Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

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Shape derivatives for the scattering by biperiodic gratings

Andreas Rathsfeld

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Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: Andreas.Rathsfeld@wias-berlin.de

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Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

Usually, the light diffraction by biperiodic grating structures is simulated by the time-harmonic Maxwell system with a constant magnetic permeability. For the optimization of the geometry parameters of the grating, a functional is defined which depends quadratically on the efficiencies of the reflected modes. The minimization of this functional by gradient based optimization schemes requires the computation of the shape derivatives of the functional with respect to the parameters of the geometry. Using classical ideas of shape calculus, formulas for these parameter derivatives are derived. In particular, these derivatives can be computed as material derivatives corresponding to a family of transformations of the underlying domain. However, the energy space $H(\mathrm{curl})$ for the electric fields is not invariant with respect to the transformation of geometry. Therefore, the formulas are derived first for the magnetic field vectors which belong to $[H^1]^3$. Afterwards, the magnetic fields in the shape-derivative formula are replaced by their electric counter parts. Numerical tests confirm the derived formulas.

1 Introduction

The diffraction of light by periodic surface structures can be simulated by the time-harmonic Maxwell system. Suppose an incoming plane wave mode with a fixed direction of incidence is scattered by the grating structure. Then the scattered field is the superposition of a finite number of propagating reflected and transmitted plane wave modes and of an evanescent light wave (cf.[18]). The efficiencies of the grating are the portions of energy which are sent to the reflected or transmitted modes. These efficiencies together with the phase shifts of the propagating plane wave modes are essential for the functionality of the grating as diffractive optical element. On the other hand, knowing the efficiencies, a reconstruction of the geometry or, at least, of some parameters of the geometry by solving an inverse problem should be possible. The corresponding measurement technique is called scatterometry. In other words, both, the optimization of diffractive optical elements (cf. e.g. [10, 2]) and the scatterometric measurement (cf. e.g. [12]), can be based on the optimization of objective functionals depending quadratically on the efficiencies of the grating. If a gradient based optimization scheme is applied, then derivatives of the objective functional with respect to the parameters of the geometry are required.

The general theory of shape calculus is well established (cf. e.g. [25]) and, using boundary integral equations, shape derivatives for three-dimensional obstacles with smooth boundaries have been derived (cf. [9]). Formulas for the shape derivatives of two-dimensional diffraction gratings have been derived in e.g. [11, 15]. It has been pointed out that, if the shape derivatives of the efficiencies are sought, then it is sufficient to compute the material derivatives of the electromagnetic field. Note that these material fields are smoother than the classical shape derivatives.

Formally, these two-dimensional techniques can be applied to biperiodic gratings too. However, the energy space of the electric field solution to the time-harmonic Maxwell equation is the space $H(\mathrm{curl})$, i.e., not all first order derivatives have a bounded L^2 norm but only a few linear combinations have this boundedness property. The geometry transformations corresponding to a change of the parameters describing the geometry, lead to a transformation of these linear combinations such that a bounded L^2 norm cannot be guaranteed after the transformation. Consequently, the integrands in the formally derived gradient formulas are not integrable.

To overcome this problem, we suppose that the magnetic permeability μ is constant. In this case, the shape calculus can be applied to the magnetic field solution which is in the smoother space $[H^1]^3$, i.e., over all subdomains filled with the same material all first order derivatives have a bounded L^2 norm (cf. [8]). A shape-derivative formula including the magnetic field can be derived. Transforming this formula, the magnetic field can be substituted by the electric field using the Maxwell equations. It is well known that the derivatives can be expressed as integrals over those interfaces of the geometry which move with the varying parameters. However, to avoid troubles with the generalized integration of unbounded integrands (cf. [11]), the formulas of the present paper will contain domain integrals as well. For each gradient of the objective functional, the original time-harmonic Maxwell system is to be solved, a solution of the adjoint Maxwell system is to be calculated, and special sesqui-linear forms including these two solutions must be evaluated.

The time-harmonic Maxwell system for the grating problem, the boundary conditions, and the incident, reflected, and transmitted plane wave modes will be introduced in Section 2. In Section 3 the variational formulation proposed by [14] (cf. also [16, 19, 13, 1, 3, 21]) is described. The objective functional and a special example, the contact hole geometry, is defined in Section 4. The main result is the shape-derivative formula of Theorem 4.1. The proof follows in the Sections 4.5–4.9. Finally, a numerical example for the contact holes is presented in Section 5.

2 The underlying boundary value problem for the time-harmonic Maxwell's equations

2.1 Geometry and electric permittivity

The biperiodic grating is a three-dimensional surface structure which is a perturbation of the plane $\{(x,y,z)^\top \in \mathbb{R}^3 : \ z = 0\}$. This perturbation is supposed to be bounded with respect to the coordinate z and periodic with respect to x and y. More precisely, the Maxwell equations are considered in $\mathbb{R}^3$ with a constant magnetic permeability μ and a piecewise constant electric permittivity $\varepsilon(x,y,z)$ such that $\varepsilon(x,y,z)$ is periodic with respect to x and y and equal to the constant values ε^+ and ε^- for $z \geq z_{\max}$ and $z \leq z_{\min}$, respectively. Here $z_{\max} > 0$ and $z_{\min} < 0$ are fixed z-coordinates such that the grating surface is contained in the set $\{(x,y,z)^\top \in \mathbb{R}^3 : \ z_{\min} < z < z_{\max}\}$.

Consequently, the variational formulation of the problem for the Maxwell equations can be restricted to a single periodicity cell, i.e., to the rectangular brick domain

$$G := [x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}] \times [z_{\min}, z_{\max}]. \tag{1}$$

The period is $\mathrm{per}_x := x_{\max} - x_{\min}$ for the x direction and $\mathrm{per}_y := y_{\max} - y_{\min}$ for the y direction. For simplicity, the domains in G with constant values ε are supposed to be polyhedral. In order to simplify the notation, we even assume periodicity across the lateral boundaries in the sense of $\varepsilon(x_{\min} + 0, y, z) = \varepsilon(x_{\max} - 0, y, z)$ and $\varepsilon(x, y_{\min} + 0, z) = \varepsilon(x, y_{\max} - 0, z)$.

2.2 Partial differential equation

Eliminating the magnetic or the electric field, the time-harmonic Maxwell equations can be reduced to two different versions of the curl-curl equations for the electric field and the magnetic field, respectively. If the electric field is sought, then the electric version should be solved. However, since $\mu = \mu_0$ is constant and ϵ only piecewise constant, the magnetic field solution has some additional smoothness properties which will be important to derive the shape-derivative formulas for the electric field equation.

In fact, for constant $\mu = \mu_0$, the magnetic field H is divergence free. The term $\nabla[\nabla \cdot H] = 0$ can be added to the curl-curl equation. Thus the magnetic field is the solution of a strongly elliptic partial differential equation over each domain with constant ε and is not only in the space $H(\mathrm{curl})$, but in $[H^1]^3$. In other words, the magnetic field solution of the magnetic curl-curl equations has square integrable first order derivatives (cf. e.g. [8, 21]). This may be not true for the electric field solution of the electric curl-curl equation.

The time-harmonic electric field can be represented as $\mathcal{E}(x, y, z, t) = \Re\mathrm{e}\{E(x, y, z)e^{-\mathbf{i}\omega t}\}$ and the magnetic field as $\mathcal{H}(x, y, z, t) = \Re\mathrm{e}\{H(x, y, z)e^{-\mathbf{i}\omega t}\}$, where $\omega > 0$ is the angular frequency. In the following, the complex valued amplitude functions E and H will be referred to as the electric and magnetic fields, respectively. The curl-curl equations look as follows. Eliminating the magnetic field H and the electric field E, respectively, from the time-harmonic Maxwell system

$$\nabla \times H - (-\mathbf{i}\omega)[\varepsilon E] = 0, \quad \nabla \times E + (-\mathbf{i}\omega)\,[\mu H] = 0,$$

yields

$$\nabla \times \nabla \times u_{el}(P) - k^2 u_{el}(P) \;=\; 0,\; P \in G, \tag{2}$$

$$\nabla \times \left[k^{-2}[\nabla \times u_{ma}(P)]\right] - u_{ma}(P) \;=\; 0,\; P \in G, \tag{3}$$

with $u_{el} = E$, $u_{ma} = H$, and wave number $k := \sqrt{\varepsilon\mu\omega^2}$. Note that (2) and (3) are satisfied at all points $P \in G$ which are located in the interior of the subdomains of G, where the piecewise constant ε takes a constant value. The two fields u_{el} and u_{ma} are connected by

$$u_{el} \;=\; \frac{\mathbf{i}\mu\omega}{k^2}[\nabla \times u_{ma}], \quad [\nabla \times u_{el}] \;=\; \mathbf{i}\mu\omega\, u_{ma}, \tag{4}$$

$$u_{ma} \;=\; -\frac{\mathbf{i}}{\mu\omega}[\nabla \times u_{el}], \quad [\nabla \times u_{ma}] \;=\; -\frac{\mathbf{i}k^2}{\mu\omega}\, u_{el}. \tag{5}$$

Note that the wave number k is given alternatively by $k = 2\pi\mathbf{n}/\lambda$, where λ is the wave length of the light in vacuum and $\mathbf{n}$ the piecewise constant refractive index describing the optical properties of the involved materials. The refractive index for the material above and below the grating will be denoted by $\mathbf{n}^{\pm}$.

2.3 Incident wave

The incident light is supposed to be a plane wave with angles of incidence θ and ϕ restricted to the ranges $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ and $0 \le \phi < 2\pi$. Thus the amplitude U^{inc} of the time harmonic wave function $U^{\mathrm{inc}}(x,y,z)e^{-\mathbf{i}\omega t}$ is

$$\begin{aligned} U_{el}^{\mathrm{inc}}(x,y,z) &:= \begin{pmatrix} e^{\mathrm{inc}} \\ f^{\mathrm{inc}} \\ g^{\mathrm{inc}} \end{pmatrix} e^{\mathbf{i}k^+(\sin\theta\cos\phi\, x + \sin\theta\sin\phi\, y - \cos\theta\, z)} \\ &= \begin{pmatrix} e_c^{\mathrm{inc}} \\ f_c^{\mathrm{inc}} \\ g_c^{\mathrm{inc}} \end{pmatrix} e^{\mathbf{i}k^+(\sin\theta\cos\phi\, x + \sin\theta\sin\phi\, y - \cos\theta\, [z - z_{\max}])}, \\ e_c^{\mathrm{inc}} := e^{\mathrm{inc}} e^{-\mathbf{i}k^+\cos\theta\, z_{\max}}, \quad f_c^{\mathrm{inc}} &:= f^{\mathrm{inc}} e^{-\mathbf{i}k^+\cos\theta\, z_{\max}}, \quad g_c^{\mathrm{inc}} := g^{\mathrm{inc}} e^{-\mathbf{i}k^+\cos\theta\, z_{\max}} \end{aligned} \tag{6}$$

for the electric field and

$$\begin{aligned} U_{ma}^{\mathrm{inc}}(x,y,z) &:= \frac{\mathbf{n}^+}{\mu c} \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ -\cos\theta \end{pmatrix} \times \begin{pmatrix} e^{\mathrm{inc}} \\ f^{\mathrm{inc}} \\ g^{\mathrm{inc}} \end{pmatrix} e^{\mathbf{i}k^+(\sin\theta\cos\phi\, x + \sin\theta\sin\phi\, y - \cos\theta\, z)} \\ &= \frac{\mathbf{n}^+}{\mu c} \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ -\cos\theta \end{pmatrix} \times \begin{pmatrix} e_c^{\mathrm{inc}} \\ f_c^{\mathrm{inc}} \\ g_c^{\mathrm{inc}} \end{pmatrix} e^{\mathbf{i}k^+(\sin\theta\cos\phi\, x + \sin\theta\sin\phi\, y - \cos\theta\, [z - z_{\max}])} \end{aligned} \tag{7}$$

for the magnetic field. Note that $\mathbf{n}^+/\mu c = k^+/\mu\omega$ implies $U_{ma}^{\mathrm{inc}} = -\mathrm{i}/\omega\mu\ \nabla \times U_{el}^{\mathrm{inc}}$ (cf. the relation (5)).

Polarization and phase are fixed by the constant complex-valued coefficients e^{inc}, f^{inc}, and g^{inc}. For TE polarization, the amplitude vector is chosen as $(e^{\mathrm{inc}}, f^{\mathrm{inc}}, g^{\mathrm{inc}})^\top = (\sin\phi, -\cos\phi, 0)^\top$ and, for TM polarization, $(e^{\mathrm{inc}}, f^{\mathrm{inc}}, g^{\mathrm{inc}})^\top = (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)^\top$. In any case, the amplitude vector $(e^{\mathrm{inc}}, f^{\mathrm{inc}}, g^{\mathrm{inc}})^\top$ must always be orthogonal to the direction of propagation $(\sin\theta\cos\phi, \sin\theta\sin\phi, -\cos\theta)^\top$, i.e., $e^{\mathrm{inc}}\sin\theta\cos\phi + f^{\mathrm{inc}}\sin\theta\sin\phi - g^{\mathrm{inc}}\cos\theta = 0$.

Exceptional formulas are needed for $\theta = 0$ since in this case the angle ϕ is not defined uniquely. Formally, ϕ is set to zero and

$$\begin{gathered} U_{el}^{\mathrm{inc}}(x,y,z) := \begin{pmatrix} e^{\mathrm{inc}} \\ f^{\mathrm{inc}} \\ g^{\mathrm{inc}} \end{pmatrix} e^{-\mathbf{i}k^+ z} = \begin{pmatrix} e_c^{\mathrm{inc}} \\ f_c^{\mathrm{inc}} \\ g_c^{\mathrm{inc}} \end{pmatrix} e^{-\mathbf{i}k^+[z - z_{\max}]}, \\ e_c^{\mathrm{inc}} := e^{\mathrm{inc}} e^{-\mathbf{i}k^+ z_{\max}}, \quad f_c^{\mathrm{inc}} := f^{\mathrm{inc}} e^{-\mathbf{i}k^+ z_{\max}}, \quad g_c^{\mathrm{inc}} := g^{\mathrm{inc}} e^{-\mathbf{i}k^+ z_{\max}} \end{gathered} \tag{8}$$

as well as

$$U_{ma}^{\mathrm{inc}}(x,y,z) := \frac{\mathbf{n}^+}{\mu c}\begin{pmatrix}0\\0\\-1\end{pmatrix}\times\begin{pmatrix}e^{\mathrm{inc}}\\f^{\mathrm{inc}}\\g^{\mathrm{inc}}\end{pmatrix}e^{-\mathbf{i}k^+z} = \frac{\mathbf{n}^+}{\mu c}\begin{pmatrix}0\\0\\-1\end{pmatrix}\times\begin{pmatrix}e_c^{\mathrm{inc}}\\f_c^{\mathrm{inc}}\\g_c^{\mathrm{inc}}\end{pmatrix}e^{-\mathbf{i}k^+[z-z_{\max}]}. \tag{9}$$

For TE polarization, the amplitude vector is given by $(e^{\mathrm{inc}}, f^{\mathrm{inc}}, g^{\mathrm{inc}})^\top = (0,-1,0)^\top$ and, for TM polarization, by $(e^{\mathrm{inc}}, f^{\mathrm{inc}}, g^{\mathrm{inc}})^\top = (1,0,0)^\top$. In general, $(e^{\mathrm{inc}}, f^{\mathrm{inc}}, g^{\mathrm{inc}})^\top$ is orthogonal to the direction of propagation $(0,0,-1)^\top$.

2.4 Boundary and transmission conditions

The incident wave is quasi-periodic, i.e., a shift by the period in the x- and y-coordinate of the argument leads to a multiplication of the vector value by the factor $e^{\mathbf{i}k^+\sin\theta\cos\phi\,\mathrm{per}_x}$ and $e^{\mathbf{i}k^+\sin\theta\sin\phi\,\mathrm{per}_y}$, respectively. Thus, according to Floquet's theorem, also the field solutions satisfy the quasi-periodic lateral conditions

$$\begin{aligned} u(x_{\max},y,z) = u(x_{\min}+\mathrm{per}_x,y,z) &= u(x_{\min},y,z)\gamma_x,\ \gamma_x := e^{\mathbf{i}k^+\sin\theta\cos\phi\,\mathrm{per}_x},\\ u(x,y_{\max},z) = u(x,y_{\min}+\mathrm{per}_y,z) &= u(x,y_{\min},z)\gamma_y,\ \gamma_y := e^{\mathbf{i}k^+\sin\theta\sin\phi\,\mathrm{per}_y}. \end{aligned}$$

In particular, for the electric field, we obtain the lateral boundary conditions

$$(1,0,0)^\top \times u_{el}(x_{\max},y,z) = (1,0,0)^\top \times u_{el}(x_{\min},y,z)\gamma_x, \tag{10}$$
$$(1,0,0)^\top \times [\nabla\times u_{el}(x_{\max},y,z)] = (1,0,0)^\top \times [\nabla\times u_{el}(x_{\min},y,z)]\gamma_x, \tag{11}$$
$$(0,1,0)^\top \times u_{el}(x,y_{\max},z) = (0,1,0)^\top \times u_{el}(x,y_{\min},z)\gamma_y, \tag{12}$$
$$(0,1,0)^\top \times [\nabla\times u_{el}(x,y_{\max},z)] = (0,1,0)^\top \times [\nabla\times u_{el}(x,y_{\min},z)]\gamma_y, \tag{13}$$

connecting the tangential components of u and $\nabla\times u$ on the lateral boundaries of G. In the case of the magnetic field, the continuity of u_{ma} and $k^{-2}\nabla\times u_{ma} = -\mathbf{i}/\mu\omega u_{el}$ yield

$$(1,0,0)^\top \times u_{ma}(x_{\max},y,z) = (1,0,0)^\top \times u_{ma}(x_{\min},y,z)\gamma_x, \tag{14}$$
$$(1,0,0)^\top \times [k^{-2}\nabla\times u_{ma}(x_{\max},y,z)] = (1,0,0)^\top \times [k^{-2}\nabla\times u_{ma}(x_{\min},y,z)]\gamma_x, \tag{15}$$
$$(0,1,0)^\top \times u_{ma}(x,y_{\max},z) = (0,1,0)^\top \times u_{ma}(x,y_{\min},z)\gamma_y, \tag{16}$$
$$(0,1,0)^\top \times [k^{-2}\nabla\times u_{ma}(x,y_{\max},z)] = (0,1,0)^\top \times [k^{-2}\nabla\times u_{ma}(x,y_{\min},z)]\gamma_y. \tag{17}$$

The normal vector at the boundary surface and at the interfaces will be denoted by ν. In other words, $\nu = (0,0,1)$ on $\Gamma^+ := \{(x,y,z)^\top \in G : \ z = z_{\max}\}$ and $\nu = (0,0,-1)$ on $\Gamma^- := \{(x,y,z)^\top \in G : \ z = z_{\min}\}$. For an interface Γ between two subdomains of G with different values of ε, an orientation is fixed. The normal ν at $P \in \Gamma$ is the unit normal at the interface pointing into the subdomain on the left of the interface. If u is a vector field over G, if $u(+P)$ is the limit at P of u from the subdomain on the right of Γ, and if $u(-P)$ is the limit from the domain on the left, then the jump of u across the interface Γ is denoted by $[u(P)]_\Gamma := u(+P) - u(-P)$.

The classical interface conditions $\nu\times[E]_\Gamma = 0$ and $\nu\times[H]_\Gamma = 0$ for the tangential jumps of the fields over interfaces Γ separating different materials turn into

$$\nu \times [u_{el}]_\Gamma \;=\; 0, \qquad \nu \times [\nabla \times u_{el}]_\Gamma \;=\; 0, \tag{18}$$

$$\nu \times [u_{ma}]_\Gamma \;=\; 0, \qquad \nu \times [k^{-2}\nabla \times u_{ma}]_\Gamma \;=\; 0. \tag{19}$$

On the upper and lower boundaries $\Gamma^\pm$, we have a similar jump condition. Left of Γ^+ and right of Γ^-, the field u is the solution in G. On the right of Γ^+ and on the left of Γ^-, we have the extension of u to the upper and lower half plane, respectively. Above Γ^+ this extension is the sum of the incoming wave u^{inc} and an upward radiating field u^+. Below Γ^- this extension is a downward radiating field u^-. In other word, the jump relation leads to the boundary condition on Γ^+

$$\nu \times u_{el} \;=\; \nu \times [u_{el}^{\text{inc}} + u_{el}^{+}], \qquad \nu \times [\nabla \times u_{el}] = \nu \times \Big[\nabla \times [u_{el}^{\text{inc}} + u_{el}^{+}]\Big], \tag{20}$$

$$\nu \times u_{ma} \;=\; \nu \times [u_{ma}^{\text{inc}} + u_{ma}^{+}], \qquad \nu \times \frac{1}{k^2}[\nabla \times u_{ma}] = \nu \times \frac{1}{k^2}\Big[\nabla \times [u_{ma}^{\text{inc}} + u_{ma}^{+}]\Big] \tag{21}$$

with an incident wave mode $u^{\text{inc}} = U^{\text{inc}}$ (cf. (6) and (7)) and a yet unknown upward radiating wave u^+ (cf. the subsequent formula (24)). On the lower boundary Γ^-, we get

$$\nu \times u_{el} \;=\; \nu \times u_{el}^{-}, \qquad \nu \times [\nabla \times u_{el}] = \nu \times \nabla \times u_{el}^{-}, \tag{22}$$

$$\nu \times u_{ma} \;=\; \nu \times u_{ma}^{-}, \qquad \nu \times \frac{1}{k^2}[\nabla \times u_{ma}] = \nu \times \frac{1}{k^2}[\nabla \times u_{ma}^{-}] \tag{23}$$

with a yet unknown downward radiating wave u^- (cf. the subsequent formula (37)). Note that the restriction to upward and downward radiating fields $u^\pm$ in (21) and (22) is the radiation condition for our Maxwell problem.

2.5 Complete boundary value problem

The solution of the Maxwell system in $\mathbb{R}^3$ splits into three parts u, u^-, and u^+. The function u is the restriction of the total field u^{tot} to the layer $\{(x, y, z) \in \mathbb{R}^3 : \; z_{\min} < z < z_{\max}\}$. Clearly, due to the quasi-periodicity $u(x + \text{per}_x, y, z) = u(x, y, z)\gamma_x$ and $u(x, y + \text{per}_y, z) = u(x, y, z)\gamma_y$, this function is determined by its restriction to G defined in (1). Since ε is constant for $z \le z_{\min}$ and $z \ge z_{\max}$, the restrictions of u^{tot} to these half spaces can be represented by the Rayleigh series expansions (cf. [18]). For $z \ge z_{\max}$, we get $u^{\text{tot}} = U^{\text{inc}} + u^+$ with the incident wave U^{inc} (cf. (6) and (7)) and with an upward radiating reflected field u^+ (cf. (24)). For $z \le z_{\min}$, we have $u^{\text{tot}} = u^-$ with a downward radiating transmitted field u^- (cf. (37)). The final electric boundary value problem is the partial differential equation (2) for u over the subdomains of G combined with the lateral boundary conditions (10)–(13), the interface conditions (18), and the conditions (20),(22) coupling u and $[\nabla \times u]$ through the yet unknown upward and downward radiating $u^\pm$. The magnetic boundary value problem is the partial differential equation (3) for u over the subdomains of G combined with the lateral boundary conditions (14)-(17), the interface conditions (19), and the coupling conditions (21),(23).

