Scattering by Biperiodic Layered Media: The Integral Equation Approach

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Habilitationsschrift
Karlsruhe
February 2010

Acknowledgements

First of all, I would like to thank my collaborators Armin Lechleiter, Kai Sandfort and Susanne Schmitt for their efforts on work related to this thesis. Our cooperation has been a great inspiration in the last phase of the writing of this work.

For many discussions and suggestions on how to pursue the research presented in this thesis, special thanks go to Simon Chandler-Wilde, Frank Hettlich and my adviser Andreas Kirsch. To Frank I am especially grateful for patiently suffering my countless interruptions of his work with some issue to discuss.

Lastly, I wish to thank my family, Anja, Charlotte and Frederik for being such a great support and a constant reminder that there is much more to life than mathematics.

Karlsruhe, November 2009

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Chapter 1

Introduction

The propagation of time-harmonic acoustic waves in a homogeneous medium is described by the Helmholtz equation

$$\Delta u + k^2 u = 0,$$

where u denotes (a potential) of the acoustic pressure field with a time dependence of $e^{-i\omega t}$ suppressed, and $k > 0$ the wave number. A detailed physical derivation is given in the introduction of [23].

A typical scattering problem is obtained, if the Helmholtz equation is posed in the exterior of some bounded domain and some boundary condition for the field is imposed on the boundary of this domain. The total field is split into the incident part describing the field in the absence of the scatterer and the scattered part which is the correction due to the presence of the scatterer.

In the case of a bounded scatterer, the scattered field asymptotically behaves like an outgoing spherical wave. This behaviour is reflected by the well-known Sommerfeld radiation condition. Physically, this condition ensures causality, mathematically it guarantees uniqueness of solution to the scattering problem.

A typical incident field is a plane wave,

$$u(x) = \exp(ik\, d \cdot x), \qquad x \in \mathbb{R}^3,$$

with $d \in \mathbb{R}^3$ a unit vector. Such a field is periodic in all spatial directions. What can we expect if we combine such a field with a scatterer also exhibiting some kind of perodicity?

Such diffraction grating problems where first considered by Lord Rayleigh [56] in 1907 and have since then received considerable attention. Firstly, due to its periodicity, the scatterer is no longer bounded and hence the Sommerfeld ratiation condition is in general not appropriate. Thus, the question of an appropriate radiation condition arises. Secondly, the problem may not be uniquely solvable, depending on the exact shape of the scatterer and the boundary condition imposed. The simple example of a flat surface with a Neumann boundary condition imposed shows this: any plane wave propagating parallel to the surface is a solution to the homogenous problem. Thirdly, it is important for applications to have efficient schemes available to compute the fields.

For two-dimensional problems, all these questions have been answered satisfactorily. Summaries of the results that have been established can be found in the monographs [7, 54]. For three-dimensional problems the question of efficient numerical schemes in particualar is still subject to on-going research. This thesis will contribute to this effort.

More generally than described above, we here consider scattering and transmission problems for the Helmholtz equation. The medium will be assumed to be biperiodic, i.e. periodic in two linearly independent spacial directions. We further make the following simplifying assumptions: that the two directions of periodicity be orthogonal, identifying them with the x_1 and x_2-coordinate directions, and that the medium be homogeneous outside a certain layer bounded in the x_3-direction.

We will also assume that the medium consists of layers in each of which the material properties are constant and, for much of this work, that the interfaces between these layers are representable as graphs of smooth functions. The wave number will be assumed to be such that the wave length is of a size comparable to the periods of the medium.

Except for special cases, there will be no common period for both medium and incident field, hence the scattered field will be only quasi-periodic, i.e. periodic up to a phase shift. Nevertheless, methods of Fourier analysis can be applied and are a common tool for the analysis of such diffraction problems.

Such problems play an important role for a number of applications. Some examples are scattering by rough surfaces such as the ocean surface, the design and simulation of thin solar cells, the structuring of surfaces in organic light emitting diodes (OLEDs) or the design of photonic crystals to have a certain band gap structure. In many of these problems, one considers periodic structures, as these on the one hand reduce the scale of the problem under consideration to just one cell of periodicity, while on the other hand the periodic nature generates a rich mathematical structure in the solutions.

We will pay particular attention to problems in which interfaces between the layers are very smooth. There are two particular reasons why we investigate this case rather than trying to develop general methods for interfaces with edges and corners: Firstly, smooth interface make it possible to develop boundary integral equation procedures with high order of convergence, as will be demonstrated by the results in this work. Secondly, for some applications such as the inverse problem of the reconstruction of a scatterer, edges and corners are not of importance as these cannot be resolved due to the ill-posedness of the problem. Here, it is more important to have highly accurate solvers available in order not to polute the results further by discretization errors.

1.1 State of the Art

As outlined above, this thesis will build on results obtained for proving uniqueness and existence of solution for scattering by biperiodic structures and on approaches for the numerical solution of the resulting boundary integral equations. Let us briefly review results currently known in these areas.

Work in the Two-Dimensional Case. Before starting the discussion of results for the three-dimensional case, let us briefly consider the case where the medium and the incident field are constant in, say, the x_2-direction. In this case, the problem reduces to a two-dimensional scattering or transmission problem for a periodic surface which has received continuous attention from researchers since the original paper by Lord Rayleigh [56] in 1907. There is a vast amount of literature on the subject available today.

Early computational approaches focused on the possibility of representing the scattered field as a Fourier series in the domain above the surface, the so-called Rayleigh hypothesis. Although this general assumption turned out to be untrue, nevertheless this approach turned out to be quite successful. A detailed account of the state of the art of such approaches in 1980 may be found in the compilation edited by R. Petit [54].

Another question receiving considerable attention was that of uniqueness and existence of solutions. For the case of a homogeneous medium bounded by an impenetrable surface with a Dirichlet or Neumann boundary condition, based on the work of Alber [3], Wilcox [65] proved that the spectrum of Laplace operator forms a sequence of discrete eigenvalues accumulating at 0. Rigorous justifications of similar results in the case of more complicated media formed by subdomains with piecewise homogeneous index of refraction were established only recently by Elschner et al. [30].

In order to say more on uniqueness of solution, geometrical assumptions on the form of the diffraction grating and a Dirichlet boundary condition, or a monotonicity property of the index of refraction are required. Bonet-Bendhia and Starling [11] give examples of non-uniqueness if such conditions are not satisfied. Chandler-Wilde and Zhang [18–20, 67] have proved uniqueness of solution for a number of problems even in the more general case of a non-periodic unbounded scatterer if such conditions are met. Similar principles apply in wave guides [4, 51, 55]. However, giving a more restrictive characterization of the eigenvalues of the problem than formulated by Wilcox even in the case of a single periodic surface with a Neumann boundary condition remains an open problem.

The application of boundary integral equation methods to such transmission or scattering problems requires the knowledge of the quasi-periodic Green's function for the Helmholtz equation. This can be thought of as being formed by a periodic array of point sources whose amplitudes differ by an appropriate phase shift. Although conceptionally simple, this Green's function turns out to be difficult to evaluate in general. One can formulate representations in terms of plane and evanescent waves or formalize the idea of a periodic array of mono-poles. Neither approach leads to expressions that are satisfactory from the point of view of numerical evaluation, at least not for all choices of arguments and parameters. Intensive research has been carried out in developing various representations for this function. The review by Linton [45] gives an excellent review of many of these methods with an extensive list of further references. Among the methods reported on by Linton is a method developed by Ewald [31], originally for the computation of three dimensional lattice potentials. This method will play an important role in the present work as well.

With the availability of the Green's function, the formulation of boundary integral equations is not substantially different from the case of scattering by bounded obstacles. Because of periodicity, the computational domain may be reduced to a single period of the grating. In the case of scattering by a single periodic surface, the resulting integral equation is in essence identical to that of scattering by a single bounded obstacle, and the same numerical methods can be applied. In the case of a grating representable as the graph of a smooth function, high order Nyström methods may be applied leading to a scheme with super-algebraic convergence [49].

Work in the Three-Dimensional Case. In the fully three-dimensional problem, the medium and the incident field are assumed to be periodic in, say, the x_1 and x_2 directions. In the x_3 direction, the medium may be variable in general, however it is usually assumed that the material properties remain constant outside some bounded layer. A simpler case called *conical diffraction* arises if the medium is assumed to be still constant in the x_2-direction but the incident field is not. Such problems essentially reduce to coupled two-dimensional ones and have been considered for Maxwell's equations in [29].

The main applications for the fully three-dimensional problem lie in area of scattering of electromagnetic fields, so the literature is strongly focused on Maxwell's equations. The Helmholtz equation appears not to have been considered so far. A series of papers in the 1990s [1,6,8,26] was written on the subject of giving variational formulations and on establishing uniqueness and existence theorems for these, although they involve more restrictive assumptions than used in [30]. The main results are similar to those in two-dimensions: There may exist an most countable set of frequencies with infinity as the only possible accumulation point for which the problem is not uniquely solvable. More specific results for certain types of scatteres appear not have been established.

Most numerical work has been based on finite element discretizations of the variational problem. Boundary integral equation methods for scattering by biperiodic media have not been used very much in the mathematical community. In [27, 52] such equations are formulated for Maxwell's equation based on a quasi-biperiodic Green's function. A Fourier series expansion of this Green's function is derived and it is proved that is converges allmost everywhere to a smooth function. However, the expression is not well suited to numerical evaluation. Thus, the main hurdle for the application of integral equations appears to be the availability of reliable and efficient numerical procedures for the evaluation of the quasi-biperiodic Green's function.

Numerical Solution of Integral Equations. It will be the goal in this work to formulate scattering and tansmission problems for biperiodic media equivalently as integral equations on the interfaces between the subdomains with homogeneous properties. There are three principle classes of methods for integral equations: Galerkin methods, collocation methods and quadrature methods (also known as Nyström methods). Of these three classes, Galerkin methods are most popular in the mathematics literature (see [57] for a recent overview of such methods). Such methods are elegant and they can build on the vast literature on Finite Element methods. Most importantly, through the Céa-Lemma and approximation results for finite element basis functions, stability of the corresponding discrete equations is assured. This is not the case for collocation methods, making their analysis much harder. However, as collocation methods are easier to implement efficiently than Galerkin methods, they are more popular in the engineering literature.

Quadrature methods conceptionally form the simplest class of methods. However, their application to boundary integral equations in three dimensions is inhibited by the inavailability of suitable quadrature rules computing integrals over weakly singular integrals to high order. For bounded obstacles globally parametrizable over a sphere, Wienert [64] proposed at Nyström method but could not prove convergence. The method was modified by Graham and Sloan [36] to a high-order Galerkin method bases on spherical harmonics. An implementation was reported on in [32]. An algorithm more similar to a Nyström method and applicable to general obstacles was proposed by Bruno and Kunyanski [13, 14]. Although many numerical experiments showed a high order of convergence was achieved, no proofs of convergence were provided. Some progress was made by Heine2008, who analysed a related method for in classical function spaces. Recently, some results in this direction have been announced [12, 28] involving a modification of the method, however no preprint or publication is available, yet.

1.2 Results Presented in this Thesis

This study of scattering problems for biperiodic layered media will start in Chapter 2 with a presentation of variational formulation of such problems. The presentation is very much in the spirit of [30]. Rather than stating many new results, this chapter provides a review of presently used methods. However, the application to the Helmholtz equation in three dimensions appears not to have been published so far, most authors being concerned with Maxwell's equations.

While the first section introduces basic notations and some preliminary results that will be used throughout this work, the second section deals with radiation conditions and the Dirichlet-Neumann operators they give rise to. The careful analysis of the mapping properties of these operators is the basis of the weak formulations of the scattering problems presented in Section 2.3. The corresponding analysis uses analytic continuation principles for operators to establish uniqueness and existence of solution for these problems for all but a countable number of wave numbers accumulating only at infinity. Corresponding results for transmission problems are provided in 2.4.

Some novel results presented in Chapter 2 are general uniqueness results for the Dirichlet scattering in Theorem 2.29 and for the transmission problem in Theorem 2.40. These are based on special geomtrical properties of the interfaces or monotonicity satisfied by the indeces of refraction. Some similar results have been reported in two spacial dimensions, for scattering problems involving rough surfaces or in wave guides [4, 11, 18–20, 51, 55, 67].

The central element for boundary integral equations is the quasi-biperiodic Green's function which we derive and analyze in Chapter 3. Representations as a Fourier series and as a superposition of point sources are presented, but these series have limited domains of convergence and are not well suited for numerical evaluation. A more general representation as the sum of two exponentially convergent series regardless of the choice of parameters is derived using Ewald's method [31]. Such expressions have so far only been derived in the physics community [40], but not with the mathematical rigour of our presentation. This material is complemented by Appendix A, in which the numerical evaluation of the Green's function is discussed. These results have been obtained in a separate effort together with Lechleiter, Sandfort and Schmitt [5].

We continue in Section 3.3 with studying analytic properties of the Green's function. Several representations needed for later numerical applications are derived. We put an emphasis on giving these representations explicitely, making it obvious that every term is indeed computable.

Chapter 4 is devoted to deriving integral equation formulations for the scattering and transmission problems. We work in fractional order Sobolev spaces on the interfaces between the layers, defining potentials and boundary operators in the spirit of [48]. Most results in this chapter are quite similar to standard results on boundary operators and boundary integral equations, although details concerning the application to biperiodic problems may differ. We use mapping properties of the boundary operators for smooth interfaces derived in [41, 42] to establish existence of solution and regularity of the densities in Theorem 4.25.

For two-dimensional problems, Fourier representations of the Green's function allow the formulation of super-algebraically convergent quadrature methods [49]. With the results of Chapter 3 we have such a representation at hand. Chapter 5 explores the application of Nyström methods based on this representation to a class of biperiodic integral equations. The stability and convergence analysis is carried out in biperiodic Sobolev spaces. Unfortunately these results are not directly applicable to the boundary integral equations arising from scattering problems: the kernels of the correpsonding integral operators contain a directional singularity that cannot be treated in this approach. Still, the results are promising in that a combination with a further approximation of the kernels may provide a high-order numerical method for solving the bounary integral equations on a simple grid.

A numerical method that can be directly applied to the boundary integral equations at hand is presented in Chapter 6. It is based on the idea of locally replacing a cartesian grid by polar coordinates to be able to integrate the weak singularities to high order [13,14]. We study a modification of this method. Except for an additional approximation in the weakly singular operator, the approach can be viewed as a collocation method in spaces of trigonometric polynomials, hence we use the term *quasi-collocation method* to describe it. We prove stability and convergence of this modified method, amounting to the result that we have convergence of any order in the case where the boundary is representable as the graph of an infintely smooth function in Corollary 6.8. No comparable published result is known to the author.

Although with establishing super-algebraic convergence of the method for arbitrarily smooth surfaces a central goal of this thesis is achieved, many open questions remain. Primarily, the numerical scheme analyzed in Chapter 6 is quite costly. It remains to establish how this cost can be reduced by suitable matrix compression schemes and further approximations. Using the results on numerical evaluation of the Green's function, a reference implementation of the scheme is then the next obvious step.

1.3 Some Notational Conventions

Throughout this thesis, we will number equations and special statements such as theorems, definitions and remarks consecutively in each chapter. A single numbering scheme will be used for theorems, definitions and remarks in order to facilitate the finding of references.

For mathematical notation we attempt to minimize the use of not generally accepted notation or to explain such notation in places where it occurs. Much general notation for domains, surfaces and spaces used throughout this work is explained or defined in Section 2.1. Although an effort has been made to avoid the use of symbols with mutiple meanings, we may have failed in a few instances.

A convention we use without further mentioning is that for vectors $x \in \mathbb{R}^d$, $d = 2, 3$, the coordinates are referenced by x_j, $j = 1, \ldots, d$, i.e. $x = (x_1, \ldots, x_d)^\top$. All vectors are column vectors unless this is explicitely stated otherwise.

In many case, we will be working with vectors $x \in \mathbb{R}^3$ and their orthogonal projections on the (x_1, x_2)-plane. Hence, for any vector $x = (x_1, x_2, x_3)^\top \in \mathbb{R}^3$, we define

$$\tilde{x} := \begin{pmatrix} x_1 \\ x_2 \\ 0 \end{pmatrix}.$$

Also, in a simplifying abuse of notation, we will sometimes identify the plane $\mathbb{R}^2 \times \{0\}$ with $\mathbb{R}^2$ in using $\tilde{x}$ as a two-dimensional vector.

For $x \in \mathbb{R}^d$, $|x|$ will denote the vector's Euclidean norm. The symbols $\|\cdot\|$ or $|||\cdot|||$ will be used to denote various norms on function spaces. Finally, the (Lebesgue)-measure of some set $M \subseteq \mathbb{R}^n$ will also be denoted by $|M|$.

Chapter 2

Problem Formulation and Uniqueness of Solution

2.1 Preliminaries

Periodic Domains and Functions. It is our objective to study the scattering of time-harmonic waves in biperiodic media. Throughout we will assume that the directions of periodicity lie in the directions of the x_1- and x_2-axis. The periods will be denoted by L_1 and L_2, respectively, and the unit cell of the underlying periodic lattice by $Q := (-L_1/2, L_1/2) \times (-L_2/2, L_2/2)$.

When working with such biperiodic media, two sets of vectors will play an important role: the *translation vectors* of the lattice, $p^{(\mu)}$, defined by

$$p^{(\mu)} := \begin{pmatrix} \mu_1 L_1 \\ \mu_2 L_2 \\ 0 \end{pmatrix}, \qquad \mu \in \mathbb{Z}^2, \tag{2.1}$$

and the *reciprocal lattice vectors*, $q^{(\nu)}$, which are given by

$$q^{(\nu)} := \begin{pmatrix} \nu_1 2\pi/L_1 \\ \nu_2 2\pi/L_2 \\ 0 \end{pmatrix}, \qquad \nu \in \mathbb{Z}^2. \tag{2.2}$$

A useful property of these vectors is that $p^{(\mu)} \cdot q^{(\nu)} \in 2\pi\mathbb{Z}$ for any μ, $\nu \in \mathbb{Z}^2$.

Of particular interest to us are functions that reflect the periodic nature of the underlying domain. A function $u : \mathbb{R}^3 \to \mathbb{C}$ is called *Q-periodic* if

$$u(x + p^{(\mu)}) = u(x) \qquad \text{for all } x \in \mathbb{R}^3,\ \mu \in \mathbb{Z}^2. \tag{2.3}$$

The function is said to be *Q-quasi-periodic with phase-shift* $\alpha \in \mathbb{R}^3$ if

$$u(x + p^{(\mu)}) = \exp(i\alpha \cdot p^{(\mu)})\, u(x) \qquad \text{for all } x \in \mathbb{R}^3,\ \mu \in \mathbb{Z}^2. \tag{2.4}$$

Note here, that the third component of the vector α does not play any role in the definition, i.e. we implicitly use only the projection of α onto the (x_1, x_2)-plane. We might have replaced α by $\tilde{\alpha}$ without changing the definition.

One important property of Q-periodic functions is that they can be expanded into a Fourier series. In our notation, this expansion takes the form

$$u(x) = \sum_{\nu \in \mathbb{Z}^2} u_\nu(x_3) \, \exp(i \, q^{(\nu)} \cdot x), \tag{2.5}$$

with some set of Fourier coefficients $(u_\nu(x_3))$ for all $x_3 \in \mathbb{R}$, given by

$$u_\nu(x_3) = \frac{1}{|Q|} \int_Q u(x) \, \exp(-i \, q^{(\nu)} \cdot x) \, d\tilde{x}.$$

The smoothness of u is reflected in the decay of the Fourier coefficient, e.g. for $(u_\nu(x_3)) \in \ell^2$, we have $u(\cdot, x_3) \in L^2(Q)$. For faster or slower decaying coefficients we obtain elements of fractional Sobolev spaces or their duals, respectively. This aspect of the Fourier series expansion will be studied in more detail later on.

For a Q-quasi-periodic function u, it is easy to check that

$$v(x) := \exp(-i\tilde{\alpha} \cdot x) \, u(x)$$

is Q-periodic. Hence, we obtain a similar Fourier expansion for the Q-quasi-periodic function u,

$$u(x) = \sum_{\nu \in \mathbb{Z}^2} u_\nu(x_3) \, \exp(i \, (\tilde{\alpha} + q^{(\nu)}) \cdot x). \tag{2.6}$$

where in this case

$$u_\nu(x_3) = \frac{1}{|Q|} \int_Q u(x) \, \exp(-i \, (\tilde{\alpha} + q^{(\nu)}) \cdot x) \, d\tilde{x}.$$

As we will use this relation between Q-quasi-periodic functions and their Q-periodic counterparts quite regularly, let us introduce the operator M_α performing a multiplication by $\exp(i\tilde{\alpha} \cdot x)$, such that with the above notation

$$v = M_{-\alpha} u.$$

Of course, we will not only be interested in Q-periodic functions defined on all of $\mathbb{R}^3$. However, we treat this case by periodic extension: A set $D \subset \mathbb{R}^3$ will be called a *cell set*, if the orthogonal projection of D onto the x_1,x_2-plane is a subset of Q. For a cell set D, we define the Q-periodic extension $E_Q(D)$ by

$$E_Q(D) := \{x \in \mathbb{R}^3 : x + p^{(\mu)} \in D \text{ for some } \mu \in \mathbb{Z}^2\}.$$

Then, the definitions of Q-periodic and Q-quasi-periodic functions can be extended to functions defined on $E_Q(D)$.

The scattering and transmission problems will be given in their weak form later on, and we will be needing appropriate Sobolev spaces for this purpose. For any open set $\Omega \subset \mathbb{R}^3$, by $C^m(\bar{\Omega})$ we denote the usual space of m times continuously differentiable functions on Ω, $m \in \mathbb{N}_0$, with continuous extensions to $\bar{\Omega}$. With the inner product

$$\langle u, v \rangle_m := \sum_{|\mu| \le m} \int_\Omega \partial^\mu u \, \overline{\partial^\mu v} \, dx,$$

where μ denotes some multi-index and ∂^μ the corresponding partial derivative, and the associated norm $\|u\|_m := (\langle u, u \rangle_m)^{1/2}$, we obtain the standard Sobolev spaces by completing $C^m(\bar{\Omega})$ in this norm,

$$H^m(\Omega) := \overline{C^m(\bar{\Omega})}^{\|\cdot\|_m}.$$

For $m = 0$, we obtain the usual space of square integrable functions, $H^0(\Omega) = L^2(\Omega)$. We will also employ the spaces

$$H^m_{\text{loc}}(\Omega) := \{u : \Omega \to \mathbb{C} : u \in H^m(\Omega') \text{ for any open, bounded set } \Omega' \text{ such that } \overline{\Omega'} \subset \Omega\}.$$

To accomodate periodic functions, spaces of such functions are required. Assume the domain D to be a cell set. We introduce

$$C^m_Q(\bar{D}) := \left\{ u|_D : u \in C^m\left(\overline{E_Q(D)}\right), \, u \text{ is } Q\text{-periodic} \right\}.$$

Obviously, $C^m_Q(\bar{D}) \subset C^m(\bar{D})$, and hence the inner product $\langle \cdot, \cdot \rangle_m$ is well defined on this space as well. Again, by a norm closure process, we obtain the Hilbert spaces

$$H^m_Q(D) := \overline{C^m_Q(\bar{D})}^{\|\cdot\|_m},$$

and the spaces

$$H^m_{Q,\text{loc}}(D) := \{u : E_Q(D) \to \mathbb{C} : u \in H^m_Q(D') \text{ for any bounded, open } D' \text{ such that } \overline{D'} \subset D\}.$$

Remark 2.1 From the definitions it is clear that $H^m_Q(D)$ forms a closed subspaces of $H^m(D)$. The two spaces are equal if $m = 0$. It follows from the trace theorem, that $H^m_Q(D)$ is a true subspace if $m \ge 1$. □

Interfaces and Layered Media. The scattering problems we will be considering, all share a common structure of the underlying medium. Besides the periodicity in the horizontal directions, we will assume that the medium consists of a finite number of distinct layers in the vertical direction. We will now define a corresponding mathematical structure of domains.

Assumption 2.2 *Let $N \in \mathbb{N}$, M_1, $M_2 \in \mathbb{R}$ with $M_1 < M_2$ and define $D := Q \times (M_1, M_2)$. For $j = 0, \dots, N$, let $\Gamma_j \subset D$ denote a Lipschitz surface such that the following conditions are satisfied:*

- *for each $y \in Q$, there exists $x \in \Gamma_j$ such that $\tilde{x} = y$, $j = 0, \dots, N$,*
- *for each $x^{(j)} \in \Gamma_j$, $x^{(j+1)} \in \Gamma_{j+1}$ such that $\tilde{x}^{(j)} = \tilde{x}^{(j+1)}$, there holds $x_3^{(j)} < x_3^{(j+1)}$, $j = 0, \dots, N-1$.*

Further introduce the plane surfaces $\Gamma^- := Q \times \{M_1\}$ and $\Gamma^+ := Q \times \{M_2\}$.

The surfaces Γ_j, $j = 0, \dots, N$ divide D into $N+2$ subdomains which we label D_j, $j = -1, \dots, N$, where D_j is bounded from below by Γ_j, or by Γ^- in the case of D_{-1} and from above by Γ_{j+1}, or by Γ^+ in the case of D_N.

We also introduce the unbounded domains $D^- := Q \times (-\infty, M_1)$ and $D^+ := Q \times (M_2, \infty)$.

The geometric relations of these surfaces and domains are shown in Figure 2.1.

Remark 2.3 With these assumptions, the domains D_j, D^-, D^+ are all Lipschitz domains (see [48, Chapter 3] for a definition). For almost every point $x \in \Gamma_j$ a unit normal vector $n(x)$ is defined, where we assume that $n(x)$ is pointing into D_j. The normal on Γ^+ and Γ^- will also be assumed to point upward, i.e. it is the third unit coordinate vector. □

More stringent assumptions will be made on the nature of the surfaces Γ_j later on, particularly regarding their smoothness. Of particular importance will be the case when each Γ_j is given as the graph of a smooth, Q-periodic function f_j.

In the scalar problems we will consider, we will be interested in functions u that are solutions to the Helmholtz equation

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

in D^+ (and D^-) while satisfying the modified Helmholtz equations

$$\Delta u + q_j k^2 u = 0$$

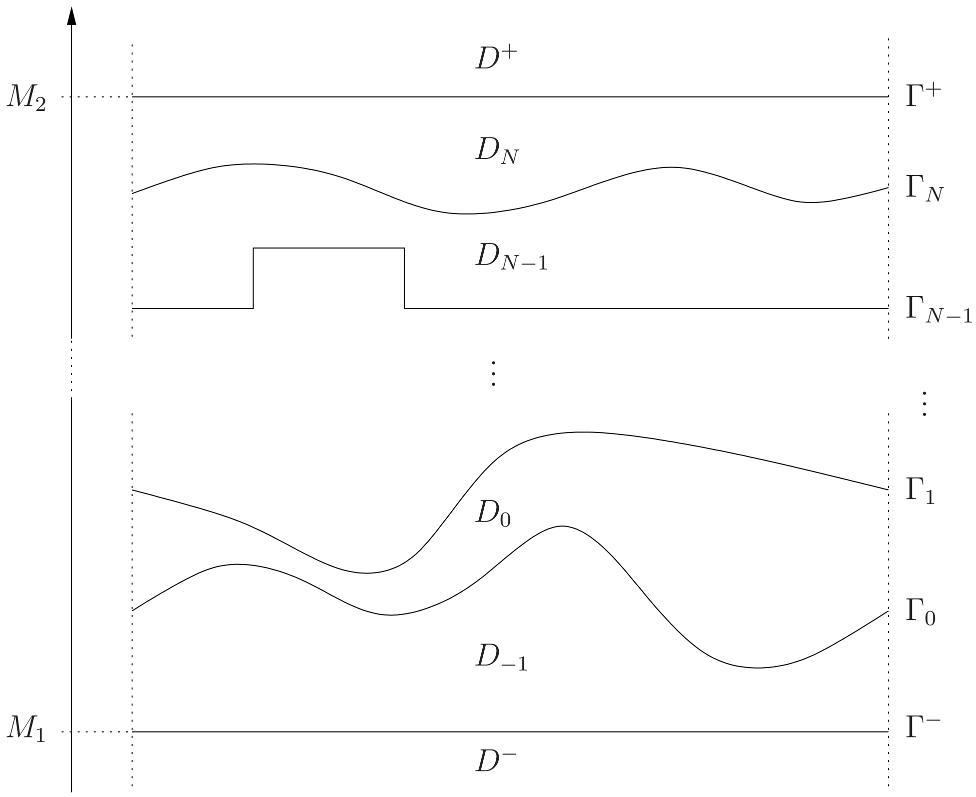


Figure 2.1: Cross section of an example for admissable surfaces Γ_j and the domains D_j generated by these.

in each domain D_j. Here k denotes the wave number and q_j the constant index of refraction of the material filling the domain D_j. The wave number is assumed to be a real positive number.

Precise assumptions on the indices of refraction will be given later in Section 2.3. However, let us state here that we will assume $q_{-1} = q_N = 1$. For each individual scattering or transmission problem, the function u will also have to satisfy appropriate transmission or boundary conditions on the interfaces Γ_j. These conditions will also be stated in Section 2.3.

Sobolev Spaces on Surfaces and Interfaces. On each Lipschitz surface $\Gamma \in \{\Gamma_0, \ldots, \Gamma_N, \Gamma^-, \Gamma^+\}$, the fractional Sobolev spaces $H^s(\Gamma)$, $0 \leq s \leq 1$ can be defined by the usual process of defining these spaces on (subsets of) $\mathbb{R}^2$ and lifting them to Γ through a piecewise parametrization (see e.g. [48, Chapter 3] for details). The dual of $H^s(\Gamma)$ is usually denoted by $\tilde{H}^{-s}(\Gamma)$, the closure of $C_0^\infty(\Gamma_j)$ in the H^{-s}-norm.

