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Spectral Methods for Direct and Inverse Scattering from Periodic Structures

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Thèse

Présentée pour obtenir le grade de

DOCTEUR DE L'ÉCOLE POLYTECHNIQUE

Spécialité : Mathématiques Appliquées

par

Dinh Liem NGUYEN

Spectral Methods for Direct and Inverse Scattering from Periodic Structures

Soutenue le 7 décembre 2012 devant le jury composé de :

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Palaiseau, November 2012

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Abstract

The main topic of the thesis are inverse scattering problems of electromagnetic waves from periodic structures. We study first the direct problem and its numerical resolution using volume integral equation methods with a focus on the case of strongly singular integral operators and discontinuous coefficients. In a second investigation of the direct problem we study conditions on the material parameters under which well-posedness is ensured for all positive wave numbers. Such conditions exclude the existence of guided waves. The considered inverse scattering problem is related to shape identification. To treat this class of inverse problems, we investigate the so-called Factorization method as a tool to identify periodic patterns from measured scattered waves. In this thesis, these measurements are always related to plane incident waves.

The outline of the thesis is the following: The first chapter is the introduction where we give the state of the art and new results of the topics studied in the thesis. The main content consists of five chapters, divided into two parts. The first part deals with the scalar case where the TM electromagnetic polarization is considered. In the second chapter we present the volume integral equation method with new results on Gårding inequalities, convergence theory and numerical validation. The third chapter is devoted to the analysis of the Factorization method for the inverse scalar problem as well as some numerical experiments. The second part is dedicated to the study of 3-D Maxwell's equations. The fourth and fifth chapters are respectively generalizations of the results of the second and third ones to the case of Maxwell's equations. The sixth chapter contains the analysis of uniqueness conditions for the direct scattering problem, that is, absence of guided modes.

Chapter 1

Introduction

Direct and inverse scattering from periodic structures has a long history. Since the first study [85] by Lord Rayleigh in 1907, it has received continuous and considerable attention from researchers not only as an interesting mathematical topic in its own right but also as a field of great interest in applications. These applications include optical filters, lenses and beam-splitters in optics, and indeed their non-destructive testing is an important issue to guarantee the functioning of such devices. An overview about this and further topics in applied mathematics related to wave propagation in periodic structures can be found in, e.g., [14, 86].

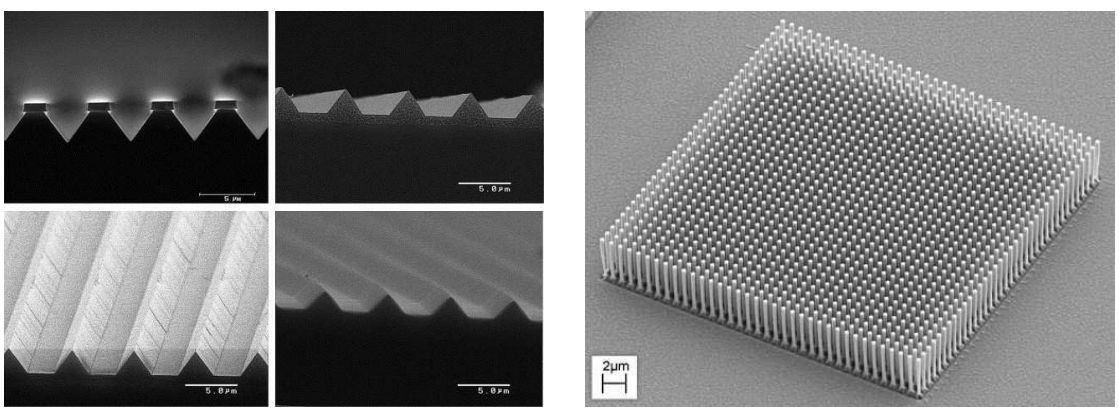


Figure 1.1: Examples of periodic structures in nanotechnology. These photos are from paper [18] (left) and *nanotechweb.org* (right).

This thesis includes three topics concerning some aspects of numerical and mathematical analysis of direct and inverse scattering problems of time-harmonic electromagnetic waves from periodic structures. The first topic which is also the main topic of the thesis is the study of the periodic inverse scattering problems in both cases of TM modes and Maxwell's equations. As a tool serving the first topic, the second topic concerns volume integral equation methods for the numerical resolution of the direct problem again in both scalar and vector

cases. Finally, we investigate in the third topic the well-posedness for all wave numbers of the direct problem for the case of Maxwell's equations.

1.1 State of the art

Let us first briefly review results from the literature in the three topics mentioned above. For each topic we indicate ongoing research subjects and new results that have been obtained in this thesis.

1.1.1 Existence and uniqueness of solutions to direct scattering problems from periodic structures

Mathematical theory for the well-posedness of electromagnetic scattering problem for periodic structures has been an active area of research in the last years. In contrast to scattering from bounded structures, uniqueness of solution for this scattering problem does not hold in general for all positive wave numbers. Instead, non-trivial solutions to the homogeneous problem might exist for a discrete set of exceptional wave numbers, and these solutions turn out to be exponentially localized surface waves.

For the scalar case, the first study can be found in [2] where the author considered a quasi-periodic boundary value problem for the Helmholtz equation arising from wave scattering by periodic structures. This paper proved existence and uniqueness of solution for all wave numbers (or, equivalently, all frequencies), under geometrical conditions on the penetrable scatterer with Dirichlet boundary conditions. Similar results are obtained in the paper [22] for more complicated periodic structures which are constituted of conducting and dielectric materials. The latter paper further gave examples of structures for which non-uniqueness of solution occurs at the so-called singular wave numbers. These wave numbers were shown to be related to guided waves (surface waves) that are exponentially localized along the structure. For a more general case of non-periodic unbounded scatterer, the authors in [29] proved uniqueness of solution and non-existence of guided waves under such geometrical conditions.

For the case of Maxwell's equations, the authors of [40] studied well-posedness of the scattering problem from a medium consisting of two homogeneous materials separated by a smooth biperiodic surface using an integral equation approach. In [12, 15, 41] the authors studied existence and uniqueness of solution for the scattering problem from penetrable biperiodic structures using a variational approach for the magnetic field formulation. Nevertheless, unlike the scalar cases, the uniqueness results in these papers were only proven for all but possibly a discrete set of wave numbers. Furthermore, they only considered the non-magnetic case, i.e, the magnetic permeability is assumed to be the same constant outside and inside the periodic structure. The case of variable magnetic permeability was investigated in the paper [1] for Maxwell's equations where the biperiodic structure consists of conducting and dielectric materials. That paper studied a variational approach, formulated in terms of the electric field, and showed that the obtained saddle point problem satisfies the Fredholm alternative, and again uniqueness of solution was proven for all but possibly a discrete set of wave

numbers. More recently, the paper [105] analyzed the well-posedness of the scattering problem for penetrable anisotropic biperiodic structures but again with the restriction of non-magnetic material. The latter paper also proved that the scattering problem is uniquely solvable for all wave numbers if the structure contains absorbing materials, and if the dielectric tensor is piecewise analytic.

Therefore, the uniqueness result for all wave numbers for Maxwell's equations with non-absorbing biperiodic materials that we have obtained in this thesis is, to the best of our knowledge, a new result in the topic.

1.1.2 Volume integral equation method and numerical discretization

Motivated by applications of periodic dielectric structures for optics it is important to construct efficient schemes to compute the electromagnetic fields involved in the associated scattering problems in the scattering problems. There are various numerical approaches to solve the direct problem. One of the two most developed and studied methods that we would like to mention first is the finite element discretization of the variational problem. One can find the results for the scalar case in, e.g., [10, 11, 13, 42, 43] as well as for the case of Maxwell's equations in [1, 12, 41, 57, 104]. This approach turns out to be advantageous in dealing with complicated materials. The system matrix is sparse even if in three dimensions number of degrees of freedoms becomes large. However, one has to take into account the quasi-periodicity of the solution and the radiation condition which might be difficult using a standard software package. The second approach mentioned above is the boundary integral equation methods. The results for both scalar and Maxwell's equations cases has been studied in, e.g., [4, 6, 82, 84, 93, 95, 111]. Also, in [4] the author provided a extensive state of the arts on boundary integral equation methods for the periodic scattering problems as well as a large amount of related publications. In this second approach the radiation condition is automatically satisfied and the resulting matrix system is smaller than the one in the first approach. However that matrix system is dense and setting up such a system matrix is hence costly both in terms of memory and CPU time. Further as we know that the main ingredient for this approach is the quasi-periodic Green's function which is also the kernel of the integral operator. Thus efficient evaluation of the integral kernel appears quite challenging due to its singularity.

We next describe the volume integral equation method which received less attention in the math community than the last two approaches. In the engineering community, volume integral equation methods are a popular tool to numerically solve scattering problems, see, e.g., [46, 75, 97, 98], since they allow to solve equations with complicated material parameters via one single integral equation, the radiation condition is automatically satisfied and the implementation is simple. The linear system resulting from the discretization of the integral operator (by, e.g., collocation or finite element methods) is large and dense. However, the convolution structure of the integral operator allows to use FFT techniques to compute matrix-vector multiplications in an order-optimal way (up to logarithmic terms), see, e.g., [94, 107, 114]. However, the discretization of the integral operator itself is sometimes done in a crude

way. The convergence analysis of the method is often missing, in particular when material parameters are not globally smooth.

Recently, volume integral equation methods also started to attract interest in the applied math community. The papers [53, 54, 80, 109] provide numerical analysis for the Lippmann-Schwinger integral equation, when the weakly singular integral operator is compact. Further, [38, 73, 90] analyze strongly singular integral equations for scattering in free space. However, [90] considers media with globally continuous material properties, and the L^2-theory in [73] does not yield physical solutions if the material parameter appearing in the highest-order coefficients are not smooth. The paper [38] proves a Gårding inequality for a strongly singular volume integral equation arising from electromagnetic scattering from a (discontinuous) dielectric. This implies the convergence of Galerkin discretizations. However, studying a finite element discretization of the volume integral equation leads to drawbacks of a large and dense matrix system where the quasi-periodic condition have to be taken into account.

We hence can see that the application of this method to periodic scattering problems for the cases of discontinuous materials and/or strongly singular integral operators (the form of the integral equations is of the second kind) is still an subject of ongoing research, and studying this subject is one of the aims of the thesis.

1.1.3 Periodic inverse scattering problems

Inverse problems in scattering by periodic structures have been an active research area in the last years. We refer to [3, 16, 17, 44, 45, 67, 112] for uniqueness results for detecting periodic scattering objects from field measurements. Furthermore, for the topic of shape identification that is investigated in this thesis, traditional approaches, e.g., Newton-type iterative methods can be found in [51, 52, 66, 76, 77]. Besides more recent approaches of non-iterative methods such as Ikehata's probe method [58–65], singular sources method [88, 89, 91, 92], the linear sampling method recently appeared as one of the most studied and developed. This method was first introduced in [33] for the scalar case of the problem of shape identification in inverse obstacle scattering. It aims to compute a picture of the shape of the scattering object from measured data. Compared to traditional approaches the linear sampling method is relatively rapid and does not need a-priori knowledge on material properties. Therefore, it has attracted much research in recent years, see, e.g., [23, 24, 26, 31, 32, 34–36]. Recent developments of the linear sampling method can be found in [25, 27]. Furthermore, the latter method has been recently extended to inverse scattering involving periodic media in [55, 56, 113]. Using complex-conjugated incident fields the authors in [55, 56] studied the periodic version of the linear sampling method for the case impenetrable periodic surfaces with mixed boundary conditions. Instead of the far field equation for the case of bounded obstacles they considered the near field equation defined on a line/plane above the periodic structure which is a linear integral equation of first kind. For penetrable periodic structures in a full space setting, the linear sampling method has been investigated in the recent paper [113] for the corresponding inverse problem. The authors studied the TE case where the incident fields used are plane incident waves.

A problem with the linear sampling method is that for a wide class of scattering problems, its complete mathematical justification still remains open, see [25]. Recently, some results on justification of this method have been obtained in [5, 9]. The so-called Factorization method, developed in [68, 74], overcomes this disadvantage. This method has a rigorous justification from a mathematical point of view, keeps the previously mentioned advantages and of course is an interesting tool for shape identification problems in inverse scattering. However, the class of scattering problems to which the Factorization method can be applied is still restricted, see [72]. We also refer to [72] for applications of the Factorization method to obstacle inverse scattering problems and impedance tomography.

The Factorization method has been recently extended to inverse scattering problems for periodic structures. The papers [7, 8] studied the method for detecting impenetrable periodic layers with Dirichlet and impedance boundary conditions. The author of [79] considered imaging of penetrable periodic interfaces between two dielectrics in two dimensions. Furthermore, the papers [7, 8, 79] investigated the Factorization method for the TE case. Using point sources as incident fields the author in [100] obtained a rigorous analysis of the Factorization method for Maxwell's equations of inverse scattering from penetrable biperiodic structures. This work extended similar results in [72] for obstacle inverse scattering of electromagnetic waves.

Therefore as a contribution to this ongoing research subject, we have developed the Factorization method for periodic inverse scattering problems for the TM case and Maxwell's equations using plane incident waves. We are interested in mathematical analysis as well as numerical implementation of the method for both scalar and vector cases.

1.2 Outline of the thesis

After the first chapter of introduction presented above, the main content of this thesis consists of five chapters, essentially divided into two parts. In each chapter, we present results obtained by studying the problems described in three topics in the state of the art above.

Part I deals with the scalar case of TM electromagnetic polarization and contains Chapters 2 and 3. In Chapter 2 we analyze electromagnetic scattering of TM polarized waves from a diffraction grating consisting of a periodic, anisotropic, and possibly negative-index dielectric material. We reformulate the periodic scattering problem as a strongly singular volume integral equation, that is, the integral operators fail to be weakly singular. Then we prove new (generalized) Gårding inequalities in weighted and unweighted Sobolev spaces for this strongly singular integral equation. These inequalities also hold for materials for which the real part of the material parameter takes negative values inside the diffraction grating, independently of the value of the imaginary part. Moreover, when the material parameter is isotropic and positive we show that trigonometric Galerkin methods applied to a periodization of the integral equation converge. Fully discrete formulas show that the numerical scheme is easy to implement and numerical examples show the performance of the method.

Chapter 3 concerns the shape identification problem of diffraction gratings from measured spectral data involving scattered electromagnetic waves in TM mode. More precisely, we con-

sider diffraction gratings consisting of a penetrable periodic dielectric mounted on a metallic plate. Using special plane incident fields introduced in [7], we study the Factorization method as a tool for reconstructing the periodic media. We propose a rigorous analysis for the method. A simple imaging criterion is also provided as well as numerical experiments to examine the performance of the method.

Part II is dedicated to the study of Maxwell's equations and consists of Chapters 4, 5 and 6.

Chapter 4 extends the volume integral equation method investigated in Chapter 1 to electromagnetic scattering problems from anisotropic biperiodic structures. These problems are governed by Maxwell's equations in a full space. We consider the case where the electric permittivity and the magnetic permeability are both matrix-valued functions. The scattering problem again can be reformulated as a strongly singular volume integral equation. Since the compact embedding $H^1 \subset L^2$ is crucially exploited for the scalar case for proving Gårding inequalities, the main difficulty in this case is that the embedding $H(\mathrm{curl}) \subset L^2$ is not compact. We overcome this by not investigating Gårding inequalities in the support of the contrast but in a bigger domain under suitable assumptions on the contrast. This turned out to be sufficient for convergence theory of a trigonometric Galerkin method appplied to the periodic integral equation. We again propose fully discrete formulas for the numerical scheme as well as numerical examples.

In Chapter 5 we extend the Factorization method studied in Chapter 2 to the electromagnetic inverse scattering problem for Maxwell's equations. Instead of a half-space setting of the problem as in the scalar case, we investigate here the vetorial problem for penetrable biperiodic structures in a full-space setting. By modifying special plane incident fields used in the scalar case and extending the approach to the vectorial problem we again propose a rigorous analysis for the Factorization method. We also provide three dimensional numerical experiments which, to the best of our knowledge, are the first numerical examples for this method in a biperiodic setting.

Finally, Chapter 6 presents results on existence and uniqueness of solution for all positive wave numbers for electromagnetic scattering problem from a biperiodic dielectric structure mounted on a perfectly conducting plate. Given that uniqueness of solution holds, existence of solution follows from a well-known Fredholm framework for the variational formulation of the problem in a suitable Sobolev space. In this chapter, we derive a Rellich identity for a solution to this variational problem under suitable smoothness conditions on the material parameter. Under additional non-trapping assumptions on the material parameter, this identity allows us to establish uniqueness of solution for all positive wave numbers (i.e. excluding the existence of surface waves).

The work of this thesis contains the results presented in the following research articles:

1. A. Lechleiter, D.-L. Nguyen: Volume Integral Equations for Scattering from Anisotropic Gratings, to appear in *Mathematical Methods in the Applied Sciences*.

2. A. Lechleiter, D.-L. Nguyen: A Galerkin Method for Strongly Singular Volume Integral Equation Arising from Grating Scattering, submitted for publication.

3. A. Lechleiter, D.-L. Nguyen: On Uniqueness in Electromagnetic Scattering from Biperiodic Structures, accepted for *ESAIM: Mathematical Modelling and Numerical Analysis*.

4. D.-L. Nguyen: On Shape Identification of Diffraction Gratings from Spectral Data: The TM Case, preprint (to be submitted).

5. A. Lechleiter, D.-L. Nguyen: Factorization Method for Inverse Electromagnetic Scattering from Biperiodic Structures, preprint (to be submitted).

Part I

The Case of TM Modes

Chapter 2

Volume Integral Equation Methods for Periodic Scattering Problems

Abstract: In Chapter 2 we analyze electromagnetic scattering of TM polarized waves from a diffraction grating consisting of a periodic, anisotropic, and possibly negative-index dielectric material (problem (2.10)–(2.12)). In Section 2.3, we reformulate the periodic scattering problem as a strongly singular volume integral equation (see equation (2.44)), that is, the integral operator of the integral equation fails to be weakly singular. Then we prove new (generalized) Gårding inequalities in weighted Sobolev spaces for this strongly singular integral equation (see Theorem 2.4.5). These inequalities also hold for materials for which the real part of the material parameter takes negative values inside the diffraction grating, independently of the value of the imaginary part. Further, when the material parameter is a scalar real-valued function we prove in Theorem 2.5.2 that such inequalities also hold for standard Sobolev spaces which is important for the numerical implementation of the method. From the latter result and the additional assumption that the scalar material parameter is positive, we show that trigonometric Galerkin methods applied to the periodized integral equation (2.46) converge (see Theorem 2.6.3). Fully discrete formulas show that the numerical scheme is easy to implement and numerical examples show the performance of the method (see Section 2.7).

2.1 Introduction

As pointed out in the introduction to this thesis, this chapter analyzes volume integral equation methods for electromagnetic scattering of TM polarized waves from a diffraction grating consisting of a periodic, anisotropic, and possibly negative-index dielectric material. We consider diffraction gratings as three-dimensional dielectric structures which are periodic in one spatial direction and invariant in a second, orthogonal, direction (compare Figure 2.1). They

are used as optical components, e.g., to split up light into beams with different directions, and they serve in optical devices as, e.g., monochromators or as optical spectrometers.

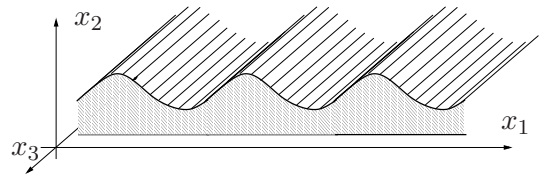


Figure 2.1: The diffraction grating is periodic in x_1, translation invariant in x_3 and bounded in x_2.

If the wave vector of an incident electromagnetic plane wave is chosen perpendicular to the invariance direction of the grating, Maxwell's equations decouple into scalar Helmholtz equations, known as transverse magnetic (TM) and transverse electric (TE) modes (these terms are not consistently used in the literature). The equation of the TM mode studied in this chapter for a non-magnetic grating has the form

$$\operatorname{div}(\varepsilon_{\mathrm{r}}^{-1}\nabla u) + k^2 u = 0, \qquad k > 0,$$

where u is a α-quasiperiodic function (that is, $u(x_1 + 2\pi, x_2) = \exp(2\pi \mathrm{i}\alpha)u(x_1, x_2)$) for all x_1, $x_2 \in \mathbb{R}$). In particular, we allow the real part of the discontinuous and matrix-valued material parameter $\varepsilon_{\mathrm{r}}^{-1}$ to be negative-definite inside the grating structure, independently of the values of the imaginary part. Negative definite material parameters are a feature that arises in the modelization of, e.g., optical metamaterials, but also for metals at certain frequencies, see, e.g., [106].

We reformulate the scattering problem using (α-quasiperiodic) volume integral equations. These turn out to be strongly singular, that is, the integral operator fails to be weakly singular. Hence, they do not fit into the standard Riesz theory, since the integral operators are not compact. Nevertheless, we prove in the first aim of this chapter Gårding inequalities for the integral equations in weighted α-quasiperiodic Sobolev spaces, which yields a Fredholm framework for the scattering problem. This result even holds if the real part $\operatorname{Re}(\varepsilon_{\mathrm{r}}^{-1})$ of the material parameter is negative definite inside the grating, independently of the imaginary part $\operatorname{Im}(\varepsilon_{\mathrm{r}}^{-1})$. Our approach extends a technique from [73], where similar volume integral equations have been analyzed for free space scattering problems in case that the scalar real-valued contrast is strictly positive. Moreover, we also prove that the Gårding inequalities in weighted Sobolev spaces can be transformed to inequalities in standard α-quasiperiodic Sobolev spaces, if the grating consists of isotropic material. Note that the restriction to the case of isotropic material is essential for our proof. Another important aspect of the analysis is that the dielectric properties of the medium are discontinuous at the air/grating interface (otherwise, the integral operators can be reduced to compact ones, see, e.g., [37, Chapter 9]).

Our second aim is to rigorously analyze a numerical method to solve the TM scattering problem by trigonometric Galerkin methods, again for discontinuous media, but with isotropic

and positive contrast. This technique originally stems from [109], where a corresponding collocation method for volume integral equations involving a compact integral operator has been analyzed. We prove that the trigonometric Galerkin method converges with optimal order, and give fully discrete formulas how to implement this method. Finally, we describe a couple of numerical experiments. In essence, the advantage of the method is that it is simple to implement, and that the linear system can be evaluated at FFT speed. Of course, the convergence order is low if the medium has jumps, due to the use of global basis functions (if the material properties are globally smooth, then the method is high-order convergent). Nevertheless, the technique is an interesting tool for numerical simulation, as we demonstrate through numerical examples.

The analysis of the integral equation for material parameters with negative real part is, to the best of our knowledge, the first application of T-coercivity (a well-known framework for variational formulations of elliptic partial differential equations with sign-changing coefficients, see [19–21]) to volume integral equations. As usual, the material parameter is, however, not allowed to take arbitrary negative values; the solvability condition for instance excludes that the relative material parameter takes the value -1 inside the grating.

The chapter is organized as follows: In Section 2.2 we give a problem setting and briefly recall variational theory for the direct scattering problem. While in Section 2.3 we introduce the corresponding integral equations, we prove in Sections 2.4 and 2.5 Gårding inequalities on a continuous level for weighted and unweighted Sobolev spaces, respectively. In Section 2.6 we prove Gårding inequalities for periodized integral equations, and error estimates for trigonometric Galerkin methods. We discretize the periodic integral equation and give gives fully discrete formulas for the implementation in Section 2.7. Finally numerical experiments are given in Section 2.8 to show the performance of the method.

For the convenience of the readers we clarify some notations used in this chapter. The trace of a function u on a boundary ∂D from the outside and from the inside of a domain D is $\gamma_{\text{ext}}(u)$ and $\gamma_{\text{int}}(u)$, respectively. The jump of u across ∂D is $[u]_{\partial D} = \gamma_{\text{ext}}(u) - \gamma_{\text{int}}(u)$. If the exterior and the interior trace of a function u coincide, we simply write $\gamma(u)$ for the trace. We denote the absolute value and the Euclidean norm by $|\cdot|$, and the spectral matrix norm by $|\cdot|_2$.

2.2 Problem Setting

Propagation of time-harmonic electromagnetic waves in an inhomogeneous and isotropic medium without free currents is described by the time-harmonic Maxwell's equations for the electric and magnetic fields E and H, respectively,

$$\operatorname{curl} H + \mathrm{i}\omega\varepsilon E = \sigma E, \qquad \operatorname{curl} E - \mathrm{i}\omega\mu_0 H = 0, \tag{2.1}$$

where $\omega > 0$ denotes the angular frequency, ε is the positive electric permittivity, μ_0 is the (scalar, constant and positive) magnetic permeability, and σ is the conductivity. The permittivity and conductivity are allowed to be anisotropic, but required to be of the special

form

$$\varepsilon = \begin{pmatrix} \varepsilon_T & 0 \\ 0 & \varepsilon_{33} \end{pmatrix}, \qquad \sigma = \begin{pmatrix} \sigma_T & 0 \\ 0 & \sigma_{33} \end{pmatrix},$$

with real and symmetric 2×2 matrices $\varepsilon_T = (\varepsilon_{ij})_{i,j=1,2}$ and $\sigma_T = (\sigma_{ij})_{i,j=1,2}$, and real functions ε_{33} and σ_{33}. Furthermore, we assume in this chapter that all three material parameters are independent of the third variable x_3 and 2π-periodic in the first variable x_1. Moreover, ε equals $\varepsilon_0 I_3 > 0$ (where I_n is the $n \times n$ identity matrix) and σ equals zero outside the grating.

If an incident electromagnetic plane wave independent of the third variable x_3 illuminates the grating, then Maxwell's equations (2.1) for the total wave field decouple into two scalar partial differential equations (see, e.g., [43]). Indeed, since both, E and H do not depend on x_3 it holds that

$$\operatorname{curl} E = \left(\frac{\partial E_3}{\partial x_2}, -\frac{\partial E_3}{\partial x_1}, \frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_1} \right)^\top, \quad \operatorname{curl} H = \left(\frac{\partial H_3}{\partial x_2}, -\frac{\partial H_3}{\partial x_1}, \frac{\partial H_2}{\partial x_1} - \frac{\partial H_1}{\partial x_2} \right)^\top.$$

Setting $a = \mathrm{i}\omega(\varepsilon + \mathrm{i}\sigma/\omega)$ and plugging these two relations in the equations of (2.1) we obtain

$$a_{11}E_1 + a_{12}E_2 + \frac{\partial H_3}{\partial x_2} = 0, \tag{2.2}$$

$$a_{21}E_1 + a_{22}E_2 - \frac{\partial H_3}{\partial x_1} = 0, \tag{2.3}$$

$$a_{33}E_3 + \frac{\partial H_2}{\partial x_1} - \frac{\partial H_1}{\partial x_2} = 0, \tag{2.4}$$

and

$$-\mathrm{i}\omega\mu_0 H_1 + \frac{\partial E_3}{\partial x_2} = 0, \tag{2.5}$$

$$-\mathrm{i}\omega\mu_0 H_2 - \frac{\partial E_3}{\partial x_1} = 0, \tag{2.6}$$

$$-\mathrm{i}\omega\mu_0 H_3 + \frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_2} = 0. \tag{2.7}$$

From these two systems we see that the knowledge of E_3 and H_3 are sufficient to determine the fields E and H. Now we plug (2.5), (2.6) into (2.4) and find that $u = E_3$ satisfies the scalar equation

$$\Delta u + \omega^2 \mu_0 \left(\varepsilon_{33} + \frac{\mathrm{i}\sigma_{33}}{\omega} \right) u = 0. \tag{2.8}$$

From (2.2) and (2.3) we obtain

$$E_1 = \frac{a_{11}\partial H_3/\partial x_1 + a_{21}\partial H_3/\partial x_2}{a_{22}a_{11} - a_{21}a_{12}}, \quad E_2 = -\frac{a_{12}\partial H_3/\partial x_1 + a_{22}\partial H_3/\partial x_2}{a_{22}a_{11} - a_{21}a_{12}}.$$

Plugging these results into (2.7) we find that $u = H_3$ satisfies

$$\operatorname{div}\left(\varepsilon_{\mathrm{r}}^{-1}\nabla u\right) + k^2 u = 0, \tag{2.9}$$

where $k := \omega\sqrt{\varepsilon_0\mu_0}$ and

$$\varepsilon_{\mathrm{r}} := \varepsilon_0^{-1}\left[\begin{pmatrix} \varepsilon_{22} & -\varepsilon_{21} \\ -\varepsilon_{12} & \varepsilon_{11} \end{pmatrix} + \mathrm{i}\begin{pmatrix} \sigma_{22} & -\sigma_{21} \\ -\sigma_{12} & \sigma_{11} \end{pmatrix}/\omega\right].$$

Solutions of the equations (2.8) and (2.9) are called *transverse electric modes* (TE mode) and *transverse magnetic modes* (TM mode), respectively. It is the aim of the first part of this thesis to study the case of TM mode. The usual jump conditions for the Maxwell's equations imply that the field u and the co-normal derivative $\nu \cdot \varepsilon_{\mathrm{r}}^{-1}\nabla u$ are continuous across interfaces with normal vector ν where ε_{r} jumps. Note that ε_{r} is 2π-periodic in x_1 and equals I_2 outside the grating.

We seek for weak solutions to (2.9) and assume that $\varepsilon_{\mathrm{r}} \in L^\infty(\mathbb{R}^2, \mathbb{C}^{2\times 2})$ takes values in the symmetric matrices, and that $\varepsilon_{\mathrm{r}}^{-1} \in L^\infty(\mathbb{R}^2, \mathbb{C}^{2\times 2})$. Moreover, we suppose that $\mathrm{Re}(\varepsilon_{\mathrm{r}}^{-1})$ is pointwise strictly positive or strictly negative definite almost everywhere. Note that we do *not* assume that $\mathrm{Re}(\varepsilon_{\mathrm{r}}^{-1})$ is positive definite in all of $\mathbb{R}^2$.

For the two-dimensional problem (2.9), incident electromagnetic waves reduce to

$$u^i(x) = \exp(\mathrm{i}k\, x \cdot d) = \exp(\mathrm{i}k(x_1 d_1 + x_2 d_2)),$$

where $|d| = 1$ and $d_2 \neq 0$. When the incident plane wave u^i illuminates the diffraction grating there arises a scattered field u^s such that the total field $u = u^i + u^s$ satisfies (2.9). Since $\Delta u^i + k^2 u^i = 0$, the scattered field satisfies

$$\mathrm{div}(\varepsilon_{\mathrm{r}}^{-1}\nabla u^s) + k^2 u^s = -\mathrm{div}(Q\nabla u^i) \quad \text{in } \mathbb{R}^2, \qquad \text{where } Q := \varepsilon_{\mathrm{r}}^{-1} - I_2 \tag{2.10}$$

is the contrast. Note that u^i is α-quasiperiodic with respect x_1, that is,

$$u^i(x_1 + 2\pi, x_2) = e^{2\pi\mathrm{i}\alpha} u^i(x_1, x_2) \quad \text{for } \alpha := kd_1.$$

Since u^i is α-quasiperiodic and ε_{r} is 2π-periodic, the total field and the scattered field both are also α-quasiperiodic in x_1. We complement this problem by a radiation condition that is set up using Fourier techniques. Since the scattered field u^s is α-quasiperiodic, the function $e^{-\mathrm{i}\alpha x_1}u^s$ is 2π-periodic in x_1, and can hence be expanded as

$$e^{-\mathrm{i}\alpha x_1}u^s(x) = \sum_{j\in\mathbb{Z}} \hat{u}_j(x_2)e^{\mathrm{i}nx_1}, \quad x = (x_1, x_2)^\top \in \mathbb{R}^2.$$

Here the Fourier coefficients $\hat{u}_j(x_2) \in \mathbb{C}$ are defined by

$$\hat{u}_j(x_2) = \frac{1}{2\pi}\int_0^{2\pi} u^s(x_1, x_2)e^{-\mathrm{i}\alpha_j x_1}\,\mathrm{d}x_1\,, \quad \alpha_j := \alpha + j, \quad j \in \mathbb{Z}.$$

We define

$$\beta_j := \begin{cases} \sqrt{k^2 - \alpha_j^2}, & k^2 \geq \alpha_j^2, \\ \mathrm{i}\sqrt{\alpha_j^2 - k^2}, & k^2 < \alpha_j^2, \end{cases}$$

In the sequel of this chapter we assume that

$$k^2 \neq \alpha_j^2 \qquad \text{for all } j \in \mathbb{Z}. \tag{2.11}$$

This assumption excludes the Rayleigh frequencies which is necessary for the definition of the Green's function used in the next section. Note that under assumption (2.11) all the β_j are non-zero.

Recall that ε_{r} equals I_2 outside the grating, that means $\varepsilon_{\mathrm{r}} = I_2$ and $Q = 0$ for $|x_2| > h$, where $h > \sup\{|x_2| : (x_1, x_2)^\top \in \operatorname{supp}(Q)\}$. Thus it holds that the equation (2.10) becomes $(\Delta + k^2)u^s = 0$ in $\{|x_2| > h\}$. Using separation of variables, and choosing the upward propagating solution, we set up a radiation condition in form of a Rayleigh expansion condition, prescribing that u^s can be written as

$$u^s(x) = \sum_{j\in\mathbb{Z}} \hat{u}_j^{\pm} e^{\mathrm{i}(\alpha_j x_1 \pm \beta_j(x_2 \mp h))} \qquad \text{for } x_2 \gtrless \pm h, \tag{2.12}$$

where $(\hat{u}_n)_{n\in\mathbb{Z}}$ are the Rayleigh sequences given by

$$\hat{u}_j^{\pm} := \hat{u}_j^{\pm}(\pm h) = \frac{1}{2\pi}\int_0^{2\pi} u^s(x_1, \pm h) e^{-\mathrm{i}\alpha_j x_1}\,\mathrm{d}x_1\,, \quad j \in \mathbb{Z}.$$

Note that we require that the series in (2.12) converges uniformly on compact subsets of $\{|x_2| > h\}$. A solution to the Helmholtz equation is called radiating if it satisfies (2.12). If $k^2 > \alpha_j^2$ then the jth mode $\exp(\mathrm{i}\alpha_j x_1 \pm \mathrm{i}\beta_j(x_2 \mp h))$ is a propagating mode, whereas $k^2 < \alpha_j^2$ means that $\exp(\mathrm{i}\alpha_j x_1 \pm \mathrm{i}\beta_j(x_2 \mp h))$ is an evanescent mode.

Variational solution theory for the scattering problem (2.10)–(2.12) is well-known, see, e.g., [22, 43, 66]. Setting

$$\Omega_h := (-\pi, \pi) \times (-h, h), \quad \Gamma_{\pm h} := (-\pi, \pi) \times \{\pm h\},$$

for $h > \sup\{|x_2| : (x_1, x_2)^\top \in \operatorname{supp}(Q)\}$, one can variationally reformulate the problem in the space

$$H^1_\alpha(\Omega_h) := \{u \in H^1(\Omega_h) : u = U|_{\Omega_h} \text{ for some } \alpha\text{-quasiperiodic } U \in H^1_{\mathrm{loc}}(\mathbb{R}^2)\}.$$

The resulting variational formulation is to find $u^s \in H^1_\alpha(\Omega_h)$ such that

$$\begin{aligned}\int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1}\nabla u^s \cdot \nabla\overline{v} - k^2 u^s \overline{v})\,\mathrm{d}x - \int_{\Gamma_h} \overline{v} T^+(u^s)\,\mathrm{d}s - \int_{\Gamma_{-h}} \overline{v} T^-(u^s)\,\mathrm{d}s \\ = -\int_{\Omega_h} Q\nabla u^i \cdot \nabla\overline{v}\,\mathrm{d}x\end{aligned} \tag{2.13}$$

for all $v \in H^1_\alpha(\Omega_h)$. The operators $T^\pm$, $\varphi \mapsto \mathrm{i}\sum_{j\in\mathbb{Z}} \beta_j \hat{\varphi}_j^{\pm} e^{\mathrm{i}\alpha_j x_1}$, are the so-called exterior Dirichlet-to-Neumann operators on $\Gamma_{\pm h}$. The sesquilinear form in (2.13) is bounded on $H^1_\alpha(\Omega_h)$ and satisfies a Gårding inequality if, e.g., $\operatorname{Re}(\varepsilon_{\mathrm{r}}^{-1})$ is positive definite, that is,

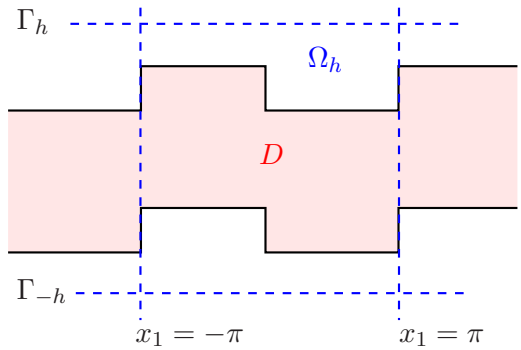


Figure 2.2: Geometric setting for scattering problem of TM-polarized electromagnetic waves from a penetrable periodic structure.

$\xi^* \mathrm{Re}(\varepsilon_\mathrm{r}^{-1})(x)\xi \geq c|\xi|^2 \geq 0$ for $\xi \in \mathbb{C}^2$ and almost every $x \in \Omega_h$. In this case, analytic Fredholm theory implies that the set of real wave numbers (excluding Rayleigh frequencies) where non-uniqueness occurs is at most countable, see [22, 66]. If $\mathrm{Re}(\varepsilon_\mathrm{r}^{-1})$ changes sign, proving Fredholm properties of the variational formulation (2.13) is non-trivial, at least if $\mathrm{Im}(\varepsilon_\mathrm{r}^{-1})$ vanishes, see [19, 21].

In this chapter, we establish a Fredholm framework for the scattering problem via integral equation techniques, that is, uniqueness of solution implies existence. We do not aim to prove the corresponding uniqueness results, since for periodic scattering problems such results are anyway not available at all frequencies, except under restrictive geometric (non-trapping) conditions, see [22] or Chapter 5.

2.3 Integral Equation Formulation

In this section, we reformulate the scattering problem (2.9) as a volume integral equation, and prove mapping properties of the integral operator between Sobolev spaces. To this end, let us recall that $Q = \varepsilon_\mathrm{r}^{-1} - I_2$ and denote by $\overline{D} \subset \Omega_h$ the support of Q, restricted to one period $\{-\pi < x_1 < \pi\}$. By G_k we denote the Green's function to the α-quasiperiodic Helmholtz equation in $\mathbb{R}^2$, see [66]. Under the assumption (2.11) the α-quasiperiodic Green's function has the series representation

$$G_k(x) := \frac{\mathrm{i}}{4\pi} \sum_{j\in\mathbb{Z}} \frac{1}{\beta_j} \exp(\mathrm{i}\alpha_j x_1 + \mathrm{i}\beta_j |x_2|), \quad x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \in \mathbb{R}^2,\ x \neq \begin{pmatrix} 2\pi m \\ 0 \end{pmatrix} \text{ for } m \in \mathbb{Z}. \tag{2.14}$$

Lemma 2.3.1 (Cf. [66])**.** *The Green's function G_k can be split into $G_k(x) = (\mathrm{i}/4)H_0^{(1)}(k|x|) + \Psi(x)$ in $\mathbb{R}^2$ where Ψ is an analytic function solving the Helmholtz equation $\Delta\Psi + k^2\Psi = 0$ in $(-2\pi, 2\pi) \times \mathbb{R}$.*

We also define a periodized Green's function, firstly setting

$$\mathcal{K}_h(x) := G_k(x), \quad x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \in \mathbb{R} \times (-h, h),\ x \neq \begin{pmatrix} 2\pi m \\ 0 \end{pmatrix} \text{ for } m \in \mathbb{Z}, \tag{2.15}$$

and secondly extending $\mathcal{K}_h(x)$ $2h$-periodically in x_2 to $\mathbb{R}^2$.

The functions

$$\varphi_j(x) := \frac{1}{\sqrt{4\pi h}} \exp\left(\mathrm{i}(j_1 + \alpha)x_1 + \mathrm{i}\frac{j_2\pi}{h}x_2\right), \quad j = \begin{pmatrix} j_1 \\ j_2 \end{pmatrix} \in \mathbb{Z}^2, \tag{2.16}$$

are orthonormal in $L^2(\Omega_h)$. They differ from the usual Fourier basis (see, e.g., [102, Section 10.5.2]) only by a phase factor $\exp(\mathrm{i}\alpha x_1)$, and hence also form a basis of $L^2(\Omega_h)$. For $f \in L^2(\Omega_h)$ and $j = (j_1, j_2)^\top \in \mathbb{Z}^2$,

$$\hat{f}(j) := \int_{\Omega_h} f\,\overline{\varphi_j}\,\mathrm{d}x$$

are the Fourier coefficients of f. For $0 \leq s < \infty$ we define a fractional Sobolev space $H^s_{\alpha,\mathrm{p}}(\Omega_h)$ as the subspace of functions in $L^2(\Omega_h)$ such that

$$\|f\|^2_{H^s_{\alpha,\mathrm{p}}(\Omega_h)} = \sum_{j\in\mathbb{Z}^2} (1 + |j|^2)^s |\hat{f}(j)|^2 < \infty. \tag{2.17}$$

It is well-known that for integer values of s, these spaces correspond to spaces of functions that are s times weakly differentiable, α-quasiperiodic in x_1, periodic in x_2, and that the above norm is then equivalent to the usual Sobolev integral norms. In particular, $H^1_{\alpha,\mathrm{p}}(\Omega_h)$ is a (strict) subspace of $H^1_\alpha(\Omega_h)$.

Lemma 2.3.1 implies in particular that $\mathcal{K}_h$ has an integrable singularity and that the Fourier coefficients $\hat{\mathcal{K}}_h(j)$ are well-defined. To compute these coefficients explicitly, we set

$$\lambda_j := k^2 - (j_1 + \alpha)^2 - \left(\frac{j_2\pi}{h}\right)^2 \quad \text{for } j \in \mathbb{Z}^2.$$

Theorem 2.3.2. *Assume that $k^2 \neq \alpha_j^2$ for all $j \in \mathbb{Z}$. Then the Fourier coefficients of the kernel $\mathcal{K}_h$ from* (2.15) *are given by*

$$\hat{\mathcal{K}}_h(j) = \begin{cases} \frac{\cos(j_2\pi)\exp(\mathrm{i}\beta_{j_1}h) - 1}{\sqrt{4\pi h}\,\lambda_j} & \textit{for } \lambda_j \neq 0, \\ \frac{\mathrm{i}}{4j_2}\left(\frac{h}{\pi}\right)^{3/2} & \textit{else}, \end{cases} \qquad j = \begin{pmatrix} j_1 \\ j_2 \end{pmatrix} \in \mathbb{Z}^2.$$

Remark 2.3.3. *Note that $\hat{\mathcal{K}}_h(j)$ is well-defined for $\lambda_j = 0$: Since $k^2 \neq \alpha_n^2$ for all $n \in \mathbb{Z}$, the definition of λ_j implies that $j_2 \neq 0$ whenever $\lambda_j = 0$. For completeness, we include a proof, noting that the case $\lambda_j \neq 0$ is also shown in [100, Section 7.1].*

Proof. It is easy to check that $(\Delta + k^2)\varphi_j = \lambda_j \varphi_j$ for $j = (j_1, j_2)^\top \in \mathbb{Z}^2$. If $\lambda_j \neq 0$, Green's second identity implies that

$$\begin{aligned}\hat{\mathcal{K}}_h(j) &= \int_{\Omega_h} \mathcal{K}_h(x)\overline{\varphi_j(x)}\,\mathrm{d}x = \lambda_j^{-1} \lim_{\delta\to 0} \int_{\Omega_h\setminus B_\delta} G_k(x)\overline{(\Delta+k^2)\varphi_j(x)}\,\mathrm{d}x \\ &= \lambda_j^{-1} \lim_{\delta\to 0} \Bigg[\left(\int_{\partial\Omega_h} + \int_{\partial B_\delta}\right) \left(G_k \frac{\partial\overline{\varphi_j}}{\partial\nu} - \frac{\partial G_k}{\partial\nu}\overline{\varphi_j}\right) \mathrm{d}s \qquad (2.18) \\ &\qquad + \int_{\Omega_h\setminus B_\delta} (\Delta+k^2) G_k(x)\overline{\varphi_j(x)}\,\mathrm{d}x \Bigg], \qquad (2.19)\end{aligned}$$

where ν denotes the exterior normal vector to $B_\delta := \{|x| < \delta\}$ and to Ω_h. The last volume integral vanishes since $(\Delta + k^2)G_k = 0$ in $\Omega_h \setminus B_\delta$ for any $\delta > 0$. Let us now consider the first integral in (2.18). The boundary of Ω_h consists of two horizontal lines $\Gamma_{\pm h}$ and two vertical lines $\{(x_1, x_2) : x_1 = \pm\pi, -h < x_2 < h\}$. Hence, the normal vector ν on these boundaries is either $(\pm 1, 0)^\top$ or $(0, \pm 1)^\top$. Straightforward computations yield that

$$G_k(x_1, \pm h) = \frac{\mathrm{i}}{4\pi} \sum_{n\in\mathbb{Z}} \frac{e^{\mathrm{i}\beta_n h}}{\beta_n} e^{\mathrm{i}\alpha_n x_1}, \quad \frac{\partial G_k}{\partial x_2}(x_1, \pm h) = \mp\frac{1}{4\pi} \sum_{n\in\mathbb{Z}} e^{\mathrm{i}\beta_n h} e^{\mathrm{i}\alpha_n x_1}, \qquad (2.20)$$

$$\overline{\varphi_j(x_1, \pm h)} = \frac{1}{\sqrt{4\pi h}} e^{-\mathrm{i}\alpha_{j_1} x_1} \cos(j_2\pi), \quad \text{and} \quad \frac{\partial\overline{\varphi_j}}{\partial x_2}(x_1, \pm h) = -\frac{\mathrm{i} j_2 \pi}{h}\overline{\varphi(x_1, \pm h)}. \qquad (2.21)$$

In consequence,

$$\begin{aligned}\int_{\Gamma_{\pm h}} \left(G_k \frac{\partial\overline{\varphi_j}}{\partial\nu} - \frac{\partial G_k}{\partial\nu}\overline{\varphi_j}\right) \mathrm{d}s &= -\int_{\Gamma_h} \frac{\partial G_k}{\partial x_2}\overline{\varphi_j}\,\mathrm{d}s + \int_{\Gamma_{-h}} \frac{\partial G_k}{\partial x_2}\overline{\varphi_j}\,\mathrm{d}s \\ &= -2\int_{\Gamma_h} \frac{\partial G_k}{\partial x_2}\overline{\varphi_j}\,\mathrm{d}s\,.\end{aligned}$$

Using the above formulas for $\partial G_k/\partial x_2$ and $\overline{\varphi_j}$ in (2.20) and (2.21), respectively, we find that

$$-2\int_{\Gamma_h} \frac{\partial G_k}{\partial x_2}\overline{\varphi_j}\,\mathrm{d}s = \frac{\cos(j_2\pi)}{\sqrt{4\pi h}} e^{\mathrm{i}\beta_{j_1} h}.$$

Computing the partial derivatives of G_k and φ_j with respect to x_1 analogously to the above computations, one finds that the integrals on the vertical boundaries of Ω_h vanish due to the α-quasiperiodicity of both functions. Thus, we obtain that

$$\int_{\partial\Omega_h} \left(G_k \frac{\partial\overline{\varphi_j}}{\partial\nu} - \frac{\partial G_k}{\partial\nu}\overline{\varphi_j}\right) \mathrm{d}s = \frac{\cos(j_2\pi)}{\sqrt{4\pi h}} e^{\mathrm{i}\beta_{j_1} h}. \qquad (2.22)$$

Now we consider the second integral in (2.18). From Lemma 2.3.1 we know that $G_k(x) = \frac{\mathrm{i}}{4} H_0^{(1)}(k|x|) + \Psi(x)$ where Ψ is a smooth function in Ω_h. Obviously,

$$\lim_{\delta\to 0} \int_{\partial B_\delta} \left(\Psi \frac{\partial\overline{\varphi_j}}{\partial\nu} - \frac{\partial\Psi}{\partial\nu}\overline{\varphi_j}\right) \mathrm{d}s = 0.$$

Using precisely the same arguments as in [102, Theorem 2.2.1] one shows that

$$\lim_{\delta\to 0}\int_{\partial B_\delta}\left(G_k\frac{\partial\overline{\varphi_j}}{\partial\nu}-\frac{\partial G_k}{\partial r}\overline{\varphi_j}\right)\,\mathrm{d}s\;=-\frac{1}{\sqrt{4\pi h}},\tag{2.23}$$

see, e.g., [102, Theorem 2.2.1]. Combining (2.22) with (2.23) yields that

$$\mathcal{K}_h(j)=\frac{1}{\sqrt{4\pi h}\lambda_j}(\cos(j_2\pi)e^{\mathrm{i}\beta_{j_1}h}-1)\quad\text{for }\lambda_j\neq 0.$$

For $\lambda_j=0$ we use de L'Hôspital's rule to find that

$$\mathcal{K}_h(j)=\lim_{\gamma\to(j_1+\alpha)^2+(j_2\pi/h)^2}\frac{\cos(j_2\pi)\exp(\mathrm{i}h\sqrt{\gamma-(j_1+\alpha)^2})-1}{\sqrt{4\pi h}\,[\gamma-(j_1+\alpha)^2-(j_2\pi/h)^2]}=\frac{\mathrm{i}h^{3/2}}{4\pi^{3/2}j_2}.$$

Note that the assumption that $k^2\neq\alpha_j^2$ for all $j\in\mathbb{Z}^2$ implies that λ_j and j_2 cannot vanish simultaneously. □

Since the Fourier coefficients of $\mathcal{K}_h$ decay quadratically,

$$|\hat{\mathcal{K}}_h(j)|\le C/(1+(j_1+\alpha)^2+(j_2\pi/h)^2)\quad\text{for }j\in\mathbb{Z}^2,$$

the convolution operator with kernel $\mathcal{K}_h$ is bounded from $L^2(\Omega_h)$ into $H^2_{\alpha,\mathrm{p}}(\Omega_h)$.

Proposition 2.3.4. *Assume that $k^2\neq\alpha_j^2$ for all $j\in\mathbb{Z}$. Then the convolution operator K_h, defined by*

$$(K_hf)(x)=\int_{\Omega_h}\mathcal{K}_h(x-y)f(y)\,\mathrm{d}y\quad\text{for }x\in\Omega_h,$$

is bounded from $L^2(\Omega_h)$ into $H^2_{\alpha,\mathrm{p}}(\Omega_h)$.

Proof. Since $\varphi_j(x-z)=\sqrt{4\pi h}\,\varphi_j(x)\overline{\varphi_j(z)}$, we exploit the periodicity of $z\mapsto\mathcal{K}_h(z)\overline{\varphi_j(z)}$ to find that

$$\begin{aligned}(K_h\varphi_j)(x)&=\int_{\Omega_h}\mathcal{K}_h(x-y)\varphi_j(y)\,\mathrm{d}y\;=\int_{x-\Omega_h}\mathcal{K}_h(z)\varphi_j(x-z)\,\mathrm{d}z\\&=\sqrt{4\pi h}\,\varphi_j(x)\int_{\Omega_h}\mathcal{K}_h(z)\overline{\varphi_j(z)}\,\mathrm{d}z\;=\sqrt{4\pi h}\,\hat{\mathcal{K}}_h(j)\varphi_j(x).\end{aligned}$$

Let $f\in L^2(\Omega_h)$ with Fourier coefficients $\hat{f}(j)$ for $j\in\mathbb{Z}^2$, and set $f_N=\sum_{|j|\le N}\hat{f}(j)\varphi_j$. Then

$$K_hf_N=\sum_{|j|\le N}\hat{f}(j)K_h\varphi_j=\sqrt{4\pi h}\sum_{|j|\le N}\hat{f}(j)\hat{\mathcal{K}}_h(j)\varphi_j$$

and

$$\|K_hf_N\|^2_{H^2_{\alpha,\mathrm{p}}(\Omega_{2h})}\le 4\sqrt{\pi h}\sum_{|j|\le N}\left[1+(j_1+\alpha)^2+(j_2\pi/h)^2\right]^2|\hat{f}(j)|^2|\hat{\mathcal{K}}_h(j)|^2.$$

From the computation of the coefficients $\hat{\mathcal{K}}_h(j)$ in Theorem 2.3.2 we know that there is $C = C(k)$ such that $|\hat{\mathcal{K}}_h(j)| \le C/(1+(j_1+\alpha)^2+(j_2\pi/h)^2)$. Hence $\|K_h f_N\|_{H^2_{\alpha,\mathrm{p}}(\Omega_{2h})} \le C\|f_N\|_{L^2(\Omega_{2h})}$ for a constant C independent of $N \in \mathbb{N}$. Passing to the limit as $N \to \infty$ shows the claim of the proposition. □

Recall that $D \subset \Omega_h$ is the support of the contrast Q. Let us additionally introduce

$$\Omega := (-\pi, \pi) \times \mathbb{R}$$

and for $\ell \in \mathbb{N}, R > 0$,

$$H^\ell_\alpha(\Omega_R) := \{u \in H^\ell(\Omega_R) : \, u = U|_{\Omega_R} \text{ for some } \alpha\text{-quasiperiodic } U \in H^\ell_{\mathrm{loc}}(\mathbb{R}^2)\}.$$

Lemma 2.3.5. *Assume that $k^2 \neq \alpha_j^2$ for all $j \in \mathbb{Z}$. Then the volume potential V defined by*

$$(Vf)(x) = \int_D G_k(x-y) f(y)\,\mathrm{d}y\,, \quad x \in \Omega,$$

is bounded from $L^2(D)$ into $H^2_\alpha(\Omega_R)$ for all $R > 0$.

Proof. Consider $\chi \in C^\infty(\Omega)$ such that $\chi = 1$ in D, $0 \le \chi \le 1$ in $\Omega_h \setminus \overline{D}$ and $\chi(x) = 0$ for $|x_2| > h$. Then $Vg = \chi Vg + (1-\chi)Vg$. Note that

$$(1-\chi)Vg = \int_D (1-\chi) G(\cdot - y) g(y)\,\mathrm{d}y$$

is an integral operator with a smooth kernel, since the series in (2.14) converges absolutely and uniformly for $|x_2| \ge h > 0$, as well as all its partial derivatives. In consequence, the integral operator $(1-\chi)V$ is bounded from $L^2(D)$ into $H^2_\alpha(\Omega_R)$, since

$$\left\| \frac{\partial^{\beta_1}}{\partial x_1} \frac{\partial^{\beta_2}}{\partial x_2} ((1-\chi)Vg) \right\|^2_{L^2(\Omega_R)} \le \int_{\Omega_R} \int_D \left| \frac{\partial^{\beta_1}}{\partial x_1} \frac{\partial^{\beta_2}}{\partial x_2} [(1-\chi(x)) G_k(x-y)] \right|^2 \mathrm{d}y\,\mathrm{d}x \;\; \|g\|^2_{L^2(D)}$$

for all $\beta_{1,2} \in \mathbb{N}$ such that $\beta_1 + \beta_2 \le 2$. It remains to show the boundedness of χV from $L^2(D)$ into $H^2(\Omega_h)$. Let $g \in L^2(D)$ and consider the operator K_{2h} from Proposition 2.3.4, mapping $L^2(\Omega_{2h})$ into $H^2_{\alpha,\mathrm{p}}(\Omega_{2h}) \subset H^2_\alpha(\Omega_{2h})$,

$$(K_{2h} g)(x) = \int_D \mathcal{K}_{2h}(x-y) g(y)\,\mathrm{d}y \quad \text{for } x \in \Omega_{2h}.$$

If $x \in \Omega_h$ and $y \in D$, then $|x_2 - y_2| \le 2h$, that is, $\mathcal{K}_{2h}(x-y) = G_k(x-y)$. Hence, $K_{2h} g = Vg$ in Ω_h, and hence $\chi K_{2h} g = \chi V g$ in Ω_h. Since χ is a smooth function, we conclude that χV is bounded from $L^2(D)$ into $H^2_\alpha(\Omega_h)$. □

Note that the potential Vf can be extended to an α-quasiperiodic function in $H^2_{\mathrm{loc}}(\mathbb{R}^2)$, due to the α-quasiperiodicity of the kernel.

Lemma 2.3.6. *For $g \in L^2(D, \mathbb{C}^2)$ the potential $w = \mathrm{div} V g$ belongs to $H^1_\alpha(\Omega_h)$ for all $h > 0$. It is the unique radiating weak solution to $\Delta w + k^2 w = -\mathrm{div} g$ in Ω, that is, it satisfies*

$$\int_\Omega (\nabla w \cdot \nabla \overline{v} - k^2 w \overline{v})\,\mathrm{d}x = -\int_D g \cdot \nabla \overline{v}\,\mathrm{d}x \tag{2.24}$$

for all $v \in H^1_\alpha(\Omega)$ with compact support, and additionally the Rayleigh expansion condition (2.12)*.*

Proof. Lemma 2.3.5 and α-quasiperiodicity of the kernel of V imply that w is a function in $H^1_\alpha(\Omega_h)$ for all $h > 0$. It is sufficient to prove (2.24) for all smooth α-quasiperiodic test functions v that are supported in $\{|x_2| < C\}$ for some $C > 0$ depending on v. It is well-known that $p = Vg$, a function in $H^2_\alpha(\Omega_h)$ for all $h > 0$, is a weak solution to the Helmholtz equation, that is,

$$\int_\Omega (\nabla p_j \cdot \nabla \partial_j \overline{v} - k^2 p_j \partial_j \overline{v})\,\mathrm{d}x = -\int_D g_j \partial_j \overline{v}\,\mathrm{d}x$$

for $j = 1, 2$. An integration by parts shows that

$$\int_\Omega (\nabla \mathrm{div} p \cdot \nabla \overline{v} - k^2 \mathrm{div} p\, \overline{v})\,\mathrm{d}x = -\int_D g \cdot \nabla \overline{v}\,\mathrm{d}x\,,$$

which implies (2.24) due to

$$\mathrm{div}\, p = \mathrm{div} V g = w.$$

Since the components of the potential $p = Vg$ satisfy the Rayleigh condition, a simple computation shows that the divergence $w = \mathrm{div}\, p$ does also satisfy the latter condition.

It remains to prove uniqueness of a radiating solution to (2.24) when g vanishes. Then w belongs to $H^1_\alpha(\Omega_h)$ for any $h > 0$ and satisfies the variational formulation (2.13) for $\varepsilon_r^{-1} = 1$ with right-hand side equal to zero. Choosing $v = u^s$ in (2.13) and taking the imaginary part of the equation shows that

$$\sum_{j:\, k^2 > \alpha_j^2} |k^2 - \alpha_j^2|^{1/2} \left(|\hat{u}_j^+|^2 + |\hat{u}_j^-|^2 \right) = 0.$$

We conclude that all the propagating modes $\{j \in \mathbb{Z} : k^2 > \alpha_j^2\}$ vanish. Hence, w can be extended by

$$w(x) = \sum_{j: k^2 < \alpha_j^2} \hat{u}_j^\pm e^{\mathrm{i}\alpha_j x_1 \mp |\alpha_j^2 - k^2|^{1/2}(x_2 \mp h)}, \quad x_2 \gtrless \pm h, \tag{2.25}$$

to a solution to the Helmholtz equation in all of Ω that decays exponentially as $x_2 \to \pm\infty$. The unique continuation property [37] for the Helmholtz equation implies that both representations of w in $x_2 \gtrless \pm h$ hold for all $x \in \Omega$, which can only be true if all coefficients $\hat{u}_n^\pm$ vanish. $\square$

Returning to the differential equation (2.10) for the scattered field u^s, let us set $f = Q\nabla u^i \in L^2(D, \mathbb{C}^2)$. (Recall that $Q = \varepsilon_{\mathrm{r}}^{-1} - I_2$.) The variational formulation of (2.10) is

$$\int_\Omega (\nabla u^s \cdot \nabla \overline{v} - k^2 u^s \overline{v})\,\mathrm{d}x = -\int_D (Q\nabla u^s + f) \cdot \nabla \overline{v}\,\mathrm{d}x \tag{2.26}$$

for all $v \in H^1_\alpha(\Omega)$ with compact support in $\overline{\Omega}$. From Lemma 2.3.6 we know that the radiating solution to this problem is given by $u^s = \mathrm{div}V(Q\nabla u^s + f)$. Hence, we aim to find $u^s : \Omega \to \mathbb{C}$ that belongs to $H^1_\alpha(\Omega_R)$ for all $R > 0$, such that

$$u^s - \mathrm{div}V(Q\nabla u^s) = \mathrm{div}V(f) \qquad \text{in } \Omega. \tag{2.27}$$

2.4 Gårding Inequalities in Weighted Sobolev Spaces

For scattering problems in free space and for scalar and positive contrast, the paper [73] investigates integral equations similar to (2.27) in weighted spaces. In this section we generalize the results from [73] to anisotropic and possibly sign-changing coefficients in a periodic setting, proving a Gårding inequality for $I - \mathrm{div}V(Q\nabla\cdot)$ in an anisotropically weighted α-quasiperiodic H^1-space.

From (2.27) it is obvious that the knowledge of u in D is sufficient to determine u in $\Omega \setminus \overline{D}$ by integration. Thus, we define the operator $L : f \mapsto \mathrm{div}Vf$ that is bounded from $L^2(D, \mathbb{C}^2)$ into $H^1_\alpha(D)$ and consider the integral equation

$$u = L(Q\nabla u + f) \quad \text{in } H^1_\alpha(D). \tag{2.28}$$

To study Gårding inequalities for volume integral equations, we introduce suitable weighted Sobolev spaces. To this end, we recall that the symmetric 2×2 matrix $\mathrm{Re}(Q)$ has pointwise almost everywhere in D an eigenvalue decomposition $\mathrm{Re}(Q) = U^*\Sigma U$ with a diagonal matrix Σ and an orthogonal matrix U. This decomposition can be used to define the absolute value $|\mathrm{Re}(Q)| = U^*|\Sigma|U$ and the square root $|\mathrm{Re}(Q)|^{1/2} = U|\Sigma|^{1/2}U^*$, where the absolute value and the square root are element-wise applied to the diagonal matrix Σ. The two eigenvalues $\lambda_{1,2}$ of $\mathrm{Re}(Q)$ define

$$\lambda_{\min}(x) = \min\{|\lambda_1(x)|, |\lambda_2(x)|\}, \quad \lambda_{\max}(x) = \max\{|\lambda_1(x)|, |\lambda_2(x)|\}, \quad x \in D. \tag{2.29}$$

We assume in the following that $\mathrm{Re}(Q)$ is pointwise either strictly positive or strictly negative definite, such that we can assign a sign function $\mathrm{sign}(\mathrm{Re}(Q)) \in L^\infty(\Omega)$ to $\mathrm{Re}(Q)$, indicating whether the eigenvalues of $\mathrm{Re}(Q)$ are positive or negative at a certain point. In the sequel, we write $\mathrm{Re}(Q) > c$ in D ($\mathrm{Re}(Q) < c$ in D) to indicate that the eigenvalues $\lambda_{1,2}$ are larger than (less than) a constant c, almost everywhere in D.