2.6 Rayleigh series expansions for the radiation condition

The Rayleigh series expansion for the reflected field takes the form

$$u^{+} = \sum_{n\in\mathbb{Z}} \sum_{m\in\mathbb{Z}} \sum_{l=0,1} B^{+}_{n,m,l} u^{+}_{n,m,l}, \tag{24}$$

where the Rayleigh coefficients $B^{+}_{n,m,l}$ are complex numbers, and the upward radiating modes $u^{+}_{n,m,l} = u^{+}_{el,n,m,l}$ in the electric case and $u^{+}_{n,m,l} = u^{+}_{ma,n,m,l}$ in the magnetic case are given by

$$u^{+}_{el,n,m,l}(x,y,z) = \begin{pmatrix} e_{n,m,l} \\ f_{n,m,l} \\ g_{n,m,l} \end{pmatrix} e^{\mathbf{i}(a_n x + b_m y + c_{n,m}[z - z_{\max}])}, \tag{25}$$

$$u^{+}_{ma,n,m,l}(x,y,z) = \frac{1}{\mu\omega} \begin{pmatrix} a_n \\ b_m \\ c_{n,m} \end{pmatrix} \times \begin{pmatrix} e_{n,m,l} \\ f_{n,m,l} \\ g_{n,m,l} \end{pmatrix} e^{\mathbf{i}(a_n x + b_m y + c_{n,m}[z - z_{\max}])}. \tag{26}$$

Here

$$a^{\mathrm{inc}} := k^{+} \sin\theta \cos\phi, \quad b^{\mathrm{inc}} := k^{+} \sin\theta \sin\phi, \tag{27}$$

$$a_n := a^{\mathrm{inc}} + n\frac{2\pi}{\mathrm{per}_x}, \quad b_m := b^{\mathrm{inc}} + m\frac{2\pi}{\mathrm{per}_y}, \quad c_{n,m} := \sqrt{(k^{+})^2 - a_n^2 - b_m^2}, \tag{28}$$

$$e_{n,m,0} := -\frac{b_m}{h_{n,m}}, \qquad f_{n,m,0} := \frac{a_n}{h_{n,m}}, \qquad g_{n,m,0} := 0, \tag{29}$$

$$h_{n,m} := \sqrt{|a_n|^2 + |b_m|^2}, \tag{30}$$

$$e_{n,m,1} := -\frac{c_{n,m} a_n}{h_{n,m,1}}, \qquad f_{n,m,1} := -\frac{c_{n,m} b_m}{h_{n,m,1}}, \qquad g_{n,m,1} := \frac{a_n^2 + b_m^2}{h_{n,m,1}}, \tag{31}$$

$$h_{n,m,1} := \sqrt{|c_{n,m}|^2 + h_{n,m}^2}\; h_{n,m}. \tag{32}$$

The square root in (28) is defined such that $c_{n,m} > 0$ if $(k^{+})^2 \geq a_n^2 + b_m^2$ and $\Im\mathrm{m}\, c_{n,m} > 0$ if $(k^{+})^2 < a_n^2 + b_m^2$. Note that

$$\left(e_{n,m,1}, f_{n,m,1}, g_{n,m,1}\right)^{\top} = \frac{h_{n,m}}{h_{n,m,1}} \left(a_n, b_m, c_{n,m}\right)^{\top} \times \left(e_{n,m,0}, f_{n,m,0}, g_{n,m,0}\right)^{\top}, \tag{33}$$

i.e., the amplitude vectors $\left(e_{n,m,l}, f_{n,m,l}, g_{n,m,l}\right)^{\top},\ l = 0, 1$ are orthogonal. In the exceptional case of $\theta = 0$, i.e., for $a_n = b_m = 0$, these amplitude vectors are defined by the formulae

$$e_{n,m,0} = 0, \qquad f_{n,m,0} = 1, \quad g_{n,m,0} = 0, \tag{34}$$

$$e_{n,m,1} = -1, \quad f_{n,m,1} = 0, \quad g_{n,m,1} = 0. \tag{35}$$

The wave mode $u^{+}_{n,m,l}$ is a propagating plane wave solution of (2) if $c_{n,m}$ is real. For imaginary $c_{n,m}$, the wave $u^{+}_{n,m,l}$ is an evanescent solution. The efficiency of the reflected propagating mode $u^{+}_{n,m,l}$ is given by

$$\mathrm{eff}^{+}_{n,m,l} := \frac{c_{n,m}}{c_{0,0}} |B^{+}_{n,m,l}|^2. \tag{36}$$

It is not hard to prove that $100\,\mathrm{eff}^+_{n,m,l}$ percent of the energy arriving with the incident plane wave onto the grating is reflected into the direction $(a_n, b_m, c_{n,m})^\top$ of the plane wave mode $u^+_{n,m,l}$. Often, functional values like $\mathrm{eff}^+_{n,m,l}$ are the most interesting entities for the solution of the boundary value problem in Section 2.5.

The Rayleigh series expansion for the transmitted field takes the form

$$u^- = \sum_{n\in\mathbb{Z}} \sum_{m\in\mathbb{Z}} \sum_{l=0,1} B^-_{n,m,l} u^-_{n,m,l}, \tag{37}$$

where the Rayleigh coefficients $B^-_{n,m,l}$ are complex numbers, and the downward radiating modes $u^-_{n,m,l} = u^-_{el,n,m,l}$ in the electric case and $u^-_{n,m,l} = u^-_{ma,n,m,l}$ in the magnetic case are given by

$$\begin{aligned} u^-_{el,n,m,l}(x,y,z) &= \begin{pmatrix} e^-_{n,m,l} \\ f^-_{n,m,l} \\ g^-_{n,m,l} \end{pmatrix} e^{\mathbf{i}(a_n x + b_m y - c^-_{n,m}[z - z_{\min}])} \\ u^-_{ma,n,m,l}(x,y,z) &= \frac{1}{\mu\omega} \begin{pmatrix} a_n \\ b_m \\ -c^-_{n,m} \end{pmatrix} \times \begin{pmatrix} e^-_{n,m,l} \\ f^-_{n,m,l} \\ g^-_{n,m,l} \end{pmatrix} e^{\mathbf{i}(a_n x + b_m y - c^-_{n,m}[z - z_{\min}])}. \end{aligned}$$

Here

$$c^-_{n,m} = \sqrt{(k^-)^2 - a_n^2 - b_m^2}, \tag{38}$$

$$e^-_{n,m,0} = \frac{b_m}{h_{n,m}}, \quad f^-_{n,m,0} = -\frac{a_n}{h_{n,m}}, \quad g^-_{n,m,0} = 0, \tag{39}$$

$$e^-_{n,m,1} = \frac{c^-_{n,m} a_n}{h^-_{n,m,1}}, f_{n,m,1} = \frac{c^-_{n,m} b_m}{h^-_{n,m,1}}, \; g^-_{n,m,1} = -\frac{a_n^2 + b_m^2}{h^-_{n,m,1}}, \tag{40}$$

$$h^-_{n,m,1} = \sqrt{|c^-_{n,m}|^2 + h^2_{n,m}}\; h_{n,m}. \tag{41}$$

In the exceptional case of $\theta = 0$, i.e., for $a_n = b_m = 0$, the amplitude vectors are defined by the formulae

$$e^-_{n,m,0} = 0, \qquad f^-_{n,m,0} = -1, \qquad g^-_{n,m,0} = 0, \tag{42}$$

$$e^-_{n,m,1} = 1, \qquad f^-_{n,m,1} = 0, \qquad g^-_{n,m,1} = 0. \tag{43}$$

The wave mode $u^-_{n,m,l}$ is a propagating plane wave solution of (2) if $c^-_{n,m}$ is real. The efficiency of such a transmitted propagating mode $u^-_{n,m,l}$ is given by

$$\mathrm{eff}^-_{n,m,l} = \frac{[\mathbf{n}^+]^2}{[\mathbf{n}^-]^2} \, \frac{c^-_{n,m}}{[c_{0,0}]_+} |B^-_{n,m,l}|^2 \tag{44}$$

with $[c_{0,0}]_+$ the last component of the wave vector $(a_0, b_0, c_{0,0})^\top$ from the reflected mode.

If the functions $u, u^\pm$ satisfy the complete boundary value problems described in Section 2.5, then u^+ and u^- is an analytic extension of u through Γ^+ and Γ^-, respectively. In other words the expansions (24) and (37) can be considered to be expansions of $u|\Gamma^\pm$, and $\mathrm{eff}^\pm_{n,m,l}$ is a functional $\mathrm{eff}^\pm_{n,m,l}(u)$ of u.

3 Variational equation for the time-harmonic curl-curl equation

3.1 Notation

Following [14], a variational equation will be set up. The coupling boundary conditions (20)-(22) and (21)-(23), respectively, will be included by a mortaring technique, and the right-hand side $U^{\mathbf{inc}}$ (cf. (20),(21)) will be included by a penalty approach. To formulate the equation, the following symbols are needed.

G	domain of grating structure given by (1) which is a rectangular solid containing one period
G^+	domain above grating structure given by the formula $G^+ := [x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}] \times [z_{\max}, z_{\max}+1]$
G^-	domain beneath grating structure given by the formula $G^- := [x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}] \times [z_{\min}-1, z_{\min}]$
Γ^+	upper boundary $\{(x,y,z) \in G : \ z = z_{\max}\}$
Γ^-	lower boundary $\{(x,y,z) \in G : \ z = z_{\min}\}$
ν	normal at boundary ∂G pointing into exterior of G, $\nu = (0,0,1)^\top$ on Γ^+, $\nu = (0,0,-1)^\top$ on Γ^-
U^{inc}	incoming wave mode from above, cf. (6) and (7)
u	electric field on domain G
u^+	electric field spanned by wave modes above G, cf. (24)
u^-	electric field spanned by wave modes below G, cf. (37)
u^{inc}	incoming wave mode u^{inc} from above included as unknown into trial space, taken from one-dimensional trial space $\mathrm{span}\{U^{\mathrm{inc}}\}$
$(\mathsf{v}, \mathsf{v}^+, \mathsf{v}^-, \mathsf{v}^{\mathrm{inc}})$	test functions
η	constant factor for mortaring, chosen as a multiple of the reciprocal meshsize
$\mathbf{p}$	factor for penalty inclusion of right-hand side, chosen as a huge value

3.2 Sesqui-linear form

A solution $(u, u^+ + u^{\mathrm{inc}}, u^-)$ of the Maxwell system is sought with $u \in H(\mathrm{curl}, G)$, with $u^+ \in H^+$, with $u^{\mathrm{inc}} \in \mathrm{span}\{U^{\mathrm{inc}}\}$, and with $u^- \in H^-$. The space $H(\mathrm{curl}, G)$ (cf. the definition in [7, 16, 4, 5, 6]) is the space of all vector functions u on G such that:

– Function u is square integrable over G.
– For all subdomains G' of G with constant ε, the curl $\nabla \times [u|_{G'}]$ is square integrable.
– For all interfaces S between subdomains of G with constant values of ε, the tangential jump $[\![\nu \times u]\!]_S$ of u over S is zero.
– Function u is quasi-periodic, i.e., u satisfies (10) and (12).

The space H^+ is the space of all Rayleigh expansions u^+ of (24) endowed with the norm of the space $H(\mathrm{curl}, G^+)$. Similarly, H^- is the space of all Rayleigh expansions u^- of (37) with bounded $H(\mathrm{curl}, G^-)$ norm.

To get the variational formulation, the partial differential equation (2) and (3), respectively, is multiplied by a test function v and integrated over the domain G. Applying partial integration, the mortar technique of Nitsche [24], and a penalty trick to include the incident wave, the variational equation is established. Note that the last trick introduces an approximation error proportional to the number $\mathbf{p}^{-1}$. In accordance with [14] (compare [16, 19, 13]), the sesqui-linear form in the electric field case, i.e., corresponding to the equations (2), (10)-(13), (18), (20), and (22), takes the form

$$
\begin{aligned}
& a_{el}\Big((u, u^+ + u^{\mathrm{inc}}, u^-), (\mathsf{v}, \mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}}, \mathsf{v}^-)\Big) \qquad (45)\\
:= \; & \int_G \nabla \times u \cdot \overline{\nabla \times \mathsf{v}} \, \mathrm{d}G - \int_G k^2 u \cdot \bar{\mathsf{v}} \, \mathrm{d}G \\
& - \int_{\Gamma^+} \nabla \times [u^+ + u^{\mathrm{inc}}] \cdot [\nu \times \bar{\mathsf{v}}] \, \mathrm{d}\Gamma^+ \\
& - \int_{\Gamma^+} \big\{\nu \times u - \nu \times [u^+ + u^{\mathrm{inc}}]\big\} \cdot \nabla \times \overline{[\mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}}]} \, \mathrm{d}\Gamma^+ \\
& + \eta \int_{\Gamma^+} \big\{\nu \times u - \nu \times [u^+ + u^{\mathrm{inc}}]\big\} \cdot \Big[\nu \times \overline{\{\mathsf{v} - [\mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}}]\}}\Big] \, \mathrm{d}\Gamma^+ \\
& - \int_{\Gamma^-} \nabla \times u^- \cdot [\nu \times \bar{\mathsf{v}}] \, \mathrm{d}\Gamma^- \\
& - \int_{\Gamma^-} \big\{\nu \times u - \nu \times u^-\big\} \cdot \nabla \times \overline{\mathsf{v}^-} \, \mathrm{d}\Gamma^- \\
& + \eta \int_{\Gamma^-} \big\{\nu \times u - \nu \times u^-\big\} \cdot \Big[\nu \times \overline{\{\mathsf{v} - \mathsf{v}^-\}}\Big] \, \mathrm{d}\Gamma^- \\
& + \mathbf{p} \int_{\Gamma^+} u^{\mathrm{inc}} \cdot \overline{\mathsf{v}^{\mathrm{inc}}} \, \mathrm{d}\Gamma^+ .
\end{aligned}
$$

Here the differential operator $\nabla\times$ over G is to be understood locally, i.e., $\nabla \times u$ is the function in $[L^2(G)]^3$ the restriction of which to the interior of the subdomains with constant values of ε is the curl of the restriction of u. The first two integrals over the domain G are the usual terms of the variational formulation of the curl-curl equation. The terms three to five are the mortar terms to couple u and $u^+ + u^{\mathrm{inc}}$ over Γ^+. Analogously, the terms six to eight are the mortar terms to couple u and u^- over Γ^-. Finally, the last term is the penalty term to enforce $u^{\mathrm{inc}} = U^{\mathrm{inc}}$.

Note that integrals of the form $\int_{\Gamma^+} \nabla \times u^+ \cdot \nu \times \overline{v} \, \mathrm{d}\Gamma^+$ are meaningful. Indeed, the Rayleigh expansions u^+ satisfy (2) such that $\nabla \times u^+$ is in $H(\mathrm{curl}, G^+)$ and its tangential trace $[\nabla \times u^+]_t$ belongs to the trace space $H^{-1/2}(\mathrm{curl}, \Gamma^+)$. The trace $\nu \times \overline{v}$ on Γ^+ belongs to the dual space $H^{-1/2}(\mathrm{div}, \Gamma^+)$ (cf. [7]). Unfortunately, the integrals with factor η are not meaningful for general $H(\mathrm{curl}, G)$ functions. Integrals like $\int_{\Gamma^+} [\nu \times u] \cdot [\nu \times \bar{\mathsf{v}}] \, \mathrm{d}\Gamma^+$ are meaningful in the mortar approach for finite element methods (cf. [14]), where u, v are finite element functions and η tends to zero with the meshsize. Alternatively, the integrals in (45) with factor η can be replaced.

For instance, the term

$$\eta \int_{\Gamma^+} \left\{ \nu \times u - \nu \times [u^+ + u^{\rm inc}] \right\} \cdot \left[\nu \times \overline{\left\{ \mathsf{v} - [\mathsf{v}^+ + \mathsf{v}^{\rm inc}] \right\}} \right] \, \mathrm{d}\Gamma^+ \tag{46}$$

can be replaced by the sum

$$\begin{aligned} &\eta \sum_{\substack{n,m,l: \\ c_{n,m}\neq 0 \text{ or } l=0 \\ n^2+m^2<N}} \int_{\Gamma^+} \nu \times [u - u^+ - u^{\rm inc}] \cdot \nu \times \overline{u}^+_{n,m,l} \, \mathrm{d}\Gamma^+ \, \overline{\int_{\Gamma^+} \nu \times [\mathsf{v} - \mathsf{v}^+ - \mathsf{v}^{\rm inc}] \cdot \nu \times \overline{u}^+_{n,m,l} \, \mathrm{d}\Gamma^+} \\ &+ \eta \sum_{\substack{n,m: \\ c_{n,m}=0}} \int_{\Gamma^+} \nu \times [u - u^+ - u^{\rm inc}] \cdot \overline{u}^+_{n,m,0} \, \mathrm{d}\Gamma^+ \, \overline{\int_{\Gamma^+} \nu \times [\mathsf{v} - \mathsf{v}^+ - \mathsf{v}^{\rm inc}] \cdot \overline{u}^+_{n,m,0} \, \mathrm{d}\Gamma^+} \end{aligned} \tag{47}$$

with a suitable large integer N. It seems that the summation in (47) can even be restricted to all n, m with $c_{n,m} = 0$ (cf. Section 4.10). For the integral over Γ_- with coefficient η, a similar modification is possible. However, to simplify the formulas of the present paper and to stick as close as possible to the numerical implementation proposed in [14], all sesqui-linear forms are written using terms like (46). For a rigorous sesqui-linear form considered in the full spaces $H(\mathrm{curl}, G)$, $H^\pm$, and $\mathrm{span}\{U^{\rm inc}\}$, the reader has to replace terms like (46) by terms like (47). Note that all these terms are not important for the shape-derivative formulas.

In the case of the magnetic field, i.e., for the equations (3), (14)-(17), (19), (21), and (23), the sesqui-linear form takes the form

$$\begin{aligned} &a_{ma}\Big((u, u^+ + u^{\rm inc}, u^-), (\mathsf{v}, \mathsf{v}^+ + \mathsf{v}^{\rm inc}, \mathsf{v}^-) \Big) \\ := \;& \mu^2\omega^2 \int_G k^{-2} \, \nabla \times u \cdot \overline{\nabla \times \mathsf{v}} \, \mathrm{d}G - \mu^2\omega^2 \int_G u \cdot \overline{\mathsf{v}} \, \mathrm{d}G \\ &- \mu^2\omega^2 \int_{\Gamma^+} k^{-2} \, \nabla \times [u^+ + u^{\rm inc}] \cdot [\nu \times \overline{\mathsf{v}}] \, \mathrm{d}\Gamma^+ \\ &- \mu^2\omega^2 \int_{\Gamma^+} k^{-2} \left\{ \nu \times u - \nu \times [u^+ + u^{\rm inc}] \right\} \cdot \nabla \times \overline{[\mathsf{v}^+ + \mathsf{v}^{\rm inc}]} \, \mathrm{d}\Gamma^+ \\ &+ \eta \, \mu^2\omega^2 \int_{\Gamma^+} k^{-2} \left\{ \nu \times u - \nu \times [u^+ + u^{\rm inc}] \right\} \cdot \left[\nu \times \overline{\left\{ \mathsf{v} - [\mathsf{v}^+ + \mathsf{v}^{\rm inc}] \right\}} \right] \, \mathrm{d}\Gamma^+ \\ &- \mu^2\omega^2 \int_{\Gamma^-} k^{-2} \, \nabla \times u^- \cdot [\nu \times \overline{\mathsf{v}}] \, \mathrm{d}\Gamma^- \\ &- \mu^2\omega^2 \int_{\Gamma^-} k^{-2} \left\{ \nu \times u - \nu \times u^- \right\} \cdot \nabla \times \overline{\mathsf{v}^-} \, \mathrm{d}\Gamma^- \\ &+ \eta \, \mu^2\omega^2 \int_{\Gamma^-} k^{-2} \left\{ \nu \times u - \nu \times u^- \right\} \cdot \left[\nu \times \overline{\left\{ \mathsf{v} - \mathsf{v}^- \right\}} \right] \, \mathrm{d}\Gamma^- \\ &+ \mathbf{p} \, \mu^2\omega^2 \int_{\Gamma^+} k^{-2} \, u^{\rm inc} \cdot \overline{\mathsf{v}^{\rm inc}} \, \mathrm{d}\Gamma^+, \end{aligned} \tag{48}$$

Note that the two sesqui-linear forms coincide in the main part, i.e., in the domain integrals (cf. the formulas (4) and (5)).

3.3 Right-hand side and variational equation

The linear functional on the right-hand side of the variational equation, for the electric and magnetic field, is given by

$$f_{el}\Big((\mathsf{v},\mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}},\mathsf{v}^-)\Big) \;:=\; \mathbf{p}\int_{\Gamma^+} U_{el}^{\mathrm{inc}}\cdot\overline{\mathsf{v}^{\mathrm{inc}}}\,\mathrm{d}\Gamma^+, \tag{49}$$

$$f_{ma}\Big((\mathsf{v},\mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}},\mathsf{v}^-)\Big) \;:=\; \mathbf{p}\,\mu^2\omega^2\int_{\Gamma^+} k^{-2}\,U_{ma}^{\mathrm{inc}}\cdot\overline{\mathsf{v}^{\mathrm{inc}}}\,\mathrm{d}\Gamma^+. \tag{50}$$

The variational equations take the form

$$a_{el}\Big((u,u^+ + u^{\mathrm{inc}},u^-),(\mathsf{v},\mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}},\mathsf{v}^-)\Big) = f_{el}\Big((\mathsf{v},\mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}},\mathsf{v}^-)\Big), \tag{51}$$

$$a_{ma}\Big((u,u^+ + u^{\mathrm{inc}},u^-),(\mathsf{v},\mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}},\mathsf{v}^-)\Big) = f_{ma}\Big((\mathsf{v},\mathsf{v}^+ + \mathsf{v}^{\mathrm{inc}},\mathsf{v}^-)\Big). \tag{52}$$

Recall that the solution u, $u^\pm$, and u^{inc} is sought such that $u\in H(\mathrm{curl},G)$ is quasi-periodic, $u^{\mathrm{inc}}\in\mathrm{span}\{U^{\mathrm{inc}}\}$, and $u^\pm\in H^\pm$ is a Rayleigh series expansions (cf. (24) and (37)). The equations (51) and (52), respectively, have to be satisfied for all quasi-periodic test functions $\mathsf{v}\in H(\mathrm{curl},G)$, for all functions $\mathsf{v}^{\mathrm{inc}}\in\mathrm{span}\{U^{\mathrm{inc}}\}$, and for all $\mathsf{v}^\pm\in H^\pm$.

Remark 3.1 *The penalty approach for the right-hand side works as follows: Suppose the penalty parameter $\mathbf{p}$ is huge. Then, choosing $\mathsf{v}=0$ and $\mathsf{v}^\pm=0$ and neglecting terms much smaller than $\mathbf{p}$, the variational system amounts to $u^{\mathrm{inc}}=U^{\mathrm{inc}}$. Setting this into the variational system with $\mathsf{v}^{\mathrm{inc}}=0$ and non-zero v and $\mathsf{v}^\pm$, a variational equation with natural right-hand side results:*

$$a\Big((u,u^+,u^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) = -a\Big((0,U^{\mathrm{inc}},0),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) \tag{53}$$

valid for all $\mathsf{v}\in H(\mathrm{curl},G)$ and $\mathsf{v}^\pm\in H^\pm$.