We will also need some appropriate Sobolev spaces of periodic functions. We start on the unit cell Q. Similarly to (2.5), we can expand a function $\varphi \in L^2(Q)$ into the Fourier series

$$\varphi(x) = \sum_{\nu \in \mathbb{Z}^2} \varphi_\nu \exp(i \widetilde{q^{(\nu)} \cdot x}), \qquad x \in Q,$$

with Fourier coefficients $(\varphi_\nu) \in \ell^2$. Using this notation, we define, for $s \geq 0$, the Sobolev spaces H_Q^s of Q-periodic functions by

$$H_Q^s := \left\{ \varphi \in L^2(Q) : \sum_{\nu \in \mathbb{Z}^2} (1 + |\nu|^2)^s \, |\varphi_\nu|^2 < \infty \right\}.$$

This space is a Hilbert space with the inner product

$$(\varphi, \psi)_{Q,s} := \sum_{\nu \in \mathbb{Z}^2} (1 + |\nu|^2)^s \, \varphi_\nu \, \overline{\psi_\nu}. \tag{2.7}$$

The elements of H_Q^s can be periodically extended to functions defined on $\mathbb{R}^2$ with the same local smoothness properties. The span of the trigononmetric polynomials $\{\exp(iq^{(\nu)} \cdot \cdot)\}$ forms a dense subspace of H_Q^s for all $s \geq 0$. By H_Q^{-s} we denote the dual space of H_Q^s with respect to the L^2 inner product. We also set

$$|||\varphi|||_{Q,s} := \sqrt{(\varphi, \varphi)_{Q,s}}.$$

Let now Γ be defined as the graph of the restriction to Q of a Q-periodic, Lipschitz continuous function $f : \mathbb{R}^2 \to \mathbb{R}$. Then each function φ defined on Γ naturally corresponds to a function φ_f defined on Q by the relation

$$\varphi_f(x_1, x_2) = \varphi(x_1, x_2, f(x_1, x_2)).$$

Using this relation, we define the Sobolev space

$$H_Q^s(\Gamma) := \left\{ \varphi \in L^2(\Gamma) : \varphi_f \in H_Q^s \right\}, \qquad s \geq 0,$$

which also becomes a Hilbert space with the induced inner product

$$\langle \varphi, \psi \rangle_{Q,s} := (\varphi_f, \psi_f)_{Q,s}.$$

In order to obtain the duals of these spaces, we define, for $\varphi \in L^2(\Gamma)$ and $s \geq 0$, the norm

$$\|\varphi\|_{Q,-s} := |||\, \varphi_f \sqrt{1 + |\nabla f|^2} \, |||_{Q,-s}. \tag{2.8}$$

Note that for a Lipschitz continuous function the gradient exists allmost everywhere and is an essentially bounded function. It then follows that

$$H_Q^{-s}(\Gamma) := \overline{L^2(\Gamma)}^{\|\cdot\|_{Q,-s}}$$

is the dual space of $H_Q^s(\Gamma)$.

Remark 2.4 The norm $\|\cdot\|_{Q,s}$ is equivalent to the Sobolev-Slobodeckiĭ norm often used to define fractional Sobolev spaces. A proof of this statement can be derived by extending the results presented in [43, Chapter 8] to two dimensional domains. It follows that $H_Q^s(\Gamma)$ forms a closed subspace of $H^s(\Gamma)$ for $s \geq 0$. The trace theorem implies that $H_Q^s(\Gamma)$ is a true subspace of $H^s(\Gamma)$ at least for $s \geq 1/2$. $\square$

In order to define boundary values for functions in Sobolev spaces, we make use of the trace operator γ. This operator is usually defined for continuous functions and it is then shown that for a Lipschitz domain Ω, it can be extended to a bounded operator from $H^1(\Omega)$ to $H^{1/2}(\Gamma)$, where Γ denotes any section of $\partial\Omega$ (see e.g. [48]). It can also be shown that the mapping $u \mapsto \partial u/\partial n := n \cdot \gamma(\nabla u)$, also called the normal derivative, can be extended to a bounded operator from the space of functions $u \in H^1(\Omega)$ such that $\Delta u \in L^2(\Omega)$ to $H^{-1/2}(\Gamma)$.

Returning to the case where Ω is one of the domains D_j, D^-, D^+ and Γ, given as the graph of a periodic Lipschitz continuous function, forms part of $\partial\Omega$, we obtain the following corollary for the periodic spaces using the results of Remarks 2.1 and 2.4.

Corollary 2.5 *Let Assumption 2.2 be satisfied and assume that* $f : \mathbb{R}^2 \to \mathbb{R}$ *is a Q-periodic Lipschitz continuous function. Assume that* $\Gamma := \{(x, f(x))^\top : x \in Q\} \subset \partial D$, *where* D *is one of the domains defined in Assumption 2.2. Then the operator*

$$\gamma : H_Q^1(D) \to H_Q^{1/2}(\Gamma)$$

is bounded. Similarly the normal derivative $\partial/\partial n$ *can be extended to a bounded operator*

$$\frac{\partial}{\partial n} : W \to H_Q^{-1/2}(\Gamma),$$

where

$$W := \{u \in H_Q^1(\Omega) : \Delta u \in L^2(\Omega)\},$$

equipped with the corresponding natural norm.

Subsequently, we will not make use of the trace operator γ explicitly but instead write $u|_\Gamma := \gamma u$ for $u \in H^1(\Omega)$. In cases, where traces of a function u can be taken from either side of a surface Γ, $u|_\Gamma^+$ will denote the trace taken with respect to the domain the normal n of Γ is pointing into while $u|_\Gamma^-$ will denote the trace taken with respect to the domain the normal n of Γ is pointing away from. If it is clear from the context, on which surface Γ the trace is taken, we will only use the $\pm$ superscript, e.g. u^+ or u^-.

2.2 Upward- and Downward Propagating Waves

Radiation Conditions. A central ingredient to any scattering problem is a suitable radiation condition. In physical terms, such a condition reflects the principle of *causality*, i.e. that the existence of the scattered field is caused by the presence of an incident field. In mathematical terms, such a condition is necessary for proving uniqueness of solution.

A well known radiation condition for scalar scattering problems is *Sommerfeld's radiation condition.* It is most often used for problems involving bounded obstacles, but is also applicable to certain cases of scattering by an unbounded obstacle. In these cases, the condition takes the form that the scattered field u satisfy the conditions

$$\left.\begin{aligned}\frac{\partial u}{\partial r}(x) - ik\,u(x) &= \mathrm{o}(r^{-1})\\ u(x) &= \mathrm{O}(r^{-1})\end{aligned}\right\} \qquad r \to \infty, \tag{2.9}$$

for all directions x/r of propagation, where we have set $r := |x|$. In the case of scattering by an unpenetrable scatterer, all directions of propagation are the directions $d \in S^2$ such that $d_3 > 0$ while in the case of a transmission problem these are all directions such that $d_3 \neq 0$.

The use of (2.9) in scattering problems involving unbounded media is limited to cases where the incident field itself satisfies this condition, e.g. when it is the field generated by a point source, or more generally a bounded source. However, we would like to study the scattering of periodic incident fields such as plane waves. A simple example shows that in this case (2.9) cannot hold: Consider the scattering of the plane wave $u^i(x) = \exp(-ik\,x_3)$ by the plane $\{x_3 = 0\}$ such that the total field u satisfies $u = 0$ on this plane. The scattered field $u^s = u - u^i$ is then given by the reflected wave $u^s(x) = \exp(ik\,x_3)$. This field certainly does not satisfy the second condition of (2.9). The first condition is also not satisfied, as the left hand side reads

$$ik\left(\frac{x_3}{|x|} - 1\right)\exp(ikx_3),$$

and this function only decays for $x_3 = |x|$, i.e. the direction of propagation of the plane wave.

An alternative radiation condition was first proposed by Lord Rayleigh [56]. To derive it, consider a bounded, Q-quasi-periodic solution u to the Helmholtz equation in D^+ that is supposed to represent a wave propagating away from Γ^+. We will make the assumption here that the phase-shift α satisfies

$$|\tilde{\alpha}| < k. \tag{2.10}$$

On any plane $\{x_3 = M\}$ such that $M > M_2$, u is then an analytic, Q-quasi-periodic function and hence can be expanded into a Fourier series of the form (2.6). After inserting this series into the Helmholtz equation, by coefficient comparison, we obtain an ordinary differential equation for the coefficients u_ν,

$$u_\nu''(x_3) + k^2(1 - |d^{(\nu)}|^2)\, u_\nu(x_3) = 0, \qquad \nu \in \mathbb{Z}^2.$$

Here, we have set

$$d^{(\nu)} := \frac{1}{k}\,(\tilde{\alpha} + q^{(\nu)}).$$

The general solution to this equation can be written as

$$u_\nu(x_3) = u_\nu^{(1)} \exp(ik\,\rho^{(\nu)}\,x_3) + u_\nu^{(2)} \exp(-ik\,\rho^{(\nu)}\,x_3)$$

with

$$\rho^{(\nu)} := \begin{cases} \sqrt{1 - |d^{(\nu)}|^2}, & |d^{(\nu)}| \le 1, \\ i\,\sqrt{|d^{(\nu)}|^2 - 1}, & |d^{(\nu)}| > 1, \end{cases}$$

and constants $u_\nu^{(j)} \in \mathbb{C}$, $j = 1, 2$, $\nu \in \mathbb{Z}^2$, to be determined.

After inserting this result back into the Fourier series, we arrive at the expression

$$u(x) = \sum_{\nu \in \mathbb{Z}^2} \left[u_\nu^{(1)} \exp(ik\,(d^{(\nu)} \cdot \tilde{x} + \rho^{(\nu)}\,x_3)) + u_\nu^{(2)} \exp(ik\,(d^{(\nu)} \cdot \tilde{x} - \rho^{(\nu)}\,x_3)) \right].$$

In the case $|d^{(\nu)}| \le 1$, the terms in this series either represent upwards or downwards propagating plane waves. Note that the case of a horizontally propagating wave ($|d^{(\nu)}| = 1$) is possible. In the case $|d^{(\nu)}| > 1$, the terms represent *evanescent waves* and are exponentially decaying or increasing as x_3 gets larger, respectively. From the assumption that u be bounded in D^+ and propagating away from Γ^+ we hence obtain that the coefficients $u_\nu^{(2)}$ in this representation must vanish.

Analogously, the above derivation could be carried out for a field u bounded in D^- and propagating away from Γ^-. In this case we take $M < M_1$ and obtain that the coefficients $u_\nu^{(1)}$ must vanish. Concluding, we obtain the following condition for upwards or downwards propagating fields, where we have introduced additional normalizing terms:

Definition 2.6 *A function $u : D^+ \to \mathbb{C}$ is said to satisfy the* upward propagating Rayleigh expansion radiation condition (URC)*, if there exists a sequence (u_ν) such that*

$$u(x) = \sum_{\nu \in \mathbb{Z}^2} u_\nu \exp(ik\,(d^{(\nu)} \cdot \tilde{x} + \rho^{(\nu)}\,(x_3 - M_2))), \qquad x \in D^+. \tag{2.11}$$

Similarly, any $u : D^- \to \mathbb{C}$ *is said to satisfy the* downward propagating Rayleigh expansion radiation condition (DRC), *if there exists a sequence* (u_ν) *such that*

$$u(x) = \sum_{\nu \in \mathbb{Z}^2} u_\nu \, \exp(ik\,(d^{(\nu)} \cdot \tilde{x} - \rho^{(\nu)}\,(x_3 + M_1))), \qquad x \in D^-. \tag{2.12}$$

Remark 2.7 The URC is closely related to the *upward propagating radiation condition (UPRC)* that has been suggested and successfully employed as a radiation condition for two-dimensional scattering problems (see e.g. [16, 17, 19, 20]). In the three-dimensional case considered here, the UPRC takes the form that for any $M > M_2$, there exists a density $\varphi \in L^\infty(\mathbb{R}^2)$ such that

$$u(x) = \int_{\Gamma^+} \frac{\partial \Phi(x,y)}{\partial x_3}\,\varphi(y)\,ds(y), \qquad x \in D^+,$$

with Φ the fundamental solution to the Helmholtz equation in free space conditions,

$$\Phi(x,y) = \frac{1}{4\pi}\,\frac{\exp(k\,|x-y|)}{|x-y|}, \qquad x, y \in \mathbb{R}^3,\ x \neq y.$$

Particularly, it is proved in [16] for the two-dimensional case that a field satisfying the URC also satisfies the UPRC, and conversely, that a quasi-periodic field satisfying the UPRC also satisfies the URC. □

Dirichlet-to-Neumann Maps. The URC and DRC can also be used to obtain explicit expressions for the *Dirichlet-to-Neumann* maps for the horizontal planes contained in Γ^+ or Γ^-, respectively. For the moment, we will concentrate on the upward propagating waves and Γ^+, but the corresponding results for downward propagating waves can be established completely analogously.

Consider a Q-quasi-periodic function φ, defined on Γ^+. We will assume that φ can be represented as the Fourier series

$$\varphi(x) = \sum_{\nu \in \mathbb{Z}^2} \varphi_\nu \, \exp(ik\,d^{(\nu)} \cdot x)$$

in some appropriate space. Consider now the boundary value problem

$$\begin{aligned} \Delta u + k^2 u = 0, &\qquad \text{in } D^+, \\ u = \varphi, &\qquad \text{on } \Gamma^+, \end{aligned}$$

where u is also assumed to be Q-quasi-periodic and to satisfy the URC. In fact, from our considerations above, we can immediately write down the solution to this problem,

$$u(x) = \sum_{\nu \in \mathbb{Z}^2} \varphi_\nu \, \exp(ik\,(d^{(\nu)} \cdot \tilde{x} + \rho^{(\nu)}\,(x_3 - M_2))).$$

Formally, the normal derivative of u on Γ^+ is now obtained as

$$\frac{\partial u}{\partial n}(x) = ik \sum_{\nu\in\mathbb{Z}^2} \varphi_\nu \, \rho^{(\nu)} \, \exp(ik\, d^{(\nu)} \cdot x), \qquad x \in \Gamma^+.$$

The convergence of this series certainly depends on the decay rate of the Fourier coefficients (φ_ν), i.e. on the smoothness of the boundary values φ, but at least for all smooth enough φ, the right hand side is well defined.

In order to define a corresponding operator, we shift the situation to Q-periodic functions: for Q-quasi-periodic φ, $\psi = M_{-\alpha}\varphi$ is Q-periodic, hence denoting by (ψ_ν) the Fourier coefficients of ψ, we can define the Dirichlet-to-Neumann map Λ^+ on Γ^+ by

$$\Lambda^+\psi(x) := ik \sum_{\nu\in\mathbb{Z}^2} \psi_\nu \, \rho^{(\nu)} \, \exp(i\, q^{(\nu)} \cdot x).$$

Hence, if u satisfies the URC, there holds

$$\Lambda^+ M_{-\alpha} u = M_{-\alpha}\frac{\partial u}{\partial n} = \frac{\partial}{\partial n} M_{-\alpha} u. \tag{2.13}$$

Conversely, we obtain the Dirichlet-to-Neumann map Λ^- on Γ^- by the expression

$$\Lambda^-\psi(x) := -ik \sum_{\nu\in\mathbb{Z}^2} \psi_\nu \, \rho^{(\nu)} \, \exp(i\, q^{(\nu)} \cdot x).$$

To see that the sign on these expressions is correct, recall that it is assumed that the normal to both Γ^+ and Γ^- points upward.

Theorem 2.8 *The Dirichlet-to-Neumann maps $\Lambda^\pm$ are bounded linear operators from $H_Q^{1/2}(\Gamma^\pm)$ to $H_Q^{-1/2}(\Gamma^\pm)$, respectively. If $\rho^{(\nu)} \neq 0$ for all $\nu \in \mathbb{Z}^2$, these operators are isomorphisms.*

Proof: We will only prove the assertion for Λ^+, the proof for Λ^- being virtually identical. Suppose that $\varphi \in H_Q^{1/2}(\Gamma^+)$. From (2.7), it then follows that

$$\sum_{\nu\in\mathbb{Z}^2} (1+|\nu|^2)^{1/2} |\varphi_\nu|^2 < \infty.$$

Recall that there is only a finite number of indices ν such that $|d^{(\nu)}| \leq 1$. For $|d^{(\nu)}| > 1$,

$$|\rho^{(\nu)}|^2 = \frac{1}{k^2}\,|\tilde{\alpha} + q^{(\nu)}|^2 - 1 \leq \frac{2}{k^2}\,\left(|\tilde{\alpha}|^2 + |q^{(\nu)}|^2\right) - 1 \leq C\,(1 + |\nu|^2),$$

where C is a constant depending on k, $\tilde{\alpha}$ and $\min\{L_1, L_2\}$. Hence

$$\sum_{\nu\in\mathbb{Z}^2}(1+|\nu|^2)^{-1/2}|\varphi_\nu\,\rho^{(\nu)}|^2 \le \sum_{\nu\in\mathbb{Z}^2}\frac{|\rho^{(\nu)}|^2}{1+|\nu|^2}\,(1+|\nu|^2)^{1/2}|\varphi_\nu|^2 \le C\;\|\varphi\|_{Q,1/2}\,.$$

However, from (2.7) and (2.8), we obtain that the left hand side of the above equality is equivalent to the $H_Q^{-1/2}(\Gamma^+)$ norm of $\Lambda^+\varphi$. Hence we have proved the first part of the Lemma.

For the second part, it is obvious that Λ^+ is injective if $\rho^{(\nu)} \neq 0$ for all $\nu \in \mathbb{Z}^2$. Now let $\psi \in H_Q^{-1/2}(\Gamma^+)$ where ψ can be expressed formally as

$$\psi(x) = \sum_{\nu\in\mathbb{Z}}\psi_\nu\,\exp(ik\,d^{(\nu)}\cdot x) \qquad \text{with} \qquad \sum_{\nu\in\mathbb{Z}^2}(1+|\nu|^2)^{-1/2}|\psi_\nu|^2 < \infty.$$

If $\rho^{(\nu)} \neq 0$ for all $\nu \in \mathbb{Z}^2$, setting

$$\varphi(x) := \sum_{\nu\in\mathbb{Z}^2}\frac{\psi_\nu}{ik\,\rho^{(\nu)}}\,\exp(ik\,d^{(\nu)}\cdot x),$$

we formally obtain $\Lambda^+\varphi = \psi$. On the other hand, a similar calculation as above shows that $\rho^{(\nu)} \neq 0$ for all $\nu \in \mathbb{Z}^2$ also implies $|\rho^{(\nu)}|^2 \ge c\,(1+|\nu|^2)$. Hence $\varphi \in H_Q^{1/2}(\Gamma^+)$. This completes the proof. ∎

Remark 2.9 The essential ingredient in the proof of Theorem 2.8 is the estimate

$$c_1(1+|\nu|^2) \le |\rho^{(\nu)}|^2 \le c_2(1+|\nu|^2)$$

with some constants c_1, c_2 depending on k, α and L_j, $j = 1, 2$. Note that the upper estimate holds unconditionally, while the lower estimate requires $\rho^{(\nu)} \neq 0$ for all $\nu \in \mathbb{Z}^2$.

When the incident field is a plane wave, the phase shift α satisfies $\alpha = kd$. In other situations, we can mimick this behaviour by setting $\alpha = k\theta$ for some $\theta \in \mathbb{R}^3$. It is then possible to obtain the following sharper lower bound for small enough wave numbers: if $\rho^{(\nu)} \neq 0$ for all $\nu \in \mathbb{Z}^2$, there exists k_0 such that for all $k \le k_0$,

$$|\rho^{(\nu)}|^2 \ge c\,(1+|\nu|^2),$$

where the constant c depends on k_0, $\hat{\alpha}$ and L_j, $j = 1, 2$. This bound follows from the fact that for small enough k_0 and $k < k_0$, for all $\nu \neq 0$, $|d^{(\nu)}| > 1$ and hence $|\rho^{(\nu)}|^2 + 1 = |\tilde{\theta} + q^{(\nu)}/k|^2$. A term $(\theta_j + q_j^{(\nu)}/k)^2$ takes its minimum at $\nu_j = \pm 1$ for small enough k, $j = 1, 2$, and asymptotically it grows at least as $(1/k_0^2)(1 + v_j^2)$. □

From the last assertion in Theorem 2.8 and from Remark 2.9, it is clear that the pairs (k, α) such that $\rho^{(\nu)} = 0$ for some $\nu \in \mathbb{Z}^2$ play a distinguished role. Hence we define

$$\mathcal{R} := \{(k, \alpha) \in \mathbb{R}_{>0} \times \mathbb{R}^3 : \ \rho^{(\nu)} = 0 \text{ for some } \nu \in \mathbb{Z}^2\}.$$

If $(k, \alpha) \in \mathcal{R}$, then there exist horizontally propagating plane waves that are Q-quasi-periodic with phase-shift α.

A further important aspect of the role of the set $\mathcal{R}$ is the dependence of $\Lambda^{\pm}$ on k. For an analysis of this we will here assume that $\alpha = k\theta$ for some $\theta \in \mathbb{R}^3$. Note that $|\tilde{\theta}| < 1$ by condition (2.10). Then,

$$k\rho^{(\nu)} = \left(k^2 - |k\tilde{\theta} + q^{(\nu)}|^2\right)^{1/2},$$

where the fractional power has been extended analytically into the complex plane except for a branch cut along the negative imaginary axis. It follows that $k\rho^{(\nu)}$ is an analytic function of k in a neighbourhood of k_0 if $(k_0, k_0\theta) \notin \mathcal{R}$. If on the other hand $(k_0, k_0\theta) \in \mathcal{R}$, then $k\rho^{(\nu)}$ is an analytic function of k in a neighbourhood of k_0 except for a branch cut $k_0 - is$, $s > 0$ and for the branch point k_0 itself. The analyticity of $k\rho^{(\nu)}$ is inherited by the operators $\Lambda^{\pm}$:

Lemma 2.10 *Suppose $\alpha = k\theta$, $\theta \in \mathbb{R}^3$ fixed. Then $\Lambda^{\pm}$ depends analytically on $k > 0$ except for a countable set of branch points k_ν, $\nu \in \mathbb{Z}^2$, satisfying $(k_\nu, k_\nu\theta) \in \mathcal{R}$, i.e. $k_\nu^2 = |k_\nu\theta + q^{(\nu)}|^2$. Furthermore $k_\nu \to \infty$ as $|\nu| \to \infty$. The branch cuts can be chosen perpendicular to the positive real axis.*

Proof: For each $\nu \in \mathbb{Z}^2$, $(k\rho^{(\nu)})^2$ is a second degree polynomial in k with two real roots given by

$$k = \frac{1}{1 - |\tilde{\theta}|^2}\left[\tilde{\theta} \cdot q^{(\nu)} \pm \left((1 - |\tilde{\theta}|^2)\, |q^{(\nu)}|^2 + (\tilde{\theta} \cdot q^{(\nu)})^2\right)^{1/2}\right].$$

Hence, $k\rho^{(\nu)}$ has exactly one branch point $k_\nu \in \mathbb{R}_{>0}$ and $k_\nu \to \infty$ as $|\nu| \to \infty$. It follows that the operators $\Lambda^{\pm}$ themselves analytically depend on k except for the countable branch points k_ν and across the corresponding branch cuts. ∎

We conclude this chapter by some observations regarding some sesquilinear forms involving the Dirichlet-to-Neumann maps that will be useful in our later considerations.

Lemma 2.11 *Assume* $u, v \in H_Q^{1/2}(\Gamma^\pm)$ *with Fourier coefficients* (u_ν), (v_ν), *respectively. Then the following identities hold:*

$$\int_{\Gamma^\pm} \bar{v}\, \Lambda^\pm u \, ds = \pm ik\, |Q| \sum_{\nu \in \mathbb{Z}^2} \rho^{(\nu)}\, u_\nu \overline{v_\nu},$$

$$\operatorname{Re} \int_{\Gamma^\pm} \bar{u}\, \Lambda^\pm u \, ds = \mp k\, |Q| \sum_{|d^{(\nu)}|>1} |\rho^{(\nu)}|\, |u_\nu|^2,$$

$$\operatorname{Im} \int_{\Gamma^\pm} \bar{u}\, \Lambda^\pm u \, ds = \pm k\, |Q| \sum_{|d^{(\nu)}|\le 1} |\rho^{(\nu)}|\, |u_\nu|^2.$$

Furthermore, for any $\zeta \in \mathbb{C}$, $\arg \zeta \in (0, \pi/2)$, *there holds*

$$\mp \operatorname{Re} \int_{\Gamma^\pm} \bar{u}\, \Lambda^\pm(\zeta u)\, ds \ge k|Q| \min\{\operatorname{Re}(\zeta), \operatorname{Im}(\zeta)\} \sum_{\nu \in \mathbb{Z}^2} |\rho^{(\nu)}|\, |u_\nu|^2.$$

Proof: We only carry out the proof for Λ^+. A simple calculation using the orthogonality of the trigonometric polynomials yields

$$\int_{\Gamma^+} \bar{v}\, \Lambda^+ u\, ds = ik \sum_{\mu,\nu \in \mathbb{Z}^2} \rho^{(\mu)}\, u_\mu\, \overline{v_\nu} \int_{\Gamma^+} \exp(i\,(q^{(\mu)} - q^{(\nu)}) \cdot x)\, ds = ik\, |Q| \sum_{\nu \in \mathbb{Z}^2} \rho^{(\nu)}\, u_\nu \overline{v_\nu}.$$

The other two identities follow directly from the definition of $\rho^{(\nu)}$ and the lower bound by combining the two. ■

2.3 Scattering Problems

Problem Formulation. As a first class of problems, we will be considering scalar scattering problems, i.e. problems where the domain D_{-1} forms an inpenetrable obstacle. We will assume throughout this section, that Assumption 2.2 is satisfied.

In classical terms, we will be interested in the following problem: Given a Q-quasi-periodic incident field u^i with phase-shift $\alpha \in \mathbb{R}^3$, find a Q-quasi-periodic function u such that

- u is a solution to the Helmholtz equations

$$\Delta\, u + q_j\, k^2\, u = 0 \tag{2.14}$$

  in each domain D_j, $j = 0, \ldots, N$, where the indices of refraction $q_j \in \mathbb{C}$ satisfy $\operatorname{Re}(q_j) > 0$ and $\operatorname{Im}(q_j) \ge 0$.

- On the interfaces Γ_j, $j = 1, \ldots, N$, the transmission conditions

$$u|_{\Gamma_j}^{+} - u|_{\Gamma_j}^{-} = 0$$
$$\text{and} \qquad \lambda_j \left.\frac{\partial u}{\partial n}\right|_{\Gamma_j}^{+} - \lambda_{j-1} \left.\frac{\partial u}{\partial n}\right|_{\Gamma_j}^{-} = 0 \tag{2.15}$$

  hold, where $\lambda_j \in \mathbb{C}$ such that

$$\operatorname{Re}(\lambda_j) > 0, \quad \operatorname{Im}(\lambda_j) \leq 0 \quad \text{and} \quad \operatorname{Im}(\lambda_j q_j) \geq 0, \qquad j = 0, \ldots, N. \tag{2.16}$$

- On Γ_0, either the Dirichlet boundary condition

$$u = 0, \tag{2.17}$$

  the Neumann boundary condition

$$\frac{\partial u}{\partial n} = 0, \tag{2.18}$$

  or the impedance boundary condition

$$\frac{\partial u}{\partial n} + i\beta u = 0 \tag{2.19}$$

  is satisfied, where in the last case $\beta \in \mathbb{C}$ such that

$$\operatorname{Re}(\lambda_0 \beta) > 0 \qquad \text{and} \qquad \operatorname{Im}(\lambda_0 \beta) \geq 0. \tag{2.20}$$

- The scattered field $u^s := u - u^i$ satisfies the URC as stated in Definition 2.6.

Remark 2.12 The assumptions on the constants λ_j are satisfied by the two particular choices $\lambda_j = 1$ and $\lambda_j = 1/(q_j k^2)$. In the case where the grating is constant in, say, the x_2 direction, the first choice, corresponds to the transverse electric (TE) mode, while the second choice, together with the Neumann boundary condition (2.18), corresponds to the transverse magnetic (TM) mode [30].

In the acoustic case, the physically correct conditions of continuous pressure and continuous normal particle velocity across an interface [38] also leads to the choice $\lambda_j = 1$. □

Variational Formulations. The basis to derive variational formulations for the scalar scattering problems is the first Green's identity. We will use the following form of Green's identities which are given with proof as [48, Theorem 4.4].

