal{K} + \chi_1\mathcal{L}\Big) \\ &\quad - \int_\Lambda (\chi - \chi(O),\nu)\left[\frac{1}{k^2}\big(\partial_{\nu,\alpha}u\,\overline{\partial_{\nu,\alpha}w} - \partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}w}\big)\right]_\Lambda \\ &= - \int_{\partial\Omega} \Big((\chi(O),\nu)\mathcal{J} + (\chi(O),\tau)\mathcal{K}\Big) \\ &\quad - \int_\Lambda (\chi - \chi(O),\nu)\left[\frac{1}{k^2}\big(\partial_{\nu,\alpha}u\,\overline{\partial_{\nu,\alpha}w} - \partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}w}\big)\right]_\Lambda , \end{aligned}$$

which proves (4.10) for $\Gamma = \partial\Omega$. On the other hand, if $G_1 \subset \Omega$ is a simply connected domain such that $O \notin \overline{G_1}$, then Remark 4.2 implies

$$\int_{\partial G_1^{\pm}} \Big((\chi(O),\nu)\mathcal{J} + (\chi(O),\tau)\mathcal{K}\Big) = 0 ,$$

where $G_1^\pm = G_1 \cap \Omega^\pm$. Hence, by the transmission conditions for u and w

$$\int_{\partial G_1} \Big((\chi(O),\nu)\mathcal{J} + (\chi(O),\tau)\mathcal{K}\Big) = -\int_{G\cap\Lambda} (\chi(O),\nu)\left[\frac{1}{k^2}\big(\partial_{\nu,\alpha} u\,\overline{\partial_{\nu,\alpha} w} - \partial_{\tau,\alpha} u\,\overline{\partial_{\tau,\alpha} w}\big)\right]_\Lambda \tag{4.12}$$

so that the right–hand side of (4.10) is in fact independent of the contour Γ. ∎

Remark 4.9. Formula (4.10) easily extends to the case of finitely many corners $O_1, \dots, O_r$ of the interface Λ. Let $\Gamma_j = \partial G_j$ be a simple piecewise smooth curve enclosing the corner point O_j only. Then the right–hand side of (4.10) has to be replaced by the sum

$$\sum_j \Bigg(\int_{\Gamma_j} \Big((\chi(O_j),\nu)\mathcal{J} + (\chi(O_j),\tau)\mathcal{K}\Big) + \int_{G_j\cap\Lambda} (\chi-\chi(O_j),\nu)\left[\frac{1}{k^2}\big(\partial_{\nu,\alpha} u\,\overline{\partial_{\nu,\alpha} w} - \partial_{\tau,\alpha} u\,\overline{\partial_{\tau,\alpha} w}\big)\right]_\Lambda \Bigg) + \int_{\Lambda\setminus(\cup G_j)} (\chi,\nu)\left[\frac{1}{k^2}\big(\partial_{\nu,\alpha} u\,\overline{\partial_{\nu,\alpha} w} - \partial_{\tau,\alpha} u\,\overline{\partial_{\tau,\alpha} w}\big)\right]_\Lambda . \tag{4.13}$$

Indeed, choosing cut–off functions ξ_j near O_j such that $\sum_j \xi_j \equiv 1$ in some neighbourhood of Λ, one applies formula (4.10) with χ replaced by $\xi_j\chi$ and summing over j then gives the result with sufficiently small discs G_j with centres O_j. Again, by virtue of (4.12), the resulting expression (4.13) is independent of the choice of the contours Γ_j.

Remark 4.10. Repeating the arguments used in the proofs of Theorem 3.3 and Corollary 4.3 one obtains the following formula for the derivative of the TE reflection and transmission coefficients $E_n^\pm$ with respect to the variations (3.2) of the interface Λ:

$$DE_n^\pm(\chi) = \int_\Lambda (\chi,\nu)\left[k^2 u\overline{w}\right]_\Lambda . \tag{4.14}$$

Here u is the solution of the direct TE problem (2.8), w solves the corresponding adjoint problem and Λ may be an arbitrary Lipschitz curve. A special case of (4.14) was first proved in [4].

5. Applications to binary gratings

For simplicity we restrict to a binary grating with two transition points t_1, $t_2 = 2\pi$ and the height t_3. Let $O_1 = (t_1, 0)$, $O_2 = (t_1, t_3)$, $O_3 = (2\pi, t_3)$ and $\Sigma_1 = \overline{O_1O_2}$, $\Sigma_2 = \overline{O_2O_3}$.