Remark 3.2 *The existence and uniqueness of the solution to the problem (2), (10)–(13), (18), (20), and (22) is still open. The unique solvability of (2), (10)–(13), (18), (20), and (22) in the case that an absorbing material is involved in the grating has been proved in [21]. If an absorbing material is included into the grating, then there should exist a unique variational solution even in the case of variable μ. Indeed, the technique of [13] for the case of a perfectly conducting substrate seems to apply also to the problem (2), (10)–(13), (18), (20), and (22).*

Remark 3.3 *The existence and uniqueness of the solution to the variational equation (53) is still open. The spirit of the mortaring technique is described in [24, 14]. Note that the consistency is easy to see. In fact, any quasi-periodic solution u of (2), (18) combined with Rayleigh expansions $u^\pm$ coupled to u by (20) and (22) is a solution of the variational equation (53) (cf. [14]). On the other hand, using (91) and (92) to define*

$$\mathcal{E} \;:=\; \Big\{\eta\in\mathbb{R}:\ \eta>0,\ \eta\neq\lambda^+_{n,m,1},\ \forall n,m \text{ s.t. } c_{n,m}\notin\mathbb{R},$$
$$\eta\neq\lambda^-_{n,m,1},\ \forall n,m \text{ s.t. } c_{n,m}\notin\mathbb{R}\Big\},$$

the parameter η can be chosen from $\mathcal{E}$. Then any solution (u, u^+, u^-) of the variational system (53) *with $u \in H(\mathrm{curl}, G)$ and Rayleigh expansions $u^\pm \in H^\pm$ solves the boundary value problem* (2)*,* (10)*–*(13)*,* (18)*,* (20)*, and* (22)*.*

A proof of the last claim in Remark 3.3 will be given in Section 4.10. Note that the just mentioned open problem for the unique solvability of the variational equation might be overcome by a coupling with boundary elements (cf. e.g. [11, 21]) or by domain decomposition techniques (cf. e.g. [19]). The formulas for the shape derivatives will not be affected by this treatment.

3.4 Formula for partial integration

For the derivation of shape-derivative formulas, we need a formula of partial integration over the upper and lower boundaries $\Gamma^\pm$. This is a version of Green's formula applied to the upward and downward radiating Rayleigh series expansions (cf. (24) and (37)). To formulate the result we introduce a modification operator for such series expansions by

$$\left[\sum_{n,m,l} B_{n,m,l} u^\pm_{n,m,l}\right]_{\mathbf{mo}} := \sum_{n,m,l:\ c_{n,m}\notin\mathbb{R}} B_{n,m,l} u^\pm_{n,m,l} - \sum_{n,m,l:\ 0\neq c_{n,m}\in\mathbb{R}} B_{n,m,l} u^\pm_{n,m,l}. \quad (54)$$

Lemma 3.1 *For any $\epsilon > 0$ and for any two absolutely convergent Rayleigh series expansions $u^\pm$ and $v^\pm$, defined on $\{(x,y,z) \in \mathbb{R}^3 :\ z \geq z_{\max} - \epsilon\}$ and $\{(x,y,z) \in \mathbb{R}^3 :\ z \leq z_{\min} + \epsilon\}$, respectively, there holds*

$$\int_{\Gamma^\pm} [\nabla \times u^\pm] \cdot [\nu \times \overline{\mathrm{v}}^\pm]\, \mathrm{d}\Gamma^\pm \;=\; \int_{\Gamma^\pm} [\nu \times u^\pm] \cdot [\nabla \times \overline{\mathrm{v}}^\pm_{\mathbf{mo}}]\, \mathrm{d}\Gamma^\pm. \quad (55)$$

Proof. Without loss of generality we consider the case of functions over the upper half plane defined by $z \geq z_{\max} - \epsilon$. The orthogonality of the exponential functions yields

$$\begin{aligned}\int_{\Gamma^+} &[\nabla \times u^+_{n,m,l}] \cdot [\nu \times \overline{u}^+_{n',m',l'}]\, \mathrm{d}\Gamma^+ \\ &= \delta_{n,n'}\delta_{m,m'} \int_{\Gamma^+} [\nabla \times u^+_{n,m,l}] \cdot [\nu \times \overline{u}^+_{n,m,l'}]\, \mathrm{d}\Gamma^+.\end{aligned}$$

For $n = n'$ and $m = m'$, we conclude

$$\begin{aligned}[\nabla\times u^+_{n,m,l}] \cdot [\nu\times\overline{u}^+_{n,m,l'}] &= \mathbf{i}\left[\begin{pmatrix} a_n \\ b_m \\ c_{n,m}\end{pmatrix} \times \begin{pmatrix} e_{n,m,l} \\ g_{n,m,l} \\ f_{n,m,l}\end{pmatrix}\right] \cdot \left[\begin{pmatrix} 0 \\ 0 \\ 1\end{pmatrix} \times \begin{pmatrix} \overline{e}_{n,m,l'} \\ \overline{g}_{n,m,l'} \\ \overline{f}_{n,m,l'}\end{pmatrix}\right] \\ &= \mathbf{i}\begin{pmatrix} 0 \\ 0 \\ 1\end{pmatrix} \cdot \left\{\begin{pmatrix} \overline{e}_{n,m,l'} \\ \overline{f}_{n,m,l'} \\ \overline{g}_{n,m,l'}\end{pmatrix} \times \left[\begin{pmatrix} a_n \\ b_m \\ c_{n,m}\end{pmatrix} \times \begin{pmatrix} e_{n,m,l} \\ f_{n,m,l} \\ g_{n,m,l}\end{pmatrix}\right]\right\} \\ &= \mathbf{i}\begin{pmatrix} 0 \\ 0 \\ 1\end{pmatrix} \cdot \left\{\begin{pmatrix} \overline{e}_{n,m,l'} \\ \overline{f}_{n,m,l'} \\ \overline{g}_{n,m,l'}\end{pmatrix} \cdot \begin{pmatrix} e_{n,m,l} \\ f_{n,m,l} \\ g_{n,m,l}\end{pmatrix} \begin{pmatrix} a_n \\ b_m \\ c_{n,m}\end{pmatrix}\right.\end{aligned}$$

$$
\begin{aligned}
& \quad - \begin{pmatrix} \overline{e}_{n,m,l'} \\ \overline{f}_{n,m,l'} \\ \overline{g}_{n,m,l'} \end{pmatrix} \cdot \begin{pmatrix} a_n \\ b_m \\ c_{n,m} \end{pmatrix} \begin{pmatrix} e_{n,m,l} \\ f_{n,m,l} \\ g_{n,m,l} \end{pmatrix} \Bigg\} \\
= & \ \mathbf{i} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \cdot \Bigg\{ \delta_{l,l'} \begin{pmatrix} a_n \\ b_m \\ c_{n,m} \end{pmatrix} \\
& \quad - \overline{g}_{n,m,l'} [c_{n,m} - \overline{c}_{n,m}] \begin{pmatrix} e_{n,m,l} \\ f_{n,m,l} \\ g_{n,m,l} \end{pmatrix} \Bigg\} \\
= & \ \mathbf{i} \{ \delta_{l,l'} c_{n,m} - g_{n,m,l} \overline{g}_{n,m,l'} [c_{n,m} - \overline{c}_{n,m}] \}.
\end{aligned}
$$

Hence, using that $c_{n,m}$ is real or purely imaginary, we get

$$
\begin{aligned}
& \int_{\Gamma^+} [\nabla \times u^+_{n,m,l}] \cdot [\nu \times \overline{u}^+_{n',m',l'}] \, \mathrm{d}\Gamma^+ = \\
& \quad \delta_{n,n'} \delta_{m,m'} \mathbf{i} \, \mathrm{per}_x \mathrm{per}_y * [\delta_{l,l'} c_{n,m} - g_{n,m,l} \overline{g_{n,m,l'}} (c_{n,m} - \overline{c}_{n,m})] \\
& \quad = \pm \int_{\Gamma^+} [\nu \times u^+_{n,m,l}] \cdot [\nabla \times \overline{u}^+_{n',m',l'}] \, \mathrm{d}\Gamma^+
\end{aligned} \tag{56}
$$

with the minus sign for the n, m with real $c_{n,m}$ and the plus otherwise. □

4 Shape-derivative formulas

4.1 Objective functional

Suppose u denotes the solution of the boundary value problem (2), (10)-(13), (18), (20), (22) or of the weak formulation (51). For an optimization and in many other applications, not u itself but a functional $\mathcal{F}(u)$ is of interest. Here, the functional $\mathcal{F}$ depending on $u = u_{el}$ is defined as follows: A set of efficiencies $\{\mathrm{eff}^+_{n,m,l} : \ (n, m, l) \in I\}$ corresponding to propagating reflected wave modes (i.e., $c_{n,m} > 0$ in (25)) is fixed, and, for each $(n, m, l) \in I$, a positive weight $w_{n,m,l}$ and a prescribed efficiency number (in percent) $0 \leq d_{n,m,l} \leq 100$ is chosen. Then (cf. (36))

$$
\begin{aligned}
\mathcal{F}(u) \ := & \sum_{(n,m,l) \in I} w_{n,m,l} \left[100 \, \mathrm{eff}^+_{n,m,l}(u) - d_{n,m,l} \right]^2 \\
= & \sum_{(n,m,l) \in I} w_{n,m,l} \left[\frac{100 \, c_{n,m}}{c_{0,0}} |B^+_{n,m,l}(u)|^2 - d_{n,m,l} \right]^2 .
\end{aligned} \tag{57}
$$

4.2 Domain transformation and derivatives

The change of geometry parameters in the grating structure can often be described by a transformation (automorphism) of the domain G. Suppose $\chi : \ G \to \mathbb{R}^3$, defined as the mapping

$(x,y,z)^\top \mapsto (\chi_x(x,y,z), \chi_y(x,y,z), \chi_z(x,y,z))^\top$, is a vector field such that:

(C1) χ is continuous and piecewise analytic

(C2) χ vanishes on the boundary ∂G of G

Then, depending on the parameter h, the transformation $\Phi_h : G \to G$ is defined by

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \mapsto \Phi_h(x,y,z) \;=\; \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} := \begin{pmatrix} x + h\chi_x(x,y,z) \\ y + h\chi_y(x,y,z) \\ z + h\chi_z(x,y,z) \end{pmatrix}. \tag{58}$$

Clearly, this is an isomorphism of G for small h. Moreover, using the inverse transformation

$$(x',y',z')^\top \mapsto \Phi_h^{-1}(x',y',z') = (x,y,z)^\top,$$

each vector function $u : G \to \mathbb{R}^3$ can be transformed to a vector function $\Psi_h u : G \to \mathbb{R}^3$ defined by

$$\Psi_h u(x',y',z') \;:=\; u(\Phi_h^{-1}(x',y',z')) \;:=\; u(x,y,z).$$

Now, for each h, there is a grating geometry over G fixed by the permittivity $\varepsilon_h := \Psi_h\varepsilon$, i.e., by the wave number $k_h := \Psi_h k$. Suppose u_h denotes the unique solution of the boundary value problem (2), (10)-(13), (18), (20), (22) with $\varepsilon_h := \Psi_h\varepsilon$ and $k_h := \Psi_h k$ or that of the weak formulation (51) with k replaced by k_h. Furthermore, suppose $u \mapsto \mathcal{F}(u)$ is the functional over the space of solutions given in (57). Then the derivative of $\mathcal{F}(u_h)$ with respect to h is sought, i.e., a formula for

$$\partial_h[\mathcal{F}(u_h)]|_{h=0} := \lim_{h\longrightarrow 0} \frac{\mathcal{F}(u_h) - \mathcal{F}(u_0)}{h}. \tag{59}$$

For an appropriate choice of χ (cf. Section 4.3), this will be the derivative of $\mathcal{F}(u)$ with respect to a parameter of the geometry.

Suppose there exists a unique solution $u = u_0$ of the boundary value problem (2), (10)-(13), (18), (20), (22). Using (4), this corresponds to the unique magnetic field solution of (3), (14)-(17), (19), (21), (23), which is the unique solution of the variational equation of [21]. Similarly to Theorem 3.1 of [11], we conclude that, if h is sufficiently small, there exist unique magnetic-field solutions of the variational equations with k replaced by $k_h := \Psi_h k$. Hence, using (4), there exist uniquely defined electric field solutions to (2), (10)-(13), (18), (20), (22) for h sufficiently small, and the derivative in (59) is well defined.

4.3 Examples of transformations for the parameter derivatives of a contact hole geometry

4.3.1 Geometry of the contact hole

For the quality check in the lithographic chip production, simple periodic test structures are manufactured and measured. One of these structures, the grating structure for a biperiodic

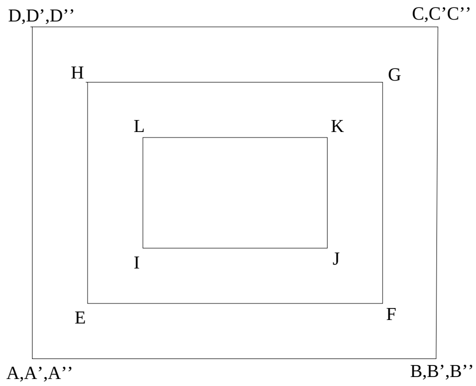

Figure 1: Geometry. View from above.

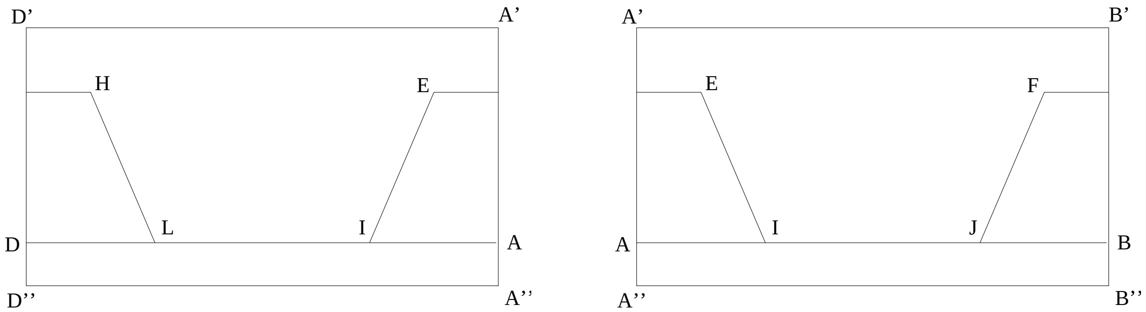

Figure 2: Geometry. left: View from left, right: Front view.

contact hole, is given in the Figures 1–3. From a layer $\{(x,y,z) \in \mathbb{R}^3 : \; 0 < z < g\}$, in each periodicity cell the central part in shape of a frustum of a pyramid is removed. This hole has the eight vertices I, J, K, L, E, F, G, H. Together with the other vertices in Figures 1–3, the points are defined by

$$
\begin{array}{lll lll}
A & := & (0,0,0), & E & := & (a,b,g), \\
I & := & (e,f,0), & A' & := & (0,0,n), \\
A" & := & (0,0,o), & B & := & (\mathrm{per}_x,0,0), \\
F & := & (\mathrm{per}_x - a,b,g), & J & := & (\mathrm{per}_x - e,f,0), \\
B' & := & (\mathrm{per}_x,0,n), & B" & := & (\mathrm{per}_x,0,o), \\
C & := & (\mathrm{per}_x,\mathrm{per}_y,0), & G & := & (\mathrm{per}_x - a,\mathrm{per}_y - b,g), \\
K & := & (\mathrm{per}_x - e,\mathrm{per}_y - f,0), & C' & := & (\mathrm{per}_x,\mathrm{per}_y,n), \\
C" & := & (\mathrm{per}_x,\mathrm{per}_y,o), & D & := & (0,\mathrm{per}_y,0), \\
H & := & (a,\mathrm{per}_y - b,g), & L & := & (e,\mathrm{per}_y - f,0), \\
D' & := & (0,\mathrm{per}_y,n), & D" & := & (0,\mathrm{per}_y,o).
\end{array}
$$

The involved parameters a, b, e, f, g, n, o, per_x, and per_y are chosen such that

$$
0 < a < \mathrm{per}_x - a < \mathrm{per}_x, \quad 0 < e < \mathrm{per}_x - e < \mathrm{per}_x, \quad 0 < b < \mathrm{per}_y - b < \mathrm{per}_y,
$$
$$
0 < f < \mathrm{per}_y - f < \mathrm{per}_y, \quad o < 0 < g < n.
$$

In the present paper, the parameters n, o, per_x, and per_y are supposed to be fixed. The shape derivatives (59) are sought with respect to the parameters a, b, e, f, and g. Therefore, the

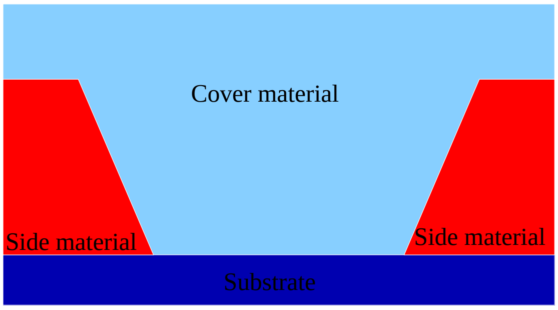

Figure 3: Geometry. Materials from lateral view.

corresponding components χ_w, $w = x, y, z$ of the transformation vector function χ are defined in Section 4.3.2. The transformation (58) is equivalent to an increase in the corresponding parameter.

4.3.2 Piecewise linear functions

Before we define the functions, let us explain the basic idea in the case of the derivative with respect to a. An increase in a means a shift of the edges EH and FG into the directions $\overrightarrow{EF}$ and $\overrightarrow{FE}$, respectively. The vertices not located on these edges remain fixed. To generate the transformation of geometry due to increased a, we need a continuous and piecewise linear vector field χ in (58) which vanishes at all vertices not located at the edges EH and FG. Over EH and FG the vector field should be of unit length and point into the direction $\overrightarrow{EF}$ and $\overrightarrow{FE}$, respectively.

More precisely, since no change of the hight z and of the lateral y coordinate is required, the only non-zero component of χ will be χ_x. The transformation should be uniform for all points with the same x and z coordinate, i.e., $\chi_x(x, y, z) = \chi_x(x, z)$ should not depend on y. To leave the points beneath $z < 0$ unchanged, the values $\chi_x(x, z)$ should vanish for $z < 0$. Since the transformation is symmetric with respect to the plane $\{(x, y, z) \in \mathbb{R}^3 : \ x = \mathrm{per}_x/2\}$, the function can be chosen such that $\chi_x(x, z) = -\chi_x(\mathrm{per}_x - x, z)$. In other words, it suffices to define $\chi_x(x, z)$ for $z \geq 0$ and $x \leq \mathrm{per}_x/2$. To move the vertices in the correct way, the values of χ_x must be zero for $z = 0, \ z = n$ and $x = 0, \ x = \mathrm{per}_x/2$. It must be one at the edge through EH, i.e., $\chi_x(a, g) = 1$. Choosing $\chi_x(x, g)$ linearly for $0 < x < a$ will keep the upper boundary of the domain surrounding the hole in the plain through E, F, G, H. Finally, choosing $\chi_x(x, z)$ linearly for (x, z) on the straight line segment connecting $(e, 0)$ and (a, g), will keep the quadrangle $ILHE$ on the lateral boundary of the domain surrounding the hole. Altogether, χ_x can be fixed as any continuous and piecewise linear function satisfying the just mentioned restrictions.

To simplify the formulas, define the parameters

$$p_x^h \ := \ \mathrm{per}_x/2, \qquad p_y^h \ := \ \mathrm{per}_y/2, \qquad n_g \ := \ n - g.$$

For the parameters a and e, it is sufficient to give the functions $\chi_w(x, y, z) = \chi_w(x, z)$ for $w = x$ and for the arguments $x \leq p_x^h$ since $\chi_y = \chi_z \equiv 0$ and $\chi_x(x, z) = -\chi_x(\mathrm{per}_x - x, z)$.