Lemma 2.13 (Green's identities) *Let the domain $\Omega \subset \mathbb{R}^3$ be Lipschitz with outward drawn unit normal n and $u,\, v \in H^1(\Omega)$.*

(a) If $\Delta v \in L^2(\Omega)$, then

$$\int_\Omega (u\,\Delta v + \nabla u \cdot \nabla v)\, dx = \int_{\partial\Omega} u\,\frac{\partial v}{\partial n}\, ds.$$

(b) If $\Delta u,\, \Delta v \in L^2(\Omega)$, then

$$\int_\Omega (u\,\Delta v - v\,\Delta u)\, dx = \int_{\partial\Omega} \left(u\,\frac{\partial v}{\partial n} - v\,\frac{\partial u}{\partial n} \right) ds.$$

The variational formulations of the scattering problems will use the setting of the spaces of periodic functions defined previously rather than in the setting of Q-quasi-periodic functions. Hence, we set

$$u_\alpha(x) := M_{-\alpha} u(x). \tag{2.21}$$

If u is a solution to the Helmholtz equation, then u_α satisfies the equation

$$(\Delta + 2i\,\tilde{\alpha} \cdot \nabla - |\tilde{\alpha}|^2)\, u_\alpha + q_j k^2\, u_\alpha = 0. \tag{2.22}$$

Setting $\nabla_\alpha := \nabla + i\tilde{\alpha}$, this equation can be rewritten as

$$\nabla_\alpha \cdot (\nabla_\alpha u_\alpha) + q_j k^2\, u_\alpha = 0.$$

Let us now introduce the spaces

$$\begin{aligned} V &:= H^1_Q(D \setminus \overline{D_{-1}}), \\ V_0 &:= \{u \in V : u = 0 \text{ on } \Gamma_0\}. \end{aligned} \tag{2.23}$$

Note, that V is identical to the space of functions u satisfying $u|_{D_j} \in H^1_Q(D_j)$, $j = 0, \ldots, N$ and $u|^+_{\Gamma_j} - u|^-_{\Gamma_j} = 0$, $j = 1, \ldots, N-1$, see [50, Lemma 5.3].

We will assume now that $u_\alpha,\, v \in V$ and also that u, related to u_α by (2.21), is a solution to the Helmholtz equation in each domain D_j in a weak sense. From (2.22), it then follows by Green's first identity and from the divergence theorem that

$$\int_{D_j} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha \bar{v}\right) dx = \int_{\partial D_j} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\, ds, \qquad j = 0, \ldots, N-1.$$

Define, for some $j \in \{0, \ldots, N-1\}$,

$$\gamma^- := \left\{x \in \partial D_j : x_1 = -\frac{L_1}{2}\right\} \quad \text{and} \quad \gamma^+ := \left\{x \in \partial D_j : x_1 = \frac{L_1}{2}\right\}.$$

Then, because of Q-periodicity,

$$\int_{\gamma^-} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds = -\int_{\gamma^-} \bar{v}\,\left(\frac{\partial u_\alpha}{\partial x_1} + i\alpha_1 u_\alpha\right)\,ds$$
$$= -\int_{\gamma^+} \bar{v}\,\left(\frac{\partial u_\alpha}{\partial x_1} + i\alpha_1 u_\alpha\right)\,ds = -\int_{\gamma^+} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds,$$

so that the contributions from γ^- and γ^+ to the integral over ∂D_j cancel. The same holds for the integrals over the other two vertical components of ∂D_j. Hence we have arrived at

$$\int_{D_j} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha \bar{v}\right)\,dx = \int_{\Gamma_{j+1}} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds - \int_{\Gamma_j} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds. \quad (2.24)$$

Similarly,

$$\int_{D_N} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - k^2\, u_\alpha\, \bar{v}\right)\,dx = \int_{\Gamma^+} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds - \int_{\Gamma_N} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds. \quad (2.25)$$

From the requirement that u satisfy also the second condition in (2.15), by multiplying the two equations by λ_j and λ_N, respectively, we obtain that

$$\sum_{j=0}^{N} \lambda_j \int_{D_j} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha \bar{v}\right)\,dx$$
$$= \lambda_N \int_{\Gamma^+} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds - \lambda_0 \int_{\Gamma_0} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds.$$

We now further require that $u^s := u - u^i$ be an upward propagating wave, i.e. by (2.13) that the relation

$$\frac{\partial u_\alpha}{\partial n} = \Lambda^+ \left[u_\alpha - M_{-\alpha} u^i\right] + M_{-\alpha} \frac{\partial u^i}{\partial n}$$

holds on Γ^+. Hence we have finally arrived at

$$\sum_{j=0}^{N} \lambda_j \int_{D_j} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha\, \bar{v}\right)\,dx - \lambda_N \int_{\Gamma^+} \bar{v}\,\Lambda^+ u_\alpha\,ds$$
$$= \lambda_N \int_{\Gamma^+} \bar{v}\,\left(M_{-\alpha} \frac{\partial u^i}{\partial n} - \Lambda^+ M_{-\alpha} u^i\right)\,ds - \lambda_0 \int_{\Gamma_0} \bar{v}\,(n \cdot \nabla_\alpha u_\alpha)\,ds. \quad (2.26)$$

From the basis of (2.26) we are now able to give variational formulations of the scalar scattering problems.

Problem 2.14 (Dirichlet Scattering Problem)
Given a Q-quasi-periodic incident field u^i, find $u_\alpha \in V_0$ such that

$$\sum_{j=0}^{N} \lambda_j \int_{D_j} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha\, \bar{v}\right) dx - \lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+ u_\alpha\, ds$$
$$= \lambda_N \int_{\Gamma^+} \bar{v} \left(M_{-\alpha} \frac{\partial u^i}{\partial n} - \Lambda^+ M_{-\alpha} u^i \right) ds \qquad \text{for all } v \in V_0.$$

This variational problem corresponds to the problem (2.14), (2.15), (2.17), (2.11).

Problem 2.15 (Neumann Scattering Problem)
Given a Q-quasi-periodic incident field u^i, find $u_\alpha \in V$ such that

$$\sum_{j=0}^{N} \lambda_j \int_{D_j} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha\, \bar{v}\right) dx - \lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+ u_\alpha\, ds$$
$$= \lambda_N \int_{\Gamma^+} \bar{v} \left(M_{-\alpha} \frac{\partial u^i}{\partial n} - \Lambda^+ M_{-\alpha} u^i \right) ds \qquad \text{for all } v \in V.$$

This variational problem corresponds to the problem (2.14), (2.15), (2.18), (2.11).

Problem 2.16 (Impedance Scattering Problem)
Given an incident field u^i, find $u_\alpha \in V$ such that

$$\sum_{j=0}^{N} \lambda_j \int_{D_j} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha\, \bar{v}\right) dx - \lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+ u_\alpha\, ds - i\lambda_0\, \beta \int_{\Gamma_0} u_\alpha\, \bar{v}\, ds$$
$$= \lambda_N \int_{\Gamma^+} \bar{v} \left(M_{-\alpha} \frac{\partial u^i}{\partial n} - \Lambda^+ M_{-\alpha} u^i \right) ds \qquad \text{for all } v \in V.$$

This variational problem corresponds to the problem (2.14), (2.15), (2.19), (2.11).

Solvability. We now face the question whether these variational problems possess solutions, and whether these solutions are unique. Unfortunately, the answer to this question is not completely known. Particularly in the case of the Neumann problem, examples of non-uniqueness are known [11], but no complete characterization is available of when the Neumann problem admits only a single solution.

To analyse the variational problems, let us define some sesquilinear forms that occur in these formulations:

$$\mathcal{A}_\alpha^{(1)}(u_\alpha, v) := \sum_{j=0}^{N} \lambda_j \int_{D_j} \left(\nabla u_\alpha \cdot \overline{\nabla v} + u_\alpha \bar{v}\right) dx - \lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+ u_\alpha \, ds,$$

$$\mathcal{A}_\alpha^{(2)}(u_\alpha, v) := \sum_{j=0}^{N} \lambda_j \int_{D_j} \nabla u_\alpha \cdot \overline{\nabla v}\, dx - \lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+ u_\alpha \, ds - i\, \lambda_0\, \beta \int_{\Gamma_0} u_\alpha \, \bar{v}\, ds,$$

$$\mathcal{A}_\alpha^{(3)}(u_\alpha, v) := \sum_{j=0}^{N} \lambda_j \int_{D_j} \left((|\tilde{\alpha}|^2 - q_j\, k^2 - 1) u_\alpha \, \bar{v} + i\tilde{\alpha} \cdot \left[u_\alpha \overline{\nabla v} - \bar{v} \nabla u_\alpha\right]\right) dx,$$

$$\mathcal{A}_\alpha^{(4)}(u_\alpha, v) := \sum_{j=0}^{N} \lambda_j \int_{D_j} \left((|\tilde{\alpha}|^2 - q_j\, k^2) u_\alpha \, \bar{v} + i\tilde{\alpha} \cdot \left[u_\alpha \overline{\nabla v} - \bar{v} \nabla u_\alpha\right]\right) dx$$

which are all bounded on $V \times V$. Hence, by the Riesz theorem, each form defines a bounded linear operator A_j on V by the relation

$$\mathcal{A}_\alpha^{(j)}(u_\alpha, v) = \langle A_j u_\alpha, v\rangle_1, \qquad j = 1, \ldots, 4.$$

In the next few lemmas, we analyse these operators further.

Lemma 2.17 *The operators $A_1 : V \to V$ and $A_2 : V \to V$ are coercive in the sense that*

$$\mathrm{Re}\langle A_j v, v\rangle_1 \geq c\, \|v\|_1^2, \qquad v \in V, \quad j = 1, 2.$$

Proof: In view of the assumption $q_N = 1$, it follows that λ_N is real and positive. Hence, from Lemma 2.11,

$$\mathrm{Re}\left(-\lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+ v\, ds\right) \geq 0. \tag{2.27}$$

This already proves coercivity for A_1.

To see that A_2 is also coercive, assume that (v_n) is a sequence in V with $\|v_n\|_1 = 1$ such that

$$\mathrm{Re}\, \mathcal{A}_\alpha^{(2)}(v_n, v_n) \longrightarrow 0 \quad (n \to \infty). \tag{2.28}$$

Without loss of generality we can assume that (v_n) converges weakly to $v \in V$. By Sobolev's imbedding theorem, this implies $v_n \to v$ in norm in L^2. On the other hand, as $\mathrm{Im}(\lambda_0 \beta) \geq 0$ and we already have (2.27), it follows from (2.28) that $\|\nabla v_n\|_0 \to 0$. Hence (v_n) is a Cauchy sequence in V and thus convergent in norm to v. Additionally we conclude $v = \text{const}$, but then $\Lambda^+ v = ik\, \rho^{(0)}\, v$, which again with (2.28) implies that $v = 0$. This contradicts the assumption $\|v_n\|_1 = 1$, hence A_2 must be coercive. ■

Lemma 2.18 *The operators $A_3 : V \to V$ and $A_4 : V \to V$ are compact.*

Proof: It is easy to see that the forms

$$\int_{D_j} v\,\bar{w}\,dx, \qquad \text{and} \qquad \int_{D_j} v\,\overline{\nabla w}\,dx$$

induce compact operators on V with respect to the argument v. The operator induced by

$$\int_{D_j} \bar{w}\,\nabla v\,dx$$

on the other hand, is the adjoint of the operator generated by the second form above, hence also compact. ■

Together, Lemmas 2.17 and 2.18 imply that the operators $A_1 + A_3$ and $A_2 + A_4$ are Fredholm operators of index 0, respectively. Hence all three variational problems are uniquely solvable whenever the homogeneous problem only admits the trivial solution. Thus, we can immediately establish unique solvability of the variational problems in certain cases which correspond to the absorption of energy by the medium:

Theorem 2.19 *(a) The Impedance Scattering Problem 2.16 is uniquely solvable.*

(b) Assume that $\mathrm{Im}(q_j) > 0$ for some $j \in \{0, \ldots, N-1\}$. Then the Dirichlet Scattering Problem 2.14 and the Neumann Scattering Problem 2.15 are uniquely solvable.

Proof: Part (a): Assume that $u_\alpha \in V$ is a solution of the homogeneous Impedance Scattering Problem 2.16. Hence,

$$\sum_{j=0}^{N} \lambda_j \int_{D_j} \left(|\nabla_\alpha u_\alpha|^2 - q_j k^2\,|u_\alpha|^2 \right) dx - \lambda_N \int_{\Gamma^+} \overline{u_\alpha}\,\Lambda^+ u_\alpha\,ds$$
$$- i\lambda_0\,\beta \int_{\Gamma_0} |u_\alpha|^2\,ds = 0$$

Taking the imaginary part of this equation, it follows from conditions (2.16) and (2.20) together with Lemma 2.11 and the fact that $\mathrm{Im}(\lambda_N) = 0$ that all terms on the left hand side of this equation are less than or equal to 0. Hence, as $\mathrm{Re}(\lambda_0\,\beta) > 0$, we have $u_\alpha = 0$ on Γ_0. We conclude that the same must hold for $u = M_\alpha u_\alpha$ and by the impedance boundary condition also for $\partial u/\partial n$. So $u = 0$ in D_0 follows from Holmgren's uniqueness theorem. Now this argument is repeated for each interface

Γ_j and the domain D_j using the transmission condition, $j = 1, \ldots, N$, to obtain the assertion.

Part (b): The proof is similar as for part (a), only now we argue that

$$\int_{D_j} |u_\alpha|^2 dx = 0$$

for that domain D_j in which $\mathrm{Im}(q_j) > 0$. Using the transmission conditions and again Holmgren's uniqueness theorem in each domain D_j, we obtain the assertion. ■

Remark 2.20 It is also possible to consider the scattering problems in the case of $\mathrm{Im}(q_N) > 0$. Doing so requires either an extension of the operator Λ^+ to complex wave numbers or considering the problem without a radiation condition. In either case, uniqueness of solution can then be established as in the proof of Theorem 2.19 (b). □

Such general uniqueness proofs are not known for the Dirichlet or Neumann scattering problems in the case where $\mathrm{Im}(q_j) = 0$, $j = 0, \ldots, N$. However, it is possible to make some general statements about the solvability of these variational problems using the theory of analytic operator families. The first step is to show that the variational problems admit a unique solution for small enough wave numbers.

Theorem 2.21 *Let $\theta \in \mathbb{R}^3$ such that $\alpha = k\theta$. Then there exists $k_0 > 0$ and a constant $c > 0$ such that for all $k \leq k_0$,*

$$\mathrm{Re}\left(\sum_{j=0}^{N} e^{i\pi/4}\lambda_j \int_{D_j} \left(|\nabla_\alpha v|^2 - q_j k^2 |v|^2\right) dx - \lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+(e^{i\pi/4} v)\, ds\right) \geq c\, \|v\|_1^2$$

for all $v \in V$.

Proof: We start by observing, for any $\varepsilon > 0$, the estimate

$$\begin{aligned}\int_{D_j} |\nabla_\alpha v|^2 dx &= \int_{D_j} \left(|\nabla v|^2 - 2k\,\mathrm{Im}(v\,\tilde{\theta} \cdot \overline{\nabla v}) + |k\tilde{\theta}|^2\,|v|^2\right) dx \\ &\geq \int_{D_j} |\nabla v|^2\, dx - 2\,|k\tilde{\theta}| \int_{D_j} |v\,\overline{\nabla v}|\, dx + |k\tilde{\theta}|^2 \int_{D_j} |v|^2\, dx \\ &\geq \left(1 - \frac{|k\tilde{\theta}|}{\varepsilon}\right) \int_{D_j} |\nabla v|^2\, dx + \left(|k\tilde{\theta}|^2 - \varepsilon|k\tilde{\theta}|\right) \int_{D_j} |v|^2\, dx.\end{aligned}$$

Hence, setting $\varepsilon = 2|k\tilde{\theta}|$, we obtain

$$\int_{D_j} |\nabla_\alpha v|^2 dx \geq \frac{1}{2} \int_{D_j} |\nabla v|^2\, dx - |k\tilde{\theta}|^2 \int_{D_j} |v|^2\, dx.$$

Led by this estimate, we define for $v,\, w \in V$,

$$\mathcal{B}_1(v,w) := \sum_{j=0}^{N} \frac{1}{2}\, e^{i\pi/4} \lambda_j \int_{D_j} \nabla v \cdot \overline{\nabla w}\, dx - \lambda_N \int_{\Gamma^+} \overline{w}\, \Lambda^+(e^{i\pi/4} v)\, ds,$$

$$\mathcal{B}_2(v,w) := \sum_{j=0}^{N} e^{i\pi/4} \lambda_j \int_{D_j} (|k\tilde{\theta}|^2 + q_j k^2)\, v\overline{w}\, dx.$$

We will prove

$$\operatorname{Re} \mathcal{B}_1(v,v) - |\mathcal{B}_2(v,v)| \geq c\, \|v\|_1^2$$

for small enough k which proves our assertion, as $\operatorname{Re}(e^{i\pi/4}\lambda_j) = (\sqrt{2}/2)\,(\operatorname{Re}(\lambda_j) - \operatorname{Im}(\lambda_j)) > 0$. Here and in the following arguments, c will denote a generic constant, which may be different in each instance it occurs.

Recall that $|\tilde{\theta}| < 1$ by (2.10). Consequently, for small enough k, it follows that $(k, k\theta) \notin \mathcal{R}$ (see also the proof of Lemma 2.10). Thus, from Lemma 2.11 we conclude

$$-\operatorname{Re} \int_{\Gamma^+} \bar{v}\, \Lambda^+(e^{i\pi/4} v)\, ds \geq \frac{\sqrt{2}}{2}\, k|Q| \sum_{\nu\in\mathbb{Z}^2} |\rho^{(\nu)}|\, |v_\nu|^2.$$

and the series on the right hand side is equivalent to $\|v|_{\Gamma^+}\|_{Q,1/2}^2$ for small enough k by Remark 2.9. Using similar arguments as employed in the proof of Lemma 2.17 to see that the operator A_2 is coercive, we obtain

$$\operatorname{Re} \mathcal{B}_1(v,v) \geq c\, k \left(\int_{D\setminus\overline{D_{-1}}} |\nabla v|^2\, dx + \|v|_{\Gamma^+}\|_{Q,1/2}^2 \right) \geq c\, k\, \|v\|_1^2\,.$$

On the other hand, there obviously holds

$$|\mathcal{B}_2(v,v)| \leq c\, k^2\, \|v\|_1^2\,.$$

Hence, for small enough k, we obtain the assertion. ■

In order to use Theorem 2.21 to deduce solvability in the case of larger wave numbers, we will employ a result on the number of linear independent solutions of a Fredholm operator equation of the second kind given in [34]. First use of this result in scattering by periodic media was made in [30]. To simplify our later arguments, we first of all prove a slight generalization of a lemma given in [34].

Lemma 2.22 (Lemma I.5.1 of [34]) *Let H denote a Hilbert space. Further let $\mu_0 \in \mathbb{C}$ and suppose that W is some neighbourhood of μ_0. Further define for fixed $\sigma \in [0, 2\pi)$*

$$\gamma := \left\{\mu = \mu_0 + te^{i\sigma} : \; t > 0\right\},$$

and set $U := W \setminus \gamma$. Assume that for all $\mu \in U$, $A_\mu : H \to H$ is a compact linear operator. Further assume that A_μ depends analytically on μ in U except possibly at μ_0, but also, that A_μ depends continuously on μ in μ_0. Then there exists $\varepsilon > 0$ such that for all $\mu \in U$ satisfying $0 < |\mu - \mu_0| < \varepsilon$, the equation

$$(I - A_\mu)\,\varphi = 0$$

has the same number of linearly independent solutions.

Proof: Let m be the dimension of the kernel of $I - A_{\mu_0}$. Denote by $\{\varphi_1, \ldots, \varphi_m\}$ an orthonormal basis of the solution space of the equation $(I - A_{\mu_0})\,\varphi = 0$ and by $\{\psi_1, \ldots, \psi_m\}$ an orthonormal basis of the orthogonal complement of the range of $I - A_{\mu_0}$. Define $B_\mu : H \to H$ by

$$B_\mu \varphi := (I - A_\mu)\,\varphi + \sum_{j=1}^{m} \langle \varphi, \varphi_j \rangle \, \psi_j.$$

Obviously, B_{μ_0} is injective, and hence, as a compact perturbation of the identity, boundedly invertible. As A_μ depends continuously on μ, so does B_μ. Hence, using a Neumann series argument, we see that there is some neighbourhood U' of μ_0, in which B_μ^{-1} exists and is bounded, except for points on γ. Note also, that as A_μ depends analytically on μ except possibly at μ_0, so does B_μ and hence also B_μ^{-1}.

Now, we rewrite $(I - A_\mu)\,\varphi = 0$ as

$$\varphi - \sum_{j=1}^{m} \langle \varphi, \varphi_j \rangle \, B_\mu^{-1} \psi_j = 0.$$

By multiplying this equation by φ_l, $l = 1, \ldots, m$, we obtain a linear system for the unknowns $\langle \varphi, \varphi_j \rangle$, $j = 1, \ldots, m$. The coefficients in the system matrix depend on μ through B_μ^{-1} and hence analytically for $\mu \in U' \setminus (\gamma \cup \{\mu_0\})$.

If the system matrix is the zero matrix in $U' \setminus \gamma$, then the number of linearly independent solutions of $(I - A_\mu)\,\varphi = 0$ is m throughout $U' \setminus \gamma$ and the lemma is proved. Otherwise, let p denote the maximal rank of the matrix for $\mu \in U' \setminus \gamma$. It follows that there is a $p \times p$ submatrix with non zero determinant. As this determinant is an analytic function of μ, it follows that it can only be zero at isolated points in U' (including μ_0). In all other points, there are $m - p$ linearly independent solutions. Take ε the largest radius such that the punctured disc with center μ_0 and radius ε includes non of these isolated points. ■

This formulation generalizes the original lemma of [34] in so far as the point μ_0 is allowed to be a branch point of an operator that depends analytically on μ away from the branch cut. A remark in [30] makes it clear that the authors of that reference in fact make use of the version we present here. Now, Lemma 2.22 is the main ingredient in the proof of the following theorem:

Theorem 2.23 (Theorem I.5.1 of [34]) *Let H denote a Hilbert space. Assume that $C \subset \mathbb{C}$ is an open connected set and that $A_\mu : H \to H$ is a compact linear operator for all $\mu \in C$ that depends analytically on μ. Then, for all $\mu \in C$ except possibly for some isolated points, the equation*

$$(I - A_\mu)\,\varphi = 0$$

has the same number of linearly independent solutions.

Using Theorem 2.23, we can obtain the following solvability theorem for the scattering problems.

Theorem 2.24 *Let $\theta \in \mathbb{R}^3$ and $\alpha = k\theta$. Then the Dirichlet and Neumann Scattering Problems are uniquely solvable except possibly for a sequence (k_j) of wave numbers such that $k_j \to \infty$ as $j \to \infty$.*

Proof: Assume $(k, \alpha) \notin \mathcal{R}$. We choose $\theta \in \mathbb{R}^3$, $|\theta| < 1$ such that $\alpha = k\theta$. Then, by Theorem 2.21, there exists a wave number K with $(K, K\theta) \notin \mathcal{R}$ such that the scattering problem is uniquely solvable in a neighbourhood of K. Without loss of generality, we assume $k > K$.

From the definition of the forms $\mathcal{A}^{(1)}_{k\theta}$ and $\mathcal{A}^{(3)}_{k\theta}$ together with Lemma 2.10 we see that there is an open neighbourhood $C \subset \mathbb{C}$ of the interval $[K, k]$ in which the operators A_1 and A_3 depend analytically on k. Typically, the set C excludes certain branch cuts starting at a finite number of wave numbers k_ν such that $(k_\nu, k_\nu\theta) \in \mathcal{R}$, see Figure 2.2. Applying Theorem 2.23, we see that both scattering problems are uniquely solvable in C except possibly for isolated points.

It remains to prove that these isolated points form a sequence tending to infinity. This however, follows from Lemma 2.22: if we assume that these points accumulate at any μ_0, we obtain a contradiction to this lemma, both in the case when $\mu_0 \in C$ and when $(\mu_0, \mu_0\theta) \in \mathcal{R}$. ■

Uniqueness of Solution in Special Cases. The solvability results of the previous section are all what is known in the case of the Neumann Scattering Problem. In case of the Dirichlet Problem more can be said in cases with a special geometry and parameters satisfying certain assumptions.

Assumption 2.25 *In addition to Assumption 2.2, let the following hold*

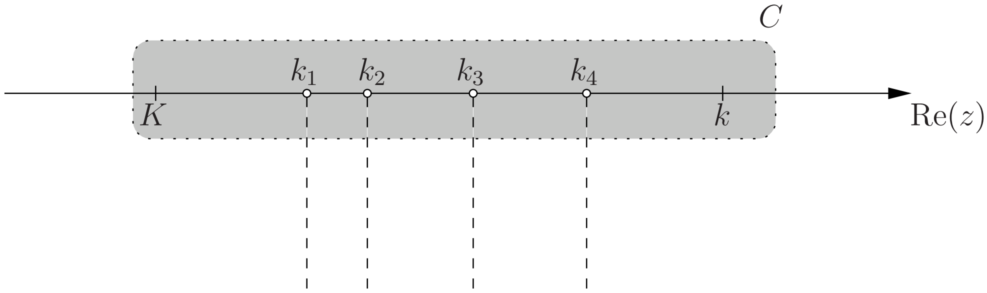


Figure 2.2: The interval $[K,k]$ and the set C with the branch points k_j and the corresponding branch cuts excluded.

- *Let each surface Γ_j, $j=0,\ldots,N$, be given as the graph of a Q-periodic Hölder continuous function f_j.*
- *Let the coefficients λ_j, $q_j > 0$ satisfy*

$$\lambda_{j-1} \geq \lambda_j \qquad \textit{and} \qquad \lambda_j q_j \geq \lambda_{j-1} q_{j-1}, \qquad j = 1,\ldots,N.$$

Remark 2.26 The additional assumptions on the constants q_j and λ_j are satisfied in the physically important cases listed in Remark 2.12. □

Lemma 2.27 *Assume $u_\alpha \in V_0$ is a solution of the Dirichlet Scattering Problem with $u^i = 0$ and that Assumption 2.25 is satisfied. Then $\Lambda^+ u_\alpha \in L^2(\Gamma^+)$ and*

$$\int_{\Gamma^+} \left(|\nabla_\alpha u_\alpha|^2 - 2\,|\Lambda^+ u_\alpha|^2 - k^2 |u_\alpha|^2 \right) ds = 0.$$

Proof: First of all note that from regularity results for elliptic partial differential equations with constant coefficients [33], we know that the first partial derivatives of u_α can be continued to Hölder continuous functions in a neighbourhood of Γ^+. Hence $\Lambda^+ u_\alpha \in L^2(\Gamma^+)$ follows so that all expressions in the assertion make sense.

Let (u_ν) denote the Fourier coefficients in the expansion of u on Γ^+. Taking the imaginary part of the variational equation of the Scalar Dirichlet Problem 2.14 for $v = u_\alpha$, we obtain

$$\operatorname{Im}\left(\int_{\Gamma^+} \overline{u_\alpha}\, \Lambda^+ u_\alpha \, ds \right) = 0,$$

and hence $\rho^{(\nu)} u_\nu = 0$ whenever $|d^{(\nu)}| \leq 1$ by Lemma 2.11.

Next, we choose $v \in V_0$ such that v is C^∞ and vanishes everywhere except for a neighborhood of Γ^+ contained in D_N. Then we obtain from the variational formulation that

$$\int_{D_N} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_N k^2\, u_\alpha\, \bar{v} \right) dx - \int_{\Gamma^+} \bar{v}\, \Lambda^+ u_\alpha \, ds = 0.$$

From regularity results for weak solutions of elliptic differential euqations with constant coefficients, we conclude that u_α is smooth on the support of v and hence we can apply Green's first identity and the divergence theorem to obtain

$$\int_{\Gamma^+} \bar{v} \left(n \cdot \nabla_\alpha u_\alpha - \Lambda^+ u_\alpha \right) ds = 0.$$

Thus we conclude $n \cdot \nabla_\alpha u_\alpha = \Lambda^+ u_\alpha$ on Γ^+, and hence,

$$\begin{aligned}
&\int_{\Gamma^+} \left(|\nabla_\alpha u_\alpha|^2 - 2\,|\Lambda^+ u_\alpha|^2 - k^2 |u_\alpha|^2 \right) ds \\
&\quad = \int_{\Gamma^+} \left(\left| \left(\frac{\partial}{\partial x_1} + i\alpha_1, \frac{\partial}{\partial x_2} + i\alpha_2, 0 \right)^\top u_\alpha \right|^2 - |\Lambda^+ u_\alpha|^2 - k^2 |u_\alpha|^2 \right) ds \\
&\quad = \sum_{\nu,\mu} \left[(iq^{(\nu)} + i\tilde{\alpha})(-iq^{(\mu)} - i\tilde{\alpha}) - k^2 \rho^{(\nu)} \overline{\rho^{(\mu)}} - k^2 \right] \\
&\qquad \times \int_{\Gamma^+} \exp(ik\,(q^{(\nu)} - q^{(\mu)}) \cdot x)\, ds\, u_\nu\, \overline{u_\mu} \\
&\quad = |Q| \sum_{|d^{(\nu)}|>1} \left[|q^{(\nu)} + \tilde{\alpha}|^2 - k^2 (1 + |\rho^{(\nu)}|^2) \right] |u_\nu|^2.
\end{aligned}$$

But for $|d^{(\nu)}| > 1$, $|\rho^{(\nu)}|^2 = |d^{(\nu)}|^2 - 1$, so the assertion is proved. ■

Remark 2.28 Note the proof of Lemma 2.27 only uses Assumption 2.25 in so far as $q_j \in \mathbb{R}$ is required, hence the arguments in fact also work for the Neumann Scattering Problem. As a consequence, we obtain the result that any solution to the homogeneous Dirichlet or Neumann problem, independently of any special geometry, does not include any plane waves propagating away from the medium in its Rayleigh expansion.

There is an interesting consequence of this result given in [30, Remark 3.4]: By obtaining the corresponding result for the adjoint problem, the authors conclude that any solution of the homogeneous adjoint problem is orthogonal on Γ^+ to a downward propagating plane wave. Hence both the Neumann and the Dirichlet Scattering Problems are always solvable for an incident plane wave, even if the solution is non-unique. □

Theorem 2.29 *Assume $u_\alpha \in V_0$ is a solution of the Dirichlet Scattering Problem with $u^i = 0$ and that Assumption 2.25 is satisfied. Then $u_\alpha = 0$.*

Proof: From regularity results for weak solutions of second order elliptic partial differential equations [33], we obtain that the first partial derivatives of u_α can be extended to Hölder continuous function on $\overline{D_j}$, $j = 0, \dots, N$. A first consequence is that we can deduce the transmission conditions (2.15) from the variational formulation.