We denote by $H^1_{\alpha,Q}(D)$ the completion of $H^1_\alpha(D)$ with respect to the norm $\|\cdot\|_{H^1_{\alpha,Q}(D)}$,

$$\|u\|^2_{H^1_{\alpha,Q}(D)} := \|\sqrt{|\mathrm{Re}(Q)|}\nabla u\|^2_{L^2(D,\mathbb{C}^2)} + \|u\|^2_{L^2(D)}. \tag{2.30}$$

Since we assumed that $\mathrm{supp}(\mathrm{Re}(Q)) = \overline{D}$, this norm is non-degenerate. Moreover, $\|u\|_{H^1_{\alpha,Q}(D)}$ is an equivalent norm in $H^1_\alpha(D)$ provided that $|\mathrm{Re}(Q)|$ is bounded from below in D by some positive constant. Note that the spectral matrix norm is denoted by $|\cdot|_2$. In general,

$$\|u\|_{H^1_{\alpha,Q}(D)} \leq (1 + \| |\sqrt{|\mathrm{Re}(Q)|}|_2 \|_{L^\infty(D)})\, \|u\|_{H^1_\alpha(D)}.$$

Note also that the norm of $H^1_{\alpha,Q}(D)$ is linked to the sesquilinear form

$$a_Q(u,v) = \int_D \left[\mathrm{sign}(\mathrm{Re}(Q))Q\nabla u \cdot \nabla \overline{v} + u\overline{v}\right] \mathrm{d}x\,, \qquad u,v \in H^1_{\alpha,Q}(D). \tag{2.31}$$

Indeed, $\|u\|^2_{H^1_{\alpha,Q}(D)} = \mathrm{Re}\,[a_Q(u,u)]$ for $u \in H^1_{\alpha,Q}(D)$. In consequence, the form a_Q is non-degenerate, that is, if $a_Q(u,v) = 0$ for all $v \in H^1_{\alpha,Q}(D)$, then $u = 0$.

If $\mathrm{Im}Q$ vanishes in D (that is, the values of $x \mapsto Q(x)$ are self-adjoint matrices), then a_Q is simply the inner product associated with the norm of $H^1_{\alpha,Q}(D)$,

$$\langle u,\, v\rangle_{H^1_{\alpha,Q}(D)} = \int_D \left[|Q|\nabla u \cdot \nabla \overline{v} + u\overline{v}\right] \mathrm{d}x\,, \qquad u,v \in H^1_{\alpha,Q}(D).$$

Lemma 2.4.1. *Assume that there exists $C > 0$ such that*

$$|\mathrm{Im}(Q(x))\xi| \leq C|\mathrm{Re}(Q(x))\xi| \quad \textit{for almost every } x \in D \textit{ and all } \xi \in \mathbb{C}^2. \tag{2.32}$$

Then $v \mapsto L(Q\nabla v)$ is bounded on $H^1_{\alpha,Q}(D)$.

Proof. Due to Theorem 2.3.5, L is bounded from $L^2(D,\mathbb{C}^2)$ into $H^1_\alpha(D)$. Furthermore, $v \mapsto Q\nabla v$ is bounded from $H^1_{\alpha,Q}(D)$ into $L^2(D,\mathbb{C}^2)$, since

$$\begin{aligned}\|Q\nabla u\|_{L^2(D,\mathbb{C}^2)} &\leq \|\mathrm{Re}(Q)\nabla u\|_{L^2(D,\mathbb{C}^2)} + \|\mathrm{Im}(Q)\nabla u\|_{L^2(D,\mathbb{C}^2)} \\ &\leq \||\mathrm{Re}(Q)|\nabla u\|_{L^2(D,\mathbb{C}^2)} + C\|\mathrm{Re}(Q)\nabla u\|_{L^2(D,\mathbb{C}^2)} \\ &\leq (1+C)\| |\sqrt{|\mathrm{Re}(Q)|}|_2\|_{L^\infty(D)}\|u\|_{H^1_{\alpha,Q}(D)}.\end{aligned} \tag{2.33}$$

Moreover, the embedding $H^1_\alpha(D) \subset H^1_{\alpha,Q}(D)$ is bounded, as mentioned above. Hence, $v \mapsto L(Q\nabla v)$ is bounded on $H^1_{\alpha,Q}(D)$. □

Remark 2.4.2. *Condition* (2.32) *is satisfied if the absolute values of the eigenvalues of* $\mathrm{Im}Q$ *are pointwise bounded by $C\lambda_{\min}$ (recall from* (2.29) *that $\lambda_{\min}$ is the minimum of the absolute values of the eigenvalues of* $\mathrm{Re}(Q)$*).*

If $u \in H^1_\alpha(D) \subset H^1_{\alpha,Q}(D)$ solves the Lippmann-Schwinger equation (2.28), then Lemma 2.4.1 implies that u solves the same equation in $H^1_{\alpha,Q}(D)$. Since a_Q is non-degenerate, solving the Lippmann-Schwinger equation in $H^1_{\alpha,Q}(D)$ is equivalent to solve

$$a_Q(u - L(Q\nabla u + f),\, v) = 0 \qquad \text{for all } v \in H^1_{\alpha,Q}(D). \tag{2.34}$$

If $u \in H^1_{\alpha,Q}(D)$ solves the latter variational problem for some $f \in L^2(D,\mathbb{C}^2)$, then $u = L(Q\nabla u + f)$ belongs to $H^1_\alpha(D)$, due to (2.33) and since L is bounded from $L^2(D,\mathbb{C}^2)$ into $H^1_\alpha(D)$.

Proposition 2.4.3. *Assume that $f \in L^2(D, \mathbb{C}^2)$. Then any solution to the Lippmann-Schwinger equation* (2.28) *in $H^1_\alpha(D)$ is a solution in $H^1_{\alpha,Q}(D)$ and vice versa.*

Our aim is now to prove a (generalized) Gårding inequality for the variational problem (2.34). The following lemma will turn out to be useful.

Lemma 2.4.4. *Suppose that X and Y are Hilbert spaces. Let $T_{1,2}$ be bounded linear operators from X into Y and consider the sesquilinear form $a : X \times X \to \mathbb{C}$, defined by $a(u, v) = \langle T_1 u, T_2 v\rangle_Y$ for $u, v \in X$. If one of the operators T_1 and T_2 is compact, then the linear operator $A : X \to X$, defined by $\langle Au, v\rangle_X = a(u, v)$ for all $u, v \in X$, is compact, too.*

Proof. It is easily seen that A is a well-defined bounded linear operator. Obviously, $|\langle Au, v\rangle_X| = |a(u, v)| \le C\|T_1 u\|_Y \|T_2 v\|_Y$ for $u, v \in X$. Assume that T_1 is compact, and note that

$$\|Au\|_X = \sup_{0\neq v\in X} \frac{|\langle Au, v\rangle_X|}{\|v\|_X} \le C\|T_1 u\|_Y.$$

If a sequence $\{u_n\}$ converges weakly to zero in X, then $\{T_1 u_n\}$ contains a strongly convergent subsequence tending to zero in Y. Consequently, $\{Au_n\}$ also contains a strongly convergent zero sequence, which means that A is compact. One can analogously derive the compactness of T in case that T_2 is compact, since $a(u, v) = \langle T_2^* T_1 u, v\rangle$ and $T_2^* T_1$ is compact. □

The next lemma proves Gårding inequalities for the operator $v \mapsto v - L(Q\nabla v)$ using the sesquilinear form a_Q from (2.31). The second part of the claim uses a periodic extension operator

$$E : H^1_\alpha(D) \to H^1_\alpha(\Omega), \quad E(u)|_D = u, \quad E(u)|_{\Omega\setminus\Omega_{2\rho}} = 0. \tag{2.35}$$

We now exemplary show how to construct such a periodic extension operator. We will only construct E for the case that the boundary of $D = \{(x_1, x_2)^\top : x_1 \in (-\pi, \pi),\ \zeta_-(x_1) < x_2 < \zeta_+(x_1)\}$ is given by two 2π-periodic Lipschitz continuous functions $\zeta_\pm : \mathbb{R} \to (-\rho, \rho)$ such that $\zeta_- < -2\rho/3$, $\zeta_+ > 2\rho/3$, and $|\zeta_\pm(x_1) - \zeta_\pm(x_1')| \le M|x_1 - x_1'|$ for $x_1, x_1' \in \mathbb{R}$. The general case can be tackled using local patches as in [81, Appendix A], see also [4, Proof of Theorem 4.22].

For $u \in H^1_\alpha(D)$, we define

$$v(x_1, x_2) = \begin{cases} u(x_1, 2\zeta_+(x_1) - x_2) & \text{if } \zeta_+(x_1) < x_2 < 2\zeta_+(x_1) - \zeta_-(x_1), \\ u(x_1, x_2) & \text{if } \zeta_-(x_1) < x_2 < \zeta_+(x_1), \\ u(x_1, 2\zeta_-(x_1) - x_2) & \text{if } 2\zeta_-(x_1) - \zeta_+(x_1) < x_2 < \zeta_-(x_1). \end{cases}$$

Note that $2\zeta_+(x_1) - \zeta_-(x_1) > 2\rho$ and that $2\zeta_-(x_1) - \zeta_+(x_1) < -2\rho$. The periodicity of ζ and α-quasi-periodicity of v in D imply that the extension belongs is also α-quasi-periodic. Additionally, straightforward computations show that $\|v\|_{H^1(\Omega_{2\rho})} \le \max(\sqrt{3}, 2\sqrt{2}M)\|u\|_{H^1_\alpha(D)}$.

To define the periodic extension operator, we use a smooth cut-off function $\chi : \mathbb{R} \to \mathbb{R}$, that satisfies $0 \le \chi \le 1$, $\chi(x_2) = 1$ for $|x_2| \le \rho$, and $\chi(2\rho) = 0$ for $|x_2| \ge 2\rho$. Then we set

$$E(u) = w, \qquad w(x) = \begin{cases} \chi(x_2)v(x) & \text{for } x \in \Omega_{2\rho}, \\ 0 & \text{else.} \end{cases}$$

Note that the operator norm of E is

$$\|E\|_{H^1_\alpha(D)\to H^1_\alpha(\Omega_{2h})} = \Big(1 + \|E\|^2_{H^1_\alpha(D)\to H^1_\alpha(\Omega_{2h}\setminus\overline{D})}\Big)^{1/2}.$$

Theorem 2.4.5. *Assume that D is a Lipschitz domain and that $Q \in L^\infty(D, \mathbb{C}^{2\times 2})$.*

(a) If $\mathrm{Re}(Q) > 0$ in D, then there exists a compact operator K_+ on $H^1_{\alpha,Q}(D)$ such that

$$\mathrm{Re}\,[a_Q(v - L(Q\nabla v),\, v)] \geq \|v\|^2_{H^1_{\alpha,Q}(D)} - \mathrm{Re}\langle K_+ v,\, v\rangle_{H^1_{\alpha,Q}(D)}, \quad v \in H^1_{\alpha,Q}(D). \tag{2.36}$$

(b) If $\mathrm{Re}(Q) < -1$, and if

$$\|E\|_{H^1_\alpha(D)\to H^1_\alpha(\Omega_{2h})} < \inf_D |\mathrm{Re}(Q)|_2^{1/2}, \tag{2.37}$$

then there exists a constant $C > 0$ and a compact operator K_- on $H^1_{\alpha,Q}(D)$ such that

$$-\mathrm{Re}\,[a_Q(v - L(Q\nabla v),\, v)] \geq C\|v\|^2_{H^1_{\alpha,Q}(D)} - \mathrm{Re}\langle K_- v,\, v\rangle_{H^1_{\alpha,Q}(D)}, \quad v \in H^1_{\alpha,Q}(D). \tag{2.38}$$

Remark 2.4.6. *If $\mathrm{Im}(Q) = 0$ in D, then both statements* (2.36) *and* (2.38) *are nothing but standard Gårding estimates: The form a_Q defines an inner product on $H^1_{\alpha,Q}(D)$, and, e.g.,* (2.36) *can be rewritten as $\mathrm{Re}\big\langle v - L(Q\nabla v),\, v\big\rangle \geq \|v\|^2 - \mathrm{Re}\langle K_+ v,\, v\rangle$ for $v \in H^1_{\alpha,Q}(D)$.*

Proof. (a) We start with the case $\mathrm{Re}(Q) > 0$ in D. Let $v \in H^1_{\alpha,Q}(D)$ and define w by

$$w = L_{\mathrm{i}}(Q\nabla v) = \mathrm{div}\int_D G_{\mathrm{i}}(\cdot - y)[Q(y)\,\nabla v(y)]\,\mathrm{d}y \quad \text{in } \Omega. \tag{2.39}$$

Then $w \in H^1_\alpha(\Omega)$ decays exponentially to zero as $|x_2|$ tends to infinity. Moreover, $\Delta w - w = -\mathrm{div}(Q\nabla v)$ holds in Ω in the weak sense due to Lemma 2.3.6, that is,

$$\int_\Omega \big[\nabla w \cdot \nabla\overline{\psi} + w\overline{\psi}\big]\,\mathrm{d}x = -\int_D Q\nabla v \cdot \nabla\overline{\psi}\,\mathrm{d}x \quad \text{for all } \psi \in H^1_\alpha(\Omega). \tag{2.40}$$

Setting $\psi = w$, we find that $-\mathrm{Re}\int_D Q\nabla v \cdot \nabla\overline{w}\,\mathrm{d}x = \|w\|^2_{H^1(\Omega)}$. Hence,

$$\begin{aligned}
&\mathrm{Re}\,[a_Q(v - L_{\mathrm{i}}(Q\nabla v),\, v)]\\
&\quad= \int_D \big[\mathrm{Re}(Q)\nabla v \cdot \nabla\overline{v} + |v|^2\big]\,\mathrm{d}x - \mathrm{Re}\int_D \big[Q\nabla w \cdot \nabla\overline{v} + w\overline{v}\big]\,\mathrm{d}x\\
&\quad= \int_D \big[|\sqrt{\mathrm{Re}(Q)}\nabla v|^2 + |v|^2 - \mathrm{Re}(w\overline{v})\big]\,\mathrm{d}x + \int_\Omega \big[|\nabla w|^2 + |w|^2\big]\,\mathrm{d}x\\
&\quad\geq \|v\|^2_{H^1_{\alpha,Q}(D)} - \frac{1}{2}\|v\|^2_{L^2(D)} + \frac{1}{2}\int_D \big[|v|^2 + |w|^2 - 2\mathrm{Re}(w\overline{v})\big]\,\mathrm{d}x\,,
\end{aligned}$$

where the last term on the right is positive. In consequence,

$$\mathrm{Re}\,[a_Q(v - L(Q\nabla v),\, v)] \geq \|v\|^2_{H^1_{\alpha,Q}(D)} - \frac{1}{2}\langle v,\, v\rangle_{L^2(D)} - \mathrm{Re}\,[a_Q((L - L_{\mathrm{i}})(Q\nabla v),\, v)]$$

for all $v \in H^1_{\alpha,Q}(D)$. Due to Lemma 2.4.4 and Rellich's embedding lemma there exists a compact operator K_1 on $H^1_{\alpha,Q}(D)$ such that $\langle v, v\rangle_{L^2(D)} = 2\mathrm{Re}\langle K_1 v,\, v\rangle_{H^1_{\alpha,Q}(D)}$. Further, the operator $(L - L_{\mathrm{i}})(Q\nabla\cdot)$ is compact on $H^1_\alpha(D)$ due to the smoothness of the kernel shown in Appendix A. Hence the operator K_2 defined by $\langle K_2 v,\, v\rangle_{H^1_{\alpha,Q}(D)} = a_Q((L - L_{\mathrm{i}})(Q\nabla v),\, v)$ is compact on $H^1_{\alpha,Q}(D)$ due to Lemma 2.4.4 and the boundedness of the embedding $H^1_\alpha(D) \subset H^1_{\alpha,Q}(D)$. Setting $K_+ := K_1 + K_2$, we obtain the claimed generalized Gårding inequality.

(b) Now we consider the case that $\mathrm{Re}(Q) < -1$ in D, and assume additionally that (2.37) holds. As in the first part of the proof, the variational formulation (2.40) for w, defined as in (2.39), yields that

$$\begin{aligned}
&-\mathrm{Re}\,[a_Q(v - L_{\mathrm{i}}(Q\nabla v),\, v)] \\
&\quad = \mathrm{Re}\int_D \big[\mathrm{Re}(Q)\nabla v\cdot\nabla\overline{v} - |v|^2 - Q\nabla w\cdot\nabla\overline{v} + w\overline{v}\big]\,\mathrm{d}x \\
&\quad = -\int_D \big[|\sqrt{|\mathrm{Re}(Q)|}\nabla v|^2 + |v|^2\big]\,\mathrm{d}x \,+ \|w\|^2_{H^1_\alpha(\Omega)} + \mathrm{Re}\int_D w\overline{v}\,\mathrm{d}x \\
&\quad \geq \|w\|^2_{H^1_\alpha(\Omega)} - \|v\|^2_{H^1_{\alpha,Q}(D)} + \mathrm{Re}\int_D w\overline{v}\,\mathrm{d}x\,.
\end{aligned}$$

We plug in $\psi = -E(v)$ into (2.40) and take the real part of that equation, to find that

$$\begin{aligned}
\|\sqrt{|\mathrm{Re}(Q)|}\nabla v\|^2_{L^2(D,\mathbb{C}^2)} &\leq \|w\|_{H^1_\alpha(\Omega)}\|E(v)\|_{H^1_\alpha(\Omega)} \\
&\leq \|E\|_{H^1_\alpha(D)\to H^1_\alpha(\Omega_{2h})}\,\|w\|_{H^1_\alpha(\Omega)}\|v\|_{H^1_\alpha(D)} \\
&\leq \|E\|\,\|w\|_{H^1_\alpha(\Omega)}\left(\||\sqrt{|\mathrm{Re}(Q)|}^{-1}|_2\|_{L^\infty(D)}\|v\|_{H^1_{\alpha,Q}(D)} + \|v\|_{L^2(D)}\right).
\end{aligned}$$

For $x \in D$, the spectral matrix norm $|\sqrt{|\mathrm{Re}(Q)|}^{-1}(x)|_2$ of the inverse of $\sqrt{|\mathrm{Re}(Q)|}(x)$ equals the reciprocal value $\lambda_{\min}(x)^{-1/2}$ ($\lambda_{\min,\max}$ are the smallest/largest eigenvalue, in magnitude, of $\mathrm{Re}(Q)$, see (2.29)). Note that

$$\begin{aligned}
\||\sqrt{|\mathrm{Re}(Q)|}^{-1}|_2\|^{-1}_{L^\infty(D)} &= [\sup_{x\in D}\lambda_{\min}(x)^{-1/2}]^{-1} = \inf_{x\in D}\lambda_{\min}(x)^{1/2} \leq \sup_{x\in D}\lambda_{\max}(x)^{1/2} \\
&\leq [1 + \sup_{x\in D}\lambda_{\max}(x)]^{1/2} = [1 + \||\mathrm{Re}(Q)|_2\|_{L^\infty(D)}]^{1/2}.
\end{aligned}$$

Next, we estimate that

$$\begin{aligned}
\|v\|^2_{H^1_{\alpha,Q}(D)} - \big[1 + \||\mathrm{Re}(Q)|_2\|_{L^\infty(D)}\big]\|v\|^2_{L^2(D)} &\leq \|v\|^2_{H^1_{\alpha,Q}(D)} - \|v\|^2_{L^2(D)} \\
&\leq \|E\|\,\||\sqrt{|\mathrm{Re}(Q)|}^{-1}|_2\|_{L^\infty(D)}\,\|w\|_{H^1_\alpha(\Omega)} \\
&\qquad \left(\|v\|_{H^1_{\alpha,Q}(D)} + [1 + \||\mathrm{Re}(Q)|_2\|_{L^\infty(D)}]^{1/2}\|v\|_{L^2(D)}\right).
\end{aligned}$$

Dividing by the term in brackets on the right, we obtain that

$$\|v\|_{H^1_{\alpha,Q}(D)} - \big[1 + \||\mathrm{Re}(Q)|_2\|_\infty\big]^{1/2}\|v\|_{L^2(D)} \leq \|E\|\,\||\sqrt{|\mathrm{Re}(Q)|}^{-1}|_2\|_{L^\infty(D)}\,\|w\|_{H^1_\alpha(\Omega)}. \quad (2.41)$$

Note that the constant

$$c := \|E\|_{H^1_\alpha(D)\to H^1_\alpha(\Omega_{2h})}\ \||\sqrt{|\mathrm{Re}(Q)|}^{-1}|_2\|_{L^\infty(D)}$$

is by assumption (2.37) less than one. If we set for a moment, $C = [1 + \||\mathrm{Re}(Q)|_2\|_\infty]^{1/2}$ then (2.41) and Cauchy's inequality imply that

$$\begin{aligned} c^2\|w\|^2_{H^1_\alpha(\Omega)} &\geq \|v\|^2_{H^1_{\alpha,Q}(D)} + C^2\|v\|^2_{L^2(D)} - 2C\|v\|_{H^1_{\alpha,Q}(D)}\|v\|_{L^2(D)} \\ &\geq (1-\varepsilon^2)\|v\|^2_{H^1_{\alpha,Q}(D)} + C^2(1-1/\varepsilon^2)\|v\|^2_{L^2(D)}, \qquad \varepsilon \in (0,1). \end{aligned}$$

In consequence,

$$\begin{aligned} -\mathrm{Re}\,[a_Q(v - L(Q\nabla v),\, v)] &\geq \left(\frac{1-\varepsilon^2}{c^2} - 1\right)\|v\|^2_{H^1_{\alpha,Q}(D)} \\ &\quad - \mathrm{Re}\int_D w\overline{v}\,\mathrm{d}x + C^2\frac{\varepsilon^2-1}{(c\varepsilon)^2}\|v\|^2_{L^2(D)} + \mathrm{Re}\,[a_Q((L-L_\mathrm{i})(Q\nabla v),\, v)] \end{aligned} \tag{2.42}$$

for $\varepsilon \in (0,1)$. Since $c < 1$ there exists $\varepsilon \in (0,1)$ such that $1-\varepsilon^2 > c^2$, that is, $(1-\varepsilon^2)/c^2 - 1 > 0$. The last three terms on the right-hand side of (2.42) can then be treated as compact perturbations, in a similar way as in the proof of the first part. □

Remark 2.4.7. *(a) If* $\mathrm{Re}(Q) < -1$ *in* D*, then solutions to* $\mathrm{div}((I_2 + Q)\nabla u) + k^2 u$ *decay exponentially in* D*. If not only the electric permittivity but also the magnetic permeability changes sign, then the corresponding solution will not decay, yielding a possibly more interesting metamaterial. Volume integral equations for such structures yield operator equations combining* L *and* V*, see, e.g., [73]. Since* V *is compact on* H^1*, the above Gårding inequalities extend to this setting. For simplicity, we restrict ourselves here to the non-magnetic case.*

(b) In the last result, we assumed that the sign of $\mathrm{Re}(Q)$ *is constant in* D*. It is possible to treat sign changes of the contrast function in* D*, but the simple choice* $\psi = -E(v)$ *that we plugged in the second part of the proof into* (2.40) *has to be adapted.*

It is a standard result that the Gårding inequalities from the last theorem imply the following consequences for the solvability of the integral equation and the scattering problem.

Theorem 2.4.8. *Suppose that the assumptions of Theorem 2.4.5(a) or (b) hold, that the boundedness condition* (2.32) *holds, and that the homogeneous equation* $v - L(Q\nabla v) = 0$ *in* $H^1_{\alpha,Q}(D)$ *has only the trivial solution. Then* (2.28) *has a unique solution for all* $f \in L^2(D, \mathbb{C}^2)$*. If* $f = Q\nabla u^i$*, then this solution can be extended by the right-hand side of* (2.28) *to a solution to the variational formulation of the scattering problem* (2.13)*. Especially, if the integral equation is uniquely solvable in* $H^1_{\alpha,Q}(D)$*, then* (2.13) *is uniquely solvable in* $H^1_\alpha(\Omega_h)$*.*

2.5 Gårding Inequalities in Standard Sobolev Spaces

The generalized Gårding inequalities from the last section imply Gårding inequalities in the standard unweighted periodic Sobolev space $H^1_\alpha(D)$ if the material parameter ε_{r} (or, equivalently, the contrast), is isotropic. Hence, in this section we assume that the contrast is a scalar real-valued function q, that is,

$$Q = qI_2 \quad \text{in } \Omega.$$

As above, $\overline{D}$ is the support of q. As mentioned in the introduction this assumption is essential for the proof of Lemma 2.5.1. Under this assumption we denote the weighted Sobolev spaces from (2.30) by $H^1_{\alpha,q}(D)$, and their norm by

$$\|u\|_{H^1_{\alpha,q}(D)} := \Big(\|\sqrt{|\mathrm{Re}(q)|}\nabla u\|^2_{L^2(D,\mathbb{C}^2)} + \|u\|^2_{L^2(D)}\Big)^{1/2}.$$

Since q is real-valued, the form a_q from (2.31) is the inner product of $H^1_{\alpha,q}(D)$, and the generalized Gårding inequalities from the last section directly transform to standard ones. Again, we assume that the sign of q is constant in D. Since we use regularity theory to prove compactness of certain commutators, we will need to require more smoothness of q and D compared to the results in the last section.

Lemma 2.5.1. *Assume that D is a domain of class $C^{2,1}$ and that $\mu \in C^{2,1}(\overline{D})$ is 2π-periodic in x_1. Then $T : H^1_\alpha(D) \to H^1_\alpha(D)$ defined by $Tv := \mathrm{div}\big[\mu V(q\nabla(v/\mu)) - V(q\nabla v)\big]$ is a compact operator.*

Proof. We denote by $\mu^* \in C^{2,1}(\overline{\Omega_h})$ a periodic extension of $\mu \in C^{2,1}(\overline{D})$ to Ω_h (see (2.35) on periodic extension operator). Then $\mu^*|_D = \mu$. Consider the two α-quasiperiodic functions

$$w_1 = V(q\nabla(v/\mu)) \quad \text{and} \quad w_2 = V(q\nabla v) \quad \text{in } \Omega_h.$$

Both functions satisfy differential equations,

$$\Delta(\mu^* w_1) + k^2(\mu^* w_1) = \begin{cases} -q\mu\nabla(v/\mu) + 2\nabla\mu\cdot\nabla w_1 + w_1\Delta\mu & \text{in } D, \\ 2\nabla\mu^*\cdot\nabla w_1 + w_1\Delta\mu^* & \text{in } \Omega_h\setminus\overline{D}, \end{cases}$$

and $\Delta w_2 + k^2 w_2 = -q\nabla v$ in D and $\Delta w_2 + k^2 w_2 = 0$ in $\Omega_h \setminus \overline{D}$. Hence, $w = \mu^* w_1 - w_2$ solves

$$\Delta w + k^2 w = \begin{cases} -q\mu\nabla(1/\mu)v + 2\nabla\mu\cdot\nabla w_1 + w_1\Delta\mu =: g_1 & \text{in } D, \\ w_1\Delta\mu^* + 2\nabla\mu^*\cdot\nabla w_1 =: g_2 & \text{in } \Omega_h\setminus\overline{D}. \end{cases}$$

The functions g_1 and g_2 belong to $H^1_\alpha(D)$ and $H^1_\alpha(\Omega_h\setminus\overline{D})$, respectively. Their norms in these spaces are bounded by the norm of μ in $C^{2,1}(\overline{D})$ times the norm of v in $H^1_\alpha(D)$. Due to Lemma 2.3.5, the jump of the trace and the normal trace of $w_{1,2}$ across ∂D vanishes. Hence, the Cauchy data of w are also continuous across the boundary of D.

Since the volume potential V is bounded from $L^2(D)$ into $H^2_\alpha(D)$, it is clear that w belongs to $H^2_\alpha(D)$. The smoothness assumptions on D and μ moreover allow to apply elliptic transmission regularity results [81, Theorem 4.20] to conclude that w is even smoother than H^2. These regularity results will in turn imply the compactness of the operator $T : v \mapsto \mathrm{div} w$ on $H^1_\alpha(D)$. Since [81, Theorem 4.20] is formulated for a bounded domain, we briefly mention how to extend this result to the periodic setting.

First, we extend w by periodicity to $\Omega'_h := (-3\pi, 3\pi) \times (-h, h)$ and proceed analogously with $g_{1,2}$. Then we choose a finite open cover $\{W_j\}_{j=1}^J$ consisting of smooth domains $W_j \subset \Omega'_h$ such that $\partial D \cap \Omega \subset \bigcup_{j=1}^J W_j$. In these smooth domains, we can then apply [81, Theorem 4.20] to obtain that

$$\|w\|_{H^3(W_j)} \leq C \left[\|w\|_{H^1_\alpha(\Omega_h)} + \|g_1\|_{H^1_\alpha(D)} + \|g_2\|_{H^1_\alpha(\Omega_h \setminus \overline{D})} \right].$$

Combining this estimate with an interior regularity result (e.g., [81, Theorem 4.18]) in a set W_0 such that $\overline{D} \subset \cup_{j=0}^J W_j$ (see Figure 2.3), we finally obtain that

$$\|w\|_{H^3(D)} \leq C \left[\|w\|_{H^1(\Omega_h)} + \|g_1\|_{H^1(D)} + \|g_2\|_{H^1(\Omega_h \setminus \overline{D})} \right] \leq C \|v\|_{H^1_\alpha(D)}.$$

□

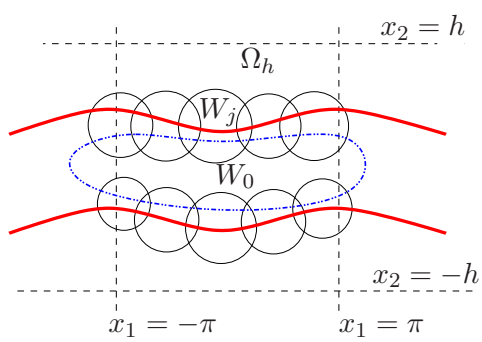


Figure 2.3: The sets W_j cover the domain D (one period of the support of the contrast q). These sets are used in the proof of Theorem 2.5.1.

The following lemma shows that the Gårding inequalities in the weighted spaces $H^1_{\alpha,q}(D)$ can be transformed into estimates in $H^1_\alpha(D)$ if, roughly speaking, the real-valued contrast q is smooth enough and if $(\nabla q)/q$ is bounded.

Theorem 2.5.2. *Assume that the scalar contrast q is real-valued, that $|q| \geq q_0 > 0$ in D, and that $\sqrt{|q|} \in C^{2,1}(\overline{D})$. Moreover, assume that D is of class $C^{2,1}$.*

(a) If $q > 0$ there exists a compact operator K_+ on $H^1_\alpha(D)$ such that

$$\mathrm{Re}\langle v - L(q\nabla v), v\rangle_{H^1_\alpha(D)} \geq \|v\|^2_{H^1_\alpha(D)} - \mathrm{Re}\langle K_+ v,\, v\rangle_{H^1_\alpha(D)}, \qquad v \in H^1_\alpha(D).$$

(b) If $q < 0$, and if

$$\|E\|_{H^1_\alpha(D)\to H^1_\alpha(\Omega_{2h})} < \inf_D |q|^{1/2}, \tag{2.43}$$

then there exists a compact operator K_- on $H^1_\alpha(D)$ such that

$$-\mathrm{Re}\langle v - L(q\nabla v), v\rangle_{H^1_\alpha(D)} \geq C\|v\|^2_{H^1_\alpha(D)} - \mathrm{Re}\langle K_- v,\, v\rangle_{H^1_\alpha(D)}, \qquad v \in H^1_\alpha(D),$$

where C is the constant from (2.38).

Proof. We only prove case (a) here, supposing that $q > q_0 > 0$ in D. The proof for case (b) is analogous, essentially one needs to replace $\sqrt{q}$ by $\sqrt{|q|}$. For simplicity, let us from now on abbreviate

$$\mu := \sqrt{q} \in C^{2,1}(\overline{D}).$$

Choose an arbitrary $u \in H^1_\alpha(D)$ and consider $v = u/\mu$. Our assumptions on q imply that $v \in H^1_{\alpha,q}(D)$, since $\|v\|^2_{H^1_{\alpha,q}(D)} \leq (2 + \|1/\mu\|^2_\infty + 2\|(\nabla\mu)/\mu\|^2_\infty)\|u\|^2_{H^1_\alpha(D)}$. In Theorem 2.4.5(a) (see also Remark 2.4.6) we showed that $\mathrm{Re}\langle v - L(q\nabla v),\, v\rangle_{H^1_{\alpha,q}(D)} \geq \|v\|^2_{H^1_{\alpha,q}(D)} - \mathrm{Re}\langle K_1 v,\, v\rangle_{H^1_{\alpha,q}(D)}$ for a compact operator K_1 on $H^1_{\alpha,q}(D)$. This implies that

$$\begin{aligned}\mathrm{Re}\langle u - L(q\nabla u),\, u\rangle_{H^1_\alpha(D)} \geq \|u\|^2_{H^1_\alpha(D)} &+ \mathrm{Re}\langle K_1(u/\mu),\, u/\mu\rangle_{H^1_{\alpha,q}(D)} \\ &+ \mathrm{Re}\langle K_2 u,\, \nabla u\rangle_{L^2(D,\mathbb{C}^2)} + \mathrm{Re}\langle K_3 u,\, u\rangle_{L^2(D)},\end{aligned}$$

with operators

$$K_2 u = \nabla\Big[\mathrm{div}\big[\mu V(q\nabla(u/\mu)) - V(q\nabla u)\big]\Big] - \nabla\Big[\nabla\mu\cdot V(q\nabla(u/\mu))\Big] + (\nabla\mu)L(q\nabla(u/\mu))$$

and

$$K_3 u = q\nabla(1/\mu)\cdot\big[\nabla L(q\nabla(u/\mu))\big] + L(q\nabla(u/\mu))/\mu - L(q\nabla u).$$

Lemma 2.5.1, the smoothness of q, and the boundedness of V and L from $L^2(D)$ and $L^2(D,\mathbb{C}^2)$ into $H^2_\alpha(D)$ and $H^1_\alpha(D)$, respectively, show that K_2 and K_3 are compact and bounded from $H^1_\alpha(D)$ into $L^2(D)$, respectively. Then the compact embedding $H^1_\alpha(D) \subset L^2(D)$ and Lemma 2.4.4 imply the claim. □

2.6 Periodization of the Integral Equation

In this section we reformulate the volume integral equation

$$u - L(q\nabla u) = L(f) \quad \text{in } H^1_\alpha(D) \tag{2.44}$$

in a periodic setting and show the equivalence of the periodized equation and the original one. The purpose of this periodization is that the resulting integral operator is, roughly speaking, diagonalized by trigonometric polynomials. This allows to use fast FFT-based schemes to discretize the periodized operator and iterative schemes to solve the discrete system. We

also prove Gårding inequalities for the periodized integral equation, which turns out to be involved. These estimates are crucial to establish convergence of the discrete schemes later on.

Recall that the periodized kernel $\mathcal{K}_h$ defined in (2.15) is not smooth at the boundaries $\{x_2 = \pm h\}$. To prove Gårding inequalities for the periodized integral equation, we additionally need to smoothen the kernel. For $R > 2h$ we choose a function $\chi \in C^3(\mathbb{R})$ that is $2R$-periodic, that satisfies $0 \leq \chi \leq 1$ and $\chi(x_2) = 1$ for $|x_2| \leq 2h$, and such that $\chi(R)$ vanishes up to order three, $\chi^{(j)}(R) = 0$ for $j = 1, 2, 3$ (compare Figure 2.4)).

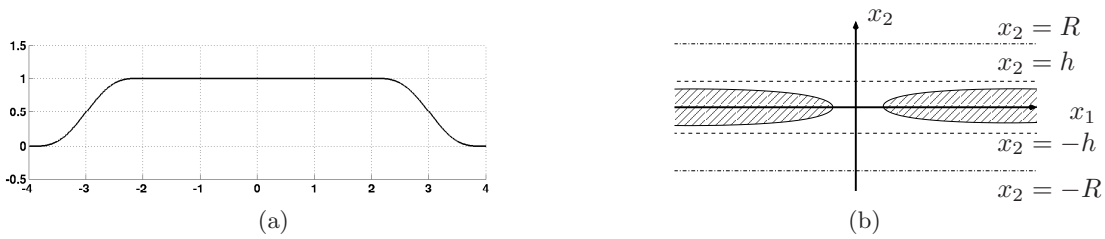


Figure 2.4: (a) The periodic function χ equals to one for $|x_2| \leq 2h$, and it vanishes at $\pm R$ up to order three. In this sketch, $h = 1$ and $R = 4$. (b) The support of the contrast (shaded) is included in Ω_h, and $R > 2h$.

Let us define a smoothed kernel $\mathcal{K}_{\mathrm{sm}}$ by

$$\mathcal{K}_{\mathrm{sm}}(x) = \chi(x_2)\mathcal{K}_R(x) \quad \text{for } x \in \mathbb{R}^2, \quad x \neq \left[2\pi m,\, 2Rn\right]^\top,\ m, n \in \mathbb{Z}, \tag{2.45}$$

where $\mathcal{K}_R$ is the kernel from (2.15). Note that $\mathcal{K}_{\mathrm{sm}}$ is α-quasiperiodic in x_1, $2R$-periodic in x_2, and a smooth function on its domain of definition (that is, away from the singularity).

Lemma 2.6.1. *The integral operator $L_{\mathrm{p}} : L^2(\Omega_R)^2 \to H^1_{\alpha,\mathrm{p}}(\Omega_R)$ defined by*

$$L_{\mathrm{p}} f = \operatorname{div} \int_D \mathcal{K}_{sm}(\cdot - y) f(y)\, \mathrm{d}y$$

is a bounded operator.

Proof. We split the integral operator in two parts,

$$\begin{aligned} L_{\mathrm{p}} f &= \operatorname{div} \int_D \mathcal{K}_{\mathrm{sm}}(\cdot - y) f(y)\, \mathrm{d}y = \operatorname{div} \int_D \chi(\cdot - y_2)\mathcal{K}_R(\cdot - y) f(y)\, \mathrm{d}y \\ &= \operatorname{div} \int_D \mathcal{K}_R(\cdot - y) f(y)\, \mathrm{d}y + \operatorname{div} \int_D [\chi(\cdot - y_2) - 1]\mathcal{K}_R(\cdot - y) f(y)\, \mathrm{d}y\,. \end{aligned}$$

By Theorem 2.3.4, the integral operator with the kernel $\mathcal{K}_R$ is bounded from $L^2(\Omega_R)^2$ into $H^1_\alpha(\Omega_R)$. Further, the definition of χ shows that $\chi(x_2 - y_2) - 1 = 0$ for $|x_2| \leq h$ and $y \in D$. The kernel $(\chi - 1)\mathcal{K}_R$ is hence smooth in Ω_R, and the corresponding integral operator is compact from $L^2(\Omega_R)^2$ into $H^1_\alpha(\Omega_R)$. Hence, L_{p} is bounded from $L^2(\Omega_R)^2$ into $H^1_\alpha(\Omega_R)$. Periodicity of the kernel $\mathcal{K}_{\mathrm{sm}}$ in the second component of its argument finally implies that $L_{\mathrm{p}} f$ belongs to $H^1_{\alpha,\mathrm{p}}(\Omega_R) \subset H^1_\alpha(\Omega_R)$. $\square$

Let us now consider the periodized integral equation

$$u - L_{\mathrm{p}}(q\nabla u) = L_{\mathrm{p}}(f) \qquad \text{in } H^1_{\alpha,\mathrm{p}}(\Omega_R). \tag{2.46}$$

Theorem 2.6.2. *(a) For $f \in L^2(\Omega_R)^2$, $L_{\mathrm{p}}(f)$ equals $L(f)$ in Ω_h.*

(b) Equation (2.44) is uniquely solvable in $H^1_\alpha(D)$ for any right-hand side $f \in L^2(D)^2$ if and only if (2.46) is uniquely solvable in $H^1_{\alpha,\mathrm{p}}(\Omega_R)$ for any right-hand side $f \in L^2(\Omega_R)^2$.

(c) If $q \in C^{2,1}(\overline{D})$ and if $f = q\nabla u^i$ for a smooth α-quasiperiodic function u^i, then any solution to (2.46) belongs to $H^s_{\alpha,\mathrm{p}}(\Omega_R)$ for any $s < 3/2$.

Proof. (a) For all x and $y \in \Omega_R$ such that $|x_2 - y_2| \le 2h$ it holds that $\mathcal{K}_{\mathrm{sm}}(x-y) = \chi(x_2 - y_2)\mathcal{K}_R(x-y) = G_k(x-y)$. In particular, for $x \in \Omega_h$ and $y \in D \subset \Omega_h$ it holds that $|x_2 - y_2| \le 2h$. Consequently,

$$\begin{aligned}(L_{\mathrm{p}}(f))(x) &= \operatorname{div} \int_D \mathcal{K}_{\mathrm{sm}}(x-y) f(y)\,\mathrm{d}y \\ &= \operatorname{div} \int_D G_k(x-y) f(y)\,\mathrm{d}y = (L(f))(x), \qquad x \in \Omega_h.\end{aligned}$$

(b) Assume that $u \in H^1_\alpha(D)$ solves (2.44) and define $\tilde{u} \in H^1_{\alpha,\mathrm{p}}(\Omega_R)$ by $\tilde{u} = L_{\mathrm{p}}(q\nabla u + f)$ (where we extended f by zero outside D). Since u solves (2.44), and due to part (a), we find that $\tilde{u}|_D = u$. Hence $L_{\mathrm{p}}(q\nabla\tilde{u} + f) = L_{\mathrm{p}}(q\nabla u + f)$ in $H^1_{\alpha,\mathrm{p}}(\Omega_R)$, which yields that

$$\tilde{u} = L_{\mathrm{p}}(q\nabla\tilde{u} + f) \text{ in } H^1_{\alpha,\mathrm{p}}(\Omega_R). \tag{2.47}$$

Now, if $f \in L^2(D)^2$ vanishes, then uniqueness of a solution to (2.44) implies that $u \in H^1_\alpha(D)$ vanishes, too. Obviously, $\tilde{u} = L_{\mathrm{p}}(q\nabla u)$ vanishes, and hence (2.47) is uniquely solvable. The converse follows directly from (a).

(c) Assume that $u \in H^1_{\alpha,\mathrm{p}}(\Omega_R)$ solves (2.46) for $f = q\nabla u^i$. Part (a) implies that the restriction of u to Ω_h solves $u - L(q\nabla u) = L(q\nabla u^i)$ in $H^1_\alpha(\Omega_h)$. Hence, Lemma 2.3.5 implies that u is a weak α-quasiperiodic solution to $\operatorname{div}((1+q)\nabla u) + k^2 u = -\operatorname{div}(q\nabla u^i)$ in Ω_h. Transmission regularity results imply that u belongs to $H^2_\alpha(D) \cap H^2_\alpha(\Omega_h \setminus \overline{D})$, and it is well-known that this implies that $u \in H^s_\alpha(\Omega_h)$ for $s < 3/2$ (see, e.g., [48, Section 1.2]). The function u is even smooth in $\Omega_R \setminus \Omega_{h-\varepsilon}$: Recall that h was chosen such that $\overline{D} \subset \Omega_h$. Hence, there is $\varepsilon > 0$ such that $D \subset \Omega_{h-2\varepsilon}$, and

$$u(x) = L_{\mathrm{p}}(q\nabla(u + u^i))(x) = \operatorname{div} \int_D \mathcal{K}_{\mathrm{sm}}(x-y) q(y) \nabla(u(y) + u^i(y))\,\mathrm{d}y\,, \quad x \in \Omega_R \setminus \Omega_{h-\varepsilon}$$

shows that the restriction of u to $\Omega_R \setminus \Omega_{h-\varepsilon}$ is a smooth α-quasiperiodic function, since the kernel of the above integral operator is smooth. □

Next we prove that the operator $I - L_{\mathrm{p}}(q\nabla\cdot)$ from (2.46) satisfies a Gårding inequality in $H^1_{\alpha,\mathrm{p}}(\Omega_R)$.

Theorem 2.6.3. *Assume that $\sqrt{q} \in C^{2,1}(\overline{D})$, that $q \geq q_0 > 0$, and that D is of class $C^{2,1}$. Then there exists $C > 0$ and a compact operator K on $H^1_{\alpha,\mathrm{p}}(\Omega_R)$ such that*

$$\mathrm{Re}\langle v - L_{\mathrm{p}}(q\nabla v), v\rangle_{H^1_{\alpha,\mathrm{p}}(\Omega_R)} \geq \|v\|^2_{H^1_{\alpha,\mathrm{p}}(\Omega_R)} - \mathrm{Re}\langle Kv,\, v\rangle_{H^1_{\alpha,\mathrm{p}}(\Omega_R)}, \quad v \in H^1_{\alpha,\mathrm{p}}(\Omega_R). \tag{2.48}$$

Remark 2.6.4. *The idea of the proof is to split the integrals defining the inner product on the left of (2.48) into the three integrals on D, $\Omega_h \setminus \overline{D}$, and on $\Omega_R \setminus \overline{\Omega_h}$. For the term on D one exploits the Gårding inequalities from Theorem 2.5.2. The terms on $\Omega_h \setminus \overline{D}$ and on $\Omega_R \setminus \overline{\Omega_h}$ can be shown to be compact or positive perturbations.*

Proof. Let $v \in H^1_{\alpha,\mathrm{p}}(\Omega_R)$. First, we split up the integrals arising from the inner product on the left of (2.48) into integrals on D, on $\Omega_h \setminus \overline{D}$, and on $\Omega_R \setminus \overline{\Omega_h}$. Second, we use the Gårding inequality from Theorem 2.5.2 to find that

$$\begin{aligned}\mathrm{Re}\langle v - L_{\mathrm{p}}(q\nabla v), v\rangle_{H^1_{\alpha,\mathrm{p}}(\Omega_R)} \geq{}& \|v\|^2_{H^1_\alpha(D)} + \langle Kv,\, v\rangle_{H^1_\alpha(D)} + \|v\|^2_{H^1_\alpha(\Omega_R\setminus\overline{D})} \\ &- \mathrm{Re}\big[\langle L_{\mathrm{p}}(q\nabla v), v\rangle_{H^1_\alpha(\Omega_R\setminus\overline{\Omega_h})} + \langle L_{\mathrm{p}}(q\nabla v), v\rangle_{H^1_\alpha(\Omega_h\setminus\overline{D})}\big]\end{aligned} \tag{2.49}$$

with a compact operator K on $H^1_\alpha(D)$. Further, the evaluation of $L_{\mathrm{p}}(q\nabla\cdot)$ on $\Omega_R \setminus \overline{\Omega_h}$ defines a compact integral operator mapping $H^1_\alpha(D)$ to $H^1_\alpha(\Omega_R \setminus \overline{\Omega_h})$, because the (periodic) kernel of this integral operator is smooth. (This argument requires the smooth kernel $\mathcal{K}_{\mathrm{sm}}$ introduced in the beginning of this section.) Lemma 2.4.4 then allows to reformulate the corresponding term in (2.49) in the way stated in the claim. Unfortunately, the last term in (2.49) does not yield a compact sesquilinear form and needs a more detailed investigation.

For $x \in \Omega_h \setminus \overline{D}$ and $y \in D$ the kernel $\mathcal{K}_{\mathrm{sm}}(x-y)$ equals $G_k(x-y)$, which is a smooth function of $x \in \Omega_h \setminus \overline{D}$ and $y \in D$. Moreover, $\Delta G_k(x-y) + k^2 G_k(x-y) = 0$ for $x \neq y$. Since $\nabla_x G_k(x-y) = -\nabla_y G_k(x-y)$, an integration by parts in $\Omega_h \setminus \overline{D}$ shows that

$$\begin{aligned}L(q\nabla v)(x) =& \mathrm{div} \int_D G_k(x-y)q(y)\nabla v(y)\,\mathrm{d}y \\ =& -\int_D \nabla_y G_k(x-y)\cdot\nabla(qv)(y)\,\mathrm{d}y + \int_D \nabla_y G_k(x-y)\cdot\nabla q(y)v(y)\,\mathrm{d}y \\ =& -k^2\int_D G_k(x-y)q(y)v(y)\,\mathrm{d}y - L(v\nabla q)(x) \\ &- \int_{\partial D} \frac{\partial G_k(x-y)}{\partial\nu(y)}\gamma_{\mathrm{int}}(q)(y)\gamma(v)(y)\,\mathrm{d}s \qquad \text{for } x \in \Omega_h \setminus \overline{D},\end{aligned}$$

where ν is the exterior normal vector to D. The integral operator appearing in the last term of the last equation is the double layer potential DL,

$$\mathrm{DL}(\psi) = \int_{\partial D} \frac{\partial G_k(\cdot - y)}{\partial\nu(y)}\psi(y)\,\mathrm{d}s \qquad \text{in } \Omega \setminus \partial D.$$

It is well-known that DL defines a bounded operator from $H^{1/2}_\alpha(\partial D)$ into $H^1_\alpha(\Omega_R \setminus \overline{D})$ and into $H^1_\alpha(D)$ (see, e.g., [4]). This implies that the jump of the double-layer potential

$$T\psi := [\mathrm{DL}\psi]_{\partial D} = \gamma_{\mathrm{ext}}(\mathrm{DL}\psi) - \gamma_{\mathrm{int}}(\mathrm{DL}\psi)$$

from the outside of D to the inside of D is a bounded operator on $H^{1/2}_\alpha(\partial D)$. It is well-known that in our case T is even a compact operator on $H^{1/2}_\alpha(\partial D)$, since D is of class $C^{2,1}$. Additionally, the equality $\gamma_{\rm int}({\rm DL}\psi) = -\psi/2 + T\psi$ holds for $\psi \in H^{1/2}_\alpha(\partial D)$.

For $v \in H^1_{\alpha,\rm p}(\Omega_R)$,

$$-\langle \nabla L(q\nabla v),\, \nabla v\rangle_{L^2(\Omega_h\setminus\overline{D})} = \langle k^2\nabla V(qv) + \nabla L(v\nabla q) + \nabla {\rm DL}(\gamma_{\rm int}(qv)),\, \nabla v\rangle_{L^2(\Omega_h\setminus\overline{D})}. \quad (2.50)$$

The mapping properties of V shown in Lemma 2.3.5 and the smoothness of q imply that $v \mapsto k^2\nabla V(qv) + \nabla L(v\nabla q)$ is compact from $H^1_{\alpha,\rm p}(\Omega_R)$ into $L^2(D)$. To finish the proof we show that the last term in (2.50) can be written as a sum of a positive and compact term. For simplicity, we define $w = {\rm DL}(\gamma_{\rm int}(qv))$ and note that $-v/2 = [\gamma_{\rm int}(w) - T(\gamma_{\rm int}(qv))]/\gamma_{\rm int}(q)$ on ∂D. Since it plays no role whether the normal derivative $\partial w/\partial\nu$ is taken from the inside or from the outside of D, we skip writing down the trace operators for the normal derivative. Then

$$\begin{aligned}\langle \nabla {\rm DL}(qv), \nabla v\rangle_{L^2(\Omega_h\setminus\overline{D})} &= \int_{\Omega_h\setminus\overline{D}} \nabla w\cdot\nabla\overline{v}\,{\rm d}x \\ &= k^2\int_{\Omega_h\setminus\overline{D}} w\overline{v}\,{\rm d}x - \int_{\partial D}\frac{\partial w}{\partial\nu}\overline{v}\,{\rm d}s + \int_{\Gamma_h}\frac{\partial w}{\partial x_2}\overline{v}\,{\rm d}s - \int_{\Gamma_{-h}}\frac{\partial w}{\partial x_2}\overline{v}\,{\rm d}s \quad (2.51)\end{aligned}$$

and the above jump relation shows that

$$\begin{aligned}-\frac{1}{2}\int_{\partial D}\frac{\partial w}{\partial\nu}\overline{v}\,{\rm d}s &= \int_{\partial D}\frac{\partial w}{\partial\nu}\frac{\gamma_{\rm int}(\overline{w})}{\gamma_{\rm int}(q)}\,{\rm d}s - \int_{\partial D}\frac{\partial w}{\partial\nu}\frac{\overline{T(\gamma_{\rm int}(qv))}}{\gamma_{\rm int}(q)}\,{\rm d}s \\ &= \int_D \nabla w\cdot\nabla\left(\frac{\overline{w}}{q}\right)\,{\rm d}x + \int_D \Delta w\frac{\overline{w}}{q}\,{\rm d}x - \int_{\partial D}\frac{\partial w}{\partial\nu}\frac{\overline{T(\gamma_{\rm int}(qv))}}{\gamma_{\rm int}(q)}\,{\rm d}s \\ &= \int_D \frac{|\nabla w|^2}{q}\,{\rm d}x + \int_D (\nabla q^{-1}\cdot\nabla w - k^2\frac{w}{q})\overline{w}\,{\rm d}x - \int_{\partial D}\frac{\partial w}{\partial\nu}\frac{\overline{T(\gamma_{\rm int}(qv))}}{\gamma_{\rm int}(q)}\,{\rm d}s\,.\end{aligned}$$

Combining the last computation with (2.51) shows that

$$\begin{aligned}&\left\langle \nabla {\rm DL}(qv|_{\partial D}),\, \nabla v|_{\Omega_h\setminus\overline{D}}\right\rangle_{L^2(\Omega_h\setminus\overline{D})} = 2\int_D\frac{|\nabla w|^2}{q}\,{\rm d}x + k^2\int_{\Omega_h\setminus\overline{D}} w\overline{v}\,{\rm d}x \quad (2.52)\\ &+ 2\int_D\left(\nabla q^{-1}\cdot\nabla w - k^2\frac{w}{q}\right)\overline{w}\,{\rm d}x - 2\int_{\partial D}\frac{\partial w}{\partial\nu}\frac{\overline{T(\gamma_{\rm int}(qv))}}{\gamma_{\rm int}(q)}\,{\rm d}s + \left(\int_{\Gamma_h} - \int_{\Gamma_{-h}}\right)\frac{\partial w}{\partial x_2}\overline{v}\,{\rm d}s\,.\end{aligned}$$

Using Lemma 2.4.4, all the terms in the second line of the last equation can be rewritten as $\langle K_1 v,\, v\rangle_{H^1_{\alpha,\rm p}(\Omega_R)}$ where K_1 is a compact operator on $H^1_{\alpha,\rm p}(\Omega_R)$. The mapping $v \mapsto \int_D |\nabla w|^2/q\,{\rm d}x$ is obviously positive if $q > 0$. In consequence, (2.49) and (2.50) show that (2.48) holds. □

2.7 Discretization of the Periodic Integral Equation

In this section we firstly consider the discretization of the periodized integral equation (2.46) in spaces of trigonometric polynomials. If the periodization satisfies certain smoothness conditions and if uniqueness of solution holds, convergence theory for the discretization is a consequence of the Gårding inequalities shown in Theorem 2.6.3. Secondly we present fully discrete formulas for implementing a Galerkin discretization of the Lippmann-Schwinger integral equation (2.46). It is also the simplicity of this method that makes it interesting for us, since we are ultimately interested in using this code to generate data for the inverse scattering problem.

For $N \in \mathbb{N}$ we define $\mathbb{Z}_N^2 = \{j \in \mathbb{Z}^2 : -N/2 < j_{1,2} \leq N/2\}$ and $\mathcal{T}_N = \operatorname{span}\{\varphi_j : j \in \mathbb{Z}_N^2\}$, where $\varphi_j \in L^2(\Omega_R)$ are the α-quasiperiodic basis functions from (2.16). Note that the union $\cup_{N\in\mathbb{N}}\mathcal{T}_N$ is dense in $H^1_{\alpha,\mathrm{p}}(\Omega_R)$. The orthogonal projection onto $\mathcal{T}_N$ is

$$P_N : H^1_{\alpha,\mathrm{p}}(\Omega_R) \to \mathcal{T}_N, \qquad P_N(v) = \sum_{j\in\mathbb{Z}_N^2} \hat{v}(j)\varphi_j,$$

where $\hat{v}(j)$ denotes as above the jth Fourier coefficient. The next proposition recalls the standard convergence result for Galerkin discretizations of equations that satisfy a Gårding inequality, see, e.g. [103, Theorem 4.2.9], combined with the regularity result from Theorem 2.6.2(c).

Proposition 2.7.1. *Assume that q satisfies the assumptions of Theorem 2.6.3 and that* (2.28) *is uniquely solvable. Then* (2.46) *has a unique solution $u \in H^1_{\alpha,\mathrm{p}}(\Omega_R)$, and then there is $N_0 \in \mathbb{N}$ such that the finite-dimensional problem to find $u_N \in \mathcal{T}_N$ such that*

$$\langle u_N - L_\mathrm{p}(q\nabla u_N), w_N\rangle_{H^1_{\alpha,\mathrm{p}}(\Omega_R)} = \langle f, w_N\rangle_{H^1_{\alpha,\mathrm{p}}(\Omega_R)} \quad \text{for all } w_N \in \mathcal{T}_N \tag{2.53}$$

possesses a unique solution for all $N \geq N_0$ and $f \in H^1_{\alpha,\mathrm{p}}(\Omega_R)$. In this case

$$\|u_N - u\|_{H^1_{\alpha,\mathrm{p}}(\Omega_R)} \leq C \inf_{w_N\in\mathcal{T}_N} \|w_N - u\|_{H^1_{\alpha,\mathrm{p}}(\Omega_R)} \leq CN^{-s}\|u\|_{H^{1+s}_{\alpha,\mathrm{p}}(\Omega_R)}, \quad 0 \leq s < 1/2,$$

with a constant C independent of $N \geq N_0$.

Remark 2.7.2. *The convergence rate increases to $s + 1 - t$ if one measures the error in the weaker Sobolev norms of $H^t_{\alpha,\mathrm{p}}(\Omega_R)$, $1/2 < t < 1$. This could be shown using adjoint estimates (see, e.g. [103, Section 4.2] for the general technique). However, the (linear) rate saturates at $t = 1/2$, since the integral operator is not bounded on $H^t_{\alpha,\mathrm{p}}(\Omega_R)$ for $t < 1/2$, that is, the L^2-error decays with a linear rate. We do not present proofs for these error estimates since those are rather technical. However, we will later on present numerical results that show exactly the indicated rates.*

Similar to the proof of Lemma 2.3.4 we have

$$\int_{\Omega_R} \mathcal{K}_\mathrm{sm}(\cdot - y)\varphi_j(y)\,\mathrm{d}y = \sqrt{4\pi R}\,\hat{\mathcal{K}}_\mathrm{sm}(j)\varphi_j \quad \text{for all } j \in \mathbb{Z}^2.$$

which implies that P_N commutes with the periodic convolution operator L_{p}, that is,

$$P_N L_{\mathrm{p}}(f) = L_{\mathrm{p}}(P_N f) \quad \text{for all } f \in L^2(\Omega_R)^2.$$

Hence applying P_N to the infinite-dimensional problem (2.46), we obtain the discrete problem to find $u_N \in \mathcal{T}_N$ such that

$$u_N - L_{\mathrm{p}}(P_N(q\nabla u_N)) = L_{\mathrm{p}}(P_N f). \tag{2.54}$$

Fast methods to evaluate the discretized operator in (2.54) exploit that the application of L_{p} to a trigonometric polynomial in $\mathcal{T}_N$ can be explicitly computed using an α-quasiperiodic discrete Fourier transform that we call $\mathcal{F}_N$. This transform maps point values of a trigonometric polynomial φ_j (see (2.16)) to the Fourier coefficients of the polynomial. If we denote by $a \bullet b$ the componentwise multiplication of two matrices, and if $t := (2\pi/N,\, 4\pi R/N)^\top$, then

$$\hat{v}_N(j) = \frac{\sqrt{4\pi R}}{N^2} \sum_{l \in \mathbb{Z}_N^2} v_N(l \bullet t) \exp\big(- 2\pi \mathrm{i}\, (j_1 + \alpha, j_2)^\top \cdot l/N\big), \qquad j \in \mathbb{Z}_N^2.$$

This defines the transform $\mathcal{F}_N$ mapping $(v_N(j \bullet t))_{j \in \mathbb{Z}_N^2}$ to $(\hat{v}_N(j))_{j \in \mathbb{Z}_N^2}$. The inverse $\mathcal{F}_N^{-1}$ is explicitly given by

$$v_N(j \bullet t) = \frac{1}{\sqrt{4\pi R}} \sum_{l \in \mathbb{Z}_N^2} \hat{v}_N(l) \exp\Big(2\pi \mathrm{i}\, (l_1 + \alpha, l_2)^\top \cdot j/N\Big), \qquad j \in \mathbb{Z}_N^2.$$

Both $\mathcal{F}_N$ and its inverse are linear operators on $\mathbb{C}_N^2 = \{(c_n)_{n \in \mathbb{Z}_N^2} : c_n \in \mathbb{C}\}$. The restriction operator $R_{N,M}$ from $\mathbb{C}_N^2$ to $\mathbb{C}_M^2$, $N > M$, is defined by $R_{N,M}(a) = b$ where $b(j) = a(j)$ for $j \in \mathbb{Z}_M^2$. The related extension operator $E_{M,N}$ from $\mathbb{C}_M^2$ to $\mathbb{C}_N^2$, $M < N$, is defined by $E_{M,N}(a) = b$ where $b(j) = a(j)$ for $j \in \mathbb{Z}_M^2$ and $b(j) = 0$ else.

Lemma 2.7.3. *The Fourier coefficients of $q\partial_\ell u_N$, $\ell = 1, 2$, are given by*

$$(\widehat{q\partial_\ell u_N}(j))_{j \in \mathbb{Z}_N^2} = R_{3N,N} \mathcal{F}_{3N} \big[\mathcal{F}_{3N}^{-1}\big(E_{2N,3N}(\hat{q}_{2N}(j))_{j \in \mathbb{Z}_N^2}\big) \bullet \mathcal{F}_{3N}^{-1}\big(E_{N,3N}(w_\ell(j)\hat{u}_N(j))_{j \in \mathbb{Z}_N^2}\big)\big]$$

where $w_1(j) = \mathrm{i}(j_1 + \alpha)$ and $w_2(j) = \mathrm{i} j_2 \pi/R$ for $j \in \mathbb{Z}^2$.