Thus, for parameter a and $x \le p_x^h$, the components of function $\chi = (\chi_w)_w$ can be defined by

$$\chi_w(x,y,z) \quad := \quad \begin{cases} \frac{x}{a} & \text{if } 0 \le z \le g,\ 0 \le x \le az/g, \text{ and } w{=}x \\ \frac{z}{g} & \text{if } 0 \le z \le g,\ az/g \le x \le [e(g-z)+az]/g, \text{ and } w{=}x \\ \frac{x+(e-p_x^h)z/g-e}{a-p_x^h} & \text{if } 0 \le z \le g,\ [e(g-z)+az]/g \le x \le [e(g-z)+p_x^h z]/g, \text{ and } w{=}x \\ \frac{x+a(n-z)/n_g-a}{a} & \text{if } g \le z \le n,\ a(z-g)/n_g \le x \le a, \text{ and } w{=}x \\ \frac{x+(a-p_x^h)(n-z)/n_g-a}{a-p_x^h} & \text{if } g \le z \le n,\ a \le x \le [a(z-g)+p_x^h(n-z)]/n_g, \text{ and } w{=}x \\ 0 & \text{else.} \end{cases}$$

Analogously, for parameter e and $x \le p_x^h$, the vector function χ is given by

$$\chi_w(x,y,z) \quad := \quad \begin{cases} \frac{x-az/g}{e} & \text{if } 0 \le z \le g,\ az/g \le x \le [e(g-z)+az]/g, \text{ and } w{=}x \\ \frac{(g-z)}{g} & \text{if } 0 \le z \le g,\ [e(g-z)+az]/g \le x \le [e(g-z)+p_x^h z]/g, \text{ and } w{=}x \\ \frac{p_x^h-x}{p_x^h-e} & \text{if } 0 \le z \le g,\ [e(g-z)+p_x^h z]/g \le x \le p_x^h, \text{ and } w{=}x \\ \frac{x-e(z-o)/o-e}{e} & \text{if } o \le z \le 0,\ ez/o \le x \le e, \text{ and } w{=}x \\ \frac{x+(e-p_x^h)(z-o)/|o|-e}{e-p_x^h} & \text{if } o \le z \le 0,\ e \le x \le [p_x^h(z-o)-ez]/|o|, \text{ and } w{=}x \\ 0 & \text{else.} \end{cases}$$

Similarly, for the parameters b and f, it is enough to define the three component functions $\chi_w(x,y,z) = \chi_w(y,z)$ for $w = y$ and for $y \le p_y^h$ since $\chi_x = \chi_z \equiv 0$ and $\chi_y(y,z) = -\chi_y(\mathrm{per}_y - y, z)$. For parameter b and $y \le p_y^h$, the vector function χ is given by

$$\chi_w(x,y,z) \quad := \quad \begin{cases} \frac{y}{b} & \text{if } 0 \le z \le g,\ 0 \le y \le bz/g, \text{ and } w{=}y \\ \frac{z}{g} & \text{if } 0 \le z \le g,\ bz/g \le y \le [f(g-z)+bz]/g, \text{ and } w{=}y \\ \frac{y+(f-p_y^h)z/g-f}{b-p_y^h} & \text{if } 0 \le z \le g,\ [f(g-z)+bz]/g \le y \le [f(g-z)+p_y^h z]/g, \text{ and } w{=}y \\ \frac{y+b(n-z)/n_g-b}{b} & \text{if } g \le z \le n,\ b(z-g)/n_g \le y \le b, \text{ and } w{=}y \\ \frac{y+(b-p_y^h)(n-z)/n_g-b}{b-p_y^h} & \text{if } g \le z \le n,\ b \le y \le [b(z-g)+p_y^h(n-z)]/n_g, \text{ and } w{=}y \\ 0 & \text{else.} \end{cases}$$

For parameter f and $y \le p_y^h$, function χ is defined by

$$\chi_w(x,y,z) \quad := \quad \begin{cases} \frac{y-bz/g}{f} & \text{if } 0 \le z \le g,\ bz/g \le y \le [f(g-z)+bz]/g, \text{ and } w{=}y \\ \frac{(g-z)}{g} & \text{if } 0 \le z \le g,\ [f(g-z)+bz]/g \le y \le [f(g-z)+p_y^h z]/g, \text{ and } w{=}y \\ \frac{p_y^h-y}{p_y^h-f} & \text{if } 0 \le z \le g,\ [f(g-z)+p_y^h z]/g \le y \le p_y^h, \text{ and } w{=}y \\ \frac{y-f(z-o)/o-f}{f} & \text{if } o \le z \le 0,\ fz/o \le y \le f, \text{ and } w{=}y \\ \frac{y+(f-p_y^h)(z-o)/|o|-f}{f-p_y^h} & \text{if } o \le z \le 0,\ f \le y \le [p_y^h(z-o)-fz]/|o|, \text{ and } w{=}y \\ 0 & \text{else.} \end{cases}$$

Finally, for parameter g, the function χ depends on z only.

$$\chi_w(x,y,z) \;:=\; \begin{cases} \frac{z}{g} & \text{if } 0 \le z \le g \text{ and } w=z \\ \frac{n-z}{n-g} & \text{if } g \le z \le n \text{ and } w=z \\ 0 & \text{else.} \end{cases}$$

4.4 The formula for the shape derivative

To formulate the result, some notation is needed. Suppose $(u_{el,0}, u^+_{el,0}, u^-_{el,0})$ is the solution of the Maxwell system, i.e., of (51). Define the new sesqui-linear form a_1 with electric fields as arguments by

$$\begin{aligned}
a_1(u_{el}, \mathsf{v}_{el}) \;:=\; & -\int_G k^2\, u_{el} \cdot \overline{\mathsf{v}_{el}}\; \nabla\cdot\chi \,\mathrm{d}G \\
& + \int_G k^2\, u_{el} \cdot \overline{\Big(\nabla\chi_x\cdot\mathsf{v}_{el}, \nabla\chi_y\cdot\mathsf{v}_{el}, \nabla\chi_z\cdot\mathsf{v}_{el}\Big)^\top}\; \mathrm{d}G \\
& + \int_G k^2 \Big(\nabla\chi_x\cdot u_{el}, \nabla\chi_y\cdot u_{el}, \nabla\chi_z\cdot u_{el}\Big)^\top \cdot \overline{\mathsf{v}_{el}}\, \mathrm{d}G \\
& - \int_G u_{el}\cdot \overline{\Big[[\nabla\times\mathsf{v}_{el}]_x \nabla\times\nabla\chi_x + [\nabla\times\mathsf{v}_{el}]_y \nabla\times\nabla\chi_y + [\nabla\times\mathsf{v}_{el}]_z \nabla\times\nabla\chi_z\Big]}\; \mathrm{d}G \\
& - \int_G \Big[[\nabla\times u_{el}]_x \nabla\times\nabla\chi_x + [\nabla\times u_{el}]_y \nabla\times\nabla\chi_y + [\nabla\times u_{el}]_z \nabla\times\nabla\chi_z\Big] \cdot \overline{\mathsf{v}_{el}}\, \mathrm{d}G \\
& + \int_G \Big[[\nabla\times u_{el}]_x \nabla\chi_x + [\nabla\times u_{el}]_y \nabla\chi_y + [\nabla\times u_{el}]_z \nabla\chi_z\Big] \cdot \overline{[\nabla\times\mathsf{v}_{el}]}\, \mathrm{d}G \\
& + \int_G [\nabla\times u_{el}] \cdot \overline{\Big[[\nabla\times\mathsf{v}_{el}]_x \nabla\chi_x + [\nabla\times\mathsf{v}_{el}]_y \nabla\chi_y + [\nabla\times\mathsf{v}_{el}]_z \nabla\chi_z\Big]}\; \mathrm{d}G \\
& - \int_G [\nabla\times u_{el}] \cdot \overline{[\nabla\times\mathsf{v}_{el}]}\; \nabla\cdot\chi \,\mathrm{d}G.
\end{aligned} \tag{60}$$

Here, the differential operators $\nabla\times$, $\nabla\cdot$, and ∇ are meant to be local derivatives, i.e., these operators are applied to the restrictions of the functions to the interior of the subdomains of G, where ε is constant and χ analytic.

Finally, by $(u_{el,ad}, u^+_{el,ad}, u^-_{el,ad})$ we denote the adjoint solution, namely the solution of (cf. (45))

$$a_{el}\Big((u_{el}, u^+_{el}, u^-_{el}), (u_{el,ad}, u^+_{el,ad}, u^-_{el,ad})\Big) \;=\; \int_{\Gamma^+} [\nu\times u_{el}]\cdot\overline{\psi}_t \,\mathrm{d}\Gamma^+ \tag{61}$$

for all quasi-periodic functions $u_{el} \in H(\mathrm{curl}, G)$ and $u^\pm_{el} \in H^\pm$. The right-hand side of (61) includes the function ψ_t defined by

$$\begin{aligned}
\psi_t \;:=\; & \frac{400[k^+]^2}{c_{0,0}\;\mathrm{per}_x \mathrm{per}_y} \sum_{(n,m,l)\in I} \frac{c_{n,m} w_{n,m,l} B^+_{n,m,l}(u_{el,0})}{\delta_{l,1}\,[a_n^2+b_m^2]+c_{n,m}^2} \left[\frac{100\, c_{n,m}}{c_{0,0}} |B^+_{n,m,l}(u_{el,0})|^2 - d_{n,m,l}\right] \\
& * [\cos\theta_{n,m}]^{2-4l} [\nu\times u^+_{el,n,m,l}] \;.
\end{aligned} \tag{62}$$

Recall that k^+ is the wave number above the grating structure, per_x and per_y are the periods of the geometry (cf. Section 2.1), $c_{n,m}$, a_n, and b_m are given in (28), and the $w_{n,m,l}$ together with the $d_{n,m,l}$ define the objective functional (57). The Rayleigh coefficient $B^+_{n,m,l}(u_{el,0})$ is that of the expansion (24) with $u^+ = u^+_{el,0}$, which is nothing else than a scaled Fourier coefficient of the quasi-periodic function $u_{el,0}$ (cf. (20), (25), and (24)). The expression $\cos\theta_{n,m}$ is defined as $c_{n,m}/\sqrt{a_n^2+b_m^2+|c_{n,m}|^2}$. For propagating modes $u_{n,m,l}$, we have $c_{n,m} > 0$, and $\theta_{n,m}$ is the angle of the propagation direction defined such that $\sin\theta_{n,m} = \sqrt{a_n^2+b_m^2}/k^+$ and $\cos\theta_{n,m} = c_{n,m}/k^+$. In particular, $\theta_{0,0} = \theta$.

In view of the similarity of the variational form (45) to those in [16, 19, 21, 11], we conjecture that the variational equation (51) and, equivalently, (61) satisfies the Fredholm alternative with index zero. Hence, if the solution of the Maxwell system (2), (10)-(13), (18), (20), and (22) is unique, then (61) is uniquely solvable, and there exists a unique adjoint solution $(u_{el,ad}, u^+_{el,ad}, u^-_{el,ad})$.

Theorem 4.1 *Suppose the boundary value problem* (2)*,* (10)–(13)*,* (18)*,* (20)*, and* (22) *for the Maxwell system is uniquely solvable, i.e., the unique electric field solution $u_{el,0}$ corresponds to the unique magnetic field solution of the variational equation in* [21]*. Suppose the objective functional $\mathcal{F}$ is defined by* (57) *and that u_h is the electric field solution of the Maxwell system with wave number function $k_h := \Psi_h k$, where the transform Ψ_h is defined as in* (58) *with a vector function χ satisfying the conditions* (C1)-(C2) *in Section* 4.2*. Finally, suppose $(u_{el,ad}, u^+_{el,ad}, u^-_{el,ad})$ is the unique solution of the adjoint equation* (61)*. Then the shape derivative $\partial_h[\mathcal{F}(u_h)]|_{h=0}$ of* (59) *is given as*

$$\partial_h[\mathcal{F}(u_h)]|_{h=0} = -\Re\mathrm{e}\, a_1(u_{el,0}, u_{el,ad}). \tag{63}$$

The Sections 4.5-4.9 are devoted to the proof of this result. For this proof, the technique of shape derivatives from [11] is adapted (compare [25]).

4.5 Transform of derivatives

Clearly, the Jacobian matrix of the transformation Φ_h is

$$J = \Big(\partial_u[\Phi_h]_v\Big)_{u,v\in\{x,y,z\}} = \begin{pmatrix} 1+h\partial_x\chi_x & h\partial_x\chi_y & h\partial_x\chi_z \\ h\partial_y\chi_x & 1+h\partial_y\chi_y & h\partial_y\chi_z \\ h\partial_z\chi_x & h\partial_z\chi_y & 1+h\partial_z\chi_z \end{pmatrix}.$$

The determinant of this Jacobian matrix and its reciprocal is given by

$$\begin{aligned} \det J \;=\; & (1+h\partial_x\chi_x)(1+h\partial_y\chi_y)(1+h\partial_z\chi_z) + (h\partial_x\chi_y)(h\partial_y\chi_z)(h\partial_z\chi_x) \\ & +(h\partial_x\chi_z)(h\partial_y\chi_x)(h\partial_z\chi_y) - (h\partial_z\chi_x)(1+h\partial_y\chi_y)(h\partial_x\chi_z) \\ & -(h\partial_y\chi_x)(h\partial_x\chi_y)(1+h\partial_z\chi_z) - (1+h\partial_x\chi_x)(h\partial_z\chi_y)(h\partial_y\chi_z) \\ =\; & 1 + h\ \{\partial_x\chi_x + \partial_y\chi_y + \partial_z\chi_z\} \\ & +h^2\{\partial_x\chi_x\partial_y\chi_y + \partial_x\chi_x\partial_z\chi_z + \partial_y\chi_y\partial_z\chi_z \\ & -\partial_z\chi_x\partial_x\chi_z - \partial_y\chi_x\partial_x\chi_y - \partial_z\chi_y\partial_y\chi_z\} \end{aligned}$$

$$
\begin{aligned}
& +h^3\{\partial_x\chi_x\partial_y\chi_y\partial_z\chi_z+\partial_x\chi_y\partial_y\chi_z\partial_z\chi_x+\partial_x\chi_z\partial_y\chi_x\partial_z\chi_y \\
& -\partial_z\chi_x\partial_y\chi_y\partial_x\chi_z-\partial_y\chi_x\partial_x\chi_y\partial_z\chi_z-\partial_x\chi_x\partial_z\chi_y\partial_y\chi_z\} \\
&= 1+h\ \nabla\cdot\chi+\mathcal{O}(h^2), \qquad (64)\\
\frac{1}{\det\ J} &= 1-h\ \nabla\cdot\chi+\mathcal{O}(h^2). \qquad (65)
\end{aligned}
$$

For the adjoint Jacobian matrix, the formula

$$
J^* = \begin{pmatrix} 1+h\partial_x\chi_x & h\partial_y\chi_x & h\partial_z\chi_x \\ h\partial_x\chi_y & 1+h\partial_y\chi_y & h\partial_z\chi_y \\ h\partial_x\chi_z & h\partial_y\chi_z & 1+h\partial_z\chi_z \end{pmatrix}
$$

holds.

Hence, a substitution of variable in integration (at least for small values of h) includes the substitution

$$
\mathrm{d}x'\mathrm{d}y'\mathrm{d}z' = |\det J(x,y,z)|\ \mathrm{d}x\mathrm{d}y\mathrm{d}z = \det J(x,y,z)\ \mathrm{d}x\mathrm{d}y\mathrm{d}z, \quad \mathrm{d}G' = \det J\ \mathrm{d}G.
$$

The first order derivatives transform according to

$$
\begin{aligned}
\partial_x &= \partial_{x'}[1+h\partial_x\chi_x]+\partial_{y'}[h\partial_x\chi_y], \quad +\partial_{z'}[h\partial_x\chi_z], \\
\partial_y &= \partial'_x[h\partial_y\chi_x] \quad +\partial'_y[1+h\partial_y\chi_y]+\partial'_z[h\partial_y\chi_z], \\
\partial_z &= \partial'_x[h\partial_z\chi_x] \quad +\partial'_y[h\partial_z\chi_y] \quad +\partial'_z[1+h\partial_z\chi_z], \\
(\partial_x,\partial_y,\partial_z)^\top &= J\ (\partial_{x'},\partial_{y'},\partial_{z'})^\top, \\
(\partial_{x'},\partial_{y'},\partial_{z'})^\top &= J^{-1}(\partial_x,\partial_y,\partial_z)^\top, \\
J^{-1} &= \frac{1}{\det\ J}\times
\end{aligned}
$$

$$
\begin{pmatrix}
\begin{matrix}(1+h\partial_y\chi_y)(1+h\partial_z\chi_z)\\ -h\partial_z\chi_y h\partial_y\chi_z\end{matrix} & \begin{matrix}h\partial_z\chi_y h\partial_x\chi_z\\ -h\partial_x\chi_y(1+h\partial_z\chi_z)\end{matrix} & \begin{matrix}h\partial_x\chi_y h\partial_y\chi_z\\ -h\partial_x\chi_z(1+h\partial_y\chi_y)\end{matrix} \\
\begin{matrix}h\partial_z\chi_x h\partial_y\chi_z\\ -h\partial_y\chi_x(1+h\partial_z\chi_z)\end{matrix} & \begin{matrix}(1+h\partial_x\chi_x)(1+h\partial_z\chi_z)\\ -h\partial_x\chi_z h\partial_z\chi_x\end{matrix} & \begin{matrix}h\partial_y\chi_x h\partial_x\chi_z\\ -h\partial_y\chi_z(1+h\partial_x\chi_x)\end{matrix} \\
\begin{matrix}h\partial_y\chi_x h\partial_z\chi_y\\ -h\partial_z\chi_x(1+h\partial_y\chi_y)\end{matrix} & \begin{matrix}h\partial_z\chi_x h\partial_x\chi_y\\ -h\partial_z\chi_y(1+h\partial_x\chi_x)\end{matrix} & \begin{matrix}(1+h\partial_x\chi_x)(1+h\partial_y\chi_y)\\ -h\partial_y\chi_x h\partial_x\chi_y\end{matrix}
\end{pmatrix}.
$$

Consequently, there holds

$$
\begin{aligned}
\partial_{x'} &= \frac{1+h\{\partial_y\chi_y+\partial_z\chi_z\}}{\det\ J}\partial_x-\frac{h\partial_x\chi_y}{\det\ J}\partial_y-\frac{h\partial_x\chi_z}{\det\ J}\partial_z+\mathcal{O}(h^2) \\
&= \frac{1}{\det\ J}\partial_x+\frac{h}{\det\ J}\{[\partial_y\chi_y+\partial_z\chi_z]\partial_x-\partial_x\chi_y\partial_y-\partial_x\chi_z\partial_z\}+\mathcal{O}(h^2), \qquad (66)\\
\partial_{y'} &= -\frac{h\partial_y\chi_x}{\det\ J}\partial_x+\frac{1+h\{\partial_x\chi_x+\partial_z\chi_z\}}{\det\ J}\partial_y-\frac{h\partial_y\chi_z}{\det\ J}\partial_z+\mathcal{O}(h^2) \\
&= \frac{1}{\det\ J}\partial_y+\frac{h}{\det\ J}\{-\partial_y\chi_x\partial_x+[\partial_x\chi_x+\partial_z\chi_z]\partial_y-\partial_y\chi_z\partial_z\}+\mathcal{O}(h^2), \qquad (67)\\
\partial_{z'} &= -\frac{h\partial_z\chi_x}{\det\ J}\partial_x-\frac{h\partial_z\chi_y}{\det\ J}\partial_y+\frac{1+h\{\partial_x\chi_x+\partial_y\chi_y\}}{\det\ J}\partial_z+\mathcal{O}(h^2) \\
&= \frac{1}{\det\ J}\partial_z+\frac{h}{\det\ J}\{-\partial_z\chi_x\partial_x-\partial_z\chi_y\partial_y+[\partial_x\chi_x+\partial_y\chi_y]\partial_z\}+\mathcal{O}(h^2). \qquad (68)
\end{aligned}
$$

This implies, for the rotation,

$$
\begin{aligned}
\nabla' \times \mathsf{v} &= \nabla' \times (\mathsf{v}_x, \mathsf{v}_y, \mathsf{v}_z)^\top = (\partial_{y'}\mathsf{v}_z - \partial_{z'}\mathsf{v}_y, \partial_{z'}\mathsf{v}_x - \partial_{x'}\mathsf{v}_z, \partial_{x'}\mathsf{v}_y - \partial_{y'}\mathsf{v}_x)^\top \\
&= \frac{1}{\det\ J}\nabla \times \mathsf{v} \\
&\quad + \frac{h}{\det\ J}\Big(- \partial_y\chi_x\partial_x\mathsf{v}_z + [\partial_x\chi_x + \partial_z\chi_z]\partial_y\mathsf{v}_z - \partial_y\chi_z\partial_z\mathsf{v}_z + \partial_z\chi_x\partial_x\mathsf{v}_y \\
&\qquad + \partial_z\chi_y\partial_y\mathsf{v}_y - [\partial_x\chi_x + \partial_y\chi_y]\partial_z\mathsf{v}_y, \\
&\qquad - \partial_z\chi_x\partial_x\mathsf{v}_x - \partial_z\chi_y\partial_y\mathsf{v}_x + [\partial_x\chi_x + \partial_y\chi_y]\partial_z\mathsf{v}_x \\
&\qquad - [\partial_y\chi_y + \partial_z\chi_z]\partial_x\mathsf{v}_z + \partial_x\chi_y\partial_y\mathsf{v}_z + \partial_x\chi_z\partial_z\mathsf{v}_z, \\
&\qquad [\partial_y\chi_y + \partial_z\chi_z]\partial_x\mathsf{v}_y - \partial_x\chi_y\partial_y\mathsf{v}_y - \partial_x\chi_z\partial_z\mathsf{v}_y \\
&\qquad + \partial_y\chi_x\partial_x\mathsf{v}_x - [\partial_x\chi_x + \partial_z\chi_z]\partial_y\mathsf{v}_x + \partial_y\chi_z\partial_z\mathsf{v}_x\Big)^\top + \mathcal{O}(h^2) \\
&= \frac{1}{\det\ J}\nabla \times \mathsf{v} \\
&\quad + \frac{h}{\det\ J}\Big\{\partial_x\chi_x(\partial_y\mathsf{v}_z - \partial_z\mathsf{v}_y, \partial_z\mathsf{v}_x, -\partial_y\mathsf{v}_x)^\top + \partial_x\chi_y(0, \partial_y\mathsf{v}_z, -\partial_y\mathsf{v}_y)^\top \\
&\qquad + \partial_x\chi_z(0, \partial_z\mathsf{v}_z, -\partial_z\mathsf{v}_y)^\top + \partial_y\chi_x(- \partial_x\mathsf{v}_z, 0, \partial_x\mathsf{v}_x)^\top \\
&\qquad + \partial_y\chi_y(- \partial_z\mathsf{v}_y, \partial_z\mathsf{v}_x - \partial_x\mathsf{v}_z, \partial_x\mathsf{v}_y)^\top + \partial_y\chi_z(- \partial_z\mathsf{v}_z, 0, \partial_z\mathsf{v}_x)^\top \\
&\qquad + \partial_z\chi_x(\partial_x\mathsf{v}_y, -\partial_x\mathsf{v}_x, 0)^\top + \partial_z\chi_y(\partial_y\mathsf{v}_y, -\partial_y\mathsf{v}_x, 0)^\top \\
&\qquad + \partial_z\chi_z(\partial_y\mathsf{v}_z, -\partial_x\mathsf{v}_z, \partial_x\mathsf{v}_y - \partial_y\mathsf{v}_x)^\top\Big\} + \mathcal{O}(h^2) \\
&= \frac{1}{\det\ J}\nabla \times \mathsf{v} \\
&\quad + \frac{h}{\det\ J}\Big\{\partial_x\chi_x([\nabla \times \mathsf{v}]_x, \partial_z\mathsf{v}_x, -\partial_y\mathsf{v}_x)^\top + \partial_x\chi_y(0, \partial_y\mathsf{v}_z, -\partial_y\mathsf{v}_y)^\top \\
&\qquad + \partial_x\chi_z(0, \partial_z\mathsf{v}_z, -\partial_z\mathsf{v}_y)^\top + \partial_y\chi_x(-\partial_x\mathsf{v}_z, 0, \partial_x\mathsf{v}_x)^\top \\
&\qquad + \partial_y\chi_y(-\partial_z\mathsf{v}_y, [\nabla \times \mathsf{v}]_y, \partial_x\mathsf{v}_y)^\top + \partial_y\chi_z(-\partial_z\mathsf{v}_z, 0, \partial_z\mathsf{v}_x)^\top \\
&\qquad + \partial_z\chi_x(\partial_x\mathsf{v}_y, -\partial_x\mathsf{v}_x, 0)^\top + \partial_z\chi_y(\partial_y\mathsf{v}_y, -\partial_y\mathsf{v}_x, 0)^\top \\
&\qquad + \partial_z\chi_z(\partial_y\mathsf{v}_z, -\partial_x\mathsf{v}_z, [\nabla \times \mathsf{v}]_z)^\top\Big\} + \mathcal{O}(h^2) \\
&= \frac{1}{\det\ J}\nabla \times \mathsf{v} \\
&\quad + \frac{h}{\det\ J}\Big\{\partial_x\chi_x\nabla \times \mathsf{v} + \partial_x\chi_x(0, \partial_x\mathsf{v}_z, -\partial_x\mathsf{v}_y)^\top + \partial_x\chi_y(0, \partial_y\mathsf{v}_z, -\partial_y\mathsf{v}_y)^\top \\
&\qquad + \partial_x\chi_z(0, \partial_z\mathsf{v}_z, -\partial_z\mathsf{v}_y)^\top + \partial_y\chi_x(-\partial_x\mathsf{v}_z, 0, \partial_x\mathsf{v}_x)^\top \\
&\qquad + \partial_y\chi_y\nabla \times \mathsf{v} + \partial_y\chi_y(-\partial_y\mathsf{v}_z, 0, \partial_y\mathsf{v}_x)^\top + \partial_y\chi_z(-\partial_z\mathsf{v}_z, 0, \partial_z\mathsf{v}_x)^\top \\
&\qquad + \partial_z\chi_x(\partial_x\mathsf{v}_y, -\partial_x\mathsf{v}_x, 0)^\top + \partial_z\chi_y(\partial_y\mathsf{v}_y, -\partial_y\mathsf{v}_x, 0)^\top \\
&\qquad + \partial_z\chi_z\nabla \times \mathsf{v} + \partial_z\chi_z(\partial_z\mathsf{v}_y, -\partial_z\mathsf{v}_x, 0)^\top\Big\} + \mathcal{O}(h^2) \\
&= \frac{1}{\det\ J}\nabla \times \mathsf{v} \\
&\quad + \frac{h}{\det\ J}\Big\{\nabla\cdot\chi_x\nabla \times \mathsf{v} + \Big(- \partial_y\chi_x\partial_x\mathsf{v}_z + \partial_z\chi_x\partial_x\mathsf{v}_y - \partial_y\chi_y\partial_y\mathsf{v}_z + \partial_z\chi_y\partial_y\mathsf{v}_y
\end{aligned}
$$

$$
\begin{aligned}
&-\partial_y\chi_z\partial_z\mathsf{v}_z + \partial_z\chi_z\partial_z\mathsf{v}_y,\\
&-\partial_z\chi_x\partial_x\mathsf{v}_x + \partial_x\chi_x\partial_x\mathsf{v}_z - \partial_z\chi_y\partial_y\mathsf{v}_x + \partial_x\chi_y\partial_y\mathsf{v}_z\\
&-\partial_z\chi_z\partial_z\mathsf{v}_x + \partial_x\chi_z\partial_z\mathsf{v}_z,\\
&-\partial_x\chi_x\partial_x\mathsf{v}_y + \partial_y\chi_x\partial_x\mathsf{v}_x - \partial_x\chi_y\partial_y\mathsf{v}_y + \partial_y\chi_y\partial_y\mathsf{v}_x\\
&-\partial_x\chi_z\partial_z\mathsf{v}_y + \partial_y\chi_z\partial_z\mathsf{v}_x\Big)^\top\Big\} + \mathcal{O}(h^2).
\end{aligned}
$$

At the end, the rotation is given by

$$
\begin{aligned}
\nabla'\times\mathsf{v} &= \frac{\nabla\times\mathsf{v}}{\det J} + \frac{h}{\det J}\Big\{\nabla\cdot\chi\ \nabla\times\mathsf{v} - \nabla\chi_x\times\partial_x\mathsf{v} - \nabla\chi_y\times\partial_y\mathsf{v} - \nabla\chi_z\times\partial_z\mathsf{v}\Big\}\\
&= \nabla\times\mathsf{v} - h\Big\{\nabla\chi_x\times\partial_x\mathsf{v} + \nabla\chi_y\times\partial_y\mathsf{v} + \nabla\chi_z\times\partial_z\mathsf{v}\Big\}\ +\ \mathcal{O}(h^2). \qquad (69)
\end{aligned}
$$

Note that, in general, the space $H(\mathrm{curl}, G)$ is not invariant under the transform Ψ_h. To treat a general χ, magnetic fields from the invariant space $[H^1]^3$ are considered, shape derivatives for these magnetic fields are computed, and the formula is converted to electric fields using (4).