As the second step in the proof, we make D_j slightly smaller, setting for some $\varepsilon > 0$ chosen small enough

$$D_j^\varepsilon = \{x \in D_j : f_j(\tilde{x}) + \varepsilon < x_3 < f_{j+1}(\tilde{x}) - \varepsilon\}.$$

Then $u_\alpha \in C^2(\overline{D_j^\varepsilon})$ and (2.24) remains valid with D replaced by D_j^ε and appropriately shifted upper and lower boundaries. Setting $v = (\partial u_\alpha)/(\partial x_3)$ and adding the complex conjugate of this equation, yields

$$\begin{aligned}&\int_{D_j^\varepsilon} \frac{\partial}{\partial x_3}\left[|\nabla_\alpha u_\alpha|^2 - q_j k^2 |u_\alpha|^2\right] dx \\ &\qquad = 2\,\mathrm{Re}\left(\int_{\Gamma_{j+1-\varepsilon}} \overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha)\,ds\right) - 2\,\mathrm{Re}\left(\int_{\Gamma_{j+\varepsilon}} \overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha)\,ds\right).\end{aligned}$$

We now make use of the fact that each surface Γ_j is given as the graph of a smooth function. A consequence is that we can apply Fubini's theorem to the domain integral to obtain

$$\begin{aligned}&\int_{\Gamma_{j+1-\varepsilon}} \left(|\nabla_\alpha u_\alpha|^2 - q_j k^2 |u_\alpha|^2\right) d\tilde{x} - 2\,\mathrm{Re}\left(\int_{\Gamma_{j+1}} \overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha)\,ds\right) \\ &\qquad - \int_{\Gamma_{j+\varepsilon}} \left(|\nabla_\alpha u_\alpha|^2 - q_j k^2 |u_\alpha|^2\right) d\tilde{x} + 2\,\mathrm{Re}\left(\int_{\Gamma_j} \overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha)\,ds\right) = 0.\end{aligned}$$

All integrals now only involve first derivative of $u_\alpha \in C^1(\overline{D_j})$, hence we can let $\varepsilon \to 0$ and this relation stays valid. Noting $n_3 ds = d\tilde{x}$, the equation can be further rewritten as

$$\begin{aligned}&\int_{\Gamma_{j+1}} \left[|\nabla_\alpha u_\alpha|^2 - 2\,\mathrm{Re}\left(\frac{1}{n_3}\overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha)\right) - q_j k^2 |u_\alpha|^2\right] d\tilde{x} \\ &\qquad - \int_{\Gamma_j} \left[|\nabla_\alpha u_\alpha|^2 - 2\,\mathrm{Re}\left(\frac{1}{n_3}\overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha)\right) - q_j k^2 |u_\alpha|^2\right] d\tilde{x} = 0.\end{aligned}$$

The same process can be applied to equation (2.25), noting also as in the proof of Lemma 2.27 that on Γ^+, $n \cdot \nabla_\alpha u_\alpha = (\partial u_\alpha)/(\partial x_3) = \Lambda^+ u_\alpha$. Multiplying all resulting equations by λ_j, respectively, and taking the sum, we obtain

$$\begin{aligned}\lambda_N \int_{\Gamma^+} &\left(|\nabla_\alpha u_\alpha|^2 - 2\,|\Lambda^+ u_\alpha|^2 - q_N k^2 |u_\alpha|^2\right) ds \\ &+ \sum_{j=1}^{N} \int_{\Gamma_j} \left\{ \lambda_{j-1} |\nabla_\alpha u_\alpha^-|^2 - \lambda_j |\nabla_\alpha u_\alpha^+|^2 - \frac{2}{n_3} \operatorname{Re}\left(\lambda_{j-1} \overline{\frac{\partial u_\alpha^-}{\partial x_3}} \,(n\cdot\nabla_\alpha u_\alpha^-) \right.\right. \\ &\qquad \left.\left. - \lambda_j \overline{\frac{\partial u_\alpha^+}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha^+)\right) + k^2\left(\lambda_j q_j - \lambda_{j-1} q_{j-1}\right)|u_\alpha|^2 \right\} d\tilde{x} \\ &\qquad - \lambda_0 \int_{\Gamma_0} \left[|\nabla_\alpha u_\alpha|^2 - \frac{2}{n_3} \operatorname{Re}\left(\overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha)\right)\right] d\tilde{x} = 0, \qquad (2.29)\end{aligned}$$

where we have used that u_α does not jump across Γ_j and where the $\pm$ superscripts denote traces taken from above or below Γ_j, respectively. We have also made use of the fact that $u_\alpha = 0$ on Γ_0 in the last integral. In (2.29), the integral over Γ^+ vanishes by Lemma 2.27.

Denoting by $\nabla_{\Gamma_j,\alpha} u_\alpha^\pm$ the tangential component of $\nabla_\alpha u_\alpha^\pm$ on Γ_j, $j = 1, \dots, N$, we write the partial derivative with respect to x_3 as a linear combination of normal and tangential compontent of $\nabla_\alpha u_\alpha^\pm$,

$$\frac{\partial u_\alpha^\pm}{\partial x_3} = n_3 (n\cdot\nabla_\alpha u_\alpha^\pm) + a\cdot\nabla_{\Gamma_j,\alpha} u_\alpha^\pm.$$

The function a only depends on Γ_j. As u_α is continuous across Γ_j, so are the tangential components of $\nabla_\alpha u_\alpha^\pm$. Hence, also making use of the transmission conditions,

$$\frac{\partial u_\alpha^-}{\partial x_3} - \frac{\partial u_\alpha^+}{\partial x_3} = n_3(n\cdot\nabla_\alpha u_\alpha^-) - n_3(n\cdot\nabla_\alpha u_\alpha^+) = n_3\left(1 - \frac{\lambda_{j-1}}{\lambda_j}\right)(n\cdot\nabla_\alpha u_\alpha^-)$$

and thus

$$\frac{2}{n_3}\operatorname{Re}\left(\lambda_{j-1}\overline{\frac{\partial u_\alpha^-}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha^-) - \lambda_j \overline{\frac{\partial u_\alpha^+}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha^+)\right) = 2\,\frac{\lambda_{j-1}}{\lambda_j}\,(\lambda_j - \lambda_{j-1})\,|n\cdot\nabla_\alpha u_\alpha^-|^2.$$

Again using the decomposition of $\nabla_\alpha u_\alpha^\pm$ in normal and tangential components, we can rewrite

$$\lambda_{j-1}|\nabla_\alpha u_\alpha^-|^2 - \lambda_j |\nabla_\alpha u_\alpha^+|^2 = \frac{\lambda_{j-1}}{\lambda_j}\,(\lambda_j - \lambda_{j-1})\,|n\cdot\nabla_\alpha u_\alpha^-|^2 + (\lambda_{j-1} - \lambda_j)\,|\nabla_{\Gamma_j,\alpha} u_\alpha|^2.$$

Combining these results, the integral over Γ_j reduces to

$$\begin{aligned}\int_{\Gamma_j} &\left(\frac{\lambda_{j-1}}{\lambda_j}\,(\lambda_{j-1} - \lambda_j)\,|n\cdot\nabla_\alpha u_\alpha^-|^2 + (\lambda_{j-1} - \lambda_j)\,|\nabla_{\Gamma_j,\alpha} u_\alpha|^2 \right. \\ &\qquad\qquad \left. + k^2\left(\lambda_j q_j - \lambda_{j-1} q_{j-1}\right)|u_\alpha|^2 \right) d\tilde{x}.\end{aligned}$$

On Γ_0, the tangential components of $\nabla_\alpha u_\alpha$ vanish because u_α does. Hence, by similar calculations as for Γ_j, $j > 0$, we obtain

$$\mathrm{Re}\left(\overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n\cdot\nabla_\alpha u_\alpha)\right) = n_3\,|\nabla_\alpha u_\alpha|^2.$$

Concluding, we have reduced (2.29) to the equation

$$\sum_{j=1}^{N}\int_{\Gamma_j}\left(\frac{\lambda_{j-1}}{\lambda_j}\,(\lambda_{j-1}-\lambda_j)\,|n\cdot\nabla_\alpha u_\alpha^-|^2 + (\lambda_{j-1}-\lambda_j)\,|\nabla_{\Gamma_j,\alpha}u_\alpha|^2 \right.$$
$$\left. + k^2\,(\lambda_j q_j - \lambda_{j-1}q_{j-1})\,|u_\alpha|^2\right)d\tilde{x} + \lambda_0\int_{\Gamma_0}|\nabla_\alpha u_\alpha|^2\,d\tilde{x} = 0.$$

By Assumption 2.25 all terms on the left hand side of this equation are non negative and thus have to vanish. So, $|\nabla_\alpha u_\alpha| \equiv 0$ on Γ_0, and this implies $u \equiv 0$ by Holmgren's uniqueness theorem and the analyticity of solutions to the Helmholtz equation applied piecewise in each domain D_j. ■

Remark 2.30 Implicitly, the proof of the previous theorem makes use of a Rellich-type identity. Examples of similar proofs for scattering by rough surfaces or wave guides in which the identity is derived and used explicitely are contained in [4, 21, 44]. □

Corollary 2.31 *Suppose that Assumption 2.25 holds. Then the scalar Dirichlet Scattering Problem 2.14 posseses a unique solution* $u_\alpha \in V_0$.

2.4 The Transmission Problem

Problem Formulations. We now consider the case where the wave field can also enter the domain D_{-1}. Instead of a boundary condition on Γ_0, we impose an additional transmission condition on Γ_0 and a radiation condition on Γ^-. Hence, we start from the following classical problem formulation: Given a Q-quasi-periodic incident field u^i with phase-shift α, find the total field u such that

- u is a solution of the Helmholtz equation (2.14) in each domain D_j, $j = -1, \ldots, N$, where we assume again $\mathrm{Re}(q_j) > 0$ and $\mathrm{Im}(q_j) \geq 0$.
- On each interface Γ_j, $j = 0, \ldots, N$, the transmission conditions (2.15) hold where the coefficients λ_j satisfy (2.16).

- The reflected field $u - u^i$ satisfies the URC and u satisfies the DRC, as stated in Definition 2.6, respectively.

The appropriate space in which to set a variational formulation for the transmission problem is the Sobolev space

$$V := H^1_Q(D).$$

To derive a variational formulation of this problem, we proceed as in Section 2.3 to obtain (2.24) and (2.25) as well as the equation

$$\int_{D_{-1}} \big(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - k^2\, u_\alpha\, \bar v\big)\, dx = \int_{\Gamma^0} \bar v\, (n \cdot \nabla_\alpha u_\alpha)\, ds - \int_{\Gamma^-} \bar v\, (n \cdot \nabla_\alpha u_\alpha)\, ds \quad (2.30)$$

for all $v \in V$. Multiplying each equation with λ_j, respectively, taking the sum and making use of the transmission conditions, we conclude

$$\sum_{j=-1}^{N} \lambda_j \int_{D_j} \big(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha \bar v\big)\, dx$$
$$= \lambda_N \int_{\Gamma^+} \bar v\, (n \cdot \nabla_\alpha u_\alpha)\, ds - \lambda_{-1} \int_{\Gamma^-} \bar v\, (n \cdot \nabla_\alpha u_\alpha)\, ds.$$

By making use of the URC and DRC, respectively, we can replace the normal derivatives on Γ^+ and Γ^- by the corresponding Dirichlet-to-Neumann maps, taking care to include the incident field in the expression for Γ^+ as in the case of the scattering problems. Hence we are led to the following variational formulation of the transmission problem:

Problem 2.32 (Transmission Problem)
Given a Q-quasi-periodic incident field u^i, find $u_\alpha \in V$ such that

$$\sum_{j=-1}^{N} \lambda_j \int_{D_j} \big(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha\, \bar v\big)\, dx - \lambda_N \int_{\Gamma^+} \bar v\, \Lambda^+ u_\alpha\, ds + \lambda_{-1} \int_{\Gamma^-} \bar v\, \Lambda^- u_\alpha\, ds$$
$$= \lambda_N \int_{\Gamma^+} \bar v\, \left(M_{-\alpha} \frac{\partial u^i}{\partial n} - \Lambda^+ M_{-\alpha} u^i \right) ds \qquad \textit{for all } v \in V.$$

Solvability. Led by the results obtained for the scattering problems, the approach for establishing solvability for the transmission problem is now straightforward. We define the sesquilinear forms

$$\mathcal{A}_\alpha^{(1)}(u_\alpha, v) := \sum_{j=-1}^{N} \lambda_j \int_{D_j} \left(\nabla u_\alpha \cdot \overline{\nabla v} + u_\alpha \bar{v}\right) dx - \lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+ u_\alpha \, ds + \lambda_{-1} \int_{\Gamma^-} \bar{v}\, \Lambda^- u_\alpha \, ds,$$

$$\mathcal{A}_\alpha^{(2)}(u_\alpha, v) := \sum_{j=-1}^{N} \lambda_j \int_{D_j} \left((|\tilde{\alpha}|^2 - q_j\, k^2 - 1) u_\alpha \bar{v} + i\tilde{\alpha} \cdot \left[u_\alpha \overline{\nabla v} - \bar{v} \nabla u_\alpha\right]\right) dx.$$

Both forms define a bounded linear operator $A_j : V \to V$, $j = 1, 2$. We obtain the following results for these operators.

Corollary 2.33 *(a) The operator $A_1 : V \to V$ is coercive, the operator $A_2 : V \to V$ is compact. Hence $A_1 + A_2$ is a Fredholm operator of index 0.*

(b) Assume that $\mathrm{Im}(q_j) > 0$ for some $j \in \{0, \dots, N-1\}$. Then the Transmission Problem 2.32 is uniquely solvable.

Proof: The proof is a simple adaptation of the proofs of Lemmas 2.17 and Theorem 2.19, additionally making use of the properties of Λ^- established in Lemma 2.11. ■

Remark 2.34 The transmission problem can also be considered for $\mathrm{Im}(q_{-1}) > 0$ or $\mathrm{Im}(q_N) > 0$. This requires considerations as outlined in Remark 2.20 for the scattering problems. Uniqueness of solution can then be established as in the proof of Corollary 2.33. □

The next step is to establish the unique solvability of the transmission problem for small enough wave numbers.

Corollary 2.35 *Let $\theta \in \mathbb{R}^3$ and $\alpha = k\theta$. Then there exists $k_0 > 0$ such that for all $k \leq k_0$ there exists a constant $c > 0$, such that*

$$\mathrm{Re}\left(\sum_{j=-1}^{N} e^{i\pi/4} \lambda_j \int_{D_j} \left(|\nabla_\alpha v|^2 - q_j k^2\, |v|^2\right) dx - \lambda_N \int_{\Gamma^+} \bar{v}\, \Lambda^+(e^{i\pi/4} v)\, ds + \lambda_{-1} \int_{\Gamma^-} \bar{v}\, \Lambda^-(e^{i\pi/4} v)\, ds\right) \geq c\, \|v\|_1^2$$

for all all $v \in V$.

Proof: The proof of the Corollary is completely similar to the proof of Theorem 2.21. The only additional argument required is that

$$\operatorname{Re} \int_{\Gamma^-} \bar{v}\, \Lambda^-(e^{i\pi/4} v)\, ds \geq \frac{\sqrt{2}}{2}\, k|Q|\ \|v\|^2_{Q,1/2}\,.$$

by Lemma 2.11. ■

We now combine the result of this corollary with Theorem 2.23 to obtain the following corollary to Theorem 2.24.

Corollary 2.36 *Let $\theta \in \mathbb{R}^3$ and $\alpha = k\theta$. Then the scalar Transmission Problem 2.32 is uniquely solvable except possibly for a sequence (k_j) of wave numbers such that $k_j \to \infty$ as $j \to \infty$.*

We will now proceed with proving a uniqueness result similar to Theorem 2.29 for the case of a transmission problem. We will require similar geometrical conditions as well as some more restrictions on the coefficients λ_j and q_j.

Assumption 2.37 *In addition to Assumption 2.2, let the following hold*

- *Let each surface Γ_j, $j = 0, \ldots, N$, be given as the graph of a Q-periodic Hölder continuous function f_j.*
- *Assume that there is an index $j_0 \in \{-1, \ldots, N\}$ such that the coefficients λ_j, $q_j > 0$ satisfy*

$$\lambda_{j-1} \geq \lambda_j \qquad \text{and} \qquad \lambda_j q_j \geq \lambda_{j-1} q_{j-1}, \qquad j = j_0 + 1, \ldots, N,$$

and

$$\lambda_{j-1} \leq \lambda_j \qquad \text{and} \qquad \lambda_j q_j \leq \lambda_{j-1} q_{j-1}, \qquad j = 0, \ldots, j_0.$$

Furthermore, we assume that there exists $c \in \mathbb{R}$ such that $Q \times \{c\} \subset D_{j_0}$.

Remark 2.38 The second condition of Assumption 2.37 has apeared frequently in the literature on scattering by unbounded inhomogenious media in two dimensions [11, 20, 59]. There it is assumed that q is a function of x and the condition in Assumption 2.37 takes the form

$$(x_3 - c)\, \frac{\partial q(x)}{\partial x_3} \geq 0, \qquad x \in D,$$

for some $c \in \mathbb{R}$. Our condition is a complete analogue in the case $\lambda_j = 1$, $j = -1, \ldots, N$. □

Lemma 2.39 *Assume* $u_\alpha \in V$ *is a solution of the Transmission Problem with* $u^i = 0$ *and that Assumption 2.37 is satisfied. Then*

$$\int_{\Gamma^\pm} \left(|\nabla_\alpha u_\alpha|^2 - 2\,|\Lambda^\pm u_\alpha|^2 - k^2 |u_\alpha|^2\right) ds = 0$$

and

$$\sum_{j=-1}^{N} \lambda_j \int_{D_j} \left(|\nabla_\alpha u_\alpha|^2 - q_j k^2\,|u_\alpha|^2\right) dx \le 0.$$

Proof: We denote the Fourier coefficients of u_α on $\Gamma^\pm$ by $(u_\nu^\pm)$, respectively. Setting $v = u_\alpha$ in the variational equation of the Transmission Problem 2.32 and taking the imaginary part, we obtain from Lemma 2.11

$$0 = \mathrm{Im}\left(\lambda_{-1} \int_{\Gamma^-} \overline{u_\alpha}\,\Lambda^- u_\alpha\,ds - \lambda_N \int_{\Gamma^+} \overline{u_\alpha}\,\Lambda^+ u_\alpha\,ds\right)$$
$$= -k|Q| \sum_{|d^{(\nu)}|\le 1} |\rho^{(\nu)}| \left(|u_\nu^-|^2 + |u_\nu^+|^2\right).$$

Hence $\rho^{(\nu)} u_\nu^\pm = 0$ for $|d^{(\nu)}| \le 1$. The first assertion now follows as in the proof of Lemma 2.27.

For the second assertion we again set $v = u_\alpha$ in the variational equation and then take the real part and apply Lemma 2.11 once more. ■

Theorem 2.40 *Assume that* $u_\alpha \in V$ *is a solution of the Transmission Problem with* $u^i = 0$ *and that Assumption 2.37 holds. Then* $u_\alpha = 0$.

Proof: As in the proof of Theorem 2.29, we argue that the first partial derivatives of u_α are Hölder continuous in $\overline{D_j}$, $j = -1, \ldots, N$. Replacing D_j by D_j^ε as in the proof of Theorem 2.29, we can insert $v(x) = (x_3 - c)\,(\partial u_\alpha)/(\partial x_3)$ in (2.24) and add the complex conjugate of this equation to obtain

$$\int_{D_j^\varepsilon} \frac{\partial}{\partial x_3} \left((x_3 - c)\,\left[|\nabla_\alpha u_\alpha|^2 - q_j k^2\,|u_\alpha|^2\right]\right) dx$$
$$+ \int_{D_j^\varepsilon} \left(2\left|\frac{\partial u_\alpha}{\partial x_3}\right|^2 - |\nabla_\alpha u_\alpha|^2 + q_j k^2\,|u_\alpha|^2\right) dx$$
$$= 2\,\mathrm{Re}\left(\int_{\Gamma_{j+1-\varepsilon}} (f_{j+1}(\tilde{x}) - \varepsilon - c)\,\overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n \cdot \nabla_\alpha u_\alpha)\,ds\right)$$
$$- 2\,\mathrm{Re}\left(\int_{\Gamma_{j+\varepsilon}} (f_j(\tilde{x}) + \varepsilon - c)\,\overline{\frac{\partial u_\alpha}{\partial x_3}}\,(n \cdot \nabla_\alpha u_\alpha)\,ds\right).$$

Recall that by f_j we denote the function representing Γ_j.

Applying Fubini's theorem letting $\varepsilon \to 0$ and performing identical manipulations as in the proof of Theorem 2.29 eventually leads to

$$\begin{aligned}
\lambda_N \int_{\Gamma^+} \left(|\nabla_\alpha u_\alpha|^2 - 2\,|\Lambda^+ u_\alpha|^2 - k^2 |u_\alpha|^2\right) ds \\
- \lambda_0 \int_{\Gamma^-} \left(|\nabla_\alpha u_\alpha|^2 - 2\,|\Lambda^- u_\alpha|^2 - k^2 |u_\alpha|^2\right) ds \\
+ \sum_{j=-1}^{N} \lambda_j \int_{D_j} \left(2 \left|\frac{\partial u_\alpha}{\partial x_3}\right|^2 - |\nabla_\alpha u_\alpha|^2 + q_j k^2\, |u_\alpha|^2\right) dx \\
+ \sum_{j=0}^{N} \int_{\Gamma_j} (f_j(\tilde{x}) - c) \left(\frac{\lambda_{j-1}}{\lambda_j} (\lambda_{j-1} - \lambda_j)\, |n \cdot \nabla_\alpha u_\alpha^-|^2 + (\lambda_{j-1} - \lambda_j)\, |\nabla_{\Gamma_j,\alpha} u_\alpha|^2 \right. \\
\left. + k^2 (\lambda_j q_j - \lambda_{j-1} q_{j-1})\, |u_\alpha|^2 \right) d\tilde{x} = 0.
\end{aligned}$$

From Lemma 2.39, we obtain that the integrals over $\Gamma^\pm$ vanish. By Assumption 2.37 and again Lemma 2.39, all other terms are non-negative and thus have to vanish. Hence, u_α and its partial derivatives are 0 along each surface Γ_j and Holmgren's uniqueness theorem together with the analyticity of solutions of the Helmholtz equation yields the assertion. ■

Theorem 2.40 together with Corollary 2.33 now immeadiately yields the following solvability result for the Scalar Transmission Problem.

Corollary 2.41 *Suppose that Assumption 2.37 holds. Then the Scalar Transmission Problem 2.32 posseses a unique solution* $u_\alpha \in V$.

Chapter 3

The Q-Quasi-Periodic Green's Function

As a first step in the development of the boundary integral equation approach for scattering by biperiodic media, it is necessary to find an expression for a Green's function with suitable periodicity properties. This task is far from trivial, in particular if the objective is to find an expression that is well suited for numerical evaluation.

For the simpler, two-dimensional case, there is a substantial amount of literature devoted to this topic. As an entry point to this subject we recommend the paper [45] which reviews several methods and points to further literature.

As will be shown in this chapter, the question of deriving expressions for the Green's function is even more delicate in three dimensions: Not only the speed of convergence of the derived expressions is an issue but also whether these expressions are only formal in nature, i.e. if they are meaningfull and converge at all.

These issues were taken up first in the physics community in the early decades of the twentieth century when methods were sought to represent and evaluate potentials of crystal structures. A method to derive Green's function representations developed and named after the physicist Ewald [31] is well known and extensively used in that community but rather less well represented in the mathematical literature. As will be shown below, this method yields both a representation that is globally convergent as well as efficiently evaluable.

3.1 Standard Expressions with Limitations

It is our aim to derive expressions for a Q-quasi-periodic Green's function of the Helmholtz equation in the entire space $\mathbb{R}^3$. Our approach to this problem is purely constructive, i.e. we derive an expression for a function with the required properties. A general existence theory for Green's functions has been carried out by many authors, see [25, pp. 253] for a historic account.

Two approaches seem very natural to attempt for this problem: seeking the Green's function in the form of a Fourier series and seeking it in the form of a periodic array of point sources. We will attempt the first approach and later try to rewrite the obtained expression to obtain the second form.

Obtaining the Fourier expansion. To formulate the problem more precisely, let us set $\Omega := Q \times \mathbb{R}$ and $\omega := \{(x, x) : x \in \Omega\}$. We seek a function $G_k : (\Omega \times \Omega) \setminus \omega \to \mathbb{C}$, depending also on the wave number k, such that for fixed y, $G_k(\cdot, y)$ has a Q-quasi-periodic extension with respect to x to $\mathbb{R}^3$ with phase-shift α, and that

$$G_k(x, y) = \Phi_k(x, y) + \Psi_k(x - y), \qquad x, y \in (\Omega \times \Omega) \setminus \omega, \tag{3.1}$$

where Φ_k denotes the fundamental solution to the Helmholtz equation in free field conditions,

$$\Phi_k(x, y) = \frac{1}{4\pi} \frac{\exp(ik\,|x - y|)}{|x - y|}, \qquad x \neq y,$$

and Ψ_k is an analytic solution to the Helmholtz equation in $(-L_1, L1) \times (-L_2, L_2) \times \mathbb{R}$. Further conditions on G_k are that $G_k(\cdot, y)$ must be propagating away from y in Ω and should be bounded on Ω except for neighbourhoods of y. We will also assume for the time being that $\arg k \in (0, \pi/2)$. In the notation of Chapter 2 this corresponds to the Helmholtz operator including an index of refraction q with positive imaginary part. However, the definition of $\rho^{(\nu)}$ must also be extended using an analytic continuation of the square root function to the complex plane cut along the negative imaginary axis.

From the condition of Q-quasi-periodicity, it follows that G_k has a formal Fourier expansion of the form

$$G_k(x, y) = \sum_{\nu \in \mathbb{Z}^2} \gamma_\nu(x_3 - y_3)\, \exp(ik\, d^{(\nu)} \cdot (x - y)) \tag{3.2}$$

with coefficients γ_ν yet to be determined. To determine these coefficients, we argue similarly as in Section 2.2. Inserting expression (3.2) into the Helmholtz equation and assuming $x_3 \neq y_3$, we obtain for $\nu \in \mathbb{Z}^2$ the differential equations

$$\gamma_\nu''(t) + k^2(1 - |d^{(\nu)}|^2)\, \gamma_\nu(t) = 0, \qquad t \in \mathbb{R},$$

with the general solution

$$\gamma_\nu(t) = a_\nu \exp(ik\, \rho^{(\nu)}\, t) + b_\nu \exp(-ik\, \rho^{(\nu)}\, t), \qquad t \in \mathbb{R}, \quad a_\nu, b_\nu \in \mathbb{C}.$$

Assuming that $x_3 > y_3$, we obtain from the condition that G_k be bounded and propagating away from y that $b_\nu = 0$. Conversely, assuming that $x_3 < y_3$, we obtain $a_\nu = 0$. We combine both cases, to obtain the representation

$$G_k(x,y) = \sum_{\nu\in\mathbb{Z}^2} c_\nu \, \exp(ik\,\rho^{(\nu)}\,|x_3 - y_3|)\,\exp(ikd^{(\nu)}\cdot(x-y)), \tag{3.3}$$

with coefficients $c_\nu \in \mathbb{C}$. To obtain expressions for these coefficients, consider the functions u_μ defined by

$$u_\mu(x) := \exp(ik\,(d^{(\mu)}\cdot x + \rho^{(\mu)}\,x_3)), \qquad x \in \mathbb{R}^3.$$

As can easily be verified, these functions are entire, Q-quasi-periodic solutions to the Helmholtz equation with phase-shift α. Hence, recalling (3.1), we obtain from Green's representation theorem, that

$$1 = u_\mu(0) = \int_{\partial\Omega_R} \left\{ G_k(0,y)\,\frac{\partial u_\mu}{\partial n}(y) - \frac{\partial G_k(0,y)}{\partial n(y)}\,u_\mu(y)\right\} ds(y),$$

where $\Omega_R := Q \times [-R,R]$, $R > 0$, and n denotes the outward-drawn normal to $\partial\Omega_R$. Because of Q-quasi-periodicity, the contributions from the vertical sections of $\partial\Omega_R$ cancel (cf. Section 2.3). Hence, setting $\Gamma_{\pm R} := Q \times \{\pm R\}$, we arrive at

$$\begin{aligned} 1 = \int_{\Gamma_R} &\left\{ G_k(0,y)\,\frac{\partial u_\mu}{\partial n}(y) - \frac{\partial G_k(0,y)}{\partial n(y)}\,u_\mu(y)\right\} ds(y) \\ &+ \int_{\Gamma_{-R}} \left\{ G_k(0,y)\,\frac{\partial u_\mu}{\partial n}(y) - \frac{\partial G_k(0,y)}{\partial n(y)}\,u_\mu(y)\right\} ds(y). \end{aligned}$$

Let us now use the Fourier expansion representations of G_k and u_ν to obtain for $y \in \Gamma_{\pm R}$,

$$\begin{aligned} G_k(0,y) &= \sum_{\nu\in\mathbb{Z}^2} c_\nu\,\exp(ik\,\rho^{(\nu)}\,R)\;\exp(-ik\,d^{(\nu)}\cdot y), \\ \frac{\partial G_k(0,y)}{\partial n(y)} &= \sum_{\nu\in\mathbb{Z}^2} c_\nu\,ik\,\rho^{(\nu)}\;\exp(ik\,\rho^{(\nu)}\,R)\,\exp(-ik\,d^{(\nu)}\cdot y), \\ u_\mu(y) &= \exp(\pm ik\,\rho^{(\mu)}\,R)\,\exp(ik\,d^{(\mu)}\cdot y), \\ \frac{\partial u_\mu}{\partial n}(y) &= \pm ik\,\rho^{(\mu)}\exp(\pm ik\rho^{(\mu)}\,R)\,\exp(ik\,d^{(\mu)}\cdot y), \end{aligned}$$

and hence,

$$\begin{aligned} 1 = \sum_{\nu\in\mathbb{Z}^2} ik\,c_\nu &\int_Q \exp(iy\cdot(q^{(\mu)} - q^{(\nu)}))\,d\tilde{y} \\ \times \Big[(\rho^{(\mu)} - \rho^{(\nu)})&\exp(ik\,R\,(\rho^{(\mu)} + \rho^{(\nu)})) - (\rho^{(\mu)} + \rho^{(\nu)})\,\exp(ik\,R\,(\rho^{(\nu)} - \rho^{(\mu)}))\Big]. \end{aligned}$$

From the orthogonality of the trigonometric monomials in $L^2(Q)$, we obtain

$$1 = -2\, ik\, |Q|\, \rho^{(\mu)}\, c_\mu,$$

which implies

$$c_\mu = \frac{i}{2|Q|}\, \frac{1}{k\, \rho^{(\mu)}}. \tag{3.4}$$

So, by inserting this result in (3.3), we have obtained the expression

$$G_k(x,y) = \frac{i}{2|Q|} \sum_{\nu\in\mathbb{Z}^2} \frac{\exp(ik\, \rho^{(\nu)}\, |x_3 - y_3|)}{k\, \rho^{(\nu)}}\, \exp(ik\, d^{(\nu)} \cdot (x-y)) \tag{3.5}$$

for the quasi-periodic fundamental solution.