Proof. For $u_N \in \mathcal{T}_N$, $j \in \mathbb{Z}^2$, and $\ell = 1, 2$,

$$\begin{aligned} 4\pi R\, \widehat{q\partial_\ell u}_N(j) &= 4\pi R \int_{\Omega_R} q\partial_\ell u_N \overline{\varphi_j}\, \mathrm{d}x = 4\pi R \sum_{m \in \mathbb{Z}_N^2} \widehat{\partial_\ell u}_N(m) \int_{\Omega_R} q\overline{\varphi_j}\varphi_m\, \mathrm{d}x \\ &= \sum_{m \in \mathbb{Z}_N^2} \widehat{\partial_\ell u}_N(m) \int_{\Omega_R} q(x) e^{-\mathrm{i}[(j_1 - m_1)x_1 + (j_2 - m_2)x_2 \pi/R]}\, \mathrm{d}x \\ &= (4\pi R)^{1/2} \sum_{m \in \mathbb{Z}_N^2} \widehat{\partial_\ell u}_N(m) \hat{q}(j - m). \end{aligned} \tag{2.55}$$

If $j \in \mathbb{Z}_N^2$, then the coefficient $\widehat{q\partial_\ell u_N}(j)$ merely depends on $\hat{q}(m)$ for $m \in \mathbb{Z}_{2N}^2$. Hence, $\widehat{q\partial_\ell u_N}(j) = \widehat{q_{2N}\partial_\ell u_N}(j)$ for $j \in \mathbb{Z}_N^2$. Obviously, $q_{2N}\partial_\ell u_N$ belongs to $\mathcal{T}_{3N}$. Hence, the Fourier coefficients of $q_{2N}\partial_\ell u_N$ are given by $\mathcal{F}_{3N}$ applied to the grid values of this function at $j \bullet h$, $j \in \mathbb{Z}_{3N}^2$. The grid values of $\widehat{\partial_\ell u_N}$ are given by $\mathcal{F}_{3N}^{-1}(E_{N,3N}(\widehat{\partial_\ell u_N}(j)_{j\in\mathbb{Z}_N^2})$, and the grid values of q_{2N} can be computed analogously. Finally, taking a partial derivative with respect to x_1 or x_2 of u yields a multiplication of the jth Fourier coefficient $\hat{u}(j)$ by $\mathrm{i}(j_1+\alpha)$ and $\mathrm{i}j_2\pi/R$, respectively. □

In Lemma 2.3.4 we computed the Fourier coefficients of the kernel $\mathcal{K}_R$. The kernel $\mathcal{K}_{\mathrm{sm}}$ used to define the periodized potential L_{p} is the product of $\mathcal{K}_R$ with the smooth function χ (see (2.45)). Hence, the Fourier coefficients of $\mathcal{K}_{\mathrm{sm}}$ are convolutions of the $\hat{\mathcal{K}}_R(j)$ with $\hat{\chi}(j_2) = (4\pi R)^{-1/2}\int_{-R}^{R}\exp(-\mathrm{i}j_2\pi x_2/R)\chi(x_2)\,\mathrm{d}x_2$,

$$\hat{\mathcal{K}}_{\mathrm{sm}}(j) = \frac{1}{(4\pi R)^{1/2}}\sum_{m\in\mathbb{Z}_N^2}\hat{\mathcal{K}}_R(j_1,m_2)\hat{\chi}(j_2-m_2), \qquad j\in\mathbb{Z}^2.$$

The latter formula can be seen by a computation similar to (2.55). Note that χ is a smooth function, which means that the Fourier coefficients $\hat{\chi}$ in the last formula are rapidly decreasing, that is, the truncation the last series converges rapidly to the exact value. The convolution structure of L_{p} finally shows that

$$\widehat{(L_{\mathrm{p}}f)}(j) = (4\pi R)^{1/2}\,\hat{\mathcal{K}}_{\mathrm{sm}}(j)\Big[\mathrm{i}(j_1+\alpha)\hat{f}_1(j) + \frac{\mathrm{i}j_2\pi}{R}\hat{f}_2(j)\Big], \quad f = \begin{pmatrix} f_1 \\ f_2\end{pmatrix} \in L^2(\Omega_R)^2. \tag{2.56}$$

The finite-dimensional operator $u_N \mapsto L_{\mathrm{p}}(P_N(q\nabla u_N))$ can now be evaluated in $O(N\log(N))$ operations by combining the formula of Lemma 2.7.3 with (2.56). The linear system (2.54) can then be solved using iterative methods. Whenever one uses iterative techniques, one would of course like to precondition the linear system. The usual multi-grid preconditioning technique for integral equations of the second kind (see, e.g., [109]) does not apply here, since the integral operator is not compact. For the numerical experiments presented in the next section, we simply used an unpreconditioned GMRES algorithm.

2.8 Numerical Experiments

In the numerical experiments 2.8.1–2.8.3 we confirm the theoretical convergence statement from Proposition 2.7.1 and Remark 2.7.2 by computing the relative error between the approximate solution and the reference solution. These experiments are carried out for different periodic structures and contrasts. In the last example of this section we present the convergence of the method using an error indicator resulting from the so-called energy conservation. All the computations in the following experiments were done on a machine with an Intel Xeon 3.20 GHz processor and 12 GB memory using MATLAB. Recall that we aim to compute the scattered field for an incident field $u^i(x_1,x_2) = \exp(\mathrm{i}k(\cos(\theta)x_1 - \sin(\theta)x_2))$ with incident angle θ.

2.8.1 Strip structure with constant contrast

In this example we consider the periodic structure as a strip (compare Figure 2.5) where the contrast q is a positive constant.

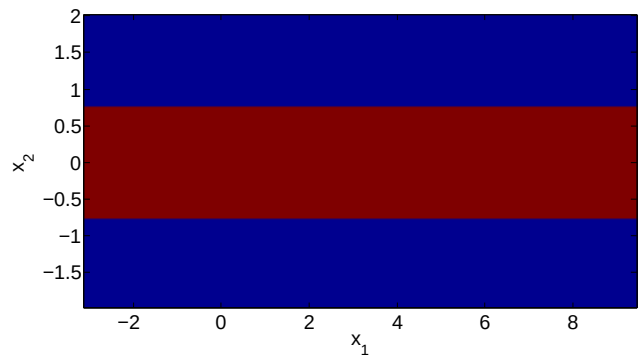


Figure 2.5: Strip structure with constant contrast plotted in $(-\pi, 3\pi) \times (-2, 2)$.

More precisely, the support $D = (-\pi, \pi) \times (-0.75, 0.75)$ and $\Omega_R = (-\pi, \pi) \times (-2, 2)$. We approximate the solution in $\mathcal{T}_N$ where $N = 2^n$ for $n = 6, ..., 11$. For this example we choose $k = \pi/2$ and $\theta = \pi/4$, the contrast q equals 2 in D. For this setting one can explicitly compute the scattered field. The GMRES iteration is stopped when the relative residual is less than 10^{-5}. In the Figure 2.6 we show the relative error between the numerical solution and the analytical solution in the norms $H^s_{\alpha,\mathrm{p}}(\Omega_R)$ where $s = 0, 0.5, 1$. The relative error measured in the norm $H^1_{\alpha,\mathrm{p}}(\Omega_R)$ fits quite well to the theoretical statement in Proposition 2.7.1. Furthermore, if one measures the relative error in the norm $H^s_{\alpha,\mathrm{p}}(\Omega_R)$ for $s = 0$ and $s = 0.5$ the experiment confirms the statement of Remark 2.7.2. To give an impression about computation times, the results in Figure 2.6 took about 0.3, 1.1, 3.7, 21.2, 131.7 and 463.7 seconds for $N = 2^n$, $n = 6, \ldots, 11$, respectively.

2.8.2 Strip structure with piecewise constant contrast

The structure in this example is again a strip where $D = (-\pi, \pi) \times (-0.75, 0.75)$, $\Omega_R = (-\pi, \pi) \times (-2, 2)$, $k = \pi/2$ and $\theta = \pi/4$ (the same to Experiment 2.8.1). However we consider the case that q is piecewise constant (compare Figure 2.7),

$$q = \begin{cases} 1 & \text{in } D_1 := (-\pi/2, \pi/2) \times (0, 0.75), \\ 2 & \text{in } D \setminus \overline{D_1}. \end{cases}$$

Since the analytical solution for this case is not available, we hence compute the relative error between the numerical solution u_N for $N = 2^n$, $n = 4, \ldots, 9$ and the reference solution u_M for $M = 3072$. Similar to the last example we compute the relative error in the norms $H^s_{\alpha,\mathrm{p}}(\Omega_R)$ where $s = 0, 0.5, 1$. Recall that D_1 and D are rectangles, the Fourier coefficients of

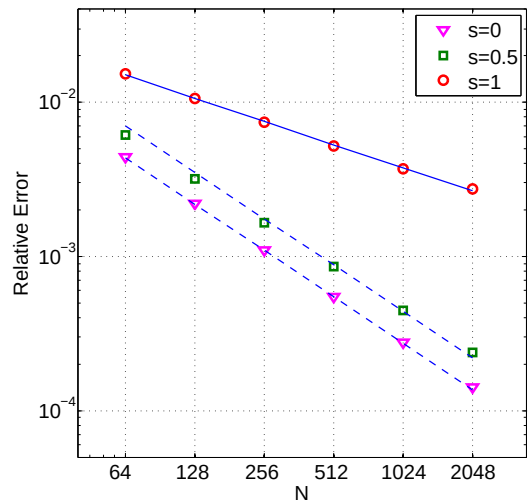


Figure 2.6: Scattering from strip structure with constant contrast. Relative error of the approximated solution u_N for $N = 2^n$, $n = 6, ..., 11$ and the analytical solution measured in $H^s_{\alpha,\mathrm{p}}$-norm for scattering from a strip. Circles, kites, triangles correspond to $s = 1$, $s = 0.5$ and $s = 0$, respectively. The continuous line and the dotted lines indicate the convergence order 0.5 and 1, respectively.

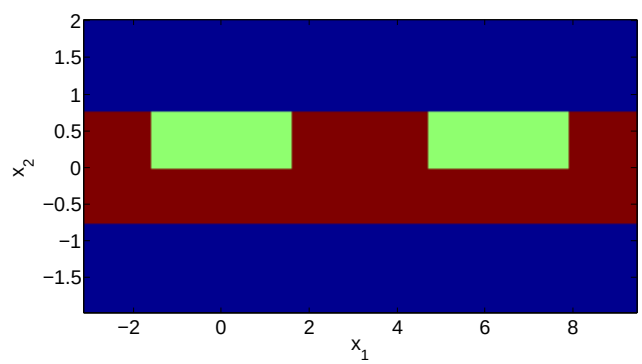


Figure 2.7: Strip structure with constant contrast plotted in $(-\pi, 3\pi) \times (-2, 2)$. The subdomain D_1 where $q = 1$ is in green.

the contrast q in this case can be computed explicitly via the formula

$$\sqrt{4\pi R}\hat{q}(j) = (q_1 - q_2)\int_{D_1} e^{-\mathrm{i}j_1x_1-\mathrm{i}j_2\pi x_2/R}\,\mathrm{d}x + q_2\int_{D} e^{-\mathrm{i}j_1x_1-\mathrm{i}j_2\pi x_2/R}\,\mathrm{d}x\,, \quad j \in \mathbb{Z}^2,$$

Similar to Experiment 2.8.1 the tolerance for GMRES solver is 10^{-5} for computing the approximate solution u_N for $N = 2^n$, $n = 4, \ldots, 9$. For the reference solution u_{3072}, the GMRES tolerance is 10^{-8} and computation time is 3076 seconds.

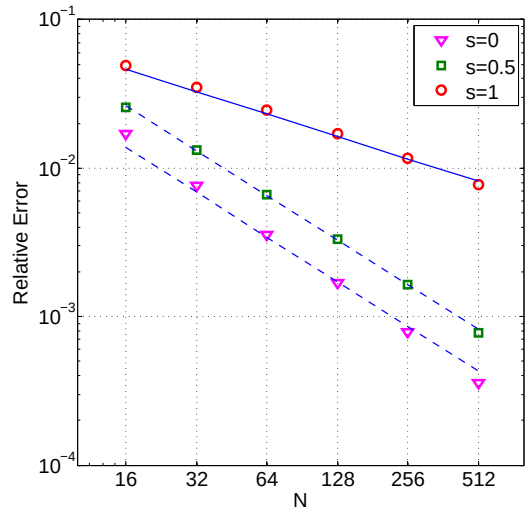


Figure 2.8: Scattering from a strip structure with piecewise constant contrast. Relative error of the approximate solution u_N for $N = 2^n$, $n = 4, ..., 9$ and the reference solution u_{3072} measured in $H^s_{\alpha,\mathrm{p}}$-norm. Circles, kites, triangles correspond to $s = 1$, $s = 0.5$ and $s = 0$, respectively. The continuous line and the dotted lines indicate the convergence order 0.5 and 1, respectively.

2.8.3 Periodic sinusoidal structure

In this example we again confirm the theoretical convergence statement from Proposition 2.7.1 and Remark 2.7.2 for a periodic sinusoidal structure (compare Figure 2.9). More precisely,

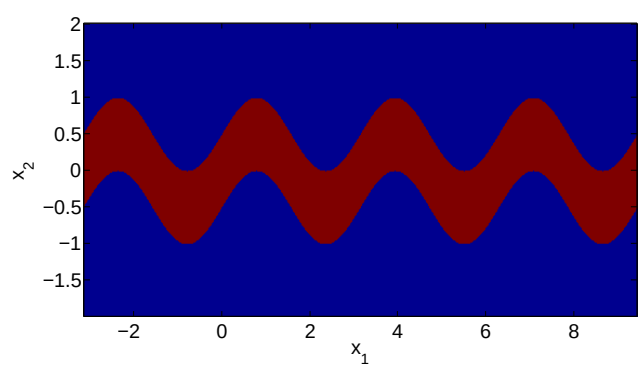


Figure 2.9: The periodic sinusoidal structure plotted in $(-\pi, 3\pi) \times (-2, 2)$.

$$D = \left\{ (x_1, x_2)^\top \in \mathbb{R}^2 : -\pi < x_1 < \pi,\ \frac{\sin(2x_1) - 1}{2} < x_2 < \frac{\sin(2x_1) + 1}{2} \right\},$$
$$\Omega_R = (-\pi, \pi) \times (-2, 2), \quad q(x_1, x_2) = \frac{e^{-x_2}}{3}, \quad (x_1, x_2)^\top \in D.$$

We choose $k = \pi/2$ and $\theta = \pi/4$. As in Experiment 2.8.2 we compute the relative error between the approximate solution u_N for $N = 2^n$, $n = 4, \ldots, 9$ and the reference solution u_M for $M = 3072$ in the norms $H^s_{\alpha,\mathrm{p}}(\Omega_R)$ where $s = 0, 0.5, 1$. The tolerance for the GMRES iteration is 10^{-5} when computing approximate solution u_N for $N = 2^n$, $n = 4, \ldots, 9$. For the reference solution u_{3072}, the GMRES tolerance is 10^{-8} and computation time is 35327 seconds. In this case the Fourier coefficients of the contrast q can be approximated using Green's formula

$$\begin{aligned}
\sqrt{4\pi R}\hat{q}(j) &= \int_{\Omega_R} q(x) e^{-\mathrm{i}j_1 x_1 - \mathrm{i}j_2 \pi x_2/R}\,\mathrm{d}x = \frac{1}{3}\int_D e^{-\mathrm{i}j_1 x_1 - (1+\mathrm{i}j_2\pi/R)x_2}\,\mathrm{d}x \\
&= \frac{-1}{3(1+\mathrm{i}j_2\pi/R)} \int_{\partial D} \nu_2(x) e^{-\mathrm{i}j_1 x_1 - (1+\mathrm{i}j_2\pi/R)x_2}\,\mathrm{d}s \\
&= \frac{-1}{3(1+\mathrm{i}j_2\pi/R)} \int_0^{2\pi} e^{-\mathrm{i}j_1 t - (1+\mathrm{i}j_2\pi/R)(\sin(2t)/2+0.5)}\,\mathrm{d}t \\
&+ \frac{1}{3(1+\mathrm{i}j_2\pi/R)} \int_0^{2\pi} e^{-\mathrm{i}j_1 t - (1+\mathrm{i}j_2\pi/R)(\sin(2t)/2-0.5)}\,\mathrm{d}t\,.
\end{aligned}$$

For the computations in this example we approximate these integrals with the fourth-order convergent composite Simpson's rule.

2.8.4 Periodic rectangle-shaped structure

This last example presents the convergence of the method using an error indicator resulting from the energy conservation for scattering from rectangle shapes that are periodically aligned (compare Figure 2.11). The rectangle support $D = (-2.5, 2.5) \times (-0.75, 0.75)$, and $\Omega_R = (-\pi, \pi) \times (-2, 2)$. The wave number k equals 2.5, we consider the contrast q given by

$$q(x_1, x_2) = 2\cos(x_1)^2(x_2 + 0.75) \quad \text{for } (x_1, x_2)^\top \in D.$$

Recall the Rayleigh coefficients $\hat{u}_j^\pm$ of the scattered field from (2.12). For the incident field, we define similar coefficients by $\hat{u}_j^i = \int_{-\pi}^{\pi} u^i(x_1, -h)\exp(-\mathrm{i}\alpha_j x_1)\,\mathrm{d}x_1$ for $j \in \mathbb{Z}$. Then Green's formula applied to (2.9) and the Rayleigh expansion condition show that

$$\sum_{j:k^2>\beta_j^2} \beta_j(|\hat{u}_j^+|^2 + |\hat{u}_j^- + \hat{u}_j^i|^2) = \beta_0. \tag{2.57}$$

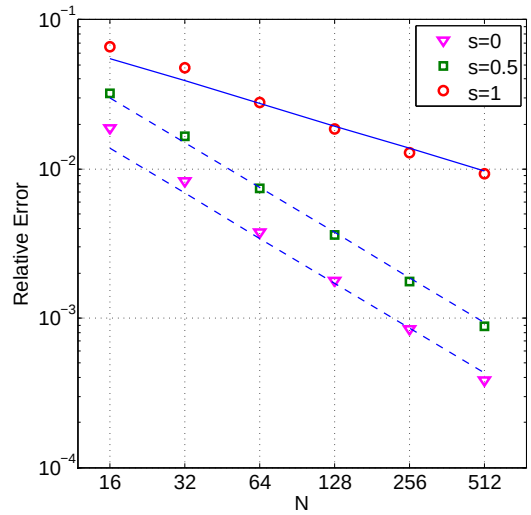


Figure 2.10: Scattering from periodic sinusoidal structure. Relative error of the approximate solution u_N for $N = 2^n$, $n = 4, ..., 9$ and the reference solution u_{3072} measured in $H^s_{\alpha,\mathrm{p}}$-norm. Circles, kites, triangles correspond to $s = 1$, $s = 0.5$ and $s = 0$, respectively. The continuous line and the dotted lines indicate the convergence order 0.5 and 1, respectively.

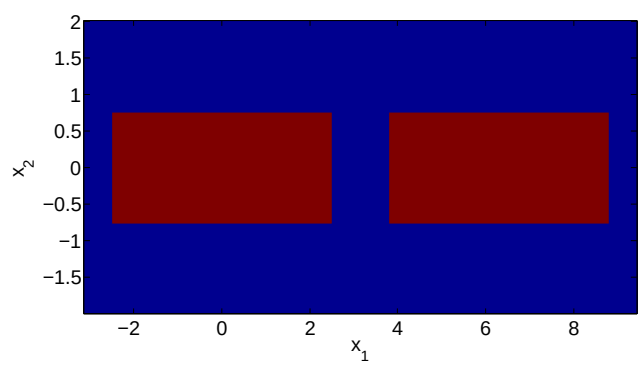


Figure 2.11: The periodic rectangle-shaped structure plotted in $(-\pi, 3\pi) \times (-2, 2)$.

Here we call (2.57) the equation of energy conservation. For an incident wave of direction $(\cos(\theta), -\sin(\theta))^\top$, the sums

$$E_{\mathrm{tra}}(\theta) := \sum_{j:k^2>\beta_j^2} \beta_j(|\hat{u}_j^- + \hat{u}_j^i|^2)/\beta_0, \quad E_{\mathrm{ref}}(\theta) := \sum_{j:k^2>\beta_j^2} \beta_j|\hat{u}_j^+|^2/\beta_0$$

correspond to transmitted and reflected wave energies. In this experiment, we use $\theta \mapsto |1 - E_{\mathrm{tra}}(\theta) - E_{\mathrm{ref}}(\theta)|$ as an error indicator for the numerical solution. The Fourier coefficients of the contrast q can be explicitly computed using integration by parts. Assume that r, ρ are

the sizes of the rectangle in x_1- and x_2-dimension, respectively. We have

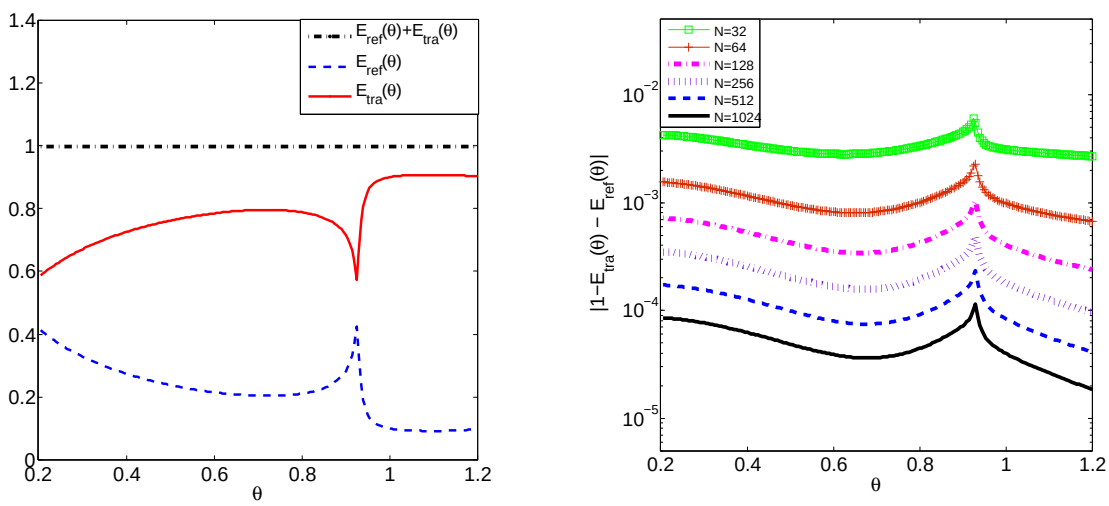
$$\hat{q}(j) = A(j_1)B(j_2)/\sqrt{4\pi R} \quad \text{for } j = (j_1, j_2) \in \mathbb{Z}^2,$$

where

$$A(j_1) = \begin{cases} \frac{\sin(rj_1)\left[(2\cos(2r)+1)/j_1 - 8/j_1^3\right] - 4\cos(j_1 r)\sin(2r)/j_1^2}{1-4/j_1^2} & j_1 \in \mathbb{Z} \setminus \{0, \pm 2\}, \\ \sin(4r)/4 + \sin(2r) + r & j_1 = \pm 2, \\ \sin(2r)/2 + r & j_1 = 0, \end{cases}$$

$$B(j_2) = \begin{cases} \frac{2\rho \mathrm{i} R}{j_2 \pi} \exp(-\mathrm{i} j_2 \pi \rho / R) - \frac{2\mathrm{i} R^2}{(j_2\pi)^2} \sin(j_2 \pi \rho / R) & j_2 \neq 0, \\ 2\rho^2 & j_2 = 0. \end{cases}$$

In these experiments the angle θ are sampled at 200 points uniformly distributed on the interval $[0.2, 1.2]$. For Figure 2.12(a) the scattered field is approximated in $\mathcal{T}_N$ where $N = 2^8$ and the computation time for solving for one fixed incident angle θ is about 2 seconds. In Figure 2.12(b) we check the energy conservation error for different N where the tolerance for the GMRES iteration is 10^{-8}. As Figure 2.12(b) shows, the error of the computed Rayleigh coefficients corresponding to propagating modes converges with order 1. This also shows an instability around Rayleigh frequencies, where $k^2 = (\alpha + n)^2$, that is, $\pi = |\pi \cos(\theta) + n|$ for some $n \in \mathbb{Z}$. We can see that the error curves in Figure 2.12(b) have a bend at the angle $\theta = \arccos(1 - 1/(2.5)) \approx 0.927$.



(a) (b)

Figure 2.12: (a) Reflected and transmitted energy curves versus the angles θ of the incident field u^i. (b) The error curves $|1 - E_{\text{tra}}(\theta) - E_{\text{ref}}(\theta)|$ for different discretization parameters N versus the angles θ of the incident field u^i.

Chapter 3

The Factorization Method for Periodic Inverse Scattering

Abstract: Chapter 3 concerns the shape identification problem of diffraction gratings from measured spectral data involving scattered electromagnetic waves in TM mode. In particular, we consider diffraction gratings consisting of a penetrable periodic dielectric mounted on a metallic plate (compare Figure 3.1). Here we model the spectral measurements which are the Rayleigh sequences of the scattered field by the near field operator N (see (3.15)). The aim of the inverse problem then is to identify the periodic scatterer when N is given. Using special plane incident fields introduced in [7] (see (3.3)), we study the Factorization method as a tool for identifying the periodic media. First, we factorize the near field operator N in Theorem 3.3.3. Second, we prove in Lemma 3.4.3 the necessary properties of the middle operator in the factorization. This allows us to apply the version of range identity theorem studied in [78] (see Theorem 3.4.1) to provide a simple imaging criterion (3.31). Finally, numerical experiments with different material parameters and periodic structures are given in Section 3.5 to examine the performance of the method.

3.1 Introduction

This chapter develops a Factorization method for the inverse scattering problem from diffraction gratings constituted by penetrable periodic dielectrics mounted on a metallic plate. As in Chapter 1 the diffraction gratings are supposed to be periodic in one direction and invariant in the perpendicular direction, and that we consider the TM mode problem in half-space setting with Neumann condition on the boundary of the metallic plate. We consider here the problem in a half-space setting instead of the full-space setting in Chapter 1 is to simplify the presentation of the technique. This technique is then extended to the full-space problem for the case of Maxwell's equations in Chapter 4. The study of our model problem is motivated

by the important applications of periodic structures in modern optical technologies such as diffractive optical filters and organic light-emitting diodes, and non-destructive testing of such structures.

As outlined in the introduction, while the papers [7, 8] studied the Factorization method for detecting impenetrable periodic layers with Dirichlet and impedance boundary conditions, the author in [79] considered imaging of penetrable periodic interfaces between two dielectrics in two dimensions. In the present chapter, the Factorization method is studied as a tool for identifying shape of diffraction gratings in the TM case. Note that the papers [7, 8, 79] investigated the Factorization method for the TE case. Furthermore, the periodic structures that we consider here are different from those studied in the latter cited papers. The measured data in the periodic inverse problem are coefficients of evanescent and propagating modes in the radiation condition. Those data are modelled by the so-called near field operator N which is central of the Factorization method. Given the operator N, the inverse problem then is to identify the shape of the diffration grating. Using the Factorization method we provide a sufficient and necessary criterion for a point z in the periodic scattering support using the eigensystem of the operator $N_\sharp = |\mathrm{Re}(N)| - \mathrm{Im}(N)$. To do that one also needs results on range identities where factorizing the near field operator in a suitable way plays an important role. Moreover, to examine the performance of the method, a number of numerical experiments are given for several kinds of diffraction gratings motivated by the ones presented in [49].

Our analysis extends approaches in [7, 72, 78] to the TM mode problem with Neumann boundary condition on the metallic plate. We use the special plane incident fields introduced in [7] which allows us to suitably factorize the near field operator. Note that this approach avoids the use of (in some sense) unphysical complex-conjugated incident fields, as in [8, 100], that are certainly non-trivial to produce in practice. To obtain the necessary properties of the middle operator for the application of range identity theorem we use the approach in [72] for obstacle inverse scattering of electromagnetic waves. Further, a modified version of the method studied in [78] treats the case that the imaginary part of the middle operator in the factorization is just semidefinite.

The chapter is organized as follows: In Section 3.2 we set up and derive the Fredholm property of the direct problem. Section 3.3 is for the factorization of the near field operator of the corresponding inverse problem. We derive the necessary properties of the middle operator and a characterization of the periodic structure in Section 3.4. Finally, Section 3.5 is devoted to the study of numerical experiments.

3.2 The Direct Scattering Problem

We consider the TM case, discussed in the previous chapter, of electromagnetic scattering problems from isotropic periodic dielectric materials mounted on a metallic plate with Neumann boundary condition. Thus we have a problem set on $\mathbb{R}^2_+ := \{(x_1, x_2)^\top, x_2 > 0\}$ as

follows

$$\operatorname{div}(\varepsilon_{\mathrm{r}}^{-1}\nabla u) + k^2 u = 0 \quad \text{in } \mathbb{R}^2_+, \tag{3.1}$$

$$\varepsilon_{\mathrm{r}}^{-1}\frac{\partial u}{\partial \nu} = 0 \quad \text{on } \{x_2 = 0\}, \tag{3.2}$$

where $k > 0$ is the wave number, ν is the outward unit normal vector to the boundary $\{x_2 = 0\}$. We assume that the material parameter $\varepsilon_{\mathrm{r}}^{-1}$ is a scalar function in $L^\infty(\mathbb{R}^2_+)$ with $\operatorname{Re}(\varepsilon_{\mathrm{r}}^{-1}) \geq c > 0$, $\operatorname{Im}(\varepsilon_{\mathrm{r}}^{-1}) \leq 0$, and that $\varepsilon_{\mathrm{r}}^{-1}$ is 2π-periodic in x_1 and equals one outside the grating. We consider the downward propagating incident field u^i, i.e.,

$$u^i(x) = e^{\mathrm{i}kx\cdot d} = e^{\mathrm{i}k(x_1 d_1 + x_2 d_2)}, \quad |d| = 1, \text{ and } d_2 < 0. \tag{3.3}$$

When the incident field u^i illuminates the diffraction grating, there arises a scattered field u^s such that the total field $u = u^i + u^s$ satisfies (3.1)–(3.2). Since $\Delta u^i + k^2 u^i = 0$ we can write (3.1)–(3.2) as

$$\operatorname{div}(\varepsilon_{\mathrm{r}}^{-1}\nabla u^s) + k^2 u^s = -\operatorname{div}(q\nabla u^i) \quad \text{in } \mathbb{R}^2_+, \tag{3.4}$$

$$\varepsilon_{\mathrm{r}}^{-1}\frac{\partial u^s}{\partial \nu} = -\varepsilon_{\mathrm{r}}^{-1}\frac{\partial u^i}{\partial \nu} \quad \text{on } \{x_2 = 0\}, \tag{3.5}$$

where q is the contrast defined by

$$q := \varepsilon_{\mathrm{r}}^{-1} - 1.$$

Similarly to the problem setting in Chapter 1, we find the α-quasiperiodic scattered field u^s to the direct problem (3.4)–(3.5), satisfying the Rayleigh expansion radiation condition

$$u^s(x) = \sum_{n\in\mathbb{Z}} \hat{u}_n e^{\mathrm{i}(\alpha_n x_1 + \beta_n(x_2 - h))} \quad \text{for } x_2 > h, \tag{3.6}$$

where $(\hat{u}_n)_{n\in\mathbb{Z}}$ are the Rayleigh sequences given by

$$\hat{u}_n := \frac{1}{2\pi}\int_0^{2\pi} u^s(x_1, h) e^{-\mathrm{i}\alpha_n x_1}\,\mathrm{d}x_1\,, \quad n \in \mathbb{Z}.$$

Note that we also require that the series in (3.6) converges uniformly on compact subsets of $\{x_2 > h\}$. Due to the periodicity of the problem (3.4)–(3.6), we can consider it in one period $\Omega := (-\pi, \pi) \times (0, \infty)$. Set $\Gamma_\rho = (-\pi, \pi) \times \{\rho\}$ for $\rho \geq 0$, we rewrite our problem as follows: Find $u^s : \mathbb{R}^2 \to \mathbb{C}$ such that

$$\operatorname{div}(\varepsilon_{\mathrm{r}}^{-1}\nabla u^s) + k^2 u^s = -\operatorname{div}(q\nabla u^i) \quad \text{in } \Omega, \tag{3.7}$$

$$\varepsilon_{\mathrm{r}}^{-1}\frac{\partial u^s}{\partial \nu} = -\varepsilon_{\mathrm{r}}^{-1}\frac{\partial u^i}{\partial \nu} \quad \text{on } \Gamma_0, \tag{3.8}$$

and u^s satisfies the radiation condition (3.6).

As mentioned in Chapter 1, the variational solution theory for the problem in full-space setting is well-known. For the convenience of the reader we give a variational formulation of problem (3.6)–(3.8) as an adaptation from the works for the full-space problem. Recall that $\Omega = (-\pi, \pi) \times (0, \infty)$, and define

$$\Omega_h := (-\pi, \pi) \times (0, h), \quad \text{for } h > \sup\{x_2 : (x_1, x_2)^\top \in \operatorname{supp}(q)\},$$
$$H^1_\alpha(\Omega_h) := \{u \in H^1(\Omega_h) : u = U|_{\Omega_h} \text{ for some } \alpha\text{-quasiperiodic } U \in H^1_{\mathrm{loc}}(\mathbb{R}^2_+)\}.$$

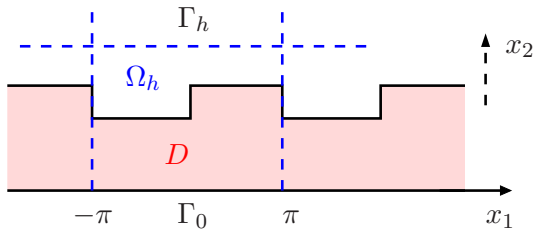


Figure 3.1: Geometric setting for inverse scattering problem of TM-polarized electromagnetic waves from periodic dielectrics mounted on a metallic plate.

The variational formulation has to couple equations (3.7)–(3.8) with the radiation condition (3.6). To this end we first define the trace space $H^s_\alpha(\Gamma_h)$ ($s \in \mathbb{R}$) which includes α-quasiperiodic functions ϕ satisfying

$$\|\phi\|^2_{H^s_\alpha(\Gamma_h)} = \sum_{n\in\mathbb{Z}} (1+n^2)^{s/2} |\hat{\phi}_n|^2 < \infty, \quad \hat{\phi}_n = \frac{1}{2\pi}\int_0^{2\pi} \phi(t) e^{-\mathrm{i}\alpha_n t}\,\mathrm{d}t\,.$$

Then we can define the Dirichlet-to-Neumann operator T^+ from $H^{1/2}_\alpha(\Gamma_h)$ into $H^{-1/2}_\alpha(\Gamma_h)$ given by

$$T^+(\phi) = \mathrm{i}\sum_{n\in\mathbb{Z}} \beta_n \hat{\phi}_n e^{\mathrm{i}\alpha_n x_1}.$$

It is easy to check that T^+ is a bounded operator. Now multiplying (3.7) by $v \in H^1_\alpha(\Omega_h)$, using Green's identities we formally have

$$\int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1} \nabla u^s \cdot \nabla \overline{v} - k^2 u^s \overline{v})\,\mathrm{d}x - \int_{\Gamma_h \cup \Gamma_0} \varepsilon_{\mathrm{r}}^{-1} \frac{\partial u^s}{\partial \nu} \overline{v}\,\mathrm{d}s = -\int_{\Omega_h} q \nabla u^i \cdot \nabla \overline{v}\,\mathrm{d}x\,. \tag{3.9}$$

Note that the boundary terms on $\{x_1 = \pm\pi\}$ vanish due to the α-quasiperiodicity. By replacing $\partial u^s/\partial\nu$ by $T^+(u^s)$ on the boundary term Γ_h, and taking into account the Neumann boundary condition (3.8), we obtain the following variational problem: Given the incident field u^i, find $u^s \in H^1_\alpha(\Omega_h)$ such that for all $v \in H^1_\alpha(\Omega_h)$ it holds

$$\begin{aligned}\mathcal{B}_p(u^s, v) := \int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1} \nabla u^s \cdot \nabla \overline{v} - k^2 u^s \overline{v})\,\mathrm{d}x - \int_{\Gamma_h} \overline{v} T^+(u^s)\,\mathrm{d}s \\ = -\int_{\Omega_h} q \nabla u^i \cdot \nabla \overline{v}\,\mathrm{d}x - \int_{\Gamma_0} \varepsilon_{\mathrm{r}}^{-1} \frac{\partial u^i}{\partial \nu} \overline{v}\,\mathrm{d}s\,.\end{aligned} \tag{3.10}$$

We can see that $\mathcal{B}_p$ is a bounded sesquilinear form on $H^1_\alpha(\Omega_h)$ because of the fact that

$$\begin{aligned}\left|\int_{\Gamma_h} \overline{v}T^+(u^s)\,\mathrm{d}s\right| &\leq \|v\|_{H^{1/2}_\alpha(\Gamma_h)}\|T^+(u^s)\|_{H^{-1/2}_\alpha(\Gamma_h)} \\ &\leq C\|v\|_{H^1_\alpha(\Omega_h)}\|u^s\|_{H^{1/2}_\alpha(\Gamma_h)} \leq C\|v\|_{H^1_\alpha(\Omega_h)}\|u^s\|_{H^1_\alpha(\Omega_h)} \qquad (3.11)\end{aligned}$$

Theorem 3.2.1. *The sesquilinear form $\mathcal{B}_p$ is of Fredholm type on $H^1_\alpha(\Omega_h)$.*

Proof. It is sufficient to show that $\mathcal{B}_p$ satisfies Gårding inequality on $H^1_\alpha(\Omega_h)$. To this end, we first use the Plancherel identity to compute

$$-\mathrm{Re}\left(\int_{\Gamma_h} \overline{u}T^+(u)\,\mathrm{d}s\right) = -\mathrm{Re}\left(\mathrm{i}\sum_{j\in\mathbb{Z}}\beta_j|\hat{u}_j|^2\right) = \sum_{j:\alpha_j^2>k^2}(\alpha_j^2-k^2)^{1/2}|\hat{u}_j|^2 \geq 0$$

Recall that the material parameter $\varepsilon_\mathrm{r}^{-1}$ satisfies $\mathrm{Re}(\varepsilon_\mathrm{r}^{-1}) \geq c > 0$. Taking the real part of the sesquilinear form we implies that

$$\mathrm{Re}(\mathcal{B}_p(u,u)) \geq c\|u\|^2_{H^1_\alpha(\Omega_h)} - \int_{\Omega_h}(\mathrm{Re}(\varepsilon_\mathrm{r}^{-1})+k^2)|u|^2\,\mathrm{d}x\,,$$

and since $H^1_\alpha(\Omega_h)$ is compactly embedded in $L^2(\Omega_h)$ (this is Rellich's compact embedding lemma in the periodic setting), $\mathcal{B}_p$ satisfies Gårding inequality. □

Fredholm theory [81] implies that existence of solution for problem (3.10) follows from uniqueness of solution. For strategies to establish uniqueness of solution by geometric conditions, one can refer to [22,66]. More generally, analytic Fredholm theory establishes uniqueness of this problem for all but possibly a discrete set of wave numbers k. In this work we assume that the wave number k is such that uniqueness of solution holds.

3.3 The Near Field Operator and Its Factorization

In this section we set up the corresponding periodic inverse problem and we introduce the near field operator. Moreover, studying the factorization of the near field operator is an important step for constructing a factorization method.

Recall that $\alpha_j = \alpha + j$ and $\beta_j = (k^2-\alpha_j^2)^{1/2} \neq 0$ for $j \in \mathbb{Z}$. To obtain data for the factorization method we use the incident fields as α-quasiperiodic plane waves

$$u_j^i = e^{\mathrm{i}(\alpha_j x_1 - \beta_j x_2)} + e^{\mathrm{i}(\alpha_j x_1 + \beta_j x_2)}, \quad j \in \mathbb{Z}. \qquad (3.12)$$

The incident fields satisfy the Neumann boundary condition $\partial u_j^i/\partial\nu = 0$ on Γ_0. These incident fields u_j^i have two parts, a downward propagating waves $\exp(\mathrm{i}(\alpha_j x_1 - \beta_j x_2))$, and $\exp(\mathrm{i}(\alpha_j x_1 + \beta_j x_2))$, which is an upward propagating wave. This choice for the corresponding incident fields for Dirichlet boundary condition has been studied in [7] regarding the analysis of the factorization method for periodic Dirichlet obstacles.

Denote by $\overline{D}$ the support of the contrast q in one period $\Omega = (-\pi,\pi)\times(0,\infty)$. The following assumption is necessary for our later frame work.

Assumption 3.3.1. *We assume that $D \subset \mathbb{R}^2$ is open and bounded with Lipschitz boundary and that there exists a positive constant c such that* $\mathrm{Re}(q) \geq c > 0$ *and* $\mathrm{Im}(q) \leq 0$ *almost everywhere in D.*

Since the incident fields u_j^i satisfies the Neumann boundary condition for all $j \in \mathbb{Z}$, replacing u^i by u_j^i in the variational form (3.10) implies

$$\int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1} \nabla u^s \cdot \nabla \overline{v} - k^2 u^s \overline{v})\,\mathrm{d}x \,-\, \int_{\Gamma_h} \overline{v} T^+(u^s)\,\mathrm{d}s \,=\, -\int_D q \nabla u_j^i \cdot \nabla \overline{v}\,\mathrm{d}x\,, \quad v \in H^1_\alpha(\Omega_h).$$

We consider a more general form as follows: Given $f \in L^2(D)^2$, find $u \in H^1_\alpha(\Omega_h)$ such that, for all $v \in H^1_\alpha(\Omega_h)$,

$$\int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1} \nabla u \cdot \nabla \overline{v} - k^2 u \overline{v})\,\mathrm{d}x \,-\, \int_{\Gamma_h} \overline{v} T^+(u)\,\mathrm{d}s \,=\, -\int_D q/\sqrt{|q|} f \cdot \nabla \overline{v}\,\mathrm{d}x\,. \tag{3.13}$$

Since the unique solvability of (3.13) has been discussed in Section 2, we then can define a solution operator

$$G : L^2(D)^2 \to \ell^2(\mathbb{Z})$$

which maps f to the Rayleigh sequence $(\hat{u}_j)_{j\in\mathbb{Z}}$ of $u \in H^1_\alpha(\Omega_h)$, solution to (3.13).

Due to the linearity of problem (3.10), a linear combination of several incident fields will lead to a corresponding linear combination of resulting scattered fields. We obtain such a linear combination using sequences $(a_j)_{j\in\mathbb{Z}} \in \ell^2(\mathbb{Z})$ and define the corresponding operator by

$$H(a_j) = \sqrt{|q|} \sum_{j\in\mathbb{Z}} \frac{a_j}{\beta_j w_j} \nabla u_j^i, \quad \text{where } w_j := \begin{cases} \mathrm{i}, & k^2 > \alpha_j^2, \\ \exp(-\mathrm{i}\beta_j h), & k^2 < \alpha_j^2, \end{cases} \tag{3.14}$$

where dividing by $\beta_j w_j$ essentially makes our later computations easier.

In our inverse problem the data measured are the Rayleigh sequences (3.6). We know that only the propagating modes are measurable far away from the structure. However, we need in this framework all the modes to be able to uniquely determine the periodic structure (the finite number of propagating modes is not enough). Hence the operator that models measurements from the periodic inhomogeneous medium of scattered fields caused by the incident fields (3.14) is referred to be the *near field* operator, denoted by N. We define $N : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ to map a sequence $(a_j)_{j\in\mathbb{Z}}$ to the Rayleigh sequences of the scattered field generated by the incident field $H(a_j)$ defined in (3.14), i.e.

$$[N(a_j)]_n := (\hat{u}_n)_{n\in\mathbb{Z}}, \tag{3.15}$$

where $u \in H^1_\alpha(\Omega_h)$ is the radiating solution to (3.13) for the source $f = H(a_j)$. Then from the definition of the solution operator G we have

$$N = GH. \tag{3.16}$$

The inverse scattering problem is now to reconstruct the support $\overline{D}$ of the contrast $q = \varepsilon_{\mathrm{r}}^{-1} - 1$ when the near field operator N is given. We solve this problem using the factorization method. Factorizing the near field operator is one of the important steps of this method. Before doing that, in the next lemma, we show some properties of operator $H : \ell^2(\mathbb{Z}) \to L^2(D)^2$ and its adjoint H^*. We rely on the sequence

$$w_j^* := \begin{cases} \exp(-\mathrm{i}\beta_j h), & k^2 > \alpha_j^2, \\ \mathrm{i}, & k^2 < \alpha_j^2. \end{cases}$$

Lemma 3.3.2. *The operator $H : \ell^2(\mathbb{Z}) \to L^2(D)^2$ is compact and injective. Its adjoint $H^* : L^2(D)^2 \to \ell^2(\mathbb{Z})$ satisfies*

$$H^*(f) = 4\pi(w_j^* \hat{u}_j)_{j\in\mathbb{Z}},$$

where $\hat{u}_j$ is the Rayleigh sequence of the radiating variational solution $u \in H^1_\alpha(\Omega_h)$ to $\Delta u + k^2 u = \operatorname{div}(\sqrt{|q|} f)$ in Ω_h and $\partial u/\partial\nu = 0$ on Γ_0, i.e.

$$\int_{\Omega_h} (\nabla u \cdot \nabla \overline{v} - k^2 u \overline{v})\,\mathrm{d}x - \int_{\Gamma_h} \overline{v} T^+(u)\,\mathrm{d}s = \int_D \sqrt{|q|} f \cdot \nabla \overline{v}\,\mathrm{d}x\,, \quad \textit{for all } v \in H^1_\alpha(\Omega_h). \tag{3.17}$$

Proof. We have

$$\int_D H(a_j)\overline{f}\,\mathrm{d}x = \sum_{j\in\mathbb{Z}} \frac{a_j}{\beta_j w_j} \int_D \sqrt{|q|} \nabla u_j^i \cdot \overline{f}\,\mathrm{d}x = \left\langle (a_j), \left(\int_D \sqrt{|q|} f \cdot \overline{\left(\frac{\nabla u_j^i}{\beta_j w_j}\right)}\,\mathrm{d}x \right) \right\rangle_{\ell^2(\mathbb{Z})}$$

Note that $\overline{w_j} = -w_j$ and $\overline{\beta_j} = \beta_j$ if $k^2 > \alpha_j^2$ but $\overline{w_j} = w_j$ and $\overline{\beta_j} = -\beta_j$ else, respectively. Therefore

$$\begin{aligned} \overline{\left(\frac{u_j^i}{\beta_j w_j}\right)} &= \begin{cases} -\frac{1}{\beta_j w_j}\left(e^{-i(\alpha_j x_1 - \beta_j x_2)} + e^{-i(\alpha_j x_1 + \beta_j x_2)}\right), & k^2 > \alpha_j^2 \\ -\frac{1}{\beta_j w_j}\left(e^{-i(\alpha_j x_1 + \beta_j x_2)} + e^{-i(\alpha_j x_1 - \beta_j x_2)}\right), & k^2 < \alpha_j^2 \end{cases} \\ &= -\frac{1}{\beta_j w_j}\left(e^{-i(\alpha_j x_1 - \beta_j x_2)} + e^{-i(\alpha_j x_1 + \beta_j x_2)}\right). \end{aligned}$$

For the unique solvability of (3.17), the Fredholm property can be obtained as in the last section. However uniqueness of solution of this problem can be deduced for all wave numbers k. Indeed, for $f = 0$, choosing smooth test functions v in (3.17) vanishing on Γ_h and Γ_0 imply that $\Delta u + k^2 u = 0$ in $L^2(\Omega_h)$. Then multiplying the latter equation by $v \in H^1_\alpha(\Omega_h)$, using the Green's first indentity, and adding the resulting expression from the variational formulation (3.17), we find that

$$\int_{\Gamma_0} \overline{v} \frac{\partial u}{\partial \nu}\,\mathrm{d}s + \int_{\Gamma_h} \overline{v} \frac{\partial u}{\partial \nu}\,\mathrm{d}s - \int_{\Gamma_h} \overline{v} T^+(u)\,\mathrm{d}s = 0, \quad \text{for all } v \in H^1_\alpha(\Omega_h).$$

Choose functions v which vanish on Γ_h we conclude that $\partial u/\partial\nu = 0$ in $H_\alpha^{-1/2}(\Gamma_0)$. Then using classical approach of separation of variables we conclude that the problem $\Delta u + k^2 u = 0$ in $L^2(\Omega_h)$ and $\partial u/\partial\nu = 0$ in $H_\alpha^{-1/2}(\Gamma_0)$ only has a trivial solution.

Now assume that u solves (3.17) and recall that $u|_{\Gamma_h} = \sum_{l\in\mathbb{Z}} \hat{u}_l \exp(\mathrm{i}\alpha_l x_1)$. Denote $v_j := u_j^i/(\beta_j w_j)$. Using the second Green's identity we have

$$\begin{aligned}\int_D \sqrt{|q|} f \cdot \nabla \overline{v_j}\,\mathrm{d}x &= \int_{\Omega_h} (\nabla u \cdot \nabla \overline{v_j} - k^2 u \overline{v_j})\,\mathrm{d}x - \int_{\Gamma_h} \overline{v_j} T^+(u)\,\mathrm{d}s \\ &= -\int_{\Omega_h} (\Delta \overline{v_j} + k^2 \overline{v_j}) u\,\mathrm{d}x + \int_{\Gamma_h} \left(u \frac{\partial \overline{v_j}}{\partial x_2} - \overline{v_j} T^+(u) \right) \mathrm{d}s \\ &= \sum_{l\in\mathbb{Z}} \hat{u}_l \int_{\Gamma_h} \left(e^{\mathrm{i}\alpha_l x_1} \frac{\partial \overline{v_j}}{\partial x_2} - \mathrm{i}\beta_l e^{\mathrm{i}\alpha_l x_1} \overline{v_j} \right) \mathrm{d}s\,.\end{aligned}$$

Further,

$$\overline{v_j}|_{\Gamma_h} = -\frac{1}{\beta_j w_j}(e^{\mathrm{i}\beta_j h} + e^{-\mathrm{i}\beta_j h}) e^{-\mathrm{i}\alpha_j x_1}, \quad \frac{\partial \overline{v_j}}{\partial x_2}|_{\Gamma_h} = -\frac{\mathrm{i}}{w_j}(e^{\mathrm{i}\beta_j h} - e^{-\mathrm{i}\beta_j h}) e^{-\mathrm{i}\alpha_j x_1}.$$

Thus we find

$$\int_D \sqrt{|q|} f \cdot \nabla \overline{v_j}\,\mathrm{d}x = 2\mathrm{i}\frac{\hat{u}_j}{w_j} \int_{\Gamma_h} e^{-\mathrm{i}\beta_j h}\,\mathrm{d}s = \begin{cases} 4\pi \hat{u}_j e^{-\mathrm{i}\beta_j h}, & k^2 > \alpha_j^2, \\ 4\pi \mathrm{i} \hat{u}_j, & k^2 < \alpha_j^2. \end{cases}$$

Hence we have shown that $H^*(f) = 4\pi(w_j^* \hat{u}_j)_{j\in\mathbb{Z}}$. Since the operations $f \mapsto u|_{\Gamma_h}$ and $u|_{\Gamma_h} \mapsto (\hat{u}_j)$ are bounded from $L^2(D)^2$ into $H_\alpha^{1/2}(\Gamma_h)$ and from $H_\alpha^{1/2}(\Gamma_h)$ into $\ell^2(\mathbb{Z})$, respectively, and since $(w_j^*)_{j\in\mathbb{Z}}$ is a bounded sequence, H^* is a bounded operator. Moreover, elliptic regularity results [81] imply that u is H^2-regular in a neighborhood of Γ_h, thus, $f \mapsto u|_{\Gamma_h}$ is a compact operation from $L^2(D)^2$ into $H_\alpha^{1/2}(\Gamma_h)$ and H^* is a compact operator. Therefore, H is compact as well.

To show that H is injective it is sufficient to show that H^* has dense range, which follows from the fact that all sequences $(\delta_{jl})_{l\in\mathbb{Z}}$ belong to the range of H^* (by definition, the Kronecker symbol δ_{jl} equals one for $j = l$ and zero otherwise). To see this, we note that $\exp(\mathrm{i}(\alpha_j x_1 + \beta_j(x_2 - h))$ has Rayleigh sequence $(\delta_{jl})_{l\in\mathbb{Z}}$. Set $\varphi_j(x_1, x_2) = \exp(\mathrm{i}(\alpha_j x_1 + \beta_j(x_2 - h))$. We choose $\chi_1, \chi_2 \in C^\infty_{\mathrm{per}}(\Omega) = \{\chi \in C^\infty(\Omega) : \chi \text{ is } 2\pi\text{-periodic in } x_1\}$ such that $\int_D \chi_2\,\mathrm{d}x \neq 0$, χ_2 vanishes on a neighborhood of boundary Γ_0 and $\Omega \setminus D$, and χ_1 vanishes for $x_2 \in \Omega \setminus D$, $(1 - \chi_1)\varphi_j$ satisfies Neumann condition on Γ_0. We set

$$\Phi_j = (1 - \chi_1)\varphi_j - \frac{\int_D (1 - \chi_1)\varphi_j\,\mathrm{d}x + \frac{1}{k^2}\int_{\partial D} \partial\varphi_j/\partial\nu\,\mathrm{d}s}{\int_D \chi_2\,\mathrm{d}x} \chi_2. \tag{3.18}$$

Then the Rayleigh sequences of Φ_j and φ_j are equal and

$$k^2 \int_D \Phi_j\,\mathrm{d}x + \int_{\partial D} \frac{\partial \varphi_j}{\partial \nu}\,\mathrm{d}s = 0. \tag{3.19}$$

Due to Lax-Milgram theorem, there exists a unique solution $v \in H^1_\diamond(D) := \{v \in H^1(D) : \int_D v\,\mathrm{d}x = 0\}$ to the equation

$$\int_D \sqrt{|q|} \nabla v \cdot \nabla \overline{\psi}\,\mathrm{d}x = \int_D (\nabla \Phi_j \cdot \nabla \overline{\psi} - k^2 \Phi_j \overline{\psi})\,\mathrm{d}x - \int_{\partial D} \frac{\partial \varphi_j}{\partial \nu} \overline{\psi}\,\mathrm{d}s$$

for all $\psi \in H^1_\diamond(D)$. This equation still holds for all the test function $\psi \in H^1(D)$ due to (3.19). From (3.18) we know that $\Phi_j = \varphi_j$ in $\Omega \setminus \overline{D}$ which implies $\Delta\Phi_j + k^2\Phi_j = 0$ in $\Omega \setminus \overline{D}$. Thus Green's first identity shows that

$$\int_{\Omega_h \setminus D} (\nabla\Phi_j \cdot \nabla\overline{\psi} - k^2\Phi_j\overline{\psi})\,\mathrm{d}x - \int_{\Gamma_h} T^+(\Phi_j)\overline{\psi}\,\mathrm{d}s = -\int_{\partial D} \frac{\partial\varphi_j}{\partial\nu}\overline{\psi}\,\mathrm{d}s$$

for all $\psi \in H^1_\alpha(\Omega_h)$. Adding the two last equations we obtain

$$\int_{\Omega_h} (\nabla\Phi_j \cdot \nabla\overline{\psi} - k^2\Phi_j\overline{\psi})\,\mathrm{d}x - \int_{\Gamma_h} T^+(\Phi_j)\overline{\psi}\,\mathrm{d}s = \int_D \sqrt{|q|}\nabla v \cdot \nabla\overline{\psi}\,\mathrm{d}x$$

for all $\psi \in H^1_\alpha(\Omega_h)$. Now we set $f = \nabla v \in L^2(D)^2$ with an extension zero outside D which shows that $H^*(f) = 4\pi(w_j^*\delta_{jl})_{l\in\mathbb{Z}}$. By a simple scaling this implies that $(\delta_{jl})_{l\in\mathbb{Z}} \in \mathrm{Rg}(H^*)$ for any $j \in \mathbb{Z}$. □

Now we show a factorization of the near field operator N in the following theorem. For simplicity we define the sign of q by

$$\mathrm{sign}(q) := \frac{q}{|q|} \quad \text{in } \Omega.$$

Theorem 3.3.3. *Let $W : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ be defined by $W(a_j) = (-4\pi w_j^* a_j)_{j\in\mathbb{Z}}$. The operator $T : L^2(D)^2 \to L^2(D)^2$ is defined by $Tf = \mathrm{sign}(q)(f + \sqrt{|q|}\nabla v)$, where $v \in H^1_\alpha(\Omega_h)$ is the solution to* (3.13)*. Then near field operator N satisfies*

$$WN = H^*TH.$$

Proof. Let us first note that W is a bounded operator on $\ell^2(\mathbb{Z})$ since $|w_j^*| = 1$ for all $j \in \mathbb{Z}$. For simplicity, we denote by Q the operator that maps $f \in L^2(D)^2$ to the Rayleigh sequence $(\hat{u}_j)_{j\in\mathbb{Z}}$ of $u \in H^1_\alpha(\Omega_h)$, radiating variational solution to $\Delta u + k^2 u = \mathrm{div}(\sqrt{|q|}f)$ in Ω_h and $\partial u/\partial\nu = 0$ on Γ_0. This operator already appeared in Lemma 3.3.2, where we showed that $H^* = -WQ$. By definition of the solution operator G we have $Gf = (\hat{u}_j)_{j\in\mathbb{Z}}$ where $u \in H^1_\alpha(\Omega_h)$ is a radiating variational solution to $\mathrm{div}(\varepsilon_\mathrm{r}^{-1}\nabla u) + k^2 u = -\mathrm{div}(q/\sqrt{|q|}f)$ in Ω_h and $\varepsilon_\mathrm{r}^{-1}\partial u/\partial\nu = 0$ on Γ_0. This means that $\Delta u + k^2 u = -\mathrm{div}(\sqrt{|q|}\,\mathrm{sign}(q)(f + \sqrt{|q|}\nabla u))$ in Ω_h and $\partial u/\partial\nu = 0$ on Γ_0, thus

$$Gf = -Q(\mathrm{sign}(q)(f + \sqrt{|q|}\nabla u)) = -(QT)f.$$

Recall that we have $N = GH$ which implies

$$WN = WGH = -WQTH = H^*TH.$$

□

3.4 Characterization of the Periodic Support

To give a characterization of the periodic support of the contrast q we need an abstract result on range identities. For the convenience of the reader, we give a rather complete proof, see also in [72,78]. First, we introduce real and imaginary part of a bounded linear operator. Let $X \subset U \subset X^*$ be a Gelfand triple, that is, U is a Hilbert space, X is a reflexive Banach space with dual X^* for the inner product of U, and the embeddings are injective and dense. Then the real and imaginary part of a bounded operator $T : X^* \to X$ are defined in accordance with the corresponding definition for complex numbers,

$$\mathrm{Re}(T) := \frac{1}{2}(T + T^*), \qquad \mathrm{Im}(T) := \frac{1}{2\mathrm{i}}(T - T^*).$$

Theorem 3.4.1. *Let $X \subset U \subset X^*$ be a Gelfand triple with Hilbert space U and reflexive Banach space X. Furthermore, let V be a second Hilbert space and $F : V \to V$, $H : V \to X$ and $T : X \to X^*$ be linear and bounded operators with*

$$F = H^*TH$$

We make the following assumptions:
a) H is compact and injective.
b) There exists $t \in [0, 2\pi]$ such that $\mathrm{Re}(e^{\mathrm{i}t}T)$ has the form $\mathrm{Re}(e^{\mathrm{i}t}T) = T_0 + T_1$ with some positive definite selfadjoint operator T_0 and some compact operator $T_1 : X \to X^*$.
c) $\mathrm{Im}T$ is non positive on X, i.e., $\langle \mathrm{Im}T\phi, \phi\rangle \le 0$ for all $\phi \in X$.
Moreover, we assume that one of the two following conditions is fullfilled
d) T is injective and the number t from b) does not equal $\pi/2$ or $3\pi/2$.
e) $\mathrm{Im}T$ is negative on the (finite dimensional) null space of $\mathrm{Re}(e^{\mathrm{i}t}T)$, i.e., for all $\phi \neq 0$ such that $\mathrm{Re}(e^{\mathrm{i}t}T)\phi = 0$ it holds $\langle \mathrm{Im}T\phi, \phi\rangle < 0$.

Then the operator $F_\sharp := |\mathrm{Re}(e^{\mathrm{i}t}F)| - \mathrm{Im}F$ is positive definite and the ranges of $H^* : X^* \to V$ and $F_\sharp^{\frac{1}{2}} : V \to V$ coincide.

Proof. We first recall from [69] that it is sufficient to assume that $X = U$ is a Hilbert space and that H has dense range in U. The reduction to the Hilbert space case follows from the introduction of the positive definite root $T_0^{1/2} : X \to U$, see, e.g., [99, Theorem 12.33], since

$$F = H^*TH = (H^*T_0^{1/2})(T_0^{-1/2}TT_0^{-1/2})(T_0^{1/2}H) =: \tilde{H}^*\tilde{T}\tilde{H}.$$

If the range $\mathrm{Rg}(H)$ of H is not dense in U, we replace U by its closed subspace $\overline{\mathrm{Rg}(H)}$ using the orthogonal projector P from U to $\overline{\mathrm{Rg}(H)}$. Since $PH = H$, the factorization $F = H^*P^*TPH$ holds and all the assumptions of the theorem are preserved. Hence, we can assume that $X = U$ and that H has dense range. We first recall from [69] that it is sufficient to assume that $X = U$ is a Hilbert space and that H has dense range in U. The reduction to the Hilbert space case follows from the introduction of the positive definite root $T_0^{1/2} : X \to U$, see, e.g., [99, Theorem 12.33], since

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If the range $\mathrm{Rg}(H)$ of H is not dense in U, we replace U by its closed subspace $\overline{\mathrm{Rg}(H)}$ using the orthogonal projector P from U to $\overline{\mathrm{Rg}(H)}$. Since $PH = H$, the factorization $F = H^*P^*TPH$ holds and all the assumptions of the theorem are preserved. Hence, we can assume that $X = U$ and that H has dense range.

The factorization of F implies that $\mathrm{Re}(e^{\mathrm{i}t}F) = H^*\mathrm{Re}(e^{\mathrm{i}t}T)H$ is compact and selfadjoint. By the spectral theorem for such operators, there exists a complete orthonormal eigensystem $(\lambda_j, \psi_j)_{j\in\mathbb{N}}$ of $\mathrm{Re}(e^{\mathrm{i}t}F)$. In consequence, the spaces

$$V^+ = \mathrm{span}\{\psi_j : \lambda_j > 0\} \qquad \text{and} \qquad V^- = \mathrm{span}\{\psi_j : \lambda_j \le 0\}$$

are invariant under $\mathrm{Re}(e^{\mathrm{i}t}F)$ and satisfy $V = V^+ \oplus V^-$. We set $U^- = HV^-$.

In the next step we show that U^- is finite dimensional. The operator $T_1 = \mathrm{Re}(e^{\mathrm{i}t}T) - T_0$ is a selfadjoint and compact operator, we denote by $(\mu_j, \phi_j)_{j\in\mathbb{N}}$ an eigensystem of T_1. By assumption of T_0, there exists $\alpha > 0$ such that $\langle T_0\varphi, \varphi\rangle \ge \alpha\|\varphi\|^2$ for all $\varphi \in U$. We set $W^+ = \mathrm{span}\{\phi_j : \mu_j > -\alpha\}$, $W^- = \mathrm{span}\{\phi_j : \mu_j \le -\alpha\}$ and note that W^- is finite dimensional since $\mu_j \to 0$. Let now $\phi = H\psi \in U^-$ with (unique) decomposition $\phi = \phi^+ + \phi^-$, $\phi^\pm \in W^\pm$. Since $\psi \in V^-$,

$$\begin{aligned} 0 \ge \langle \mathrm{Re}(e^{\mathrm{i}t}F)\psi, \psi\rangle &= \langle \mathrm{Re}(e^{\mathrm{i}t}T)H\psi, H\psi\rangle = \langle \mathrm{Re}(e^{\mathrm{i}t}T)(\phi^+ + \phi^-), \phi^+ + \phi^-\rangle \\ &= \langle \mathrm{Re}(e^{\mathrm{i}t}T)\phi^+, \phi^+\rangle + \langle \mathrm{Re}(e^{\mathrm{i}t}T)\phi^-, \phi^-\rangle \ge c\|\phi^+\|^2 - \|\mathrm{Re}(e^{\mathrm{i}t}T)\|\|\phi^-\|^2, \end{aligned}$$

thus, $\|\phi\|^2 = \|\phi^+\|^2 + \|\phi^-\|^2 \le C\|\phi^-\|^2$. This shows that the mapping $\phi \mapsto \phi^-$ is boundedly invertible from U^- into W^-. Consequently, U^- is finite dimensional.