4.6 Asymptotic expansion of variational form

In this subsection all functions u and v are magnetic fields. For each h, a perturbed variational equation (52) is defined replacing k by $k_h := \Psi_h k$, i.e., by

$$
k_h(x',y',z') \ = \ k_h\Big(\Phi_h(x,y,z)\Big) \ := \ k\Big(\Phi_h^{-1}\Phi_h(x,y,z)\Big) \ = \ k(x,y,z).
$$

The corresponding sesqui-linear form is denoted by a_h, and the variational equation equivalent to (53) is considered with a_h. This a_h takes the form

$$
\begin{aligned}
&a_h\Big((u,u^+,u^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) \ =\\
&\mu^2\omega^2\int_G k_h^{-2}\ \nabla\times u\cdot\overline{\nabla\times\mathsf{v}}\ \mathrm{d}G - \mu^2\omega^2\int_G\ u\cdot\bar{\mathsf{v}}\ \mathrm{d}G\ + a_R\Big((u,u^+,u^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big).
\end{aligned}
$$

The remainder form a_R consists of boundary integrals over $\Gamma^\pm$ and is independent of h. Similarly, the right-hand sides

$$
f_h\Big((\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) := -a_h\Big((0,U^{\mathrm{inc}},0),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) = -a\Big((0,U^{\mathrm{inc}},0),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big)
$$

are independent of h. Now (69) and (64) lead, for $h\to 0$, to the asymptotic expansion of the variational form

$$
a_h\Big((\Psi_h u,u^+,u^-),(\Psi_h\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) \qquad (70)
$$

$$
= \ \mu^2\omega^2\int_G k^{-2}(\Phi_h^{-1}(x',y',z'))\ \nabla\times u(\Phi_h^{-1}(x',y',z'))\cdot \overline{\nabla\times\mathsf{v}(\Phi_h^{-1}(x',y',z'))}\ \mathrm{d}G' \qquad (71)
$$

$$
\begin{aligned}
&-\mu^2\omega^2 \int_G u(\Phi_h^{-1}(x',y',z')) \cdot \overline{\mathsf{v}(\Phi_h^{-1}(x',y',z'))}\, \mathrm{d}G' \\
&+a_R\Big((u,u^+,u^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) \\
=\;& \mu^2\omega^2 \int_G k^{-2} \left\{\nabla\times u - h\Big[\nabla\chi_x\times\partial_x u + \nabla\chi_y\times\partial_y u + \nabla\chi_z\times\partial_z u\Big] + \mathcal{O}(h^2)\right\} \\
&\cdot\overline{\left\{\nabla\times \mathsf{v} - h\Big[\nabla\chi_x\times\partial_x \mathsf{v} + \nabla\chi_y\times\partial_y \mathsf{v} + \nabla\chi_z\times\partial_z \mathsf{v}\Big] + \mathcal{O}(h^2)\right\}} \det J \,\mathrm{d}G \\
&-\mu^2\omega^2 \int_G u\cdot\bar{\mathsf{v}}\, \det J\,\mathrm{d}G + a_R\Big((u,u^+,u^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) \\
=\;& a\Big((u,u^+,u^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big) + \; h\, a_1(u,\mathsf{v}) + \mathcal{O}(h^2)
\end{aligned}
$$

with a_1 defined as

$$
\begin{aligned}
a_1(u,\mathsf{v}) \;:=\;& \mu^2\omega^2 \int_G k^{-2}\,[\nabla\times u]\cdot\overline{[\nabla\times \mathsf{v}]}\;\nabla\cdot\chi\,\mathrm{d}G \\
&-\mu^2\omega^2 \int_G k^{-2}\,[\nabla\times u]\cdot\overline{\Big[\nabla\chi_x\times\partial_x \mathsf{v} + \nabla\chi_y\times\partial_y \mathsf{v} + \nabla\chi_z\times\partial_z \mathsf{v}\Big]}\;\mathrm{d}G \\
&-\mu^2\omega^2 \int_G k^{-2}\,\Big[\nabla\chi_x\times\partial_x u + \nabla\chi_y\times\partial_y u + \nabla\chi_z\times\partial_z u\Big]\;\cdot\overline{[\nabla\times \mathsf{v}]}\,\mathrm{d}G \\
&-\mu^2\omega^2 \int_G u\cdot\bar{\mathsf{v}}\;\;\nabla\cdot\chi\,\mathrm{d}G.
\end{aligned}
$$

Note that the magnetic field solutions of the Maxwell equations u and v are in $[H^1]^3$ such that the last definition is meaningful. The values of the form a_1 applied to solutions of the Maxwell equations coincide with those in (60). This fact will be shown in the remainder of this section.

In view of the identities $\partial_s u = \nabla u_s - e_s\times[\nabla\times u],\; s=x,y,z$ as well as $\nabla\chi_s\times e_s\times[\nabla\times u] = \nabla\chi_s\cdot[\nabla\times u]\;e_s - \nabla\chi_s\cdot e_s\;[\nabla\times u]$ with $e_s := (\delta_{x,s},\delta_{y,s},\delta_{z,s})^\top$, the form a_1 is equal to

$$
\begin{aligned}
a_1(u,\mathsf{v}) \;=\;& -\mu^2\omega^2 \int_G k^{-2}\,[\nabla\times u]\cdot\overline{[\nabla\times \mathsf{v}]}\;\nabla\cdot\chi\,\mathrm{d}G \\
&-\mu^2\omega^2 \int_G k^{-2}\,[\nabla\times u]\cdot\overline{\Big[\nabla\chi_x\times\nabla \mathsf{v}_x + \nabla\chi_y\times\nabla \mathsf{v}_y + \nabla\chi_z\times\nabla \mathsf{v}_z\Big]}\;\mathrm{d}G \\
&+\mu^2\omega^2 \int_G k^{-2}\,[\nabla\times u]\cdot\overline{\Big(\nabla\chi_x\cdot[\nabla\times \mathsf{v}], \nabla\chi_y\cdot[\nabla\times \mathsf{v}], \nabla\chi_z\cdot[\nabla\times \mathsf{v}]\Big)^\top}\;\mathrm{d}G \\
&-\mu^2\omega^2 \int_G k^{-2}\,\Big[\nabla\chi_x\times\nabla u_x + \nabla\chi_y\times\nabla u_y + \nabla\chi_z\times\nabla u_z\Big]\;\cdot\overline{[\nabla\times \mathsf{v}]}\,\mathrm{d}G \\
&+\mu^2\omega^2 \int_G k^{-2}\,\Big(\nabla\chi_x\cdot[\nabla\times u], \nabla\chi_y\cdot[\nabla\times u], \nabla\chi_z\cdot[\nabla\times u]\Big)^\top\cdot\overline{[\nabla\times \mathsf{v}]}\,\mathrm{d}G \\
&-\mu^2\omega^2 \int_G u\cdot\bar{\mathsf{v}}\;\;\nabla\cdot\chi\,\mathrm{d}G.
\end{aligned}
$$

The identities

$$
\nabla\cdot\{[\nabla\times u]\times[\bar{\mathsf{v}}_s\nabla\chi_s]\} \;=\; [\nabla\times\nabla\times u]\cdot[\bar{\mathsf{v}}_s\nabla\chi_s]
$$

$$
\begin{aligned}
& & & -[\nabla\times u]\cdot\{\nabla\overline{\mathsf{v}}_s\times\nabla\chi_s+\overline{\mathsf{v}}_s\nabla\times\nabla\chi_s\},\\
&[\nabla\times u]\cdot[\nabla\chi_s\times\nabla\overline{\mathsf{v}}_s] &=& \nabla\cdot\{[\nabla\times u]\times[\overline{\mathsf{v}}_s\nabla\chi_s]\}\\
& & & -[\nabla\times\nabla\times u]\cdot[\overline{\mathsf{v}}_s\nabla\chi_s]+[\nabla\times u]\cdot[\overline{\mathsf{v}}_s\nabla\times\nabla\chi_s],\\
&[\nabla\chi_s\times\nabla u_s]\cdot[\nabla\times\overline{\mathsf{v}}] &=& -\nabla\cdot\{[u_s\nabla\chi_s]\times[\nabla\times\overline{\mathsf{v}}]\}\\
& & & -[u_s\nabla\chi_s]\cdot[\nabla\times\nabla\times\overline{\mathsf{v}}]+[u_s\nabla\times\nabla\chi_s]\cdot[\nabla\times\overline{\mathsf{v}}]
\end{aligned}
$$

lead to

$$
\begin{aligned}
a_1(u,\mathsf{v}) \;:=\; & -\mu^2\omega^2\int_G k^{-2}\,[\nabla\times u]\cdot\overline{[\nabla\times\mathsf{v}]}\;\nabla\cdot\chi\,\mathrm{d}G\\
& -\mu^2\omega^2\int_G k^{-2}\,[\nabla\times u]\cdot\overline{\Big[\mathsf{v}_x\nabla\times[\nabla\chi_x]+\mathsf{v}_y\nabla\times[\nabla\chi_y]+\mathsf{v}_z\nabla\times[\nabla\chi_z]\Big]}\;\mathrm{d}G\\
& +\mu^2\omega^2\int_G k^{-2}\,\nabla\times[\nabla\times u]\cdot\overline{\Big[\mathsf{v}_x\nabla\chi_x+\mathsf{v}_y\nabla\chi_y+\mathsf{v}_z\nabla\chi_z\Big]}\;\mathrm{d}G\\
& -\mu^2\omega^2\int_G k^{-2}\,\nabla\cdot\Big\{[\nabla\times u]\times\overline{\Big[\mathsf{v}_x\nabla\chi_x+\mathsf{v}_y\nabla\chi_y+\mathsf{v}_z\nabla\chi_z\Big]}\Big\}\,\mathrm{d}G\\
& +\mu^2\omega^2\int_G k^{-2}\,[\nabla\times u]\cdot\overline{\Big(\nabla\chi_x\cdot[\nabla\times\mathsf{v}],\nabla\chi_y\cdot[\nabla\times\mathsf{v}],\nabla\chi_z\cdot[\nabla\times\mathsf{v}]\Big)^\top}\;\mathrm{d}G\\
& -\mu^2\omega^2\int_G k^{-2}\,\Big[u_x\nabla\times[\nabla\chi_x]+u_y\nabla\times[\nabla\chi_y]+u_z\nabla\times[\nabla\chi_z]\Big]\;\cdot\overline{[\nabla\times\mathsf{v}]}\,\mathrm{d}G\\
& +\mu^2\omega^2\int_G k^{-2}\,\Big[u_x\nabla\chi_x+u_y\nabla\chi_y+u_z\nabla\chi_z\Big]\;\cdot\overline{\nabla\times[\nabla\times\mathsf{v}]}\,\mathrm{d}G\\
& +\mu^2\omega^2\int_G k^{-2}\,\nabla\cdot\Big\{\Big[u_x\nabla\chi_x+u_y\nabla\chi_y+u_z\nabla\chi_z\Big]\times\overline{[\nabla\times\mathsf{v}]}\Big\}\,\mathrm{d}G\\
& +\mu^2\omega^2\int_G k^{-2}\,\Big(\nabla\chi_x\cdot[\nabla\times u],\nabla\chi_y\cdot[\nabla\times u],\nabla\chi_z\cdot[\nabla\times u]\Big)^\top\cdot\overline{[\nabla\times\mathsf{v}]}\,\mathrm{d}G\\
& -\mu^2\omega^2\int_G u\cdot\overline{\mathsf{v}}\;\;\nabla\cdot\chi\,\mathrm{d}G.
\end{aligned}
$$

Now suppose Γ^I is the collection of $\Gamma^\pm$ and all interfaces with jumps in k^{-2} and $\nabla\chi_s,\ s=x,y,z$ and that ν is the normal to Γ^I. Recall the definition of the jump $[\![\ldots]\!]_{\Gamma^I}$ in Section 2.4. The jump over $\Gamma^\pm$ is defined simply by setting the undefined functions above Γ^+ and below Γ^- to zero. If the u and v are solutions of the curl-curl equation (3), then the divergence theorem $\int_\Omega\nabla\cdot w=\int_{\partial\Omega}w\cdot\nu$ implies

$$
\begin{aligned}
a_1(u,\mathsf{v}) \;=\; & -\mu^2\omega^2\int_G k^{-2}\,[\nabla\times u]\cdot\overline{[\nabla\times\mathsf{v}]}\;\nabla\cdot\chi\,\mathrm{d}G \qquad (72)\\
& -\mu^2\omega^2\int_G k^{-2}\,[\nabla\times u]\cdot\overline{\Big[\mathsf{v}_x\nabla\times[\nabla\chi_x]+\mathsf{v}_y\nabla\times[\nabla\chi_y]+\mathsf{v}_z\nabla\times[\nabla\chi_z]\Big]}\;\mathrm{d}G\\
& +\mu^2\omega^2\int_G u\cdot\overline{\Big[\mathsf{v}_x\nabla\chi_x+\mathsf{v}_y\nabla\chi_y+\mathsf{v}_z\nabla\chi_z\Big]}\;\mathrm{d}G\\
& -\mu^2\omega^2\int_{\Gamma^I}[\![\,k^{-2}\,\Big[\nu\times[\nabla\times u]\Big]\cdot\overline{\Big[\mathsf{v}_x\nabla\chi_x+\mathsf{v}_y\nabla\chi_y+\mathsf{v}_z\nabla\chi_z\Big]}\,]\!]_{\Gamma^I}\,\mathrm{d}\Gamma^I
\end{aligned}
$$

$$
\begin{aligned}
&+\mu^2\omega^2 \int_G k^{-2}\,[\nabla\times u]\cdot \overline{\Big(\nabla\chi_x\cdot[\nabla\times \mathsf{v}],\nabla\chi_y\cdot[\nabla\times \mathsf{v}],\nabla\chi_z\cdot[\nabla\times \mathsf{v}]\Big)^\top}\,\mathrm{d}G\\
&-\mu^2\omega^2 \int_G k^{-2}\,\Big[u_x\nabla\times[\nabla\chi_x]+u_y\nabla\times[\nabla\chi_y]+u_z\nabla\times[\nabla\chi_z]\Big]\cdot\overline{[\nabla\times \mathsf{v}]}\,\mathrm{d}G\\
&+\mu^2\omega^2 \int_G \Big[u_x\nabla\chi_x+u_y\nabla\chi_y+u_z\nabla\chi_z\Big]\cdot\bar{\mathsf{v}}\,\mathrm{d}G\\
&-\mu^2\omega^2 \int_{\Gamma^I} [\![\, k^{-2}\,\Big[u_x\nabla\chi_x+u_y\nabla\chi_y+u_z\nabla\chi_z\Big]\cdot\Big[\nu\times\overline{[\nabla\times \mathsf{v}]}\Big]\,]\!]_{\Gamma^I}\,\mathrm{d}\Gamma^I\\
&+\mu^2\omega^2 \int_G k^{-2}\,\Big(\nabla\chi_x\cdot[\nabla\times u],\nabla\chi_y\cdot[\nabla\times u],\nabla\chi_z\cdot[\nabla\times u]\Big)^\top\cdot\overline{[\nabla\times \mathsf{v}]}\,\mathrm{d}G\\
&-\mu^2\omega^2 \int_G u\cdot\bar{\mathsf{v}}\;\;\nabla\cdot\chi\,\mathrm{d}G.
\end{aligned}
$$

The integrals over Γ^I take the form

$$
\begin{aligned}
&\int_{\Gamma^I} [\![\, k^{-2}\,\Big[\nu\times[\nabla\times u]\Big]\cdot\overline{\Big[\mathsf{v}_x\nabla\chi_x+\mathsf{v}_y\nabla\chi_y+\mathsf{v}_z\nabla\chi_z\Big]}\,]\!]_{\Gamma^I}\,\mathrm{d}\Gamma^I\\
&\qquad=\sum_{w\in\{x,y,z\}}\int_{\Gamma^I} [\![\,\bar{\mathsf{v}}_w\,k^{-2}\,\Big[\nu\times[\nabla\times u]\Big]\cdot[\nabla\chi_w]_t\,]\!]_{\Gamma^I}\,\mathrm{d}\Gamma^I.
\end{aligned}
$$

Here, for a vector function $[\ldots]$, the expression $[\ldots]_t$ denotes the tangential part of $[\ldots]$.

Now, by Γ^i we denote the union of the boundaries $\Gamma^\pm$ and all the interfaces between the subdomains of G, where the permittivity ε is constant. On the surface $\Gamma^I\setminus\Gamma^i$, the wave number k and the Maxwell solutions $\nabla\times u$ and v are continuous. Since χ_w is continuous and piecewise analytic (cf. condition (C1) at the beginning of Section 4.2), the tangential derivative $[\nabla\chi_w]_t$ is continuous too. The interface normal ν in the jump expression changes sign. Consequently, the jump $[\![\,\bar{\mathsf{v}}_w\,k^{-2}\,[\nu\times[\nabla\times u]]\cdot[\nabla\chi_w]_t\,]\!]_{\Gamma^I}$ over $\Gamma^I\setminus\Gamma^i$ is zero and we can replace the surface integrals over Γ^I in (72) by integrals over Γ^i. Over Γ^i, the tangential parts of the Maxwell solutions $k^{-2}[\nabla\times u]_t$ and $[\mathsf{v}]_t$ are continuous. Again $[\nabla\chi_w]_t$ is continuous. Thus splitting v into the continuous tangential part $[\mathsf{v}]_t$ and the normal part $[\mathsf{v}\cdot\nu]\,\nu$, we can drop the zero jump of the continuous parts and obtain

$$
\begin{aligned}
&\int_{\Gamma^i} [\![\, k^{-2}\,\Big[\nu\times[\nabla\times u]\Big]\cdot\overline{\Big[\mathsf{v}_x\nabla\chi_x+\mathsf{v}_y\nabla\chi_y+\mathsf{v}_z\nabla\chi_z\Big]}\,]\!]_{\Gamma^i}\,\mathrm{d}\Gamma^i\\
&=\int_{\Gamma^i} [\![\,\Big(k^{-2}\Big[\nu\times[\nabla\times u]\Big]\cdot\nabla\chi_x\,,\;k^{-2}\Big[\nu\times[\nabla\times u]\Big]\cdot\nabla\chi_y\,,\;k^{-2}\Big[\nu\times[\nabla\times u]\Big]\cdot\nabla\chi_z\Big)^\top\\
&\qquad\cdot\bar{\mathsf{v}}\,]\!]_{\Gamma^i}\,\mathrm{d}\Gamma^i\\
&=\int_{\Gamma^i} [\![\,\Big(k^{-2}\Big[\nu\times[\nabla\times u]\Big]\cdot\nabla\chi_x\,,\;k^{-2}\Big[\nu\times[\nabla\times u]\Big]\cdot\nabla\chi_y\,,\;k^{-2}\Big[\nu\times[\nabla\times u]\Big]\cdot\nabla\chi_z\Big)^\top\\
&\qquad\cdot[\bar{\mathsf{v}}\cdot\nu]\,\nu\,]\!]_{\Gamma^i}\,\mathrm{d}\Gamma^i\\
&=\sum_{w\in\{x,y,z\}}\int_{\Gamma^i} [\![\,[\bar{\mathsf{v}}\cdot\nu]\nu_w\,k^{-2}\,\Big[\nu\times[\nabla\times u]\Big]\cdot[\nabla\chi_w]_t\,]\!]_{\Gamma^i}\,\mathrm{d}\Gamma^i\\
&=\int_{\Gamma^i} [\![\,k^{-2}\,\Big[\nu\times[\nabla\times u]\Big]\cdot[\nabla(\nu\cdot\chi)]\;\;[\nu\cdot\bar{\mathsf{v}}]\,]\!]_{\Gamma^i}\,\mathrm{d}\Gamma^i. \qquad (73)
\end{aligned}
$$

For the magnetic field solution $\bar{\mathsf{v}}$, the substitution (5) and the splitting $\mathsf{v}_{el} = [\mathsf{v}_{el}]_t + [\mathsf{v}_{el} \cdot \nu]\nu$ yield

$$\begin{aligned}\nu \cdot \mathsf{v} &= \frac{-\mathbf{i}}{\mu\omega}\left\{\nu \cdot \Big[\nabla \times [\mathsf{v}_{el}]_t\Big] + \nu \cdot \Big[\nabla \times \{[\mathsf{v}_{el} \cdot \nu]\nu\}\Big]\right\}\\ &= \frac{-\mathbf{i}}{\mu\omega}\left\{[\nu \times \nabla] \cdot [\mathsf{v}_{el}]_t + \nu \cdot \Big[\nabla[\mathsf{v}_{el} \cdot \nu] \times \nu + [\mathsf{v}_{el} \cdot \nu]\ \nabla \times \nu\Big]\right\}\\ &= \frac{-\mathbf{i}}{\mu\omega}[\nu \times \nabla] \cdot [\mathsf{v}_{el}]_t,\end{aligned}$$

since $\nabla \times \nu = 0$. Now $[\nu \times \nabla]\cdot$ is a tangential derivative, where only the sign depends on the side of the interface. The tangential derivative of the function $[\mathsf{v}_{el}]_t$ is continuous and the jump of $\nu \cdot \mathsf{v}$ over the interface vanishes. Consequently, the interface integral (73) is zero.