Expression (3.5) can be regarded as a formal Fourier expansion and hence as an element of an appropriately chosen quasi-periodic Sobolev space. However, absolute convergence of the series is only guaranteed for $x_3 \neq y_3$. Note however, that (3.5) can be continued analytically to real k as long as $(k,\alpha) \notin \mathcal{R}$ and $x_3 \neq y_3$.

Obtaining a superposition of point sources. Alternatively, the Green's function can be expressed as a Q-quasi-periodic superposition of point sources, which also gives an explicit expression for the function Ψ in (3.1). We start by observing the following lemma, in whose formulation for ease of notation vectors in $\mathbb{R}^2 \times \{0\}$ have been identified with vectors in $\mathbb{R}^2$.

Lemma 3.1 (Possion Summation Formula) *Let the function f be an element of the Schwartz space $S(\mathbb{R}^2)$. Then*

$$\sum_{\mu\in\mathbb{Z}^2} f(\tilde{x} - p^{(\mu)}) = \frac{1}{|Q|} \sum_{\nu\in\mathbb{Z}^2} \hat{f}(q^{(\nu)})\, \exp(-i\, q^{(\nu)} \cdot \tilde{x}), \qquad \tilde{x} \in \mathbb{R}^2,$$

where $\hat{f}$ denotes the Fourier transform of f with respect to $\tilde{x}$,

$$\hat{f}(q) = \int_{\mathbb{R}^2} f(\tilde{x})\, \exp(iq \cdot \tilde{x})\, d\tilde{x}, \qquad q \in \mathbb{R}^2\,.$$

The series on both sides converge absolutely and uniformly on compact subsets of $\mathbb{R}^2$.

Remark 3.2 The Poisson summation formula, particularly in one dimension, is often formulated as an equality of distributions. For some other formulations we refer to [58, 66]. We have here chosen a classical formulation which is well suited to the applications we intend. □

Proof: The left hand side of the equation is clearly a Q-periodic function. Hence it can be represented as a Fourier series

$$\sum_{\mu\in\mathbb{Z}^2} f(\tilde{x}-p^{(\mu)}) = \sum_{\nu\in\mathbb{Z}^2} \gamma_\nu \exp(i\, q^{(\nu)}\cdot\tilde{x}).$$

The coefficients γ_ν are given by

$$\begin{aligned}\gamma_\nu &= \frac{1}{|Q|}\int_Q \left(\sum_{\mu\in\mathbb{Z}^2} f(\tilde{x}-p^{(\mu)})\right) \exp(-i\, q^{(\nu)}\cdot\tilde{x})\, d\tilde{x}\\ &= \frac{1}{|Q|}\sum_{\mu\in\mathbb{Z}^2}\int_Q f(\tilde{x}-p^{(\mu)})\, \exp(-i\, q^{(\nu)}\cdot(\tilde{x}-p^{(\mu)}))\, d\tilde{x}\\ &= \frac{1}{|Q|}\int_{\mathbb{R}^2} f(\tilde{x})\, \exp(-i\, q^{(\nu)}\cdot\tilde{x})\, d\tilde{x} = \frac{1}{|Q|}\hat{f}(-q^{(\nu)}).\end{aligned}$$

The second line holds as $p^{(\mu)}\cdot q^{(\nu)} \in 2\pi\mathbb{Z}$. From the last line we now obtain the formula of the lemma by replacing ν by $-\nu$. The assertion on the convergence of the series follows from the fact that f is an element of the Schwartz space. ■

To apply Lemma 3.1 to the situation at hand, we consider the function

$$f(\tilde{x};x_3) := \frac{1}{4\pi}\,\frac{\exp(ik\,(|\tilde{x}|^2+x_3^2)^{1/2})}{(|\tilde{x}|^2+x_3^2)^{1/2}}, \qquad \tilde{x}\in\mathbb{R}^2, \tag{3.6}$$

with $x_3 \in \mathbb{R}\setminus\{0\}$. Note the earlier assumption that $\mathrm{Im}(k) > 0$ which implies $f(\cdot;x_3)\in S(\mathbb{R}^2)$. Hence we can apply the lemma. From tables of Fourier transforms [53], we find that

$$\hat{f}(\xi;x_3) = \frac{1}{2}\frac{\exp(-|x_3|\,(|\xi|^2-k^2)^{1/2})}{(|\xi|^2-k^2)^{1/2}}, \qquad \xi\in\mathbb{R}^2. \tag{3.7}$$

Setting $g(\tilde{x};x_3) := \exp(i\tilde{\alpha}\cdot\xi)\, f(\tilde{x};x_3)$, we obtain

$$\hat{g}(\xi;x_3) = \hat{f}(\tilde{\alpha}+\xi;x_3).$$

Substituting g for f in the lemma, some elementary manipulations starting from (3.5) now yield

$$G_k(x,y) = \frac{1}{4\pi}\sum_{\mu\in\mathbb{Z}^2}\exp(i\alpha\cdot p^{(\mu)})\,\frac{\exp(ik\,|x-y-p^{(\mu)}|)}{|x-y-p^{(\mu)}|}. \tag{3.8}$$

This series is exponentially convergent for all $(x,y)\in(\Omega\times\Omega)\setminus\omega$ and hence shows, that the Green's function can be extended analytically to the line $x_3 = y_3$ for $x\neq y$. However, the series does not converge for real k.

3.2 An Application of Ewald's method

In this section we will derive an alternative expression for the Q-quasi-periodic Green's function which can be extended analytically to real k and is well suited for numerical evaluation. This method was first developed by the physicist EWALD in the context of evaluating potentials on crystal lattices [31] and is well known in that research area. As was pointed out in the introduction, it is rather less well known in the mathematics community.

We start with a representation of the Hankel function. This representation can be found in mathematical handbooks such as [35]. However we give a complete proof here for the convenience of the reader.

Lemma 3.3 *For $\nu \in \mathbb{R}$, $r > 0$ and $k \in \mathbb{C}$ such that $\arg(k) \in (0, \pi/2)$, there holds*

$$H_\nu^{(1)}(kr) = \frac{2}{i\,\pi}\, e^{-i\pi\nu} \left(\frac{k}{2r}\right)^\nu \int_{\gamma_1} t^{-2\nu-1} \exp\left(-r^2t^2 + \frac{k^2}{4t^2}\right) dt,$$

where γ_1 is an integration path in the complex plane starting at the origin in the direction $e^{-i\pi/4}$ and approaching infinity in any direction $e^{i\varphi}$ with $-\pi/4 < \varphi < \pi/4$.

Proof: We start with the well-known representation of the Hankel function of the first kind of order ν [2, formula 9.1.25],

$$H_\nu^{(1)}(z) = \frac{1}{i\,\pi} \int_{-\infty}^{\infty+\pi i} e^{z\,\sinh\omega - \nu\omega}\, d\omega, \qquad |\arg(z)| < \frac{\pi}{2}. \tag{3.9}$$

A possible path of integration is shown in blue in Figure 3.1.

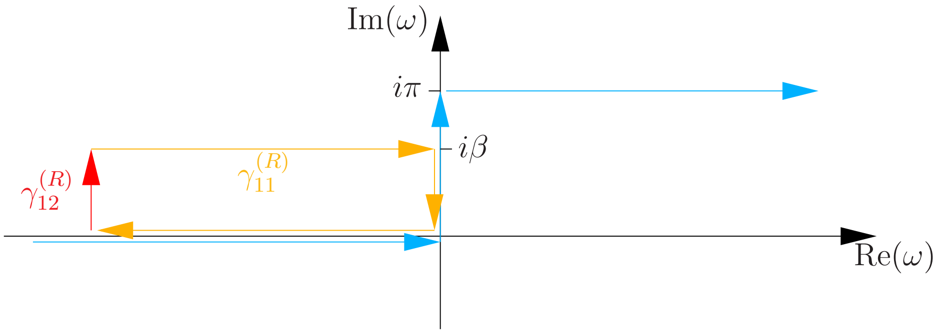


Figure 3.1: Contours for the line integrals in the complex plane

We now consider a different contour integral for the same integrand: Suppose $\beta > 0$ and set

$$\gamma_{11}^{(R)} := \big\{-t : 0 \le t \le R\big\} \cup \big\{i\,t : 0 < t < \beta\big\} \cup \big\{-t + i\beta : 0 \le t \le R\big\},$$
$$\gamma_{12}^{(R)} := \big\{-R + i\,t : 0 < t < \beta\big\},$$

with the orientation of both contours shown in Figure 3.1. As the integrand of the integral in (3.9) is holomorphic in ω, by Cauchy's integral theorem we have

$$\int_{\gamma_{11}^{(R)}} e^{z\,\sinh\omega-\nu\omega}\,d\omega = \int_{\gamma_{12}^{(R)}} e^{z\,\sinh\omega-\nu\omega}\,d\omega.$$

We work out the integral on the right-hand side in detail, obtaining

$$\begin{aligned}\int_{\gamma_{12}^{(R)}} e^{z\,\sinh\omega-\nu\omega}\,d\omega &= \int_0^\beta e^{z\,\sinh(-R+it)-\nu(-R+it)}\,dt\\ &= \int_0^\beta e^{\nu R}\,e^{-i\nu t}\,e^{z\sinh(-R+it)}\,dt.\end{aligned}$$

Suppose now that $0 < \arg(z) < \pi/2$ and also $0 < \beta < \pi/2$. In this case, for $t \in (0, \beta)$,

$$\mathrm{Re}(z\sinh(-R+it)) = -\,\mathrm{Re}(z)\,\cos(t)\,\sinh(R) - \mathrm{Im}(z)\,\sin(t)\,\cosh(R) < 0,$$

and the absolute value of both terms on the right grows exponentially in R. Consequently, $\nu R + \mathrm{Re}(z\sinh(-R+it)) < 0$ for any R large enough and we obtain

$$\lim_{R\to\infty}\int_{\gamma_{11}^{(R)}} e^{z\,\sinh\omega-\nu\omega}\,d\omega = \lim_{R\to\infty}\int_{\gamma_{12}^{(R)}} e^{z\,\sinh\omega-\nu\omega}\,d\omega = 0.$$

Choosing $\beta = \pi/2 - \arg(z)$ for $0 < \arg(z) < \pi/2$, and combining the integrals along both contours, we obtain the representation

$$H_\nu^{(1)}(z) = \frac{1}{i\,\pi}\int_{-\infty+\left(\frac{\pi}{2}-\arg(z)\right)i}^{\infty+\pi i} e^{z\,\sinh\omega-\nu\omega}\,d\omega, \qquad 0 < \arg(z) < \frac{\pi}{2}. \tag{3.10}$$

We rewrite this expression for the Hankel function as

$$H_\nu^{(1)}(z) = \frac{1}{i\,\pi}\int_{-\infty+\left(\frac{\pi}{2}-\arg(z)\right)i}^{\infty+\pi i} (e^\omega)^{-\nu}\,\exp\left(\frac{z}{2}\,(e^\omega - e^{-\omega})\right)d\omega.$$

The substitution $u = e^\omega$ yields

$$H_\nu^{(1)}(z) = \frac{1}{i\,\pi}\int_{\gamma_2} u^{-\nu-1}\,\exp\left(\frac{z}{2}\left(u-\frac{1}{u}\right)\right)du,$$

where γ_2 is a contour in the complex plane starting at the origin with direction $e^{i\,(\pi/2-\arg(z))}$, tending to minus infinity in the direction of the negative real axis and performing a positively oriented arc around the origin along its course (see Figure 3.2).

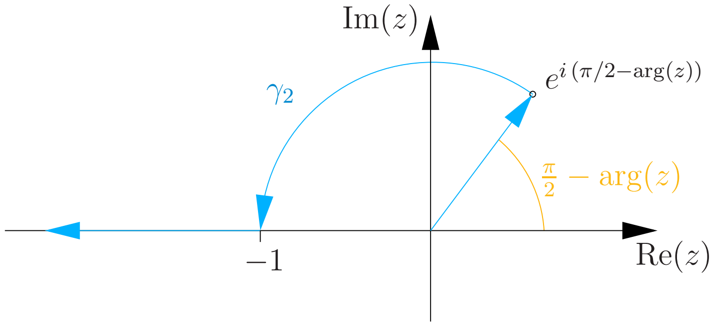


Figure 3.2: Contour path γ_2 obtained by the substitution $u = e^{i\omega}$.

Setting $z = kr$ with $r > 0$, we obtain

$$H_\nu^{(1)}(kr) = \frac{1}{i\,\pi}\int_{\gamma_2} u^{-\nu-1}\,\exp\left(\frac{kr}{2}\left(u-\frac{1}{u}\right)\right)du,$$

We perform a second substitution, $u = -2r\,t^2/k$, to derive

$$H_\nu^{(1)}(kr) = \frac{2}{i\,\pi}\,e^{-i\pi\nu}\left(\frac{k}{2r}\right)^\nu\int_{\gamma_3} t^{-2\nu-1}\,\exp\left(-r^2t^2+\frac{k^2}{4t^2}\right)dt.$$

The new path of integration γ_3 again starts at the origin in the direction $e^{-i\pi/4}$ and approaches infinity in the direction $e^{i\,\arg(k)/2}$, see Figure 3.3. The path of integration may deviate from γ_3 as long as two conditions are met: The direction at which the path leaves the origin must not change and the path must go to infinity at a direction $e^{i\varphi}$ with $-\pi/4 < \varphi < \pi/4$. This ensures $\mathrm{Re}(t^2) > 0$ so that the integrand decays exponentially for $|t| \to \infty$. These are the conditions given for γ_1 in the assumptions of the lemma. ■

From the previous lemma, we immediately obtain a representation of the Green's function for the Helmholtz equation in free field conditions:

Lemma 3.4 *Let $r > 0$ and $k \in \mathbb{C}$ such that* $\arg(k) \in (0, \pi/2)$. *Then*

$$\frac{1}{4\pi}\frac{\exp(ikr)}{r} = \frac{1}{2\pi^{3/2}}\int_{\gamma_1}\exp\left(-r^2z^2+\frac{k^2}{4z^2}\right)dz,$$

where γ_1 is the contour from Lemma 3.3.

Proof: From formulae in chapters 9 and 10 of [2], we find that

$$\frac{1}{4\pi}\frac{\exp(ikr)}{r} = \frac{1}{4\sqrt{2\pi}}\sqrt{\frac{k}{r}}\,H_{-1/2}^{(1)}(kr).$$

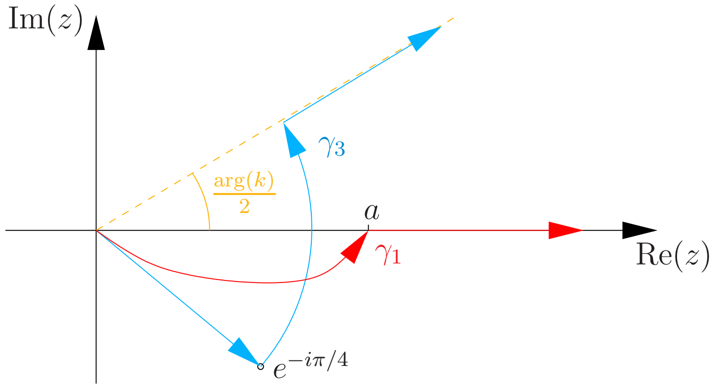


Figure 3.3: Contour paths γ_3 and γ_1 (one example).

Hence the assertion follows directly from Lemma 3.3. ∎

Inserting the formula from Lemma 3.4 into the expression found in (3.8), we obtain

$$G_k(x,y) = \frac{1}{2\pi^{3/2}} \int_{\gamma_1} \sum_{\mu\in\mathbb{Z}^2} \exp(i\,\alpha\cdot p^{(\mu)}) \exp\left(-|x-y-p^{(\mu)}|^2 z^2 + \frac{k^2}{4z^2}\right) dz.$$

Let now γ_1 be chosen as in Figure 3.3 with some $a > 0$. By γ_4 we denote that part of γ_1 connecting the origin with a. We can then split the expression for G_k into two parts,

$$G_k(x,y) = G_k^{(1)}(x,y) + G_k^{(2)}(x,y), \tag{3.11}$$

where

$$G_k^{(1)}(x,y) := \frac{1}{2\pi^{3/2}} \int_a^\infty \sum_{\mu\in\mathbb{Z}^2} \exp(i\,\alpha\cdot p^{(\mu)}) \exp\left(-|x-y-p^{(\mu)}|^2 z^2 + \frac{k^2}{4z^2}\right) dz\,,$$

$$G_k^{(2)}(x,y) := \frac{1}{2\pi^{3/2}} \int_{\gamma_4} \sum_{\mu\in\mathbb{Z}^2} \exp(i\,\alpha\cdot p^{(\mu)}) \exp\left(-|x-y-p^{(\mu)}|^2 z^2 + \frac{k^2}{4z^2}\right) dz\,.$$

In the next step, the expression of $G_k^{(1)}$ will be rewritten in a straight forward manner to obtain a quickly converging series with the speed of convergence increasing as the parameter a gets large. The expression for $G_k^{(2)}$ on the other hand is only very slowly convergent as it stands. The central idea of Ewald's method is to rewrite this expression using the Poisson summation formula. As the integrand is a smooth function, the Fourier series will be quickly convergent. These manipulations will be carried out in a further step.

In order to rewrite the expression for $G_k^{(1)}$, we will make use of the following lemma.

Lemma 3.5 *For $r > 0$ and $b \in \mathbb{C}$ there holds*

$$\int_a^\infty \exp\left(-r^2 z^2 + \frac{b^2}{z^2}\right) dz = \frac{a}{2} \sum_{j=0}^\infty \frac{1}{j!} \left(\frac{b}{a}\right)^{2j} \int_1^\infty t^{-j-1/2} \exp(-a^2 r^2 t)\, dt.$$

Proof: From the power series expansion of the exponential function, we see

$$\exp\left(\frac{b^2}{z^2}\right) = \sum_{j=0}^\infty \frac{1}{j!} \left(\frac{b}{z}\right)^{2j}.$$

Next, substituting $t = z^2/a^2$, we obtain

$$\int_a^\infty \left(\frac{b}{z}\right)^{2j} \exp(-r^2 z^2)\, dz = \frac{a}{2} \left(\frac{b}{a}\right)^{2j} \int_1^\infty t^{-j-1/2} \exp(-a^2 r^2 t)\, dt.$$

■

Remark 3.6 The integral on the right hand side of the expression in Lemma 3.5 can be viewed as an extension to non-integer indices of the Exponential Integral E_n, which is defined by

$$E_n(r) := \int_1^\infty t^{-n} \exp(-rt)\, dt, \qquad \mathrm{Re}(r) > 0, \quad n \in \mathbb{N}.$$

For real r, there is also a relation to the incomplete Gamma function Γ,

$$\int_1^\infty t^{-\sigma} \exp(-rt)\, dt = r^{\sigma-1}\, \Gamma(1-\sigma, r).$$

□

We can now rewrite the expression for $G_k^{(1)}$, obtaining

$$\begin{aligned} G_k^{(1)}(x,y) = {} & \frac{a}{4\pi^{3/2}} \sum_{\mu \in \mathbb{Z}^2} \exp(i\,\alpha \cdot p^{(\mu)}) \\ & \times \sum_{j=0}^\infty \frac{1}{j!} \left(\frac{k}{2a}\right)^{2j} \int_1^\infty t^{-j-1/2} \exp\left(-a^2 |x-y-p^{(\mu)}|^2 t\right)\, dt. \end{aligned} \quad (3.12)$$

We now perform the application of the Poisson summation formula to transform the expression of $G_k^{(2)}$ which is the key idea in the proof of the following lemma.

Lemma 3.7 *The function $G_k^{(2)}$ can be expressed as*

$$G_k^{(2)}(x,y) = -\frac{1}{2\sqrt{\pi}|Q|}\sum_{\nu\in\mathbb{Z}^2} \exp(ik\,d^{(\nu)}\cdot(x-y))$$
$$\times \int_{\gamma_5} \exp\left(-\frac{|x_3-y_3|^2}{s^2} + \frac{s^2}{4}(k\rho^{(\nu)})^2\right) ds,$$

and the integration path is defined by $\gamma_5 := \{z \in \mathbb{C} : 1/z \in \gamma_4\}$.

Proof: Consider for fixed $z \in \mathbb{C}$ with $0 \le \arg z < \pi/4$, the function

$$F(\xi) := \sum_{\mu\in\mathbb{Z}^2} \exp(-i\,\tilde{\alpha}\cdot(\xi - p^{(\mu)}))\,\exp(-|\xi - p^{(\mu)}|^2\,z^2), \qquad \xi \in \mathbb{R}^3.$$

This function has exactly the correct form to apply the Poisson summation formula Lemma 3.1. Suppressing the term $\exp(-\xi_3^2 z^2)$ for the moment, we need to compute the Fourier transform of

$$f(\xi) = \exp(-i\tilde{\alpha}\cdot\tilde{\xi})\,\exp(-|\tilde{\xi}|^2\,z^2).$$

This we obtain as

$$\begin{aligned}\hat{f}(\tilde{q}) &= \int_{\mathbb{R}^2} \exp(-i\,\tilde{\xi}\cdot(\tilde{\alpha}-\tilde{q}))\,\exp(-|\tilde{\xi}|^2\,z^2)\,d\tilde{\xi} \\ &= \exp\left(-\frac{|\tilde{\alpha}-\tilde{q}|^2}{4z^2}\right)\int_{\mathbb{R}^2} \exp\left(-\left(z\,\tilde{\xi} + i\frac{\tilde{\alpha}-\tilde{q}}{2z}\right)\cdot\left(z\,\tilde{\xi} + i\frac{\tilde{\alpha}-\tilde{q}}{2z}\right)\right) d\tilde{\xi}.\end{aligned}$$

This last integral separates into the product of two integrals over the real line which both take the form

$$I := \int_{-\infty}^{\infty} \exp\left(-\left(zs + i\,\frac{c}{z}\right)^2\right) ds$$

with some real constant c. The integrand is exponentially decaying for our choice of u and all $c \in \mathbb{R}$ as $|s|$ becomes large. Hence, by Cauchy's integral theorem we can transform the integral to obtain

$$I = \int_{-\infty}^{\infty} \exp(-z^2 s^2)\,ds = \frac{\sqrt{\pi}}{z}.$$

Concluding, we apply Lemma 3.1 to see that

$$F(\xi) = \frac{\pi}{|Q|}\sum_{\nu\in\mathbb{Z}^2} \exp\left(-\frac{|kd^{(\nu)}|^2}{4z^2}\right)\frac{\exp(-z^2\xi_3^2)}{z^2}\,\exp(i\,q^{(\nu)}\cdot\xi).$$

We now return to the definition of $G_k^{(2)}$ and reformulate using F,

$$\begin{aligned}
G_k^{(2)}(x,y) &= \frac{1}{2\pi^{3/2}} \exp(i\,\tilde{\alpha}\cdot(x-y)) \int_{\gamma_4} F(x-y) \exp\left(\frac{k^2}{4z^2}\right) dz \\
&= \frac{1}{2\pi^{1/2}|Q|} \sum_{\nu\in\mathbb{Z}^2} \exp(ik\,d^{(\nu)}\cdot(x-y)) \\
&\qquad \times \int_{\gamma_4} \frac{\exp(-z^2|x_3-y_3|^2)}{z^2} \exp\left(\frac{k^2}{4z^2}\,(\rho^{(\nu)})^2\right) dz.
\end{aligned}$$

The substitution $z = 1/s$ now yields

$$\begin{aligned}
G_k^{(2)}(x,y) = -\frac{1}{2\pi^{1/2}|Q|} &\sum_{\nu\in\mathbb{Z}^2} \exp(ik\,d^{(\nu)}\cdot(x-y)) \\
&\times \int_{\gamma_5} \exp\left(-\frac{|x_3-y_3|^2}{s^2} + \frac{s^2}{4}\,(k\rho^{(\nu)})^2\right) ds,
\end{aligned}$$

which is the assertion of the lemma. ■

We now analyse the individual summands in the expression found in Lemma 3.7 depending on the sign of $\mathrm{Re}((k\rho^{(\nu)})^2)$. The simpler case is when $\mathrm{Re}((k\rho^{(\nu)})^2) < 0$. In this case, we can shift the path of integration from γ_5 to the interval $(1/a,\infty)$ on the real line. Then, from formula (7.4.34) in [2], we obtain

$$\begin{aligned}
&\int_{\gamma_5} \exp\left(-\frac{|x_3-y_3|^2}{s^2} + \frac{s^2}{4}(k\rho^{(\nu)})^2\right) ds \\
&\quad = -\frac{\sqrt{\pi}i}{2\,k\rho^{(\nu)}} \Bigg[\exp(-i\,k\rho^{(\nu)}\,(x_3-y_3))\ \mathrm{erfc}\left(-i\,\frac{k\rho^{(\nu)}}{2a} + (x_3-y_3)\,a\right) \\
&\qquad + \exp(i\,k\rho^{(\nu)}\,(x_3-y_3))\ \mathrm{erfc}\left(-i\,\frac{k\rho^{(\nu)}}{2a} - (x_3-y_3)\,a\right)\Bigg]. \quad (3.13)
\end{aligned}$$

Here, $\mathrm{erfc}(\cdot)$ denotes the complimentary error function, defined by

$$\mathrm{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty \exp(-\xi^2)\,d\xi, \qquad z\in\mathbb{C}.$$

In this definition, the path of integration must approach ∞ such that $\arg(z) \in (-\pi/4,\pi/4)$.

In the case $\mathrm{Re}((k\rho^{(\nu)})^2) > 0$, we first perform the substitution $s = it$, which yields

$$\begin{aligned}
&\int_{\gamma_5} \exp\left(-\frac{|x_3-y_3|^2}{s^2} + \frac{s^2}{4}(k\rho^{(\nu)})^2\right) ds \\
&\qquad = i \int_{\gamma_6} \exp\left(\frac{|x_3-y_3|^2}{t^2} - \frac{t^2}{4}(k\rho^{(\nu)})^2\right) dt, \quad (3.14)
\end{aligned}$$

where γ_6 is obtained from γ_5 by a counter-clockwise rotation with an angle of $\pi/2$ in the complex plane. Now we can again apply formula (7.4.34) in [2]. Thus

$$\int_{\gamma_6} \exp\left(\frac{|x_3-y_3|^2}{t^2} - \frac{t^2}{4}(k\rho^{(\nu)})^2\right) dt$$
$$= -\frac{\sqrt{\pi}}{2\,k\rho^{(\nu)}}\Bigg[\exp(-i\,k\rho^{(\nu)}\,(x_3-y_3))\ \mathrm{erfc}\left(-i\,\frac{k\rho^{(\nu)}}{2a} + (x_3-y_3)\,a\right)$$
$$+ \exp(i\,k\rho^{(\nu)}\,(x_3-y_3))\ \mathrm{erfc}\left(-i\,\frac{k\rho^{(\nu)}}{2a} - (x_3-y_3)\,a\right)\Bigg]. \quad (3.15)$$

Combining (3.13) – (3.15) with Lemma 3.7 we arrive at

$$G_k^{(2)}(x,y) = \frac{i}{4\,|Q|}\sum_{\nu\in\mathbb{Z}^2}\frac{1}{k\rho^{(\nu)}}\ \exp(ik\,d^{(\nu)}\cdot(x-y))$$
$$\times\Bigg[\exp(-i\,k\rho^{(\nu)}\,(x_3-y_3))\ \mathrm{erfc}\left(-i\,\frac{k\rho^{(\nu)}}{2a} + (x_3-y_3)\,a\right)$$
$$+ \exp(i\,k\rho^{(\nu)}\,(x_3-y_3))\ \mathrm{erfc}\left(-i\,\frac{k\rho^{(\nu)}}{2a} - (x_3-y_3)\,a\right)\Bigg]. \quad (3.16)$$

This representation of $G_k^{(2)}$ should be compared to the expression (3.5) for G_k. In a sense, (3.16) constitutes an approximation to (3.5) with Fourier coefficients with an exponential decay rate, even for real k and for $x_3 = y_3$. The speed of convergence increases as the parameter a gets smaller.