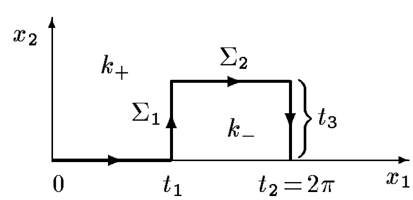

Figure 1: Cross section of a simple binary grating

We first compute the derivative $D_1 H_n^\pm$ of the Rayleigh coefficients with respect to the variation of t_1. Then the mapping (3.2) takes the form

$$\Phi_h(x) = x + h\,\chi(x)\,, \quad \chi(x) = (\chi_1(x), 0)\,,$$

where $\chi_1 \equiv 1$ in some neighbourhood of Σ_1 and $\chi \in C_o^\infty(U)$ for a somewhat larger neighbourhood U (not containing other corners of the profile curve Λ). Since

$$\chi - \chi(O_1) = \chi - \chi(O_2) = 0 \quad \text{on } \Sigma_1\,, \quad (\chi, \nu) = 0 \quad \text{on } \Lambda \setminus \Sigma_1\,,$$

from Remark 4.9 we easily obtain

Corollary 5.1. *Let Γ be an arbitrary simple closed piecewise smooth curve around Σ_1, which does not encircle corner points on Λ different from O_1, O_2. Then*

$$\begin{aligned} D_1 H_n^\pm \;&=\; \int_\Gamma \Big(\nu_1\big(-u\,\overline{w} + \frac{1}{k^2}(\partial_2 u\,\partial_2\overline{w} - \partial_{1,\alpha} u\,\overline{\partial_{1,\alpha} w})\big) \\ &\qquad + \frac{\nu_2}{k^2}(\partial_2 u\,\overline{\partial_{1,\alpha} w} + \partial_{1,\alpha} u\,\partial_2\overline{w})\Big), \end{aligned} \tag{5.1}$$

where u and w denote the solutions of the direct and adjoint diffraction problems (2.9), (3.10), *respectively.*

To prove (5.1), one may choose, for example rectangles G_j $(j = 1, 2)$ around O_j with a common side such that $\Gamma = \partial(G_1 \cup G_2)$ encloses the segment Σ_1. Then formula (5.1) follows immediately from Remark 4.9. Note that (4.13) reduces to

$$\sum_{j=1,2}\int_{\partial G_j} \big((\chi(O_j), \nu)\mathcal{J} + (\chi(O_j), \tau)\mathcal{K}\big) = \int_\Gamma \big(\nu_1 \mathcal{J} - \nu_2 \mathcal{K}\big)$$

with $\mathcal{J}$, $\mathcal{K}$ defined in (4.1). The fact that the integral in (5.1) is path–independent is an easy consequence of Remark 4.2.

Define $O_{j,\pm\varepsilon}$ as in Sec. 3, and let $\Sigma_{1,\varepsilon} = \overline{O_{1,\varepsilon} O_{2,-\varepsilon}}$. Let further λ_0 be the root of equation (4.3) with $\delta = \pi/2$, lying in the strip $0 < \operatorname{Re}\lambda < 1$. Note that for all corner points of a binary grating the same transcendental equation occurs. Since $\nu = (1,0), \tau = (0,1)$ on Σ_1 and $(\chi, \nu) = 0$ on $\Lambda \setminus \Sigma_1$, Remark 4.6 implies immediately

Corollary 5.2. *With* $\mathcal{G} := \left[\frac{1}{k^2}(\partial_{1,\alpha} u\,\overline{\partial_{1,\alpha} w} - \partial_2 u\,\overline{\partial_2 w})\right]_\Lambda$ *we have*

$$D_1 H_n^\pm = \lim_{\varepsilon \to 0}\Big(\int_{\Sigma_{1,\varepsilon}} \mathcal{G} + \frac{\varepsilon}{2\lambda_0 - 1}\big(\mathcal{G}(O_{1,\varepsilon}) + \mathcal{G}(O_{2,-\varepsilon})\big)\Big)\,.$$

This result has been stated, without proof, in [5, Remark 4.3].

We now compute the derivative $D_1 H_n^\pm$ with respect to the height of the binary grating. In this case the mapping (3.2) is of the form

$$\Phi_h(x) = x + h\,\chi(x)\,, \quad \chi(x) = (0, \chi_2(x))\,,$$

where $\chi_2 \equiv 1$ near Σ_2 and $\chi_2 \in C_o^\infty(U)$ for a sufficiently small neighbourhood U of Σ_2. Note that $\nu = (0,-1), \tau = (1,0)$ on Σ_2 and $\chi - \chi(O_2) = \chi - \chi(O_3) = 0$ on Σ_2 and $(\chi, \nu) = 0$ on $\Lambda \setminus \Sigma_2$. As above we then obtain