Substituting the solution of the magnetic equation in (72) by that of the electric equation (cf. (5)), i.e., substituting $u = u_{ma} = -\mathbf{i}/\mu\omega\ [\nabla \times u_{el}]$ and $[\nabla \times u] = -\mathbf{i}k^2/\mu\omega\ u_{el}$ as well as $\mathsf{v} = \mathsf{v}_{ma} = -\mathbf{i}/\mu\omega\ [\nabla \times \mathsf{v}_{el}]$ and $[\nabla \times \mathsf{v}] = -\mathbf{i}k^2/\mu\omega\ \mathsf{v}_{el}$, the formula (60) follows.

4.7 Asymptotic expansion of solution

Suppose u_h, u_h^+, and u_h^- are the magnetic field solutions of the system

$$a_h\Big((u_h, u_h^+, u_h^-), (\mathsf{v}_h, \mathsf{v}^+, \mathsf{v}^-)\Big) = f_h\Big((\mathsf{v}_h, \mathsf{v}^+, \mathsf{v}^-)\Big) := -a\Big((0, U^{\mathrm{inc}}, 0), (\mathsf{v}_h, \mathsf{v}^+, \mathsf{v}^-)\Big).$$

Since $\nabla \cdot u_h = 0$ for a constant μ, the term $\int_G \nabla \cdot u_h \overline{\nabla \cdot v_h}\ \mathrm{d}G$ can be added to the variational equation leading to a strongly elliptic sesqui-linear form. In other words $u_h \in [H^1]^3$ over the subdomains with constant ε. However, $[H^1]^3$ is invariant under the action of Ψ_h. The classical theory of asymptotics yields (compare the two-dimensional case treated in [11])

$$\begin{aligned}\Psi_h^{-1} u_h &= u_0 + h u_1 + \mathcal{O}(h^2),\\ u_h^+ &= u_0^+ + h u_1^+ + \mathcal{O}(h^2),\\ u_h^- &= u_0^- + h u_1^- + \mathcal{O}(h^2).\end{aligned} \qquad (74)$$

Of course, the derivation requires the unique solvability of the boundary value problem (3), (14)-(17), (19), (21), and (23).

The field derivatives u_1, u_1^+, and u_1^- can be characterized as the solution of a variational equation (cf. the subsequent variational equation (75)). Indeed, substituting (74) into the variational form over the transformed domain, the equation changes to

$$\begin{aligned}a_h\Big((\Psi_h[u_0 + h u_1 + \mathcal{O}(h^2)], [u_0^+ + h u_1^+ + \mathcal{O}(h^2)], [u^- + h u_1^- + \mathcal{O}(h^2)]), (\Psi_h \mathsf{v}, \mathsf{v}^+, \mathsf{v}^-)\Big)\\ = f_h\Big((\Psi_h \mathsf{v}, \mathsf{v}^+, \mathsf{v}^-)\Big) = f\Big((\mathsf{v}, \mathsf{v}^+, \mathsf{v}^-)\Big).\end{aligned}$$

From (70), there follows

$$a_h\Big((\Psi_h[u_0 + h u_1 + \mathcal{O}(h^2)], [u_0^+ + h u_1^+ + \mathcal{O}(h^2)], [u_0^- + h u_1^- + \mathcal{O}(h^2)]), (\Psi_h \mathsf{v}, \mathsf{v}^+, \mathsf{v}^-)\Big)$$

$$
\begin{aligned}
&= a\Big(([u_0+hu_1+\mathcal{O}(h^2)],[u_0^+ +hu_1^+ +\mathcal{O}(h^2)],[u_0^- +hu_1^- +\mathcal{O}(h^2)]),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big)\\
&\quad +ha_1\Big([u_0+hu_1+\mathcal{O}(h^2)],\mathsf{v}\Big)+\mathcal{O}(h^2)\\
&= a\Big((u_0,u_0^+,u_0^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big)+ha\Big((u_1,u_1^+,u_1^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big)\\
&\quad +ha_1(u_0,\mathsf{v})+\mathcal{O}(h^2)\\
&= f\Big(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-\Big)+ha\Big((u_1,u_1^+,u_1^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big)+ha_1(u_0,\mathsf{v})+\mathcal{O}(h^2).
\end{aligned}
$$

Here, a_1 is the form (72) depending on the magnetic field solutions. In view of the last two formulas, the derivatives u_1, u_1^+, and u_1^- of (74) are the solution of the equation

$$
a\Big((u_1,u_1^+,u_1^-),(\mathsf{v},\mathsf{v}^+,\mathsf{v}^-)\Big)=-a_1(u_0,\mathsf{v}). \tag{75}
$$

Note that this characterization of the material derivative u_1 cannot be converted directly into an equation for the electric fields. In fact, the test functionals v are not the solutions of Maxwell's equation and do not necessarily satisfy (4) and (5). For the final formula, the general test function v will be replaced by the adjoint solution of the Maxwell's equations, and the conversion will be done in Section 4.9.

4.8 Derivative of objective functional

In order to define the adjoint solution, a formula for the derivative of the objective functional (57) is needed. The first step to get such a formula is to derive an expression for the derivative of the Rayleigh coefficient $B_{n,m,l}^+$ of the magnetic field u_h with respect to h.

Again the magnetic field functions are considered. Suppose $u_{n',m',l'}^+$ is propagating into the upper half space ($c_{n',m'}>0$). Then

$$
\begin{aligned}
&\frac{1}{\mu\omega}\nu\times\left[\begin{pmatrix}a_n\\b_m\\c_{n,m}\end{pmatrix}\times\begin{pmatrix}e_{n,m,l}\\f_{n,m,l}\\g_{n,m,l}\end{pmatrix}\right]\cdot\overline{\frac{1}{\mu\omega}\nu\times\left[\begin{pmatrix}a_n\\b_m\\c_{n,m}\end{pmatrix}\times\begin{pmatrix}e_{n,m,l'}\\f_{n,m,l'}\\g_{n,m,l'}\end{pmatrix}\right]}\\
&\quad=\frac{1}{\mu^2\omega^2}\left[\nu\cdot\begin{pmatrix}e_{n,m,l}\\f_{n,m,l}\\g_{n,m,l}\end{pmatrix}\begin{pmatrix}a_n\\b_m\\c_{n,m}\end{pmatrix}-\nu\cdot\begin{pmatrix}a_n\\b_m\\c_{n,m}\end{pmatrix}\begin{pmatrix}e_{n,m,l}\\f_{n,m,l}\\g_{n,m,l}\end{pmatrix}\right]\cdot\\
&\qquad\overline{\left[\nu\cdot\begin{pmatrix}e_{n,m,l'}\\f_{n,m,l'}\\g_{n,m,l'}\end{pmatrix}\begin{pmatrix}a_n\\b_m\\c_{n,m}\end{pmatrix}-\nu\cdot\begin{pmatrix}a_n\\b_m\\c_{n,m}\end{pmatrix}\begin{pmatrix}e_{n,m,l'}\\f_{n,m,l'}\\g_{n,m,l'}\end{pmatrix}\right]}\\
&\quad=\frac{1}{\mu^2\omega^2}\left[g_{n,m,l}\begin{pmatrix}a_n\\b_m\\c_{n,m}\end{pmatrix}-c_{n,m}\begin{pmatrix}e_{n,m,l}\\f_{n,m,l}\\g_{n,m,l}\end{pmatrix}\right]\cdot\\
&\qquad\overline{\left[g_{n,m,l'}\begin{pmatrix}a_n\\b_m\\c_{n,m}\end{pmatrix}-c_{n,m}\begin{pmatrix}e_{n,m,l'}\\f_{n,m,l'}\\g_{n,m,l'}\end{pmatrix}\right]}
\end{aligned}
$$

$$= \frac{1}{\mu^2\omega^2}\Big[g_{n,m,l}\,\overline{g_{n,m,l'}}\,k^2 + |c_{n,m}|^2\delta_{l,l'}\Big] = \frac{\delta_{l,l'}}{\mu^2\omega^2}\Big[\delta_{l',1}\,[a_n^2+b_m^2] + c_{n,m}^2\Big].$$

Consequently,

$$\begin{aligned}\int_{\Gamma^+}[\nu\times u^+_{n,m,l}]\cdot[\nu\times\overline{u}^+_{n',m',l'}]\,\mathrm{d}\partial G^+ &= \delta_{n,n'}\delta_{m,m'}\delta_{l,l'}\;\kappa_{n',m',l'}\;,\\ \kappa_{n',m',l'} &:= \frac{1}{\mu^2\omega^2}\Big[\delta_{l',1}\,[a_{n'}^2+b_{m'}^2]+c_{n',m'}^2\Big]\;\mathrm{per}_x\mathrm{per}_y.\end{aligned}$$

For a mode $u^+_{n,m,l}$ in (57) with $(n,m,l)\in I$, the relation $c_{n,m}>0$ is assumed. Hence $u^+_{n,m,l}$ is propagating into the upper half space. The boundary value $u=u^++u^{\mathrm{inc}}$ on Γ^+ satisfies

$$\begin{aligned}\int_{\Gamma^+}[\nu\times u]\cdot[\nu\times\overline{u}^+_{n,m,l}]\,\mathrm{d}\Gamma^+ &= \Big\{B^+_{n,m.l}+\delta_{n,0}\delta_{m,0}\,\kappa_l^{\mathrm{inc}}\Big\}\;\kappa_{n,m,l},\\ \kappa_l^{\mathrm{inc}} &:= \frac{1}{\mu^2\omega^2}\,\frac{\mathrm{per}_x\mathrm{per}_y}{\kappa_{0,0,l}}\Big[\delta_{l,1}g_c^{\mathrm{inc}}\,\overline{g}_{0,0,1}\,\big[a_0^2+b_0^2-c_{0,0}^2\big]\\ &\qquad -c_{0,0}^2\,\big[e_c^{\mathrm{inc}}\overline{e}_{0,0,l}+f_c^{\mathrm{inc}}\overline{f}_{0,0,l}+g_c^{\mathrm{inc}}\overline{g}_{0,0,l}\big]\\ &\qquad -g_c^{\mathrm{inc}}c_{0,0}\,\big[a_0\overline{e}_{0,0,l}+b_0\overline{f}_{0,0,l}-c_{0,0}\overline{g}_{0,0,l}\big]\\ &\qquad +c_{0,0}\overline{g}_{0,0,l}\,\big[e_c^{\mathrm{inc}}a_0+f_c^{\mathrm{inc}}b_0+g_c^{\mathrm{inc}}c_{0,0}\big]\Big],\\ B^+_{n,m.l} &= \frac{1}{\kappa_{n,m,l}}\int_{\Gamma^+}[\nu\times u]\cdot[\nu\times\overline{u}^+_{n,m,l}]\,\mathrm{d}\Gamma^+ - \delta_{n,0}\delta_{m,0}\,\kappa_l^{\mathrm{inc}}.\end{aligned}$$

In other words, $B^+_{n,m.l}(u)$ is an affine function of the magnetic solution u. Hence, the derivative of $B^+_{n,m.l}(u_h)$ with respect to h is

$$\partial_h[B^+_{n,m.l}(u_h)]|_{h=0} = \frac{1}{\kappa_{n,m,l}}\int_{\Gamma^+}[\nu\times u_1]\cdot[\nu\times\overline{u}^+_{n,m,l}]\,\mathrm{d}\Gamma^+,$$

where the function u_1 (cf. the asymptotic expansion (74)) is the derivative of the field solution u_h with respect to parameter h.

For the derivative of the objective functional (57) depending on $u=u_{ma}$, the last formula implies

$$\begin{aligned}\partial_h[\mathcal{F}(u_h)]|_{h=0} &:= \sum_{n,m,l} w_{n,m,l}2\left[\frac{100\,c_{n,m}}{c_{0,0}}|B^+_{n,m,l}(u_0)|^2-d_{n,m,l}\right]\frac{100\,c_{n,m}}{c_{0,0}}\\ &\qquad *2\Re\mathrm{e}\left[\overline{B^+_{n,m,l}(u_0)}\frac{1}{\kappa_{n,m,l}}\int_{\Gamma^+}[\nu\times u_1]\cdot[\nu\times\overline{u}^+_{n,m,l}]\,\mathrm{d}\Gamma^+\right]\\ &= \Re\mathrm{e}\int_{\Gamma^+}[\nu\times u_1]\cdot\Bigg\{4\sum_{n,m,l}w_{n,m,l}\left[\frac{100\,c_{n,m}}{c_{0,0}}|B^+_{n,m,l}(u_0)|^2-d_{n,m,l}\right]\\ &\qquad *\frac{100\,c_{n,m}}{c_{0,0}}\overline{B^+_{n,m,l}(u_0)}\frac{1}{\kappa_{n,m,l}}[\nu\times\overline{u}^+_{n,m,l}]\Bigg\}\,\mathrm{d}\Gamma^+.\end{aligned}$$

Hence, there holds $\partial_h[\mathcal{F}(u_h)]|_{h=0} = \Re\mathrm{e}\, \widetilde{\mathcal{F}}(u_1)$ with

$$\begin{aligned}\widetilde{\mathcal{F}}(u) &:= \mu^2\omega^2 \int_{\Gamma^+} k^{-2}\, [\nu \times u] \cdot \overline{\varphi}_t \, \mathrm{d}\Gamma^+, \\ \varphi_t &:= \frac{4k^2}{\mu^2\omega^2} \sum_{n,m,l} \frac{w_{n,m,l}}{\kappa_{n,m,l}} \left[\frac{100\, c_{n,m}}{c_{0,0}} |B^+_{n,m,l}(u_0)|^2 - d_{n,m,l} \right] \\ &\qquad * \frac{100\, c_{n,m}}{c_{0,0}} B^+_{n,m,l}(u_0)[\nu \times u^+_{ma,n,m,l}].\end{aligned} \tag{76}$$

Furthermore, if $u_{ma,ad}$, $u^{\pm}_{ma,ad}$, $u^{\mathrm{inc}}_{ma,ad}$ is the adjoint solution defined by the variational equation

$$a_{ma}\Big((u, u^+, u^-), (u_{ma,ad}, u^+_{ma,ad}, u^-_{ma,ad})\Big) \;=\; \widetilde{\mathcal{F}}(u) \tag{77}$$

with test functions u, u^+, and u^-, then (75) implies

$$\begin{aligned}\partial_h[\mathcal{F}(u_h)]|_{h=0} &= \Re\mathrm{e}\, a_{ma}\Big((u_1, u_1^+, u_1^-), (u_{ma,ad}, u^+_{ma,ad}, u^-_{ma,ad})\Big) \\ &= -\Re\mathrm{e}\, a_1(u_0, u_{ma,ad}),\end{aligned}$$

with a_1 defined in (72).

4.9 Adjoint electric-field solution

Recall from Section 4.6 that the form (60) is just the form (72) after substituting the magnetic $u = u_{ma}$ and $v = v_{ma}$ by the electric u_{el} and v_{el} using (5). Hence, to finish the proof of Theorem 4.1, it suffices to show that the adjoint solutions $u_{ma,ad}$ of (77) and $u_{el,ad}$ of (61) are connected by (5).

Now choose the test functions $u^{\pm} = 0$ and u with a support disjoint to the boundaries $\Gamma^{\pm}$ and the interfaces between the subdomains defined by different values of ε. Then, the Green's formula over the subdomain G' with zero boundary values

$$\mu^2\omega^2 \int_{G'} k^{-2}\, [\nabla \times u] \cdot [\nabla \times \overline{u_{ma,ad}}] \;=\; \mu^2\omega^2 \int_{G'} u \cdot \Big[\nabla \times [k^{-2}\, \nabla \times \overline{u_{ma,ad}}] \Big],$$

and the variational equation (77) yield that $\mu^2\omega^2 \int_{G'} u \cdot \{\nabla \times [k^{-2} \nabla \times \overline{u_{ma,ad}}] - \overline{u_{ma,ad}}\} \mathrm{d}G' = 0$, i.e., that $u_{ma,ad}$ satisfies (3) over each domain G' with constant ε. The transmission condition $\nu \times [\![u_{ma,ad}]\!]_\Gamma = 0$ (cf. the first condition in (19)) holds since the variational solution $u_{ma,ad}$ is in $H(\mathrm{curl}, G)$. Choosing the test function u non-zero also over a single fixed interface S, substituting (3), and using the Green's formula

$$\begin{aligned}\mu^2\omega^2 \int_S k^{-2}\, [\nu \times u] \cdot [\nabla \times \overline{u_{ma,ad}}] &= \mu^2\omega^2 \int_{G'} k^{-2}\, [\nabla \times u] \cdot [\nabla \times \overline{u_{ma,ad}}] \\ &\quad - \mu^2\omega^2 \int_{G'} u \cdot \Big[\nabla \times [k^{-2}\, \nabla \times \overline{u_{ma,ad}}] \Big]\end{aligned} \tag{78}$$

over the two subdomains $G' \subseteq G$ adjacent to S, the variational equation (77) implies that $-\mu^2\omega^2 \int_S [\![u \cdot \{\nu \times [k^{-2}\nabla \times \overline{u_{ma,ad}}]\}]\!]_S \mathrm{d}S = 0$, i.e., that $\nu \times [\![k^{-2}\nabla \times u_{ma,ad}]\!]_S = 0$ which is the second transmission condition in (19). In other words, the transmission condition (19) is satisfied.

Substituting (78), (3), and (19) into (77), the variational equation turns into

$$\begin{aligned}
&\mu^2\omega^2 \int_{\Gamma^+} k^{-2}\, [\nu \times u] \cdot \overline{\varphi}_t \,\mathrm{d}\Gamma^+ \qquad (79)\\
&= \mu^2\omega^2 \int_{\Gamma^+} k^{-2}\, \nu \times u \cdot \overline{\nabla \times u_{ma,ad}} \,\mathrm{d}\Gamma^+ \\
&\quad + \mu^2\omega^2 \int_{\Gamma^-} k^{-2}\, \nu \times u \cdot \overline{\nabla \times u_{ma,ad}} \,\mathrm{d}\Gamma^- \\
&\quad -\mu^2\omega^2 \int_{\Gamma^+} k^{-2}\, \nabla \times u^+ \cdot [\nu \times \overline{u_{ma,ad}}] \,\mathrm{d}\Gamma^+ \\
&\quad -\mu^2\omega^2 \int_{\Gamma^+} k^{-2} \left\{\nu \times u - \nu \times u^+\right\} \cdot \nabla \times \overline{u^+_{ma,ad}} \,\mathrm{d}\Gamma^+ \\
&\quad +\eta\, \mu^2\omega^2 \int_{\Gamma^+} k^{-2} \left\{\nu \times u - \nu \times u^+\right\} \cdot \left\{\nu \times \overline{\left[u_{ma,ad} - u^+_{ma,ad}\right]}\right\} \mathrm{d}\Gamma^+ \\
&\quad -\mu^2\omega^2 \int_{\Gamma^-} k^{-2}\, \nabla \times u^- \cdot [\nu \times \overline{u_{ma,ad}}] \,\mathrm{d}\Gamma^- \\
&\quad -\mu^2\omega^2 \int_{\Gamma^-} k^{-2} \left\{\nu \times u - \nu \times u^-\right\} \cdot \nabla \times \overline{u^-_{ma,ad}} \,\mathrm{d}\Gamma^- \\
&\quad +\eta\, \mu^2\omega^2 \int_{\Gamma^-} k^{-2} \left\{\nu \times u - \nu \times u^-\right\} \cdot \left\{\nu \times \overline{\left[u_{ma,ad} - u^-_{ma,ad}\right]}\right\} \mathrm{d}\Gamma^- .
\end{aligned}$$

To derive all the boundary conditions for the solution $u_{ma,ad}$ hidden in the variational equation, a technical definition is needed. At first, we define the tangential part of a vector field v by $[\mathrm{v}]_t := -\nu \times [\nu \times \mathrm{v}]$. If $c_{n,m} = 0$, then $\nu \times u^+_{el,n,m,1} = 0$ and $\nu \times [\nabla \times u^+_{el,n,m,0}] = 0$. Similarly, $\nu \times u^+_{ma,n,m,0} = 0$ and $\nu \times [\nabla \times u^+_{ma,n,m,1}] = 0$. For a general expansion of a quasi-periodic tangential vector function F_t over $\Gamma^\pm$

$$\begin{aligned}
F_t &= \sum_{n,m,l:\, c_{n,m}\neq 0 \text{ or } l=1} C^{F_t,ma}_{n,m,l} [\nu \times u^\pm_{ma,n,m,l}] + \sum_{n,m:\, c_{n,m}=0} C^{F_t,ma}_{n,m,0}\, [u^\pm_{ma,n,m,1}]_t \\
&= \sum_{n,m,l:\, c_{n,m}\neq 0 \text{ or } l=0} C^{F_t,el}_{n,m,l} [\nu \times u^\pm_{el,n,m,l}] + \sum_{n,m:\, c_{n,m}=0} C^{F_t,el}_{n,m,1}\, [u^\pm_{el,n,m,0}]_t, \qquad (80)
\end{aligned}$$

the projections $P^{ma}_{\Gamma^\pm}$ and $P^{el}_{\Gamma^\pm}$ are introduced by

$$\begin{aligned}
P^{ma}_{\Gamma^\pm} F_t &:= \sum_{n,m,l:\, c_{n,m}\neq 0 \text{ or } l=1} C^{F_t,ma}_{n,m,l} [\nu \times u^\pm_{ma,n,m,l}], \\
P^{el}_{\Gamma^\pm} F_t &:= \sum_{n,m,l:\, c_{n,m}\neq 0 \text{ or } l=0} C^{F_t,el}_{n,m,l} [\nu \times u^\pm_{el,n,m,l}].
\end{aligned}$$

Clearly, there holds $P^{ma}_{\Gamma^\pm}[\nu \times u^\pm_{ma}] = [\nu \times u^\pm_{ma}]$ and $P^{el}_{\Gamma^\pm}[\nu \times u^\pm_{el}] = [\nu \times u^\pm_{el}]$. Introducing the operators $\Pi^{ma}_{\Gamma^\pm} F := -\nu \times P^{ma}_{\Gamma^\pm}(\nu \times F)$ and $\Pi^{el}_{\Gamma^\pm} F := -\nu \times P^{el}_{\Gamma^\pm}(\nu \times F)$, we get

$P^{ma}_{\Gamma^\pm}(\nu \times F) = \nu \times \Pi^{ma}_{\Gamma^\pm} F$ and $P^{el}_{\Gamma^\pm}(\nu \times F) = \nu \times \Pi^{el}_{\Gamma^\pm} F$. Note that the restrictions of $\Pi^{ma}_{\Gamma^\pm}$ and $\Pi^{el}_{\Gamma^\pm}$ to tangential fields are projections.