The combination (3.11), (3.12) and (3.16) for expressing G_k is the central result of this section. As it turns out this expression is very well suited both to analysis of the Green's function as carried out below and for numerical evaluation. Firstly, all series appearing in (3.12) and (3.16) converge absolutely, regardless of the choice of parameters. This can easily be shown using asymptotic estimates available for the Complementary Error Function and for the Incomplete Gamma Function. We will discuss such estimates in more detail when we report on the numerical evaluation of G_k in the appendix. Secondly, all functions appearing in these expressions are analytic, as long as $(k,\alpha) \notin \mathcal{R}$. Hence we can see that G_k allows an analytic extension both to the line $x_3 = y_3$ and to real wave numbers k. Thus, from now on we will consider once more the case $k > 0$.

3.3 Analytic Properties of the Green's Function

It is necessary to study the properties of the Q-quasi-periodic Green's function in more detail, particularly its exact behaviour near the singularity at $x = y$. Of course, we postulated (3.1), however we have not yet checked that the expression for G_k that we have found indeed satisfies this equation.

In fact, it is easy to see that (3.1) holds for $\operatorname{Im} k > 0$ from (3.8). Here, the singularity is isolated in just one term of the series while the remainder is analytic in $x - y$. One property of the expressions found by Ewald's method is that this isolation of the singularity is preserved.

Theorem 3.8 *Let $k \in \mathbb{C}$, $\arg k \in [0, \pi/2)$ such that $(k, \alpha) \notin \mathcal{R}$. Then*

$$G_k(x, y) = \frac{1}{4\pi} \frac{1}{|x - y|} H_1(x, y) + H_2(x, y),$$

where

$$H_1(x, y) = \cos(k\,|x - y|)$$

and

$$\begin{aligned} H_2(x, y) = -\frac{a}{4\pi^{3/2}} \Bigg[&\cos(k|x - y|) \sum_{l=0}^{\infty} \frac{(-1)^l}{(l - 1/2)\, l!} (a\,|x - y|)^{2l} \\ &+ e^{-(a|x-y|)^2} \sum_{l=0}^{\infty} \left(\frac{k\,|x - y|}{2} \right)^{2l} \sum_{j=1}^{\infty} \frac{c_{j+l,l+1}}{(j + l)!} \left(\frac{k}{2a} \right)^{2j} \Bigg] \\ &+ \sum_{\mu \in \mathbb{Z}^2 \setminus \{0\}} \exp(i\,\alpha \cdot p^{(\mu)}) S(|x - y - p^{(\mu)}|) + G_k^{(2)}(x, y)\,, \end{aligned}$$

with

$$S(r) = \frac{a}{4\pi^{3/2}} \sum_{j=0}^{\infty} \frac{1}{j!} \left(\frac{k}{2a} \right)^{2j} \int_1^{\infty} t^{-j-1/2} \exp(-a^2 r^2 t)\, dt.$$

and the coefficients $c_{j,l}$ given by

$$c_{j,l} = \frac{(-1)^l}{\prod_{m=0}^{l-1} (j - m - 1/2)}, \qquad j = 0, 1, 2, \ldots, \quad l = 0, \ldots, j\,.$$

Proof: We rewrite (3.12) in the form

$$G_1^{(k)}(x, y) = \sum_{\mu \in \mathbb{Z}^2} \exp(i\,\alpha \cdot p^{(\mu)}) S(|x - y - p^{(\mu)}|)\,.$$

It is then clear from (3.11) that we only have to show $S(|x - y|)$ equals the first summand in the representation of H_2 stated in the theorem. We define

$$I_j(\tau) = \int_1^{\infty} s^{-j-1/2} e^{-\tau s}\, ds, \qquad j = 0, 1, 2, \ldots\,.$$

Integration by parts yields

$$I_{j+1}(\tau) = \frac{e^{-\tau}}{j+1/2} - \frac{\tau}{j+1/2}\, I_j(\tau), \qquad j = 0,1,2,\dots, \tag{3.17}$$

and a simple induction argument leads to the explicit formula

$$I_j(\tau) = c_{j,j}\,\tau^j\, I_0(\tau) - e^{-\tau} \sum_{l=1}^{j} c_{j,l}\,\tau^{l-1}, \qquad j = 0,1,2,\dots.$$

With these notations, we can rewrite S as

$$\begin{aligned}
S(r) &= \frac{a}{4\pi^{3/2}} \sum_{j=0}^{\infty} \frac{1}{j!} \left(\frac{k}{2a}\right)^{2j} I_j(a^2r^2) \\
&= \frac{a}{4\pi^{3/2}} \Bigg[I_0(a^2r^2) \sum_{j=0}^{\infty} \frac{c_{j,j}}{j!} \left(\frac{k}{2a}\right)^{2j} (ar)^{2j} \\
&\qquad\qquad - e^{-(ar)^2} \sum_{j=0}^{\infty} \sum_{l=0}^{j-1} \frac{c_{j,l+1}}{j!} \left(\frac{k}{2a}\right)^{2j} (ar)^{2l} \Bigg] \\
&= \frac{a}{4\pi^{3/2}} \Bigg[I_0(a^2r^2) \sum_{j=0}^{\infty} \frac{c_{j,j}}{j!} \left(\frac{kr}{2}\right)^{2j} \\
&\qquad\qquad - e^{-(ar)^2} \sum_{l=0}^{\infty} \left(\frac{kr}{2}\right)^{2l} \sum_{j=1}^{\infty} \frac{c_{j+l,l+1}}{(j+l)!} \left(\frac{k}{2a}\right)^{2j} \Bigg]
\end{aligned}$$

A direct computation using the explicit formula above gives

$$I_0(a^2r^2) = \frac{\sqrt{\pi}}{ar} - \sum_{l=0}^{\infty} \frac{(-1)^l}{(l-1/2)\,l!}\,(ar)^{2l}.$$

Furthermore, another simple induction yields

$$\frac{c_{j,j}}{j!\,4^j} = \frac{(-1)^j}{(2j)!}\,.$$

Hence

$$\begin{aligned}
&S(r) + \frac{a}{4\pi^{3/2}}\, e^{-(ar)^2} \sum_{l=0}^{\infty} \left(\frac{kr}{2}\right)^{2l} \sum_{j=1}^{\infty} \frac{c_{j+l,l+1}}{(j+l)!} \left(\frac{k}{2a}\right)^{2j} \\
&= \frac{1}{4\pi\, r} \sum_{j=0}^{\infty} \frac{(-1)^j}{(2j)!}\,(kr)^{2j} - \frac{a}{4\pi^{3/2}} \sum_{j=0}^{\infty} \frac{(-1)^j}{(2j)!}\,(kr)^{2j} \sum_{l=0}^{\infty} \frac{(-1)^l}{(l-1/2)\,l!}\,(ar)^{2l} \\
&= \frac{1}{4\pi\, r}\, \cos(kr) - \frac{a}{4\pi^{3/2}}\, \cos(kr) \sum_{l=0}^{\infty} \frac{(-1)^l}{(l-1/2)\,l!}\,(ar)^{2l}\,.
\end{aligned}$$

This completes the proof. ■

Remark 3.9 From the definitions, we see that H_1 is an analytic function with respect to both variables in $\mathbb{R}^2 \times \mathbb{R}^2$. The function H_2 is analytic with respect to both variables in $Q \times Q$. □

Theorem 3.8 plays a very important role in the analysis of surface potentials and integral operators with G_k as a kernel. It allows us to directly transfer properties of the corresponding potentials and operators from standard potential theory. Some fundamental results in this respect will be presented below.

Furthermore, we will use Theorem 3.8 to obtain a representation of G_k and its derivatives if both x and y are located on a surface that is the graph of a smooth function. This will be the subject of the next few theorems.

Theorem 3.10 *Let Γ denote one of the interfaces Γ_j, $j = 0, \dots, N$, defined as the graph of a Q-periodic function $f \in C^m(\overline{Q})$. Then there exist functions F_1, F_2, $F_3 \in C^{m-1}(\mathbb{R}^2 \times \mathbb{R}^2)$ with F_1 Q-periodic and F_2, F_3 Q-quasi-periodic such that*

$$G_k(x,y) = G_k(\tilde{x},\tilde{y})\,\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\,F_1(\tilde{x},\tilde{y}) + \frac{|\tilde{x}-\tilde{y}|}{|x-y|}\,F_2(\tilde{x},\tilde{y}) + F_3(\tilde{x},\tilde{y})$$

for all x, $y \in \Gamma$ such that $\tilde{x} \neq \tilde{y} + p^{(\mu)}$ for all $\mu \in \mathbb{Z}^2$.

Proof: Set $\rho := \min\{\pi/(4k), L_1/2, L_2/2)$ and denote by $\chi \in C^\infty(Q)$ a function satisfying $\chi(\xi) = 0$ for $|\xi| \geq \rho$ and $\chi \equiv 1$ in a neighborhood of 0.

We will now use the notation $x = (\tilde{x}, f(\tilde{x}))^\top$ and $y = (\tilde{y}, f(\tilde{y}))^\top$. Define

$$F_1(\tilde{x},\tilde{y}) := \begin{cases} \chi(\tilde{x}-\tilde{y})\,\dfrac{H_1(x,y)}{H_1(\tilde{x},\tilde{y})}, & |\tilde{x}-\tilde{y}| < \rho, \\ 0, & \text{otherwise.} \end{cases}$$

It follows that $F_1 \in C^{m-1}(Q \times Q)$ as $H_1(\tilde{x},\tilde{y}) \geq \sqrt{2}/2 > 0$ on the support of χ. Note that the closure of the support of F_1 is a compact subset of $Q \times Q$. Hence we can extend F_1 to a Q-periodic function in $C^{m-1}(\mathbb{R}^2 \times \mathbb{R}^2)$.

We next define

$$F_2(\tilde{x},\tilde{y}) := \begin{cases} -\chi(\tilde{x}-\tilde{y})\,\dfrac{H_1(x,y)\,H_2(\tilde{x},\tilde{y})}{H_1(\tilde{x},\tilde{y})}, & |\tilde{x}-\tilde{y}| < \rho, \\ 0, & \text{otherwise.} \end{cases}$$

Obviously, F_2 can be extended to a Q-quasi-periodic function and we can argue as for H_1 that it is an element of $C^{m-1}(\mathbb{R}^2 \times \mathbb{R}^2)$. Now, Theorem 3.8 shows that

$$F_3(\tilde{x},\tilde{y}) := G_k(x,y) - G_k(\tilde{x},\tilde{y})\,\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\,F_1(\tilde{x},\tilde{y}) - \frac{|\tilde{x}-\tilde{y}|}{|x-y|}\,F_2(\tilde{x},\tilde{y})$$

is an element of $C^{m-1}(\mathbb{R}^2 \times \mathbb{R}^2)$, and it is Q-quasi-periodic by definition. ■

Lemma 3.11 *Let $f \in C^m(\mathbb{R})$ and set*

$$g(s,t) := \frac{f(s) - f(t)}{s - t}, \qquad s,t \in \mathbb{R}, \quad s \neq t$$

as well as

$$h(s,t) := \frac{f(s) - f(t) - f'(t)\,(s-t)}{(s-t)^2}, \qquad s,t \in \mathbb{R}, \quad s \neq t\,.$$

Then g can be extended to a function in $C^{m-1}(\mathbb{R} \times \mathbb{R})$ and h to a function in $C^{m-2}(\mathbb{R} \times \mathbb{R})$.

Proof: As $g(s,t) = g(t,s)$, it suffices to study derivatives of g with respect to t. We assert that

$$\frac{\partial^l g}{\partial t^l}\,(s,t) = l!\,(s-t)^{-(l+1)} \left[f(s) - \sum_{j=0}^{l} \frac{1}{j!}\, f^{(j)}(t)\,(s-t)^j \right].$$

Indeed, for $l = 0$, this is the definition of g. Using induction, we obtain

$$\begin{aligned}
\frac{\partial^{l+1} g}{\partial t^{l+1}}\,(s,t) &= (l+1)!\,(s-t)^{-(l+2)} \left[f(s) - \sum_{j=0}^{l} \frac{1}{j!}\, f^{(j)}(t)\,(s-t)^j \right] \\
&\quad + l!\,(s-t)^{-(l+1)} \left[\sum_{j=1}^{l} \frac{1}{(j-1)!}\, f^{(j)}(t)\,(s-t)^{j-1} \right. \\
&\qquad\qquad \left. - \sum_{j=0}^{l} \frac{1}{j!}\, f^{(j+1)}(t)\,(s-t)^j \right] \\
&= (l+1)!\,(s-t)^{-(l+2)} \left[f(s) - \sum_{j=0}^{l} \frac{1}{j!}\, f^{(j)}(t)\,(s-t)^j \right] \\
&\quad - l!\,(s-t)^{-(l+1)} \frac{1}{l!}\, f^{(l+1)}(t)\,(s-t)^l \\
&= (l+1)!\,(s-t)^{-(l+2)} \left[f(s) - \sum_{j=0}^{l+1} \frac{1}{j!}\, f^{(j)}(t)\,(s-t)^j \right].
\end{aligned}$$

Hence the representation of the derivatives of g is proved. Using Taylor's theorem, we obtain that the derivatives of g up to order $m-1$ can be continuously extended to $t = s$.

Noting that $h(s,t) = \partial g(s,t)/\partial t$, the assertion for h follows immediately. ■

Theorem 3.12 *Let* Γ *denote one of the interfaces* Γ_j, $j = 0, \dots, N$, *defined as the graph of a* Q*-periodic function* $f \in C^m(\overline{Q})$ *and* $n(y)$ *the unit normal to* Γ *at* y. *Then there exists a* 2×2*-matrix valued function* $E_1 \in C^{m-2}(\mathbb{R}^2 \times \mathbb{R}^2)$ *with all components* Q*-periodic with respect to both variables as well as scalar functions* $E_j \in C^{m-1}(\mathbb{R}^2 \times \mathbb{R}^2)$, $j = 2, \dots, 6$, *where* E_2, E_3 *are* Q*-periodic and* E_4, E_5, E_6 *are* Q*-quasi-periodic with respect to both arguments, such that*

$$\begin{aligned} n(y) \cdot \nabla_y G_k(x,y) = \left(\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\right)^3 \nabla_{\tilde{y}} G_k(\tilde{x},\tilde{y}) \cdot [E_1(\tilde{x},\tilde{y})\,(\tilde{x}-\tilde{y})] \\ + \left(\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\right)^3 G_k(\tilde{x},\tilde{y})\, E_2(\tilde{x},\tilde{y}) + \frac{|\tilde{x}-\tilde{y}|}{|x-y|}\, G_k(\tilde{x},\tilde{y})\, E_3(\tilde{x},\tilde{y}) \\ + \left(\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\right)^3 E_4(\tilde{x},\tilde{y}) + \frac{|\tilde{x}-\tilde{y}|}{|x-y|}\, E_5(\tilde{x},\tilde{y}) + E_6(\tilde{x},\tilde{y}) \end{aligned}$$

for all x, $y \in \Gamma$ *such that* $\tilde{x} \neq \tilde{y} + p^{(\mu)}$ *for all* $\mu \in \mathbb{Z}^2$.

Proof: By Theorem 3.8, for x, $y \in \Gamma$, we obtain

$$\nabla_y G_k(x,y) = \frac{x-y}{4\pi\,|x-y|^3}\, H_1(x,y) + \frac{1}{4\pi\,|x-y|}\, \nabla_y H_1(x,y) + \nabla_y H_2(x,y),$$

Using the expression $n(y) = (-f_{y_1}(\tilde{y}), -f_{y_2}(\tilde{y}), 1)^\top / \sqrt{1 + |\nabla f(\tilde{y})|^2}$, we write

$$\begin{aligned} \sqrt{1 + |\nabla f(\tilde{y})|^2}\, n(y) \cdot (x-y) &= f(\tilde{x}) - f(\tilde{y}) - \nabla f(\tilde{y}) \cdot (\tilde{x}-\tilde{y}) \\ &= (\tilde{x}-\tilde{y}) \cdot [V(\tilde{x},\tilde{y})(\tilde{x}-\tilde{y})]\,, \end{aligned}$$

where V is a 2×2-matrix valued function with components given by

$$V_{11}(\tilde{x},\tilde{y}) = \frac{f(x_1,x_2) - f(y_1,x_2) - \dfrac{\partial f}{\partial y_1}(y_1,x_2)\,(x_1-y_1)}{(x_1-y_1)^2}\,,$$

$$V_{12}(\tilde{x},\tilde{y}) = \frac{\dfrac{\partial f}{\partial y_1}(y_1,x_2) - \dfrac{\partial f}{\partial y_1}(y_1,y_2)}{x_2-y_2}\,,$$

$$V_{22}(\tilde{x},\tilde{y}) = \frac{f(y_1,x_2) - f(y_1,y_2) - \dfrac{\partial f}{\partial y_2}(y_1,y_2)(x_2-y_2)}{(x_2-y_2)^2}\,,$$

$$V_{2,1}(\tilde{x},\tilde{y}) = 0\,.$$

Lemma 3.11 implies that $V \in C^{m-2}(\overline{Q} \times \overline{Q})$.

We now compare the expression for $\nabla_y G_k(x, y)$ with

$$\nabla_{\tilde{y}} G_k(\tilde{x}, \tilde{y}) = \frac{\tilde{x} - \tilde{y}}{4\pi\, |\tilde{x} - \tilde{y}|^3}\, H_1(\tilde{x}, \tilde{y}) + \frac{1}{4\pi\, |\tilde{x} - \tilde{y}|} \nabla_{\tilde{y}} H_1(\tilde{x}, \tilde{y}) + \nabla_{\tilde{y}} H_2(\tilde{x}, \tilde{y})\,.$$

Letting χ be as in the proof of Theorem 3.10, we set

$$E_1(\tilde{x}, \tilde{y}) := \chi(\tilde{x} - \tilde{y}) \left(1 + |\nabla f(\tilde{y})|^2\right)^{-1/2} V(\tilde{x}, \tilde{y})\, \frac{H_1(x, y)}{H_1(\tilde{x}, \tilde{y})}\,.$$

It follows that E_1 is of class C^{m-2}. Furthermore, we set

$$E_2(\tilde{x}, \tilde{y}) = -\frac{\nabla_{\tilde{y}} H_1(\tilde{x}, \tilde{y}) \cdot [E_1(\tilde{x}, \tilde{y})\, (\tilde{x} - \tilde{y})]}{H_1(\tilde{x}, \tilde{y})}\,,$$

$$E_3(\tilde{x}, \tilde{y}) = \chi(\tilde{x} - \tilde{y})\, \frac{\nabla_y H_1(x, y)}{H_1(\tilde{x}, \tilde{y})}\,,$$

$$E_4(\tilde{x}, \tilde{y}) = -\nabla_{\tilde{y}} H_2(\tilde{x}, \tilde{y}) \cdot [E_1(\tilde{x}, \tilde{y})(\tilde{x} - \tilde{y})]$$

$$E_5(\tilde{x}, \tilde{y}) = -H_2(\tilde{x}, \tilde{y})\, E_3(\tilde{x}, \tilde{y})\,.$$

A short investigation of the term $E_1(\tilde{x}, \tilde{y})\, (\tilde{x} - \tilde{y})$ reveals by similar arguments as above that E_2 and E_4 are of class C^{m-1}. For E_3 the argument is easy and hence it follows for E_5 also. All functions have the same support as χ has and hence can be extended to $\mathbb{R}^2 \times \mathbb{R}^2$ with the asserted periodicity conditions.

Defining E_6 by

$$\begin{aligned} E_6(\tilde{x}, \tilde{y}) = n(y) \cdot \nabla_y G_k(x, y) - \left(\frac{|\tilde{x} - \tilde{y}|}{|x - y|}\right)^3 \nabla_{\tilde{y}} G_k(\tilde{x}, \tilde{y}) \cdot [E_1(\tilde{x}, \tilde{y})\, (\tilde{x} - \tilde{y})] \\ - \left(\frac{|\tilde{x} - \tilde{y}|}{|x - y|}\right)^3 G_k(\tilde{x}, \tilde{y})\, E_2(\tilde{x}, \tilde{y}) - \frac{|\tilde{x} - \tilde{y}|}{|x - y|}\, G_k(\tilde{x}, \tilde{y})\, E_3(\tilde{x}, \tilde{y}) \\ - \left(\frac{|\tilde{x} - \tilde{y}|}{|x - y|}\right)^3 E_4(\tilde{x}, \tilde{y}) - \frac{|\tilde{x} - \tilde{y}|}{|x - y|}\, E_5(\tilde{x}, \tilde{y}), \end{aligned}$$

gives the assertion, as a straightforward calculation shows that E_6 is of class C^{m-1} as well. ■

In Chapter 5 we will discuss some numerical methods for solving integral equations of the second kind with certain kernels involving G_k. Theorems 3.13 and 3.14 show that because of the non-smooth function

$$\frac{|\tilde{x} - \tilde{y}|}{|x - y|}\,,$$

the integral equations arising from the scattering problems of Chapter 2 are not of the type considered in Chapter 5. However, a regularization technique might consist of approximating- the above function by a smooth counterpart and then applying the methods of Chapter 5. A similar approach for a potential problem has for example been considered in [9]. The analysis of such an approach remains an interesting open question.

The key observation that forms the basis of the methods discussed in Chapter 5 is that the Fourier coefficients of G_k and of derivatives of G_k are known.

Theorem 3.13 *Let $k \in \mathbb{C}$, $\arg k \in [0, \pi/4)$ such that $(k, \alpha) \notin \mathcal{R}$. Then*

$$\int_Q G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, d\tilde{y} = \frac{i}{2\, k\rho^{(\nu)}} \exp(ik\, d^{(\nu)} \cdot \tilde{x}), \qquad \tilde{x} \in Q.$$

Proof: Let $y := (\tilde{y}, \varepsilon)^\top$ for some $\varepsilon > 0$. Then, by (3.5), we have

$$\int_Q G_k(\tilde{x}, y) \exp(ik\, d^{(\nu)} \cdot y)\, d\tilde{y} = \frac{i \exp(ik\rho^{(\nu)}\, |\varepsilon|)}{2\, k\rho^{(\nu)}} \exp(ik\, d^{(\nu)} \cdot \tilde{x}).$$

By Theorem 3.8, the integrand becomes weakly singular for $\varepsilon \to 0$, hence we can apply the Lebesgue dominated convergence theorem and let ε tend to 0 to prove the assertion. ■

Theorem 3.14 *Let $k \in \mathbb{C}$, $\arg k \in [0, \pi/4)$ such that $(k, \alpha) \notin \mathcal{R}$. Then*

$$\int_Q \nabla_{\tilde{y}} G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, d\tilde{y} = \frac{\widetilde{d^{(\nu)}}}{2\, \rho^{(\nu)}} \exp(ik\, d^{(\nu)} \cdot \tilde{x}), \qquad \tilde{x} \in Q,$$

where the integral exists as a finite part integral.

Proof: Let $\tilde{x} \in Q$ and define

$$Q_\varepsilon := \{\tilde{y} \in Q : |\tilde{x} - \tilde{y}| < \varepsilon\}.$$

We will assume that ε is small enough such that Q_ε is the interior of a circle. Then, using partial integration, we have

$$\begin{aligned} \int_{Q \setminus \overline{Q_\varepsilon}} \nabla_{\tilde{y}} \left(G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y}) \right) d\tilde{y} &= \int_{\partial Q} G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, n^{(0)}(\tilde{y})\, ds(\tilde{y}) \\ &+ \int_{\partial Q_\varepsilon} G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, n^{(0)}(\tilde{y})\, ds(\tilde{y}). \end{aligned}$$

Here, $n^{(0)}(\tilde{y})$ denotes the outward drawn unit normal to the domain $Q \setminus \overline{Q_\varepsilon}$ at $(\tilde{y})$ in the $y_1 y_2$-plane. The function $G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})$ is Q-periodic with respect to $\tilde{y}$, hence the contributions to the integral over ∂Q from opposite edges cancel.

Using Theorem 3.8, we obtain

$$\int_{Q\setminus\overline{Q_\varepsilon}} \nabla_{\tilde{y}} \left(G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y}) \right) d\tilde{y}$$
$$= \frac{1}{4\pi\varepsilon} \int_{\partial Q_\varepsilon} H_1(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, n^{(0)}(\tilde{y})\, ds(\tilde{y})$$
$$+ \int_{\partial Q_\varepsilon} H_2(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, n^{(0)}(\tilde{y})\, ds(\tilde{y}).$$

Both integrands on the right hand side are now smooth. Hence, applying [22, Theorem 2.1] again, we obtain two domain integrals over Q_ε which are both $O(\varepsilon^2)$. Consequently, the right hand side tends to 0 for $\varepsilon \to 0$. It follows, that the integral in the assertion exists as a finite part integral and we obtain using Theorem 3.13

$$\int_Q \nabla_{\tilde{y}} G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, d\tilde{y} = -\int_Q G_k(\tilde{x}, \tilde{y})\, \nabla_{\tilde{y}} \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, d\tilde{y}$$
$$= -ik\, \widetilde{d^{(\nu)}} \int_Q G_k(\tilde{x}, \tilde{y}) \exp(ik\, d^{(\nu)} \cdot \tilde{y})\, d\tilde{y} = \frac{\widetilde{d^{(\nu)}}}{2\,\rho^{(\nu)}} \exp(ik\, d^{(\nu)} \cdot \tilde{x}).$$

This completes the proof. ∎

As the final consideration in this chapter, we discuss Green's representation formula in connection with the quasi-periodic Green's function. Assume that D_j, $j = 0, \ldots, N-1$ is one of the domains from Assumption 2.2, with Γ_j as a boundary from below and Γ_{j+1} as a boundary from above. Furthermore, assume that u is such that $M_{-\alpha} u \in H^1_Q(D_j)$ and that $\Delta u \in L^2(D_j)$. Hence, we can apply the standard Green's representation formula (see e.g. [48, Theorem 6.10]) to obtain

$$u(x) = \int_{\partial D_j} \left(\Phi_k(x, y) \frac{\partial u}{\partial n}(y) - \frac{\partial \Phi_k(x, y)}{\partial n(y)} u(y) \right) ds(y)$$
$$- \int_{D_j} \left(\Delta u(y) + k^2 u(y) \right) \Phi_k(x, y)\, dy, \qquad \text{f.a.a. } x \in D_j.$$

Note here that the Laplace operator in the domain integral is to be understood in a distributional sense. Using Theorem 3.8, we immediately conclude that also

$$u(x) = \int_{\partial D_j} \left(G_k(x, y) \frac{\partial u}{\partial n}(y) - \frac{\partial G_k(x, y)}{\partial n(y)} u(y) \right) ds(y)$$
$$- \int_{D_j} \left(\Delta u(y) + k^2 u(y) \right) G_k(x, y)\, dy, \qquad \text{f.a.a. } x \in D_j.$$

In this representation, the contributions over the vertical components of ∂D_j cancel because of the Q-quasi-periodicity of u and G_k — note that $G_k(x,\cdot)$ is Q-quasi-periodic with phase-shift $-\alpha$. Hence, we obtain the representation

$$\begin{aligned} u(x) = \int_{\Gamma_{j+1}} &\left(G_k(x,y)\,\frac{\partial u}{\partial n}(y) - \frac{\partial G_k(x,y)}{\partial n(y)}\,u(y)\right) ds(y) \\ &- \int_{\Gamma_j} \left(G_k(x,y)\,\frac{\partial u}{\partial n}(y) - \frac{\partial G_k(x,y)}{\partial n(y)}\,u(y)\right) ds(y) \\ &\qquad - \int_{D_j} \left(\Delta u(y) + k^2 u(y)\right) G_k(x,y)\,dy, \qquad \text{f.a.a. } x \in D_j. \end{aligned}$$

Deriving the corresponding result for $x \notin D_j$ in a similar fashion we obtain the following variant of the representation formula, that for allmost all $x \in \Omega$,

$$\begin{aligned} \int_{\Gamma_{j+1}} &\left(G_k(x,y)\,\frac{\partial u}{\partial n}(y) - \frac{\partial G_k(x,y)}{\partial n(y)}\,u(y)\right) ds(y) \\ &- \int_{\Gamma_j} \left(G_k(x,y)\,\frac{\partial u}{\partial n}(y) - \frac{\partial G_k(x,y)}{\partial n(y)}\,u(y)\right) ds(y) \\ &- \int_{D_j} \left(\Delta u(y) + k^2 u(y)\right) G_k(x,y)\,dy = \begin{cases} u(x), & x \in D_j, \\ 0, & x \in \Omega \setminus \overline{D_j}. \end{cases} \end{aligned} \tag{3.18}$$

To make this formula compatible with the variational formulations of Chapter 2 and the potentials to be defined in Chapter 4, we set $u_\alpha := M_{-\alpha} u$ to obtain the following corollary.