Denseness of the range of H implies that the sum $\overline{HV^+} + U^-$ is dense in U. Since U^- is a finite dimensional and therefore complemented subspace, we can choose a closed subspace U^+ of $\overline{HV^+}$ such that the (non-orthogonal) sum $U = U^+ \oplus U^-$ is direct. Let moreover $U^0 := \overline{HV^+} \cap U^-$ be the intersection of $\overline{HV^+}$ and U^-, we will show that U^0 is contained in the kernel of $\mathrm{Re}(e^{\mathrm{i}t}T)$. We denote $P_{U^\pm} : U \to U^\pm$ the canonical projections, that is, every $\phi \in U$ has the unique decomposition $\phi = P_{U^+}\phi + P_{U^-}\phi$. Both operators $P_{U^\pm}$ are bounded and $P_{U^+} - P_{U^-}$ is an isomorphism, since

$$(P_{U^+} - P_{U^-})^2 = P_{U^+}^2 + P_{U^-}^2 - P_{U^+}P_{U^-} - P_{U^-}P_{U^+} = P_{U^+} + P_{U^-} = \mathrm{Id}\,.$$

From the factorization $\mathrm{Re}(e^{\mathrm{i}t}F) = H^*\mathrm{Re}(e^{\mathrm{i}t}T)H$ and the definition of $U^\pm$ we obtain that $H^*\mathrm{Re}(e^{\mathrm{i}t}T)(U^-) = \mathrm{Re}(e^{\mathrm{i}t}F)(V^-) \subset V^-$. Note also that, by definition we have $U^+ \subset \overline{HV^+}$. In consequence, for $\phi^- \in U^-$ and $\psi^+ \in V^+$ we have

$$0 = \langle H^*(\mathrm{Re}(e^{\mathrm{i}t}T))\phi^-, \psi^+\rangle = \langle \mathrm{Re}(e^{\mathrm{i}t}T)\phi^-, H\psi^+\rangle = \langle \phi^-, (\mathrm{Re}(e^{\mathrm{i}t}T))H\psi^+\rangle. \tag{3.20}$$

We conclude that $\mathrm{Re}(e^{\mathrm{i}t}T)U^- \subset (HV^+)^\perp = (U^+ \oplus U^0)^\perp \subset (U^+)^\perp$ and, $\mathrm{Re}(e^{\mathrm{i}t}T)U^+ \subset \mathrm{Re}(e^{\mathrm{i}t}T)\overline{HV^+} \subset (U^-)^\perp$. Indeed, for $\phi^+ \in \overline{HV^+}$ there is a sequence $\psi_n^+ \in V^+$ such that $H\psi_n^+ \to \phi^+$ and $\mathrm{Re}(e^{\mathrm{i}t}T)H\psi_n^+ \subset (U^-)^\perp$ by (3.20), thus, $\mathrm{Re}(e^{\mathrm{i}t}T)\phi^+ \subset (U^-)^\perp$. For $\phi^0 \in \overline{HV^+} \cap U^-$, these mapping properties of $\mathrm{Re}(e^{\mathrm{i}t}T)$ imply that $\mathrm{Re}(e^{\mathrm{i}t}T)\phi^0$ is orthogonal both to U^- and U^+. Therefore $\mathrm{Re}(e^{\mathrm{i}t}T)\phi^0 = 0$ and we conclude that $U^0 = \overline{HV^+} \cap U^-$ is contained in the kernel of $\mathrm{Re}(e^{\mathrm{i}t}T)$. This inclusion allows to show a factorization of $F_\sharp$ in the next step.

Let $\psi \in V$ and $\psi^{\pm}$ be its orthogonal projection on $V^{\pm}$. Then

$$\begin{aligned}
|\mathrm{Re}(e^{\mathrm{i}t}F)|\psi &= H^*\mathrm{Re}(e^{\mathrm{i}t}T)H(\psi^+ - \psi^-) \\
&= H^*\mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+}H\psi^+ + P_{U^-}H\psi^+ - P_{U^+}H\psi^- - P_{U^-}H\psi^-) \\
&= H^*\mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+}H\psi + 2 \underbrace{P_{U^-}H\psi^+}_{\in U^0 \subset \ker(\mathrm{Re}(e^{\mathrm{i}t}T))} - P_{U^+}H\psi) \\
&= H^*\mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-})H\psi
\end{aligned}$$

This factorization of $|\mathrm{Re}(e^{\mathrm{i}t}F)|$ yields a factorization of $F_\sharp$,

$$F_\sharp = |\mathrm{Re}(e^{\mathrm{i}t}F)| - \mathrm{Im}F = H^*(\mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-}) - \mathrm{Im}T)H = H^*T_\sharp H,$$

where $T_\sharp = \mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-}) - \mathrm{Im}T$. Due to the fact that $\langle \mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-})H\phi, H\phi\rangle = \langle |\mathrm{Re}(e^{\mathrm{i}t}F)|\phi, \phi\rangle \geq 0$ for all $\phi \in V$ and denseness of the range of H in U we conclude that $\mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-})$ is nonnegative on U. Since $T_\sharp$ is therefore a nonnegative operator, we can apply the inequality [69, Estimate (4.5)] for bounded nonnegative operators,

$$\langle T_\sharp\psi, \psi\rangle \geq \frac{1}{\|T_\sharp\|}\|T_\sharp\psi\|^2, \quad \psi \in U \tag{3.21}$$

Now, we show that assumption d) implies assumption e). Under the assumption d), let ϕ belong to the null space of $\mathrm{Re}(e^{\mathrm{i}t}T)$ and suppose that $\langle \mathrm{Im}T\phi, \phi\rangle = 0$. We need to show that this implies that $\phi = 0$. By definition of the real part of an operator,

$$e^{\mathrm{i}t}T\phi + e^{-\mathrm{i}t}T^*\phi = 0 \tag{3.22}$$

Furthermore, $-\mathrm{Im}T$ is a bounded nonnegative operator so the application of (3.21) to $-\mathrm{Im}T$ yields

$$0 = \langle -\mathrm{Im}T\phi, \phi\rangle \geq \frac{1}{\|\mathrm{Im}T\|}\|\mathrm{Im}T\phi\|^2, \quad \phi \in U,$$

hence $\|\mathrm{Im}T\phi\| = 0$ and $\mathrm{Im}\phi = 0$. By definition of the imaginary part, this is to say that $T\phi - T^*\phi = 0$. Combine this equation with (3.22) yields that $(1 + e^{\mathrm{i}2t})T\phi = 0$. Since $t \in [0, 2\pi] \setminus \{\frac{\pi}{2}, \frac{3\pi}{2}\}$, this implies $T\phi = 0$ and $\phi = 0$ by assumption d). We have hence proven that $\langle \mathrm{Im}T\phi, \phi\rangle < 0$ for all $0 \neq \phi \in \ker(\mathrm{Re}(e^{\mathrm{i}t}T))$. This is precisely assumption e) which is considered next.

Assuming e), we will show that $T_\sharp$ is injective. Suppose that $T_\sharp\phi = 0$, then we have $\langle \mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-})\phi, \phi\rangle - \langle \mathrm{Im}T\phi, \phi\rangle = 0$. Boths terms on the left are nonnegative so we have

$$\begin{cases} \langle \mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-})\phi, \phi\rangle = 0 \\ \langle \mathrm{Im}T\phi, \phi\rangle = 0 \end{cases} \tag{3.23}$$

From this and application of (3.21) to $\mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-})$ yield $\mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-})\phi = 0$. Moreover, due to the selfadjointness we obtain

$$\mathrm{Re}(e^{\mathrm{i}t}T)(P_{U^+} - P_{U^-}) = (P_{U^+} - P_{U^-})^*\mathrm{Re}(e^{\mathrm{i}t}T)$$

and since $P_{U^+} - P_{U^-}$ is an isomorphism so is $(P_{U^+} - P_{U^-})^*$. Consequently, $\mathrm{Re}(e^{\mathrm{i}t}T)\phi = 0$. Assumption e) now implies that $\langle \mathrm{Im}T\phi, \phi\rangle < 0$ if $\phi \neq 0$. However, we showed, in (3.23), that $\langle -\mathrm{Im}T\phi, \phi\rangle = 0$, that is, $\phi = 0$ and therefore $T_\sharp$ is injective.

Hence, by assumption d) or e), $T_\sharp$ is an injective Fredholm operator on index 0 (Fredholmness is due to assumption b)) and hence boundedly invertible. By (3.21) we obtain

$$\langle T_\sharp\psi, \psi\rangle \geq \frac{1}{\|T_\sharp\|}\|T_\sharp\psi\|^2 \geq C\|\psi\|^2 \quad \text{for all } \psi \in U$$

Now, as $T_\sharp$ has been show to be positive definite, the square root $T_\sharp^{1/2}$ of $T_\sharp$ is also positive definite on U, see, e.g., [99], hence the inverse $T_\sharp^{-1/2}$ is bounded and we can write

$$F_\sharp = F_\sharp^{1/2}\big(F_\sharp^{1/2}\big)^* = H^*T_\sharp H = \big(H^*T_\sharp^{1/2}\big)\big(H^*T_\sharp^{1/2}\big)^*$$

However, if two positive operators agree, then the ranges of their square root agree, as the following well known lemma shows.

Lemma 3.4.2. *(Lemma 2.4 in [69]). Let V, U_1 and U_2 be Hilbert spaces and $A_j : U_j \to V$, $j = 1, 2$, bounded and injective such that $A_1A_1^* = A_2A_2^*$. Then the ranges of A_1 and A_2 coincide and $A_1^{-1}A_2$ is an isomorphism from U_2 onto U_1.*

Setting $A_1 = F_\sharp^{1/2}$ and $A_2 = H^*T_\sharp^{1/2}$, the last lemma states that the ranges of $F_\sharp^{1/2}$ and $H^*T_\sharp^{1/2}$ agree and that $F_\sharp^{-1/2}H^*T_\sharp^{1/2}$ is an isomorphism from U to V. Since $T_\sharp^{1/2}$ is an isomorphism on U, we conclude that the range of $H^*T_\sharp^{1/2}$ equals the range of H^* and that $F_\sharp^{-1/2}H^* : U \to V$ is bounded with bounded inverse. □

For an application of the Theorem 3.4.1, we need to study properties of the middle operator T in the factorization of Theorem 3.3.3

Lemma 3.4.3. *Suppose that the contrast q satisfies the Assumption 3.3.1 and that the direct scattering problem* (3.13) *is uniquely solvable for any $f \in L^2(D)^2$. Let $T : L^2(D)^2 \to L^2(D)^2$ be the operator defined as in Theorem 3.3.3, i.e.*

$$Tf = \mathrm{sign}(q)(f + \sqrt{|q|}\nabla u),$$

where $u \in H^1_\alpha(\Omega_h)$ is the radiating variational solution to $\mathrm{div}(\varepsilon_\mathrm{r}^{-1}\nabla u) + k^2u = -\mathrm{div}(q/\sqrt{|q|}f)$ *in Ω_h and $\varepsilon_\mathrm{r}^{-1}\partial u/\partial\nu = 0$ on Γ_0, i.e., for all $\psi \in H^1_\alpha(\Omega_h)$,*

$$\int_{\Omega_h}(\varepsilon_\mathrm{r}^{-1}\nabla u \cdot \nabla\overline{\psi} - k^2u\overline{\psi})\,\mathrm{d}x - \int_{\Gamma_h}\overline{\psi}T^+(u)\,\mathrm{d}s = -\int_D q/\sqrt{|q|}f \cdot \nabla\overline{\psi}\,\mathrm{d}x\,. \tag{3.24}$$

Then we have

(a) T is injective and $\langle \mathrm{Im}(T)f, f\rangle \leq 0$ for all $f \in L^2(D)^2$.

(b) Define the operator $T_0 : L^2(D)^2 \to L^2(D)^2$ *by* $T_0 f = \operatorname{sign}(q)(f + \sqrt{|q|}\nabla\tilde{u})$ *where* $\tilde{u} \in H^1_\alpha(\Omega_h)$ *solves* (3.24) *for* $k = \mathrm{i}$ *and* $f \in L^2(D)^2$. *Then we have that* $T - T_0$ *is compact in* $L^2(D)^2$.

(c) For T_0 *defined as in (b), if* $\operatorname{Re}(q) > 0$ *on* $L^2(D)^2$ *then* $\operatorname{Re}(T_0)$ *is coercive in* $L^2(D)^2$, *i.e., there exists a constant* $\gamma > 0$ *such that*

$$\langle \operatorname{Re}(T_0) f, f\rangle_{L^2(D)^2} \geq \gamma \|f\|_{L^2(D)^2}.$$

Proof. (a) We show the injectivity of T by assuming that $Tf = \operatorname{sign}(q)(f + \sqrt{|q|}\nabla u) = 0$, then u is a radiating variational solution to the homogeneous problem $\Delta u + k^2 u = 0$ in Ω_h and $\partial u/\partial\nu = 0$ on Γ_0. However, we showed in the proof of Lemma 3.3.2 that the latter problem has only the trivial solution which implies that $u = 0$ in Ω_h. Thus, $f = 0$ or T is injective.

Now we set $w = f + \sqrt{|q|}\nabla u$, then $Tf = \operatorname{sign}(q) w$ and

$$\begin{aligned}
\langle Tf, f\rangle_{L^2(D)^2} &= \int_D \operatorname{sign}(q) w \cdot (\overline{w} - \sqrt{|q|}\nabla\overline{u})\,\mathrm{d}x \\
&= \int_D (\operatorname{sign}(q)|w|^2 - q/\sqrt{|q|} w \cdot \nabla\overline{u})\,\mathrm{d}x \\
&= \int_D \operatorname{sign}(q)|w|^2\,\mathrm{d}x + \int_{\Omega_h} (|\nabla u|^2 - k^2|u|^2)\,\mathrm{d}x - \int_{\Gamma_h} \overline{u} T^+(u)\,\mathrm{d}s
\end{aligned} \tag{3.25}$$

Now recall Theorem 3.2.1, using Plancherel identity implies that

$$-\operatorname{Im}\left(\int_{\Gamma_h} \overline{u} T^+(u)\,\mathrm{d}s\right) = -\operatorname{Im}\left(\mathrm{i}\sum_{j\in\mathbb{Z}} \beta_j |\hat{u}_j|^2\right) = -\sum_{j:k^2>\alpha_j^2} (k^2 - \alpha_j^2)^{1/2} |\hat{u}_j|^2 \leq 0$$

Together with the fact that $\operatorname{Im}(q) \leq 0$ in D, we hence obtain

$$\langle \operatorname{Im}(T) f, f\rangle_{L^2(D)^2} = \int_D \frac{\operatorname{Im}(q)}{|q|}|w|^2 - \operatorname{Im}\left(\int_{\Gamma_h} \overline{v} T^+(v)\,\mathrm{d}s\right) \leq 0.$$

(b) From the definitions of T and T_0 we note that $Tf - T_0 f = q/\sqrt{|q|}\nabla(u - \tilde{u})$ where $u, \tilde{u} \in H^1_\alpha(\Omega_h)$ are the solutions, for k and $k = \mathrm{i}$, of

$$\int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1}\nabla u \cdot \nabla\overline{\psi} - k^2 u\overline{\psi})\,\mathrm{d}x - \int_{\Gamma_h} \overline{\psi} T^+(u)\,\mathrm{d}s = -\int_{\Omega_h} q/\sqrt{|q|} f \cdot \nabla\overline{\psi}\,\mathrm{d}x\,, \tag{3.26}$$

$$\int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1}\nabla \tilde{u} \cdot \nabla\overline{\psi} + \tilde{u}\overline{\psi})\,\mathrm{d}x - \int_{\Gamma_h} \overline{\psi} T^+(\tilde{u})\,\mathrm{d}s = -\int_{\Omega_h} q/\sqrt{|q|} f \cdot \nabla\overline{\psi}\,\mathrm{d}x\,, \tag{3.27}$$

for all $\psi \in H^1_\alpha(\Omega_h)$. Consider now the sequence f_j which converges weakly to zero in $L^2(D)^2$, and denote by u_j, $\tilde{u}_j$ the corresponding solutions in (3.26),(3.27), respectively. It is sufficient to prove that $\|(T - T_0) f_j\|_{L^2(D)^2} \to 0$. Due to the boundedness of the solution operator from $L^2(D)^2$ into $H^1_\alpha(\Omega_h)$ we imply that u_j and $\tilde{u}_j$ converge weakly to zero in $H^1_\alpha(\Omega_h)$. That means

that $w_j := u_j - \tilde{u}_j$ converge strongly to zero in $L^2(\Omega_h)$ because of the compact embedding $H^1_\alpha(\Omega_h) \subset L^2(\Omega_h)$.

Now consider (3.26),(3.27) for u_j, $\tilde{u}_j$ and f_j, making a subtraction we have

$$\int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1} \nabla w_j \cdot \nabla \overline{\psi} - k^2 w_j \overline{\psi})\, \mathrm{d}x \, - \int_{\Gamma_h} \overline{\psi} T^+(w_j)\, \mathrm{d}s \, = (k^2+1) \int_{\Omega_h} \tilde{u}_j \overline{\psi}\, \mathrm{d}x\,.$$

Choose $\psi = w_j$ we obtain

$$\int_{\Omega_h} (\varepsilon_{\mathrm{r}}^{-1} |\nabla w_j|^2 - k^2 |w_j|^2)\, \mathrm{d}x \, - \int_{\Gamma_h} \overline{w_j} T^+(w_j)\, \mathrm{d}s \, = (k^2+1) \int_{\Omega_h} \tilde{u}_j \overline{w_j}\, \mathrm{d}x\,, \tag{3.28}$$

We know that $\|w_j\|_{L^2(\Omega_h)} \to 0$, and $\tilde{u}_j, T^+(w_j)$ are bounded sequences. Moreover we recall that u_j and $\tilde{u}_j$ are smooth in a neighborhood of Γ_h, and hence $w_j = u_j - \tilde{u}_j$ converge uniformly to zero on Γ_h. The latter facts allow us to conclude that $\|\nabla w_j\|_{L^2(\Omega_h)} \to 0$ as j tends to infinity. Thus we have $\|(T - T_0) f_j\|_{L^2(D)^2} \to 0$.

(c) If $\mathrm{Re}(q) > 0$, we return to (3.25) for $\tilde{u}$ instead of u. Then taking the real part implies that

$$\begin{aligned}
\langle \mathrm{Re} T_0 f, f \rangle_{L^2(D)^3} &= \mathrm{Re} \int_D \mathrm{sign}(q) |f + \sqrt{|q|} \nabla \tilde{u}|^2\, \mathrm{d}x \\
&\quad + \int_{\Omega_h} (|\nabla \tilde{u}|^2 + |\tilde{u}|^2)\, \mathrm{d}x \, - \mathrm{Re} \int_{\Gamma_h} \overline{\tilde{u}} T^+(\tilde{u})\, \mathrm{d}s \\
&\geq \mathrm{Re} \int_D \mathrm{sign}(q) |f + \sqrt{|q|} \nabla \tilde{u}|^2\, \mathrm{d}x \, + \int_{\Omega_h} (|\nabla \tilde{u}|^2 + |\tilde{u}|^2)\, \mathrm{d}x
\end{aligned} \tag{3.29}$$

since we know in Theorem 3.2.1 that $-\mathrm{Re} \int_{\Gamma_h} \overline{\tilde{u}} T^+(\tilde{u})\, \mathrm{d}s \, \geq 0$. Now assume that there is no such a constant $\gamma > 0$ for the statement of (c), then we can find a sequence $\{f_j\}$ such that $\|f_j\|_{L^2(D)^2} = 1$ and $\langle \mathrm{Re} T_0 f_j, f_j \rangle_{L^2(D)^2} \to 0$. Due to (3.29), we imply that $f_j + \sqrt{|q|} \nabla \tilde{u}_j \to 0$ in $L^2(D)^2$ where $\tilde{u}_j$ denotes the solution of (3.24) for f and k replaced by f_j and i, respectively. Also, we have from the variational formulation for $\tilde{u}_j$ that

$$\int_{\Omega_h} (|\nabla \tilde{u}_j|^2 + |\tilde{u}_j|^2)\, \mathrm{d}x \, \leq -\mathrm{Re} \int_D q/\sqrt{|q|} (f_j + \sqrt{|q|} \nabla \tilde{u}_j) \cdot \nabla \overline{\tilde{u}_j}\, \mathrm{d}x\,,$$

which let us obtain that $\|\tilde{u}_j\|_{H^1_\alpha(\Omega_h)} \to 0$. Hence $f_j \to 0$ in $L^2(D)^2$ which is a contradiction to $\|f_j\|_{L^2(D)^2} = 1$. Therefore $\mathrm{Re}(T_0)$ is coercive. □

Next, by using a special test sequence, we show a characterization of a point z belonging to the support $\overline{D}$ of the contrast q.

Lemma 3.4.4. *Let $H^* : L^2(D)^2 \to \ell^2(\mathbb{Z})$ be the operator defined as in Theorem 3.3.2. Suppose that the contrast q satisfies Assumption 3.3.1 and that the direct problem* (3.13) *is*

uniquely solvable for any $f \in L^2(D)^2$. Moreover, the complement of D in Ω_h is assumed to be connected. Then for $z \in \Omega_h$, the sequence $(r_j(z))_{j\in\mathbb{Z}}$ given by

$$r_j(z) = \frac{\mathrm{i}}{4\pi\beta_j} e^{-\mathrm{i}(\alpha_j z_1 + \beta_j(z_2-h))}, \tag{3.30}$$

belongs to $\mathrm{Rg}(H^*)$ *if and only if z belongs to the interior of the support $\overline{D}$ of q.*

Proof. From (2.14) we see that

$$G_k(x,z) = \sum_{j\in\mathbb{Z}} \frac{\mathrm{i}}{4\pi\beta_j} e^{-\mathrm{i}(\alpha_j z_1 + \beta_j(z_2-h))} e^{\mathrm{i}(\alpha_j x_1 + \beta_j(x_2-h))}, \quad z \in \Omega_h,\ x_2 > h.$$

Then $(r_j(z))_{j\in\mathbb{Z}}$ is the Rayleigh sequence of $G_k(\cdot, z)$. Now we assume that z is not in D and $(r_j(z))_{j\in\mathbb{Z}} \in \mathrm{Rg}(H^*)$. Then there exists $u \in H^1_\alpha(\Omega_h)$ solving the problem (3.17) with the source function $f \in L^2(D)^2$ in the right hand side. Further $\hat{u}_j = r_j(z)$ for $j \in \mathbb{Z}$. Since the Rayleigh sequences of $G_k(\cdot, z)$ and u are equal, both functions coincide in $(-\pi, \pi) \times (h, \infty)$. Due to the analyticity of u and $G_k(\cdot, z)$ in $\Omega \setminus D$ and $\Omega \setminus \{z\}$, respectively, and the analytic continuation we conclude that $u = G_k(\cdot, z)$ in $\Omega \setminus (D \cup \{z\})$. However from [8] we know that $G_k(\cdot, z)$ has a logarithmic singularity at z. This is hence a contradiction since $u \in H^1(B)$ for some neighborhood B of z but $G_k(\cdot, z) \notin H^1(B)$ due to the singularity at z.

To show that for $z \in D$ there exists $f \in L^2(D)^2$ such that $H^*(f) = (r_j(z))_{j\in\mathbb{Z}}$, we just apply the proof of the injectivity of H in Lemma 3.3.2 to the Green function $G_k(\cdot, z)$ instead of $\exp(\mathrm{i}(\alpha_j x_1 + \beta_j(x_2 - h))$. □

Theorem 3.4.5. *Suppose that the contrast q satisfies Assumption 3.3.1 and that the direct problem* (3.13) *is uniquely solvable for any $f \in L^2(D)^2$. For $j \in \mathbb{Z}$, denote by $(\lambda_n, \psi_{j,n})_{n\in\mathbb{N}}$ an orthonormal eigensystem of $(WN)_\sharp = |\mathrm{Re}(WN)| + \mathrm{Im}(WN)$ and by $(r_j(z))_{j\in\mathbb{Z}}$ the test sequence from* (3.30)*. Then a point $z \in \Omega_h$ belongs to the support of q if and only if*

$$\sum_{n=1}^{\infty} \frac{|\langle r_j(z), \psi_{j,n}\rangle_{\ell^2(\mathbb{Z})}|^2}{\lambda_n} < \infty. \tag{3.31}$$

Proof. As we assumed in the theorem, let $(\lambda_n^{1/2}, \psi_{j,n})_{n\in\mathbb{N}}$ be an orthonormal eigensystem of $(WN)_\sharp^{1/2}$. The assumptions of Theorem 3.4.1 on H, H^* and T have been checked in Lemma 3.4.4 and Lemma 3.3.2. Therefore, an application of Theorem 3.4.1 to the factorization $WN = H^*TH$ yields that $\mathrm{Rg}((WN)_\sharp^{1/2}) = \mathrm{Rg}(H^*)$. Combine the latter range identities with the characterization given in Lemma 3.4.4 we obtain that $(r_j(z))_{j\in\mathbb{Z}} \in \mathrm{Rg}((WN)_\sharp^{1/2})$ if and only if $z \in D$. Then the criterion (3.31) follows from the Picard's range criterion. □

3.5 Numerical Experiments

The study of numerical examples in this section mainly focuses on the dependence of the reconstructions on the number of the incident fields used, and the perfomance of the method

when the data is perturbed by artificial noise. We also indicate the number of the evanescent modes which are used for each reconstruction. Furthermore, different incident directions d_1 in (3.3) are considered for the reconstructions for each structure. These experiments are studied via three periodic structures motivated by the ones presented in [49]. More specific, for $-\pi \le x_1 \le \pi$, we consider the following diffraction gratings represented by the support $\overline{D}$ of the contrast q in one period Ω:

$$
\begin{aligned}
(a)\ \tau_1(x_1) &= \frac{-\sin(x_1)}{2} + 1,\ q = 1.5 \quad \text{in } D = \{(x_1,x_2)^\top \in \Omega : 0 < x_2 < \tau_1(x_1)\}.\\
(b)\ \tau_2(x_1) &= \frac{3}{2}\mathbf{1}_{[-\pi,-3\pi/4]\cup[3\pi/4,\pi]} + \frac{1}{2}\mathbf{1}_{[-\pi/2,\pi/2]} + \left(\frac{4}{\pi}x_1 - 1.5\right)\mathbf{1}_{[\pi/2,3\pi/4]}\\
&\quad + \left(-\frac{4}{\pi}x_1 - 1.5\right)\mathbf{1}_{[-3\pi/4,-\pi/2]},\\
q &= (x_2+1)(\sin^2(x_1)+0.5)/3 - 2\mathrm{i} \quad \text{in } D = \{(x_1,x_2)^\top \in \Omega : 0 < x_2 < \tau_2(x_1)\}.\\
(c)\ \tau_3(x_1) &= \frac{1}{2}\mathbf{1}_{(-\pi/2,\pi/2)} + \frac{3}{2}\mathbf{1}_{[-\pi,\pi/2]\cup[\pi/2,\pi]},\ D = \{(x_1,x_2)^\top \in \Omega : 0 < x_2 < \tau_3(x_1)\},\\
q &= \begin{cases} 1-3\mathrm{i} & \text{in } D_1 = \{(x_1,x_2)^\top \in D : -\pi/2 < x_1 < \pi/2\},\\ 0.5 & \text{in } D \setminus D_1. \end{cases}
\end{aligned}
$$

Here the functions $\tau_{1,2,3}$ have 2π-periodic extensions in x_1 direction. Note that, in our numerical examples, we consider different kinds of the contrast q for different structures. Specifically, in the case (a) the contrast q is considered to be homogeneous (constant) and non-absorbed in its support $\overline{D}$. The case (b) studies an inhomogeneous and absorbing contrast, and a partially absorbing contrast having jumps in its support is investigated in the case (c).

We use the data of the direct scattering problem implemented by the volume integral equation method studied in Chapter 1. For the numerical experiments we solve the direct problem for a finite number $j = -M_1, ..., M_2$ of incident fields $u_j^i = e^{\mathrm{i}(\alpha_j x_1 - \beta_j x_2)} + e^{\mathrm{i}(\alpha_j x_1 + \beta_j x_2)}$ where $M_1, M_2 \in \mathbb{N}$. For $-M_1 \le n, j \le M_2$, the near field operator N then corresponds to the matrix $[\hat{u}_{n,j}]$ of Rayleigh sequences $\hat{u}_n$ corresponding to the incident fields u_j^i. Denote by $\mathcal{N}_{M_1,M_2}$ the matrix corresponding to the discretization of the operator WN. Then the symmetric matrix $\mathrm{Re}(\mathcal{N}_{M_1,M_2})$ can be decomposed as

$$\mathrm{Re}(\mathcal{N}_{M_1,M_2}) = VDV^{-1},$$

where D, V are the matrices of eigenvalues and corresponding eigenvectors of $\mathrm{Re}(\mathcal{N}_{M_1,M_2})$, respectively. Note that D is a diagonal matrix and we denote by $|D|$ the absolute value of D which is taken componentwise. Then we have

$$(\mathcal{N}_{M_1,M_2})_\sharp := V|D|V^{-1} + \mathrm{Im}(\mathcal{N}_{M_1,M_2}).$$

Computing the singular value decomposition of $(\mathcal{N}_{M_1,M_2})_\sharp$ implies that

$$(\mathcal{N}_{M_1,M_2})_\sharp^{1/2} = U|S|^{1/2}V^{-1},$$

where S is the diagonal matrix of singular values λ_l of $(\mathcal{N}_{M_1,M_2})_\sharp$. Also $U = [\psi_{j,l}]$ is a $(M_1+M_2+1)\times(M_1+M_2+1)$ matrix of "left" singular vectors. Then the criterion (3.31) for computing the image P can be approximated as follows

$$P(z) = \left[\sum_{l=1}^{M_1+M_2+1} \frac{1}{\lambda_l}\left|\sum_{j=-M_1}^{M_2} r_j(z)\overline{\psi}_{j+M_1+1,l}\right|^2\right]^{-1/2}, \tag{3.32}$$

Note that P should be small outside of the support $\overline{D}$ of the contrast and big inside of D.

To show the performance of the method with noisy data, we pertub our synthetic data by artificial noise. More particularly, we add the noise matrix $\mathcal{X}$ of uniformly distributed random entries to the data matrix $(\mathcal{N}_{M_1,M_2})_\sharp^{1/2}$. Denote by δ the noise level, then the noised data matrix $(\mathcal{N}_{M_1,M_2})_{\sharp,\delta}^{1/2}$ is given by

$$(\mathcal{N}_{M_1,M_2})_{\sharp,\delta}^{1/2} := (\mathcal{N}_{M_1,M_2})_\sharp^{1/2} + \delta\frac{\mathcal{X}}{\|\mathcal{X}\|_2}\|(\mathcal{N}_{M_1,M_2})_\sharp^{1/2}\|_2,$$

where $\|\cdot\|_2$ is the matrix 2-norm. Note that from the latter equation we also have

$$\frac{\|(\mathcal{N}_{M_1,M_2})_{\sharp,\delta}^{1/2} - (\mathcal{N}_{M_1,M_2})_\sharp^{1/2}\|_2}{\|(\mathcal{N}_{M_1,M_2})_\sharp^{1/2}\|_2} = \delta.$$

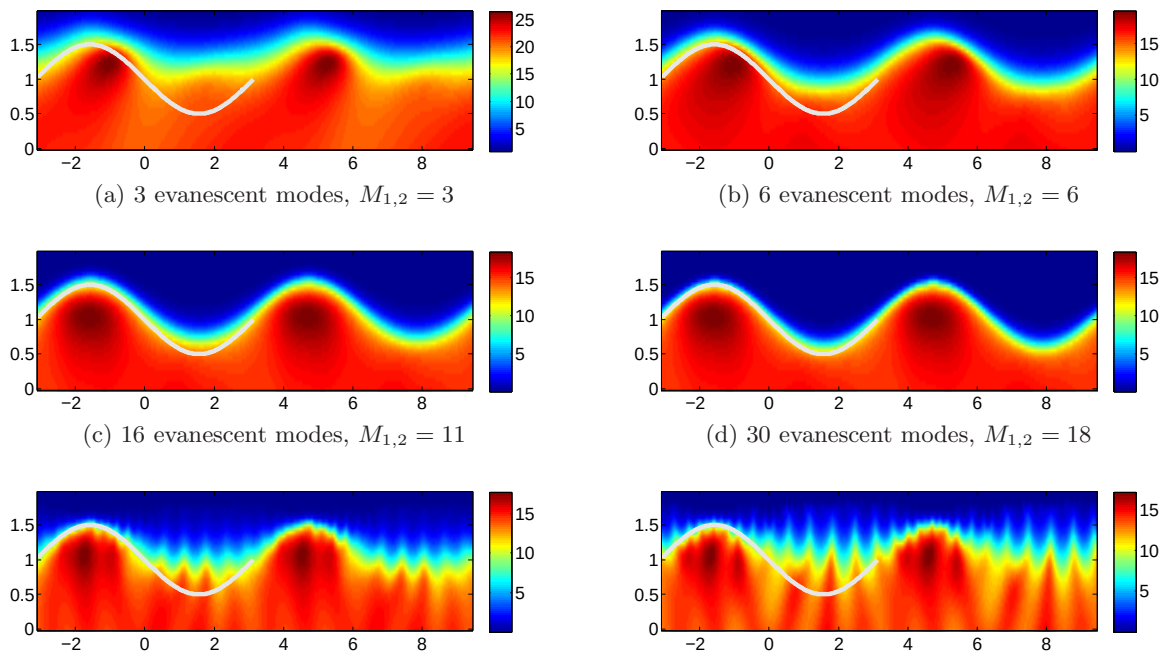
We apply Tikhonov regularization [30], then instead of implementing (3.32) we consider

$$P(z) = \left[\sum_{l=1}^{M_1+M_2+1} \left(\frac{\lambda_l^{1/2}}{\lambda_l+\gamma}\right)^2\left|\sum_{j=-M_1}^{M_2} r_j(z)\overline{\psi}_{j+M_1+1,l}\right|^2\right]^{-1/2}, \tag{3.33}$$

Here λ_l, $\psi_{j,l}$ are the singular values and vectors of $(-\mathcal{N}_{M_1,M_2})_{\sharp,\delta}$, respectively. The parameter γ is chosen by Morozov's generalized discrepancy principle which can be obtained by solving the equation

$$\sum_{l=1}^{M_1+M_2+1} \frac{\gamma^2-\delta^2\lambda_l}{(\lambda_l+\gamma)^2}\left|\sum_{j=-M_1}^{M_2} r_j(z)\overline{\psi}_{j+M_1+1,l}\right|^2 = 0$$

for some fixed sampling point z. For the numerical examples in this section, we choose the wave number $k = 3.5$. The number of the incident fields used is M_1+M_2+1. The exact geometry is the domain below the white line (in one period), and the pictures are plotted in two periods.



(a) 3 evanescent modes, $M_{1,2} = 3$

(b) 6 evanescent modes, $M_{1,2} = 6$

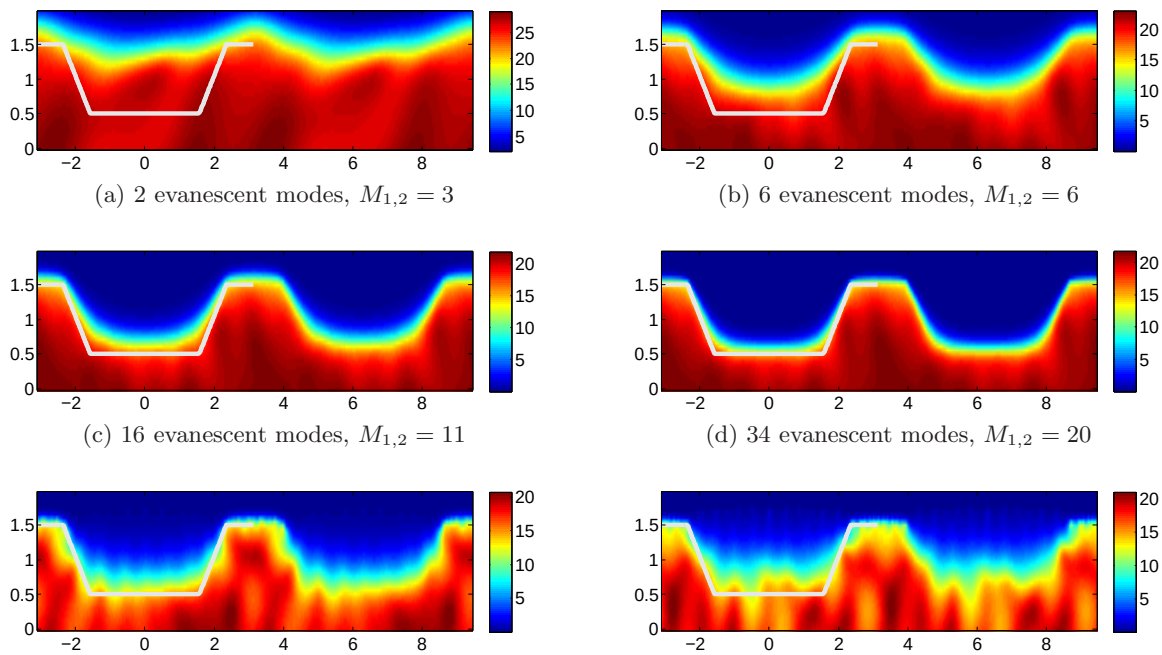
(c) 16 evanescent modes, $M_{1,2} = 11$

(d) 30 evanescent modes, $M_{1,2} = 18$

(e) 30 evanescent modes, $M_{1,2} = 18$, 2% noise

(f) 30 evanescent modes, $M_{1,2} = 18$, 5% noise

Figure 3.2: Reconstructions for the case of function τ_1, $q = 1.5$ in D, $k = 3.5$, $d_1 = \cos(\pi/6)$, 4 propagating modes for (a) and 7 propagating modes for the rest.



(a) 2 evanescent modes, $M_{1,2} = 3$

(b) 6 evanescent modes, $M_{1,2} = 6$

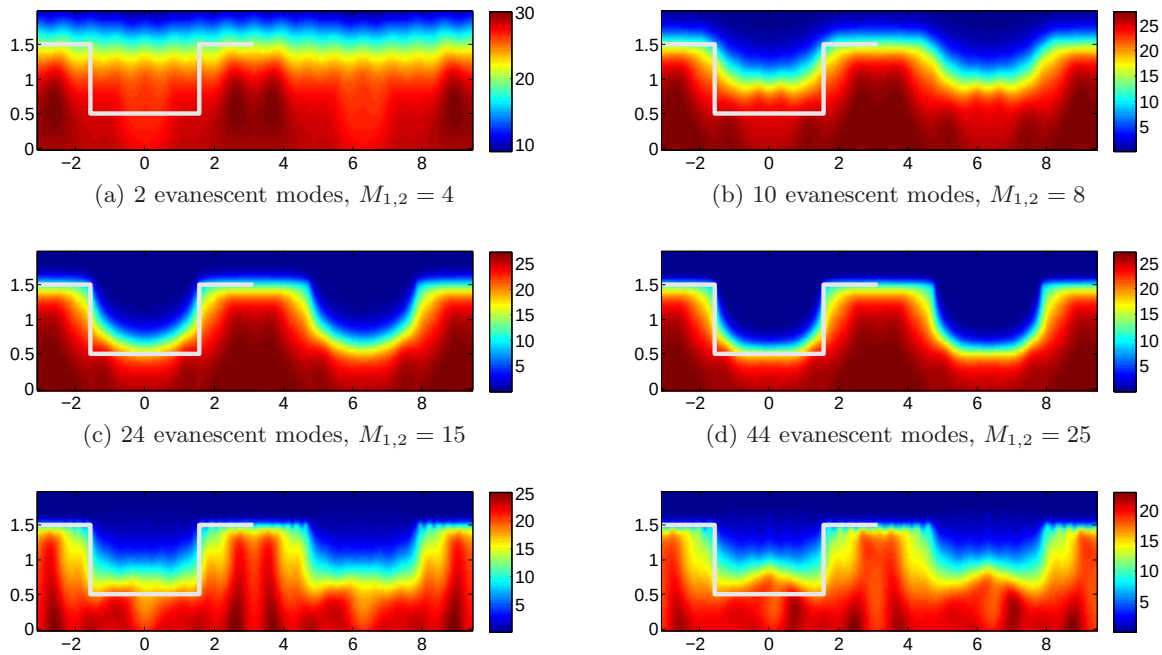
(c) 16 evanescent modes, $M_{1,2} = 11$

(d) 34 evanescent modes, $M_{1,2} = 20$

(e) 34 evanescent modes, $M_{1,2} = 20$, 2% noise

(f) 44 evanescent modes, $M_{1,2} = 25$, 5% noise

Figure 3.3: Reconstructions for the case of function τ_2, $q = (x_2 + 1)(\sin^2(x_1) + 0.5)/3 - 2\mathrm{i}$ in D, $k = 3.5$, $d_1 = \cos(\pi/4)$, 5 propagating modes for (a) and 7 propagating modes for the rest.



(a) 2 evanescent modes, $M_{1,2} = 4$

(b) 10 evanescent modes, $M_{1,2} = 8$

(c) 24 evanescent modes, $M_{1,2} = 15$

(d) 44 evanescent modes, $M_{1,2} = 25$

(e) 44 evanescent modes, $M_{1,2} = 25$, 2% noise

(f) 54 evanescent modes, $M_{1,2} = 30$, 5% noise

Figure 3.4: Reconstructions for the case of function τ_3, $q = 1 - 3\mathrm{i}$ in $D_1 = \{(x_1, x_2)^\top \in D : -\pi/2 < x_1 < \pi/2\}$ and $q = 0.5$ in $D \setminus D_1$, $k = 3.5$, $d_1 = \cos(\pi/2)$, 7 propagating modes.

Part II

The Case of Maxwell's Equations

Chapter 4

Volume Integral Equation Methods for Biperiodic Scattering Problems

Abstract: In Chapter 4, we extend the volume integral equation method investigated in Chapter 1 to electromagnetic scattering problems from anisotropic biperiodic structures. These problems are governed by Maxwell's equations in a full space. We consider the case where the electric permittivity and the magnetic permeability are both matrix-valued functions. The scattering problem again can be reformulated as a strongly singular volume integral equation (see equation (4.23)). Since the compact embedding $H^1 \subset L^2$ is crucially exploited for the scalar case for proving Gårding inequalities, the main difficulty in this case is that the embedding $H(\mathrm{curl}) \subset L^2$ is not compact. We overcome this by not investigating Gårding inequalities in the support of the contrast but in a bigger domain under suitable assumptions on the contrast (see Theorem 4.4.2). This turned out to be sufficient for convergence theory of a trigonometric Galerkin method appplied to the periodized integral equation (see Theorem 4.5.3 and Theorem 4.6.1). We again propose fully discrete formulas for the numerical scheme as well as numerical examples (see Section 4.6–4.7).

4.1 Introduction

In this chapter we extend the volume integral equation method investigated in Chapter 1 to the case of Maxwell's equations for the direct scattering problem from biperiodic structures. By biperiodic, we mean that the structure is periodic in the, say, x_1- and x_2-direction, while it is bounded in the x_3 direction (compare Figure 4.1).

Central to the study is again to prove Gårding inequalities for strongly singular integral equations (again, "strongly singular" simply means that the kernels of the corresponding integral operators fail to be weakly singular, and the integral operators in general fails to be

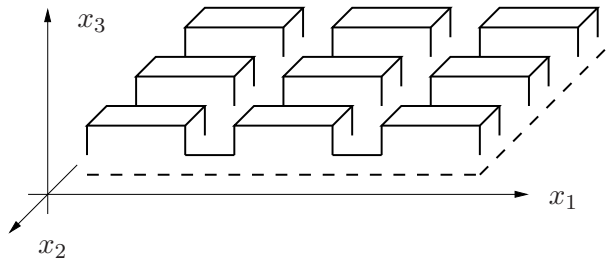


Figure 4.1: Sketch of the biperiodic structure under consideration.

compact). In this chapter we do not aim to investigate such inequalities for negative-index dielectric material as in the scalar case. Instead we study such inequalities for the case that the electric permittivity and the magnetic permeability are both positive-semidefinite matrix-valued functions. We again exploit the technique studied for the case of positive contrast of Theorem 2.4.5 in Chapter 1. Obviously, in the $H(\text{curl})$-formulation studied for the Maxwell's equations, the embedding $H(\text{curl}) \subset L^2$ is not compact. Therefore, a straightforward extension from the proof of Theorem 2.4.5 does not seem to work since the compact embedding $H^1 \subset L^2$ is crucially exploited in the proof. We overcome this by not investigating Gårding inequalities in the support of the contrasts but in a bigger domain using the technique of Theorem 2.4.5. In this way we can directly obtain the Gårding inequality for standard Sobolev spaces without studying weighted spaces. Further from this result one can easily prove that such an inequality also holds for the periodized integral equation which leads to convergence theory of the Galerkin method. It turns out also that we need weaker assumptions on the contrasts as well as on their support. However, a price we have to pay for the Maxwell case is that for discontinuous material parameters the solution is less regular than the scalar case which does not allow us to obtain the order of convergence estimate as in the case of TM modes. Anyway the approach can be applied to obstacle scattering problems for both scalar and vector cases. Finally we propose fully discrete formulas for the numerical scheme as well as numerical examples to indicate the performance of the method.

The chapter is organized as follows: In Section 4.2 we give a problem setting for the direct scattering problem. While in Section 4.3 we give the volume integral equation formulation of the problem, we prove in Sections 4.4 the Gårding inequality on a continuous level. In Section 4.5 we periodize the integral equation, prove Gårding inequalities for periodized integral equation, and error estimates for trigonometric Galerkin methods. We discretize the periodic integral equation and give fully discrete formulas in Section 4.6. Finally, we give some numerical experiments in Section 4.7 to examine the performance of the method.

4.2 Problem Setting

We consider scattering of time-harmonic electromagnetic waves from a biperiodic structure. The electric field E and the magnetic field H are governed by the time-harmonic Maxwell

equations at frequency $\omega > 0$ in $\mathbb{R}^3$

$$\operatorname{curl} H + \mathrm{i}\omega\varepsilon E = \sigma E \quad \text{in } \mathbb{R}^3, \tag{4.1}$$

$$\operatorname{curl} E - \mathrm{i}\omega\mu H = 0 \quad \text{in } \mathbb{R}^3, \tag{4.2}$$

where the electric permittivity ε, the magnetic permeability μ and the conductivity σ are matrix-valued functions in $L^\infty(\mathbb{R}^3, \mathbb{R}^{3\times 3})$. We assume that ε and μ are 2π-periodic in x_1 and x_2, and that there are positive constants ε_0 and μ_0 such that $\varepsilon \equiv \varepsilon_0 I_3$, $\mu \equiv \mu_0 I_3$, and that $\sigma \equiv 0 I_3$ outside the biperiodic structure. As usual, the problem (4.1)–(4.2) has to be completed by a radiation condition that we set up using Fourier techniques.

The biperiodic structure is illuminated by an electromagnetic plane wave with wave vector $d = (d_1, d_2, d_3) \in \mathbb{R}^3$, $d_3 \neq 0$ such that $d \cdot d = \omega^2 \varepsilon_0 \mu_0$. The polarizations $p, s \in \mathbb{R}^3$ of the incident wave satisfy $p \cdot d = 0$ and $s = 1/(\omega\varepsilon_0)(p \times d)$. With these definitions, the incident plane waves E^i and H^i given by

$$E^i = s e^{\mathrm{i} d\cdot x}, \quad H^i = p e^{\mathrm{i} d \cdot x}, \quad x \in \mathbb{R}^3. \tag{4.3}$$

For $d = (d_1, d_2, d_3) \in \mathbb{R}^3$ defined in (4.3), we set $\alpha = (\alpha_1, \alpha_2, 0) = (d_1, d_2, 0)$. Similar to the scalar case a function $u : \mathbb{R}^3 \to \mathbb{C}^3$ is called α-quasiperiodic if, for all $(x_1, x_2, x_3)^\top \in \mathbb{R}^3$,

$$u(x_1 + 2\pi, x_2, x_3) = e^{2\pi\mathrm{i}\alpha_1} u(x_1, x_2, x_3), \quad u(x_1, x_2 + 2\pi, x_3) = e^{2\pi\mathrm{i}\alpha_2} u(x_1, x_2, x_3).$$

Note that the incident fields E^i, H^i defined in (4.3) are α-quasiperiodic functions. The relative material parameters are defined by

$$\varepsilon_{\mathrm{r}} = \frac{\varepsilon + \mathrm{i}\sigma/\omega}{\varepsilon_0}, \qquad \mu_{\mathrm{r}} = \frac{\mu}{\mu_0}.$$

Then ε_{r} and μ_{r} equal I_3 outside the biperiodic structure. In the rest of this chapter, we will work with the magnetic field H. This is motivated by the important case of non-magnetic media where we also have the divergence-free condition $\operatorname{div}(H) = 0$. Hence, introducing the wave number $k = \omega(\varepsilon_0\mu_0)^{1/2}$, and eliminating the electric field E from (4.1)–(4.2), we find that

$$\operatorname{curl}\left(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl} H\right) - k^2 \mu_{\mathrm{r}} H = 0 \quad \text{in } \mathbb{R}^3. \tag{4.4}$$

We wish to reformulate the last equation in terms of the scattered field H^s, defined by $H^s := H - H^i$. Since, by construction, $\operatorname{curl}\operatorname{curl} H^i - k^2 H^i = 0$, subtracting the latter equation and (4.4) implies that

$$\operatorname{curl}\left(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl} H^s\right) - k^2 \mu_{\mathrm{r}} H^s = -\operatorname{curl}\left(Q \operatorname{curl} H^i\right) + k^2 P H^i \quad \text{in } \mathbb{R}^3, \tag{4.5}$$

where the contrasts Q, P are defined by

$$Q := \varepsilon_{\mathrm{r}}^{-1} - I_3, \qquad P := \mu_{\mathrm{r}} - I_3.$$

As in the scalar case ε_{r}, μ_{r} are 2π-periodic in x_1 and x_2, the incident field H^i is α-quasiperiodic, thus the solution H^s that we seek for is α-quasiperiodic as well. We next complement this problem by a radiation condition for the scattered field H^s that is set up using Fourier techniques. This step is carried out similarly to the scalar case. Indeed due to the α-quasiperiodicity of H^s, we obtain that $e^{-\mathrm{i}\alpha\cdot x}H^s$ is 2π-periodic in x_1 and x_2, and can hence be expanded as

$$e^{-\mathrm{i}\alpha\cdot x}H^s(x) = \sum_{n\in\mathbb{Z}^2} \hat{H}_n(x_3)e^{\mathrm{i}(n_1x_1+n_2x_2)}, \quad x = (x_1, x_2, x_3)^\top \in \mathbb{R}^3.$$

Here the Fourier coefficients $\hat{H}_n(x_3)$ are defined by

$$\hat{H}_n(x_3) = \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} H^s(x_1, x_2, x_3)e^{-\mathrm{i}\alpha_n\cdot x}\,\mathrm{d}x_1\,\mathrm{d}x_2\,, \quad n \in \mathbb{Z}^2.$$

where

$$\alpha_n := (\alpha_{1,n}, \alpha_{2,n}, 0) = (\alpha_1 + n_1, \alpha_2 + n_2, 0).$$

Define, for $n \in \mathbb{Z}^2$,

$$\beta_n := \begin{cases} \sqrt{k^2 - |\alpha_n|^2}, & k^2 \geq |\alpha_n|^2, \\ \mathrm{i}\sqrt{|\alpha_n|^2 - k^2}, & k^2 < |\alpha_n|^2. \end{cases}$$

Note that we also exclude the Rayleigh frequencies as in the scalar case, that is, all β_n are supposed to be nonzero.

Recall that $\varepsilon_{\mathrm{r}}^{-1}$ and μ_{r} equal I_3 outside the structure that implies $\varepsilon_{\mathrm{r}}^{-1} = \mu_{\mathrm{r}} = I_3$ and $Q = P = 0I_3$ for $|x_3| > h$ where $h > \sup\{|x_3| : (x_1, x_2, x_3)^\top \in \operatorname{supp}(Q) \cup \operatorname{supp}(P)\}$. Thus, from equation (4.5) it holds that $\operatorname{div} H^s$ vanishes for $|x_3| > h$, and $(\Delta + k^2)H^s = 0$ in $\{|x_3| > h\}$. Using separation of variables, and choosing the upward propagating solution, we set up a radiation condition in form of a Rayleigh expansion condition, prescribing that H^s can be written as

$$H^s(x) = \sum_{n\in\mathbb{Z}^2} \hat{H}_n^{\pm} e^{\mathrm{i}(\alpha_n\cdot x \pm \beta_n(x_3 \mp h))} \quad \text{for } x_3 \gtrless \pm h, \tag{4.6}$$

where

$$\hat{H}_n^{\pm} = \hat{H}_n(\pm h) = \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} H^s(x_1, x_2, \pm h)e^{-\mathrm{i}\alpha_n\cdot x}\,\mathrm{d}x_1\,\mathrm{d}x_2\,.$$

From now, a function which satisfies (4.6) is called to be radiating. Note that we require that the series in (4.6) converges uniformly in compact subsets of $\{|x_3| > h\}$. Further, note that only a finite number of terms in (4.6) are propagating plane waves which are called propagating modes, the rest are evanescent modes which correspond to exponentially decaying terms.

The problem (4.5)–(4.6) can be reduced to one period $\Omega := (-\pi, \pi)^2 \times \mathbb{R}$ due to its periodicity. Consider a more general following problem: Given f, $g \in L^2(D)^3$, find $u : \Omega \to \mathbb{C}^3$ such that

$$\operatorname{curl}\left(\varepsilon_{\mathrm{r}}^{-1}\operatorname{curl} u\right) - k^2\mu_{\mathrm{r}}u = -\operatorname{curl} f + k^2 g \quad \text{in } \Omega, \tag{4.7}$$

and

$$u(x) = \sum_{n\in\mathbb{Z}^2} \hat{u}_n^{\pm} e^{\mathrm{i}(\alpha_n\cdot x \pm \beta_n(x_3\mp h))} \quad \text{for } x_3 \gtrless \pm h, \tag{4.8}$$

where the Rayleigh sequences $\hat{u}_n^{\pm}$ are defined as in (4.6).

4.3 Integral Equation Formulation

In this section, we reformulate the scattering problem (4.7)–(4.8) as a volume integral equation, and prove mapping properties between Sobolev spaces of the integral operators that are involved. As in two-dimensional case, we denote by G_k the Green's function to the α-quasiperiodic Helmholtz equation in $\mathbb{R}^3$, see [4]. Recall that all β_j are nonzero, the α-quasiperiodic Green's function has the series representation

$$G_k(x) := \frac{\mathrm{i}}{8\pi^2} \sum_{j\in\mathbb{Z}^2} \frac{1}{\beta_j} \exp(\mathrm{i}\alpha_j\cdot x + \mathrm{i}\beta_j|x_3|), \tag{4.9}$$

for $x = (x_1, x_2, x_3)^\top \in \mathbb{R}^3$, $x \neq (2\pi m_1, 2\pi m_2, 0)$, $(m_1, m_2) \in \mathbb{Z}^2$. Similar to Lemma 2.3.1 we also have

$$G_k(x) = \frac{e^{\mathrm{i}k|x|}}{4\pi|x|} + \Psi(x) \quad \text{in } \mathbb{R}^3, \tag{4.10}$$

where Ψ is an analytic function solving the Helmholtz equation $\Delta\Psi + k^2\Psi = 0$ in $(-2\pi, 2\pi)^2 \times \mathbb{R}$.

Now recall that $\Omega = (-\pi,\pi)^2 \times \mathbb{R}$ and $h > \sup\{|x_3| : (x_1, x_2, x_3)^\top \in \mathrm{supp}(Q) \cup \mathrm{supp}(P)\}$ we set

$$\overline{D} := [\mathrm{supp}(Q) \cup \mathrm{supp}(P)] \cap \Omega.$$

We also define a periodized Green's function, firstly, setting

$$\mathcal{K}_h(x) := G_k(x), \tag{4.11}$$

for $x = (x_1, x_2, x_3)^\top \in \mathbb{R}^2 \times (-h, h)$, $x \neq (2\pi m_1, 2\pi m_2, 0)$, $(m_1, m_2) \in \mathbb{Z}^2$, and secondly extending $\mathcal{K}_h(x)$ $2h$-periodically in x_3 to $\mathbb{R}^3$. We define

$$\Omega_h := (-\pi,\pi)^2 \times (-h, h), \quad \tilde{j} := (j_1, j_2)^\top \text{ for } j = (j_1, j_2, j_3)^\top \in \mathbb{Z}^3.$$

Then, similar to the scalar case, the trigonometric polynomials

$$\varphi_j(x) := \frac{1}{\sqrt{8\pi^2 h}} \exp\Big(\mathrm{i}\alpha_{\tilde{j}}\cdot x + \mathrm{i}\frac{j_3\pi}{h}x_3\Big), \tag{4.12}$$

form an orthonormal basis in $L^2(\Omega_h)$, and the Fourier coefficients of $f \in L^2(\Omega_h)$ are given by

$$\hat{f}(j) = \int_{\Omega_h} f\,\overline{\varphi_j}\,\mathrm{d}x\,, \quad j = (j_1, j_2, j_3)^\top \in \mathbb{Z}^3.$$

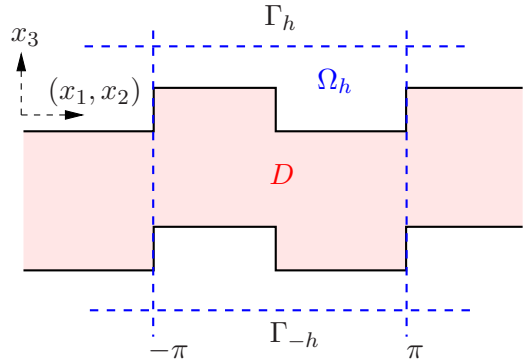


Figure 4.2: Geometric setting for scattering problem of electromagnetic waves from a penetrable biperiodic structure (in two dimentions, for simplicity).

For $0 \leq s < \infty$ we recall from (2.17) the fractional Sobolev space $H^s_{\alpha,\mathrm{p}}(\Omega_h)$ consisting of functions in $L^2(\Omega_h)$ such that

$$\|f\|^2_{H^s_{\alpha,\mathrm{p}}(\Omega_h)} = \sum_{j\in\mathbb{Z}^3} (1+|j|^2)^{s/2} |\hat{f}(j)|^2 < \infty.$$

To compute the Fourier coefficients $\hat{\mathcal{K}}_h(j)$ of the periodic Green's function $\mathcal{K}_h$ explicitly, we set

$$\lambda_j := k^2 - |\alpha_{\tilde{j}}|^2 - \left(\frac{j_3\pi}{h}\right)^2 \quad \text{for } j \in \mathbb{Z}^3.$$

and carry out similarly to the two-dimensional case.

Theorem 4.3.1. *The Fourier coefficients of the kernel $\mathcal{K}_h$ from* (4.11) *are given by*

$$\hat{\mathcal{K}}_h(j) = \begin{cases} \frac{\cos(j_3\pi)\exp(\mathrm{i}\beta_{\tilde{j}}h)-1}{\sqrt{8\pi^2 h}\,\lambda_j} & \textit{for } \lambda_j \neq 0, \\ \frac{\mathrm{i}h^{3/2}}{4\sqrt{2}\pi^2 j_3} & \textit{else}, \end{cases} \qquad j = \begin{pmatrix} j_1 \\ j_2 \\ j_3 \end{pmatrix} \in \mathbb{Z}^3.$$

Remark 4.3.2. *Note that $\hat{\mathcal{K}}_h(j)$ is well-defined for $\lambda_j = 0$: Since $k^2 \neq |\alpha_{\tilde{j}}|^2$ for all $j \in \mathbb{Z}^3$, the definition of λ_j implies that $j_3 \neq 0$ whenever $\lambda_j = 0$.*

Proof. It is easy to check that $(\Delta + k^2)\varphi_j = \lambda_j \varphi_j$ for $j = (j_1, j_2, j_3)^\top \in \mathbb{Z}^3$. If $\lambda_j \neq 0$, Green's second identity implies that

$$\begin{aligned} \hat{\mathcal{K}}_h(j) &= \int_{\Omega_h} \mathcal{K}_h(x)\overline{\varphi_j(x)}\,\mathrm{d}x = \lambda_j^{-1} \lim_{\delta\to 0} \int_{\Omega_h\setminus B(0,\delta)} G_k(x)\overline{(\Delta+k^2)\varphi_j(x)}\,\mathrm{d}x \\ &= \lambda_j^{-1} \lim_{\delta\to 0} \Bigg[\left(\int_{\partial\Omega_h} + \int_{\partial B(0,\delta)} \right) \left(G_k \frac{\partial\overline{\varphi_j}}{\partial\nu} - \frac{\partial G_k}{\partial\nu}\overline{\varphi_j} \right) \mathrm{d}s \qquad (4.13) \\ &\qquad + \int_{\Omega_h\setminus B(0,\delta)} (\Delta+k^2) G_k(x)\overline{\varphi_j(x)}\,\mathrm{d}x \Bigg], \qquad (4.14) \end{aligned}$$

where ν denotes the exterior normal vector to $B(0,\delta)$. The last volume integral vanishes since $(\Delta + k^2)G_k = 0$ in $\Omega_h \setminus B(0,\delta)$ for any $\delta > 0$. Let us now consider the first integral in (4.13). The boundary of Ω_h consists of two horizontal planes $\Gamma_{\pm h}$ and four vertical planes $\{(x_1, x_2, x_3) : x_1 = \pm, x_2 = \pm\pi, -h < x_3 < h\}$. Hence, the normal vector ν on these boundaries can be $(\pm 1, 0, 0)^\top$ or $(0, \pm 1, 0)^\top$ or $(0, 0, \pm 1)^\top$. Straightforward computations yield that

$$G_k(x_1, x_2, \pm h) = \frac{\mathrm{i}}{8\pi^2} \sum_{n\in\mathbb{Z}^2} \frac{e^{\mathrm{i}\beta_n h}}{\beta_n} e^{\mathrm{i}\alpha_n\cdot x}, \quad \frac{\partial G_k}{\partial x_3}(x_1, x_2, \pm h) = \mp\frac{1}{8\pi^2} \sum_{n\in\mathbb{Z}^2} e^{\mathrm{i}\beta_n h} e^{\mathrm{i}\alpha_n\cdot x}, \tag{4.15}$$

$$\overline{\varphi_j}(x_1, x_2, \pm h) = \frac{e^{-\mathrm{i}\alpha_{\tilde{j}}\cdot x}}{\sqrt{8\pi^2 h}} \cos(j_3\pi), \quad \text{and} \quad \frac{\partial \overline{\varphi_j}}{\partial x_3}(x_1, x_2, \pm h) = -\frac{\mathrm{i} j_3 \pi}{h} \overline{\varphi_j}(x_1, x_2, \pm h). \tag{4.16}$$

In consequence,

$$\begin{aligned}\int_{\Gamma_{\pm h}} \left(G_k \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial G_k}{\partial \nu} \overline{\varphi_j} \right) \mathrm{d}s &= -\int_{\Gamma_h} \frac{\partial G_k}{\partial x_3} \overline{\varphi_j}\, \mathrm{d}s + \int_{\Gamma_{-h}} \frac{\partial G_k}{\partial x_3} \overline{\varphi_j}\, \mathrm{d}s \\ &= -2 \int_{\Gamma_h} \frac{\partial G_k}{\partial x_3} \overline{\varphi_j}\, \mathrm{d}s\,.\end{aligned}$$

Using the above formulas for $\partial G_k/\partial x_3$ and $\overline{\varphi_j}$ in (4.15) and (4.16), respectively, we find that

$$-2 \int_{\Gamma_h} \frac{\partial G_k}{\partial x_3} \overline{\varphi_j}\, \mathrm{d}s = \frac{\cos(j_3\pi)}{\sqrt{8\pi^2 h}} e^{\mathrm{i}\beta_{\tilde{j}} h}.$$

Computing the partial derivatives of G_k and φ_j with respect to x_1, x_2 analogously to the above computations, one finds that the integrals on the vertical boundaries of Ω_h vanish due to the α-quasiperiodicity of both functions. Thus, we obtain that

$$\int_{\partial\Omega_h} \left(G_k \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial G_k}{\partial \nu} \overline{\varphi_j} \right) \mathrm{d}s = \frac{\cos(j_3\pi)}{\sqrt{8\pi^2 h}} e^{\mathrm{i}\beta_{\tilde{j}} h}. \tag{4.17}$$

Now we consider the second integral in (4.13). From (4.10) we know that $G_k(x) = \exp(\mathrm{i}k|x|)/(4\pi|x|) + \Psi(x)$ where Ψ is a smooth function in Ω_h. Obviously,

$$\lim_{\delta\to 0} \int_{\partial B(0,\delta)} \left(\Psi \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial \Psi}{\partial \nu} \overline{\varphi_j} \right) \mathrm{d}s = 0.$$

Taking into account the asymptotics of $\exp(\mathrm{i}k|x|)/(4\pi|x|)$ for small $|x|$ allow to show that

$$\lim_{\delta\to 0} \int_{\partial B(0,\delta)} \left(G_k \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial G_k}{\partial r} \overline{\varphi_j} \right) \mathrm{d}s = -\frac{1}{\sqrt{8\pi^2 h}}, \tag{4.18}$$

see, e.g., [102, Theorem 2.2.1]. Combining (4.17) with (4.18) yields that

$$\mathcal{K}_h(j) = \frac{1}{\sqrt{8\pi^2 h}\lambda_j} \Big[\cos(j_3\pi) e^{\mathrm{i}\beta_{\tilde{j}} h} - 1 \Big] \quad \text{for } \lambda_j \neq 0.$$

For $\lambda_j = 0$ we use de L'Hôspital's rule to find that

$$\mathcal{K}_h(j) = \lim_{\gamma \to |\alpha_{\tilde{j}}|^2 + (j_3\pi/h)^2} \frac{\cos(j_3\pi)\exp\left(\mathrm{i}h[\gamma - |\alpha_{\tilde{j}}|^2]^{1/2}\right) - 1}{\sqrt{8\pi^2 h}\,[\gamma - |\alpha_{\tilde{j}}|^2 - (j_3\pi/h)^2]} = \frac{\mathrm{i}h^{3/2}}{4\sqrt{2}\pi^2 j_3}.$$

Note that the assumption that $k^2 \neq \alpha_j^2$ for all $j \in \mathbb{Z}^3$ implies that λ_j and j_3 cannot vanish simultaneously. □

As in the scalar case, the Fourier coefficients of $\mathcal{K}_h$ decay quadratically,

$$|\hat{\mathcal{K}}_h(j)| \leq C/(1 + |\alpha_{\tilde{j}}|^2 + (j_3\pi/h)^2)$$

for $j \in \mathbb{Z}^3$, thus the convolution operator with kernel $\mathcal{K}_h$ is bounded from $L^2(\Omega_h)$ into $H^2_{\alpha,\mathrm{p}}(\Omega_h)$.