Now look at the third term on the right-hand side of (79). We would like to apply a partial integration similar to (55). Clearly, $\nu \times u_{ma,ad}|_{\Gamma^+}$ is a general quasi-periodic tangential vector field and can be split into $\nu \times \Pi^{ma}_{\Gamma^+}(u_{ma,ad}|_{\Gamma^+})$ and $(I - P^{ma}_{\Gamma^+})(\nu \times u_{ma,ad}|_{\Gamma^+})$. Since $\nu \times \Pi^{ma}_{\Gamma^+}(u_{ma,ad}|_{\Gamma^+})$ is in the span of the functions $\nu \times u^+_{ma,n,m,l}$, formula (55) implies

$$\begin{aligned}\int_{\Gamma^+} \nabla \times u^+ \cdot [\nu \times \overline{u_{ma,ad}}] \, \mathrm{d}\Gamma^+ \;=\; & \int_{\Gamma^+} \nu \times u^+ \cdot \Big[\nabla \times [\Pi^{ma}_{\Gamma^+}(u_{ma,ad}|_{\Gamma^+})]_{\mathbf{mo}}\Big] \, \mathrm{d}\Gamma^+ \\ & + \int_{\Gamma^+} \nabla \times u^+ \cdot (I - P^{ma}_{\Gamma^+})(\nu \times \overline{u_{ma,ad}}|_{\Gamma^+}) \, \mathrm{d}\Gamma^+\end{aligned}$$

However, $\nu \times [\nabla \times u^+_{ma,n,m,1}] = 0$ implies $\nabla \times \Pi^{ma}_{\Gamma^+} F_t = \nabla \times F_t$, and the projector in the first term on the right-hand side can be dropped. Furthermore, the image of $(I - P^{ma}_{\Gamma^+})$ is spanned by the $u^+_{ma,n,m,1}$ with $c_{n,m} = 0$. In view of $\nu \times [\nabla \times u^+_{ma,n,m,1}] = 0$ and due to the orthogonality of the $\nu \times u^+_{n,m,l}$ to $u^+_{n',m',l'}$ for (n, m) different from (n', m'), we can replace u^+ in the second term on the right-hand side by $Q^{ma}_{\Gamma^+} u^+$. We get

$$\begin{aligned}\int_{\Gamma^+} \nabla \times u^+ \cdot [\nu \times \overline{u_{ma,ad}}] \, \mathrm{d}\Gamma^+ \;=\; & \int_{\Gamma^+} \nu \times u^+ \cdot \Big[\nabla_+ \times [\overline{u_{ma,ad}}|_{\Gamma^+}]_{\mathbf{mo}}\Big] \, \mathrm{d}\Gamma^+ + \\ & \int_{\Gamma^+} \nabla \times Q^{ma}_{\Gamma^+} u^+ \cdot (I - P^{ma}_{\Gamma^+})(\nu \times \overline{u_{ma,ad}}|_{\Gamma^+}) \, \mathrm{d}\Gamma^+\end{aligned}$$

Note that $[\overline{u_{ma,ad}}|_{\Gamma^+}]_{\mathbf{mo}}$ stands for the following. Firstly, the tangential trace $[\overline{u_{ma,ad}}|_{\Gamma^+}]_t$ is represented as a quasi-periodic Fourier series expansion with respect to the basis functions $[u^+_{n,m,l}]_t$ for all $n, m \in \mathbb{Z}$ such that $c_{n,m} \neq 0$ or $l = 0$ together with the basis functions $\nu \times u^+_{n,m,1}$ for all $n, m \in \mathbb{Z}$ such that $c_{n,m} = 0$. Secondly, the modification operator (54) is applied to this representation. All the terms with functions corresponding to $c_{n,m} = 0$ are deleted. By $\nabla_+ \times [\overline{u_{ma,ad}}|_{\Gamma^+}]_{\mathbf{mo}}$ we denote the curl operator applied to the modified function, i.e., to the wave expansion in the upper half plane. A similar formula with an analogous notation holds over Γ^-.

Now substituting the last equation and the analogous formula for Γ^- into (79), the variational equation turns into

$$\begin{aligned}\mu^2\omega^2 & \int_{\Gamma^+} k^{-2} \, [\nu \times u] \cdot \overline{\varphi}_t \, \mathrm{d}\Gamma^+ \qquad (81) \\ = \;& \mu^2\omega^2 \int_{\Gamma^+} k^{-2} \, \nu \times u \cdot \overline{\nabla \times u_{ma,ad}} \, \mathrm{d}\Gamma^+ \\ & -\mu^2\omega^2 \int_{\Gamma^+} k^{-2} \, \nu \times u^+ \cdot \Big[\nabla_+ \times [\overline{u_{ma,ad}}|_{\Gamma^+}]_{\mathbf{mo}}\Big] \, \mathrm{d}\Gamma^+ \\ & -\mu^2\omega^2 \int_{\Gamma^+} k^{-2} \, \nabla \times Q^{ma}_{\Gamma^+} u^+ \cdot (I - P^{ma}_{\Gamma^+})(\nu \times \overline{u_{ma,ad}}|_{\Gamma^+}) \, \mathrm{d}\Gamma^+ \\ & -\mu^2\omega^2 \int_{\Gamma^+} k^{-2} \left\{\nu \times u - \nu \times u^+\right\} \cdot \nabla \times \overline{u^+_{ma,ad}} \, \mathrm{d}\Gamma^+ \\ & +\eta \, \mu^2\omega^2 \int_{\Gamma^+} k^{-2} \left\{\nu \times u - \nu \times u^+\right\} \cdot \left\{\nu \times \overline{\left[u_{ma,ad} - u^+_{ma,ad}\right]}\right\} \mathrm{d}\Gamma^+\end{aligned}$$

$$
\begin{aligned}
&+\mu^2\omega^2 \int_{\Gamma^-} k^{-2}\, \nu\times u \cdot \overline{\nabla\times u_{ma,ad}}\, \mathrm{d}\Gamma^- \\
&-\mu^2\omega^2 \int_{\Gamma^-} k^{-2}\, \nu\times u^- \cdot \Big[\nabla_-\times[\overline{u_{ma,ad}}|_{\Gamma^-}]_{\mathbf{mo}}\Big]\, \mathrm{d}\Gamma^- \\
&-\mu^2\omega^2 \int_{\Gamma^-} k^{-2}\, \nabla\times Q^{ma}_{\Gamma^-}u^- \cdot (I-P^{ma}_{\Gamma^-})(\nu\times\overline{u_{ma,ad}}|_{\Gamma^-})\, \mathrm{d}\Gamma^- \\
&-\mu^2\omega^2 \int_{\Gamma^-} k^{-2}\, \big\{\nu\times u-\nu\times u^-\big\}\cdot\nabla\times\overline{u^-_{ma,ad}}\, \mathrm{d}\Gamma^- \\
&+\eta\, \mu^2\omega^2 \int_{\Gamma^-} k^{-2}\, \big\{\nu\times u-\nu\times u^-\big\}\cdot\Big\{\nu\times\overline{\big[u_{ma,ad}-u^-_{ma,ad}\big]}\Big\}\, \mathrm{d}\Gamma^- \,.
\end{aligned}
$$

Now consider the variational equation (81) and choose the magnetic test functions according to the following six cases:

- choose an arbitrary u with $[\nu\times u]|_{\Gamma^-}=0$ as well as $u^\pm=0$
- choose an arbitrary u^+ with $Q^+_{\Gamma^+}u^+=0$ and $u^-=0$ as well as $u=0$
- choose $u^+=Q^+_{\Gamma^+}u^+$ and $u=0$ as well as $u^-=0$
- choose an arbitrary u with $[\nu\times u]|_{\Gamma^+}=0$ as well as $u^\pm=0$
- choose an arbitrary u^- with $Q^-_{\Gamma^-}u^-=0$ and $u^+=0$ as well as $u=0$
- choose $u^-=Q^-_{\Gamma^-}u^-$ and $u=0$ as well as $u^+=0$

The following six relations can be derived.

$$
\begin{aligned}
\varphi_t &= [\nabla\times u_{ma,ad}]_t-[\nabla\times u^+_{ma,ad}]_t+\eta\,\big[\nu\times\{u_{ma,ad}-u^+_{ma,ad}\}\big]_t && \text{on }\Gamma^+,\\
0 &= -\Big[\nabla_+\times[u_{ma,ad}|_{\Gamma^+}]_{\mathbf{mo}}\Big]_t+P^{ma}_{\Gamma^+}[\nabla\times u^+_{ma,ad}]_t \\
&\quad -\eta P^{ma}_{\Gamma^+}\big[\nu\times\{u_{ma,ad}-u^+_{ma,ad}\}\big]_t && \text{on }\Gamma^+,\\
0 &= (I-P^{ma}_{\Gamma^+})\Big[[\nu\times u_{ma,ad}]|_{\Gamma^+}\Big] && \text{on }\Gamma^+,\\
0 &= [\nabla\times u_{ma,ad}]_t-[\nabla\times u^-_{ma,ad}]_t+\eta\,\big[\nu\times\{u_{ma,ad}-u^-_{ma,ad}\}\big]_t && \text{on }\Gamma^-,\\
0 &= -\Big[\nabla_-\times[u_{ma,ad}|_{\Gamma^-}]_{\mathbf{mo}}\Big]_t+P^{ma}_{\Gamma^-}[\nabla\times u^-_{ma,ad}]_t \\
&\quad -\eta P^{ma}_{\Gamma^-}\big[\nu\times\{u_{ma,ad}-u^-_{ma,ad}\}\big]_t && \text{on }\Gamma^-,\\
0 &= (I-P^{ma}_{\Gamma^-})\Big[[\nu\times u_{ma,ad}]|_{\Gamma^-}\Big] && \text{on }\Gamma^-.
\end{aligned}
\tag{82}
$$

In other words, applying $P^{ma}_{\Gamma^\pm}$ to the first and fourth equation, adding the resulting first to the second, and adding the resulting fourth to the fifth, we get the boundary conditions

$$
\begin{aligned}
\varphi_t &= \Big[(\nabla\times u_{ma,ad})|_{\Gamma^+}\Big]_t-\sum_{n,m:\,c_{n,m}=0}\frac{\int_{\Gamma^+}[\nabla\times u_{ma,ad}]\cdot[\overline{u}^+_{ma,n,m,1}]_t\,\mathrm{d}\Gamma^+}{\int_{\Gamma^+}\|[u^+_{ma,n,m,1}]_t\|^2\,\mathrm{d}\Gamma^+}\,[u^+_{ma,n,m,1}]_t \\
&\quad -\Big[\nabla_+\times[u_{ma,ad}|_{\Gamma^+}]_{\mathbf{mo}}\Big]_t \qquad \text{on }\Gamma^+,\\
0 &= \Big[(\nabla\times u_{ma,ad})|_{\Gamma^-}\Big]_t-\sum_{n,m:\,c_{n,m}=0}\frac{\int_{\Gamma^-}[\nabla\times u_{ma,ad}]\cdot[\overline{u}^-_{ma,n,m,1}]_t\,\mathrm{d}\Gamma^-}{\int_{\Gamma^-}\|[u^-_{ma,n,m,1}]_t\|^2\,\mathrm{d}\Gamma^-}\,[u^+_{n,m,1}]_t
\end{aligned}
$$

$$
\begin{aligned}
&\quad -\Big[\nabla_- \times [u_{ma,ad}|_{\Gamma^-}]_{\mathbf{mo}}\Big]_t && \text{on } \Gamma^-, && (83)\\
0 &= \int_{\Gamma^-} [\nu \times u_{ma,ad}|_{\Gamma^+}] \cdot \overline{u}^+_{ma,n,m,1} \, \mathrm{d}\Gamma^+ && \forall (n,m) \text{ s.t. } c_{n,m}=0,\\
0 &= \int_{\Gamma^-} [\nu \times u_{ma,ad}|_{\Gamma^-}] \cdot \overline{u}^-_{ma,n,m,1} \, \mathrm{d}\Gamma^- && \forall (n,m) \text{ s.t. } c_{n,m}=0.
\end{aligned}
$$

Now, switching to the electric field $u_{el,ad} = \frac{\mathbf{i}\mu\omega}{k^2}\nabla \times u_{ma,ad}$ (cf. (4)) and taking into account that $u^{\pm}_{ma,n,m,1}$ is proportional to $u^{\pm}_{el,n,m,0}$, the adjoint solution $u_{el,ad}$ is the solution of (2), (18) together with the boundary conditions

$$
\begin{aligned}
\frac{\mathbf{i}\mu\omega}{k^2}\varphi_t &= \left[u_{el,ad}|_{\Gamma^+} - \sum_{n,m:\, c_{n,m}=0} \frac{\int_{\Gamma^+} [u_{el,ad}]_t \cdot [\overline{u}^+_{el,n,m,0}]_t \, \mathrm{d}\Gamma^+}{\int_{\Gamma^+} \|[u^+_{el,n,m,0}]_t\|^2 \, \mathrm{d}\Gamma^+} [u^+_{el,n,m,0}]_t \right]_t\\
&\quad - k^{-2}\Big[\nabla_+ \times [(\nabla \times u_{el,ad})|_{\Gamma^+}]_{\mathbf{mo}}\Big]_t \qquad \text{on } \Gamma^+,\\
0 &= \left[u_{el,ad}|_{\Gamma^-} - \sum_{n,m:\, c_{n,m}=0} \frac{\int_{\Gamma^-} [u_{el,ad}]_t \cdot [\overline{u}^-_{el,n,m,0}]_t \, \mathrm{d}\Gamma^-}{\int_{\Gamma^-} \|[u^-_{el,n,m,0}]_t\|^2 \, \mathrm{d}\Gamma^-} [u^+_{el,n,m,0}]_t \right]_t\\
&\quad - k^{-2}\Big[\nabla_- \times [(\nabla \times u_{el,ad})|_{\Gamma^-}]_{\mathbf{mo}}\Big]_t \qquad \text{on } \Gamma^-, \qquad (84)\\
0 &= \int_{\Gamma^+} \Big[\nu \times [\nabla \times u_{el,ad}]|_{\Gamma^+}\Big] \cdot \overline{u}^+_{el,n,m,0} \, \mathrm{d}\Gamma^+ \qquad \forall (n,m) \text{ s.t. } c_{n,m}=0,\\
0 &= \int_{\Gamma^-} \Big[\nu \times [\nabla \times u_{el,ad}]|_{\Gamma^-}\Big] \cdot \overline{u}^-_{el,n,m,0} \, \mathrm{d}\Gamma^- \qquad \forall (n,m) \text{ s.t. } c_{n,m}=0.
\end{aligned}
$$

Obviously, there is a Dirichlet-to-Neumann operator $u_t \mapsto [\nabla_+ \times u_t]_t := [(\nabla \times u)|_{\Gamma^+}]_t$, mapping the tangential traces u_t, orthogonal to the functions $[\nu \times u^+_{el,n,m,0}]$ with $c_{n,m} = 0$, to the tangential traces of the curl function $[(\nabla \times u)|_{\Gamma^+}]_t$ of the solution u to (2) over the half space above Γ^+ and to the boundary condition $[u|_{\Gamma^+}]_t = u_t$. Taking into account that $\nu \times [\nabla \times u^+_{el,n,m,l}] = 0$ if and only if $l = 0$ and $c_{n,m} = 0$, we get $[\nabla_+ \times u^+_{el,n,m,0}]_t = 0$ for $c_{n,m} = 0$ and the one-to-one correspondence of the Dirichlet-to-Neumann mapping for all tangential traces u_t orthogonal to the functions $[u^+_{el,n,m,0}]_t$ and $[\nu \times u^+_{el,n,m,0}]$ with $c_{n,m} = 0$. Consequently, the first of the boundary conditions (84) is equivalent to (cf. (54))

$$
\begin{aligned}
0 &= \int_{\Gamma^+} \Big[u_{el,ad}|_{\Gamma^+}\Big]_t \cdot [\nu \times \overline{u}^+_{el,n,m,0}] \, \mathrm{d}\Gamma^+ \quad \forall (n,m) \text{ s.t. } c_{n,m}=0,\\
\frac{\mathbf{i}\mu\omega}{k^2}\Big[\nabla_+ \times \varphi_t\Big]_t &= \left[\nabla_+ \times \left[u_{el,ad}|_{\Gamma^+} - \sum_{n,m:\, c_{n,m}=0} \frac{\int_{\Gamma^+} [u_{el,ad}]_t \cdot [\overline{u}^+_{el,n,m,0}]_t \, \mathrm{d}\Gamma^+}{\int_{\Gamma^+} \|[u^+_{el,n,m,0}]_t\|^2 \, \mathrm{d}\Gamma^+} u^+_{el,n,m,0} \right]_t \right]_t\\
&\quad - k^{-2}\Big[\nabla_+ \times \nabla_+ \times [(\nabla \times u_{el,ad})|_{\Gamma^+}]_{\mathbf{mo}}\Big]_t\\
&= \Big[\nabla_+ \times [u_{el,ad}|_{\Gamma^+}]_t\Big]_t - \Big[(\nabla \times u_{el,ad})|_{\Gamma^+}\Big]_{\mathbf{mo}} \quad \text{on } \Gamma^+ .
\end{aligned}
$$

In other words, applying the modification operator (54) to the left and right-hand sides of the last condition and using the notation $C^{[(\nabla \times u_{el,ad})|_{\Gamma^+}]_t}_{n,m,l}$ for the Fourier coefficients of the tangential field

$F_t = [(\nabla\times u_{el,ad})|_{\Gamma^+}]_t$ (cf. the Fourier series expansion in (80)), the last boundary condition is equivalent to

$$
\begin{aligned}
0 \;&=\; \int_{\Gamma^+} \Big[u_{el,ad}|_{\Gamma^+}\Big]_t \cdot [\nu\times\overline{u}^+_{el,n,m,0}]\,\mathrm{d}\Gamma^+ \quad \forall(n,m) \text{ s.t. } c_{n,m}=0,\\
\frac{\mathbf{i}\mu\omega}{k^2}[\nabla_+\times\varphi_t]_t &= -\Big[\frac{\mathbf{i}\mu\omega}{k^2}[\nabla_+\times\varphi_t]_t\Big]_{\mathbf{mo}}\\
&= \Big[(\nabla\times u_{el,ad})|_{\Gamma^+}\Big]_t - \\
&\quad \sum_{n,m:\, c_{n,m}=0}\Big\{C^{[(\nabla\times u_{el,ad})|_{\Gamma^+}]_t}_{n,m,0}[\nu\times u^+_{el,n,m,0}] + C^{[(\nabla\times u_{el,ad})|_{\Gamma^+}]_t}_{n,m,1}[u^+_{el,n,m,0}]_t\Big\}\\
&\quad -\Big[\nabla_+\times[u_{el,ad}|_{\Gamma^+}]_{\mathbf{mo}}\Big]_t \qquad\qquad \text{on } \Gamma^+.
\end{aligned}
\tag{85}
$$

We observe that the third relation of (84) is nothing else than $C^{[(\nabla\times u_{el,ad})|_{\Gamma^+}]_t}_{n,m,0} = 0$. Thus, if we drop the first term in the sum on the right hand-side of the second equation in (85), then this last equation in (85) includes the third relation of (84). This way, all the four boundary conditions (84) are equivalent to

$$
\begin{aligned}
\frac{\mathbf{i}\mu\omega}{k^2}[\nabla_+\times\varphi_t]_t \;&=\; \Big[(\nabla\times u_{el,ad})|_{\Gamma^+}\Big]_t - \sum_{n,m:\, c_{n,m}=0} C^{[(\nabla\times u_{el,ad})|_{\Gamma^+}]_t}_{n,m,1}[u^+_{el,n,m,0}]_t\\
&\quad -\Big[\nabla_+\times[u_{el,ad}|_{\Gamma^+}]_{\mathbf{mo}}\Big]_t \qquad\qquad \text{on } \Gamma^+,\\
0 \;&=\; \Big[(\nabla\times u_{el,ad})|_{\Gamma^-}\Big]_t - \sum_{n,m,l:\, c_{n,m}=0} C^{[(\nabla\times u_{el,ad})|_{\Gamma^-}]_t}_{n,m,1}[u^-_{el,n,m,0}]_t\\
&\quad -\Big[\nabla_-\times[u_{el,ad}|_{\Gamma^-}]_{\mathbf{mo}}\Big]_t \qquad\qquad \text{on } \Gamma^-,\\
0 \;&=\; \int_{\Gamma^+}\Big[\nu\times u_{el,ad}|_{\Gamma^+}\Big]\cdot\overline{u}^+_{el,n,m,0}\,\mathrm{d}\Gamma^+ \quad \forall(n,m) \text{ s.t. } c_{n,m}=0,\\
0 \;&=\; \int_{\Gamma^-}\Big[\nu\times u_{el,ad}|_{\Gamma^-}\Big]\cdot\overline{u}^-_{el,n,m,0}\,\mathrm{d}\Gamma^- \quad \forall(n,m) \text{ s.t. } c_{n,m}=0.
\end{aligned}
\tag{86}
$$

Now, similarly to the derivation of (83), it is easy to see that the adjoint solution $u_{el,ad}$ of (61) satisfies the equation (2) with the boundary conditions (86) provided that the function ψ_t of (62) is equal to $\mathbf{i}\mu\omega\; k^{-2}\;[\nabla_+\times\varphi_t]_t$.

Suppose the angle $\theta_{n,m}$ is defined as before Theorem 4.1. Then, from the definitions (25)–(32), it is easy to conclude that

$$
\nu\times u^+_{el,n,m,l} \;=\; \begin{cases} (-1)^l[\cos\theta_{n,m}]^{2l-1}[u^+_{el,n,m,1-l}]_t & \text{if } c_{n,m}\neq 0 \text{ or } l=1\\ -\begin{pmatrix} a_n/h_{n,m}\\ b_m/h_{n,m}\\ 0\end{pmatrix} e^{\mathbf{i}(a_n x+b_m y+c_{n.m}[z-z_{\max}])} & \text{else ,}\end{cases}
\tag{87}
$$

$$
\nabla\times u^+_{el,n,m,l} \;=\; (-1)^l\mathbf{i}\frac{[k^+]^{2l}}{\sqrt{a_n^2+b_m^2+|c_{n,m}|^2}^{2l-1}}\;u^+_{el,n,m,1-l}.
\tag{88}
$$

For $c_{n,m} > 0$, the relation $\sqrt{a_n^2 + b_m^2 + |c_{n,m}|^2} = k^+$ holds, and (87) and (88) imply

$$\begin{aligned}
\Big[\nabla_+ \times [\nu \times u^+_{el,n,m,l}]\Big]_t &= (-1)^l [\cos\theta_{n,m}]^{2l-1} \nabla_+ \times [u^+_{el,n,m,1-l}]_t \\
&= (-1)^l [\cos\theta_{n,m}]^{2l-1} [\nabla \times u^+_{el,n,m,1-l}]_t \\
&= -\mathbf{i}k^+ \, [\cos\theta_{n,m}]^{2l-1} \, [u^+_{el,n,m,l}]_t, \\
\Big[\nabla_+ \times [\nu \times u^+_{ma,n,m,l}]\Big]_t &= \frac{-\mathbf{i}}{\mu\omega} \Big[\nabla_+ \times [\nu \times \nabla \times u^+_{el,n,m,l}]\Big]_t \\
&= \frac{(-1)^l k^+}{\mu\omega} \Big[\nabla_+ \times [\nu \times u^+_{el,n,m,1-l}]\Big]_t \\
&= \frac{(-1)^{1+l}\mathbf{i}[k^+]^2}{\mu\omega} [\cos\theta_{n,m}]^{1-2l} \, [u^+_{el,n,m,1-l}]_t \\
&= -\frac{\mathbf{i}[k^+]^2}{\mu\omega} [\cos\theta_{n,m}]^{2-4l} \, [\nu \times u^+_{el,n,m,l}].
\end{aligned}$$

Substituting the last relation into $\nabla_+ \times \varphi_t$ with φ_t given by (76), the required formula $\psi_t = \mathbf{i}\mu\omega \, k^{-2} \, [\nabla_+ \times \varphi_t]_t$ follows for ψ_t from (62).