Corollary 3.15 *Assume that Assumption 2.2 holds, that $u_\alpha \in H^1_Q(D_j)$ and that $\Delta u_\alpha \in L^2(D_j)$ for some $j \in \{0,\dots,N-1\}$. Then, for almost all $x \in \Omega$,*

$$\begin{aligned} \int_{\Gamma_{j+1}} &\exp(i\tilde{\alpha}\cdot(y-x)) \left(G_k(x,y)\, n\cdot\nabla_\alpha u_\alpha(y) - \frac{\partial G_k(x,y)}{\partial n(y)}\,u_\alpha(y)\right) ds(y) \\ &- \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x)) \left(G_k(x,y)\, n\cdot\nabla_\alpha u_\alpha(y) - \frac{\partial G_k(x,y)}{\partial n(y)}\,u_\alpha(y)\right) ds(y) \\ -\int_{D_j} &\left(\nabla_\alpha\cdot\nabla_\alpha u(y) + k^2 u(y)\right) \exp(i\tilde{\alpha}\cdot(y-x))\, G_k(x,y)\,dy = \begin{cases} u(x), & x \in D_j, \\ 0, & x \in \Omega \setminus \overline{D_j}. \end{cases} \end{aligned}$$

Remark 3.16 Of course this result extends to D_N and D_{-1} with Γ_{j+1} replaced by Γ^+ and Γ_j replaced by Γ^-, respectively. □

Chapter 4

The Boundary Integral Equation Approach

The scattering and transmission problems discussed in Chapter 2 are ideally suited to the application of the boundary integral equation method. We will investigate this approach by first studying the properties of Q-periodic potentials and the corresponding boundary operators. We will then use these potentials to make an ansatz for the solution of the scattering or transmission problem. This approach is often referred to as the *indirect approach* as opposed to the *direct approach* in which a representation of the solution is obtained from Green's representation formula.

As a minimum requirement for the derivation of the results in this section we will require that Assumption 2.2 holds and that all interfaces Γ_j are given as graphs of corresponding Lipschitz functions f_j, $j = 0, \dots, N$. We recall that this assumption is necessary because of the way the Q-periodic fractional order Sobolev spaces on surfaces were defined in Chapter 2.

4.1 Q-Periodic Layer Potentials and Boundary Operators

The objects of interest in this section are Q-periodic single- and double-layer potentials. For a given interface Γ_j, $j = 0, \dots, N$, such potentials will be defined on two domains associated with the interface

$$\Omega_j^- := \{x \in \mathbb{R}^3 : \tilde{x} \in Q, M_1 < x_3 < f_j(\tilde{x})\},$$
$$\Omega_j^+ := \{x \in \mathbb{R}^3 : \tilde{x} \in Q, f_j(\tilde{x}) < x_3 < M_2\}.$$

Recall that f_j is the Q-periodic Lipschitz function defining Γ_j and $M_{1/2}$ are the constants from Assumption 2.2.

Given a density φ on Γ_j we formally define the Q-periodic single-layer potentials

$$\mathrm{SL}_j^+\varphi(x) := \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x))\, G_{q_j^{1/2}k}(x,y)\,\varphi(y)\,ds(y), \qquad x \in \Omega_j^- \cup \Omega_j^+,$$

$$\mathrm{SL}_j^-\varphi(x) := \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x))\, G_{q_{j-1}^{1/2}k}(x,y)\,\varphi(y)\,ds(y), \qquad x \in \Omega_j^- \cup \Omega_j^+.$$

Note that the superscript $\pm$ is associated with the refractive index of the medium, q_j in the case of "+" and q_{j-1} in the case of "−".

Likewise, we define the Q-periodic double-layer potentials

$$\mathrm{DL}_j^+\varphi(x) := \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x))\, \frac{\partial G_{q_j^{1/2}k}(x,y)}{\partial n(y)}\,\varphi(y)\,ds(y), \qquad x \in \Omega_j^- \cup \Omega_j^+,$$

$$\mathrm{DL}_j^-\varphi(x) := \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x))\, \frac{\partial G_{q_{j-1}^{1/2}k}(x,y)}{\partial n(y)}\,\varphi(y)\,ds(y), \qquad x \in \Omega_j^- \cup \Omega_j^+.$$

In subsequent sections of this chapter, when deriving boundary integral equations, it will be important to distinguish between the "+" and "−" versions of these potentials. In the remainder of this section, however, we will derive results which are identical for both versions. Hence we will leave out this superscript whenever possible without creating ambiguity and assume that the wave numbers on both sides of the surface Γ_j are identical. This wave number will be denoted by k, however values of k such that $\arg(k) \in [0, \pi/2)$ are allowed.

As a first step, we establish mapping properties for the operators SL_j and DL_j, respectively. These, of course, also clarify to which spaces the densities are required to belong.

Theorem 4.1 *The single layer potentials give rise to bounded operators*

$$\mathrm{SL}_j : H_Q^{-1/2}(\Gamma_j) \to H_Q^1(\Omega_j^- \cup \Gamma_j \cup \Omega_j^+).$$

The double layer potentials give rise to bounded operators

$$\mathrm{DL}_j : H_Q^{1/2}(\Gamma_j) \to \begin{cases} H_Q^1(\Omega_j^-), \\ H_Q^1(\Omega_j^+). \end{cases}$$

Proof: By Theorem 3.8, we know that G_k has the same singularity as the fundamental solution $G^{(0)}$ of Laplace's equation. The corresponding result for potentials based on $G^{(0)}$ in Sobolev spaces $H^1(D_j)$, $H^{1/2}(\Gamma_j)$ and $H^{-1/2}(\Gamma_j)$ are well known, see e.g. [48, Theorem 6.11]. If $\varphi \in H_Q^{\pm 1/2}(\Gamma_j)$, then, by the Q-quasi-periodicity of G_k, it follows that the corresponding potentials are Q-periodic as well. ■

An immediate consequence of these mapping properties can be deduced from the trace theorem and from Green's representation formula.

Theorem 4.2 *Assume that* $\varphi \in H_Q^{-1/2}(\Gamma_j)$, $j = 0, \ldots, N$. *Then*

$$\mathrm{SL}_j\varphi|_{\Gamma_j} \in H_Q^{1/2}(\Gamma_j) \qquad \textit{and} \qquad n \cdot \nabla_\alpha \mathrm{SL}_j\varphi|_{\Gamma_j}^{\pm} \in H_Q^{-1/2}(\Gamma_j).$$

Furthermore, the jump relations

$$\mathrm{SL}_j\varphi|_{\Gamma_j}^{+} - \mathrm{SL}_j\varphi|_{\Gamma_j}^{-} = 0, \qquad n \cdot \nabla_\alpha \mathrm{SL}_j\varphi|_{\Gamma_j}^{+} - n \cdot \nabla_\alpha \mathrm{SL}_j\varphi|_{\Gamma_j}^{-} = -\varphi$$

are satisfied. Assuming that $\psi \in H_Q^{1/2}(\Gamma_j)$, $j = 0, \ldots, N$, *there holds*

$$\mathrm{DL}_j\psi|_{\Gamma_j} \in H_Q^{1/2}(\Gamma_j) \qquad \textit{and} \qquad n \cdot \nabla_\alpha \mathrm{DL}_j\psi|_{\Gamma_j}^{\pm} \in H_Q^{-1/2}(\Gamma_j),$$

and the jump relations

$$\mathrm{DL}_j\psi|_{\Gamma_j}^{+} - \mathrm{DL}_j\psi|_{\Gamma_j}^{-} = \psi, \qquad n \cdot \nabla_\alpha \mathrm{DL}_j\psi|_{\Gamma_j}^{+} - n \cdot \nabla_\alpha \mathrm{DL}_j\psi|_{\Gamma_j}^{-} = 0$$

are satisfied.

Proof: The correct spaces for these traces are obtained by combining Theorem 4.1 and Corollary 2.5.

The jump relations could also be deduced directly from the corresponding results from standard potential theory. However, we here want to present the very elegant functional analytic approach that can be found in [48] and which originally was derived in [24].

The fact that the single layer potential does not jump follows directly from Theorem 4.1. To derive the jump of the normal derivative of the single layer potential, we first introduce set $D := Q \times (M_1, M_2)$ and denote by V the space of Q-periodic functions in $C^\infty(D)$ that vanish both in a neighborhood of Γ^+ and of Γ^-. Assume that $\chi \in V$ also satisfies $\chi = 1$ in a neighborhood of Γ_j. Applying Corollary 3.15 to $\chi \mathrm{SL}_j\varphi$ both in Ω_j^- and in Ω_j^+ and taking the difference of both formulae, we obtain, in the neighborhood of Γ_j where $\chi = 1$,

$$\mathrm{SL}_j\varphi = \mathrm{DL}_j[\mathrm{SL}_j\varphi] - \mathrm{SL}_j\left[n \cdot \nabla_\alpha \mathrm{SL}_j\varphi\right] = -\mathrm{SL}_j\left[n \cdot \nabla_\alpha\, \mathrm{SL}_j\varphi\right], \tag{4.1}$$

where the square brackets denote a jump across Γ_j. Next we choose an arbitrary function $\psi \in V$ and obtain, interpreting all derivatives as distributional derivatives, that

$$\begin{aligned}
((\nabla_\alpha \cdot \nabla_\alpha + k^2)\mathrm{SL}_j\varphi, \psi) &= \int_D \int_{\Gamma_j} \exp(i\tilde{\alpha} \cdot (y - x))\, G_k(x, y)\, \varphi(y)\, ds(y) \\
&\qquad\qquad \times (\nabla_\alpha \cdot \nabla_\alpha + k^2)\, \psi(x)\, dx \\
&= \int_{\Gamma_j} \varphi(y) \int_D \exp(i\tilde{\alpha} \cdot (y - x)) \\
&\qquad\qquad \times G_k(x, y)\, (\nabla_\alpha \cdot \nabla_\alpha + k^2)\, \psi(x)\, dx\, ds(y) \\
&= (\varphi, \psi|_{\Gamma_j}).
\end{aligned}$$

As the traces of functions in V are dense in $H_Q^{1/2}(\Gamma_j)$, it follows that $(\nabla_\alpha \cdot \nabla_\alpha + k^2)\mathrm{SL}_j$ is injective and hence SL_j itself is injective. Thus, from (4.1), we conclude

$$[n \cdot \nabla_\alpha \mathrm{SL}_j \varphi] = -\varphi.$$

To derive the corresponding results for the double layer potentials, consider the boundary value problem

$$\Delta w + (k^2 - \lambda)\, w = 0 \quad \text{in } \Omega_j^-, \qquad \begin{aligned} w &= 0 \quad \text{on } \Gamma^-, \\ w &= M_\alpha \psi \quad \text{on } \Gamma_j, \end{aligned}$$

with some $\psi \in H_Q^{1/2}(\Gamma_j)$. By choosing λ appropriately, standard results on solvability of elliptic boundary value problems yield that this problem has a unique weak Q-quasi-periodic solution w.

We now set

$$v(x) := \begin{cases} M_{-\alpha} w(x), & x \in \Omega_j^-, \\ 0, & x \in \Omega_j^+. \end{cases}$$

Then

$$[v] = -\psi \qquad \text{and} \qquad [n \cdot \nabla_\alpha v] = -\left.\frac{\partial w}{\partial n}\right|_{\Gamma_j}.$$

Proceeding as above by applying Green's representation in Ω_j^+ and Ω_j^+ to v, we obtain

$$\begin{aligned} v(x) = \mathrm{DL}_j[v](x) - \mathrm{SL}_j\,[n \cdot \nabla_\alpha v]\,(x) \\ - \lambda \int_D \exp(i\tilde{\alpha} \cdot (y - x))\, G_k(x, y)\, v(y)\, dy, \quad x \in D. \end{aligned}$$

The integral in this equation is known as a volume potential. As for the single and double layer potential, Theorem 3.8 allows the transfer of standard mapping properties of such potentials on bounded domains to the Q-periodic case. Thus, the volume potential is seen to be an element of $H^2(D)$ (c.f. [48, Theorem 6.1]) and hence it and its normal derivative do not jump across Γ_j. From the result for the single layer potential, we now obtain

$$\psi = -[v] = -[\mathrm{DL}_j[v](x)] = [\mathrm{DL}_j \psi]$$

and

$$\begin{aligned} 0 = [n \cdot \nabla_\alpha v] - [n \cdot \nabla_\alpha v] = [n \cdot \nabla_\alpha v] + [n \cdot \nabla_\alpha \mathrm{SL}_j\,[n \cdot \nabla_\alpha v]] \\ = [n \cdot \nabla_\alpha \mathrm{DL}_j[v]] = -\,[n \cdot \nabla_\alpha \mathrm{DL}_j \psi]\,. \end{aligned}$$

This completes the proof. ■

Of course, the reason to use these potentials is that they form weak solutions of the differential operator at hand. As this follows directly from their definition, for completeness and later reference we will state this fact here without detailed proof.

Theorem 4.3 *Let $j \in \{0, \ldots, N-1\}$ and $\varphi_j \in H_Q^{-1/2}(\Gamma_j)$, $\psi_j \in H_Q^{1/2}(\Gamma_j)$, $\varphi_{j+1} \in H_Q^{-1/2}(\Gamma_{j+1})$ and $\psi_{j+1} \in H_Q^{1/2}(\Gamma_{j+1})$. Denote by P one of the potentials $\mathrm{SL}_j^+\varphi_j$, $\mathrm{DL}_j^+\psi_j$, $\mathrm{SL}_{j+1}^-\varphi_{j+1}$, $\mathrm{DL}_{j+1}^-\psi_{j+1}$. Then,*

$$\int_{D_j} \left(\nabla_\alpha P \cdot \overline{\nabla_\alpha v} - k^2 P \overline{v}\right) dx$$
$$= \int_{\Gamma_{j+1}} n \cdot \nabla_\alpha P \, \overline{v} \, ds - \int_{\Gamma_j} n \cdot \nabla_\alpha P \, \overline{v} \, ds \qquad \text{for all } v \in H_Q^1(D_j),$$

Of course, the assertion also holds for D_{-1} and D_N with the appropriate boundary replaced by Γ^- or Γ^+, respectively.

One further important feature of potentials which is also essential in the treatment of exterior scattering problems, is that these functions automatically satisfy the radiation condition. For scattering by biperiodic media we express the fact that the potentials satisfy the Rayleigh expansion radiation condition of Definition 2.6 using the Dirichlet-to-Neumann maps $\Lambda^\pm$:

Theorem 4.4 *Let $\varphi^+ \in H_Q^{-1/2}(\Gamma_N)$, $\psi^+ \in H_Q^{1/2}(\Gamma_N)$, $\varphi^- \in H_Q^{-1/2}(\Gamma_0)$ and $\psi^- \in H_Q^{1/2}(\Gamma_0)$, respectively. Then*

$$n \cdot \nabla_\alpha \mathrm{SL}_N^+\varphi^+\big|_{\Gamma^+} = \Lambda^+ \mathrm{SL}_N^+\varphi^+|_{\Gamma^+}, \qquad n \cdot \nabla_\alpha \mathrm{SL}_0^-\varphi^-\big|_{\Gamma^-} = \Lambda^- \mathrm{SL}_0^-\varphi^-|_{\Gamma^-},$$
$$n \cdot \nabla_\alpha \mathrm{DL}_N^+\psi^+\big|_{\Gamma^+} = \Lambda^+ \mathrm{DL}_N^+\psi^+|_{\Gamma^+}, \qquad n \cdot \nabla_\alpha \mathrm{DL}_0^-\psi^-\big|_{\Gamma^-} = \Lambda^- \mathrm{DL}_0^-\psi^-|_{\Gamma^-}.$$

Note again the convention that the normal n on Γ_j is always assumed to be pointing into D_j.

Proof: We only give the proof here for SL_N^+, the proofs of the other identities being similar.

The normal derivative on Γ^+ corresponds to the partial derivative with respect to x_3. For $x \in \Gamma^+$, $y \in \Gamma_N$, the representation (3.5) can be used, so that we can rewrite the potential as

$$\mathrm{SL}_N^+\varphi^+(x) = \frac{i}{2|Q|} \sum_{\nu \in \mathbb{Z}^2} \int_{\Gamma_N} \frac{\exp(ik\,\rho^{(\nu)}\,(x_3 - y_3))}{k\,\rho^{(\nu)}} \exp(ik\,q^{(\nu)} \cdot (x-y))\,\varphi^+(y)\,ds(y)$$
$$= \sum_{\nu \in \mathbb{Z}^2} c_\nu(x_3)\,\exp(ik\,q^{(\nu)} \cdot x), \qquad x \in \Gamma^+,$$

where we have defined the Fourier coefficients

$$c_\nu(x_3) := \frac{i}{2|Q|} \exp(ik\,\rho^{(\nu)}\,x_3) \int_{\Gamma_N} \frac{\exp(-ik\,\rho^{(\nu)}\,y_3)}{k\,\rho^{(\nu)}} \exp(-ik\,q^{(\nu)}\cdot y)\,\varphi^+(y)\,ds(y).$$

Taking the partial derivative with respect to x_3 now immediately yields

$$\frac{\partial}{\partial x_3}\mathrm{SL}_N^+\varphi^+(x) = \sum_{\nu\in\mathbb{Z}^2} ik\,\rho^{(\nu)}\,c_\nu(x_3)\,\exp(ik\,q^{(\nu)}\cdot x) = \Lambda^+\mathrm{SL}_N^+\varphi^+(x), \qquad x\in\Gamma^+.$$

Noting that $\partial/\partial x_3 = n_3\,\partial/\partial x_3 = n\cdot\nabla_\alpha$ on Γ^+ completes the proof. ■

The traces of the potentials on the surfaces Γ_j give rise to boundary operators. We will later see that these operators can be represented as integral operators provided that the surface and the densities are smooth enough. The mapping properties of these operators do not rely on this representation but are an immediate consequence of their definition and of the jump relations of the potentials.

Definition 4.5 *Let $\varphi\in H_Q^{-1/2}(\Gamma_j)$ and $\psi\in H_Q^{1/2}(\Gamma_j)$, $j\in\{0,\dots,N\}$. We define the boundary operators*

$$S_j^\pm : H_Q^{-1/2}(\Gamma_j)\to H_Q^{1/2}(\Gamma_j), \qquad K_j^\pm : H_Q^{1/2}(\Gamma_j)\to H_Q^{1/2}(\Gamma_j),$$
$$\tilde{K}_j^\pm : H_Q^{-1/2}(\Gamma_j)\to H_Q^{-1/2}(\Gamma_j), \qquad T_j^\pm : H_Q^{1/2}(\Gamma_j)\to H_Q^{-1/2}(\Gamma_j)$$

by

$$S_j^\pm\varphi := \mathrm{SL}_j^\pm\varphi|_{\Gamma_j}, \qquad K_j^\pm\psi := \frac{1}{2}\left[\mathrm{DL}_j^\pm\psi|_{\Gamma_j}^+ + \mathrm{DL}_j^\pm\psi|_{\Gamma_j}^-\right],$$
$$\tilde{K}_j^\pm\varphi := \frac{1}{2}\left[n\cdot\nabla_\alpha\mathrm{SL}_j^\pm\varphi\Big|_{\Gamma_j}^+ + n\cdot\nabla_\alpha\mathrm{SL}_j^\pm\varphi\Big|_{\Gamma_j}^-\right], \qquad T_j^\pm\varphi := -\,n\cdot\nabla_\alpha\mathrm{DL}_j^\pm\psi\Big|_{\Gamma_j}.$$

From Theorem 4.2 we immediately obtain the classical relations of these boundary operators to the traces of the potentials. In the formulation of this corollary we will again suppress the superscripts $\pm$.

Corollary 4.6 *Let $\varphi\in H_Q^{-1/2}(\Gamma_j)$ and $\psi\in H_Q^{1/2}(\Gamma_j)$, $j\in\{0,\dots,N\}$. Then the following relations are satisfied:*

$$\mathrm{SL}_j\varphi|_{\Gamma_j} = S_j\varphi, \qquad \mathrm{DL}_j\psi|_{\Gamma_j}^\pm = K_j\psi \pm \frac{1}{2}\,\psi$$
$$n\cdot\nabla_\alpha\mathrm{SL}_j\varphi|_{\Gamma_j}^\pm = \tilde{K}_j\varphi \mp \frac{1}{2}\,\varphi, \qquad n\cdot\nabla_\alpha\mathrm{DL}_j\psi|_{\Gamma_j} = -T_j\psi.$$

In order to implement a numerical method, the question arises how these boundary operators can be represented in a computable fashion, i.e. as proper integral operators. Results in this respect are usually derived by studying the corresponding operators for Laplace's equation and then arguing that the fundamental solution of the problem at hand differs from that for the latter equation by a smooth function. The basis for this line of argument in our case is Theorem 3.8, hence we state the following Theorem without proof and not in maximal generality, refering the reader to [57, Chapter 3.3] for details, or to [48, Chapter 7] for comparable results.

Theorem 4.7 *Assume that Γ_j is piecewise C^2, $x \in \Gamma_j$ and that $\psi \in C_Q(\Gamma_j)$, $j \in \{0,\dots,N\}$ and piecewise continuously differentiable. Then there hold the representations*

$$\begin{aligned}
S_j\psi(x) &= \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x))\, G_{q^{1/2}k}(x,y)\,\psi(y)\,ds(y),\\
K_j\psi(x) &= \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x))\, \frac{\partial G_{q^{1/2}k}(x,y)}{\partial n(y)}\,\psi(y)\,ds(y),\\
\tilde{K}_j\psi(x) &= \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x))\, \frac{\partial G_{q^{1/2}k}(x,y)}{\partial n(x)}\,\psi(y)\,ds(y),
\end{aligned}$$

Here, the integrals exist as improper integrals. The superscripts "±" on the operators and the corresponding indices on q have been dropped for ease of presentation.

A similar representation can be shown for the hypersingular operators $T_j^{\pm}$ [48, Theorem 7.4], with the integral existing as a finite parts integral. However, as will be demonstrated in the subsequent sections of this chapter, only differences $T_j^+ - T_j^-$ will be of interest in the boundary integral equations considered here. Using Theorem 3.8 and regularity results for boundary operators defined using the fundamental solution for the Helmholtz equation, we obtain that the kernel of this operator has a weak singularity. Hence we obtain a similar representation as in Theorem 4.7.

Theorem 4.8 *Assume that Γ_j is piecewise C^2, $x \in \Gamma_j$ and that $\psi \in C_Q(\Gamma_j)$, $j \in \{0,\dots,N\}$ and is continuously differentiable. Then there holds the representation*

$$(T_j^+ - T_j^-)\,\psi(x) = \int_{\Gamma_j} \exp(i\tilde{\alpha}\cdot(y-x))\, \frac{\partial^2\big(G_{q_j^{1/2}k}(x,y) - G_{q_{j-1}^{1/2}k}(x,y)\big)}{\partial n(x)\,\partial n(y)}\,\psi(y)\,ds(y),$$

where the integral exists as an improper integral.

4.2 Deriving Boundary Integral Equations

As outlined earlier, we chose to derive boundary integral equation formulations of the scattering and transmission problems based on an indirect approach: the solution u_α of Problems 2.14 – 2.16 or of Problem 2.32 will be sought as a suitable superposition of single- and double-layer potentials in the individual domains D_j. Regularity considerations and the variational formulation will then lead to a boundary equation formulation of these problems.

Preliminary Considerations. All of the scalar scattering and transmission problems share some common features: the medium consists of a stack of layers with varying indices of refraction. The problems only differ in the condition to be satisfied on the lowest surface.

This common structure of the problems will be reflected in the ansatzes to be made for the solution: these will also only differ in the lowest layers of the medium. Hence, the conditions to be derived for the upper layers will be identical for all problems and we will derive them here in a generic way in order to simplify the arguments later on.

Let us consider only a section of the full medium consisting of two layers D_{j-1}, D_j and the related interfaces Γ_{j-1}, Γ_j and Γ_{j+1}. By D we denote the domain $D_{j-1} \cup \Gamma_j \cup D_j$. We will make the following ansatz for the restriction of the solution u_α of one of the variational problems to D_l, $l = j-1,\, j$:

$$u_\alpha = \frac{1}{\lambda_l}\left(\mathrm{DL}_l^+ \psi_l + \mathrm{SL}_l^+ \varphi_l + \mathrm{DL}_{l+1}^- \psi_{l+1} + \mathrm{SL}_{l+1}^- \varphi_{l+1}\right),$$

where $\varphi_l \in H_Q^{-1/2}(\Gamma_l)$, $\psi_l \in H_Q^{1/2}(\Gamma_l)$, $l = j-1,\, j,\, j+1$.

As was pointed out in Chapter 2, the restriction of u_α to D has to be an element of $H^1(D)$ and hence automatically satisfies the condition

$$u_\alpha|^+ - u_\alpha|^- = 0 \quad \text{on } \Gamma_j. \tag{4.2}$$

Applying Corollary 4.6, we obtain an equation on Γ_j involving the boundary operators,

$$\begin{aligned}\left[\frac{\lambda_{j-1}+\lambda_j}{2\lambda_{j-1}\lambda_j}\, I + \frac{1}{\lambda_j}\, K_j^+ - \frac{1}{\lambda_{j-1}}\, K_j^-\right]\psi_j - \frac{1}{\lambda_{j-1}}\,\mathrm{DL}_{j-1}^+\psi_{j-1} + \frac{1}{\lambda_j}\,\mathrm{DL}_{j+1}^-\psi_{j+1} \\ + \left[\frac{1}{\lambda_j}\, S_j^+ - \frac{1}{\lambda_{j-1}}\, S_j^-\right]\varphi_j - \frac{1}{\lambda_{j-1}}\,\mathrm{SL}_{j-1}^+\varphi_{j-1} + \frac{1}{\lambda_j}\,\mathrm{SL}_{j+1}^-\varphi_{j+1} = 0.\end{aligned} \tag{4.3}$$

When considering the complete layered medium, we obtain an entire system of equations of this form. In order to represent this system, we introduce the following two auxiliary matrix operators, for $m \geq l$:

$$A_{l,m}^{(1,1)} := \begin{pmatrix} \frac{(\lambda_{l-1}+\lambda_l)\,I}{2\lambda_{l-1}\lambda_l} + \frac{K_l^+}{\lambda_l} - \frac{K_l^-}{\lambda_{l-1}} & -\frac{\mathrm{DL}_{l+1}^-}{\lambda_l} & & \\ -\frac{\mathrm{DL}_1^+}{\lambda_1} & \ddots & \ddots & \\ & \ddots & \ddots & \frac{\mathrm{DL}_m^-}{\lambda_{m-1}} \\ & & -\frac{\mathrm{DL}_{m-1}^+}{\lambda_{m-1}} & \frac{(\lambda_{m-1}+\lambda_m)\,I}{2\lambda_{m-1}\lambda_m} + \frac{K_m^+}{\lambda_m} - \frac{K_m^-}{\lambda_{m-1}} \end{pmatrix}$$

and

$$A_{l,m}^{(1,2)} := \begin{pmatrix} \frac{S_l^+}{\lambda_l} - \frac{S_l^-}{\lambda_{l-1}} & \frac{\mathrm{SL}_{l+1}^-}{\lambda_l} & & \\ -\frac{\mathrm{SL}_l^+}{\lambda_l} & \ddots & \ddots & \\ & \ddots & \ddots & \frac{\mathrm{SL}_m^-}{\lambda_{m-1}} \\ & & -\frac{\mathrm{SL}_{m-1}^+}{\lambda_{m-1}} & \frac{S_m^+}{\lambda_m} - \frac{S_m^-}{\lambda_{m-1}} \end{pmatrix}.$$

Because the potentials already are weak solutions to the Helmholtz equation in the individual layers, the variational formulation of the scattering and transmission problems reduces to conditions for the jumps of the Neumann traces across the interfaces. This will be shown in detail below for the individual problems. For the generic subproblem discussed here, we obtain exactly the second transmission condition on Γ_j of the classical problem (2.15) formulated for the Q-periodic function u_α, i.e.

$$\lambda_j\, n \cdot \nabla_\alpha u_\alpha\big|_{\Gamma_j}^+ - \lambda_{j-1}\, n \cdot \nabla_\alpha u_\alpha\big|_{\Gamma_j}^- = 0 \tag{4.4}$$

Applying once more Corollary 4.6, we obtain a second boundary equation,

$$\begin{aligned} \left(T_j^+ - T_j^-\right)\psi_j + n \cdot \nabla_\alpha \mathrm{DL}_{j-1}^+ \psi_{j-1} - n \cdot \nabla_\alpha \mathrm{DL}_{j+1}^- \psi_{j+1} \\ + \left(I - \tilde{K}_j^+ + \tilde{K}_j^-\right)\varphi_j + n \cdot \nabla_\alpha \mathrm{SL}_{j-1}^+ \varphi_{j-1} - n \cdot \nabla_\alpha \mathrm{SL}_{j+1}^- \varphi_{j+1} = 0. \end{aligned} \tag{4.5}$$

Again, we wish to introduce generic operators that represent this type of equation in the general situation of a layered medium. Here, this goal is achieved by introducing the operators

$$A_{l,m}^{(2,1)} := \begin{pmatrix} T_l^+ - T_l^- & -n \cdot \nabla_\alpha \mathrm{DL}_{l+1}^- & & \\ n \cdot \nabla_\alpha \mathrm{DL}_l^+ & \ddots & \ddots & \\ & \ddots & \ddots & -n \cdot \nabla_\alpha \mathrm{DL}_m^- \\ & & n \cdot \nabla_\alpha \mathrm{DL}_{m-1}^+ & T_m^+ - T_m^- \end{pmatrix}$$

and

$$A_{l,m}^{(2,2)} := \begin{pmatrix} I - \tilde{K}_l^+ + \tilde{K}_l^- & -n\cdot\nabla_\alpha \mathrm{SL}_{l+1}^- & & \\ n\cdot\nabla_\alpha \mathrm{SL}_l^+ & \ddots & \ddots & \\ & \ddots & \ddots & -n\cdot\nabla_\alpha \mathrm{SL}_m^- \\ & & n\cdot\nabla_\alpha \mathrm{SL}_{m-1}^+ & I - \tilde{K}_m^+ + \tilde{K}_m^- \end{pmatrix}.$$

The Case of the Dirichlet Scattering Problem. We will make the following ansatz for the solution

$$u_\alpha = \begin{cases} \dfrac{1}{\lambda_0}\,(\mathrm{DL}_0^+ - i\mathrm{SL}_0^+)\psi_0 & \\ \qquad + \dfrac{1}{\lambda_0}\,(\mathrm{DL}_1^-\psi_1 + \mathrm{SL}_1^-\varphi_1) & \text{in } D_0 \\ \dfrac{1}{\lambda_j}\,(\mathrm{DL}_j^+\psi_j + \mathrm{SL}_j^+\varphi_j) & \\ \qquad + \dfrac{1}{\lambda_j}\,(\mathrm{DL}_{j+1}^-\psi_{j+1} + \mathrm{SL}_{j+1}^-\varphi_{j+1}) & \text{in } D_j,\ j = 1,\dots,N-1 \\ \dfrac{1}{\lambda_N}\,(\mathrm{DL}_N^+\psi_N + \mathrm{SL}_N^+\varphi_N + M_{-\alpha}u^i) & \text{in } D_N \end{cases} \tag{4.6}$$

with $\psi_j \in H_Q^{1/2}(\Gamma_j)$, $j = 0,\dots,N$, and $\varphi_j \in H_Q^{-1/2}(\Gamma_j)$, $j = 1,\dots,N$. We collect these densities in the vectors $\boldsymbol{\psi} := (\psi_0,\dots,\psi_N)^\top$ and $\boldsymbol{\varphi} := (\varphi_1,\dots,\varphi_N)^\top$, respectively.