Proposition 4.3.3. *The convolution operator K_h defined by*

$$(K_h f)(x) = \int_{\Omega_h} \mathcal{K}_h(x-y) f(y)\,\mathrm{d}y \quad \textit{for } x \in \Omega_h,$$

is bounded from $L^2(\Omega_h)$ into $H^2_{\alpha,\mathrm{p}}(\Omega_h)$.

Again, similar to Lemma 2.3.5 for the scalar case we have

Lemma 4.3.4. *The volume potential V defined by*

$$(Vf)(x) = \int_D G_k(x-y) f(y)\,\mathrm{d}y\,, \quad x \in \Omega,$$

is bounded from $L^2(D)$ into $H^2_\alpha(\Omega_R)$ for all $R > 0$.

Note that the potential Vf can be extended to a quasiperiodic function in $H^2_{\mathrm{loc}}(\mathbb{R}^3)$, due to the quasiperiodicity of the kernel. Now we define

$$H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega) := \{u \in H_{\mathrm{loc}}(\mathrm{curl},\Omega) : u = U|_\Omega \text{ for some } \alpha\text{-quasiperiodic } U \in H_{\mathrm{loc}}(\mathrm{curl},\mathbb{R}^3)\}, \tag{4.19}$$

Lemma 4.3.5. *Let V be the volume potential defined in Lemma 4.3.4. Then the potentials $\mathrm{curl}\,V$ and $(k^2 + \nabla\mathrm{div})V$ are bounded from $L^2(D)^3$ into $H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$. Further, for $g \in L^2(D)^3$, $w_1 = \mathrm{curl}\,Vg$ and $w_2 = (k^2 + \nabla\mathrm{div})Vg$ are the unique radiating variational solutions to $\mathrm{curl}^2 w - k^2 w = \mathrm{curl}\,g$ and $\mathrm{curl}^2 w - k^2 w = k^2 g$ in Ω, respectively, that is, they satisfy*

$$\int_\Omega (\mathrm{curl}\,w_1 \cdot \mathrm{curl}\,\overline{\psi} - k^2 w_1 \overline{\psi})\,\mathrm{d}x = \int_D g \cdot \mathrm{curl}\,\overline{\psi}\,\mathrm{d}x \tag{4.20}$$

$$\int_\Omega (\mathrm{curl}\,w_2 \cdot \mathrm{curl}\,\overline{\psi} - k^2 w_2 \overline{\psi})\,\mathrm{d}x = k^2 \int_D g \cdot \overline{\psi}\,\mathrm{d}x \tag{4.21}$$

for all $\psi \in H_\alpha(\mathrm{curl},\Omega)$ with compact support, and additionally the Rayleigh expansion condition (4.6).

Proof. We first consider the potential w_1. Lemma 4.3.4 and quasi-periodicity of the kernel of V imply that w_1 is a function in $H_\alpha(\mathrm{curl}, \Omega_R)$ for all $R > 0$. It is sufficient to prove (4.20) for all smooth quasiperiodic test functions ψ that are supported in $\{|x_3| < C\}$ for some $C > 0$ depending on ψ. Since smooth functions with compact support in D is dense in $L^2(D)^3$, it is sufficient to consider $g \in C_0^\infty(D)^3$. It is well-known that $u = Vg \in H^2_\alpha(\Omega)$ solves $\Delta u + k^2 u = -g$. In the other hand, see also in [71], we have

$$\begin{aligned} w(x) &= \mathrm{curl} \int_D G_k(x,y) g(y)\,\mathrm{d}y \;= \int_D \mathrm{curl}_x (G_k(x,y) I_3) g(y)\,\mathrm{d}y \\ &= -\int_D \mathrm{curl}_y (G_k(x,y) I_3) g(y)\,\mathrm{d}y \;= \int_D G_k(x,y)\,\mathrm{curl}\, g(y)\,\mathrm{d}y\,. \end{aligned}$$

Consequently, $w_1 = \mathrm{curl}\, Vg = V(\mathrm{curl}\, g)$ solves $\Delta w_1 + k^2 w_1 = -\,\mathrm{curl}\, g$. Further, the potential w_1 is by construction divergence free which implies that $\mathrm{curl}^2\, w_1 = -\Delta w_1$. Hence, we obtain that

$$\mathrm{curl}^2\, w_1 - k^2 w_1 = \mathrm{curl}\, g, \quad \text{in } \Omega.$$

By substituting the expression of $G_k(x,y)$ into the latter expression, it follows that

$$w_1(x) = \sum_{j\in\mathbb{Z}^2} \frac{\mathrm{i}}{8\pi^2\beta_j} \int_D \mathrm{curl}\, g(y) e^{-\mathrm{i}\alpha_j\cdot y \mp \mathrm{i}\beta_j(y_3\mp h)}\,\mathrm{d}y\, e^{\mathrm{i}\alpha_j\cdot x \pm \mathrm{i}\beta_j(x_3\mp h)} \quad \text{for } x_3 \gtrless \pm h,$$

which shows that w_1 satisfies the Rayleigh expansion (4.6). Uniqueness of a radiating solution to (4.20) when $g = 0$ can be shown using integral representation formulas from Theorem 3.1 of [100].

Now we prove the claim concerning w_2. Since $\mathrm{curl}\,\nabla = 0$, we imply that $\mathrm{curl}(k^2 + \nabla\mathrm{div})V = k^2\,\mathrm{curl}\, V$ which shows the boundedness of $(k^2 + \nabla\mathrm{div})V$ from $L^2(D)^3$ into $H_\alpha(\mathrm{curl}, \Omega_R)$ for all $R > 0$ due to part (a). Furthermore, we have

$$\mathrm{curl}^2\, w_2 = k^2\,\mathrm{curl}^2\, Vg = k^2(k^2 + \nabla\mathrm{div} - (\Delta + k^2))Vg = k^2 w_2 + k^2 g,$$

which implies (4.21). The uniqueness of w_2 follows from uniqueness of solution of (4.20), and the Rayleigh expansion condition for w_2 can be checked similarly as for w_1. □

Return to the differential equation (4.7), and recall that $Q = \varepsilon_\mathrm{r}^{-1} - I_3$, and $P = \mu_\mathrm{r} - I_3$. We write its variational formulation as

$$\int_\Omega (\mathrm{curl}\, u \cdot \mathrm{curl}\, \overline{\psi} - k^2 u \overline{\psi})\,\mathrm{d}x \;= -\int_D (Q\,\mathrm{curl}\, u + f)\cdot \mathrm{curl}\, \overline{\psi}\,\mathrm{d}x \;+ k^2 \int_D (Pu + g)\cdot\overline{\psi}\,\mathrm{d}x\,, \quad (4.22)$$

for all $\psi \in H_\alpha(\mathrm{curl}, \Omega)$ with compact support. Now we define, for $f \in L^2(D)^3$,

$$\begin{aligned} Af &= \mathrm{curl}\, Vf = \mathrm{curl} \int_D G_k(\cdot - y) f(y)\,\mathrm{d}y\,, \\ Bf &= (k^2 + \nabla\mathrm{div})Vf = (k^2 + \nabla\mathrm{div}) \int_D G_k(\cdot - y) f(y)\,\mathrm{d}y\,, \end{aligned}$$

which are bounded operators from $L^2(D)^3$ into $H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$ due to Lemma 4.3.5. We next show that the problem (4.22) is equivalent to the integral equation

$$u + A(Q\,\mathrm{curl}\,u + f) - B(Pu + g) = 0 \quad \text{in } \Omega. \tag{4.23}$$

The proof of the next theorem is similar to the one of Theorem 2.3 in [70] for the free space case. However, for convenience, we also give a proof for the periodic case.

Theorem 4.3.6. *Assume that $u \in H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$ is a radiating solution to* (4.22)*, then u solves* (4.23)*, and vice versa.*

Proof. Let $u \in H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$ be a radiating solution to (4.22). We rewrite (4.7) as

$$\mathrm{curl}^2\,u - k^2 u = \mathrm{curl}(Q\,\mathrm{curl}\,u + f) + k^2(Pu + g)$$

Define u_1 and u_2 by

$$u_1 = A(Q\,\mathrm{curl}\,u + f), \qquad u_2 = B(Pu + g).$$

Then, due to Lemma 4.3.5, we imply that u_1 and u_2 satisfy

$$\mathrm{curl}^2\,u_1 - k^2 u_1 = \mathrm{curl}(Q\,\mathrm{curl}\,u + f), \qquad \mathrm{curl}^2\,u_2 - k^2 u_2 = k^2(Pu + g),$$

in the variational sense. From the last two equations we obtain

$$\mathrm{curl}^2(u_1 + u_2) - k^2(u_1 + u_2) = \mathrm{curl}(Q\,\mathrm{curl}\,u + f) + k^2(Pu + g) = \mathrm{curl}^2\,u - k^2 u$$

Since $u_1 + u_2$ and u are radiating solutions, and due to Lemma 4.3.5, the equation $\mathrm{curl}^2(u_1 + u_2 - u) - k^2(u_1 + u_2 - u) = 0$ has only the trivial solution or $u_1 + u_2 = u$. The converse direction can be obtained using Lemma 4.3.5. □

4.4 Gårding Inequality

We recall that $D \subset \Omega_h$. Due to the structure of the operators A and B in (4.23), one can see that the knowledge of u in Ω_h is sufficient to determine u in $\Omega \setminus \overline{\Omega_h}$ by integration. Thus, we consider the integral equation

$$u + A(Q\,\mathrm{curl}\,u) - B(Pu) = -Af + Bg \quad \text{in } H_\alpha(\mathrm{curl},\Omega_h). \tag{4.24}$$

The goal of this section is to prove the Gårding inequality for the operator in the left hand side of equation (4.24). As pointed out in the introduction the main difference from the scalar case is that we investigate a Gårding inequality for the corresponding integral equation in Ω_h instead of D. Exploiting the smoothness of the biperiodic Green's function away from its singularity we treat the boundary terms arising from using Green's identities. Compared to the scalar case this approach only needs the contrasts P and Q to satisfy the following assumption.

Assumption 4.4.1. *We assume that the support $D \subset \Omega_h$ is open and bounded with Lipschitz boundary. Furthermore, $\overline{z}^\top \mathrm{Re}(Q)(x)z \geq 0$ and $\overline{z}^\top \mathrm{Re}(P)(x)z \geq 0$ for all $z \in \mathbb{C}^3$ and almost all $x \in D$.*

We also need to define, for $f \in L^2(D)^3$,

$$A_{\mathrm{i}} f = \mathrm{curl} \int_D G_{\mathrm{i}}(\cdot - y) f(y)\,\mathrm{d}y\,, \quad B_{\mathrm{i}} f = (k^2 + \nabla \mathrm{div}) \int_D G_{\mathrm{i}}(\cdot - y) f(y)\,\mathrm{d}y\,.$$

These are bounded operators from $L^2(D)^3$ into $H_{\alpha,\mathrm{loc}}(\mathrm{curl}, \Omega)$ due to Lemma 4.3.5.

Theorem 4.4.2. *Assume that the contrasts Q and P satisfy Assumption 4.4.1. Then there exists a compact operator K on $H_\alpha(\mathrm{curl}, \Omega_h)$ such that*

$$\mathrm{Re}\langle u + A(Q\,\mathrm{curl}\,u) - B(Pu), u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)} \geq \|u\|^2_{H_\alpha(\mathrm{curl},\Omega)} - \mathrm{Re}\langle Ku,\, u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)},$$

for all $u \in H_\alpha(\mathrm{curl}, \Omega_h)$.

Proof. Let $u \in H_\alpha(\mathrm{curl}, \Omega_h)$ and define w_1, w_2 by

$$w_1 = A_{\mathrm{i}}(Q\,\mathrm{curl}\,u) = \mathrm{curl} \int_D G_{\mathrm{i}}(\cdot - y) Q(y)\,\mathrm{curl}\,u(y)\,\mathrm{d}y \quad \text{in } \Omega, \tag{4.25}$$

$$w_2 = B_{\mathrm{i}}(Pu) = (-1 + \nabla \mathrm{div}) \int_D G_{\mathrm{i}}(\cdot - y) P(y) u(y)\,\mathrm{d}y \quad \text{in } \Omega. \tag{4.26}$$

Due to Lemma 4.3.5 we obtain that $w_1, w_2 \in H_{\alpha,\mathrm{loc}}(\mathrm{curl}, \Omega)$ are variational solutions to $\mathrm{curl}^2\, w_1 + w_1 = \mathrm{curl}(Q\,\mathrm{curl}\,u)$, $\mathrm{curl}^2\, w_2 + w_2 = Pu$, respectively. Now recall that $C^\infty_{\mathrm{p}}(\Omega) = \{\chi \in C^\infty(\Omega) : \chi \text{ is } 2\pi\text{-periodic in } x_1 \text{ and } x_2\}$, consider $\chi \in C^\infty_{\mathrm{p}}(\Omega)$ such that $\chi = 1$ in Ω_h, and $\chi(x) = 0$ for $|x_3| > 2h$. Then the test function χu belongs to $H_\alpha(\mathrm{curl}, \Omega)$, it has compact support, and

$$\int_{\Omega_h} (\mathrm{curl}\, w_1 \cdot \mathrm{curl}\,\overline{u} + w_1 \cdot \overline{u})\,\mathrm{d}x + \int_{\Omega_{2h}\setminus\Omega_h} (\mathrm{curl}\, w_1 \cdot \mathrm{curl}(\overline{\chi u}) + w_1 \cdot \overline{\chi u})\,\mathrm{d}x = \int_D \mathrm{curl}\,\overline{u}^\top Q\,\mathrm{curl}\,u\,\mathrm{d}x\,.$$

Now using Green's theorems and exploiting the fact that w_1 satisfies $\mathrm{curl}^2\, w_1 + w_1 = 0$ in $\Omega \setminus \Omega_h$, we obtain that

$$\int_{\Omega_h} (\mathrm{curl}\, w_1 \cdot \mathrm{curl}\,\overline{u} + w_1 \cdot \overline{u})\,\mathrm{d}x + \int_{\Gamma_{\pm h}} (\nu \times \mathrm{curl}\, w_1) \cdot (\nu \times \overline{u}) \times \nu\,\mathrm{d}s = \int_D \mathrm{curl}\,\overline{u}^\top Q\,\mathrm{curl}\,u\,\mathrm{d}x\,.$$

Similarly for w_2 we also have

$$\int_{\Omega_h} (\mathrm{curl}\, w_2 \cdot \mathrm{curl}\,\overline{u} + w_2 \cdot \overline{u})\,\mathrm{d}x + \int_{\Gamma_{\pm h}} (\nu \times \mathrm{curl}\, w_2) \cdot (\nu \times \overline{u}) \times \nu\,\mathrm{d}s = -\int_D \overline{u}^\top Pu\,\mathrm{d}x\,.$$

Note that, for $y \in D$, $G_{\mathrm{i}}(\cdot - y)$ is smooth on $\Gamma_{\pm h}$. Therefore, the kernels of the potentials w_1 and w_2 is smooth on $\Gamma_{\pm h}$, and the traces on $\Gamma_{\pm h}$ in the variational equations above are well defined. Now we have

$$\begin{aligned}
\mathrm{Re}\langle u + A_{\mathrm{i}}(Q\,\mathrm{curl}\,u) - B_{\mathrm{i}}(Pu), u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)} &= \mathrm{Re}\langle u + w_1 - w_2, u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)} \\
&= \|u\|^2_{H_\alpha(\mathrm{curl},\Omega_h)} + \mathrm{Re}\int_{\Omega_h} \left[\mathrm{curl}(w_1 - w_2)\cdot \mathrm{curl}\,\overline{u} + (w_1 - w_2)\cdot\overline{u}\right] \mathrm{d}x \\
&= \|u\|^2_{H_\alpha(\mathrm{curl},\Omega_h)} - \mathrm{Re}\int_{\Gamma_{\pm h}} (\nu \times \mathrm{curl}(w_1 - w_2))\cdot(\nu\times\overline{u})\times\nu\,\mathrm{d}s \\
&\quad + \int_D (\mathrm{curl}\,\overline{u}^\top \mathrm{Re}(Q)\,\mathrm{curl}\,u + \overline{u}^\top \mathrm{Re}(P)u)\,\mathrm{d}x \\
&\geq \|u\|^2_{H_\alpha(\mathrm{curl},\Omega_h)} - \mathrm{Re}\int_{\Gamma_{\pm h}} (\nu \times \mathrm{curl}(w_1 - w_2))\cdot(\nu\times\overline{u})\times\nu\,\mathrm{d}s
\end{aligned}$$

In consequence, we obtain that

$$\begin{aligned}
\mathrm{Re}\langle u + A(Q\,\mathrm{curl}\,u) - B(Pu), u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)} &\geq \|u\|^2_{H_\alpha(\mathrm{curl},\Omega_h)} \\
+\mathrm{Re}\langle (A - A_{\mathrm{i}})(Q\,\mathrm{curl}\,u) - (B - B_{\mathrm{i}})(Pu), u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)} \\
-\mathrm{Re}\int_{\Gamma_{\pm h}} (\nu \times \mathrm{curl}(w_1 - w_2))\cdot(\nu\times\overline{u})\times\nu\,\mathrm{d}s\,.
\end{aligned}$$

Now recall from (4.10) that the Green function $G_k(x,y) = \Phi_k(x,y) + \Psi(x,y)$ where $\Phi_k(x,y) = \exp(\mathrm{i}k|x-y|)/(4\pi|x-y|)$ and $\Psi(x,y)$ is an analytic function. Furthermore, from Appendix A we have

$$\Phi_k(x,y) - \Phi_{\mathrm{i}}(x,y) = \alpha(|x-y|^2) + |x-y|\beta(|x-y|^2)$$

where α and β are analytic functions. Therefore, the singularities of the kernels of the operators $(A - A_{\mathrm{i}})(Q\,\mathrm{curl}\,\cdot)$, $(B - B_{\mathrm{i}})(P\,\cdot)$ which are as strong as $\partial^2[\Phi_k(x,y) - \Phi_{\mathrm{i}}(x,y)]/\partial x_j \partial x_l$ for $j,l = 1,2,3$, are at most as strong as $1/|x-y|$. They are hence compact operators on $H_\alpha(\mathrm{curl},\Omega_h)$ due to their weakly singular kernels. Now the operator K_1 defined by $\langle K_1 u,\, u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)} = \langle (A - A_{\mathrm{i}})(Q\,\mathrm{curl}\,u) - (B - B_{\mathrm{i}})(Pu), u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)}$ is compact on $H_\alpha(\mathrm{curl},\Omega_h)$ due to Lemma 2.4.4. Similarly, the operator K_2 defined by $\langle K_1 u,\, u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)} = \int_{\Gamma_{\pm h}} (\nu \times \mathrm{curl}(w_1 - w_2))\cdot(\nu\times\overline{u})\times\nu\,\mathrm{d}s$ is also compact on $H_\alpha(\mathrm{curl},\Omega_h)$ due to the smoothness of the kernel G_{i} on $\Gamma_{\pm h}$. Setting $K := K_1 + K_2$, we obtain the claimed Gårding inequality. □

4.5 Periodization of the Integral Equation

In this section we reformulate the volume integral equation

$$u + A(Q\,\mathrm{curl}\,u) - B(Pu) = -Af + Bg \quad \text{in } H_\alpha(\mathrm{curl},\Omega_h). \tag{4.27}$$

in a periodic setting and show the equivalence of the periodized equation and the original one. The purpose of this periodization is that the resulting integral operator is, roughly speaking, diagonalized by trigonometric polynomials. This allows to use fast FFT-based schemes to discretize the periodized operator and iterative schemes to solve the discrete system. We also prove Gårding inequalities for the periodized integral equation, which are crucial to establish convergence of the discrete schemes later on.

The periodized kernel $\mathcal{K}_h$ is not smooth at the boundaries $\{x_3 = \pm h\}$. To prove Gårding inequalities for the periodized integral equation, we additionally need to smoothen the kernel (as we did for the scalar case, see (2.45)). For $R > 2h$ we choose a function $\chi \in C^3(\mathbb{R})$ that is $2R$-periodic, that satisfies $0 \le \chi \le 1$ and $\chi(x_3) = 1$ for $|x_3| \le 2h$, and such that $\chi(R)$ vanishes up to order three, $\chi^{(j)}(R) = 0$ for $j = 1, 2, 3$ (compare Figure 2.4)).

Let us define a smoothed kernel $\mathcal{K}_{\mathrm{sm}}$ by

$$\mathcal{K}_{\mathrm{sm}}(x) = \chi(x_3)\mathcal{K}_R(x) \quad \text{for } x \in \mathbb{R}^3, \quad x \neq \left[2\pi m,\, 2Rn\right]^\top,\, m \in \mathbb{Z}^2,\, n \in \mathbb{Z}, \tag{4.28}$$

where $\mathcal{K}_R$ is the periodic kernel defined in (4.11). Note that $\mathcal{K}_{\mathrm{sm}}$ is α-quasiperiodic in x_1 and x_2, $2R$-periodic in x_3, and a smooth function on its domain of definition (that is, away from the singularity). To study the periodization of equation (4.27) we define the space $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$ as a subspace in $L^2(\Omega_R)^3$ containning those $f \in L^2(\Omega_R)^3$ such that

$$\|f\|^2_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)} = \sum_{j\in\mathbb{Z}^3} \left(|\hat{f}(j)|^2 + |(\alpha_{1,j}, \alpha_{2,j}, j_3\pi/R) \times \hat{f}(j)|^2\right) < \infty. \tag{4.29}$$

Note that a function $f \in H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$ is α-quasiperiodic in x_1 and x_2, $2R$-periodic in x_3, and that the norm $\|\cdot\|_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)}$ on $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$ is equivalent to the usual integral norm $\|\cdot\|_{H(\mathrm{curl},\Omega_R)}$.

Lemma 4.5.1. *Let the integral operators A_{p}, B_{p} from $L^2(\Omega_R)^3$ into $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$ be defined by*

$$A_{\mathrm{p}} f = \mathrm{curl} \int_D \mathcal{K}_{sm}(\cdot - y) f(y)\,\mathrm{d}y \quad \textit{in } \Omega,$$
$$B_{\mathrm{p}} f = (k^2 + \nabla\mathrm{div}) \int_D \mathcal{K}_{sm}(\cdot - y) f(y)\,\mathrm{d}y \quad \textit{in } \Omega.$$

Then A_{p}, B_{p} are bounded operators.

Proof. We split the integral operator A_{p} into two parts,

$$\begin{aligned} A_{\mathrm{p}} f &= \mathrm{curl} \int_D \mathcal{K}_{\mathrm{sm}}(\cdot - y) f(y)\,\mathrm{d}y = \mathrm{curl} \int_D \chi(\cdot - y_3)\mathcal{K}_R(\cdot - y) f(y)\,\mathrm{d}y \\ &= \mathrm{curl} \int_D \mathcal{K}_R(\cdot - y) f(y)\,\mathrm{d}y + \mathrm{curl} \int_D [\chi(\cdot - y_3) - 1]\mathcal{K}_R(\cdot - y) f(y)\,\mathrm{d}y\,. \end{aligned}$$

By Theorem 4.3.3, the integral operator with the kernel $\mathcal{K}_R$ is bounded from $L^2(\Omega_R)^3$ into $H^1_\alpha(\Omega_R)^3$. Further, the definition of χ shows that $\chi(x_3 - y_3) - 1 = 0$ for $|x_3| \le h$ and $y \in D$.

The kernel $(\chi - 1)\mathcal{K}_R$ is hence smooth in Ω_R, and the corresponding integral operator is compact from $L^2(\Omega_R)^3$ into $H^1_\alpha(\Omega_R)^3$. Hence, A_p is bounded from $L^2(\Omega_R)^3$ into $H^1_\alpha(\Omega_R)^3$. Periodicity of the kernel $\mathcal{K}_\mathrm{sm}$ in the third component of its argument finally implies that $A_\mathrm{p} f$ belongs to $H^1_{\alpha,\mathrm{p}}(\Omega_R)^3 \subset H^1_\alpha(\Omega_R)^3$. Then the boundedness of A_p from $L^2(\Omega_R)^3$ into $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$ follows from the bounded embedding $H^1_{\alpha,\mathrm{p}}(\Omega_R)^3 \subset H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$. Now we have $\mathrm{curl}\,\nabla = 0$, thus we deduce that $\mathrm{curl}\, B_\mathrm{p} = k^2\, \mathrm{curl}\, A_\mathrm{p}$ which also implies the boundedness of B_p from $L^2(\Omega_R)^3$ into $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$. □

Let us now consider the periodized integral equation

$$u + A_\mathrm{p}(Q\,\mathrm{curl}\, u) - B_\mathrm{p}(Pu) = -A_\mathrm{p} f + B_\mathrm{p} g \quad \text{in } H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R). \tag{4.30}$$

Theorem 4.5.2. *(a) For $f \in L^2(\Omega_R)^3$, $A_\mathrm{p} f = Af$ and $B_\mathrm{p} f = Bf$ in Ω_h.*

(b) Equation (4.27) is uniquely solvable in $H_\alpha(\mathrm{curl}, \Omega_h)$ for any right-hand side $f, g \in L^2(D)^3$ if and only if (4.30) is uniquely solvable in $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$ for any right-hand side $f, g \in L^2(\Omega_R)^3$.

Proof. (a) We only prove the case of A_p, the proof for the case of B_p is analogous. For all x and $y \in \Omega_R$ such that $|x_3 - y_3| \le 2h$ it holds that $\mathcal{K}_\mathrm{sm}(x-y) = \chi(x_3 - y_3)\mathcal{K}_R(x-y) = G_\alpha(x-y)$. In particular, for $x \in \Omega_h$ and $y \in D \subset \Omega_h$ it holds that $|x_3 - y_3| \le 2h$. Consequently,

$$\begin{aligned}(A_\mathrm{p} f)(x) &= \mathrm{curl} \int_D \mathcal{K}_\mathrm{sm}(x-y) f(y)\,\mathrm{d}y \\ &= \mathrm{curl} \int_D G_\alpha(x-y) f(y)\,\mathrm{d}y \;= (Af)(x), \qquad x \in \Omega_h.\end{aligned}$$

(b) Assume that $u \in H_\alpha(\mathrm{curl}, \Omega_h)$ solves (4.27) and define $\tilde{u} \in H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$ by $\tilde{u} = -A_\mathrm{p}(Q\,\mathrm{curl}\, u + f) + B_\mathrm{p}(Pu + g)$ (where we extended f, g by zero outside D). Since u solves (4.27), and due to part (a), we find that $\tilde{u}|_{\Omega_h} = u$. Hence $A_\mathrm{p}(Q\,\mathrm{curl}\,\tilde{u} + f) = A_\mathrm{p}(Q\,\mathrm{curl}\, u + f)$, and $B_\mathrm{p}(P\tilde{u} + g) = B_\mathrm{p}(Pu + g)$ in $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$, which yields that

$$\tilde{u} = -A_\mathrm{p}(Q\,\mathrm{curl}\,\tilde{u} + f) + B_\mathrm{p}(P\tilde{u} + g) \text{ in } H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R). \tag{4.31}$$

Now, if $f, g \in L^2(D)^3$ vanish, then uniqueness of a solution to (4.27) implies that $u \in H_\alpha(\mathrm{curl}, \Omega_h)$ vanishes, too. Obviously, $\tilde{u} = -A_\mathrm{p}(Q\,\mathrm{curl}\, u) + B_\mathrm{p}(Pu)$ vanishes, and hence (4.31) is uniquely solvable. The converse follows directly from (a). □

Next we prove that the operator $I + A_\mathrm{p}(Q\,\mathrm{curl}\,\cdot) - B_\mathrm{p}(P\,\cdot)$ from (4.30) satisfies a Gårding inequality in $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$.

Theorem 4.5.3. *Assume that the contrasts Q and P satisfy the Assumption 4.4.1. Then there exists a compact operator K on $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$ such that*

$$\mathrm{Re}\langle u + A_\mathrm{p}(Q\,\mathrm{curl}\, u) - B_\mathrm{p}(Pu), u\rangle_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)} \ge \|u\|^2_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)} - \mathrm{Re}\langle Ku,\, u\rangle_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)}, \tag{4.32}$$

for all $u \in H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$.

Proof. Let $u \in H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$. First, we split up the integrals arising from the inner product on the left of (4.32) into integrals on Ω_h, and on $\Omega_R \setminus \overline{\Omega_h}$. Second, we use the Gårding inequality from Theorem 4.4.2 to find that

$$\begin{aligned}\mathrm{Re}\langle u + A_\mathrm{p}(Q\,\mathrm{curl}\,u) - B_\mathrm{p}(Pu), u\rangle_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)} &\geq \|u\|^2_{H_\alpha(\mathrm{curl},\Omega_h)} + \mathrm{Re}\langle K_1 u,\, u\rangle_{H_\alpha(\mathrm{curl},\Omega_h)} \\ &\quad + \|u\|^2_{H_\alpha(\mathrm{curl},\Omega_R\setminus\Omega_h)} + \mathrm{Re}\langle A_\mathrm{p}(Q\,\mathrm{curl}\,u) - B_\mathrm{p}(Pu), u\rangle_{H_\alpha(\mathrm{curl},\Omega_R\setminus\Omega_h)} \quad (4.33)\end{aligned}$$

with a compact operator K_1 on $H_\alpha(\mathrm{curl}, \Omega_h)$. Further, the evaluation of $A_\mathrm{p}(Q\,\mathrm{curl}\,\cdot) - B_\mathrm{p}(P\,\cdot)$ on $\Omega_R \setminus \overline{\Omega_h}$ defines a compact integral operator mapping $H_\alpha(\mathrm{curl}, \Omega_h)$ to $H_\alpha(\mathrm{curl}, \Omega_R \setminus \Omega_h)$, because the (periodic) kernel of these integral operators is smooth. (This argument requires the smooth kernel $\mathcal{K}_\mathrm{sm}$ introduced in the beginning of this section.) Lemma 2.4.4 then allows to reformulate the corresponding term in (4.33) in the way stated in the claim. □

4.6 Discretization of the Periodic Integral Equation

In this section we firstly consider the discretization of the periodized integral equation (4.30) in spaces of trigonometric polynomials. If the periodization satisfies certain smoothness conditions and if uniqueness of solution holds, convergence theory for the discretization is a consequence of the Gårding inequalities shown in Theorem 4.5.3. Secondly we present fully discrete formulas for implementing a Galerkin discretization of the Lippmann-Schwinger integral equation (4.30), together with a couple of numerical examples that we computed using these formulas.

For $N \in \mathbb{N}$ we define

$$\mathbb{Z}^3_N = \{j \in \mathbb{Z}^3 : -N/2 < j_{1,2,3} \leq N/2\}, \quad \mathcal{T}_N = \mathrm{span}\{\varphi_j : j \in \mathbb{Z}^3_N\},$$

where $\varphi_j \in L^2(\Omega_R)^3$ are the α-quasiperiodic basis functions from (2.16). Note that the union $\cup_{N\in\mathbb{N}}\mathcal{T}_N$ is dense in $H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$. The orthogonal projection onto $\mathcal{T}_N$ is

$$P_N : H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R) \to \mathcal{T}_N, \qquad P_N(v) = \sum_{j\in\mathbb{Z}^3_N} \hat{v}(j)\varphi_j,$$

where $\hat{v}(j)$ denotes as above the jth Fourier coefficient.

The next proposition recalls the standard convergence result for Galerkin discretizations of equations that satisfy a Gårding inequality, see, e.g. [103, Theorem 4.2.9].

Proposition 4.6.1. *Assume that Q and P satisfy Assumption 4.4.1 and that* (2.28) *is uniquely solvable. Then* (4.30) *has a unique solution $u \in H_{\alpha,\mathrm{p}}(\mathrm{curl}, \Omega_R)$, and then there is $N_0 \in \mathbb{N}$ such that the finite-dimensional problem to find $u_N \in \mathcal{T}_N$ such that*

$$\langle u_N + A_\mathrm{p}(Q\,\mathrm{curl}\,u_N) - B_\mathrm{p}(Pu_N), w_N\rangle_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)} = \langle -A_\mathrm{p} f + B_\mathrm{p} g, w_N\rangle_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)} \quad (4.34)$$

for all $w_N \in \mathcal{T}_N$, possesses a unique solution for all $N \geq N_0$ and $f, g \in L^2(\Omega_R)^3$. In this case

$$\|u_N - u\|_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)} \leq C \inf_{w_N\in\mathcal{T}_N} \|w_N - u\|_{H_{\alpha,\mathrm{p}}(\mathrm{curl},\Omega_R)},$$

with a constant C independent of $N \geq N_0$.

Remark 4.6.2. *The solution u can be in H^1 if the contrast P satisfies some global smoothness, see, e.g., [47, 83, 101]. However H^1-regularity is not sufficient to conclude convergence rates as in Proposition 2.7.1. To prove such rates one can probably follow the technique of duality estimates for solutions to Maxwell's equations in the book [83, Chapter 7]. This is out of the scope of this thesis.*

It is also obvious that if the solution has higher regularity H^s with $s > 1$, then one could have convergence rates in H^1 as in Proposition 2.7.1. We can have more regularity on the solution by assumming global smoothness of P and Q. That is somehow unattractive, since this is what we wanted to avoid in the beginning, and also since in this case, the integral equation could be reduced to a weakly singular integral equation following the integration by parts trick in the book [37, Chapter 9.1 and 9.2].

Similar to the scalar case, the operator P_N commutes with the periodic convolution operators A_p, B_p. We apply P_N to the infinite-dimensional problem (4.30) and obtain the discrete problem to find $u_N \in \mathcal{T}_N$ such that

$$u_N + A_\mathrm{p}(P_N(Q \operatorname{curl} u_N)) - B_\mathrm{p}(P_N(P u_N)) = -A_\mathrm{p}(P_N f) + B_\mathrm{p}(P_N g) \tag{4.35}$$

Fast methods to evaluate the discretized operator in (4.35) exploit that the application of A_p and B_p to a trigonometric polynomial in $\mathcal{T}_N$ can be explicitly computed using an α-quasiperiodic discrete Fourier transform that we call $\mathcal{F}_N$. This transform maps point values of a trigonometric polynomial φ_j (see (2.16)) to the Fourier coefficients of the polynomial. Now recall that $\alpha_{1,j} = j_1 + \alpha_1$, $\alpha_{2,j} = j_2 + \alpha_2$ for $j \in \mathbb{Z}^3$. If we denote by $a \bullet b$ the componentwise multiplication of two matrices, and if $t := (2\pi/N, 2\pi/N, 2R/N)^\top$, then

$$\hat{v}_N(j) = \frac{\sqrt{8\pi^2 R}}{N^3} \sum_{l \in \mathbb{Z}_N^3} v_N(l \bullet t) \exp\big(-2\pi \mathrm{i} (\alpha_{1,j}, \alpha_{2,j}, j_3)^\top \cdot l/N \big), \qquad j \in \mathbb{Z}_N^3.$$

This defines the transform $\mathcal{F}_N$ mapping $(v_N(j \bullet t))_{j \in \mathbb{Z}_N^3}$ to $(\hat{v}_N(j))_{j \in \mathbb{Z}_N^3}$. The inverse $\mathcal{F}_N^{-1}$ is explicitly given by

$$v_N(j \bullet t) = \frac{1}{\sqrt{8\pi^2 R}} \sum_{l \in \mathbb{Z}_N^3} \hat{v}_N(l) \exp\Big(2\pi \mathrm{i} (\alpha_{1,l}, \alpha_{2,l}, l_3)^\top \cdot j/N \Big), \qquad j \in \mathbb{Z}_N^3.$$

Both $\mathcal{F}_N$ and its inverse are linear operators on $\mathbb{C}_N^3 = \{(c_n)_{n \in \mathbb{Z}_N^3} : c_n \in \mathbb{C}\}$. The restriction operator $R_{N,M}$ from $\mathbb{C}_N^3$ to $\mathbb{C}_M^3$, $N > M$, is defined by $R_{N,M}(a) = b$ where $b(j) = a(j)$ for $j \in \mathbb{Z}_M^3$. The related extension operator $E_{M,N}$ from $\mathbb{C}_M^3$ to $\mathbb{C}_N^3$, $M < N$, is defined by $E_{M,N}(a) = b$ where $b(j) = a(j)$ for $j \in \mathbb{Z}_M^3$ and $b(j) = 0$ else.

Lemma 4.6.3. *For $\mu \in L^2(\Omega_R)^3$ and $u_N \in \mathcal{T}_N$, the Fourier coefficients of $\mu \partial_\ell u_N$, $\ell = 1, 2, 3$, are given by*

$$(\widehat{\mu \partial_\ell u}_N(j))_{j \in \mathbb{Z}_N^3} = R_{3N,N} \mathcal{F}_{3N} \big[\mathcal{F}_{3N}^{-1}\big(E_{2N,3N}(\hat{\mu}_{2N}(j))_{j \in \mathbb{Z}_N^3}\big) \bullet \mathcal{F}_{3N}^{-1}\big(E_{N,3N}(w_\ell(j) \hat{u}_N(j))_{j \in \mathbb{Z}_N^3}\big) \big]$$

where $w_1(j) = \mathrm{i}\alpha_{1,j}$, $w_2(j) = \mathrm{i}\alpha_{2,j}$ and $w_3(j) = \mathrm{i} j_3 \pi/R$ for $j \in \mathbb{Z}^3$.

Proof. For $u_N \in \mathcal{T}_N$, $j \in \mathbb{Z}^3$, and $\ell = 1, 2, 3$,

$$\begin{aligned} 8\pi^2 R\, \widehat{\mu\partial_\ell u}_N(j) &= 8\pi^2 R \int_{\Omega_R} \mu \partial_\ell u_N \overline{\varphi_j}\, \mathrm{d}x \;= 8\pi^2 R \sum_{m\in\mathbb{Z}^3_N} \widehat{\partial_\ell u}_N(m) \int_{\Omega_R} \mu \overline{\varphi_j} \varphi_m \,\mathrm{d}x \\ &= \sum_{m\in\mathbb{Z}^3_N} \widehat{\partial_\ell u}_N(m) \int_{\Omega_R} \mu(x) e^{-\mathrm{i}[(j_1-m_1)x_1+(j_2-m_2)x_2+(j_3-m_3)x_3\pi/R]}\,\mathrm{d}x \\ &= \sqrt{8\pi^2 R} \sum_{m\in\mathbb{Z}^3_N} \widehat{\partial_\ell u}_N(m) \hat{\mu}(j-m). \end{aligned} \tag{4.36}$$

If $j \in \mathbb{Z}^3_N$, then the coefficient $\widehat{\mu\partial_\ell u_N}(j)$ merely depends on $\hat{\mu}(m)$ for $m \in \mathbb{Z}^3_{2N}$. Hence, $\widehat{\mu\partial_\ell u_N}(j) = \widehat{\mu_{2N}\partial_\ell u_N}(j)$ for $j \in \mathbb{Z}^3_N$. Obviously, $\mu_{2N}\partial_\ell u_N$ belongs to $\mathcal{T}_{3N}$. Hence, the Fourier coefficients of $\mu_{2N}\partial_\ell u_N$ are given by $\mathcal{F}_{3N}$ applied to the grid values of this function at $j \bullet h$, $j \in \mathbb{Z}^3_{3N}$. The grid values of $\widehat{\partial_\ell u_N}$ are given by $\mathcal{F}_{3N}^{-1}(E_{N,3N}(\widehat{\partial_\ell u}_N(j)_{j\in\mathbb{Z}^3_N})$, and the grid values of μ_{2N} can be computed analogously. Finally, taking a partial derivative with respect to x_1 or x_2 or x_3 of u yields a multiplication of the jth Fourier coefficient $\hat{u}(j)$ by $\mathrm{i}\alpha_{1,j}$ or $\mathrm{i}\alpha_{2,j}$ or $\mathrm{i}j_3\pi/R$, respectively. □

In Lemma 4.3.3 we computed the Fourier coefficients of the kernel $\mathcal{K}_R$. The kernel $\mathcal{K}_{\mathrm{sm}}$ used to define the periodized potentials A_{p} and B_{p} is the product of $\mathcal{K}_R$ with the smooth function χ (see (4.28)). Hence, the Fourier coefficients of $\mathcal{K}_{\mathrm{sm}}$ are convolutions of the $\hat{\mathcal{K}}_R(j)$ with $\hat{\chi}(j_3) = (8\pi^2 R)^{-1/2} \int_{-R}^{R} \exp(-\mathrm{i}j_3\pi x_3/R)\chi(x_3)\,\mathrm{d}x_3$,

$$\hat{\mathcal{K}}_{\mathrm{sm}}(j) = \frac{1}{\sqrt{8\pi^2 R}} \sum_{m\in\mathbb{Z}^3_N} \hat{\mathcal{K}}_R(j_1, j_2, m_3)\hat{\chi}(j_3 - m_3), \qquad j \in \mathbb{Z}^3.$$

The latter formula can be seen by a computation similar to (4.36). Note that χ is a smooth function, which means that the Fourier coefficients $\hat{\chi}$ in the last formula are rapidly decreasing, that is, the truncation of the last series converges rapidly to the exact value. The convolution structure of A_{p} and B_{p} finally shows that, for $f = (f_1, f_2, f_3) \in L^2(\Omega_R)^2$,

$$\widehat{(A_{\mathrm{p}} f)}(j) = \sqrt{8\pi^2 R} \begin{pmatrix} \mathrm{i}\alpha_{2,j}\big[\mathrm{i}\alpha_{1,j}\hat{f}_2(j) - \mathrm{i}\alpha_{2,j}\hat{f}_1(j)\big] - \frac{\mathrm{i}j_3\pi}{R}\big[\frac{\mathrm{i}j_3\pi}{R}\hat{f}_1(j) - \mathrm{i}\alpha_{1,j}\hat{f}_3(j)\big] \\ \frac{\mathrm{i}j_3\pi}{R}\big[\mathrm{i}\alpha_{2,j}\hat{f}_3(j) - \frac{\mathrm{i}j_3\pi}{R}\hat{f}_2(j)\big] - \mathrm{i}\alpha_{1,j}\big[\mathrm{i}\alpha_{1,j}\hat{f}_2(j) - \mathrm{i}\alpha_{2,j}\hat{f}_1(j)\big] \\ \mathrm{i}\alpha_{1,j}\big[\frac{\mathrm{i}j_3\pi}{R}\hat{f}_1(j) - \mathrm{i}\alpha_{1,j}\hat{f}_3(j)\big] - \mathrm{i}\alpha_{2,j}\big[\mathrm{i}\alpha_{2,j}\hat{f}_3(j) - \frac{\mathrm{i}j_3\pi}{R}\hat{f}_2(j)\big] \end{pmatrix} \hat{\mathcal{K}}_{\mathrm{sm}}(j), \tag{4.37}$$

$$\widehat{(B_{\mathrm{p}} f)}(j) = \sqrt{8\pi^2 R} \begin{pmatrix} (k^2 - \alpha_{1,j}^2)\hat{f}_1(j) - \alpha_{1,j}\alpha_{2,j}\hat{f}_2(j) - \frac{\alpha_{1,j}j_3\pi}{R}\hat{f}_3(j) \\ -\alpha_{2,j}\alpha_{1,j}\hat{f}_1(j) + (k^2 - \alpha_{2,j}^2)\hat{f}_2(j) - \frac{\alpha_{2,j}j_3\pi}{R}\hat{f}_3(j) \\ -\frac{\alpha_{1,j}j_3\pi}{R}\hat{f}_1(j) - \frac{\alpha_{2,j}j_3\pi}{R}\hat{f}_2(j) + (k^2 - (\frac{j_3\pi}{R})^2)\hat{f}_3(j) \end{pmatrix} \hat{\mathcal{K}}_{\mathrm{sm}}(j). \tag{4.38}$$

The finite-dimensional operators $u_N \mapsto A_{\mathrm{p}}(P_N(Q \operatorname{curl} u_N))$ and $u_N \mapsto B_{\mathrm{p}}(P_N(Pu_N))$ can now be evaluated in $O(N\log(N))$ operations by combining the formula of Lemma 4.6.3 with (4.37)

and (4.38). Similar to the scalar case the linear system (4.35) can then be solved using iterative methods. The usual multi-grid preconditioning technique for integral equations of the second kind (see, e.g., [109]) does not apply here, since the integral operator is not compact. For the numerical experiments presented below, we simply used an unpreconditioned GMRES algorithm.

4.7 Numerical Experiments

In this section we describe the convergence of the method using the energy error presented in Experiment 2.8.4. For simplicity we consider the case that the material is non-magnetic and isotropic, that is, $Q = qI_3$ and $P = 0$ or the terms of the operator B_{p} in (4.35) vanish. As in the scalar case all the computations in the following experiments were done on a machine with an Intel Xeon 3.20 GHz processor and 12 GB memory using MATLAB. The scattered field in the examples of this section is computed for an incident field

$$u^i(x) = (-\sin(\theta_2), \cos(\theta_2), 0)e^{\mathrm{i}k[\cos(\theta_1)\cos(\theta_2)x_1 + \cos(\theta_1)\sin(\theta_2)x_2 - |\sin(\theta_1)|x_3]},$$

where $\theta_1 \in (0, \pi)$, $\theta_2 \in [0, 2\pi)$. As in the scalar case we compute the energy error for 'many' incidence angles of u^i. For simplicity we fix $\theta_2 = \pi/4$, the energy conservation error is then tested for θ_1 sampled at 75 points uniformly distributed on the interval $[1.2, 1.95]$. Further, the numerical examples below do not show the effect of the Rayleigh frequencies as in the scalar case. This is probably can be seen when one considers a larger interval of θ_1 where the number of sample points are big enough. This is out of the scope of this section. Now recall the Rayleigh coefficients $\hat{u}_j^{\pm}$ of the scattered field from (4.6). We define Rayleigh coefficients for the incident field u^i by

$$\hat{u}_j^i = \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} u^i(x_1, x_2, -h)e^{-\mathrm{i}(\alpha_{1,j}x_1 + \alpha_{2,j}x_2)}\,\mathrm{d}x_1\,\mathrm{d}x_2\,.$$

As in the scalar case the equation of energy conservation is

$$\sum_{j:k^2>\beta_j^2} \beta_j(|\hat{u}_j^+|^2 + |\hat{u}_j^- + \hat{u}_j^i|^2) = \beta_0. \tag{4.39}$$

where the transmitted and reflected wave energies are again given by

$$E_{\mathrm{tra}}(\theta_1) := \sum_{j:k^2>\beta_j^2} \beta_j(|\hat{u}_j^- + \hat{u}_j^i|^2)/\beta_0, \quad E_{\mathrm{ref}}(\theta_1) := \sum_{j:k^2>\beta_j^2} \beta_j|\hat{u}_j^+|^2/\beta_0.$$

Similar to Experiment 2.8.4, we use $\theta_1 \mapsto |1 - E_{\mathrm{tra}}(\theta_1) - E_{\mathrm{ref}}(\theta_1)|$ as an error indicator for the numerical solution in the three experiments considered in this section.

4.7.1 Flat structure with piecewise constant contrast

In this example we consider the biperiodic structure as a flat plane (compare Figure 4.3) where $D = (-\pi, \pi)^2 \times (-0.5, 0.5)$, $\Omega_R = (-\pi, \pi)^2 \times (-1, 1)$, and the contrast q is piecewise constant

$$q = \begin{cases} 0.5 & \text{in } D_1 := (-\pi/2, \pi/2)^2 \times (0, 0.5), \\ 1 & \text{in } D \setminus \overline{D_1}. \end{cases}$$

As in Experiment 2.8.2 the Fourier coefficients of the contrast q can be explicitly computed

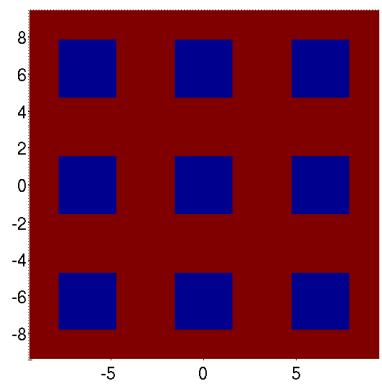


Figure 4.3: Flat structure with piecewise constant contrast viewed down x_3 axis. The domains where $q = 0.5$ and $q = 1$ are in blue and red, respectively. This is plotted in $(-3\pi, 3\pi)^2$.

via the formula

$$\hat{q}(j) = \frac{(q_1 - q_2)}{\sqrt{8\pi^2 R}} \int_{D_1} \phi_j \, \mathrm{d}x + \frac{q_2}{\sqrt{8\pi^2 R}} \int_D \phi_j \, \mathrm{d}x \,, \quad j \in \mathbb{Z}^3,$$

where $\phi_j(x) = \exp(-\mathrm{i}(j_1 x_1 + j_2 x_2 + j_3 \pi x_3 / R))$. The wave number k is $2\pi/3$ in this experiment. In Figure 4.4 we check the energy conservation error for $N = 2^n$, $n = 3, \ldots, 6$ where the tolerance for the GMRES iteration is 10^{-8}. We can see in Figure 4.4 that the error of the computed Rayleigh coefficients corresponding to propagating modes converges with order 1.

4.7.2 Biperiodic structure of cubes

In this example we consider the biperiodic structure of cubes (compare Figure 4.5) where $D = (-2.5, 2.5)^2 \times (-1, 1)$, $\Omega_R = (-\pi, \pi)^2 \times (-2, 2)$, and the contrast q is given by

$$q(x) = \frac{1}{2} \cos(x_1)^2 (x_3 + 1), \quad x = (x_1, x_2, x_3) \in D.$$

In this experiment the wave number k is $\pi/2$. Similar to the case in Experiment 2.8.4, the

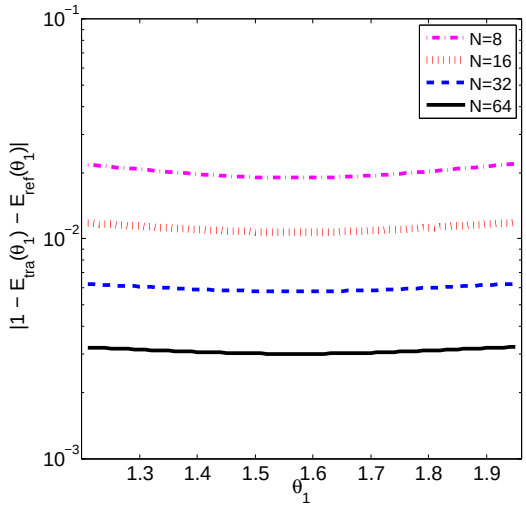
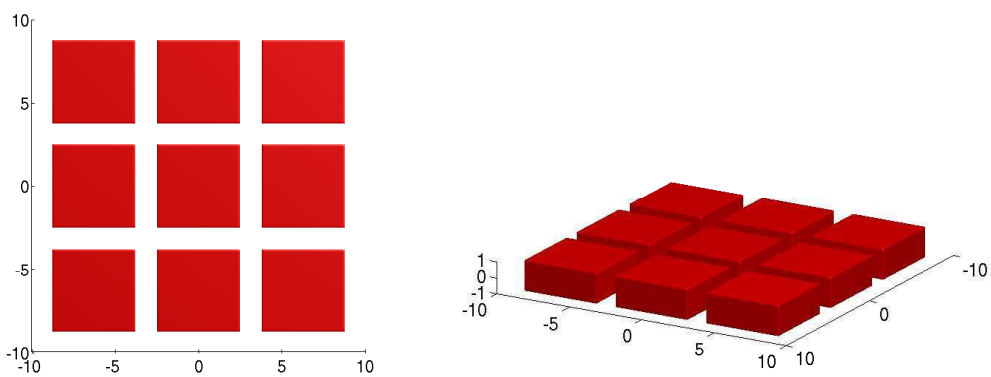


Figure 4.4: Scattering from flat structure with piecewise constant contrast. The error curves $|1 - E_{\text{tra}}(\theta_1) - E_{\text{ref}}(\theta_1)|$ for different discretization parameters N versus the angles θ_1 of the incident field u^i.



(a) View down x_3 axis (b) 3D view

Figure 4.5: Biperiodic structure of cubes of size $2.5 \times 2.5 \times 1$ plotted in $(-3\pi, 3\pi)^2 \times (-1, 1)$.

Fourier coefficients of q can be computed explicitly. Assume that r is the size of the cube in x_1- and x_2-dimensions, ρ is the size of the cube in x_3-dimension. We have

$$\hat{q}(j) = \frac{A(j_1)B(j_2)C(j_3)}{4\sqrt{8\pi^2 R}} \quad \text{for } j = (j_1, j_2, j_3) \in \mathbb{Z}^3,$$

where

$$A(j_1) = \begin{cases} \frac{\sin(rj_1)\left[(2\cos(2r)+1)/j_1 - 8/j_1^3\right] - 4\cos(j_1 r)\sin(2r)/j_1^2}{1-4/j_1^2} & j_1 \in \mathbb{Z}\setminus\{0,\pm 2\}, \\ \sin(4r)/4 + \sin(2r) + r & j_1 = \pm 2, \\ \sin(2r)/2 + r & j_1 = 0, \end{cases}$$

$$B(j_2) = \begin{cases} 2\sin(j_2 r)/j_2 & j_2 \neq 0, \\ 2r & j_2 = 0, \end{cases}$$

$$C(j_3) = \begin{cases} \frac{2\rho \mathrm{i} R}{j_3 \pi}\exp(-\mathrm{i} j_3 \pi \rho/R) - \frac{2\mathrm{i}R^2}{(j_3\pi)^2}\sin(j_3\pi\rho/R) & j_3 \neq 0, \\ 2\rho^2 & j_3 = 0. \end{cases}$$

In Figure 4.4 we check the energy conservation error for $N = 2^n$, $n = 3, \ldots, 6$ where the tolerance for the GMRES iteration is 10^{-8}.

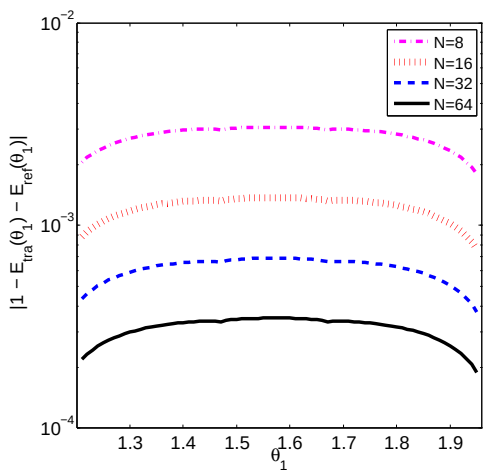


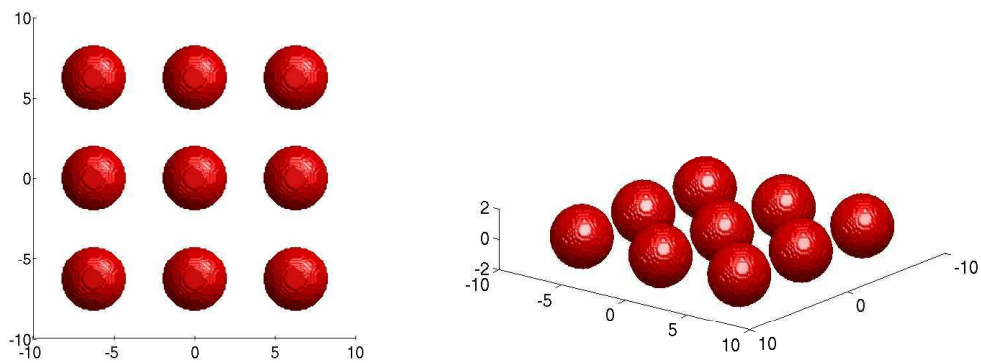
Figure 4.6: Scattering from biperiodic structure of cubes. The error curves $|1 - E_{\mathrm{tra}}(\theta_1) - E_{\mathrm{ref}}(\theta_1)|$ for different discretization parameters N versus the angles θ_1 of the incident field u^i.

4.7.3 Biperiodic structure of spheres

This last example deals with scattering from the biperiodic structure of spheres (compare Figure 4.7). We have

$$D = \{(x_1, x_2, x_3)^\top \in \mathbb{R}^3 : (|x_1|^2 + |x_2|^2 + |x_3|^2)^{1/2} < 2\},$$
$$\Omega_R = (-\pi, \pi)^2 \times (-4, 4), \quad q(x) = 0.5, \text{ for } x \in D.$$

In this experiment the wave number k is $\pi/2$. The Fourier coefficients of constant contrast q



(a) View down x_3 axis (b) 3D view

Figure 4.7: Biperiodic structure of spheres of radius 2 plotted in $(-3\pi, 3\pi)^2 \times (-2, 2)$.

in this case can be computed explicitly, see [87]. Assume that $q = q_0 > 0$, r is the radius of the sphere, and $I(j) = |j_1|^2 + |j_2|^2 + |j_3\pi/R|^2$ for $j = (j_1, j_2, j_3) \in \mathbb{Z}^3$, we have

$$\sqrt{8\pi^2 R}\hat{q}(j) = \begin{cases} 4\pi r^3 q_0/3 & I(j) = 0, \\ q_0 4\pi\big[-r\cos(I(j)r)/I(j) + \sin(I(j)r)/I(j)^2\big]/I(j) & I(j) \neq 0. \end{cases}$$

As in the last two experiments we check in Figure 4.4 the energy conservation error for $N = 2^n$, $n = 3, \ldots, 6$ where the tolerance for the GMRES iteration is 10^{-8}.

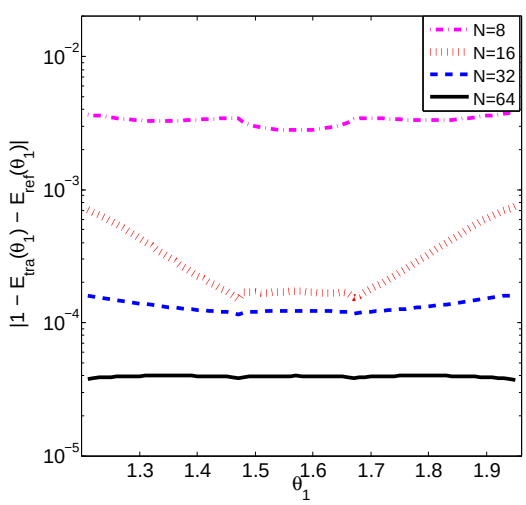


Figure 4.8: Scattering from biperiodic structures of spheres. The error curves $|1 - E_{\mathrm{tra}}(\theta) - E_{\mathrm{ref}}(\theta)|$ for different discretization parameters N versus the angles θ of the incident field u^i.

Chapter 5

The Factorization Method for Biperiodic Inverse Scattering

Abstract: In this chapter, we extend the Factorization method studied in Chapter 2 to the electromagnetic inverse scattering problem for Maxwell's equations. Instead of a half-space setting of the problem as in the scalar case, we investigate here the vectorial problem for penetrable biperiodic structures in a full-space setting (compare Figure 5.1). To extend the technique of the scalar problem to the vectorial problem, we first introduce special plane incident fields that, basically, are suitable modifications of the fields used in the scalar case (see (5.9)). Second, we again factorize the near field operator N and prove necessary properties of the middle operator in the factorization (see Theorem 5.3.2 and Theorem 5.4.1). Again, this allows us to apply Theorem 3.4.1 of range identity to provide a simple imaging criterion (5.30). In Section 5.5, we also provide three dimensional numerical experiments which, to the best of our knowledge, are the first numerical examples for this method in a biperiodic setting.

5.1 Introduction

This chapter is the extension of the Factorization method studied in Chapter 2 to inverse biperiodic medium scattering for Maxwell's equations. We consider penetrable biperiodic structures similar to the one in Chapter 3. Further, Chapter 2 investigates the problem in a half-space setting with Neumann boundary condition. We study in the present chapter the vectorial problem for penetrable biperiodic structures in a full-space setting. The inverse problem that we treat in this paper is again the shape reconstruction of a biperiodic medium from measured data consisting of scattered electromagnetic waves. We consider plane electromagnetic waves as incident fields.