Corollary 5.3. *Let Γ be an arbitrary simple closed piecewise smooth curve enclosing Σ_2 but no other corner points of Λ. Then*

$$\begin{aligned} D_2 H_n^\pm \;&=\; \int_\Gamma \Big(\nu_2\big(-u\,\overline{w} + \frac{1}{k^2}(\partial_{1,\alpha} u\,\overline{\partial_{1,\alpha} w} - \partial_2 u\,\overline{\partial_2 w})\big) \\ &\qquad - \frac{\nu_1}{k^2}(\partial_2 u\,\overline{\partial_{1,\alpha} w} + \partial_{1,\alpha} u\,\partial_2\overline{w})\Big) \\ &= \lim_{\varepsilon \to 0}\Big(\int_{\Sigma_{2,\varepsilon}} \mathcal{G} + \frac{\varepsilon}{2\lambda_0 - 1}\big(\mathcal{G}(O_{2,\varepsilon}) + \mathcal{G}(O_{3,-\varepsilon})\big)\Big)\,, \end{aligned}$$

where $\Sigma_{2,\varepsilon} = \overline{O_{2,\varepsilon} O_{3,-\varepsilon}}$ *and* $\mathcal{G}$ *is defined as in Corollary* 5.2.

Finally, we remark that for $\operatorname{Re} \lambda_0 > 1/2$ we have

$$D_i H_n^{\pm} = \int_{\Sigma_i} \left[\frac{1}{k^2} \left(\partial_{1,\alpha} u \, \overline{\partial_{1,\alpha} w} - \partial_2 u \, \overline{\partial_2 w} \right) \right]_{\Lambda} ,$$

which gives

$$\begin{aligned} D_1 H_n^{\pm} &= \frac{1}{k_+^2} \int_{\Sigma_1} \left(\partial_{1,\alpha} u|_{\Lambda}^{+} \, \overline{\partial_{1,\alpha} w}|_{\Lambda}^{+} - \partial_2 u \, \partial_2 \overline{w} \right) \\ &\quad - \frac{1}{k_-^2} \int_{\Sigma_1} \left(\partial_{1,\alpha} u|_{\Lambda}^{-} \, \overline{\partial_{1,\alpha} w}|_{\Lambda}^{-} - \partial_2 u \, \partial_2 \overline{w} \right) \\ &= \frac{k_+^2 - k_-^2}{(k_+ k_-)^2} \int_{\Sigma_1} \left(\partial_{1,\alpha} u|_{\Lambda}^{+} \, \overline{\partial_{1,\alpha} w}|_{\Lambda}^{-} + \partial_2 u \, \partial_2 \overline{w} \right) , \end{aligned}$$

$$\begin{aligned} D_2 H_n^{\pm} &= \frac{1}{k_+^2} \int_{\Sigma_2} \left(\partial_{1,\alpha} u \, \overline{\partial_{1,\alpha} w} - \partial_2 u|_{\Lambda}^{+} \, \partial_2 \overline{w}|_{\Lambda}^{+} \right) \\ &\quad - \frac{1}{k_-^2} \int_{\Sigma_2} \left(\partial_{1,\alpha} u \, \overline{\partial_{1,\alpha} w} - \partial_2 u|_{\Lambda}^{-} \, \partial_2 \overline{w}|_{\Lambda}^{-} \right) \\ &= \frac{k_-^2 - k_+^2}{(k_+ k_-)^2} \int_{\Sigma_2} \left(\partial_{1,\alpha} u \, \overline{\partial_{1,\alpha} w} + \partial_2 u|_{\Lambda}^{+} \, \partial_2 \overline{w}|_{\Lambda}^{-} \right) . \end{aligned}$$

These formulas have been proved in [5, Sec. 4.3] using another approach.

References

[1] A.-S. Bonnet-Bendhia and F. Starling, Guided waves by electromagnetic gratings and non–uniqueness examples for the diffraction problem. *Math. Meth. Appl. Sci.* **17** (1994), 305–338.

[2] G. Bao, D. C. Dobson, and J. A. Cox, Mathematical studies in rigorous grating theory. *J. Opt. Soc. Amer.* **A 12** (1995), 1029–1042.

[3] M. Costabel and E. Stephan, A direct boundary integral equation method for transmission problems, *J. Math. Anal. Appl.* **106** (1985), 367–413.

[4] D. C. Dobson, Optimal shape design of blazed diffraction gratings, *Appl. Math. Opt.* **40** (1999), 61-78.

[5] J. Elschner and G. Schmidt, Diffraction in periodic structures and optimal design of binary gratings I. Direct problems and gradient formulas, *Math. Meth. Appl. Sci* **21** (1998), 1297–1342.

[6] J. Elschner , R. Hinder, F. Penzel, and G. Schmidt, Existence, uniqueness and regularity for solutions of the conical diffraction problem, M^3AS (to appear).

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

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