Note that if, as supposed in Theorem 4.1, there exists an adjoint solution $(u_{el,ad}, u^+_{el,ad}, u^-_{el,ad})$ of (61), then an adjoint magnetic field $u_{ma,ad}$ can be defined by (5). Using (87) and (88), it is not hard to find $u^\pm_{ma,ad}$ such that (82) is satisfied. Hence, there exists an adjoint magnetic field solution $(u_{ma,ad}, u^+_{ma,ad}, u^-_{ma,ad})$ satisfying (77). Moreover, the solution $u_{ma,ad}$ is not only in $H(\mathrm{curl}, G)$ but also in $[H^1]^3$ over each subdomain of G with constant ε. Indeed, the solution $u_{ma,ad}$ fulfills (83) and, in view of (3), also $\nabla \cdot u_{ma,ad} \equiv 0$. Consequently, the boundary conditions (12) of [21] are satisfied with a slight modification of the right-hand side. Similarly to the H^1 regularity of the original solution of the Maxwell problem shown in [21], the H^1 regularity of $u_{ma,ad}$ follows.

4.10 Proof of last assertion in Remark 3.3

We proceed analogously to the the treatment in the beginning of Section 4.9. Suppose u and $u^\pm$ are the solutions of (53). Choosing the test functions in (53) such that $\mathrm{v}^\pm = 0$ and that the support of v is located in the interior of a material domain with constant ε, we conclude that u satisfies (2). Fixing an interface between the subdomains of constant ε and choosing a test functional v which is smooth on S but vanishes over all other interfaces, then the variational equation yields the interface condition (18).

Choosing $\mathrm{v} = 0$, v^-, and v^+ either as an $u^+_{el,n,m,0}$ with $c_{n,m} = 0$ or as the linear combination of all other $u^+_{el,n,m,l}$, there follows

$$0 = \eta \int \nu \times [u - u^+ - u^{\mathrm{inc}}] \cdot [\nu \times \overline{u}^+_{el,n,m,0}], \quad \forall n, m \text{ s.t. } c_{n,m} = 0, \tag{89}$$

$$0 = \Big[\nabla_+ \times \Big[[(u - u^+ - u^{\mathrm{inc}})|_{\Gamma^+}]_t\Big]_{\mathbf{mo}}\Big]_t - \eta \, P^{el}_{\Gamma^+} \nu \times [u - u^+ - u^{\mathrm{inc}}]_t \,. \tag{90}$$

Expanding the tangential component $[u]_t$ into the Fourier series

$$[u]_t = \sum_{n,m,l:\ c_{n,m}\neq 0\ or\ l=0} C_{n,m,l}\,[u^+_{el,n,m,l}]_t + \sum_{n,m:\ c_{n,m}=0} C_{n,m,1}\,[\nu \times u^+_{el,n,m,0}],$$

using the expansion (24) of u^+ and $U^{\rm inc} = D_0 u^+_{0,0,0} + D_1 u^+_{0,0,1}$, and taking into account (87), (88), and (54), the equations (89) and (90) turn into

$$\begin{aligned}
0 &= \Big[C_{n,m,0} - B^+_{n,m,0} - \delta_{(n,m,0),(0,0,0)} D_0\Big]\eta, && \forall n,m:\ c_{n,m}=0,\\
0 &= \Big[C_{n,m,l} - B^+_{n,m,l} - \sum_{l=0}^{1} \delta_{(n,m,l),(0,0,l)} D_l\Big]\eta_{n,m,l}, && \forall n,m,l:\ c_{n,m}>0,\\
&\quad \eta_{n,m,l} := \lambda^+_{n,m,l} - \eta,\ \lambda^+_{n,m,l} := -\mathbf{i}k^+[\cos\theta_{n,m}]^{1-2l},\\
0 &= \Big[C_{n,m,l} - B^+_{n,m,l} - \sum_{l=0}^{1} \delta_{(n,m,l),(0,0,l)} D_l\Big]\eta_{n,m,l}, && \forall n,m,l:\ c_{n,m}\notin\mathbb{R},\\
&\quad \eta_{n,m,l} := \lambda^+_{n,m,l} - \eta,\ \lambda^+_{n,m,l} := \frac{(-1)^{l+1}[k^+]^{4l-1}}{[\Im\mathrm{m}\, c_{n,m}]^{2l-1}\sqrt{2[\Im\mathrm{m}\, c_{n,m}]^2+[k^+]^2}^{\,2l-1}}, \qquad (91)\\
0 &= C_{n,m,1}\eta, && \forall n,m:\ c_{n,m}=0.
\end{aligned}$$

If the numbers $\eta_{n,m,l}$ are nonzero, then the last equalities imply $[u-u^+-u^{\rm inc}]_t = 0$, i.e., the left equation of (20). Clearly, we have $\eta_{n,m,0}\neq 0$. On the other hand, $\Im\mathrm{m}\, c_{n,m} \sim \sqrt{1+n^2+m^2}$ for $|n|+|m| \longrightarrow \infty$. In other words, the only cluster point of the $\lambda^+_{n,m,1}$ is zero. Choosing η sufficiently large or at least different from $\lambda^+_{n,m,1}$ for all $n,m\in\mathbb{Z}$, we get $\eta_{n,m,l}\neq 0$ and $[u-u^+-u^{\rm inc}]_t = 0$. Note that if (46) is replaced by (47), then we get $\eta_{n,m,l}$ as above if $n^2+m^2<N$ and $\eta_{n,m,l} = \lambda^+_{n,m,l}$ for all n,m with $n^2+m^2\geq N$. In this case, we have to choose $\eta>0$ different to the numbers $\lambda^+_{n,m,1}$ for all n,m with $n^2+m^2<N$.

Choosing the test functions in (53) such that $\mathrm{v}^\pm = 0$, using (2) and the Green formula

$$\int_{\partial G} [\nabla\times u]\cdot[\nu\times\bar{\mathrm{v}}] \;=\; \int_G [\nabla\times u]\cdot[\nabla\times\bar{\mathrm{v}}] + \int_G \Big[\nabla\times[\nabla\times\overline{u}]\Big]\cdot\bar{\mathrm{v}},$$

we arrive at

$$0 \;=\; \big[\nabla\times[u-u^+-u^{\rm inc}] + \eta\,\nu\times[u-u^+-u^{\rm inc}]\big]_t\,,$$

i.e., the tangential trace of $\nabla\times[u-u^+-u^{\rm inc}]$ is zero and we get the right equation of (20). Similarly, we can derive (22). In particular, the $\lambda^+_{n,m,l}$ for $c_{n.m}\notin\mathbb{R}$ are to be replaced by

$$\lambda^-_{n,m,l} := \frac{(-1)^{l+1}[k^-]^{4l-1}}{[\Im\mathrm{m}\, c^-_{n,m}]^{2l-1}\sqrt{2[\Im\mathrm{m}\, c^-_{n,m}]^2+[k^-]^2}^{\,2l-1}}, \qquad (92)$$

Altogether u, $u^\pm$ are solutions of the boundary value problem (2), (10)-(13), (18), (20), and (22).

5 Numerical example

5.1 Numerical gradients

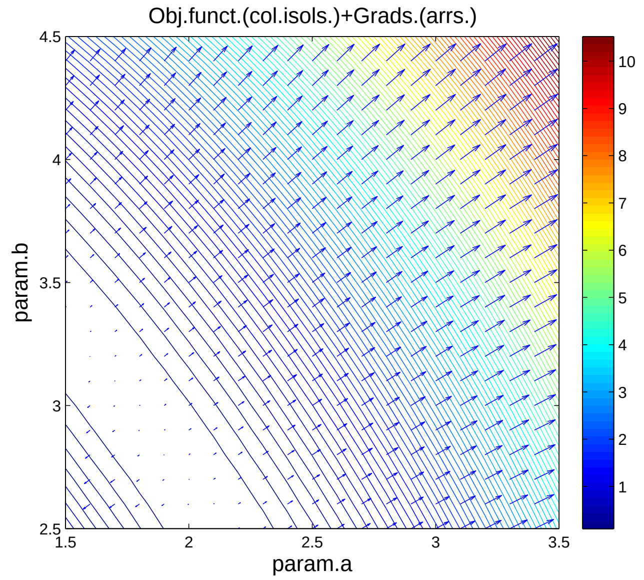

Figure 4: Functional $\mathcal{F}$ for $2.5 \le a \le 3.5$, $3.5 \le b \le 4.5$, $e = 4$, $f = 5$, and $g = 3$. Corresponding 2D gradient vectors.

We consider the structure of a biperiodic array of contact holes (cf. Section 4.3.1). The parameters are chosen in accordance to

$$\begin{array}{ccc} a \in [1.5, 3.5], & b \in [2.5, 4.5], & e \in [2.5, 4.5], \\ f \in [3.5, 5.5], & g \in [2.5, 3.5], & n = 5, \\ \mathrm{per}_y = 12, & \mathrm{per}_x = 10 \quad , & o = -2. \end{array}$$

We assume an incoming plane wave under TE polarization with wave length $\lambda = 25$ and with angles of incidence $\theta = 35^\circ$ and $\phi = 30^\circ$ (cf. Section 2.3). The refractive index of the cover material and of the material in the hole is set to 1, that for the substrate to 1.5, and that for the material surrounding the hole to 2. For the electro-magnetic field reflected by the structure, we consider the quadratic functional

$$\mathcal{F}(u) \quad := \quad \left[100\,\mathrm{eff}^{+}_{0,0,0}(u) - 22.0\right]^2$$

with the efficiency $\mathrm{eff}^{+}_{0,0,0}$ defined by (36). We have computed the fields numerically using (51) (cf. (45)) and the quadratic edge elements of NGSOLVE (cf. [14, 22, 23]). The Rayleigh series expansions in the trial functions (cf. (24),(37)) have been reduced to terms with $|n| \le 4$ and $|m| \le 4$. The stepsize of the FEM grid has been chosen such that the number of unknowns is about $80\,000$. Of course, the grid is chosen such that the derivatives of the vector function χ (cf. (58) and (60)) are continuous over the tetrahedra of the

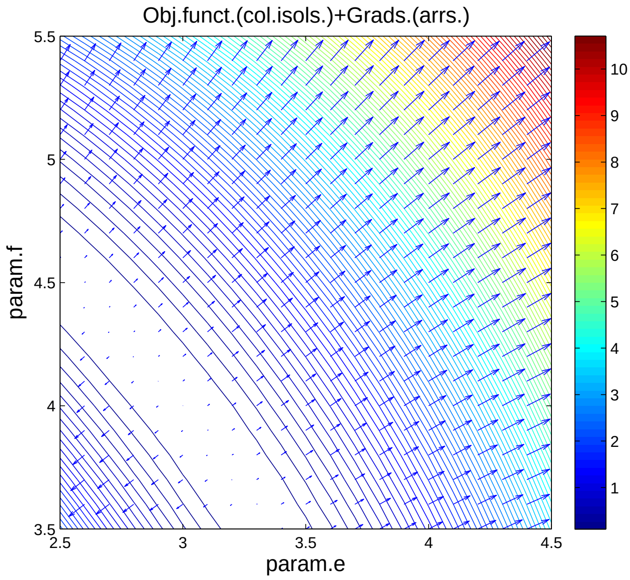

Figure 5: Functional $\mathcal{F}$ for $a = 3$, $b = 4$, $3.5 \le e \le 4.5$, $4.5 \le f \le 5.5$, and $g = 3$. Corresponding 2D gradient vectors.

grid. The systems of linear equations have been solved by PARDISO (cf. [20]). Note that a single LU factorization is needed to solve for the approximate solution as well as for the adjoint solution.

First, we look at the derivative with respect to parameter a for $a = 3$, $b = 4$, $e = 4$, $f = 5$, and $g = 3$. The value of (63) computed with the approximate solution and the approximate adjoint solution is $\partial_a[\mathcal{F}(u)]_{a=3} \approx 4.267$. Using a simple central difference formula of stepsize 0.25 we have obtained $([\mathcal{F}(u)]_{a=3.25} - [\mathcal{F}(u)]_{a=2.75})/0.5 \approx 4.399$ for the same value. This suggests that the error is less than 3%. For a difference formula with a smaller stepsize, we have got

$$\begin{aligned}
\frac{[\mathcal{F}(u)]_{a=3} - [\mathcal{F}(u)]_{a=2.975}}{0.025} &\approx 0.222\,00,\\
\frac{[\mathcal{F}(u)]_{a=3} - \Big\{[\mathcal{F}(u)]_{a=2.975} - 0.025\,\partial_a[\mathcal{F}(u)]_{a=3}\Big\}}{0.025} &\approx 0.008\,66.
\end{aligned}$$

Computing the same values with an FEM grid of halved meshsize, we have obtained $\partial_a[\mathcal{F}(u)]_{a=3} \approx 4.373$ and

$$\begin{aligned}
\frac{[\mathcal{F}(u)]_{a=3} - [\mathcal{F}(u)]_{a=2.975}}{0.025} &\approx 0.220\,19,\\
\frac{[\mathcal{F}(u)]_{a=3} - \Big\{[\mathcal{F}(u)]_{a=2.975} - 0.025\,\partial_a[\mathcal{F}(u)]_{a=3}\Big\}}{0.025} &\approx 0.001\,51.
\end{aligned}$$

Finally, we present the functional $\mathcal{F}$ and its gradients in the Figures 4–6. The gradient vectors computed approximately by formula (63) fit nicely to the isolines of $\mathcal{F}$.

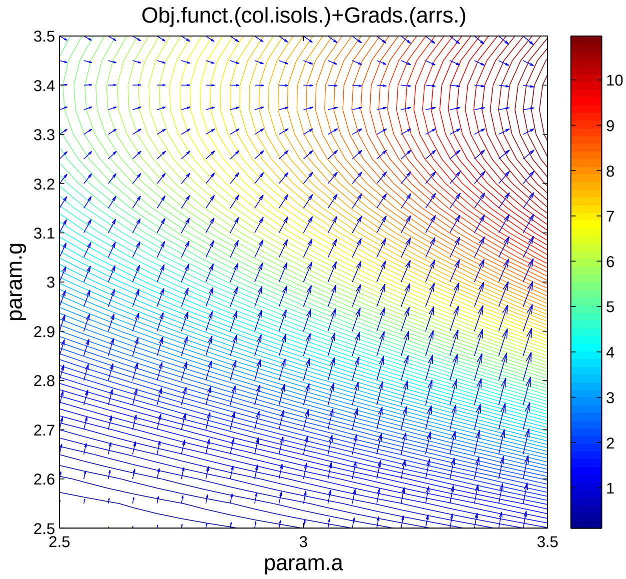

Figure 6: Functional $\mathcal{F}$ for $2.5 \le a \le 3.5$, $b = 4$, $e = 4$, $f = 5$, and $2.5 \le g \le 3.5$. Corresponding 2D gradient vectors.

5.2 Gradients in the reconstruction method

Now we reconstruct a contact hole geometry with three unknown parameters from efficiency data. This example should be closer to the application in EUV scatterometry (cf. e.g. [12] and the papers cited there). Therefore, we choose the wave length $\lambda = 13.7\,\mathrm{nm}$ and illuminate the contact hole under TE polarization directly from above, i.e., $\theta = 0$ and $\phi = 0$. We fix the parameters (cf. Section 4.3.1)

$$\begin{array}{ccc} a \in [3.15\,\mathrm{nm}, 3.85\,\mathrm{nm}], & b \in [4.55\,\mathrm{nm}, 5.25\,\mathrm{nm}], & e = 5.6\,\mathrm{nm}, \\ f = 7\,\mathrm{nm}, & g \in [3.85\,\mathrm{nm}, 4.55\,\mathrm{nm}], & n = 7\,\mathrm{nm}, \\ \mathrm{per}_y = 16.8\,\mathrm{nm}, & \mathrm{per}_x = 14\,\mathrm{nm} \quad , & o = -2\,\mathrm{nm}. \end{array} \tag{93}$$

The material above the grating and in the hole is described by the refractive index of vacuum. The material around the hole is SiO_2 and that of the layer beneath the hole is Ta. Additionally, we assume a multi-layer structure beneath the contact-hole grating. Under two capping layers of SiO_2 and Si with a thickness of 1.234 nm and 12.869 nm, respectively, we assume 49 identical groups of four layers. Each group consists of a Mo/Si, a Mo, a Mo/Si, and a Si layer with a thickness of 0.147 nm, 2.141 nm, 1.972 nm, and 2.838 nm, respectively. Note that Mo/Si is a mixture of Mo and Si with an interpolated refractive index to model a non-strict transition from Si to Mo.

The contact hole to be reconstructed is that with $a = 3.5\,\mathrm{nm}$, $b = 4.9\,\mathrm{nm}$, and $g = 4.2\,\mathrm{nm}$. For this we simulate measurement data by an FEM solution with a stepsize of $0.37\,\mathrm{nm}$ and with quadratic edge elements. So we get approximate values $d_{n,m,l}$ for the efficiencies $\mathrm{eff}^+_{n,m,l}$ (cf. (36)) with (n, m, l) equal to (-1,0,0), (0,-1,1), (0,0,0), (0,1,1), and (1,0,0). In order to reconstruct a, b, and g, we determine the minimum of the least-square deviation

$\mathcal{F}$ in (57) with $w_{-1,0,0} = w_{1,0,0} = 1000$, $w_{0,-1,1} = w_{0,1,1} = 2000$, and $w_{0,0,0} = 4$. Note that the weights have been chosen such that the terms in (57) have almost the same range of values over (93). The values of $\mathcal{F}$ and their numerical gradients for fixed $g = 4.2\,$nm and the FEM meshsizes $2.95\,$nm and $1.47\,$nm are shown in Figures 7 and 8.

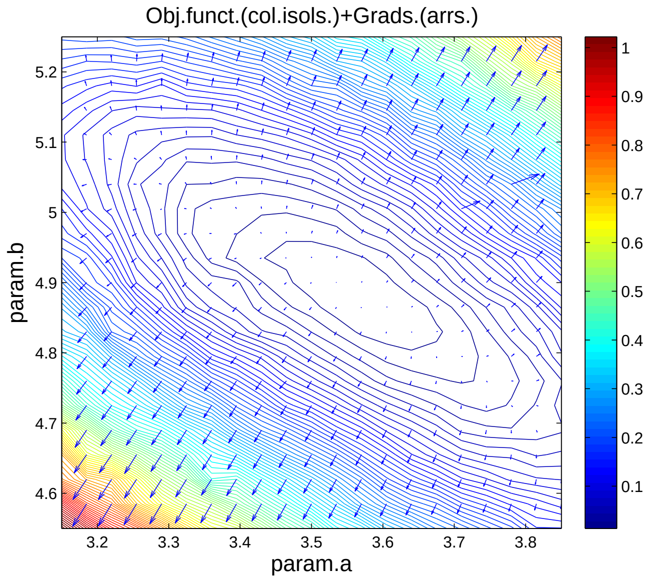

Figure 7: Objective functional $\mathcal{F}$ for $3.15\,\mathrm{nm} \leq a \leq 3.85\,\mathrm{nm}$, $4.55\,\mathrm{nm} \leq b \leq 5.25\,\mathrm{nm}$, $e = 5.6\,$nm, $f = 7\,$nm, as well as $g = 4.2\,$nm. Meshsize $2.95\,$nm. Corresponding 2D gradient vectors.

For the optimization of $\mathcal{F}$ we have applied the Gauss-Newton method (cf. e.g. [17]). Though we actually have used a variant of SQP type to satisfy the prescribed interval bounds in (93), the components of the iterative solutions remained between the upper and lower bounds such that the optimization steps were pure Gauss-Newton steps. Each step requires the computation of the Jacobian matrix for the mapping of the geometry parameters to the efficiencies. The entries of the Jacobian can be computed with formulas similarly to Theorem 4.1. In our numerical experiment the initial solution was $a = 3.8\,$nm, $b = 4.6\,$nm, and $g = 3.9\,$nm, and the results are shown in Table 1. Note that a good initial solution is realistic in scatterometry since the manufacturing process results in small perturbations of the ideal parameters only. With a small number of iterations, the exact solution has been reconstructed perfectly.

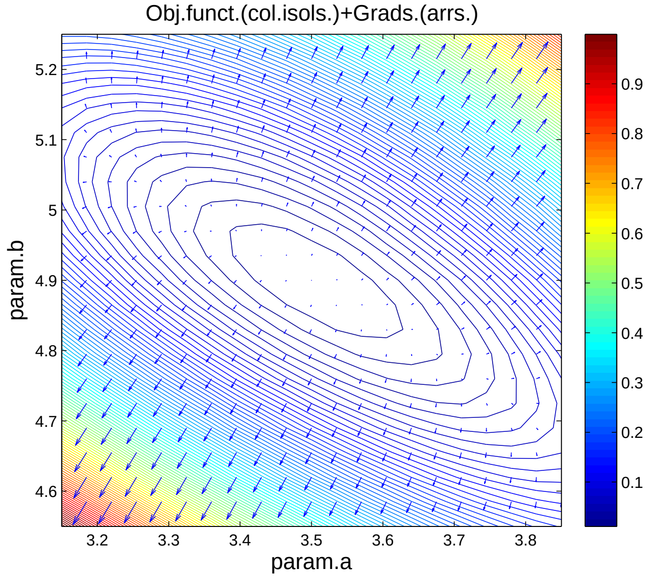

Figure 8: Objective functional $\mathcal{F}$ for $3.15\,\mathrm{nm} \le a \le 3.85\,\mathrm{nm}$, $4.55\,\mathrm{nm} \le b \le 5.25\,\mathrm{nm}$, $e = 5.6$ nm, $f = 7$ nm, as well as $g = 4.2$ nm. Meshsize 1.47 nm. Corresponding 2D gradient vectors.

meshsize	nmb.of its.	a	b	g
initial vals.		3.90000 nm	4.60000 nm	3.90000 nm
2.95	8	3.52643 nm	4.89211 nm	4.20601 nm
1.47	5	3.49339 nm	4.90394 nm	4.20270 nm
0.73	5	3.49984 nm	4.90018 nm	4.20011 nm
exact		3.50000 nm	4.90000 nm	4.20000 nm

Table 1: Number of iterations and reconstruction of parameters for contact hole.

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