The aim again is to study the Factorization method as a tool for reconstructing three-dimensional biperiodic structures from measurements related to scattered waves. More pre-

cisely, the measured data that we consider here are the coefficients of propagating and evanescent modes of the scattered fields. Given those coefficients of the tangential components of the electromagnetic scattered fields, the inverse problem is then to determine the three-dimensional penetrable biperiodic scatterer. As presented in the rest of the chapter, the Factorization method is shown to be an efficient tool to our imaging problem. From a full mathematical justification of the method, a simple criterion for imaging is shown to work accurately in the three-dimensional numerical experiments which, to the best of our knowledge, are the first numerical examples for this method in a biperiodic setting. Besides the difficult technicalities of the Maxwell case, the vectorial problem in a full-space setting requires measurements from above and below of the biperiodic structure. Thus we need to suitably adapt the special plane incident waves used in Chapter 2 for the case of Maxwell's equations.

Similar to the scalar case, the imaginary part of the middle operator in the factorization is just semidefinite. Therefore we need a modified version of the central range identity of the Factorization to overcome that. This modification follows again [78] in a comparable way to Chapter 2. Again the neccessary properties of the middle operator are obtained by the approach in [72] for obstacle inverse scattering of electromagnetic waves.

The chapter is organized as follows: In Section 5.2 we introduce the direct problem and set up the corresponding inverse problem. Section 5.3 is dedicated to study the factorization of the near field operator. We derive the neccessary properties of the middle operator in the factorization in Section 5.4. Finally, a characterization of the biperiodic structure and numerical experiments are given in Section 5.5.

5.2 Problem Setting

As in the previous chapter the electric field E and the magnetic field H are governed by the time-harmonic Maxwell equations at frequency $\omega > 0$ in $\mathbb{R}^3$,

$$\operatorname{curl} H + \mathrm{i}\omega\varepsilon E = \sigma E \quad \text{in } \mathbb{R}^3, \tag{5.1}$$

$$\operatorname{curl} E - \mathrm{i}\omega\mu_0 H = 0 \quad \text{in } \mathbb{R}^3. \tag{5.2}$$

Compared to Chapter 3 we restrict ourselves here to the case that the electric permittivity ε and the conductivity σ are scalar bounded measurable functions which are 2π-periodic in x_1 and x_2, and that the magnetic permeability μ_0 is a positive constant. We assume that ε equals $\varepsilon_0 > 0$ and that σ vanishes outside the biperiodic structure. The relative material parameter is again

$$\varepsilon_{\mathrm{r}} := \frac{\varepsilon + \mathrm{i}\sigma}{\varepsilon_0}.$$

Note that ε_{r} equals 1 outside the biperiodic structure. Recall that the magnetic permeability μ_0 is constant which motivates us to work with the divergence-free magnetic field. Hence, introducing the wave number $k = \omega(\varepsilon_0\mu_0)^{1/2}$, and eliminating the electric field E from (5.1)–(5.2), we find that

$$\operatorname{curl}\left(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl} H\right) - k^2 H = 0 \quad \text{in } \mathbb{R}^3. \tag{5.3}$$

Assume that the biperiodic structure is illuminated by α-quasiperiodic incident electric and magnetic fields E^i and H^i, respectively, satisfying

$$\operatorname{curl} H^i + \mathrm{i}\omega\varepsilon_0 E^i = 0, \qquad \operatorname{curl} E^i - \mathrm{i}\omega\mu_0 H^i = 0 \quad \text{in } \mathbb{R}^3.$$

Simple examples for such α-quasiperiodic fields are certain plane waves that we introduce below. We wish to reformulate (5.3) in terms of the scattered field H^s, defined by $H^s := H - H^i$. Straightforward computations show that $\operatorname{curl}\operatorname{curl} H^i - k^2 H^i = 0$, and

$$\operatorname{curl}\left(\varepsilon_{\mathrm{r}}^{-1}\operatorname{curl} H^s\right) - k^2 H^s = -\operatorname{curl}\left(q \operatorname{curl} H^i\right) \quad \text{in } \mathbb{R}^3, \tag{5.4}$$

where q is the scalar contrast defined by

$$q := \varepsilon_{\mathrm{r}}^{-1} - 1.$$

Similarly to the problem setting in Chapter 3, we find the α-quasiperiodic scattered field H^s to the direct problem (5.4), satisfying the Rayleigh expansion radiation condition

$$H^s(x) = \sum_{n\in\mathbb{Z}^2} \hat{H}_n^{\pm} e^{\mathrm{i}(\alpha_n\cdot x + \beta_n|x_3-h|)} \quad \text{for } x_3 \gtrless \pm h, \tag{5.5}$$

where $(\hat{H}_n^{\pm})_{n\in\mathbb{Z}^2}$ are the Rayleigh sequences given by

$$\hat{H}_n^{\pm} := \hat{H}_n(\pm h) = \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} H^s(x_1,x_2,\pm h)e^{-\mathrm{i}\alpha_n\cdot x}\,\mathrm{d}x_1\,\mathrm{d}x_2\,, \quad n\in\mathbb{Z}^2.$$

Note that we require that the series in (5.5) converges uniformly on compact subsets of $\{|x_3| > h\}$. Recall that, for $n \in \mathbb{Z}^2$, $\alpha_n = (\alpha_{1,n}, \alpha_{2,n}, 0) = (\alpha_1 + n_1, \alpha_2 + n_2, 0)$ and

$$\beta_n = \begin{cases} \sqrt{k^2 - |\alpha_n|^2}, & k^2 \geq |\alpha_n|^2, \\ \mathrm{i}\sqrt{|\alpha_n|^2 - k^2}, & k^2 < |\alpha_n|^2, \end{cases}$$

and β_n is assumed to be nonzero for all $n \in \mathbb{Z}^2$. Further, only a finite number of terms in (5.5) are propagating plane waves which are called propagating modes, the rest are evanescent modes which correspond to exponentially decaying terms.

Denote by $\overline{D}$ the support of the contrast q in one period $\Omega = (-\pi,\pi)^2 \times \mathbb{R}$. We make an assumption which is neccessary for the subsequent factorization framework.

Assumption 5.2.1. *We assume that the support $D \subset \Omega$ is open and bounded with Lipschitz boundary and that there exists a positve constant c such that* $\operatorname{Re}(q) \geq c > 0$ *and* $\operatorname{Im}(q) \leq 0$ *almost everywhere in Ω.*

Considering a more general source term on the right hand side of (5.4), we have the following direct problem: Given $f \in L^2(D)^3$, find $u : \Omega \to \mathbb{C}^3$ in a suitable function space such that

$$\operatorname{curl}\left(\varepsilon_{\mathrm{r}}^{-1}\operatorname{curl} u\right) - k^2 u = -\operatorname{curl}\left(q/\sqrt{|q|}f\right) \quad \text{in } \Omega, \tag{5.6}$$

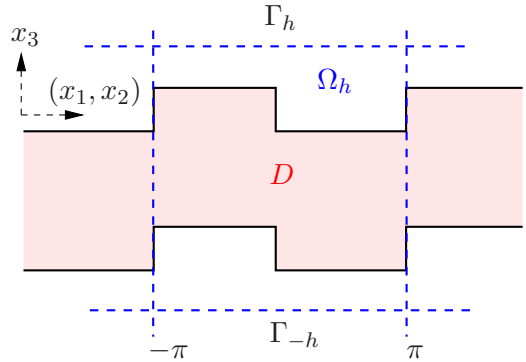


Figure 5.1: Geometric setting for inverse scattering problem of electromagnetic waves from a penetrable biperiodic structure (in two dimentions, for simplicity).

and u satisfies the Rayleigh expansion condition (5.5). In the following, a function which satisfies (5.5) is said to be radiating. It is also seen that if u is a solution of (5.4) then u solves (5.6) for the right hand side of $f = \operatorname{curl} H^i/\sqrt{|q|}$.

For a variational formulation of the problem we recall from (4.19) that

$$H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega) = \{u \in H_{\mathrm{loc}}(\mathrm{curl},\Omega) : u = U|_\Omega \text{ for some } \alpha\text{-quasiperiodic } U \in H_{\mathrm{loc}}(\mathrm{curl},\mathbb{R}^3)\},$$

and $\Omega_h = (-\pi,\pi)^2 \times (-h,h)$ for $h > \sup\{|x_3| : (x_1,x_2,x_3)^\top \in \operatorname{supp}(q)\}$ with boundaries $\Gamma_{\pm h} = (-\pi,\pi)^2 \times \{\pm h\}$. The variational formulation to the problem (5.6) is to find a radiating solution $u \in H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$ such that

$$\int_\Omega (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl} u \cdot \operatorname{curl} \overline{\psi} - k^2 u \cdot \overline{\psi})\,\mathrm{d}x = -\int_\Omega q/\sqrt{|q|} f \cdot \operatorname{curl} \overline{\psi}\,\mathrm{d}x\,, \tag{5.7}$$

for all $\psi \in H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$ with compact support. Existence and uniqueness of this problem can be obtained for all but possibly a discrete set of wave numbers k, see e.g. [12, 41, 105]. In the sequel we assume that (5.7) is uniquely solvable for any $f \in L^2(D)^3$ and fixed $k > 0$. Then we define a solution operator

$$G : L^2(D)^3 \to \ell^2(\mathbb{Z}^2)^4$$

which maps f to the Rayleigh sequences $(\hat{u}^+_{1,j}, \hat{u}^-_{1,j}, \hat{u}^+_{2,j}, \hat{u}^-_{2,j})_{j\in\mathbb{Z}^2}$ of the first two components of $u \in H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$, solution to (5.7). Note that the Rayleigh sequences $\hat{u}^\pm_{(1,2),j}$ are given by

$$\hat{u}^\pm_{(1,2),j} = \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} u_{(1,2)}(x_1,x_2,\pm h) e^{-\mathrm{i}\alpha_j\cdot x}\,\mathrm{d}x_1\,\mathrm{d}x_2\,, \quad j \in \mathbb{Z}^2. \tag{5.8}$$

Now we introduce the notation $\tilde{b} = (b_1, b_2, -b_3)^\top$ for $b = (b_1,b_2,b_3)^\top \in \mathbb{C}^3$. To obtain the data for the factorization method we consider the following α-quasiperiodic plane waves

$$\varphi_j^{(l)\pm} = p_j^{(l)} e^{\mathrm{i}(\alpha_j\cdot x + \beta_j x_3)} \pm \tilde{p}_j^{(l)} e^{\mathrm{i}(\alpha_j\cdot x - \beta_j x_3)}, \quad l = 1,2, \quad j \in \mathbb{Z}^2, \tag{5.9}$$

where $p_j^{(l)} = (p_{1,j}^{(l)}, p_{2,j}^{(l)}, p_{3,j}^{(l)}) \in \mathbb{C}^3 \setminus \{0\}$ are complex polarizations chosen such that, for all $j \in \mathbb{Z}^2$,

$$i)\ p_j^{(1)} \times p_j^{(2)} = c_j(\alpha_{1,j}, \alpha_{2,j}, \beta_j)^\top, \quad \text{for } c_j \in \mathbb{C} \setminus \{0\}. \tag{5.10}$$

$$ii)\ |p_j^{(1)}| = |p_j^{(2)}| = 1. \tag{5.11}$$

Together with the assumption that $\beta_j \neq 0$ for all $j \in \mathbb{Z}^2$, such polarizations are linear independent. One possible choice is

$$p_j^{(1)} = (0, \beta_j, -\alpha_{2,j})/(|\beta_j|^2 + \alpha_{2,j}^2)^{1/2}, \quad p_j^{(2)} = (-\beta_j, 0, \alpha_{1,j})/(|\beta_j|^2 + \alpha_{1,j}^2)^{1/2}.$$

Note that $\varphi_j^{(l)\pm}$ are propagating plane waves if β_j are real, and evanescent waves if β_j are complex. Further $\varphi_j^{(l)\pm}$ are divergence-free functions for all $j \in \mathbb{Z}^2$, $l = 1, 2$. Due to the linearity of the problem, a linear combination of several incident fields will lead to a corresponding linear combination of the resulting scattered fields. We obtain such a linear combination using sequences $(a_j)_{j\in\mathbb{Z}^2} = \left(a_j^{(1)+}, a_j^{(1)-}, a_j^{(2)+}, a_j^{(2)-}\right)_{j\in\mathbb{Z}^2} \in \ell^2(\mathbb{Z}^2)^4$ and define the corresponding operator $H : \ell^2(\mathbb{Z}^2)^4 \to L^2(D)^3$ by

$$H(a_j) = \sqrt{|q|} \sum_{j\in\mathbb{Z}^2} \frac{1}{\beta_j w_j} \Big[a_j^{(1)+} \operatorname{curl} \varphi_j^{(1)+} + a_j^{(2)+} \operatorname{curl} \varphi_j^{(2)+} + a_j^{(1)-} \operatorname{curl} \varphi_j^{(1)-} + a_j^{(2)-} \operatorname{curl} \varphi_j^{(2)-} \Big], \tag{5.12}$$

where

$$w_j := \begin{cases} \mathrm{i}, & k^2 > \alpha_j^2, \\ \exp(-\mathrm{i}\beta_j h), & k^2 < \alpha_j^2. \end{cases}$$

Note that we divide by $\beta_j w_j$ to make later computations easier.

In our inverse problem the data that we measure are the Rayleigh sequences defined in (5.8). Similar to the scalar case we need both propagating and evanescent modes to be able to uniquely determine the periodic structure. Hence the operator that models measurements of fields scattered from the periodic inhomogeneous medium caused by the incident fields (5.12) is referred to be the *near field* operator, denoted by N. We define $N : \ell^2(\mathbb{Z}^2)^4 \to \ell^2(\mathbb{Z}^2)^4$ to map a sequence $(a_j)_{j\in\mathbb{Z}^2}$ to the Rayleigh sequences of the first two components of the scattered field generated by the incident field $H(a_j)$ defined in (5.12), i.e.

$$[N(a_j)]_n := (\hat{u}_{1,n}^+, \hat{u}_{1,n}^-, \hat{u}_{2,n}^+, \hat{u}_{2,n}^-)_{n\in\mathbb{Z}^2},$$

where $u \in H_{\alpha,\mathrm{loc}}(\operatorname{curl}, \Omega)$ is the radiating solution to (5.7) for the source $f = H(a_j)$. Then from the definition of the solution operator we have

$$N = GH. \tag{5.13}$$

The inverse scattering problem is now to reconstruct the support $\overline{D}$ of the contrast $q = \varepsilon_\mathrm{r}^{-1} - 1$ when the near field operator N is given. Note that it is not clear yet that N is a bounded linear operator, but we will prove this in the next section.

5.3 Factorization of the Near Field Operator

We study the inverse problem of the previous section using the factorization method. One of the important steps of the latter method that this section is devoted to is factorizing the near field operator. Before doing that, in the next lemma, we show some properties of the operator $H : \ell^2(\mathbb{Z}^2)^4 \to L^2(D)^3$ and its adjoint H^*. We need the sequence

$$w_j^* := \begin{cases} \exp(-\mathrm{i}\beta_j h), & k^2 > \alpha_j^2, \\ \mathrm{i}, & k^2 < \alpha_j^2. \end{cases}$$

Lemma 5.3.1. *For $p_j^{(l)} = (p_{1,j}^{(l)}, p_{2,j}^{(l)}, p_{3,j}^{(l)})$, $j \in \mathbb{Z}^2$, $l = 1, 2$, defined as in* (5.10) *and* (5.11)*, the operator $H : \ell^2(\mathbb{Z}^2)^4 \to L^2(D)^3$ is compact and injective, and its adjoint $H^* : L^2(D)^3 \to \ell^2(\mathbb{Z}^2)^4$ satisfies*

$$(H^* f)_j = 8\pi^2 w_j^* \begin{pmatrix} \overline{p_{1,j}^{(1)}}(\hat{u}_{1,j}^+ + \hat{u}_{1,j}^-) + \overline{p_{2,j}^{(1)}}(\hat{u}_{2,j}^+ + \hat{u}_{2,j}^-) \\ \overline{p_{1,j}^{(2)}}(\hat{u}_{1,j}^+ + \hat{u}_{1,j}^-) + \overline{p_{2,j}^{(2)}}(\hat{u}_{2,j}^+ + \hat{u}_{2,j}^-) \\ \overline{p_{1,j}^{(1)}}(\hat{u}_{1,j}^+ - \hat{u}_{1,j}^-) + \overline{p_{2,j}^{(1)}}(\hat{u}_{2,j}^+ - \hat{u}_{2,j}^-) \\ \overline{p_{1,j}^{(2)}}(\hat{u}_{1,j}^+ - \hat{u}_{1,j}^-) + \overline{p_{2,j}^{(2)}}(\hat{u}_{2,j}^+ - \hat{u}_{2,j}^-) \end{pmatrix}^\top, \quad j \in \mathbb{Z}^2, \tag{5.14}$$

where $(\hat{u}_{1,j}^+, \hat{u}_{1,j}^-, \hat{u}_{2,j}^+, \hat{u}_{2,j}^-)_{j\in\mathbb{Z}^2}$ are the Rayleigh sequences of the first two components of $u \in H_{\alpha,loc}(\mathrm{curl}, \Omega)$, the radiating variational solution to $\mathrm{curl}^2 u - k^2 u = \mathrm{curl}(\sqrt{|q|} f)$ in Ω.

Proof. For $l = 1, 2$ and $j \in \mathbb{Z}^2$, we have

$$\begin{aligned} \int_D H(a_j)\overline{f}\,\mathrm{d}x &= \sum_{j\in\mathbb{Z}^2} \left[\sum_{l=1,2} \frac{a_j^{(l)+}}{\beta_j w_j} \int_D \sqrt{|q|}\overline{f} \cdot \mathrm{curl}\,\varphi_j^{(l)+}\,\mathrm{d}x + \sum_{l=1,2} \frac{a_j^{(l)-}}{\beta_j w_j} \int_D \sqrt{|q|}\overline{f} \cdot \mathrm{curl}\,\varphi_j^{(l)-}\,\mathrm{d}x \right] \\ &= \left\langle (a_j), \left(\int_D \sqrt{|q|} f \cdot \overline{\left(\frac{\mathrm{curl}\,\varphi_j^{(l)+}}{\beta_j w_j} \right)}\,\mathrm{d}x\,, \int_D \sqrt{|q|} f \cdot \overline{\left(\frac{\mathrm{curl}\,\varphi_j^{(l)-}}{\beta_j w_j} \right)}\,\mathrm{d}x \right) \right\rangle_{\ell^2(\mathbb{Z}^2)^4}. \end{aligned}$$

Note that the equation $\mathrm{curl}^2 u - k^2 u = \mathrm{curl}(\sqrt{|q|} f)$ in Ω with Rayleigh expansion condition is uniquely solvable for all wave numbers $k > 0$. The Fredholm property can be obtained as in [12, 41, 105], and using integral representation formulas from Theorem 3.1 in [100] one shows the uniqueness. Now we define $v_j^{(l)\pm} = \varphi_j^{(l)\pm}/(\beta_j w_j)$ and consider a smooth function $\phi \in C^\infty(\mathbb{R})$ such that $\phi = 1$ in $(-h, h)$, $\phi = 0$ in $\mathbb{R} \setminus \overline{(-2h, 2h)}$. Then $\phi v_j^{(l)\pm}$ belongs to $H_\alpha(\mathrm{curl}, \Omega)$ with compact support in $\{|x_3| < 2h\}$. Assume that $u \in H_{\alpha,\mathrm{loc}}(\mathrm{curl}, \Omega)$ is the variational radiating solution to $\mathrm{curl}^2 u - k^2 u = -\mathrm{curl}(\sqrt{|q|} f)$ in Ω. We have

$$\begin{aligned} \int_D \sqrt{|q|} f \cdot \mathrm{curl}\,\overline{v_j^{(l)\pm}}\,\mathrm{d}x &= \int_{\Omega_h} (\mathrm{curl}\,u \cdot \mathrm{curl}\,\overline{v_j^{(l)\pm}} - k^2 u \cdot \overline{v_j^{(l)\pm}})\,\mathrm{d}x \\ &\quad + \int_{\Omega_{2h}\setminus\Omega_h} (\mathrm{curl}\,u \cdot \mathrm{curl}(\overline{\phi v_j^{(l)\pm}}) - k^2 u \cdot \overline{\phi v_j^{(l)\pm}})\,\mathrm{d}x\,. \end{aligned}$$

Now using Green's theorems and exploiting the fact that $v_j^{(l)\pm}$ and u are divergence-free solutions to the Hemholtz equation in $\mathbb{R}^3$ and $\Omega \setminus \Omega_h$, respectively, we obtain that

$$\begin{aligned}\int_D \sqrt{|q|} f \cdot \operatorname{curl} \overline{v_j^{(l)\pm}} \,\mathrm{d}x &= \int_{\Gamma_h} (e_3 \times \operatorname{curl} u \cdot \overline{v_j^{(l)\pm}} - e_3 \times \operatorname{curl} \overline{v_j^{(l)\pm}} \cdot u) \,\mathrm{d}s \\ &\quad + \int_{\Gamma_{-h}} (e_3 \times \operatorname{curl} \overline{v_j^{(l)\pm}} \cdot u - e_3 \times \operatorname{curl} u \cdot \overline{v_j^{(l)\pm}}) \,\mathrm{d}s \\ &= \left(\int_{\Gamma_h} - \int_{\Gamma_{-h}} \right) \left[\frac{\partial \overline{v_{2,j}^{(l)\pm}}}{\partial x_3} u_2 - \frac{\partial u_2}{\partial x_3} \overline{v_{2,j}^{(l)\pm}} + \frac{\partial \overline{v_{1,j}^{(l)\pm}}}{\partial x_3} u_1 - \frac{\partial u_1}{\partial x_3} \overline{v_{1,j}^{(l)\pm}} \right] \mathrm{d}s \,. \end{aligned} \tag{5.15}$$

Note that we have

$$\begin{aligned} \overline{v_{1,j}^{(l)+}} &= \overline{\left(\frac{p_{1,j}^{(l)}}{\beta_j w_j} \right)} (e^{\mathrm{i}\beta_j x_3} + e^{-\mathrm{i}\beta_j x_3}) e^{-\mathrm{i}\alpha_j \cdot x}, \\ \frac{\partial \overline{v_{1,j}^{(l)+}}}{\partial x_3} &= \mathrm{i}\beta_j \overline{\left(\frac{p_{1,j}^{(l)}}{\beta_j w_j} \right)} (e^{\mathrm{i}\beta_j x_3} - e^{-\mathrm{i}\beta_j x_3}) e^{-\mathrm{i}\alpha_j \cdot x}. \end{aligned}$$

Then by straightforward computation we obtain

$$\begin{aligned} \int_{\Gamma_h} \left(\frac{\partial \overline{v_{1,j}^{(l)+}}}{\partial x_3} u_1 - \frac{\partial u_1}{\partial x_3} \overline{v_{1,j}^{(l)+}} \right) \mathrm{d}s &= \sum_{n \in \mathbb{Z}^2} \hat{u}_{1,n}^+ \int_{\Gamma_h} e^{\mathrm{i}\alpha_n \cdot x} \left[\frac{\partial \overline{v_{1,j}^{(l)+}}}{\partial x_3} - i\beta_n \overline{v_{1,j}^{(l)+}} \right] \mathrm{d}s \\ &= 8\pi^2 w_j^* \overline{p_{1,j}^{(l)}} \hat{u}_{1,j}^+. \end{aligned}$$

Similarly we also have

$$\begin{aligned} \int_{\Gamma_h} \left(\frac{\partial \overline{v_{2,j}^{(l)+}}}{\partial x_3} u_2 - \frac{\partial u_2}{\partial x_3} \overline{v_{2,j}^{(l)+}} \right) \mathrm{d}s &= 8\pi^2 w_j^* \overline{p_{2,j}^{(l)}} \hat{u}_{2,j}^+, \\ \int_{\Gamma_{-h}} \left(\frac{\partial \overline{v_{2,j}^{(l)+}}}{\partial x_3} u_2 - \frac{\partial u_2}{\partial x_3} \overline{v_{2,j}^{(l)+}} + \frac{\partial \overline{v_{1,j}^{(l)+}}}{\partial x_3} u_1 - \frac{\partial u_1}{\partial x_3} \overline{v_{1,j}^{(l)+}} \right) \mathrm{d}s &= -8\pi^2 w_j^* (\overline{p_{1,j}^{(l)}} \hat{u}_{1,j}^- + \overline{p_{2,j}^{(l)}} \hat{u}_{2,j}^-). \end{aligned}$$

Now substituting the last two equations into (5.15) we derive

$$\int_D \sqrt{|q|} f \cdot \operatorname{curl} \overline{v_j^{(l)+}} \,\mathrm{d}x = 8\pi^2 w_j^* (\overline{p_{1,j}^{(l)}} \hat{u}_{1,j}^- + \overline{p_{2,j}^{(l)}} \hat{u}_{2,j}^- + \overline{p_{1,j}^{(l)}} \hat{u}_{1,j}^+ + \overline{p_{2,j}^{(l)}} \hat{u}_{2,j}^+).$$

Similarly we have

$$\int_D \sqrt{|q|} f \cdot \operatorname{curl} \overline{v_j^{(l)-}} \,\mathrm{d}x = 8\pi^2 w_j^* (-\overline{p_{1,j}^{(l)}} \hat{u}_{1,j}^- - \overline{p_{2,j}^{(l)}} \hat{u}_{2,j}^- + \overline{p_{1,j}^{(l)}} \hat{u}_{1,j}^+ + \overline{p_{2,j}^{(l)}} \hat{u}_{2,j}^+)$$

which shows that H^* satisfies (5.14). Next we show the compactness of H^*. This relies on the operator $W : \ell^2(\mathbb{Z}^2)^4 \to \ell^2(\mathbb{Z}^2)^4$ defined by

$$W((a_l)_{l\in\mathbb{Z}^2}) = -8\pi^2 w_j^* \begin{pmatrix} \overline{p_{1,j}^{(1)}}(a_j^{(1)+} + a_j^{(1)-}) + \overline{p_{2,j}^{(1)}}(a_j^{(2)+} + a_j^{(2)-}) \\ \overline{p_{1,j}^{(2)}}(a_j^{(1)+} + a_j^{(1)-}) + \overline{p_{2,j}^{(2)}}(a_j^{(2)+} + a_j^{(2)-}) \\ \overline{p_{1,j}^{(1)}}(a_j^{(1)+} - a_j^{(1)-}) + \overline{p_{2,j}^{(1)}}(a_j^{(2)+} - a_j^{(2)-}) \\ \overline{p_{1,j}^{(2)}}(a_j^{(1)+} - a_j^{(1)-}) + \overline{p_{2,j}^{(2)}}(a_j^{(2)+} - a_j^{(2)-}) \end{pmatrix}^\top, \quad j \in \mathbb{Z}^2. \tag{5.16}$$

Since $(w_j^*)_{j\in\mathbb{Z}^2}$ is a bounded sequence, and since the sequences $(p_j^{(l)})_{j\in\mathbb{Z}^2}$ are bounded for $l = 1, 2$ due to (5.11), the operator W is bounded. Now we define the operator

$$Q : L^2(D)^3 \to \ell^2(\mathbb{Z}^2)^4 \tag{5.17}$$

which maps f to $(\hat{u}_{1,j}^+, \hat{u}_{1,j}^-, \hat{u}_{2,j}^+, \hat{u}_{2,j}^-)$ where u is the radiating variational solution to $\operatorname{curl}^2 u - k^2 u = \operatorname{curl}(\sqrt{|q|} f)$ in Ω. Then we have

$$H^* = -WQ. \tag{5.18}$$

The following trace spaces are neccessary for our proof: We define

$$Y(\Gamma_{\pm h}) = \{f \in H^{-1/2}(\Gamma_{\pm h})^3 | \text{ there exists } u \in H_\alpha(\operatorname{curl}, \Omega_h) \text{ with } \pm e_3^\top \times u|_{\Gamma_{\pm h}} = f\}$$

with norm

$$\|f\|_{Y(\Gamma_{\pm h})} = \inf_{u\in H_\alpha(\operatorname{curl},\Omega_h), \pm e_3^\top \times u|_{\Gamma_{\pm h}} = f} \|u\|_{H_\alpha(\operatorname{curl},\Omega_h)}.$$

The trace spaces $Y(\Gamma_{\pm h})$ are Banach spaces with this norm, see [83, Chapter 3]. Note that the results in latter reference are presented for bounded Lipschitz domains which are certainly valid for Ω_h. Further the operation $u \mapsto ((0, 0, \pm 1) \times u|_{\Gamma_{\pm h}}) \times (0, 0, \pm 1)$ is bounded from $H_\alpha(\operatorname{curl}, \Omega_h)$ into $Y'(\Gamma_{\pm h})$ which is the dual space of $Y(\Gamma_{\pm h})$.

Now we know that the operation which maps $f \in L^2(D)^3$ into $u \in H_{\alpha,\mathrm{loc}}(\operatorname{curl}, \Omega)$, radiating variational solution to $\operatorname{curl}^2 u - k^2 u = \operatorname{curl}(\sqrt{|q|} f)$, is bounded. Note that $((0, 0, \pm 1) \times u|_{\Gamma_{\pm h}}) \times (0, 0, \pm 1) = (u_1, u_2, 0)$. We obtain that the operations $f \mapsto (u_1, u_2, 0)|_{\Gamma_h}$ and $(u_1, u_2, 0)|_{\Gamma_h} \mapsto (\hat{u}_{1,j}^+, \hat{u}_{2,j}^+)$ are bounded from $L^2(D)^3$ into $Y'(\Gamma_h)$ and from $Y'(\Gamma_h)$ into $\ell^2(\mathbb{Z}^2)^2$, respectively. Similarly for Γ_{-h} we obtain that $f \mapsto (\hat{u}_{1,j}^-, \hat{u}_{2,j}^-)$ are bounded from $L^2(D)^3$ into $\ell^2(\mathbb{Z}^2)^2$. Together with the boundedness of the sequence $(w_j^*)_{j\in\mathbb{Z}^2}$, Q is a bounded operator. We know that in a neighbourhood of $\Gamma_{\pm h}$ u solves the Hemholtz equation. Hence elliptic regularity results [81] imply that u is H^2-regular in a neighbourhood of $\Gamma_{\pm h}$, thus, $f \mapsto (u_1, u_2, 0)|_{\Gamma_{\pm h}}$ is a compact operation from $L^2(D)^3$ into $Y'(\Gamma_{\pm h})$. Then Q is a compact operator and H^* is compact. Therefore H is compact as well.

To obtain the injectivity of H, we prove that H^* has dense range. It is sufficient to prove that W has dense range and all sequences $((\delta_{jl})_{l\in\mathbb{Z}^2}, 0, 0, 0), (0, (\delta_{jl})_{l\in\mathbb{Z}^2}, 0, 0), (0, 0, (\delta_{jl})_{l\in\mathbb{Z}^2}, 0)$

and $(0,0,0,(\delta_{jl})_{l\in\mathbb{Z}^2})$ belong to the range of Q (by definition, the Kronecker symbol δ_{jl} equals one for $j=l$ and zero otherwise). The operator W has dense range due to the fact that

$$\det\begin{pmatrix} \overline{p_{1,j}^{(1)}} & \overline{p_{1,j}^{(1)}} & \overline{p_{2,j}^{(1)}} & \overline{p_{2,j}^{(1)}} \\ \overline{p_{1,j}^{(2)}} & \overline{p_{1,j}^{(2)}} & \overline{p_{2,j}^{(2)}} & \overline{p_{2,j}^{(2)}} \\ \overline{p_{1,j}^{(1)}} & -\overline{p_{1,j}^{(1)}} & \overline{p_{2,j}^{(1)}} & -\overline{p_{2,j}^{(1)}} \\ \overline{p_{1,j}^{(2)}} & -\overline{p_{1,j}^{(2)}} & \overline{p_{2,j}^{(2)}} & -\overline{p_{2,j}^{(2)}} \end{pmatrix} = -4\left(\overline{p_{1,j}^{(2)}p_{2,j}^{(1)}} - \overline{p_{2,j}^{(2)}p_{1,j}^{(1)}}\right)^2 = 4(\overline{c_j\beta_j})^2 \neq 0,$$

due to the property (5.10) of the polarizations. Now we show that $((\delta_{jl})_{l\in\mathbb{Z}^2},0,0,0)$ belongs to the range of Q, and the other cases can be done in a similar way. We choose a cut-off function $\chi_{1,j}\in\mathbb{C}^\infty(\mathbb{R})$ such that $\chi_{1,j}(t)=0$ for $t<0$ and $\chi(t)=1$ for $t>h/2$. Then $(x_1,x_2,x_3)\mapsto\chi_{1,j}(x_3)\exp(\mathrm{i}(\alpha_j\cdot x+\beta_j(x_3-h))$ has Rayleigh sequence $((\delta_{jl})_{l\in\mathbb{Z}^2},0)$. For all $j\in\mathbb{Z}^2$, we define

$$\varphi_j(x)=(\chi_{1,j}(x_3),0,\chi_{3,j}(x_3))^\top\exp(\mathrm{i}(\alpha_j\cdot x+\beta_j(x_3-h)),$$

where

$$\chi_{3,j}(x_3)=-\mathrm{i}\alpha_{1,j}e^{-\mathrm{i}\beta_j x_3}\int_0^{x_3}e^{\mathrm{i}\beta_j t}\chi_{1,j}(t)\,\mathrm{d}t\,.$$

Then $\mathrm{div}\varphi_j=0$ in Ω and the Rayleigh sequences of the first two components of φ_j are $((\delta_{jl})_{l\in\mathbb{Z}^2},0,0,0)$. Next we show that there exists $f_j\in L^2(D)^3$ such that $\mathrm{curl}^2\,\varphi_j-k^2\varphi_j=\mathrm{curl}(\sqrt{|q|}f_j)$ in Ω holds in the variational sense. Set

$$g_j(x):=\mathrm{curl}^2\,\varphi_j(x)-k^2\varphi_j(x),\quad x\in\Omega,$$

then we have $\mathrm{div}(g_j)=0$ in Ω which also implies that

$$\int_{\partial\Omega_h}g_j\cdot\nu\,\mathrm{d}s\;=0.$$

Therefore, due to Theorem 3.38 in [83], there exists $\psi_j\in H^1(\Omega_h)^3$ such that

$$g_j=\mathrm{curl}\,\psi_j\quad\text{ in }\Omega_h.$$

Define $f_j=\sqrt{|q|}^{-1}\psi_j$, then $f_j\in L^2(D)^3$ and we have, in the weak sense,

$$\mathrm{curl}^2\,\varphi_j-k^2\varphi_j=\mathrm{curl}(\sqrt{|q|}f_j)\quad\text{ in }\Omega_h.$$

Together with $\mathrm{curl}^2\,\varphi_j-k^2\varphi_j=0$ in $\Omega\setminus\Omega_h$, we complete the proof. □

Now we show a factorization of the near field operator N in the following theorem. To this end, we define the sign of q by

$$\mathrm{sign}(q):=\frac{q}{|q|}.$$

Theorem 5.3.2. *Assume that q satisfies the Assumption 5.2.1. The operator W is defined as in* (5.16)*. Let $T : L^2(D)^3 \to L^2(D)^3$ be defined by $Tf = \operatorname{sign}(q)(f + \sqrt{|q|}\operatorname{curl} v)$, where $v \in H_{\alpha,loc}(\operatorname{curl},\Omega)$ is the radiating solution to* (5.7)*. Then the near field operator satisfies*

$$WN = H^*TH.$$

Proof. We recall the operator Q in (5.17) that maps $f \in L^2(D)^3$ to the Rayleigh sequences $(\hat{u}^+_{1,j}, \hat{u}^-_{1,j}, \hat{u}^+_{2,j}, \hat{u}^-_{2,j})$ where u is the radiating variational solution to $\operatorname{curl}^2 u - k^2 u = \operatorname{curl}(\sqrt{|q|}f)$ in Ω. By definition of the solution operator G we have $Gf = (\hat{u}^+_{1,j}, \hat{u}^-_{1,j}, \hat{u}^+_{2,j}, \hat{u}^-_{2,j})$ where $u \in H_{\alpha,\mathrm{loc}}(\operatorname{curl},\Omega)$ is a radiating weak solution to

$$\operatorname{curl}(\varepsilon_{\mathrm{r}}^{-1}\operatorname{curl} u) - k^2 u = -\operatorname{curl}(q/\sqrt{|q|}f)$$

. This means that $\operatorname{curl}^2 u - k^2 u = -\operatorname{curl}(\sqrt{|q|}\operatorname{sign}(q)(f + \sqrt{|q|}\operatorname{curl} v))$, thus, $Gf = -(QT)f$. Now due to the fact that $N = GH$ we have

$$WN = WGH = -WQTH.$$

Additionally we know from (5.18) that $H^* = -WQ$ which completes the proof. □

5.4 Study of the Middle Operator

In this section we analyze the middle operator T in the factorization of Theorem 5.3.2 and derive its neccessary properties for the application of the Theorem 3.4.1. This is seen in the following lemma.

Lemma 5.4.1. *Suppose that the contrast q satisfies the Assumption 5.2.1 and that the direct scattering problem* (5.7) *is uniquely solvable for any $f \in L^2(D)^3$. Let $T : L^2(D)^3 \to L^2(D)^3$ be the operator defined as in Theorem 5.3.2, i.e.*

$$Tf = \operatorname{sign}(q)(f + \sqrt{|q|}\operatorname{curl} v),$$

where $v \in H_{\alpha,loc}(\operatorname{curl},\Omega)$ is the radiating variational solution to

$$\operatorname{curl}(\varepsilon_{\mathrm{r}}^{-1}\operatorname{curl} u) - k^2 u = -\operatorname{curl}(q/\sqrt{|q|}f). \tag{5.19}$$

Then we have

(a) T is injective and $\langle \operatorname{Im} Tf, f\rangle \le 0$ for all $f \in L^2(D)^3$.

(b) Define the operator $T_0 : L^2(D)^3 \to L^2(D)^3$ by $T_0 f = \operatorname{sign}(q)(f + \sqrt{|q|}\operatorname{curl}\tilde{v})$ where $\tilde{v} \in H_{\alpha,\mathrm{loc}}(\operatorname{curl},\Omega)$ solves (5.19) *for $k = \mathrm{i}$, $f \in L^2(D)^3$, in the variational sense. Then we have that $T - T_0$ is compact in $L^2(D)^3$.*

(c) For T_0 defined as in (b), if $\operatorname{Re}(q) > 0$ on $L^2(D)^3$ then $\operatorname{Re}(T_0)$ is coercive in $L^2(D)^3$, i.e, there exists a constant $\gamma > 0$ such that

$$\langle \operatorname{Re}(T_0)f, f\rangle_{L^2(D)^3} \ge \gamma \|f\|_{L^2(D)^3}.$$

Note that the proofs of (b) and (c) can be found in Theorem 4.9 [100] or Theorem 5.12 [72]. Here, for convenience, we repeat the proofs in [72] with slight modifications.

Proof. (a) We show the injectivity of T by assuming that $Tf = \operatorname{sign}(q)(f + \sqrt{|q|}\operatorname{curl} v) = 0$, then v is a radiating variational solution to the homogeneous problem $\operatorname{curl}^2 v - k^2 v = 0$. However, we showed in the proof of Lemma 5.3.1 that the latter problem has only the trivial solution which implies that $v = 0$ in Ω. Thus, $f = 0$ or T is injective.

Now we set $w = f + \sqrt{|q|}\operatorname{curl} v$, then $Tf = \operatorname{sign}(q)w$ and

$$\begin{aligned}\langle Tf, f\rangle_{L^2(D)^3} &= \int_D \operatorname{sign}(q) w \cdot (\overline{w} - \sqrt{|q|}\operatorname{curl}\overline{v})\,\mathrm{d}x \\ &= \int_D (\operatorname{sign}(q)|w|^2 - q/\sqrt{|q|} w \cdot \operatorname{curl}\overline{v})\,\mathrm{d}x\end{aligned}$$

For $r > \sup\{|x_3| : (x_1, x_2, x_3)^\top \in D\}$, we consider a smooth function $\chi \in C^\infty(\mathbb{R})$ such that $\chi = 1$ in Ω_r, $\chi = 0$ in $\Omega \setminus \Omega_{2r}$. Then χv belongs to $H_{\alpha,\mathrm{loc}}(\operatorname{curl}, \Omega)$ with compact support in Ω_{3r}. Since $v \in H_{\alpha,\mathrm{loc}}(\operatorname{curl}, \Omega)$ is the radiating solution to (5.19), we have

$$\begin{aligned}-\int_D q/\sqrt{|q|} w \cdot \operatorname{curl}\overline{v}\,\mathrm{d}x &= \int_{\Omega_r} (|\operatorname{curl} v|^2 - k^2|v|^2)\,\mathrm{d}x \\ &\quad + \int_{\Omega_{2r}\setminus\Omega_r} (\operatorname{curl} v \cdot \operatorname{curl}(\overline{\chi v}) - k^2 v \cdot \overline{\chi v})\,\mathrm{d}x\end{aligned}$$

Now using Green's theorems and exploiting the fact that v solve the Hemholtz equation in $\Omega \setminus \Omega_h$, we obtain that

$$\begin{aligned}-\int_D q/\sqrt{|q|} w \cdot \operatorname{curl}\overline{v}\,\mathrm{d}x &= \int_{\Omega_r} (|\operatorname{curl} v|^2 - k^2|v|^2)\,\mathrm{d}x + \left(\int_{\Gamma_r} - \int_{\Gamma_{-r}}\right)(e_3 \times \operatorname{curl} v \cdot \overline{v})\,\mathrm{d}s \\ &= \int_{\Omega_r} (|\operatorname{curl} v|^2 - k^2|v|^2)\,\mathrm{d}x + \left(\int_{\Gamma_r} - \int_{\Gamma_{-r}}\right)\left(-\overline{v_1}\frac{\partial v_1}{\partial x_1} - \overline{v_2}\frac{\partial v_2}{\partial x_3} + v_3\frac{\partial \overline{v_3}}{\partial x_3}\right)\mathrm{d}s\,.\end{aligned} \tag{5.20}$$

Taking the imaginary part of the latter equation we have

$$-\operatorname{Im}\int_D q/\sqrt{|q|} w \cdot \operatorname{curl}\overline{v}\,\mathrm{d}x = \operatorname{Im}\left(\int_{\Gamma_r} - \int_{\Gamma_{-r}}\right)\left(-\overline{v_1}\frac{\partial v_1}{\partial x_3} - \overline{v_2}\frac{\partial v_2}{\partial x_3} + v_3\frac{\partial \overline{v_3}}{\partial x_3}\right)\mathrm{d}s\,.$$

Recall that v satisfies the radiating Rayleigh condition for $|x_3| > r$. Thus all the terms corresponding to evanescent modes tend to zero as r tends to infinity. Then due to a straightforward computation we derive

$$\begin{aligned}-\operatorname{Im}\int_D q/\sqrt{|q|} w \cdot \operatorname{curl}\overline{v}\,\mathrm{d}x &= \lim_{r\to\infty} \operatorname{Im}\left(\int_{\Gamma_r} - \int_{\Gamma_{-r}}\right)\left(-\overline{v_1}\frac{\partial v_1}{\partial x_3} - \overline{v_2}\frac{\partial v_2}{\partial x_3} + v_3\frac{\partial \overline{v_3}}{\partial x_3}\right)\mathrm{d}s \\ &= -4\pi^2 \sum_{j:k^2>\alpha_j^2} \beta_j(|\hat{v}_j^+|^2 + |\hat{v}_j^-|^2),\end{aligned}$$

which implies that

$$\begin{aligned}\langle \mathrm{Im} Tf, f\rangle_{L^2(D)^3} &= \int_D \mathrm{Im} q/|q||w|^2\,\mathrm{d}x \,-\mathrm{Im}\int_D q/\sqrt{|q|}w\cdot\mathrm{curl}\,\overline{v}\,\mathrm{d}x\\ &= \int_D \mathrm{Im} q/|q||w|^2\,\mathrm{d}x \,-4\pi^2\sum_{j:k^2>\alpha_j^2}\beta_j(|\hat{v}_j^+|^2+|\hat{v}_j^-|^2)\le 0,\end{aligned}$$

since $\mathrm{Im}(q)\le 0$ in D.

(b) From the definitions of T and T_0 we note that $Tf-T_0f = q/\sqrt{|q|}\,\mathrm{curl}(v-\tilde{v})$ where $v,\tilde{v}\in H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$ are the solutions, for k and $k=\mathrm{i}$, of

$$\int_\Omega(\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}\,v\cdot\mathrm{curl}\,\overline{\psi}-k^2v\cdot\overline{\psi})\,\mathrm{d}x \,=-\int_\Omega q/\sqrt{|q|}f\cdot\mathrm{curl}\,\overline{\psi}\,\mathrm{d}x\,, \tag{5.21}$$

$$\int_\Omega(\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}\,\tilde{v}\cdot\mathrm{curl}\,\overline{\psi}+\tilde{v}\cdot\overline{\psi})\,\mathrm{d}x \,=-\int_\Omega q/\sqrt{|q|}f\cdot\mathrm{curl}\,\overline{\psi}\,\mathrm{d}x\,, \tag{5.22}$$

respectively, for all $\psi\in H_\alpha(\mathrm{curl},\Omega)$ with compact support. By substituting $\psi=\nabla\varphi$ for scalar functions $\varphi\in C^\infty(\Omega)$ with compact support we obtain that $\int_\Omega v\cdot\nabla\overline{\varphi}\,\mathrm{d}x\,=0$ for all $\varphi\in C^\infty(\Omega)$ with compact support which means that $\mathrm{div}v=0$, and analogously, $\mathrm{div}\tilde{v}=0$ in Ω. The difference $w=v-\tilde{v}$ solves

$$\int_\Omega(\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}\,w\cdot\mathrm{curl}\,\overline{\psi}-k^2w\cdot\overline{\psi})\,\mathrm{d}x \,=(k^2+1)\int_\Omega\tilde{v}\cdot\overline{\psi}\,\mathrm{d}x\,,$$

for all $\psi\in H_\alpha(\mathrm{curl},\Omega)$ with compact support.

Let now the sequence f_j converge weakly to zero in $L^2(D)^3$ and denote by $v_j,\tilde{v}_j\in H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$ the corresponding radiating solutions of (5.21) and (5.22), respectively. Define $w_j\in H_{\alpha,\mathrm{loc}}(\mathrm{curl},\Omega)$ again by the difference $w_j=v_j-\tilde{v}_j$. Set $R>\mathrm{supp}\{|x_3|:(x_1,x_2,x_3)^\top\in D\}$, then $\overline{D}\subset\Omega_R$. By the boundedness of the solution operator we conclude that v_j and $\tilde{v}_j$ converge weakly to zero in $H_\alpha(\mathrm{curl},\Omega_R)$. Furthermore, v_j and $\tilde{v}_j$ are smooth outside of $\overline{D}$ and converges uniformly (with all of its derivatives) to zero on $\Gamma_{\pm h}$. In consequence, w_j converges to zero in $C(\partial\Omega_R)$. We determine $p_j\in H^1_{\alpha,\diamond}(\Omega_R)$ as the solution of

$$\int_{\Omega_R}\nabla p_j\cdot\nabla\varphi\,\mathrm{d}x \,=\int_{\partial\Omega_R}(\nu\cdot w_j)\overline{\varphi}\,\mathrm{d}s \tag{5.23}$$

for all $\varphi\in H^1_{\alpha,\diamond}(\Omega_R)$. Here the subspace $H^1_{\alpha,\diamond}(\Omega_R)$ of $H^1_\alpha(\Omega_R)$ is defined as $H^1_{\alpha,\diamond}(\Omega_R)=\{\varphi\in H^1_\alpha(\Omega_R):\int_{\Omega_R}\varphi\,\mathrm{d}s\,=0\}$. The solution of (5.23) exists and is unique since the form $(p,\varphi)\mapsto\int_{\Omega_R}\nabla p\cdot\nabla\varphi\,\mathrm{d}x$ is bounded and coercive on $H^1_{\alpha,\diamond}(\Omega_R)$ by the inequality of Poincaré (cf. [108]). The latter states that there exists a constant $c>0$ with

$$\int_{\Omega_R}|\nabla\varphi|^2\,\mathrm{d}x\,\ge c\|\varphi\|^2_{H^1_\alpha(\Omega_R)}\text{ for all }\varphi\in H^1_{\alpha,\diamond}(\Omega_R). \tag{5.24}$$

Problem (5.23) is the variational form of the Neumann boundary value problem

$$\Delta p_j = \mathrm{div} w_j = 0 \text{ in } \Omega_R, \quad \frac{\partial p_j}{\partial \nu_j} = \nu \cdot w_j \text{ on } \partial\Omega_R.$$

We observe that (5.23) holds even for all $\varphi \in H^1_\alpha(\Omega_R)$ since $\int_{\partial\Omega_R}(\nu \cdot w_j)\,\mathrm{d}s$ vanishes by the divergence theorem and the fact that $\mathrm{div} w_j = 0$. Substituting $\varphi = p_j$ into (5.23) yields, using (5.24) and the trace theorem,

$$c\|p_j\|^2_{H^1_\alpha(\Omega_R)} \le \int_{\Omega_R} |\nabla p_j|^2\,\mathrm{d}x = \int_{\partial\Omega_R} (\nu \cdot w_j)\overline{p_j}\,\mathrm{d}s \le \tilde{c}\|w_j\|_{C(\partial\Omega_R)}\|p_j\|_{H^1_\alpha(\Omega_R)},$$

i.e. $\|p_j\|_{H^1_\alpha(\Omega_R)} \le (\tilde{c}/c)\|w_j\|_{C(\partial\Omega_R)}$ which converges to zero. Therefore, the functions $\tilde{w}_j := w_j - \nabla p_j \in H_\alpha(\mathrm{curl}, \Omega_R)$ satisfy

- $\tilde{w}_j \in H_{\alpha,\mathrm{div}}(\mathrm{curl}, \Omega_R) := \{u \in H_\alpha(\mathrm{curl}, \Omega_R) : \int_{\Omega_R} \nabla\varphi \cdot u\,\mathrm{d}x = 0 \text{ for all } \varphi \in H^1_\alpha(\Omega_R)\}$
- $\tilde{w}_j \rightharpoonup 0$ weakly in $L^2(\Omega_R)^3$,
- $\mathrm{curl}\,\tilde{w}_j = \mathrm{curl}\, w_j \rightharpoonup 0$ weakly in $L^2(\Omega_R)^3$.

These three conditions assure that $\tilde{w}_j$ converges to zero in the norm of $L^2(\Omega_R)^3$ since the closed subspace $H_{\alpha,\mathrm{div}}(\mathrm{curl}, \Omega_R)$ of $H_\alpha(\mathrm{curl}, \Omega_R)$ is compactly imbedded in $L^2(\Omega)^3$. We refer to [110], see also [83], Theorem 4.7. Since also $\|\nabla p_j\|_{L^2(\Omega_R)^3} \to 0$ this yields $\|w_j\|_{L^2(\Omega_R)} \to 0$ as j tends to infinity. Now we return to the variational equation for w_j and substitute $\psi = \phi\overline{w_j}$ where $\phi \in C^\infty(\Omega)$ is some function with compact support such that $\phi = 1$ on Ω_R. This yields

$$\begin{aligned}\int_{\Omega_R} (\varepsilon_\mathrm{r}^{-1}|\,\mathrm{curl}\, w_j|^2 - k^2|w_j|^2)\,\mathrm{d}x &= \int_{\Omega\setminus\Omega_R} (\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}\, w_j \cdot \mathrm{curl}(\phi\overline{w_j}) - k^2\phi|w_j|^2)\,\mathrm{d}x \\ &\quad + (k^2+1)\int_\Omega \phi\tilde{v}_j \cdot \overline{w_j}\,\mathrm{d}x\,.\end{aligned}$$

We note that w_j is smooth in $\Omega \setminus \Omega_R$. Green's theorem in $\Omega_{mR} \setminus \Omega_R$ (for a sufficiently large value of m) and application of $\mathrm{curl}^2 w_j - k^2 w_j = (k^2+1)\tilde{v}_j$ in this region yields

$$\int_{\Omega_R} (\varepsilon_\mathrm{r}^{-1}|\,\mathrm{curl}\, w_j|^2 - k^2|w_j|^2)\,\mathrm{d}x = \int_{\partial\Omega_R} (\nu \times \mathrm{curl}\, w_j) \cdot \overline{w_j}\,\mathrm{d}s + (k^2+1)\int_{\Omega_R} \tilde{v}_j \cdot \overline{w_j}\,\mathrm{d}x$$

which tends to zero as j tends to infinity since $\tilde{v}_j$ and $\mathrm{curl}\, w_j$ are bounded sequences and $\|w_j\|_{L^2(\Omega_R)}$, $\|w_j\|_{C(\partial\Omega_R)}$ tend to zero. Therefore, also $\mathrm{curl}\, w_j$ tends to zeros in $L^2(\Omega_R)^3$ which complete the proof.

(c) If $\mathrm{Re}(q) > 0$, we return to (5.20) for $\tilde{v}$ instead of v. Since $\tilde{v}$ decays exponentially to zero as $|x_3|$ tends to infinity we conclude, by letting r tend to infinity,

$$\langle \mathrm{Re} T_0 f, f\rangle_{L^2(D)^3} = \mathrm{Re}\int_D \mathrm{sign}(q)|f + \sqrt{|q|}\,\mathrm{curl}\,\tilde{v}|^2\,\mathrm{d}x + \int_\Omega (|\,\mathrm{curl}\,\tilde{v}|^2 + |\tilde{v}|^2)\,\mathrm{d}x\,. \tag{5.25}$$

Now assume that there is no such a constant $\gamma > 0$ for the statement of (c), then we can find a sequence $\{f_j\}$ such that $\|f_j\|_{L^2(D)^3} = 1$ and $\langle \mathrm{Re} T_0 f_j, f_j\rangle_{L^2(D)^3} \to 0$. Due to (5.25), we have that $f_j + \sqrt{|q|}\,\mathrm{curl}\,\tilde{v}_j \to 0$ in $L^2(D)^3$ where $\tilde{v}_j$ denotes the solution of (5.19) for f and k replaced by f_j and i, respectively. Then we have

$$\int_\Omega (|\,\mathrm{curl}\,\tilde{v}_j|^2 + |\tilde{v}_j|^2)\,\mathrm{d}x = -\int_\Omega q/\sqrt{|q|}(f_j + \sqrt{|q|}\,\mathrm{curl}\,\tilde{v}_j)\cdot \mathrm{curl}\,\overline{\tilde{v}_j}\,\mathrm{d}x\,,$$

which let us obtain that $\|\tilde{v}_j\|_{H_\alpha(\mathrm{curl},\Omega)} \to 0$. Hence $f_j \to 0$ in $L^2(D)^3$ which is a contradiction to $\|f_j\|_{L^2(D)^3} = 1$. Therefore $\mathrm{Re}(T_0)$ is coercive. □

5.5 Characterization of the Biperiodic Support

In this section, we give a characterization when a point z belongs to the support of the contrast q by exploiting special test sequences. A simple criterion for imaging the periodic support is also proposed.

First recall from (4.9) that the α-quasiperiodic Green's function $G_k(x,y)$ of the Hemholtz operator in three dimensions is given

$$G_k(x,y) = \frac{\mathrm{i}}{8\pi^2}\sum_{j\in\mathbb{Z}} \frac{1}{\beta_j} e^{\mathrm{i}\alpha_j\cdot(x-y)+\mathrm{i}\beta_j|x_3-y_3|}, \quad x,y\in\Omega,\ x_3\neq y_3. \tag{5.26}$$

Further from (4.10) $G_k(x,y)$ can be decomposed as

$$G_k(x,y) = \frac{e^{\mathrm{i}k|x-y|}}{4\pi|x-y|} + \Psi_k(x-y), \tag{5.27}$$

where Ψ_k is the analytic solution to the Hemholtz equation in $(-2\pi,2\pi)^2\times\mathbb{R}$.

The α-quasiperiodic Green's tensor $\mathbb{G}_k(x,y)$ defined by

$$\mathbb{G}_k(x,y) = G_k(x,y)I_3 + k^{-2}\nabla_x \mathrm{div}_x(G_k(x,y)I_3), \quad x,y\in\Omega,\ x_3\neq y_3,$$

solves

$$\mathrm{curl}_x^2\,\mathbb{G}_k(x,y) - k^2\mathbb{G}_k(x,y) = \delta_y(x)I_3, \qquad x\in\Omega,$$

where I_3 is again the 3×3 identity matrix. Here, the curl of a matrix is taken columnwise, the div of a matrix and the ∇ are meant to be taken columnwise and componentwise, respectively. Note that $\mathbb{G}_k$ satisfies the Rayleigh expansion condition.

Lemma 5.5.1. *Let the operator W be defined as in* (5.16)*. For any $z\in\Omega$ and fixed nonzero $p=(p_1,p_2,p_3)\in\mathbb{C}^3$ we denote by $(\hat{\Psi}^{\pm}_{z,j})_{j\in\mathbb{Z}^2}\in\ell^2(\mathbb{Z}^2)^4$ the Rayleigh coefficients of the first two components of*

$$\begin{aligned}\Psi_z(x) &:= k^2\mathbb{G}_k(x,z)p\\ &= \begin{pmatrix} \left[k^2G_k(x,z) + \frac{\partial^2 G_k(x,z)}{\partial x_1^2}\right]p_1 + \frac{\partial^2 G_k(x,z)}{\partial x_1\partial x_2}p_2 + \frac{\partial^2 G_k(x,z)}{\partial x_1\partial x_3}p_3\\ \frac{\partial^2 G_k(x,z)}{\partial x_2\partial x_1}p_1 + \left[k^2G_k(x,z) + \frac{\partial^2 G_k(x,z)}{\partial x_2^2}\right]p_2 + \frac{\partial^2 G_k(x,z)}{\partial x_2\partial x_3}p_3\\ \frac{\partial^2 G_k(x,z)}{\partial x_3\partial x_1}p_1 + \frac{\partial^2 G_k(x,z)}{\partial x_3\partial x_2}p_2 + \left[k^2G_k(x,z) + \frac{\partial^2 G_k(x,z)}{\partial x_3^2}\right]p_3\end{pmatrix},\end{aligned} \tag{5.28}$$

for $x \in \Omega,\ x \neq z$. Then z belongs to D if and only if $W(\hat{\Psi}^{\pm}_{j,z}) \in \mathrm{Rg}(H^*)$.

Remark 5.5.2. *Note that the Rayleigh sequences $\hat{G}^{\pm}_{k,j}(z)$ of the α-quasiperiodic Green's function $G_k(\cdot, z)$ can be obtained from the representation of $G_k(\cdot, z)$ in* (5.26)

$$\hat{G}^{\pm}_{k,j}(z) = \frac{\mathrm{i}}{8\pi^2\beta_j} e^{-\mathrm{i}[\alpha_{1,j}z_1 + \alpha_{2,j}z_2 \pm \beta_j(z_3 \mp h)]}.$$

Then the Rayleigh sequences $(\hat{\Psi}^{\pm}_{z,j})_{j\in\mathbb{Z}^2} \in \ell^2(\mathbb{Z}^2)^4$ of the first two components of Ψ_z can be given as

$$\hat{\Psi}^{\pm}_{z,j} = \begin{pmatrix} (k^2 - \alpha_{1,j}^2)\hat{G}^{\pm}_{k,j}(z)p_1 - \alpha_{1,j}\alpha_{2,j}\hat{G}^{\pm}_{k,j}(z)p_2 \mp \alpha_{1,j}\beta_j\hat{G}^{\pm}_{k,j}(z)p_3 \\ -\alpha_{2,j}\alpha_{1,j}\hat{G}^{\pm}_{k,j}(z)p_1 + (k^2 - \alpha_{2,j}^2)\hat{G}^{\pm}_{k,j}(z)p_2 \mp \alpha_{2,j}\beta_j\hat{G}^{\pm}_{k,j}(z)p_3 \end{pmatrix}. \tag{5.29}$$

From (5.27) *and* (5.28) *we can see that the Green's tensor $\mathbb{G}_k$ has the same singularity to the function $\partial^2\Phi_k/\partial x_i\partial x_j$ where $\Phi_k(x,y) = \exp(\mathrm{i}k|x-y|)/(4\pi|x-y|)$ and $i,j = 1,2,3$. Further denote by δ_{ij} the Kronecker symbol ($\delta_{ij} = 1$ for $i = j, \delta_{ij} = 0$ for $i \neq j$), we have*

$$\begin{aligned}\frac{\partial^2\Phi_k(x,y)}{\partial x_i\partial x_j} = \Phi_k(x,y)\Bigg(&\frac{\mathrm{i}k\delta_{ij}}{|x-y|} + \frac{4\pi(\mathrm{i}k)^2(x_i-y_i)(x_j-y_j) - \delta_{ij}}{4\pi|x-y|^2} \\ &- \frac{8\pi\mathrm{i}k(x_i-y_i)^2 + \mathrm{i}k(x_i-y_i)(x_j-y_j)}{4\pi|x-y|^3} + \frac{3(x_i-y_i)^2}{4\pi|x-y|^4}\Bigg)\end{aligned}$$

which implies that the singularity of $\partial^2\Phi_k/\partial x_i\partial x_j$ is as strong as $1/|x-y|^3$.

Proof. First, let $z \in D$. Recall the operator Q defined in (5.17). Due to the fact that $H^* = -WQ$, it is sufficient to show that $(\hat{\Psi}_{z,j})_{j\in\mathbb{Z}^2} \in \mathrm{Rg}(Q)$. Choose $r > 0$ such that $B(z,r) \in D$ and consider a cut-off function $\varphi \in C^\infty(\mathbb{R}^3)$ with $\varphi(x) = 0$ for $|x-z| \leq r/2$ and $\varphi(x) = 1$ for $|x-z| \geq r$. We define

$$w(x) = \mathrm{curl}^2(\varphi(x)\mathbb{G}_k(x,z)p), \quad x \in \Omega.$$

Note that, for $|x-z| \geq r$, we have

$$w(x) = \mathrm{curl}^2(\varphi(x)\mathbb{G}_k(x,z)p) = k^2\mathbb{G}_k(x,z)p,$$

and further $(\hat{w}_j)_{j\in\mathbb{Z}^2} = (\hat{\Psi}_{z,j})_{j\in\mathbb{Z}^2}$. Using Green's theorem we obtain

$$\begin{aligned}\int_\Omega (\mathrm{curl}\, w \cdot \mathrm{curl}\,\overline{\psi} - k^2 w\cdot\overline{\psi})\,\mathrm{d}x &= \int_\Omega (\mathrm{curl}\, w - k^2\,\mathrm{curl}(\varphi(x)\mathbb{G}_k(x,z)p)) \cdot \mathrm{curl}\,\overline{\psi}\,\mathrm{d}x \\ &= \int_\Omega g \cdot \mathrm{curl}\,\overline{\psi}\,\mathrm{d}x\,,\end{aligned}$$

for all $\psi \in H_\alpha(\mathrm{curl}, \Omega)$ with compact support, and $g := \mathrm{curl}\, w - k^2 \,\mathrm{curl}(\varphi(x)\mathbb{G}_k(x,z)p)$. Since g is smooth and vanishes for $|z-x| \geq r$, thus $\mathrm{supp}(g) \subset D$. Set $f = \sqrt{|q|}^{-1} g \in L^2(D)^3$. Then we have

$$\int_\Omega (\mathrm{curl}\, w \cdot \mathrm{curl}\, \overline{\psi} - k^2 w \cdot \overline{\psi})\, \mathrm{d}x \;=\; \int_D \sqrt{|q|} f \cdot \mathrm{curl}\, \overline{\psi}\, \mathrm{d}x\,,$$

which implies that $(\hat{\Psi}_{z,j})_{j\in\mathbb{Z}^2} \in \mathrm{Rg}(Q)$.

Now let $z \notin D$, and on the contrary, assume that $\hat{\Psi}_{z,j} \in \mathrm{Rg}(Q)$. That means there exists $u \in H_{\alpha,\mathrm{loc}}(\mathrm{curl}, \Omega)$ and $f \in L^2(D)^3$ such that u is the variational radiating solution to $\mathrm{curl}^2 u - k^2 u = \mathrm{curl}(\sqrt{|q|} f)$ and $\hat{u}_j = \hat{\Psi}_{z,j}$ for all $j \in \mathbb{Z}^2$. Since the Rayleigh sequences of u and Ψ_z are equal, both functions coincide in $(-\pi,\pi)^2 \times \{|x_3| > h\}$ where $h > \mathrm{supp}\{|x_3| : (x_1,x_2,x_3)^\top \in D\}$. Due to the analyticity of u and Ψ_z in $\Omega \setminus D$ and $\Omega \setminus \{z\}$, respectively, and the analytic continuation we conclude that $u = \Psi_z$ in $\Omega \setminus (D \cup \{z\})$. This is a contradiction since $u \in H(\mathrm{curl}, B)$ for any ball B containing z but $\mathrm{curl}(k^2 \mathbb{G}_k(\cdot, z)p) \notin H(\mathrm{curl}, B)$ due to a strongly singularity at z. □

Theorem 5.5.3. *Suppose that the contrast q satisfies the Assumption 5.2.1 and that the direct scattering problem* (5.7) *is uniquely solvable. For $j \in \mathbb{Z}^2$, denote by $(\lambda_n, \psi_{n,j})_{n\in\mathbb{N}}$ the orthonormal eigensystem of $(WN)_\sharp = |\mathrm{Re}(WN)| + \mathrm{Im}(WN)$ and by $(\hat{\Psi}^\pm_{z,j})_{j\in\mathbb{Z}^2}$ the test sequence defined in* (5.29)*. A point z belongs to the support of q if and only if*

$$\sum_{n=1}^{\infty} \frac{|\langle \hat{\Psi}^\pm_{z,j}, \psi_{j,n}\rangle_{\ell^2(\mathbb{Z}^2)^4}|^2}{\lambda_n} < \infty. \tag{5.30}$$

Proof. As we assumed in the theorem, $(\lambda_n, \psi_{n,j})_{n\in\mathbb{N}}$ is an orthonormal eigensystem of $(WN)_\sharp$. The assumptions of Theorem 3.4.1 on H, H^* and T in the factorization $WN = H^*TH$ have been checked in Lemmas 5.3.1 and 5.4.1. Therefore, an application of Theorem 3.4.1 yields that $\mathrm{Rg}((WN)_\sharp^{1/2}) = \mathrm{Rg}(H^*)$. Combining this range identity with the characterization given in Lemma 5.5.1 we obtain that $(\hat{\Psi}^\pm_{z,j})_{j\in\mathbb{Z}^2} \in \mathrm{Rg}((WN)_\sharp^{1/2})$ if and only if $z \in D$. Then the criterion (5.30) follows from Picard's range criterion. □

5.6 Numerical Experiments

As mentioned in the introduction, these are to the best of our knowledge the first three-dimensional examples of the Factorization method in a biperiodic setting. These numerical examples focus on the dependence of the reconstructions on the number of the incident fields (or, equivalently, the evanescent modes), and the performance of the method when the data is perturbed by artificial noise. Further, we also indicate the number of the evanescent and propagating modes which are used for each reconstruction. These experiments use three biperiodic structures presented in one period $\Omega = (-\pi,\pi)^2 \times \mathbb{R}$ in terms of the support $\overline{D}$ of the contrast q as follows:

(i) Biperiodic structures of ellipsoids,

$$\overline{D} = \{(x_1, x_2, x_3)^\top \in \Omega : \frac{x_1^2}{2.5^2} + \frac{x_2^2}{2.5^2} + \frac{x_3^2}{0.4^2} \leq 1\},$$
$$q = 0.5 \quad \text{in } D.$$

(ii) Biperiodic structures of cubes,

$$\overline{D} = \{(x_1, x_2, x_3)^\top \in \Omega : |x_1| \leq 2.5, |x_2| \leq 2.5, |x_3| \leq 0.45\},$$
$$q = (x_3 + 1)(\sin(x_1)^2 \sin(x_2)^2 + 0.3)/4 - 0.4\mathrm{i} \quad \text{in } D.$$

(iii) Biperiodic structures of plus signs,

$$\overline{D} = \Omega \cap [(\{|x_1| \leq 1.75\} \cup \{|x_2| \leq 1.75\}) \cap \{|x_3| \leq 0.45\}],$$
$$q = \begin{cases} 0.5 - 0.6\mathrm{i} & \text{in } D_1 = \{(x_1, x_2)^\top \in D : -1 < x_1 < 1\}, \\ 0.3 & \text{in } D \setminus D_1. \end{cases}$$

The data of the direct scattering problem has been obtained by the volume integral equation method studied in Chapter 3 for the case of the Maxwell's equations. Of course it is not possible to numerically compute data for all incident fields $(\varphi_j^{(l)\pm})_{j\in\mathbb{Z}^2}$ in (5.9). Denote

$$\mathbb{Z}^2_{M_1,M_2} = \{j = (j_1, j_2) \in \mathbb{Z}^2 : -M_1 \leq j_1, j_2 \leq M_2\}, \quad \text{for } M_1, M_2 \in \mathbb{N}.$$

For the numerical experiments here we solve the direct problem for a number $j = (j_1, j_2)$ of incident fields $\varphi_j^{(l)\pm}$ where $j \in \mathbb{Z}^2_{M1,M2}$. Now recall that $\hat{u}^{\pm}_{(1,2),n}$ are the Rayleigh sequences defined in (5.8). For $l = 1, 2$, we denote by $(\hat{u}^{\pm}_{(1,2),n})_j^{(l)\pm}$ the Rayleigh sequences corresponding to the the incident fields $\varphi_j^{(l)\pm}$. Denote by $\mathcal{N}_{M_1,M_2}$ the block matrix corresponding to the discretization of the near field operator N. Then $\mathcal{N}_{M_1,M_2}$ is given by

$$\mathcal{N}_{M_1,M_2} = \begin{pmatrix} (\hat{u}^+_{1,n})_j^{(1)+} & (\hat{u}^+_{1,n})_j^{(1)-} & (\hat{u}^+_{1,n})_j^{(2)+} & (\hat{u}^+_{1,n})_j^{(2)-} \\ (\hat{u}^+_{2,n})_j^{(1)+} & (\hat{u}^+_{2,n})_j^{(1)-} & (\hat{u}^+_{2,n})_j^{(2)+} & (\hat{u}^+_{2,n})_j^{(2)-} \\ (\hat{u}^-_{1,n})_j^{(1)+} & (\hat{u}^-_{1,n})_j^{(1)-} & (\hat{u}^-_{1,n})_j^{(2)+} & (\hat{u}^-_{1,n})_j^{(2)-} \\ (\hat{u}^-_{2,n})_j^{(1)+} & (\hat{u}^-_{2,n})_j^{(1)-} & (\hat{u}^-_{2,n})_j^{(2)+} & (\hat{u}^-_{2,n})_j^{(2)-} \end{pmatrix}, \quad j, n \in \mathbb{Z}^2_{M_1,M_2}. \tag{5.31}$$

Note that each component of $\mathcal{N}_{M_1,M_2}$ is a matrix of size $(M_1 + M_2 + 1)^2$, thus $\mathcal{N}_{M_1,M_2}$ is a $4(M_1 + M_2 + 1)^2 \times 4(M_1 + M_2 + 1)^2$ matrix. The matrix $\mathcal{W}\mathcal{N}_{M_1,M_2}$ which corresponds to the discretization of WN can be computed using (5.14), the symetric matrix $\mathrm{Re}(\mathcal{W}\mathcal{N}_{M_1,M_2})$ can be decomposed as

$$\mathrm{Re}(\mathcal{W}\mathcal{N}_{M_1,M_2}) = VDV^{-1},$$

where D, V are the matrices of eigenvalues and corresponding eigenvectors of $\mathrm{Re}(\mathcal{W}\mathcal{N}_{M_1,M_2})$, respectively. Denote by $|D|$ the absolute value of D which is taken componentwise. Then we have

$$(\mathcal{W}\mathcal{N}_{M_1,M_2})_\sharp := V|D|V^{-1} + \mathrm{Im}(\mathcal{W}\mathcal{N}_{M_1,M_2}).$$

Computing singular value decomposition of $(\mathcal{WN}_{M_1,M_2})_\sharp$ implies that

$$(\mathcal{WN}_{M_1,M_2})_\sharp^{1/2} = U|S|^{1/2}V^{-1},$$

where S is the diagonal matrix of singular values λ_m of $(\mathcal{WN}_{M_1,M_2})_\sharp$. Also $U = [\psi_{n,m}]$ is a $4(M_1+M_2+1)^2 \times 4(M_1+M_2+1)^2$ matrix of "left" singular vectors . We now reshape $[\psi_{n,m}]$ into 4 arrays $[\psi^{(l)}_{j+M_1+1,m}]$, $l = 1,...,4$, $j \in \mathbb{Z}^2_{M_1,M_2}$, where each of them consists of $4(M_1+M_2+1)^2$ square matrices of size M_1+M_2+1. Note that the elements of $[\psi^{(l)}_{j+M_1+1,m}]$ are taken columnwise from $[\psi_{n,m}]$.

Now recall that we have $\hat{\Psi}^{\pm}_{z,j} = (\hat{\Psi}^{+}_{1,z,j}, \hat{\Psi}^{+}_{2,z,j}, \hat{\Psi}^{-}_{1,z,j}, \hat{\Psi}^{-}_{2,z,j})^\top$ which can be rewritten as $\hat{\Psi}_{z,j} = (\hat{\Psi}^{(1)}_{z,j}, \hat{\Psi}^{(2)}_{z,j}, \hat{\Psi}^{(3)}_{z,j}, \hat{\Psi}^{(4)}_{z,j})^\top$. Then the criterion (5.30) for computing the image can be approximated as follows

$$P(z) = \left[\sum_{n=1}^{4(M_1+M_2+1)^2} \frac{A_n(z)}{\lambda_n} \right]^{-1}, \tag{5.32}$$

where

$$A_n(z) = \left| \sum_{l=1}^{4} \sum_{j\in\mathbb{Z}^2_{M_1,M_2}} \hat{\Psi}^{(l)}_{z,j} \overline{\psi}^{(l)}_{j+M_1+1,n} \right|^2.$$

Note that P should be small outside of D and big inside of D.

To show the performance of the method with noisy data, we pertub our synthetic data by artificial noise. More particularly, we add the noise matrix $\mathcal{X}$ of uniformly distributed random entries to the data matrix $(\mathcal{WN}_{M_1,M_2})_\sharp^{1/2}$. Denote by δ the noise level, then the noise data matrix $(\mathcal{WN}_{M_1,M_2})_{\sharp,\delta}^{1/2}$ is given by

$$(\mathcal{WN}_{M_1,M_2})_{\sharp,\delta}^{1/2} := (\mathcal{WN}_{M_1,M_2})_\sharp^{1/2} + \delta \frac{\mathcal{X}}{\|\mathcal{X}\|_2} \|(\mathcal{WN}_{M_1,M_2})_\sharp^{1/2}\|_2,$$

where $\|\cdot\|_2$ is the matrix 2-norm. Note that from the latter equation we also have

$$\frac{\|(\mathcal{WN}_{M_1,M_2})_{\sharp,\delta}^{1/2} - (\mathcal{WN}_{M_1,M_2})_\sharp^{1/2}\|_2}{\|(\mathcal{WN}_{M_1,M_2})_\sharp^{1/2}\|_2} = \delta.$$

Since we apply Tikhonov regularisation [30], instead of implementing (5.32) we consider

$$P(z) = \left[\sum_{n=1}^{4(M_1+M_2+1)^2} \left(\frac{\lambda_n^{1/2}}{\lambda_n + \gamma} \right)^2 A_n(z) \right]^{-1}, \tag{5.33}$$

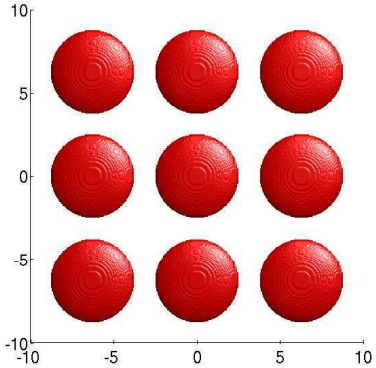
where

$$A_n(z) = \left| \sum_{l=1}^{4} \sum_{j\in\mathbb{Z}^2_{M_1,M_2}} \hat{\Psi}^{(l)}_{z,j} \overline{\psi}^{(l)}_{j+M_1+1,n} \right|^2.$$

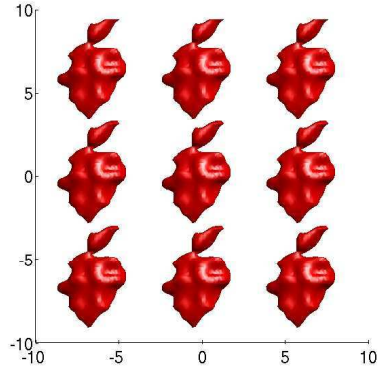
Here λ_n, $\psi_{j,n}$ are the singular values and vectors of $(\mathcal{WN}_{M_1,M_2})_{\sharp,\delta}$, respectively. The parameter γ is chosen by Morozov's generalized discrepancy principle which can be obtained by solving the equation

$$\sum_{n=1}^{4(M_1+M_2+1)^2} \frac{\gamma^2 - \delta^2\lambda_n}{(\lambda_n+\gamma)^2} A_n(z) = 0.$$

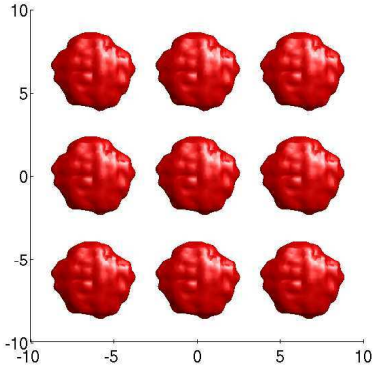
for each sampling point z. For the following experiments, we choose the wave number $k = 2\pi/3$. The number of the incident fields used is $4(M_1+M_2+1)^2$. Further, the reconstructions have been smoothened using the command smooth3 in Matlab, and we plot the pictures in 3×3 periods.



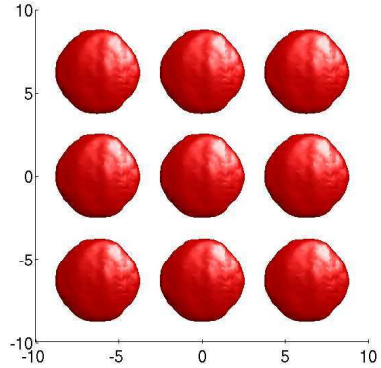
(a) Exact geometry (view down x_3 axis)



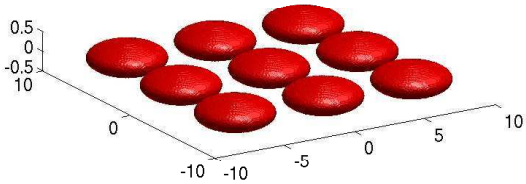
(b) $M_{1,2} = 2$ (view down x_3 axis)



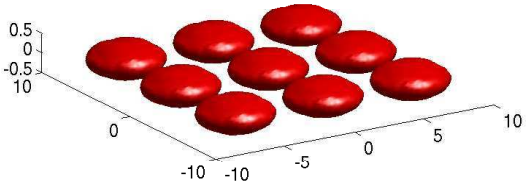
(c) $M_{1,2} = 4$ (view down x_3 axis)



(d) $M_{1,2} = 8$ (view down x_3 axis)

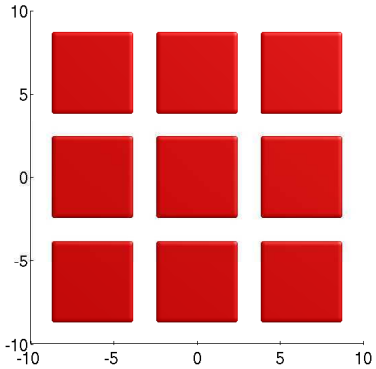


(e) Exact geometry (3D view)

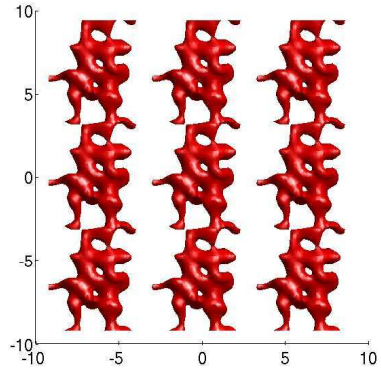


(f) $M_{1,2} = 8$ (3D view)

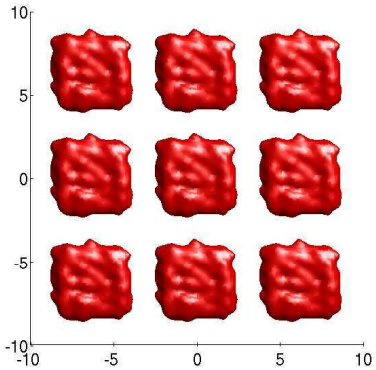
Figure 5.2: Reconstructions of biperiodic shapes of ellipsoids for different number of incident fields without noise. The number of Rayleigh coefficients measured in each reconstruction is $4(M_1+M_2+1)^2$. The contrast $q = 0.5$ in D. (b) 48 propagating modes, 52 evanescent modes, isovalue 7 (c) 52 propagating modes, 312 evanescent modes, isovalue 0.1 (d) 52 propagating modes, 1104 evanescent modes, isovalue 0.01.



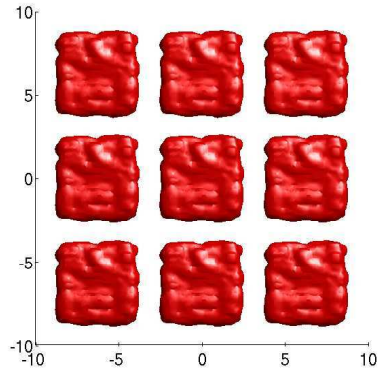
(a) Exact geometry (view down x_3 axis)



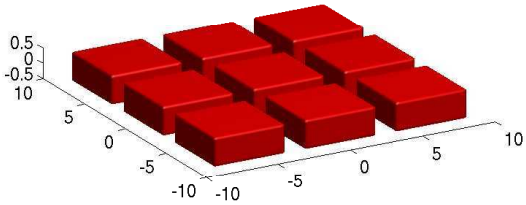
(b) $M_{1,2} = 2$ (view down x_3 axis)



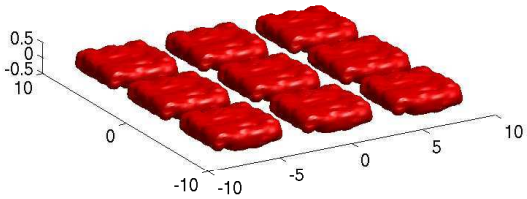
(c) $M_{1,2} = 4$ (view down x_3 axis)



(d) $M_{1,2} = 8$ (view down x_3 axis)

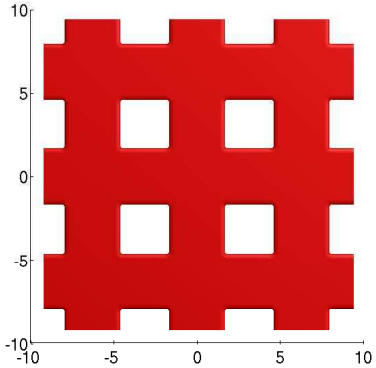


(e) Exact geometry (3D view)

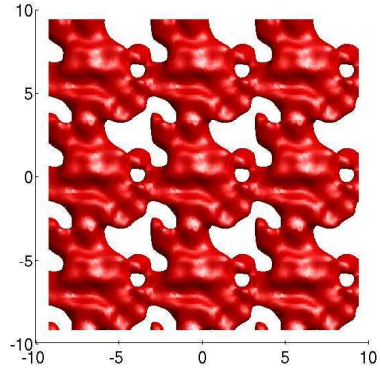


(f) $M_{1,2} = 8$ (3D view)

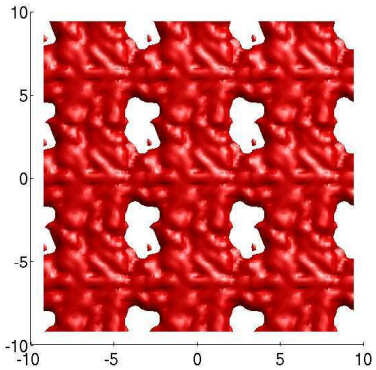
Figure 5.3: Reconstructions of biperiodic shapes of cubes for different number of incident fields without noise. The number of Rayleigh coefficients measured in each reconstruction is $4(M_1 + M_2 + 1)^2$. The contrast $q = (x_3 + 1)(\sin(x_1)^2 \sin(x_2)^2 + 0.3)/4 - 0.4\mathrm{i}$ in D. (b) 48 propagating modes, 52 evanescent modes, isovalue 40 (c) 52 propagating modes, 312 evanescent modes, isovalue 1.8 (d) 52 propagating modes, 1104 evanescent modes, isovalue 0.008.



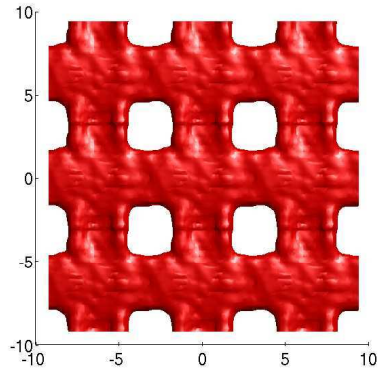
(a) Exact geometry (view down x_3 axis)



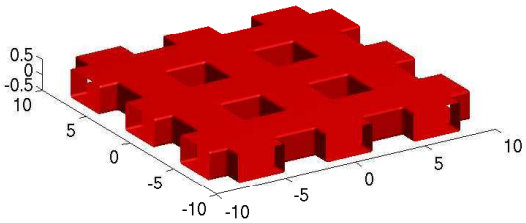
(b) $M_{1,2} = 2$ (view down x_3 axis)



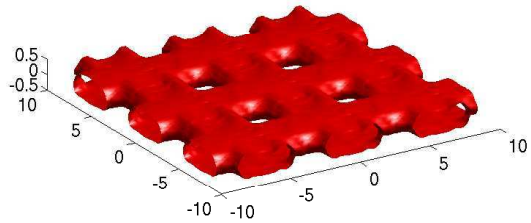
(c) $M_{1,2} = 4$ (view down x_3 axis)



(d) $M_{1,2} = 8$ (view down x_3 axis)

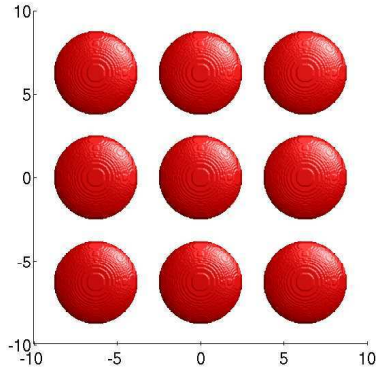


(e) Exact geometry (3D view)

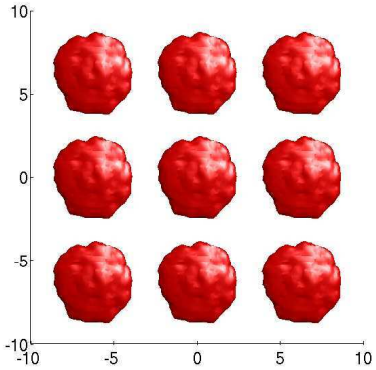


(f) $M_{1,2} = 8$ (3D view)

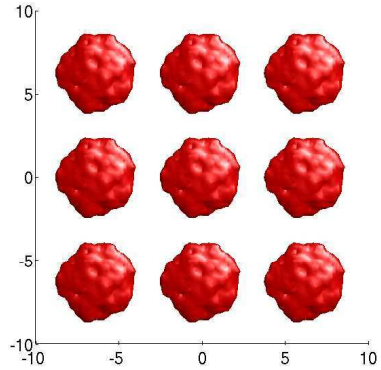
Figure 5.4: Reconstructions of biperiodic shapes of plus signs for different number of incident fields without noise. The number of Rayleigh coefficients measured in each reconstruction is $4(M_1 + M_2 + 1)^2$. The contrast $q = 0.5 - 0.6\mathrm{i}$ in $D_1 = \{(x_1, x_2)^\top \in D : -1 < x_1 < 1\}$ and $q = 0.3$ in $D \setminus D_1$. (b) 48 propagating modes, 52 evanescent modes, isovalue 15 (c) 52 propagating modes, 312 evanescent modes, isovalue 2 (d) 52 propagating modes, 1104 evanescent modes, isovalue 0.05.



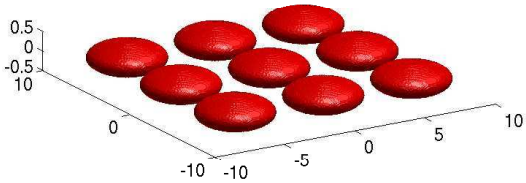
(a) Exact geometry (view down x_3 axis)



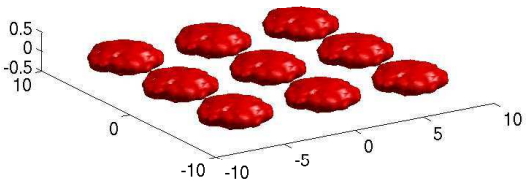
(b) 2% artificial noise, $M_{1,2} = 8$ (view down x_3 axis)



(c) 5% artificial noise, $M_{1,2} = 8$ (view down x_3 axis)

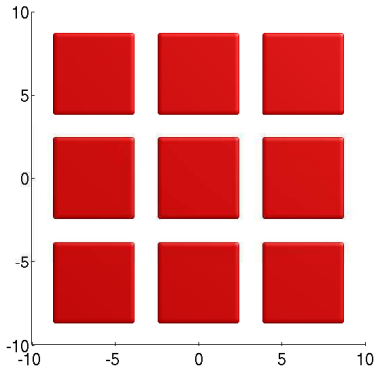


(d) Exact geometry (3D view)

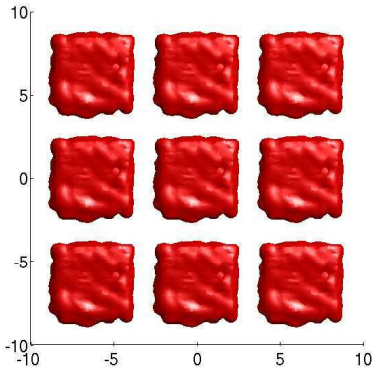


(e) 5% artificial noise, $M_{1,2} = 8$ (3D view)

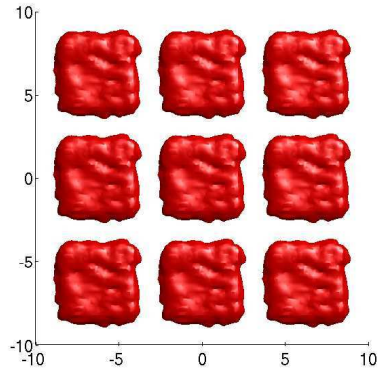
Figure 5.5: Reconstructions of biperiodic shapes of ellipsoids for artificial noise. The number of Rayleigh coefficients measured in each reconstruction is $4(M_1 + M_2 + 1)^2$. The contrast $q = 0.5$ in D. (b) 52 propagating modes, 1104 evanescent modes, isovalue 0.0012 (c) 52 propagating modes, 1104 evanescent modes, isovalue 0.0023.



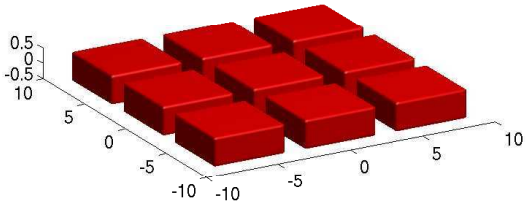
(a) Exact geometry (view down x_3 axis)



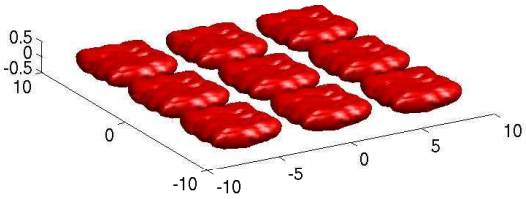
(b) 2% artificial noise, $M_{1,2} = 8$ (view down x_3 axis)



(c) 5% artificial noise, $M_{1,2} = 8$ (view down x_3 axis)

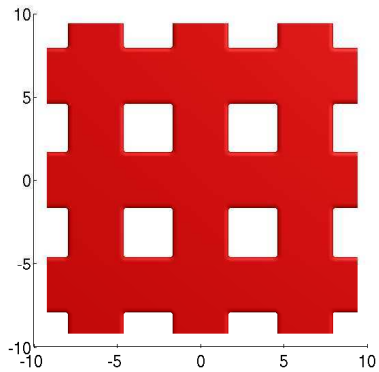


(d) Exact geometry (3D view)

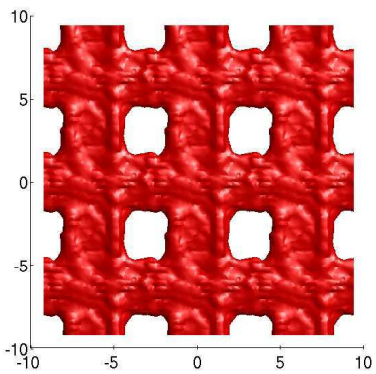


(e) 5% artificial noise, $M_{1,2} = 8$ (3D view)

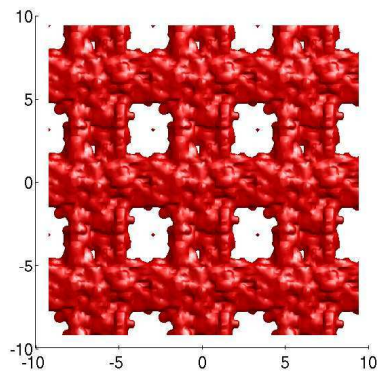
Figure 5.6: Reconstructions of biperiodic shapes of cubes for artificial noise. The number of Rayleigh coefficients measured in each reconstruction is $4(M_1 + M_2 + 1)^2$. The contrast $q = (x_3+1)(\sin(x_1)^2 \sin(x_2)^2 + 0.3)/4 - 0.4\mathrm{i}$ in D. (b) 52 propagating modes, 1104 evanescent modes, isovalue 0.1 (c) 52 propagating modes, 1104 evanescent modes, isovalue 0.02.



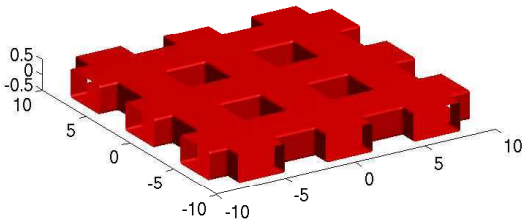
(a) Exact geometry (view down x_3 axis)



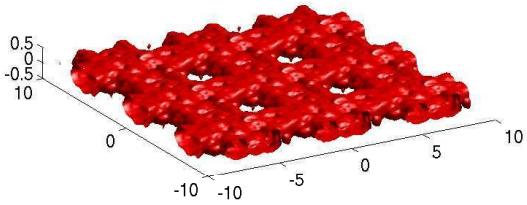
(b) 2% artificial noise, $M_{1,2} = 8$ (view down x_3 axis)



(c) 5% artificial noise, $M_{1,2} = 8$ (view down x_3 axis)



(d) Exact geometry (3D view)



(e) 5% artificial noise, $M_{1,2} = 8$ (3D view)

Figure 5.7: Reconstructions of biperiodic shapes of plus signs for artificial noise. The number of Rayleigh coefficients measured in each reconstruction is $4(M_1 + M_2 + 1)^2$. The contrast $q = 0.5 - 0.6\mathrm{i}$ in $D_1 = \{(x_1, x_2)^\top \in D : -1 < x_1 < 1\}$ and $q = 0.3$ in $D \setminus D_1$. (b) 52 propagating modes, 1104 evanescent modes, isovalue 0.1 (c) 52 propagating modes, 1104 evanescent modes, isovalue 0.02.

Chapter 6

Uniqueness for All Wave Numbers in Biperiodic Scattering Problems

Abstract: In this chapter, we present results on existence and uniqueness of solution for all positive wave numbers for an electromagnetic scattering problem from a biperiodic dielectric structure mounted on a perfectly conducting plate. Given that uniqueness of solution holds, existence of solution follows from a Fredholm framework for the variational formulation of the problem in a suitable Sobolev space (see Section 6.3). In Section 6.4 we obtain integral identities which are necessary for establishing a Rellich identity for a solution to the variational problem (see Lemma 6.5.1). This identity is obtained under suitable smoothness conditions on the material parameter. Under additional non-trapping assumptions on the material parameter (see (6.32)), the Rellich identity allows us to obtain a solution estimate in Lemma 6.5.4. This solution estimate is the key point to derive uniqueness of solution for all positive wave numbers, that is, to be able to exclude the existence of surface waves (see Section 6.6).

6.1 Introduction

As mentioned in the state of the art of the introduction that uniqueness of solution for this scattering problem does not hold in general for all wave numbers. Instead, non-trivial solutions to the homogeneous problem might exist for a discrete set of exceptional wave numbers, and these solutions turn out to be exponentially localized surface waves. Further the introduction also pointed out that uniqueness results for all wave numbers for the case of Maxwell's equations still remains as an open problem if the biperiodic materials is non-absorbing. In this chapter we aim to study this open problem for the model of electromagnetic scattering from a dielectric biperiodic structure mounted on a perfectly conducting plate in three dimensions. More precisely we prove that the electromagnetic scattering problem for non-absorbing biperiodic dielectric structures mounted on a perfectly conducting plate is

uniquely solvable for all positive wave numbers if the material parameter satisfies non-trapping and smoothness conditions. This also means that materials satisfying the latter conditions cannot guide surface waves.

We formulate the Maxwell's equations variationally in terms of the magnetic field in a suitable Sobolev space. We further restrict ourselves to the case of non-magnetic and isotropic materials. The variational problem is well-known to fit into a Fredholm framework, see, e.g., [12, 41, 105]. (These works deal with periodic scattering in the full space, but can be adapted to the half-space setting that we consider here.) To prove the uniqueness result we derive a so-called Rellich identity for a solution to the homogeneous variational problem. The solution estimates resulting from this integral identity allow us to show that the homogeneous variational problem has only the trivial solution for *all* positive wave numbers.

Our analysis extends the approach in [50] that was motivated by an existence and uniqueness proof for solutions to rough surface scattering problems via Rellich identities in [28]. For scalar periodic problems, a related technique has been used in [22]. The paper [50] studied electromagnetic scattering from rough, unbounded penetrable layers. Such scattering problems are considered to be more complicated than those for periodic structures since the problem to find the scattered field cannot reduced, e.g., to a bounded domain. The applications of rough scattering problems include for instance outdoor noise propagation, oceanography or even optical technologies when the dielectric lacks periodicity. The authors in [50] formulated the latter scattering problem in terms of the electric field. We will instead choose a formulation in terms of the magnetic field, which somewhat changes the role of the dielectric material parameter in the integral identities since the material is non-magnetic. The paper [50] establishes existence and uniqueness of solution under non-trapping and smoothness conditions on the material parameter. While a priori estimates resulting from the Rellich identity allowed the authors in [50] to deduce uniqueness of solution, existence of solution has been obtained using a limiting absorption argument. The approach studied in the present chapter is, from the technical point of view, somewhat similar to the one introduced in [50]. However, the analysis of the biperiodic case is definitely simpler since uniqueness of solution directly implies existence. Therefore, one only needs to investigate the Rellich identity and estimates for solutions to the homogeneous problem. It turns out also that this procedure produces weaker assumptions on the material parameter than those found in [50]. More precisely, uniqueness and existence of solution for all wave numbers are obtained under the following (non-trapping and smoothness) assumptions on the biperiodic relative material parameter $\varepsilon_{\mathrm{r}} : \mathbb{R}^3_+ := \{x \in \mathbb{R}^3,\, x_3 > 0\} \to \mathbb{R}$. First, we assume that $\varepsilon_{\mathrm{r}}^{-1} \in L^\infty(\mathbb{R}^3_+)$ equals one in $\{x_3 > h\}$ for some $h > 0$ and possesses essentially bounded and measurable first weak derivatives. Second, we require that

(a) $\dfrac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \leq 0$ in $\mathbb{R}^3_+$,

(b) It holds that $\dfrac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} < 0$ in some non-empty open subset of $\mathbb{R}^3_+$,

(c) There exists $\delta > 1/2$ such that $\dfrac{\delta}{2}\|\nabla_T \varepsilon_{\mathrm{r}}^{-1}\|^2_{L^\infty(\mathbb{R}^3_+)^3} + \dfrac{\sqrt{2}}{h}\left\|\dfrac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3}\right\|_{L^\infty(\mathbb{R}^3_+)} < \dfrac{2}{h^2}$,

where $\nabla_T \varepsilon_{\mathrm{r}}^{-1} := (\partial\varepsilon_{\mathrm{r}}^{-1}/\partial x_1, \partial\varepsilon_{\mathrm{r}}^{-1}/\partial x_2, 0)^\top$. Under these conditions, the existence of surface waves is automatically ruled out. While conditions (a) and (c) are similar to conditions (a) and (d) in [50, Eq. (7.2)], condition (b) is weaker and clearly simpler than the corresponding conditions (b) and (c) in [50, Eq. (7.2)].

The half-space setting that we consider in this chapter is somewhat special, and it seems worth to mention that the Rellich identity itself generalizes to a corresponding periodic scattering problem in full space. The resulting estimate for a solution H to the scattering problem has a similar structure to the estimate in Lemma 6.5.4. However, in the half-space setting, the term $2\mathrm{Re}\int_\Omega (\partial\varepsilon_{\mathrm{r}}^{-1}/\partial x_3)\,(\partial H_3/\partial x_3)\overline{H_3}\,\mathrm{d}x$ can be treated without integration by parts using a Poincaré lemma. In contrast, in the full-space setting the only obvious way of treating this term is to integrate by parts. Since we seek for solution estimates, this introduces the condition that $x_3 \mapsto \varepsilon_{\mathrm{r}}^{-1}(x_1, x_2, x_3)$ needs to be concave to conclude. Since this is a somewhat unnatural condition, we do not present this result in more detail.

One can further generalize the results presented here to certain anisotropic structures. However, already for the simpler case of isotropic coefficients the derivation of the Rellich identity is a technical matter. Again, we have opted to try to keep the presentation simple instead of treating the most general setting that could be considered.

The chapter is organized as follows: In Section 6.2 we present setting of the problem. Section 6.3 is dedicated to a variational formulation and to the Fredholm property of the latter. Section 6.4 contains a couple of technical lemmas. We derive the integral inequalities resulting from the Rellich identity in Section 6.5. Finally, the uniqueness of the variational problem for all wave numbers is proven in Section 6.6.

6.2 Problem Setting

We consider scattering of time-harmonic electromagnetic waves from a biperiodic structure which models a dielectric layer mounted on a perfectly conducting plate. The electric field E and the magnetic field H are governed by the time-harmonic Maxwell's equations at frequency $\omega > 0$ in $\mathbb{R}^3_+ = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 > 0\}$,

$$\operatorname{curl} H + i\omega\varepsilon E = 0 \quad \text{in } \mathbb{R}^3_+, \tag{6.1}$$

$$\operatorname{curl} E - i\omega\mu H = 0 \quad \text{in } \mathbb{R}^3_+, \tag{6.2}$$

$$e_3 \times E = 0 \quad \text{on } \{x_3 = 0\}, \tag{6.3}$$

where $e_3 = (0, 0, 1)^\top$. The electric permittivity ε is a real-valued bounded measurable function that is 2π-periodic in x_1 and x_2. Further, we assume that ε equals $\varepsilon_0 > 0$ outside the biperiodic structure, that is, for $x_3 \geq h$ where $h > 0$ is chosen larger than $\sup\{x_3 : (x_1, x_2, x_3)^\top \in \operatorname{supp}(\varepsilon - \varepsilon_0)\}$. The magnetic permeability $\mu = \mu_0$ is assumed to be a positive constant and the conductivity is assumed to vanish. As usual, the problem (6.1)–(6.3) has to be completed by a radiation condition that we set up using Fourier series.

The biperiodic structure is illuminated by an electromagnetic plane wave with wave vector $d = (d_1, d_2, d_3) \in \mathbb{R}^3$, $d_3 < 0$, such that $d \cdot d = \omega^2\varepsilon_0\mu_0$. The polarizations $p, q \in \mathbb{R}^3$ of the

incident wave satisfy $p \cdot d = 0$ and $q = 1/(\omega\varepsilon_0)(p \times d)$. With these definitions, the incident plane waves E^i and H^i are given by

$$E^i := qe^{id\cdot x}, \quad H^i := pe^{id\cdot x}, \quad x \in \mathbb{R}^3_+.$$

In the following we will exploit that one can explicitly compute the corresponding reflected field at $\{x_3 = 0\}$. To this end, we introduce the notation $\tilde{a} = (a_1, a_2, -a_3)^\top$ for $a = (a_1, a_2, a_3)^\top \in \mathbb{R}^3$. The reflected waves at the plane $\{x_3 = 0\}$ are

$$E^r(x) := -\tilde{q}e^{\mathrm{i}\tilde{d}\cdot x}, \quad H^r(x) := \tilde{p}e^{\mathrm{i}\tilde{d}\cdot x}, \quad x \in \mathbb{R}^3_+,$$

since $\mathrm{div} E^r = 0$, $\mathrm{div} H^r = 0$, and $e_3 \times (E^i + E^r) = 0$, $e_3 \cdot (H^i + H^r) = 0$ on $\{x_3 = 0\}$. From now on, we denote the sum of the incident and reflected plane waves by

$$E^{ir} := E^i + E^r \quad \text{and} \quad H^{ir} := H^i + H^r.$$

To support technical computations that this chapter will deal with we need some change of variables as follows: Set

$$\alpha = (\alpha_1, \alpha_2, \alpha_3)^\top := (d_1, d_2, 0)^\top$$

and define E^{ir}_α and H^{ir}_α by

$$E^{ir}_\alpha := e^{-\mathrm{i}\alpha\cdot x}E^{ir}(x), \quad H^{ir}_\alpha := e^{-\mathrm{i}\alpha\cdot x}H^{ir}(x), \quad x \in \mathbb{R}^3_+,$$

such that E^{ir}_α and H^{ir}_α are 2π-periodic in x_1 and x_2. If we apply the same phase shift to solutions E and H of the Maxwell's equations (6.1)–(6.3),

$$E_\alpha = e^{-\mathrm{i}\alpha\cdot x}E(x), \quad H_\alpha = e^{-\mathrm{i}\alpha\cdot x}H(x),$$

and if we denote

$$\nabla_\alpha f = \nabla f + \mathrm{i}\alpha f, \quad \mathrm{curl}_\alpha F = \mathrm{curl}\, F + \mathrm{i}\alpha \times F, \quad \mathrm{div}_\alpha F = \mathrm{div} F + \mathrm{i}\alpha \cdot F$$

for scalar functions f and vector fields F, then E_α and H_α satisfy

$$\mathrm{curl}_\alpha H_\alpha + i\omega\varepsilon E_\alpha = 0 \quad \text{in } \mathbb{R}^3_+, \tag{6.4}$$

$$\mathrm{curl}_\alpha E_\alpha - i\omega\mu_0 H_\alpha = 0 \quad \text{in } \mathbb{R}^3_+, \tag{6.5}$$

$$e_3 \times E_\alpha = 0 \quad \text{on } \{x_3 = 0\}. \tag{6.6}$$

Note that we still have $\mathrm{div}_\alpha \mathrm{curl}_\alpha = 0$ and $\mathrm{curl}_\alpha \nabla_\alpha = 0$. Let us denote the relative material parameter by

$$\varepsilon_\mathrm{r} := \frac{\varepsilon}{\varepsilon_0}.$$

Obviously, ε_r equals one outside the biperiodic dielectric structure. Recall that the magnetic permeability μ_0 is constant which motivates us to work with the divergence-free magnetic field, that is, $\mathrm{div}_\alpha H_\alpha = 0$.

Note that (6.4) plugged in into (6.6) implies that $e_3 \times (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H_\alpha) = 0$ on $\{x_3 = 0\}$ and that the condition $e_3 \cdot H_\alpha = 0$ on $\{x_3 = 0\}$ can be derived by plugging (6.6) into (6.5). Hence, introducing the wave number $k = \omega(\varepsilon_0\mu_0)^{1/2}$, and eliminating the electric field E_α from (6.4)–(6.6), we find that

$$\operatorname{curl}_\alpha \left(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H_\alpha\right) - k^2 H_\alpha = 0 \quad \text{in } \mathbb{R}^3_+, \tag{6.7}$$

$$e_3 \times (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H_\alpha) = 0 \quad \text{on } \{x_3 = 0\}, \tag{6.8}$$

$$e_3 \cdot H_\alpha = 0 \quad \text{on } \{x_3 = 0\}. \tag{6.9}$$

We wish to reformulate the last three equations in terms of the scattered field H_α^s, defined by $H_\alpha^s := H_\alpha - H_\alpha^{ir}$. Since, by construction, $\operatorname{curl}_\alpha \operatorname{curl}_\alpha H_\alpha^{ir} - k^2 H_\alpha^{ir} = 0$ in $\mathbb{R}^3_+$, $H_\alpha^{ir} \cdot e_3 = 0$ and $e_3 \times (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H_\alpha^{ir}) = 0$ on $\{x_3 = 0\}$, a simple computation shows that

$$\begin{aligned} \operatorname{curl}_\alpha \left(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H_\alpha^s\right) - k^2 H_\alpha^s &= -\operatorname{curl}_\alpha \left((\varepsilon_{\mathrm{r}}^{-1} - 1) \operatorname{curl}_\alpha H_\alpha^{ir}\right) \quad \text{in } \mathbb{R}^3_+, \\ e_3 \times (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H_\alpha^s) &= 0 \quad \text{on } \{x_3 = 0\}, \\ e_3 \cdot H_\alpha^s &= 0 \quad \text{on } \{x_3 = 0\}. \end{aligned} \tag{6.10}$$

Due to the biperiodicity of the right-hand side and of ε_{r}, we seek for a biperiodic solution H_α^s, and reduce the problem to the domain $(0, 2\pi)^2 \times (0, \infty)$. We complement this boundary value problem by a radiation condition that we set up using Fourier series. The scattered field H_α^s is 2π-periodic in x_1 and x_2 and can hence be expanded as

$$H_\alpha^s(x) = \sum_{n \in \Lambda} \hat{H}_n(x_3) e^{\mathrm{i} n \cdot x}, \quad x = (x_1, x_2, x_3)^\top \in \mathbb{R}^3_+, \ \Lambda = \mathbb{Z}^2 \times \{0\},$$

where the Fourier coefficients $\hat{H}_n(x_3)$ are defined by

$$\hat{H}_n(x_3) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} H_\alpha^s(x_1, x_2, x_3) e^{-\mathrm{i} n \cdot x} \, \mathrm{d}x_1 \, \mathrm{d}x_2 \,, \quad n \in \Lambda.$$

Define

$$\beta_n := \begin{cases} \sqrt{k^2 - |n + \alpha|^2}, & k^2 \geq |n + \alpha|^2, \\ \mathrm{i}\sqrt{|n + \alpha|^2 - k^2}, & k^2 < |n + \alpha|^2, \end{cases} \quad n \in \Lambda.$$

Since $\varepsilon_{\mathrm{r}}^{-1}$ equals one for $x_3 > h$ it holds that $\operatorname{div}_\alpha H_\alpha^s$ vanishes for $x_3 > h$, and equation (6.10) becomes $(\Delta_\alpha + k^2) H_\alpha^s = 0$ in $\{x_3 > h\}$, where $\Delta_\alpha = \Delta + 2\mathrm{i}\alpha \cdot \nabla - |\alpha|^2$. Using separation of variables, and choosing the upward propagating solution, we set up a radiation condition in form of a Rayleigh expansion condition, prescribing that H_α^s can be written as

$$H_\alpha^s(x) = \sum_{n \in \Lambda} \hat{H}_n e^{\mathrm{i}\beta_n (x_3 - h) + \mathrm{i} n \cdot x} \quad \text{for } \{x_3 > h\}, \quad \text{where } \hat{H}_n := \hat{H}_n(h), \tag{6.11}$$

and that the series converges uniformly in compact subsets of $\{x_3 > h\}$.

The scattering problem to find a scattered field H_α^s that satisfies the boundary value problem (6.10) and the expansion (6.11) is in the following section reformulated variationally in a suitable Sobolev space.

6.3 Variational Formulation

We solve the scattering problem presented in the last section variationally, and briefly recall in this section a variational formulation of the problem in a suitable Sobolev space. Our framework is an adaption of the results from [105] to our half-space setting. In contrast to the variational formulation in $H(\mathrm{curl})$ in [1], the papers [12, 15, 41, 105] set up a variational formulation in H^1 for the magnetic field. Indeed, since the latter is divergence-free, any solution that is locally $H(\mathrm{curl})$ indeed belongs locally to H^1. For our purposes, the H^1 formulation has the additional advantage that it is well-defined at Rayleigh-Wood frequencies, as it was noted in [105]. We define a bounded domain

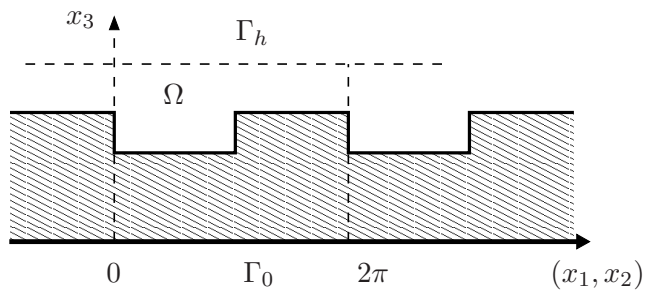


Figure 6.1: Geometric setting for electromagnetic scattering problem from a biperiodic dielectric structure mounted on a perfectly conducting plate (in two dimensions, for simplicity).

$$\Omega = (0, 2\pi)^2 \times (0, h) \qquad \text{for } h > \sup\{x_3 : (x_1, x_2, x_3)^\top \in \operatorname{supp}(\varepsilon_\mathrm{r} - 1)\},$$

with boundaries $\Gamma_0 := (0, 2\pi)^2 \times \{0\}$ and $\Gamma_h := (0, 2\pi)^2 \times \{h\}$, and Sobolev spaces

$$\begin{aligned} H^\ell_\mathrm{p}(\Omega)^3 &:= \{F \in H^\ell(\Omega)^3 : F = \tilde{F}|_\Omega \text{ for some } 2\pi\text{-biperiodic } \tilde{F} \in H^\ell_\mathrm{loc}(\mathbb{R}^3)^3\}, \quad \ell \in \mathbb{N}, \\ H^1_\mathrm{p,T}(\Omega)^3 &:= \{F = (F_1, F_2, F_3)^\top \in H^1_\mathrm{p}(\Omega)^3 : F_3 = 0 \text{ on } \Gamma_0\}, \end{aligned}$$

equipped with the usual integral norm, e.g.,

$$\|F\|^2_{H^1_\mathrm{p}(\Omega)^3} = \|F\|^2_{L^2(\Omega)^3} + \|\nabla_\alpha F\|^2_{L^2(\Omega)^3}.$$

The space $H^1_\mathrm{p,T}(\Omega)^3$ of periodic vector fields that are tangential on Γ_0 is well-defined due to the standard trace theorem in H^1. We also define periodic Sobolev spaces of functions with $d = 1, 2, 3$ components on Γ_h: for $s \in \mathbb{R}$,

$$H^s_\mathrm{p}(\Gamma_h)^d := \{F \in H^s(\Gamma_h)^d : F = \tilde{F}|_{\Gamma_h} \text{ for some } 2\pi\text{-biperiodic } \tilde{F} \in H^s_\mathrm{loc}(\{x_3 = h\})^d\}.$$

A periodic vector field $F \in H^s(\Gamma_h)^d$ can be developed in a Fourier series, $F(x) = \sum_{n\in\Lambda} \hat{F}_n \exp(\mathrm{i}n\cdot x)$, and $\|F\|_{H^s_\mathrm{p}(\Gamma_h)^d} = (\sum_{n\in\Lambda}(1+n^2)^s|\hat{F}_n|^2)^{1/2}$ defines a norm on $H^s_\mathrm{p}(\Gamma_h)^d$.

We define a non-local boundary operator T_α (the exterior Dirichlet-Neumann operator) by

$$(T_\alpha f)(x) = \sum_{n\in\Lambda} \mathrm{i}\beta_n \hat{f}_n e^{\mathrm{i}n\cdot x}, \quad \text{for } f = \sum_{n\in\Lambda} \hat{f}_n \exp(\mathrm{i}n\cdot x) \in H^{1/2}_{\mathrm{p}}(\Gamma_h).$$

It is a classical result that T_α is bounded from $H^{1/2}_{\mathrm{p}}(\Gamma_h)$ into $H^{-1/2}_{\mathrm{p}}(\Gamma_h)$, see, e.g., [4]. Using T_α, we define a vector of (pseudo-)differential operators $R_\alpha := (\partial^\alpha/\partial x_1, \partial^\alpha/\partial x_2, T_\alpha)$. For a vector field $F \in H^{1/2}_{\mathrm{p}}(\Gamma_h)^3$,

$$R_\alpha \times F = (\partial^\alpha/\partial x_1, \partial^\alpha/\partial x_2, T_\alpha) \times F, \quad R_\alpha \cdot F = (\partial^\alpha/\partial x_1, \partial^\alpha/\partial x_2, T_\alpha) \cdot F.$$

Since all components of R_α are bounded operators from $H^{1/2}_{\mathrm{p}}(\Gamma_h)$ into $H^{-1/2}_{\mathrm{p}}(\Gamma_h)$, the operator $F \mapsto R_\alpha \times F$ is bounded from $H^{1/2}_{\mathrm{p}}(\Gamma_h)^3$ into $H^{-1/2}_{\mathrm{p}}(\Gamma_h)^3$, and $F \mapsto R_\alpha \cdot F$ is bounded from $H^{1/2}_{\mathrm{p}}(\Gamma_h)^3$ into $H^{-1/2}_{\mathrm{p}}(\Gamma_h)$. If a biperiodic function $H \in H^1_{\mathrm{loc}}(\mathbb{R}^3_+)$ satisfies the Rayleigh expansion condition, then $T_\alpha H_3 = \partial H_3/\partial x_3$ on Γ_h. This implies that $e_3 \times (\operatorname{curl}_\alpha H) = e_3 \times (R_\alpha \times H)$ on Γ_h (see, e.g., [105]).

Assume that H^s_α is a distributional periodic solution to the boundary value problem (6.10) such that H^s_α, $\operatorname{curl}_\alpha H^s_\alpha$, and $\operatorname{div}_\alpha H^s_\alpha$ are locally square-integrable, such that the radiation condition (6.11) is satisfied, and such that $\nu \cdot (H^s_\alpha + H^{ir}_\alpha)$ and $\nu \times (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}(H^s_\alpha + H^{ir}_\alpha))$ are continuous over interfaces with normal vector ν where ε_{r} jumps. As noted in [105], this implies that, following the above notation, $H^s_\alpha \in H^1_{\mathrm{p,T}}(\Omega)$. Then the Stokes formula [1, 105] implies that

$$\begin{aligned}
&\int_\Omega (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H^s_\alpha \cdot \overline{\operatorname{curl}_\alpha F} - k^2 H^s_\alpha \cdot \overline{F})\,\mathrm{d}x \\
&- \int_{\Gamma_0} e_3 \times (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H^s_\alpha) \cdot \overline{F}\,\mathrm{d}x + \int_{\Gamma_h} e_3 \times (R_\alpha \times H^s_\alpha) \cdot \overline{F}\,\mathrm{d}s \\
&= \int_\Omega (1 - \varepsilon_{\mathrm{r}}^{-1}) \operatorname{curl}_\alpha H^{ir}_\alpha \cdot \overline{\operatorname{curl}_\alpha F}\,\mathrm{d}x - \int_{\Gamma_0} (e_3 \times (1 - \varepsilon_{\mathrm{r}}^{-1}) \operatorname{curl}_\alpha H^{ir}_\alpha) \cdot \overline{F}\,\mathrm{d}x
\end{aligned}$$

for all test functions $F \in H^1_{\mathrm{p,T}}(\Omega)^3$. Since we assumed that

$$0 = e_3 \times (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H_\alpha) = e_3 \times (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha (H^s_\alpha + H^{ir}_\alpha)) \quad \text{on } \Gamma_0,$$

the above identity simplifies to

$$\begin{aligned}
\int_\Omega (\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H^s_\alpha \cdot \overline{\operatorname{curl}_\alpha F} - k^2 H^s_\alpha \cdot \overline{F})\,\mathrm{d}x + \int_{\Gamma_h} e_3 \times (R_\alpha \times H^s_\alpha) \cdot \overline{F}\,\mathrm{d}s \\
= \int_\Omega (1 - \varepsilon_{\mathrm{r}}^{-1}) \operatorname{curl}_\alpha H^{ir}_\alpha \cdot \overline{\operatorname{curl}_\alpha F}\,\mathrm{d}x - \int_{\Gamma_0} (e_3 \times \operatorname{curl}_\alpha H^{ir}_\alpha) \cdot \overline{F}\,\mathrm{d}x\,.
\end{aligned}$$

By construction, $e_3 \times \operatorname{curl}_\alpha H^{ir}_\alpha$ vanishes on Γ_0, that is, we can neglect the last term in the

last equation. The divergence constraint $\mathrm{div}_\alpha H^s_\alpha = 0$ that follows from (6.10) shows that

$$\begin{aligned}\mathcal{B}(H^s_\alpha, F) := &\int_\Omega (\varepsilon_{\mathrm{r}}^{-1}\,\mathrm{curl}_\alpha\, H^s_\alpha \cdot \overline{\mathrm{curl}_\alpha\, F} - k^2 H^s_\alpha \cdot \overline{F})\,\mathrm{d}x + \rho \int_\Omega (\mathrm{div}_\alpha H^s_\alpha)(\overline{\mathrm{div}_\alpha F})\,\mathrm{d}x \\ &+ \int_{\Gamma_h} e_3 \times (R_\alpha \times H^s_\alpha) \cdot \overline{F}\,\mathrm{d}s - \int_{\Gamma_h} (R_\alpha \cdot H^s_\alpha)(e_3 \cdot \overline{F})\,\mathrm{d}s \\ &= \int_\Omega (1 - \varepsilon_{\mathrm{r}}^{-1})\,\mathrm{curl}_\alpha\, H^{ir}_\alpha \cdot \overline{\mathrm{curl}_\alpha\, F}\,\mathrm{d}x\,, \end{aligned} \tag{6.12}$$

where ρ is some complex constant with $\mathrm{Re}(\rho) \geq c > 0$ and $\mathrm{Im}(\rho) < 0$.

We next prove that the bounded sesquilinear form $\mathcal{B}:\ H^1_{\mathrm{p,T}}(\Omega)^3 \times H^1_{\mathrm{p,T}}(\Omega)^3 \to \mathbb{C}$ satisfies a Gårding inequality (this goes back to [1]), i.e. there exist strictly positive constants c_1 and c_2 such that

$$\mathrm{Re}(\mathcal{B}(H,H)) \geq c_1 \int_\Omega |\nabla_\alpha H|^2\,\mathrm{d}x - c_2 \int_\Omega |H|^2\,\mathrm{d}x\,. \tag{6.13}$$

for all $H \in H^1_{\mathrm{p,T}}(\Omega)^3$.

Theorem 6.3.1. *Assume that $\varepsilon_{\mathrm{r}}^{-1} \in L^\infty(\Omega)$ is positive and bounded away from zero. Set $\mathrm{Re}\rho = \inf_\Omega \varepsilon_{\mathrm{r}}^{-1} > 0$ and choose $\mathrm{Im}\rho < 0$. Then $\mathcal{B}$ satisfies* (6.13).

Proof. As in [105, proof of Theorem 1] one shows that

$$\begin{aligned}\mathrm{Re}(\mathcal{B}(H,H)) \geq \mathrm{Re}(\rho) &\int_\Omega (|\,\mathrm{curl}_\alpha\, H|^2 + |\mathrm{div}_\alpha H|^2)\,\mathrm{d}x - k^2 \int_\Omega |H|^2\,\mathrm{d}x \\ &- \mathrm{Re}\int_{\Gamma_h} T_\alpha H \cdot \overline{H}\,\mathrm{d}s - 2\mathrm{Re}\int_{\Gamma_h} \left(\overline{H_3}\frac{\partial^\alpha H_1}{\partial x_1} + \overline{H_3}\frac{\partial^\alpha H_2}{\partial x_2}\right)\mathrm{d}s\,.\end{aligned}$$

The following identity follows from integrations by parts, the periodicity, and the vanishing normal component of H on Γ_0,

$$\int_\Omega (|\,\mathrm{curl}_\alpha\, H|^2 + |\mathrm{div}_\alpha H|^2)\,\mathrm{d}x = \int_\Omega |\nabla_\alpha H|^2\,\mathrm{d}x + 2\mathrm{Re}\int_{\Gamma_h} \left(\overline{H_3}\frac{\partial^\alpha H_1}{\partial x_1} + \overline{H_3}\frac{\partial^\alpha H_2}{\partial x_2}\right)\mathrm{d}s\,.$$

In consequence,

$$\begin{aligned}\mathrm{Re}(\mathcal{B}(H,H)) \geq \mathrm{Re}(\rho) &\int_\Omega |\nabla_\alpha H|^2\,\mathrm{d}x - k^2 \int_\Omega |H|^2\,\mathrm{d}x \\ &- \mathrm{Re}\int_{\Gamma_h} T_\alpha H \cdot \overline{H}\,\mathrm{d}s - 2(1 - \mathrm{Re}(\rho))\,\mathrm{Re}\int_{\Gamma_h} \left(\frac{\partial^\alpha H_1}{\partial x_1} + \frac{\partial^\alpha H_2}{\partial x_2}\right)\overline{H_3}\,\mathrm{d}s\,.\end{aligned}$$

Precisely as in [105] one shows now by a Fourier series argument that

$$\begin{aligned}-\mathrm{Re}\int_{\Gamma_h} T_\alpha H \cdot \overline{H}\,\mathrm{d}s - 2(1 - \mathrm{Re}(\rho))\mathrm{Re}\int_{\Gamma_h} \left(\frac{\partial^\alpha H_1}{\partial x_1} + \frac{\partial^\alpha H_2}{\partial x_2}\right)\overline{H_3}\,\mathrm{d}s &\geq \mathrm{Re}\int_{\Gamma_h} K(H) \cdot \overline{H}\,\mathrm{d}s \\ &\geq -C\int_\Omega |H|^2\,\mathrm{d}x\end{aligned}$$

for a finite-dimensional operator K on $H_{\mathrm{p}}^{1/2}(\Gamma_h)^3$. Note that the last inequality follows from $|\int_{\Gamma_h} K(H)\cdot\overline{H}\,\mathrm{d}s| \le C\int_\Omega |H|^2\,\mathrm{d}x$ due to the finite-dimensional range of K and the fact that on finite-dimensional spaces all norms are equivalent. The last inequality implies a Gårding inequality for $\mathcal{B}$. □

For simplicity we write from now on H for the searched-for scattered field H_α^s in (6.12) and replace the source function $\operatorname{curl} H_\alpha^{ir}$ by a $G \in H_{\mathrm{p}}^1(\Omega)^3$. The last theorem implies the following corollary.

Corollary 6.3.2. *The variational problem to find $H \in H_{\mathrm{p,T}}^1(\Omega)^3$ such that*

$$\mathcal{B}(H,F) = \int_\Omega (1-\varepsilon_{\mathrm{r}}^{-1})G\cdot\overline{\operatorname{curl}_\alpha F}\,\mathrm{d}x \quad \textit{for all } F \in H_{\mathrm{p,T}}^1(\Omega)^3 \tag{6.14}$$

satisfies the Fredholm alternative, i.e., uniqueness of solution implies existence of solution.

Note that this formulation corresponds to the usual variational formulation of the Maxwell's equations with perfectly conducting magnetic boundary conditions in smooth bounded domains, see, e.g., [39, Section 4.5(b)]. For special material parameters $\varepsilon_{\mathrm{r}}^{-1}$ in

$$W_{\mathrm{p}}^{1,\infty}(\Omega) := \{f \in L^\infty(\Omega) : f = \tilde{f}|_\Omega \text{ for some } 2\pi\text{-biperiodic } \tilde{f} \in W^{1,\infty}(\mathbb{R}^3)\}$$

we will in the sequel of the chapter establish a uniqueness result via a Rellich identity. The next lemma will be useful when proving this identity.

Lemma 6.3.3. *Assume that $\varepsilon_{\mathrm{r}}^{-1} \in W_{\mathrm{p}}^{1,\infty}(\Omega)$ is positive and bounded away from zero, and that $G \in H_{\mathrm{p}}^1(\Omega)^3$. Then a solution $H \in H_{\mathrm{p,T}}^1(\Omega)^3$ to problem* (6.14) *satisfies*

$$\operatorname{curl}_\alpha(\varepsilon_{\mathrm{r}}^{-1}\operatorname{curl}_\alpha H) - k^2 H = \operatorname{curl}_\alpha((1-\varepsilon_{\mathrm{r}}^{-1})G) \qquad \textit{in } L^2(\Omega)^3, \tag{6.15}$$

$$\operatorname{div}_\alpha H = 0 \qquad \textit{in } L^2(\Omega), \tag{6.16}$$

$$e_3 \times (\varepsilon_{\mathrm{r}}^{-1}\operatorname{curl}_\alpha H) = e_3 \times ((1-\varepsilon_{\mathrm{r}}^{-1})G) \qquad \textit{in } H_{\mathrm{p}}^{-1/2}(\Gamma_0)^3, \tag{6.17}$$

$$e_3 \cdot H = 0 \qquad \textit{in } H_{\mathrm{p}}^{1/2}(\Gamma_0). \tag{6.18}$$

Moreover,

$$e_3 \times R_\alpha \times H = e_3 \times \operatorname{curl}_\alpha H \quad \textit{in } H_{\mathrm{p}}^{-1/2}(\Gamma_h)^3 \textit{ and } \quad R_\alpha \cdot H = 0 \quad \textit{in } H_{\mathrm{p}}^{-1/2}(\Gamma_h), \tag{6.19}$$

and $\partial H/\partial x_3 = T_\alpha(H)$ holds in $H_{\mathrm{p}}^{-1/2}(\Gamma_h)$.

Proof. The proof that $\operatorname{div}_\alpha H = 0$ is analogous to the proof of [105, Theorem 2]. In consequence, using a test function $F \in C_0^\infty(\Omega)^3$ in the variational problem (6.14) shows that the solution H satisfies the differential equation (6.15) in the distributional sense. Since $H \in H_{\mathrm{p,T}}^1(\Omega)^3$, (6.15) holds in the L^2-sense if the right-hand side belongs to $L^2(\Omega)^3$, which holds if $\varepsilon_{\mathrm{r}}^{-1} \in W_{\mathrm{p}}^{1,\infty}(\Omega)$ and $G \in H_{\mathrm{p}}^1(\Omega)^3$.

Multiplying (6.15) by $F \in H^1_{\mathrm{p,T}}(\Omega)^3$, using the Stokes formula, and subtracting the resulting expression from the variational formulation (6.14), we find that

$$\int_{\Gamma_h} e_3 \times (R_\alpha \times H) \cdot \overline{F}\,\mathrm{d}s - \int_{\Gamma_h} (R_\alpha \cdot H)(e_3 \cdot \overline{F})\,\mathrm{d}s - \int_{\Gamma_h} e_3 \times \mathrm{curl}_\alpha H \cdot \overline{F}\,\mathrm{d}s$$
$$+ \int_{\Gamma_0} e_3 \times (\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}_\alpha H) \cdot \overline{F}\,\mathrm{d}s - \int_{\Gamma_0} e_3 \times ((1-\varepsilon_\mathrm{r}^{-1})G) \cdot \overline{F}\,\mathrm{d}s = 0.$$

If we choose F such that $F|_{\Gamma_h} = 0$, then we see that $e_3 \times (\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}_\alpha H - (1-\varepsilon_\mathrm{r}^{-1})G) = 0$ in $H_\mathrm{p}^{-1/2}(\Gamma_0)$. If $e_3 \cdot F|_{\Gamma_h} = 0$, it follows that $e_3 \times (R_\alpha \times H) = e_3 \times \mathrm{curl}_\alpha H$ in $H_\mathrm{p}^{-1/2}(\Gamma_h)^3$. Hence, $R_\alpha \cdot H = 0$ in $H_\mathrm{p}^{-1/2}(\Gamma_h)$. These identities imply that $\partial H/\partial x_3 = T_\alpha(H)$ in $H_\mathrm{p}^{-1/2}(\Gamma_h)$ due to [105, Lemma 1]. □

Remark 6.3.4. *Instead of the above variational formulation in $H^1_{\mathrm{p,T}}(\Omega)^3$, one can also consider formulations in $H_\mathrm{p}(\mathrm{curl}_\alpha,\Omega)^3$, the natural energy space for the second-order Maxwell equations* (6.10)*, see, e.g., [1]. In $H_\mathrm{p}(\mathrm{curl}_\alpha,\Omega)^3$ there is no bounded trace operator for the normal component of the field, and in consequence, the formulation* (6.14) *needs to be adapted. Usually, one replaces $F \mapsto e_3 \times (R_\alpha \times F) \times e_3$ by $Q(e_3 \times H)$, where Q is a bounded operator between the natural trace spaces $H^{-1/2}_{\mathrm{p,div}}(\Gamma_h)$ and $H^{-1/2}_{\mathrm{p,curl}}(\Gamma_h)$, defined by*

$$(QF)(x) = -\sum_{n\in\Lambda} \frac{1}{\mathrm{i}\beta_n}\{k^2 \hat{F}_{T,n} - [(n+\alpha)\cdot \hat{F}_n](n+\alpha)\}e^{\mathrm{i}n\cdot x}, \quad \textit{for } F(x) = \sum_{n\in\Lambda} \hat{F}_n e^{\mathrm{i}n\cdot x}, \tag{6.20}$$

see, e.g., [1]. Obviously this definition only makes sense if all β_n are non-zero. If this is the case, then the variational formulation (6.14) *is equivalent to the formulation in $H_\mathrm{p}(\mathrm{curl}_\alpha,\Omega)^3$ obtained using Q. Under the assumption that $\beta_n \neq 0$, all subsequent results could also be obtained via the formulation in $H_\mathrm{p}(\mathrm{curl}_\alpha,\Omega)^3$.*

6.4 Integral Identities

This section is concerned with technical lemmas that will be used to derive the Rellich identity and solution bounds subsequently. Roughly speaking, for deriving the Rellich identity, we will multiply the Maxwell equations (6.15) by $x_3\partial H/\partial x_3$ and integrate by parts. Therefore, it is the aim of the technical lemmas in this section to analyze the term $\mathrm{Re}\int_\Omega x_3 \partial H/\partial x_3 \cdot \overline{\mathrm{curl}_\alpha(\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}_\alpha H)}\,\mathrm{d}x$ for a solution $H \in H^1_{\mathrm{p,T}}(\Omega)^3$ to the problem (6.14). Note that the first two lemmas need the function H to be in $H^2_\mathrm{p}(\Omega)^3$. These lemmas for the magnetic field formulation actually correspond to the ones for the electric field formulation in [50, Section 3].

We need to introduce some notation. For a vector field $F = (F_1, F_2, F_3)^\top$ we denote by $F_T = (F_1, F_2, 0)^\top$ its transverse part. Recall that $\partial^\alpha f/\partial x_j = \partial f/\partial x_j + \mathrm{i}\alpha_j f$ for a scalar

function f and $j = 1, 2, 3$. Further, we introduce

$$\nabla_T f := \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, 0\right)^\top, \quad \nabla_{\alpha,T} f := \left(\frac{\partial^\alpha f}{\partial x_1}, \frac{\partial^\alpha f}{\partial x_2}, 0\right)^\top, \quad \overrightarrow{\operatorname{curl}}_{\alpha,T} f := \left(\frac{\partial^\alpha f}{\partial x_2}, -\frac{\partial^\alpha f}{\partial x_1}, 0\right)^\top,$$

and, for a vector field $F = (F_1, F_2, F_3)^\top$,

$$\operatorname{div}_{\alpha,T} F := \frac{\partial^\alpha F_1}{\partial x_1} + \frac{\partial^\alpha F_2}{\partial x_2} \quad \text{and} \quad \operatorname{curl}_{\alpha,T} F := \frac{\partial^\alpha F_2}{\partial x_1} - \frac{\partial^\alpha F_1}{\partial x_2}.$$

It is straightforwards to show that $\operatorname{div}_{\alpha,T} \overrightarrow{\operatorname{curl}}_{\alpha,T} = 0$ as well as $\operatorname{curl}_{\alpha,T} \nabla_{\alpha,T} = 0$. Moreover, a tedious computation shows that

$$\operatorname{curl}_\alpha F = (\operatorname{curl}_{\alpha,T} F_T) e_3 + \overrightarrow{\operatorname{curl}}_{\alpha,T} F_3 - \frac{\partial (F \times e_3)}{\partial x_3},$$

and further

$$|\operatorname{curl}_\alpha F|^2 = |\operatorname{curl}_{\alpha,T} F_T|^2 + |\overrightarrow{\operatorname{curl}}_{\alpha,T} F_3|^2 + \left|\frac{\partial F_T}{\partial x_3}\right|^2 - 2\mathrm{Re}\left(\overline{\nabla_{\alpha,T} F_3} \cdot \frac{\partial F_T}{\partial x_3}\right). \tag{6.21}$$

Lemma 6.4.1. *Assume that $\varepsilon_{\mathrm{r}}^{-1} \in W_{\mathrm{p}}^{1,\infty}(\Omega)$ is positive and bounded away from zero and that $H \in H_{\mathrm{p}}^2(\Omega)^3$. Then*

$$\begin{aligned} 2\mathrm{Re} \int_\Omega x_3 \frac{\partial H}{\partial x_3} \cdot \overline{\operatorname{curl}_\alpha(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H)} \,\mathrm{d}x &= -\int_\Omega \frac{\partial (x_3 \varepsilon_{\mathrm{r}}^{-1})}{\partial x_3} |\operatorname{curl}_\alpha H|^2 \,\mathrm{d}x + h \int_{\Gamma_h} |\operatorname{curl}_\alpha H|^2 \,\mathrm{d}s \\ &\quad + 2\mathrm{Re} \int_\Omega \varepsilon_{\mathrm{r}}^{-1} \left(e_3 \times \frac{\partial H}{\partial x_3}\right) \cdot \overline{\operatorname{curl}_\alpha H} \,\mathrm{d}x + 2h\mathrm{Re} \int_{\Gamma_h} \frac{\partial H_T}{\partial x_3} \cdot (e_3 \times \overline{\operatorname{curl}_\alpha H}) \,\mathrm{d}s\,. \end{aligned} \tag{6.22}$$

Proof. Denote by ν the outward unit normal to Ω. Using integration by parts and noting that $\nu = e_3$ on Γ_h, and that the boundary term on Γ_0 vanishes since $x_3 = 0$ on Γ_0, we find that

$$\begin{aligned} &2\mathrm{Re} \int_\Omega x_3 \frac{\partial H}{\partial x_3} \cdot \overline{\operatorname{curl}_\alpha(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H)} \,\mathrm{d}x \\ &\quad = 2\mathrm{Re} \int_\Omega \varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha \left(x_3 \frac{\partial H}{\partial x_3}\right) \cdot \overline{\operatorname{curl}_\alpha H} \,\mathrm{d}x + 2\mathrm{Re} \int_{\partial\Omega} x_3 \frac{\partial H}{\partial x_3} \cdot (\nu \times \overline{\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H}) \,\mathrm{d}s \\ &\quad = \int_\Omega \varepsilon_{\mathrm{r}}^{-1} x_3 \frac{\partial |\operatorname{curl}_\alpha H|^2}{\partial x_3} \,\mathrm{d}x + 2\mathrm{Re} \int_\Omega \varepsilon_{\mathrm{r}}^{-1} \left(e_3 \times \frac{\partial H}{\partial x_3}\right) \cdot \overline{\operatorname{curl}_\alpha H} \,\mathrm{d}x \\ &\qquad\qquad + 2h\mathrm{Re} \int_{\Gamma_h} \frac{\partial H_T}{\partial x_3} \cdot (e_3 \times \overline{\operatorname{curl}_\alpha H}) \,\mathrm{d}s \\ &\quad = -\int_\Omega \frac{\partial (x_3 \varepsilon_{\mathrm{r}}^{-1})}{\partial x_3} |\operatorname{curl}_\alpha H|^2 \,\mathrm{d}x + 2\mathrm{Re} \int_\Omega \varepsilon_{\mathrm{r}}^{-1} \left(e_3 \times \frac{\partial H}{\partial x_3}\right) \cdot \overline{\operatorname{curl}_\alpha H} \,\mathrm{d}x \\ &\qquad\qquad + h \int_{\Gamma_h} |\operatorname{curl}_\alpha H|^2 \,\mathrm{d}s + 2h\mathrm{Re} \int_{\Gamma_h} \frac{\partial H_T}{\partial x_3} \cdot (e_3 \times \overline{\operatorname{curl}_\alpha H}) \,\mathrm{d}s\,. \end{aligned}$$

□

The next lemma continues the analysis of the term $\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}(e_3\times\partial H/\partial x_3)\cdot\overline{\mathrm{curl}_\alpha H}\,\mathrm{d}x$ in the right hand side of (6.22).

Lemma 6.4.2. *Assume that $\varepsilon_\mathrm{r}^{-1}\in W_\mathrm{p}^{1,\infty}(\Omega)$ is positive and bounded away from zero. Then for all $H\in H_\mathrm{p}^2(\Omega)^3$ the following identity holds,*

$$\begin{aligned}2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\left(e_3\times\frac{\partial H}{\partial x_3}\right)\cdot\overline{\mathrm{curl}_\alpha H}\,\mathrm{d}x &= 2\int_\Omega \varepsilon_\mathrm{r}^{-1}\left|\frac{\partial H}{\partial x_3}\right|^2\mathrm{d}x + 2\mathrm{Re}\int_\Omega \nabla\varepsilon_\mathrm{r}^{-1}\cdot\frac{\partial H}{\partial x_3}\overline{H_3}\,\mathrm{d}x\\ &-2\mathrm{Re}\int_\Omega \frac{\partial(\varepsilon_\mathrm{r}^{-1}\overline{H_3})}{\partial x_3}\mathrm{div}_\alpha H\,\mathrm{d}x - 2\mathrm{Re}\int_{\Gamma_h}\left(\frac{\partial H_3}{\partial x_3}-\mathrm{div}_\alpha H\right)\overline{H_3}\,\mathrm{d}s\\ &-2\mathrm{Re}\int_{\Gamma_0}\varepsilon_\mathrm{r}^{-1}\overline{H_3}\mathrm{div}_{\alpha,T}H_T\,\mathrm{d}s\,. \qquad (6.23)\end{aligned}$$

Proof. First, we have

$$\begin{aligned}2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\left(e_3\times\frac{\partial H}{\partial x_3}\right)\cdot\overline{\mathrm{curl}_\alpha H}\,\mathrm{d}x &= 2\int_\Omega \varepsilon_\mathrm{r}^{-1}\left|\frac{\partial H_T}{\partial x_3}\right|^2\mathrm{d}x\\ &-2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial H_T}{\partial x_3}\cdot\nabla_T\overline{H_3}\,\mathrm{d}x + 2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial H_T}{\partial x_3}\cdot\mathrm{i}\alpha\overline{H_3}\,\mathrm{d}x\,. \qquad (6.24)\end{aligned}$$

Second, we compute that

$$\begin{aligned}-2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial H_T}{\partial x_3}\cdot\nabla_T\overline{H_3}\,\mathrm{d}x &= 2\mathrm{Re}\int_\Omega \mathrm{div}_T\left(\varepsilon_\mathrm{r}^{-1}\frac{\partial H_T}{\partial x_3}\right)\overline{H_3}\,\mathrm{d}x\\ &= 2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\mathrm{div}_T\left(\frac{\partial H_T}{\partial x_3}\right)\overline{H_3}\,\mathrm{d}x + 2\mathrm{Re}\int_\Omega \nabla_T\varepsilon_\mathrm{r}^{-1}\cdot\frac{\partial H_T}{\partial x_3}\overline{H_3}\,\mathrm{d}x\\ &= -2\mathrm{Re}\int_\Omega \frac{\partial\varepsilon_\mathrm{r}^{-1}}{\partial x_3}\overline{H_3}\mathrm{div}_T H_T\,\mathrm{d}x - 2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial\overline{H_3}}{\partial x_3}\mathrm{div}_T H_T\,\mathrm{d}x\\ &+ 2\mathrm{Re}\int_\Omega \nabla_T\varepsilon_\mathrm{r}^{-1}\cdot\frac{\partial H_T}{\partial x_3}\overline{H_3}\,\mathrm{d}x + 2\mathrm{Re}\int_{\Gamma_h}\overline{H_3}\mathrm{div}_T H_T\,\mathrm{d}s - 2\mathrm{Re}\int_{\Gamma_0}\varepsilon_\mathrm{r}^{-1}\overline{H_3}\mathrm{div}_T H_T\,\mathrm{d}s\end{aligned}$$

Now, using the identity $\mathrm{div}_T H_T = -\partial H_3/\partial x_3 + \mathrm{div}_\alpha H - \mathrm{i}\alpha\cdot H$, we obtain that

$$\begin{aligned}-2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial H_T}{\partial x_3}\cdot\nabla_T\overline{H_3}\,\mathrm{d}x &= 2\mathrm{Re}\int_\Omega \frac{\partial\varepsilon_\mathrm{r}^{-1}}{\partial x_3}\overline{H_3}(\mathrm{i}\alpha\cdot H)\,\mathrm{d}x + 2\mathrm{Re}\int_\Omega \frac{\partial\varepsilon_\mathrm{r}^{-1}}{\partial x_3}\overline{H_3}\frac{\partial H_3}{\partial x_3}\,\mathrm{d}x\\ &- 2\mathrm{Re}\int_\Omega \frac{\partial\varepsilon_\mathrm{r}^{-1}}{\partial x_3}\overline{H_3}\mathrm{div}_\alpha H\,\mathrm{d}x + 2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial\overline{H_3}}{\partial x_3}(\mathrm{i}\alpha\cdot H)\,\mathrm{d}x + 2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\left|\frac{\partial H_3}{\partial x_3}\right|^2\mathrm{d}x\\ &- 2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial\overline{H_3}}{\partial x_3}\mathrm{div}_\alpha H\,\mathrm{d}x + 2\mathrm{Re}\int_\Omega \nabla_T\varepsilon_\mathrm{r}^{-1}\cdot\frac{\partial H_T}{\partial x_3}\overline{H_3}\,\mathrm{d}x + 2\mathrm{Re}\int_{\Gamma_h}\overline{H_3}\mathrm{div}_T H_T\,\mathrm{d}x\\ &- 2\mathrm{Re}\int_{\Gamma_0}\varepsilon_\mathrm{r}^{-1}\overline{H_3}\mathrm{div}_T H_T\,\mathrm{d}s\end{aligned}$$

Applying Green formula to the term $2\mathrm{Re}\int_\Omega(\partial\varepsilon_\mathrm{r}^{-1}/\partial x_3)\overline{H_3}(\mathrm{i}\alpha\cdot H)\,\mathrm{d}x$, we have

$$\begin{aligned}-2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial H_T}{\partial x_3}\cdot\nabla_T\overline{H_3}\,\mathrm{d}x &= -2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial H_T}{\partial x_3}\cdot\mathrm{i}\alpha\overline{H_3}\,\mathrm{d}x + 2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\left|\frac{\partial H_3}{\partial x_3}\right|^2\mathrm{d}x\\ &- 2\mathrm{Re}\int_\Omega \frac{\partial\varepsilon_\mathrm{r}^{-1}}{\partial x_3}\overline{H_3}\mathrm{div}_\alpha H\,\mathrm{d}x - 2\mathrm{Re}\int_\Omega \varepsilon_\mathrm{r}^{-1}\frac{\partial\overline{H_3}}{\partial x_3}\mathrm{div}_\alpha H\,\mathrm{d}x + 2\mathrm{Re}\int_\Omega \nabla\varepsilon_\mathrm{r}^{-1}\cdot\frac{\partial H}{\partial x_3}\overline{H_3}\,\mathrm{d}x\\ &- 2\mathrm{Re}\int_{\Gamma_h}\left(\frac{\partial H_3}{\partial x_3}-\mathrm{div}_\alpha H\right)\overline{H_3}\,\mathrm{d}s - 2\mathrm{Re}\int_{\Gamma_0}\varepsilon_\mathrm{r}^{-1}\overline{H_3}\mathrm{div}_{\alpha,T}H_T\,\mathrm{d}s\end{aligned}$$

Now the claim follows from substituting this identity into equation (6.24). □

In the following final lemma of this section we will reformulate the term

$$\mathrm{Re}\int_\Omega x_3\partial H/\partial x_3\cdot\overline{\mathrm{curl}_\alpha(\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}_\alpha H)}\,\mathrm{d}x$$

for a solution $H\in H^1_{\mathrm{p,T}}(\Omega)^3$ to the problem (6.14) using the last two lemmas.

Lemma 6.4.3. *Assume that $\varepsilon_\mathrm{r}^{-1}\in W^{1,\infty}_\mathrm{p}(\Omega)$ is positive and bounded away from zero. Then any solution $H\in H^1_{\mathrm{p,T}}(\Omega)^3$ to the problem* (6.14) *satisfies*

$$\begin{aligned}2\mathrm{Re}\int_\Omega x_3\frac{\partial H}{\partial x_3}\cdot\overline{\mathrm{curl}_\alpha(\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}_\alpha H)}\,\mathrm{d}x &= -\int_\Omega\frac{\partial(x_3\varepsilon_\mathrm{r}^{-1})}{\partial x_3}|\,\mathrm{curl}_\alpha H|^2\,\mathrm{d}x + h\int_{\Gamma_h}|\,\mathrm{curl}_\alpha H|^2\,\mathrm{d}s\\ &+2\int_\Omega\varepsilon_\mathrm{r}^{-1}\left|\frac{\partial H}{\partial x_3}\right|^2\mathrm{d}x + 2\mathrm{Re}\int_\Omega\nabla\varepsilon_\mathrm{r}^{-1}\cdot\frac{\partial H}{\partial x_3}\overline{H_3}\,\mathrm{d}x - 2\mathrm{Re}\int_{\Gamma_h}\overline{H_3}\frac{\partial H_3}{\partial x_3}\,\mathrm{d}s\\ &+2h\mathrm{Re}\int_{\Gamma_h}\frac{\partial H_T}{\partial x_3}\cdot(e_3\times\overline{\mathrm{curl}_\alpha H})\,\mathrm{d}s\,.\end{aligned}$$

Proof. It is sufficient to prove that H satisfies (6.22) and

$$\begin{aligned}2\mathrm{Re}\int_\Omega\varepsilon_\mathrm{r}^{-1}\left(e_3\times\frac{\partial H}{\partial x_3}\right)\cdot\overline{\mathrm{curl}_\alpha H}\,\mathrm{d}x &= 2\int_\Omega\varepsilon_\mathrm{r}^{-1}\left|\frac{\partial H}{\partial x_3}\right|^2\mathrm{d}x + 2\mathrm{Re}\int_\Omega\nabla\varepsilon_\mathrm{r}^{-1}\cdot\frac{\partial H}{\partial x_3}\overline{H_3}\,\mathrm{d}x\\ &- 2\mathrm{Re}\int_{\Gamma_h}\overline{H_3}\frac{\partial H_3}{\partial x_3}\,\mathrm{d}s\,. \qquad (6.25)\end{aligned}$$

Recall that, for $h>\sup\{x_3:\,(x_1,x_2,x_3)^\top\in\mathrm{supp}(\varepsilon_\mathrm{r}-1)\}$, there exists a constant $0<\eta\ll 1$ such that $\varepsilon_\mathrm{r}=1$ in $(0,2\pi)^2\times(h-\eta,h)$. Hence, a solution $H\in H^1_{\mathrm{p,T}}(\Omega)^3$ to the problem (6.14) belongs to $H^1_{\mathrm{p,T}}(\Omega)^3\cap H^2_\mathrm{p}((0,2\pi)^2\times(h-\eta,h))^3$ due to interior elliptic regularity theory. Then one can extend H to a function defined in all of $\mathbb{R}^3$ that is 2π-biperiodic and belongs to $H^1_\mathrm{p}((0,2\pi)^2\times(-\infty,h))^3\cap H^2_\mathrm{p}((0,2\pi)^2\times(h-\eta,\infty))^3$ (This can be seen using [81] combined with suitable cut-off arguments.) By abuse of notation, we still denote the extended function by H. Let $\phi\in C^\infty(\mathbb{R}^3)$ be a smooth and non-negative function supported in the unit ball and

$\int_{\mathbb{R}^3} \phi \, \mathrm{d}x = 1$. For $\delta > 0$ and $x \in \mathbb{R}^3$ let $\phi^\delta(x) = \delta^{-3}\phi(x/\delta)$. The convolution $H^\delta := \phi^\delta * H$ belongs to $H^2_{\mathrm{p}}(\Omega)^3$ and thus satisfies (6.22). Then, from Lemma 6.3.3 and the fact that $H^\delta \to H$ in $H^1_{\mathrm{p,T}}(\Omega)^3 \cap H^2_{\mathrm{p}}((0,2\pi)^2 \times (h-\eta,h))^3$ we obtain that

$$\operatorname{curl}_\alpha(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H^\delta) \overset{\delta\to 0}{\to} \operatorname{curl}_\alpha(\varepsilon_{\mathrm{r}}^{-1} \operatorname{curl}_\alpha H) \quad \text{in } L^2(\Omega)^3.$$

Moreover, the convergence in $H^2_{\mathrm{p}}((0,2\pi)^2 \times (h-\eta,h))^3$ implies that $\operatorname{curl}_\alpha H^\delta \to \operatorname{curl}_\alpha H$ in $L^2(\Gamma_h)^3$ as $\delta \to 0$. Consequently, H satisfies (6.22).

It remains to show that H also satisfies (6.25). The function H^δ satisfies (6.23) and we consider the limit of this identity as $\delta \to 0$. It is easily seen that $\operatorname{div}_\alpha H^\delta \to \operatorname{div}_\alpha H = 0$ in $L^2(\Omega)$. Thus, we have

$$e_3 \cdot H^\delta \overset{\delta\to 0}{\to} e_3 \cdot H = 0 \quad \text{in } H^{1/2}_{\mathrm{p}}(\Gamma_0), \qquad \operatorname{div}_{\alpha,T} H^\delta_T \overset{\delta\to 0}{\to} \operatorname{div}_{\alpha,T} H_T \quad \text{in } H^{-1/2}_{\mathrm{p}}(\Gamma_0),$$

due to the convergence of H^δ to H in $H^1_{\mathrm{p}}(\Omega)^3$. Further, the convergence of H^δ to H in $H^2_{\mathrm{p}}((0,2\pi)^2 \times (h-\eta,h))^3$ and the fact $\operatorname{div}_\alpha H = 0$ on Γ_h imply that

$$\frac{\partial H^\delta}{\partial x_3} - \operatorname{div}_\alpha H^\delta \to \frac{\partial H_3}{\partial x_3} - \operatorname{div}_\alpha H = \frac{\partial H_3}{\partial x_3} \quad \text{in } H^{-1/2}_{\mathrm{p}}(\Gamma_h).$$

Plugging in these limits into (6.23) shows that (6.25) holds. □

6.5 Rellich Identity and Solution Estimate

For establishing uniqueness of solution to the variational problem (6.14), we derive in this section the so-called Rellich identity relating $|\operatorname{curl}_\alpha H|^2$ and $|\partial H/\partial x_3|^2$ where H is a solution to the homogeneous variational problem corresponding to (6.14). Then, under suitable non-trapping and smoothness conditions on the material parameter, integral inequality resulting from this identity allow us to obtain estimate for a solution to the homogeneous problem. As mentioned in the introduction, the Rellich identity and solution estimate obtained in this section are much simpler than the ones in [50, Section 4]. It turns out also that the non-trapping assumptions on the parameter material are weaker than the ones in the latter paper.

The proof of the Rellich identity is based on an integration-by-parts technique that goes back to Rellich [96]. Typically, this technique requires more regularity of a solution than just to belong to the energy space. In our case we will roughly speaking multiply the Maxwell's equations (6.15), for $G = 0$ in the right hand side, by $x_3 \partial H/\partial x_3$ and integrate by parts.

Lemma 6.5.1 (Rellich Identity)**.** *Assume that $\varepsilon_{\mathrm{r}}^{-1} \in W^{1,\infty}_{\mathrm{p}}(\Omega)$ is positive and bounded away from zero. Then the following identity holds for all solutions $H \in H^1_{\mathrm{p,T}}(\Omega)^3$ to the homogeneous problem corresponding to* (6.14)*,*

$$\int_\Omega \left[2\varepsilon_{\mathrm{r}}^{-1} \left| \frac{\partial H}{\partial x_3} \right|^2 - x_3 \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} |\operatorname{curl}_\alpha H|^2 + 2\mathrm{Re}\left(\nabla \varepsilon_{\mathrm{r}}^{-1} \cdot \frac{\partial H}{\partial x_3} \overline{H_3} \right) \right] \mathrm{d}x$$
$$+ \mathrm{Re} \int_{\Gamma_h} e_3 \times (R_\alpha \times H) \cdot \overline{H} \, \mathrm{d}s - 2\mathrm{Re} \int_{\Gamma_h} T_\alpha(H_3) \overline{H_3} \, \mathrm{d}s = 0. \tag{6.26}$$

Proof. Let $H \in H^1_{\mathrm{p,T}}(\Omega)^3$ be a solution to the homogeneous problem corresponding to (6.14). First, using integration by parts we have

$$\mathrm{Re}\int_{\Gamma_h} \frac{\partial H_T}{\partial x_3} \cdot (e_3 \times \overline{\mathrm{curl}_\alpha H})\,\mathrm{d}s \;=\; \int_{\Gamma_h} \left|\frac{\partial H_T}{\partial x_3}\right|^2 \mathrm{d}s \;+ \mathrm{Re}\int_{\Gamma_h} \frac{\partial H_T}{\partial x_3} \cdot \overline{\nabla_{\alpha,T} H_3}\,\mathrm{d}s\,.$$

Note that H satisfies the assumptions of Lemma 6.4.3. Together with the latter equation we obtain

$$\begin{aligned}
2\mathrm{Re}\int_\Omega x_3 \frac{\partial H}{\partial x_3} \cdot \overline{\mathrm{curl}_\alpha(\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}_\alpha H)}\,\mathrm{d}x \;&= -\int_\Omega \frac{\partial(x_3\varepsilon_\mathrm{r}^{-1})}{\partial x_3}|\,\mathrm{curl}_\alpha H|^2\,\mathrm{d}x \;+ h\int_{\Gamma_h} |\,\mathrm{curl}_\alpha H|^2\,\mathrm{d}s \\
&\quad + 2\int_\Omega \varepsilon_\mathrm{r}^{-1}\left|\frac{\partial H}{\partial x_3}\right|^2 \mathrm{d}x \;+ 2\mathrm{Re}\int_\Omega \nabla\varepsilon_\mathrm{r}^{-1} \cdot \frac{\partial H}{\partial x_3}\overline{H_3}\,\mathrm{d}x \;- 2\mathrm{Re}\int_{\Gamma_h} \frac{\partial H_3}{\partial x_3}\overline{H_3}\,\mathrm{d}s \\
&\quad - 2h\int_{\Gamma_h} \left|\frac{\partial H_T}{\partial x_3}\right|^2 \mathrm{d}s \;+ 2h\mathrm{Re}\int_{\Gamma_h} \frac{\partial H_T}{\partial x_3} \cdot \overline{\nabla_{\alpha,T} H_3}\,\mathrm{d}s\,.
\end{aligned}$$

We exploit that H solves (6.15) for $G = 0$,

$$\begin{aligned}
2\mathrm{Re}\int_\Omega x_3 \frac{\partial H}{\partial x_3} \cdot \overline{\mathrm{curl}_\alpha(\varepsilon_\mathrm{r}^{-1}\,\mathrm{curl}_\alpha H)}\,\mathrm{d}x \;&= k^2 2\mathrm{Re}\int_\Omega x_3 \frac{\partial \overline{H}}{\partial x_3} \cdot H\,\mathrm{d}x \;= k^2\int_\Omega x_3 \frac{\partial |H|^2}{\partial x_3}\,\mathrm{d}x \\
&= -k^2\int_\Omega |H|^2\,\mathrm{d}x \;+ k^2 h\int_{\Gamma_h} |H|^2\,\mathrm{d}s\,.
\end{aligned}$$

From the last two equations we conclude that

$$\begin{aligned}
&-\int_\Omega \left(\frac{\partial(x_3\varepsilon_\mathrm{r}^{-1})}{\partial x_3}|\,\mathrm{curl}_\alpha H|^2 - k^2|H|^2\right)\mathrm{d}x \;+ 2\int_\Omega \varepsilon_\mathrm{r}^{-1}\left|\frac{\partial H}{\partial x_3}\right|^2 \mathrm{d}x \;+ 2\mathrm{Re}\int_\Omega \nabla\varepsilon_\mathrm{r}^{-1} \cdot \frac{\partial H}{\partial x_3}\overline{H_3}\,\mathrm{d}x \\
&\quad - 2\mathrm{Re}\int_{\Gamma_h} \overline{H_3}\frac{\partial H_3}{\partial x_3}\,\mathrm{d}s \;- 2h\int_{\Gamma_h} \left|\frac{\partial H_T}{\partial x_3}\right|^2 \mathrm{d}s \;+ 2h\mathrm{Re}\int_{\Gamma_h} \frac{\partial H_T}{\partial x_3} \cdot \overline{\nabla_{\alpha,T} H_3}\,\mathrm{d}s \\
&\quad + h\int_{\Gamma_h} (|\,\mathrm{curl}_\alpha H|^2 - k^2|H|^2)\,\mathrm{d}s \;= 0.
\end{aligned}$$

Due to the variational formulation (6.14) for $G = 0$,

$$\int_\Omega (\varepsilon_\mathrm{r}^{-1}|\,\mathrm{curl}_\alpha H|^2 - k^2|H|^2)\,\mathrm{d}x \;+ \mathrm{Re}\int_{\Gamma_h} e_3 \times (R_\alpha \times H) \cdot \overline{H}\,\mathrm{d}s \;= 0 \tag{6.27}$$

since $\mathrm{div}_\alpha H = 0$ in Ω and $R_\alpha \cdot H = 0$ in $H^{-1/2}_\mathrm{p}(\Gamma_h)$ due to Lemma 6.3.3. Adding the last two equations yields that the term $\int_\Omega k^2|H|^2\,\mathrm{d}x$ cancels, and further exploiting $\partial H_3/\partial x_3 = T_\alpha H_3$

on Γ_h to yields that

$$
\begin{aligned}
&-\int_\Omega x_3 \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} |\operatorname{curl}_\alpha H|^2 \,\mathrm{d}x + 2\int_\Omega \varepsilon_{\mathrm{r}}^{-1} \left|\frac{\partial H}{\partial x_3}\right|^2 \mathrm{d}x + 2\mathrm{Re}\int_\Omega \nabla \varepsilon_{\mathrm{r}}^{-1} \cdot \frac{\partial H}{\partial x_3} \overline{H_3}\,\mathrm{d}x \\
&\quad - 2\mathrm{Re}\int_{\Gamma_h} T_\alpha(H_3)\overline{H_3}\,\mathrm{d}s + \mathrm{Re}\int_{\Gamma_h} e_3 \times (R_\alpha \times H)\cdot \overline{H}\,\mathrm{d}s + 2h\mathrm{Re}\int_{\Gamma_h} \frac{\partial H_T}{\partial x_3}\cdot \overline{\nabla_{\alpha,T} H_3}\,\mathrm{d}s \\
&\qquad\qquad + h\int_{\Gamma_h}\left(|\operatorname{curl}_\alpha H|^2 - k^2|H|^2 - 2\left|\frac{\partial H_T}{\partial x_3}\right|^2\right)\mathrm{d}s = 0.
\end{aligned}
$$

Recall equality (6.21),

$$
|\operatorname{curl}_\alpha H|^2 = |\operatorname{curl}_{\alpha,T} H|^2 + |\overrightarrow{\operatorname{curl}}_{\alpha,T} H_3|^2 + \left|\frac{\partial H_T}{\partial x_3}\right|^2 - 2\mathrm{Re}\left(\frac{\partial H_T}{\partial x_3}\cdot \overline{\nabla_{\alpha,T} H_3}\right).
$$

Combining the last two equations yields

$$
L(H) = h\int_{\Gamma_h}\left(\left|\frac{\partial H_T}{\partial x_3}\right|^2 + k^2|H|^2 - |\operatorname{curl}_{\alpha,T} H|^2 - |\overrightarrow{\operatorname{curl}}_{\alpha,T} H_3|^2\right)\mathrm{d}s
$$

where $L(H)$ is the left hand side of (6.26). It remains now to prove that the right hand side of the latter equation vanishes. First, we recall from Lemma 6.3.3 that $\partial H/\partial x_3 = T_\alpha H$ in $H_{\mathrm{p}}^{-1/2}(\Gamma_h)$ which yields that

$$
\int_{\Gamma_h}\left|\frac{\partial H_T}{\partial x_3}\right|^2 = \sum_{n\in\Lambda} |\beta_n \hat{H}_{T,n}|^2, \quad \int_{\Gamma_h}\left|\frac{\partial H_3}{\partial x_3}\right|^2 = \sum_{n\in\Lambda} |\beta_n \hat{H}_{3,n}|^2.
$$

Using the latter formulas and replacing k^2 by $|n+\alpha|^2+\beta_n^2$ in the first boundary term in (6.26) yields

$$
\begin{aligned}
&\int_{\Gamma_h}\left(\left|\frac{\partial H_T}{\partial x_3}\right|^2 + k^2|H|^2 - |\operatorname{curl}_{\alpha,T} H|^2 - |\overrightarrow{\operatorname{curl}}_{\alpha,T} H_3|^2\right)\mathrm{d}s \\
&= \sum_{n\in\Lambda}\Big[|\beta_n \hat{H}_{T,n}|^2 + (|n+\alpha|^2+\beta_n^2)(|\hat{H}_{T,n}|^2 + |\hat{H}_{3,n}|^2) - |(n+\alpha)\times \hat{H}_{T,n}|^2 - |n+\alpha|^2|\hat{H}_{3,n}|\Big] \\
&= \sum_{n\in\Lambda}\Big[(\beta_n^2 + |\beta_n|^2)|\hat{H}_{T,n}|^2 + |n+\alpha|^2|\hat{H}_{T,n}|^2 - |(n+\alpha)\times \hat{H}_{T,n}|^2 + \beta_n^2|\hat{H}_{3,n}|\Big]. \qquad (6.28)
\end{aligned}
$$

On the other hand, due to the divergence-free condition, we have

$$
\begin{aligned}
\sum_{n\in\Lambda}\Big[|n+\alpha|^2|\hat{H}_{T,n}|^2 - |(n+\alpha)\times \hat{H}_{T,n}|^2\Big] &= \sum_{n\in\Lambda} |(n_1+\alpha_1)\hat{H}_{1,n} + (n_2+\alpha_2)\hat{H}_{2,n}|^2 \\
&= \|\operatorname{div}_{\alpha,T} H_T\|^2_{L^2(\Gamma_h)} = \|\partial H_3/\partial x_3\|^2_{L^2(\Gamma_h)} = \sum_{n\in\Lambda} |\beta_n \hat{H}_{3,n}|^2.
\end{aligned}
$$

Now substituting the latter equation into (6.28) leads to

$$\int_{\Gamma_h} \left(\left| \frac{\partial H_T}{\partial x_3} \right|^2 + k^2 |H|^2 - |\operatorname{curl}_{\alpha,T} H|^2 - |\overrightarrow{\operatorname{curl}}_{\alpha,T} H_3|^2 \right) \mathrm{d}s = 2 \sum_{\beta_n \geq 0} \beta_n^2 |\hat{H}_n|^2, \tag{6.29}$$

where we exploited that β_n is either a non-negative or a purely imaginary number. The proof is hence finished if we show that $\sum_{\beta_n \geq 0} \beta_n^2 |\hat{H}_n|^2 = 0$ (since then $L(H) = 0$, which is the claim of the theorem). First, we compute that

$$\begin{aligned} \langle e_3 \times (R_\alpha \times H), H \rangle_{\Gamma_h} &= \sum_{n \in \Lambda} \mathrm{i}(n+\alpha) \cdot \overline{\hat{H}_{T,n}} \hat{H}_{3,n} - \sum_{n \in \Lambda} \mathrm{i}\beta_n |\hat{H}_{T,n}|^2 \\ &= - \sum_{n \in \Lambda} \mathrm{i}\overline{\beta_n} |\hat{H}_{3,n}|^2 - \sum_{n \in \Lambda} \mathrm{i}\beta_n |\hat{H}_{T,n}|^2. \end{aligned}$$

Since $\operatorname{Re}(\beta_n) \geq 0$ this implies that

$$\operatorname{Im}\langle e_3 \times (R_\alpha \times H), H \rangle_{\Gamma_h} = - \sum_{n \in \Lambda} \operatorname{Re}(\beta_n) |\hat{H}_n|^2 \leq 0, \text{ and} \tag{6.30}$$

$$\operatorname{Re}\langle e_3 \times (R_\alpha \times H), H \rangle_{\Gamma_h} = \sum_{n \in \Lambda} \operatorname{Im}(\overline{\beta_n}) |\hat{H}_{3,n}|^2 + \sum_{n \in \Lambda} \operatorname{Im}(\beta_n) |\hat{H}_{T,n}|^2. \tag{6.31}$$

(The second equation will be exploited later on.) Taking the imaginary part of the variational formulation (6.14) with $G = 0$ and $F = H$, and exploiting Lemma 6.3.3, we obtain that

$$0 = \operatorname{Im}\langle e_3 \times (R_\alpha \times H), H \rangle_{\Gamma_h} \overset{(6.30)}{=} - \sum_{n \in \Lambda} \operatorname{Re}(\beta_n) |\hat{H}_n|^2.$$

This implies that $|\hat{H}_n|^2 = 0$ for all n such that $\operatorname{Re}(\beta_n) > 0$. Since β_n is either purely imaginary or non-negative, we conclude that $\sum_{\beta_n \geq 0} \beta_n^2 |\hat{H}_n|^2 = 0$. □

The next Poincaré-like result is classical (see, e.g., [28] for a proof).

Lemma 6.5.2. *For $u \in \{v \in H^1_{\mathrm{p}}(\Omega) : v|_{\Gamma_0} = 0\}$ there holds $2\|u\|^2_{L^2(\Omega)} \leq h^2 \|\partial u / \partial x_3\|^2_{L^2(\Omega)}$.*

The following assumptions on $\varepsilon_{\mathrm{r}}^{-1}$ will guarantee a stability estimate and a uniqueness statement for a solution to the variational problem (6.14):

$$\begin{aligned} &(a) \quad \varepsilon_{\mathrm{r}}^{-1} \in W^{1,\infty}_{\mathrm{p}}(\Omega) \text{ satisfies } \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \leq 0 \text{ in } \Omega, \\ &(b) \quad \text{It holds that } \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} < 0 \text{ in a non-empty open ball } B \subset \Omega, \\ &(c) \quad \text{There exists } \delta > 1/2 \text{ such that } \frac{\delta}{2} \|\nabla_T \varepsilon_{\mathrm{r}}^{-1}\|^2_{L^\infty(\Omega)^2} + \frac{\sqrt{2}}{h} \left\| \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \right\|_{L^\infty(\Omega)} < \frac{2}{h^2}. \end{aligned} \tag{6.32}$$

Remark 6.5.3. *Note that* (6.32)*(a) implies that* $\varepsilon_{\mathrm{r}}^{-1} \geq 1$*, since, by construction,* $\varepsilon_{\mathrm{r}}^{-1} = 1$ *in* $\{h - \eta < x_3 < h\}$ *for some small* $\eta > 0$*. For the case of periodic non-absorbing structures, the main difference between these non-trapping conditions and the ones for the scalar case in [22] is the additional condition* (6.32)*(c). This condition arises from estimating the term* $2\mathrm{Re}\int_\Omega (\nabla\varepsilon_{\mathrm{r}}^{-1} \cdot \partial H/\partial x_3 \overline{H_3})\,\mathrm{d}x$ *in the Rellich identity* (6.26) *using the Poincaré-like result above. This is natural since the Rellich identity resulting from a similar technique for the scalar case [22] does not have a corresponding term.*

Let us construct a function $\varepsilon_{\mathrm{r}}^{-1}$ *that satisfies the above assumptions* (6.32)*. Choose constants* $0 < h_1 < h_2 < h$*,* $\lambda > 0$*, and a* C^1*-smooth cut-off function* $\chi \in C^1((0,2\pi)^2)$ *with compact support in* $(0,2\pi)^2$ *such that* $0 \leq \chi \leq 1$ *and* $\chi = 1$ *in* $(\pi/2, 3\pi/2)^2$*. For* $x = (x_1, x_2, x_3)^\top \in \Omega$*, we define*

$$\varepsilon_{\mathrm{r}}^{-1}(x_1,x_2,x_3) = \begin{cases} \lambda\chi(x_1,x_2) + 1, & 0 < x_3 < h_1, \\ \lambda\left(\frac{x_3-h_2}{h_1-h_2}\right)\chi(x_1,x_2) + 1, & h_1 < x_3 < h_2, \\ 1, & h_2 < x_3 < h. \end{cases}$$

Then $\varepsilon_{\mathrm{r}}^{-1}$ *is a decreasing function that satisfies* (6.32)*(a), and condition* (6.32)*(c) is satisfied when* $\lambda > 0$ *is small enough. Moreover,* $\varepsilon_{\mathrm{r}}^{-1}$ *also satisfies condition* (6.32)*(b) in* $(\pi/2, 3\pi/2)^2 \times (h_1, h_2)$*. However,* $\varepsilon_{\mathrm{r}}^{-1}$ *does not satisfy the corresponding conditions (7.2)(b,c) in [50], which require, roughly speaking, strict positivity of* $\partial\varepsilon_{\mathrm{r}}/\partial x_3$ *in* $(0,2\pi)^2 \times (h_1,h_2)$ *(an arbitrary ball* $B \subset \Omega$ *as in* (6.32)*(b) is not sufficient for the proof in [50]).*

Lemma 6.5.4. *Assume that* $\varepsilon_{\mathrm{r}}^{-1}$ *satisfies the three assumptions in* (6.32)*. Then there exists* $C > 0$ *(independent of* $k > 0$*) such that*

$$C\int_\Omega \left|\frac{\partial H}{\partial x_3}\right|^2 \mathrm{d}x \leq \int_\Omega x_3 \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} |\operatorname{curl}_\alpha H|^2\,\mathrm{d}x$$

for all solutions $H \in H^1_{\mathrm{p,T}}(\Omega)^3$ *to the homogeneous problem corresponding to* (6.14)*.*

Proof. We first estimate the two boundary terms in (6.26). We find that

$$-2\mathrm{Re}\int_{\Gamma_h} T_\alpha(H_3)\overline{H_3}\,\mathrm{d}s = 2\sum_{n\in\Lambda} \mathrm{Im}(\beta_n)|\hat{H}_{3,n}|^2 \geq 0.$$

Together with (6.31) we obtain

$$\mathrm{Re}\langle e_3 \times (R_\alpha \times H), H\rangle_{\Gamma_h} - 2\mathrm{Re}\int_{\Gamma_h} T_\alpha(H_3)\overline{H_3}\,\mathrm{d}s = \sum_{n\in\Lambda} \mathrm{Im}(\beta_n)|\hat{H}_n|^2 \geq 0.$$

Therefore, from the Rellich identity (6.26) we deduce $V(H) \leq 0$ where $V(H)$ is the volumetric

terms in (6.26). We need now to bound $V(H)$ from below,

$$V(H) = \int_\Omega \left[2\varepsilon_{\mathrm{r}}^{-1} \left| \frac{\partial H}{\partial x_3} \right|^2 - x_3 \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} |\operatorname{curl}_\alpha H|^2 + 2\mathrm{Re}\left(\nabla_T \varepsilon_{\mathrm{r}}^{-1} \cdot \frac{\partial H_T}{\partial x_3} \overline{H_3} + \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \frac{\partial H_3}{\partial x_3} \overline{H_3} \right) \right] \mathrm{d}x$$

$$\geq \int_\Omega \left[2 \left| \frac{\partial H}{\partial x_3} \right|^2 - x_3 \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} |\operatorname{curl}_\alpha H|^2 \, \mathrm{d}x \right] \mathrm{d}x - \gamma^{-1} \left\| \frac{\partial H_3}{\partial x_3} \right\|^2_{L^2(\Omega)} - \gamma \left\| \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \right\|^2_{L^\infty(\Omega)} \|H_3\|^2_{L^2(\Omega)}$$

$$- \delta \|\nabla_T \varepsilon_{\mathrm{r}}^{-1}\|^2_{L^\infty(\Omega)^2} \|H_3\|^2_{L^2(\Omega)} - \delta^{-1} \left\| \frac{\partial H_T}{\partial x_3} \right\|^2_{L^2(\Omega)^2}$$

for arbitrary $\delta, \gamma > 0$. Poincaré's inequality from Lemma 6.5.2 and the binomial formula imply that

$$V(H) \geq \int_\Omega \left[\left(2 - \frac{\delta h^2}{2} \|\nabla_T \varepsilon_{\mathrm{r}}^{-1}\|^2_{L^\infty(\Omega)^2}\right) \left| \frac{\partial H_3}{\partial x_3} \right|^2 + \frac{2\delta - 1}{\delta} \left| \frac{\partial H_T}{\partial x_3} \right|^2 - x_3 \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} |\operatorname{curl}_\alpha H|^2 \, \mathrm{d}x \right] \mathrm{d}x$$

$$- \gamma^{-1} \left\| \frac{\partial H_3}{\partial x_3} \right\|^2_{L^2(\Omega)} - \gamma \left\| \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \right\|^2_{L^\infty(\Omega)} \|H_3\|^2_{L^2(\Omega)}$$

Again, we exploit Poincaré's inequality, to find that

$$\gamma^{-1} \left\| \frac{\partial H_3}{\partial x_3} \right\|^2_{L^2(\Omega)} + \gamma \left\| \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \right\|^2_{L^\infty(\Omega)} \|H_3\|^2_{L^2(\Omega)} \leq \left(\gamma^{-1} + \gamma \frac{h^2}{2} \left\| \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \right\|^2_{L^\infty(\Omega)} \right) \left\| \frac{\partial H_3}{\partial x_3} \right\|^2_{L^2(\Omega)} .$$

The minimum of $\gamma \mapsto \gamma^{-1} + C\gamma$ is $2\sqrt{C}$. In consequence,

$$V(H) \geq \left[2 - \frac{\delta h^2}{2} \|\nabla_T \varepsilon_{\mathrm{r}}^{-1}\|^2_{L^\infty(\Omega)^2} - \sqrt{2} h \left\| \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} \right\|_{L^\infty(\Omega)} \right] \int_\Omega \left| \frac{\partial H_3}{\partial x_3} \right|^2 \mathrm{d}x$$

$$+ \frac{2\delta - 1}{\delta} \int_\Omega \left| \frac{\partial H_T}{\partial x_3} \right|^2 \mathrm{d}x - \int_\Omega x_3 \frac{\partial \varepsilon_{\mathrm{r}}^{-1}}{\partial x_3} |\operatorname{curl}_\alpha H|^2 \, \mathrm{d}x .$$

Finally, assumption (6.32)(c) implies that there exists $\delta > 1/2$ such that the first bracket on the right-hand side is positive. □

6.6 Uniqueness of Solution for All Wave Numbers

In this section, we prove our main uniqueness result for the electromagnetic scattering problem (6.14), under the assumption that ε_{r} satisfies (6.32). As mentioned above, corresponding uniqueness results that hold for all wave numbers currently exist, to the best of our knowledge, only for absorbing materials, see [105], or simpler two-dimensional structures, see [22].

Theorem 6.6.1. *Assume that $\varepsilon_{\mathrm{r}}^{-1}$ satisfies the assumptions* (6.32)*. Then problem* (6.14) *is uniquely solvable for all right-hand sides $G \in H^1_{\mathrm{p}}(\Omega)$ and for all wave numbers $k > 0$.*

Proof. Consider a solution $H \in H^1_{\mathrm{p,T}}(\Omega)^3$ to the homogeneous problem corresponding to (6.14). Due to Lemma 6.5.4 and the assumptions on $\varepsilon_{\mathrm{r}}^{-1}$ we obtain that $\partial H/\partial x_3 = 0$ in Ω and $\mathrm{curl}_\alpha H = 0$ in the ball B (see assumption (6.32)(b)). Equation (6.15) implies that H vanishes in B, too.

Since H is independent of x_3, it is sufficient to show that H vanishes on $\Gamma_{h-\eta} = \{(x_1, x_2, x_3) \in \Omega : x_3 = h - \eta\}$ for some (small) $\eta > 0$ to conclude that H vanishes entirely in Ω. If η is small enough, then all three components H_j, $j = 1, 2, 3$, satisfy

$$\Delta_\alpha H_j + k^2 H_j = 0, \qquad \Delta_\alpha H_j := \Delta H_j + 2i\alpha \cdot \nabla H_j - |\alpha|^2 H_j,$$

in some neighborhood of $\Gamma_{h-\eta}$. Let us denote by $\Delta_2 = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2$ the two-dimensional Laplacian. Since $\partial^2 H_j/\partial x_3^2$ vanishes, $H_j|_{\Gamma_{h-\eta}} \in H^1_{\mathrm{p}}(\Gamma_{h-\eta})$ is a weak solution to the two-dimensional equation

$$\Delta_2 H_j + 2i\alpha \cdot \nabla_T H_j + (k^2 - |\alpha|^2) H_j = 0 \quad \text{on } \Gamma_{h-\eta}, \quad j = 1, 2, 3.$$

Standard elliptic regularity results imply that $H_j|_{\Gamma_{h-\eta}}$ belongs to $H^2_{\mathrm{p}}(\Gamma_{h-\eta})$. Moreover, since H vanishes in the open ball B and since H is independent of x_3, H_j vanish in a non-empty relatively open subset of $\Gamma_{h-\eta}$.

In this situation, the unique continuation principle stated in Theorem 6.6.2 (see, e.g., [83]) implies that H_j vanishes on $\Gamma_{h-\eta}$ for $j = 1, 2, 3$, and hence H vanishes in Ω. □

Theorem 6.6.2. *Let $\mathcal{O}$ be an open and simply connected set in $\mathbb{R}^2$, and let $u_1, ..., u_m \in H^2(\mathcal{O})$ be real-valued such that*

$$|\Delta u_j| \le C \sum_{l=1}^{m} (|u_l| + |\nabla u_l|) \text{ in } \mathcal{O} \text{ for } j = 1, ..., m. \tag{6.33}$$

If u_j vanishes in some open and non-empty subset of $\mathcal{O}$ for all $j = 1, ..., m$, then u_j vanish identically in $\mathcal{O}$ for all $j = 1, ..., m$.

Appendix A

Smoothness of the Difference of Periodic Green's Functions

The following lemma is a consequence of the corresponding result for the fundamental solution to the Helmholtz equation in free-space (see Lemma 2.3.1).

Lemma A.0.3. *Assume that $k^2 \neq \alpha_j^2$ for all $j \in \mathbb{Z}$. Then the difference $G_{k,\alpha} - G_{\mathrm{i},\alpha}$ can be written as*

$$G_{k,\alpha}(x) - G_{\mathrm{i},\alpha}(x) = \alpha(|x|^2) + C|x|^2 \ln(|x|)\beta(|x|^2)$$

where α and β are analytic functions and C is a constant.

Proof. Recall that the Bessel function

$$J_n(t) = \sum_{p=0}^{\infty} \frac{(-1)^p}{p!(n+p)!}\left(\frac{t}{2}\right)^{n+2p} \qquad n = 0, 1, 2, ...$$

is an analytic function for all $t \in \mathbb{R}$. It is moreover well-known that the Neumann function

$$\begin{aligned} Y_n(t) = \frac{2}{\pi}\left\{ \ln\frac{t}{2} + C \right\} J_n(t) - \frac{1}{\pi}\sum_{p=0}^{n-1} \frac{(n-1-p)!}{p!}\left(\frac{2}{t}\right)^{n-2p} \\ - \frac{1}{\pi}\sum_{p=0}^{\infty} \frac{(-1)^p}{p!(n+p)!}\left(\frac{t}{2}\right)^{n+2p} \{\psi(n+p) + \psi(p)\} \end{aligned}$$

is analytic for $t \in (0, \infty)$. (Here $\psi(0) := 0$, $\psi(p) := \sum_{m=1}^{p} \frac{1}{m}$ for $p = 1, 2, \ldots$, and C is Euler's constant.) If $n = 0$ the finite sum in the expression of Y_n is set equal to zero. From [66] we know that the Green's function $G_{k,\alpha}$ can be split as $G_{k,\alpha}(x) = \frac{\mathrm{i}}{4}H_0^1(k|x|) + \Psi_k(x)$, where Ψ_k is an analytic function. The same decomposition holds for $G_{\mathrm{i},\alpha}$, with a different analytic function Ψ_{i}. Hence, it only remains to consider the difference $H_0^1(k|x|) - H_0^1(\mathrm{i}|x|)$. To this

end, we note that

$$\begin{aligned} J_0(k|x|) - J_0(\mathrm{i}|x|) &= \sum_{p=0}^{\infty} \frac{(-1)^p}{(p!)^2 4^p} \Big[(k|x|)^{2p} - (\mathrm{i}|x|)^{2p} \Big] \\ &= |x|^2 \sum_{p=0}^{\infty} \frac{(-1)^{p+1}}{[(p+1)!]^2 4^{p+1}} \Big[(k)^{2p+2} - (\mathrm{i})^{2p+2} \Big] (|x|^2)^p. \end{aligned} \tag{A.1}$$

Use the ratio test one can check that the power series in (A.1) converges to some analytic function of the variable $|x|^2$ in $\mathbb{R}$. Moreover, due to the expression of Y_0 we can see that

$$Y_0(k|x|) - Y_0(\mathrm{i}|x|) = \frac{2}{\pi} \ln(|x|) \Big[J_0(k|x|) - J_0(\mathrm{i}|x|) \Big] + \Psi_1(|x|^2), \tag{A.2}$$

where Ψ_1 is an analytic function. Furthermore, we have

$$\begin{aligned} G_{k,\alpha}(x) - G_{\mathrm{i},\alpha}(x) &= \frac{\mathrm{i}}{2} \Big[H_0^1(k|x|) - H_0^1(\mathrm{i}|x|) \Big] \\ &= J_0(k|x|) - J_0(\mathrm{i}|x|) + \mathrm{i} \Big[Y_0(k|x|) - Y_0(\mathrm{i}|x|) \Big]. \end{aligned}$$

Substitution of (A.1) and (A.2) into the last equation finishes the proof. □

Now we prove a similar result for the fundamental solution to the three-dimensional Helmholtz equation in free-space.

Lemma A.0.4. *Assume that* $\Phi_k(x) = \exp(\mathrm{i}k|x|)/(4\pi|x|)$ *for* $x \neq 0$. *We have*

$$\Phi_k(x) - \Phi_{\mathrm{i}}(x) = \alpha(|x|^2) + |x|\beta(|x|^2)$$

where α *and* β *are analytic functions.*

Proof. First we have

$$e^{-|x|} = \sum_{n=0}^{\infty} \frac{(-1)^n |x|^n}{n!} = \sum_{n=0}^{\infty} \frac{|x|^{2n}}{(2n)!} - \sum_{n=0}^{\infty} \frac{|x|^{2n+1}}{(2n+1)!} \tag{A.3}$$

By the ratio test the last sum in (A.3) can be rewritten as $|x|f(|x|^2)$ where f is an analytic function. Therefore,

$$e^{-|x|} = 1 + \sum_{n=1}^{\infty} \frac{|x|^{2n}}{(2n)!} - |x|f(|x|^2)$$

In the other hand we know that

$$e^{\mathrm{i}k|x|} = \cos(k|x|) + \mathrm{i}\sin(k|x|) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n k^{2n} |x|^{2n}}{(2n)!} + \mathrm{i} \sum_{n=0}^{\infty} \frac{(-1)^n k^{2n+1} |x|^{2n+1}}{(2n+1)!} \tag{A.4}$$

Similarly the last sum in (A.4) converges to $|x|g(|x|^2)$ where g is an analytic function. We hence obtain

$$\begin{aligned} e^{\mathrm{i}k|x|} - e^{-|x|} &= \sum_{n=1}^{\infty} \frac{[(-1)^n k^{2n} - 1]|x|^{2n}}{(2n)!} + |x|(f+g)(|x|^2), \\ &= |x|^2 \sum_{n=0}^{\infty} \frac{[(-1)^{n+1} k^{2n+2} - 1]|x|^{2n}}{(2n+2)!} + |x|(f+g)(|x|^2) \end{aligned}$$

Now the ratio test deduces that the first sum converges to $|x|^2 l(|x|^2)$ where l is an analytic function. This implies that

$$\frac{e^{\mathrm{i}k|x|}}{4\pi|x|} - \frac{e^{-|x|}}{4\pi|x|} = \frac{(f+g)(|x|^2)}{4\pi} + |x|\frac{l(|x|^2)}{4\pi},$$

which completes the proof.

□

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