A necessary condition for u_α to be a solution of Problem 2.14 is that $u_\alpha \in V_0$, where the space V_0 was defined in (2.23). Hence, we obtain the condition

$$u_\alpha = 0 \quad \text{on } \Gamma_0$$

as well as (4.2) for $j = 1,\dots,N$.

In order for u_α to be a solution of the Dirichlet scattering problem, it has to be a solution of the variational equation

$$\sum_{j=0}^{N} \lambda_j \int_{D_j} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2\, u_\alpha\, \bar{v}\right) dx - \lambda_N \int_{\Gamma^+} \bar{v}\,\Lambda^+ u_\alpha\, ds$$
$$= \lambda_N \int_{\Gamma^+} \bar{v}\,\left(M_{-\alpha}\frac{\partial u^i}{\partial n} - \Lambda^+ M_{-\alpha}u^i\right) ds \qquad \text{for all } v \in V_0.$$

Applying Theorems 4.3 and 4.4, we obtain, for all $v \in V_0$,

$$\sum_{j=1}^{N} \int_{\Gamma_j} \bar{v}\,\left(\lambda_{j-1}\, n\cdot\nabla_\alpha u_\alpha|^- - \lambda_j\, n\cdot\nabla_\alpha u_\alpha|^+\right) ds = 0.$$

Choosing a test function v that is identical to 1 in a neighborhood of Γ_j and vanishes in a neighborhood of all other surfaces for each $j = 1, \dots, N$ in turn, we obtain (4.4) on Γ_j, $j = 1, \dots, N$. Hence we have derived a total of $2N + 1$ equations for the unknowns $\boldsymbol{\psi}$, $\boldsymbol{\varphi}$, which we write in concise notation as

$$\begin{aligned} A_{\mathrm{D}}^{(1,1)} \boldsymbol{\psi} + A_{\mathrm{D}}^{(1,2)} \boldsymbol{\varphi} &= b^{(1)}, \\ A_{\mathrm{D}}^{(2,1)} \boldsymbol{\psi} + A_{\mathrm{D}}^{(2,2)} \boldsymbol{\varphi} &= b^{(2)}, \end{aligned} \tag{4.7}$$

with the operators and right hand sides defined using the operators from the preliminary considerations as follows:

$$A_{\mathrm{D}}^{(1,1)} := \left(\begin{array}{c|c} \frac{1}{\lambda_0} \left(\frac{1}{2} I + K_0^+ - i S_0^+ \right) & \frac{1}{\lambda_0} \mathrm{DL}_1^- \quad 0 \quad \cdots \quad 0 \\ \hline -\frac{1}{\lambda_0} \left(\mathrm{DL}_0^+ - i \mathrm{SL}_0^+ \right) & \\ 0 & \\ \vdots & A_{1,N}^{(1,1)} \\ 0 & \end{array} \right),$$

$$A_{\mathrm{D}}^{(1,2)} := \left(\begin{array}{c} \frac{1}{\lambda_0} \mathrm{SL}_1^- \quad 0 \quad \cdots \quad 0 \\ \hline A_{1,N}^{(1,2)} \end{array} \right),$$

$$A_{\mathrm{D}}^{(2,1)} := \left(\begin{array}{c|c} n \cdot \nabla_\alpha (\mathrm{DL}_0^+ - i \mathrm{SL}_0^+) & \\ 0 & \\ \vdots & A_{1,N}^{(2,1)} \\ 0 & \end{array} \right),$$

and

$$A_{\mathrm{D}}^{(2,2)} := A_{1,N}^{(2,2)}$$

as well as

$$\begin{aligned} b^{(1)} &:= \left(0\,, \ \dots\,, \ 0\,, \ -\frac{1}{\lambda_N} M_{-\alpha} u^i \right)^\top, \\ b^{(2)} &:= \left(0\,, \ \dots\,, \ 0\,, \ n \cdot \nabla_\alpha M_{-\alpha} u^i \right)^\top. \end{aligned}$$

The sizes of the rows and columns of zeros are clear from the context.

The Cases of the Neumann and Impedance Scattering Problems. To derive a boundary integral equation formulation for these problems, it is only necessary to modify the approach of the previous section slightly. We will make the ansatz

$$u_\alpha = \begin{cases} \dfrac{1}{\lambda_0}\,\mathrm{SL}_0^+\varphi_0 + \dfrac{1}{\lambda_0}\,(\mathrm{DL}_1^-\psi_1 + \mathrm{SL}_1^-\varphi_1) & \text{in } D_0 \\ \dfrac{1}{\lambda_j}\,(\mathrm{DL}_j^+\psi_j + \mathrm{SL}_j^+\varphi_j) & \\ \qquad\qquad + \dfrac{1}{\lambda_j}\,(\mathrm{DL}_{j+1}^-\psi_{j+1} + \mathrm{SL}_{j+1}^-\varphi_{j+1}) & \text{in } D_j,\ j = 1,\ldots,N-1 \\ \dfrac{1}{\lambda_N}\,(\mathrm{DL}_N^+\psi_N + \mathrm{SL}_N^+\varphi_N + M_{-\alpha}u^i) & \text{in } D_N \end{cases} \tag{4.8}$$

with $\psi_j \in H_Q^{1/2}(\Gamma_j)$, $j = 1,\ldots,N$, and $\varphi_j \in H_Q^{-1/2}(\Gamma_j)$, $j = 0,\ldots,N$. We again collect these densities vectors $\boldsymbol{\psi} := (\psi_1,\ldots,\psi_N)^\top$ and $\boldsymbol{\varphi} := (\varphi_0,\ldots,\varphi_N)^\top$.

For u_α to be an element of the correct space V, we obtain condition (4.2) on the interfaces Γ_j, $j = 1,\ldots,N$. The variational formulation leads to the further conditions (4.4) on Γ_j, $j = 1,\ldots,N$, as well as an additional condition on Γ_0, the boundary condition. Inserting the ansatz for u_α, for the Neumann case, this takes the form

$$\left(\frac{1}{2}I - \tilde{K}_0^+\right)\varphi_0 - \frac{\partial}{\partial n}\mathrm{DL}_1^-\psi_1 - \frac{\partial}{\partial n}\mathrm{SL}_1^-\varphi_1 = 0.$$

In the case of the impedance boundary condition, the boundary equation on Γ_0 is

$$\left(\frac{1}{2}I - \tilde{K}_0^+ - i\beta S_0^+\right)\varphi_0 - \frac{\partial}{\partial n}\mathrm{DL}_1^-\psi_1 - \frac{\partial}{\partial n}\mathrm{SL}_1^-\varphi_1 = 0.$$

Again, we have obtained $2N+1$ conditions for the $2N+1$ unknowns $\boldsymbol{\psi}$, $\boldsymbol{\varphi}$, which we write as the system

$$\begin{aligned} A_{\mathrm{N}}^{(1,1)}\boldsymbol{\psi} + A_{\mathrm{N}}^{(1,2)}\boldsymbol{\varphi} &= b^{(1)}, \\ A_{\mathrm{N}}^{(2,1)}\boldsymbol{\psi} + A_{\mathrm{N/I}}^{(2,2)}\boldsymbol{\varphi} &= b^{(2)}, \end{aligned} \tag{4.9}$$

with the operators defined as

$$A_{\mathrm{N}}^{(1,1)} := A_{1,N}^{(1,1)}$$

$$A_{\mathrm{N}}^{(1,2)} := \left(\begin{array}{c|c} -\frac{1}{\lambda_0}\,\mathrm{SL}_0^+ & \\ 0 & \\ \vdots & A_{1,N}^{(1,2)} \\ 0 & \end{array}\right),$$

$$A_{\mathrm{N}}^{(2,1)} := \left(\begin{array}{c} -n\cdot\nabla_\alpha \mathrm{DL}_1^- \quad 0 \quad \cdots \quad 0 \\ \hline A_{1,N}^{(2,1)} \end{array}\right),$$

and

$$A_{\mathrm{N}}^{(2,2)} := \left(\begin{array}{c|c} \frac{1}{2}I - \tilde{K}_0^+ & -n\cdot\nabla_\alpha \mathrm{SL}_1^- \quad 0 \quad \cdots \quad 0 \\ \hline n\cdot\nabla_\alpha \mathrm{SL}_0^+ & \\ 0 & \\ \vdots & A_{1,N}^{(2,2)} \\ 0 & \end{array}\right)$$

as well as

$$A_{\mathrm{I}}^{(2,2)} := \left(\begin{array}{c|c} \frac{1}{2}I - \tilde{K}_0^+ - i\beta S_0^+ & -n\cdot\nabla_\alpha \mathrm{SL}_1^- \quad 0 \quad \cdots \quad 0 \\ \hline n\cdot\nabla_\alpha \mathrm{SL}_0^+ & \\ 0 & \\ \vdots & A_{1,N}^{(2,2)} \\ 0 & \end{array}\right)$$

The right hand side vectors $b^{(j)}$ are again given by

$$b^{(1)} := \left(0\,,\ \ldots\ ,\ 0\,,\ -\frac{1}{\lambda_N}\, M_{-\alpha}u^i\right)^\top,$$

$$b^{(2)} := \left(0\,,\ \ldots\ ,\ 0\,,\ n\cdot\nabla_\alpha M_{-\alpha}u^i\right)^\top,$$

however, note that their size differs from the Dirichlet scattering problem case.

The Case of the Transmission Problem. The modifications to the ansatz necessary for obtaining boundary integral equations for the Transmission Problem 2.32 effect only the representation of u_α in D_0 and in the additional subdomain D_{-1}. In fact, we set

$$u_\alpha = \begin{cases} \dfrac{1}{\lambda_{-1}}\left(\mathrm{DL}_0^-\psi_0 + \mathrm{SL}_0^-\varphi_0\right) & \text{in } D_{-1} \\ \dfrac{1}{\lambda_j}\left(\mathrm{DL}_j^+\psi_j + \mathrm{SL}_j^+\varphi_j\right) & \\ \qquad\qquad + \dfrac{1}{\lambda_j}\left(\mathrm{DL}_{j+1}^-\psi_{j+1} + \mathrm{SL}_{j+1}^-\varphi_{j+1}\right) & \text{in } D_j,\ j = 0,\ldots,N-1 \\ \dfrac{1}{\lambda_N}\left(\mathrm{DL}_N^+\psi_N + \mathrm{SL}_N^+\varphi_N + M_{-\alpha}u^i\right) & \text{in } D_N \end{cases} \tag{4.10}$$

with $\psi_j \in H_Q^{1/2}(\Gamma_j)$, $j = 0,\ldots,N$, and $\varphi_j \in H_Q^{-1/2}(\Gamma_j)$, $j = 0,\ldots,N$. We again collect these densities vectors $\boldsymbol{\psi} := (\psi_0,\ldots,\psi_N)^\top$ and $\boldsymbol{\varphi} := (\varphi_0,\ldots,\varphi_N)^\top$.

The conditions for the correct space are (4.2) on Γ_j, $j = 0, \ldots, N$ and the variational formulation leads to (4.4) on Γ_j, $j = 0, \ldots, N$. Hence, in this case, the system of boundary equations is

$$\begin{aligned} A_{0,N}^{(1,1)} \boldsymbol{\psi} + A_{0,N}^{(1,2)} \boldsymbol{\varphi} &= b^{(1)}, \\ A_{0,N}^{(2,1)} \boldsymbol{\psi} + A_{0,N}^{(2,2)} \boldsymbol{\varphi} &= b^{(2)}, \end{aligned} \tag{4.11}$$

with the operators exactly as in the section on preliminary considerations. The right hand sides are again defined formally as in the case of the Dirichlet or Neumann scattering problems, with the length of the zero columns adjusted to the correct size.

4.3 Uniqueness of Solution

Solvability of systems of integral equations can in simple cases conveniently be proved through the application of Fredholm theory. This section is devoted to the first step of this process, establishing injectivity of the matrix integral operators introduced in Section 4.2.

We will here reverse the usual order in which we have considered the individual problems and start with the Transmission Problem. It provides the general framework in which we will also treat the scattering problems.

The Transmission Problem. The technique for establishing injectivity of the matrix operator encountered in (4.11) consists of formulating transmission problems with just one interface Γ_j and involving only a single pair of densities φ_j, ψ_j and establishing $\varphi_j = 0$, $\psi_j = 0$ for each of these. To this end, we make the following definition:

Definition 4.9 *Suppose $j \in \{0, \ldots, N\}$ and denote by V_j the space $H^1_Q(\Omega_j^+ \cup \Gamma_j \cup \Omega_j^-)$. The* auxiliary transmission problem *associated with Γ_j is to find $u_\alpha \in V_j$ such that*

$$\int_{\Omega_j^+} \big(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_{j-1} k^2 \, u_\alpha \, \bar{v}\big) \, dx + \int_{\Omega_j^-} \big(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_j k^2 \, u_\alpha \, \bar{v}\big) \, dx$$
$$- \int_{\Gamma^+} \bar{v} \, \Lambda_\alpha^+ u_\alpha \, ds + \int_{\Gamma^-} \bar{v} \, \Lambda_\alpha^- u_\alpha \, ds = 0 \qquad \textit{for all } v \in V_j.$$

Remark 4.10 The auxiliary transmission problem corresponds to the following classical formulation for $u = M_\alpha u_\alpha$:

- $\Delta u + q_{j-1} k^2 u = 0$ in Ω_j^+ and $\Delta u + q_j k^2 u = 0$ in Ω_j^-,

- $u|^+ = u|^-$ and $\partial u/\partial n|^+ = \partial u/\partial n|^-$ on Γ_j,
- u satisfies the URC and the DRC.

Hence, this is a homogeneous transmission problem with just one interface. Solvability of this problem has been studied in Chapter 2. For complex indices of refraction q_{j-1}, q_j, bear in mind Remark 2.34. □

The basis for establishing injectivity of the matrix operator associated with the transmission problem is the following assumption.

Assumption 4.11 *Suppose that the interface Γ_j is such that the auxiliary transmission problem associated with Γ_j only admits the trivial solution, where $j \in \{0, \ldots, N\}$.*

Remark 4.12 Note that for a general Lipschitz interface Γ_j, there may exist a countable set of wave numbers such that the auxiliary transmission problem admits non-trivial solutions. If, however, Assumption 2.37 is satisfied, then 4.11 is automatically satisfied for all $j = 0, \ldots, N$. □

Theorem 4.13 *Assume that the Transmission Problem 2.32 is uniquely solvable and let Assumption 4.11 hold for all $j \in \{0, \ldots, N\}$. Then the matrix operator associated with the transmission problem is injective.*

Proof: Let $\boldsymbol{\psi}$, $\boldsymbol{\varphi}$ be vectors of densities that are a solution to (4.11) for $u^i \equiv 0$. From uniqueness for the Transmission Problem 2.32 it follows that u_α defined by (4.10) is equal to 0 almost everywhere.

We now define

$$w := \begin{cases} \mathrm{DL}_N^- \psi_N + \mathrm{SL}_N^- \varphi_N + \mathrm{DL}_{N-1}^+ \psi_{N-1} + \mathrm{SL}_{N-1}^+ \varphi_{N-1} & \text{in } \Omega_N^+ \\ -\mathrm{DL}_N^+ \psi_N - \mathrm{SL}_N^+ \varphi_N & \text{in } \Omega_N^- \end{cases}$$

Using the fact that $u_\alpha = 0$ and the jump relations from Theorem 4.2, we conclude

$$\begin{aligned} w|^+ &= w|^+ - \lambda_{N-1} u_\alpha|^- = \psi_N, \\ w|^- &= w|^- + \lambda_N u_\alpha|^+ = \psi_N \end{aligned}$$

and

$$\begin{aligned} n \cdot \nabla_\alpha w|^+ &= n \cdot \nabla_\alpha w|^+ - \lambda_{N-1}\, n \cdot \nabla_\alpha u_\alpha|^- = -\varphi_N, \\ n \cdot \nabla_\alpha w|^- &= n \cdot \nabla_\alpha w|^- + \lambda_N\, n \cdot \nabla_\alpha u_\alpha|^+ = -\varphi_N. \end{aligned}$$

Hence w satisfies the transmission conditions

$$w|^{+} - w|^{-} = 0 \qquad \text{and} \qquad n \cdot \nabla_\alpha w|^{+} - n \cdot \nabla_\alpha w|^{-} = 0.$$

From these conditions and the definition, it follows that w is a solution of the auxiliary transmission problem associated with Γ_N. Hence from Assumption 4.11 we conclude $w \equiv 0$ and thus $\psi_N = 0$ and $\varphi_N = 0$.

This process can now be repeated for each interface Γ_j with $j = N-1, \ldots, 0$, respectively, to eventually obtain $\boldsymbol{\psi} = 0$ and $\boldsymbol{\varphi} = 0$, so the proof is complete. ∎

The Scattering Problems. Most aspects of treating the matrix operators associated with the three scattering problems are rather similar to the case of the transmission problem. Again, the auxiliary transmission problems for $j = 1, \ldots, N$ play a role, and additionally an auxiliary boundary value problem.

Definition 4.14 *Denote by W the space $\{u \in H^1_Q(\Omega_0^-) : u = 0 \text{ on } \Gamma_0\}$. The* auxiliary Dirichlet problem *associated with Γ_0 is to find $u_\alpha \in W$ such that*

$$\int_{\Omega_0^-} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_0 k^2 \, u_\alpha \, \bar{v} \right) dx + \int_{\Gamma^-} \bar{v} \, \Lambda_\alpha^- u_\alpha \, ds = 0$$

Remark 4.15 The auxiliary Dirichlet problem corresponds to the following classical formulation for $u = M_\alpha u_\alpha$:

- $\Delta u + q_0 k^2 u = 0$ in Ω_0^-,
- $u = 0$ on Γ_0,
- u satisfies the DRC.

For real q_0, this is exactly a homogeneous Dirichlet Scattering problem posed in a domain obtained from the cases studied here by a reflection at a horizontal plane. Hence Theorem 2.29 ensures that this problem only admits the trivial solution whenever Γ_0 is the graph of a function with Hölder continuous first partial derivatives. In more general cases, the results of Chapter 2 guarantee this result for all but a countable set of wave numbers.

For q_0 with positive imaginary part we remind the reader of Remark 2.20 which implies that the auxiliary Dirichlet problem only admits the trivial solution in this case. □

We can turn straight to the proofs of the injectivity theorems for the matrix operators associated with the Neumann and Impedance Scattering Problems.

Theorem 4.16 *Assume that the Neumann Scattering Problem 2.14 is uniquely solvable, that Assumption 4.11 holds for all $j \in \{1, \ldots, N\}$ and that the auxiliary Dirichlet problem admits only the trivial solution. Then the matrix operator defined in* (4.9) *for the Neumann Scattering Problem is injective.*

Proof: Assume that $\boldsymbol{\psi}$, $\boldsymbol{\varphi}$ solve (4.9) for the Neumann Scattering Problem with $u^i \equiv 0$. By the same argument as in the proof of Theorem 4.13 we obtain that $\psi_j = 0$, $\varphi_j = 0$ for $j = 1, \ldots, N$. Thus the problem reduces to the boundary equation

$$\left(\frac{1}{2} I - \tilde{K}_0^+\right) \varphi_0 = 0.$$

We now set $w := \mathrm{SL}_0^+ \varphi_0$ in Ω_0^-. By the jump relation for the single layer potential we conclude that $w = 0$ on Γ_0, and consequently w is a solution of the auxiliary Dirichlet problem. Hence $w \equiv 0$ and

$$n \cdot \nabla_\alpha w|^- = \left(\frac{1}{2} I + \tilde{K}_0^-\right) \varphi_0 = 0 \qquad \text{on } \Gamma_0.$$

Thus, by adding both equations on Γ_0, we obtain $\varphi_0 = 0$. ■

Theorem 4.17 *Assume that Assumption 4.11 holds for all $j \in \{1, \ldots, N\}$ and that the auxiliary Dirichlet problem admits only the trivial solution. Then the matrix operator defined in* (4.9) *for the Impedance Scattering Problem is injective.*

Proof: Assume that $\boldsymbol{\psi}$, $\boldsymbol{\varphi}$ solve (4.9) for the Impedance Scattering Problem with $u^i \equiv 0$. By the same argument as in the proof of Theorem 4.13 we obtain that $\psi_j = 0$, $\varphi_j = 0$ for $j = 1, \ldots, N$. Thus the problem reduces to the boundary equation

$$\left(\frac{1}{2} I - \tilde{K}_0^+ + i\beta S_0^+\right) \varphi_0 = 0.$$

Set $w = \mathrm{SL}_0^+ \varphi_0$ in Ω_0^+ and Ω_0^-. Then

$$n \cdot \nabla_\alpha w|^+ + i\beta w|^+ = 0 \qquad \text{on } \Gamma_0.$$

By uniqueness for the Impedance Scattering Problem in Ω_0^+, we obtain $w \equiv 0$ in Ω_0^+ and hence $w|^- = 0$ on Γ_0 from the jump relations for the single layer potential. Uniqueness of solution for the auxiliary Dirichlet problem implies $w \equiv 0$ in Ω_0^-, hence $n \cdot \nabla_\alpha w|^- = 0$ on Γ_0. The jump relations for the normal derivative of the single layer potential now yield $\varphi_0 = 0$. ■

Because of the Brakhage/Werner type ansatz for the solution of the Dirichlet Scattering Problem (4.6), this problem is in a certain sense dual to the case of the Impedance Scattering Problem. We will need an auxiliary impedance boundary value problem.

Definition 4.18 *The* auxiliary impedance problem *associated with* Γ_0 *is to find* $u_\alpha \in H^1_Q(\Omega_0^-)$ *such that*

$$\int_{\Omega_0^-} \left(\nabla_\alpha u_\alpha \cdot \overline{\nabla_\alpha v} - q_0 k^2\, u_\alpha\, \bar{v}\right) dx + \int_{\Gamma^-} \bar{v}\, \Lambda^- u_\alpha\, ds - i\beta \int_{\Gamma_0} u_\alpha\, \bar{v}\, ds = 0$$

for all $v \in H^1_Q(\Omega_0^-)$.

Remark 4.19 The auxiliary impedance problem is nearly identical to the classical problem of Remark 4.15 with the Dirichlet boundary condition $u = 0$ on Γ_0 replaced by $(\partial u)/(\partial n) - i\beta u = 0$. Note that the normal here is assumed to point out of Ω_0^-.

By reflection at a horizontal plane, from Theorem 2.19 (a) we conclude that the auxiliary Impedance problem only admits the trivial solution. □

Theorem 4.20 *Assume that the Dirichlet Scattering Problem 2.14 is uniquely solvable, that Assumption 4.11 holds for all* $j \in \{1, \ldots, N\}$. *Then the matrix operator defined in* (4.7) *is injective.*

Proof: Let $\boldsymbol{\psi}$, $\boldsymbol{\varphi}$ be vectors of densities that are a solution to (4.7) for $u^i \equiv 0$. From uniqueness of the Dirichlet Scattering Problem we obtain that u_α defined by (4.6) is equal to 0 almost everywhere.

As in the proof of Theorem 4.13, we now conclude that $\psi_j = 0$, $\varphi_j = 0$ for $j = 1, \ldots, N$. Hence we are left with the single boundary equation on Γ_0,

$$\left(\frac{1}{2}\, I + K_0^+ - iS_0^+\right) \psi_0 = 0.$$

We now set $w := (\mathrm{DL}_0^+ - i\mathrm{SL}_0^+)\psi_0$ in Ω_0^-. Hence we obtain

$$n \cdot \nabla_\alpha w|^- = n \cdot \nabla_\alpha w|^- - n \cdot \nabla_\alpha u_\alpha|^+ = -i\psi_0 \qquad \text{and} \qquad w|^- = w|^- - u_\alpha|^+ = -\psi_0$$

on Γ_0, concluding that w satisfies the boundary condition

$$n \cdot \nabla_\alpha w|^- - iw|^- = 0.$$

Thus, w is a solution to the auxiliary impedance problem and consequently $w \equiv 0$ in Ω_0^-. The jump relations for the single and double layer potentials now imply $\psi_0 = 0$. ■

4.4 Regularity and Existence of Solution

Existence of solution to the systems of integral equations under consideration will be proved via the Riesz-Fredholm theory. This approach requires sufficient regularity of interfaces such that the matrix operators introduced in Section 4.2 are Fredholm of index 0. Hence, our initial concern will be to establish mapping properties of the boundary integral operators provided the interfaces satisfy additional smoothness assumptions. Our approach is to extend results in this line for standard boundary integral operators on closed surfaces to the Q-periodic case using the results established for the Q-quasi-periodic Green's function in Chapter 3. We will be able to immediately conclude regularity results for the solutions to the systems of boundary integral equations encountered in the preceding sections.

Two approaches to establishing smoothing properties of boundary operators in Sobolev spaces are known in the literature. Using the theory of pseudo-differential operators, by classification of the singularity of the operator's symbol, the mapping properties can be deduced [61–63]. To derive the principal symbol of the operators, expansions of the singularities in local coordinate systems are required [46]. The second approach, introduced by Kirsch in his Habilitation thesis [41] (see also [42]), is to first establish the mapping properties for densities in Hölder spaces and then to use Lax's Theorem [43, Thorem 4.11] to extend these properties for densities in Sobolev spaces. It is this approach that we will make use of here.

We will start with a general assumption on the smoothness of the interfaces that will be required for the regularity and existence theory.

Assumption 4.21 *Assume that for some $m \in \mathbb{N}$, $m \geq 3$, the interfaces Γ_j, $j = 0, \ldots, N$, are graphs of Q-periodic functions in the Hölder class $C^{m,\alpha}$, $\alpha \in (0,1)$.*

Theorem 4.22 *Assume that Assumption 4.21 holds.*

- *The operators $S_j^{\pm}$ and $K_j^{\pm}$ map $H_Q^s(\Gamma_j)$ continuously into $H_Q^{s+1}(\Gamma_j)$ for all $s \in \mathbb{R}$ such that $-m+1 \leq s \leq m-1$.*
- *The operator $\tilde{K}_j^{\pm}$ maps $H_Q^s(\Gamma_j)$ continuously into $H_Q^{s+1}(\Gamma_j)$ for all $s \in \mathbb{R}$ such that $-m+2 \leq s \leq m-2$.*

Proof: Let us first consider the situation of a bounded domain D of class $C^{m,\alpha}$. Then the assertion is given in [41, Theorem 2.14] for all three operators.

We now return to periodic interfaces, denoting by A any of the operators in the theorem. Choose a partition of unity made up of compactly supported C^∞ functions $\{\phi_\nu : \nu = 1, \ldots, M\}$ such that $Q \subset \cup_{\nu=1}^{k} \operatorname{supp} \phi_\nu$ with the following additional property: if $\operatorname{supp} \phi_\nu \cap \operatorname{supp} \phi_\mu \neq \emptyset$, then there exists a translation $\tilde{Q}$ of Q such that $\operatorname{supp} \phi_\nu \cup \operatorname{supp} \phi_\mu \subset \tilde{Q}$.

Recall that by f_j we denote the function such that Γ_j is the graph of $f_j|_Q$. For each pair of indices (ν, μ) such that $\operatorname{supp}\phi_\nu \cap \operatorname{supp}\phi_\mu \neq \emptyset$ we define a closed surface $\Gamma_{\nu,\mu}$ of class $C^{m,\alpha}$ such that the set $\{x \in \mathbb{R}^3 : \tilde{x} \in \operatorname{supp}\phi_\nu \cup \operatorname{supp}\phi_\mu, x_3 = f_j(\tilde{x})\} \subset \Gamma_{\nu,\mu}$.

We now write, for $\varphi \in H^s_Q(\Gamma_j)$,

$$A\varphi = \sum_{\mu,\nu=1}^{M} \phi_\mu A(\phi_\nu \varphi).$$

For μ, ν such that $\operatorname{supp}\phi_\nu \cap \operatorname{supp}\phi_\mu = \emptyset$, the operators on the right hand side are integral operators with an analytical kernel, hence compact. Otherwise, we extend $\phi_\nu\varphi$ by 0 to a function in $H^s(\Gamma_{\nu,\mu})$. Denote by $\mathcal{A}$ the boundary operator corresponding to A for the closed surface $\Gamma_{\nu,\mu}$. By Theorem 3.8, the kernel of $\phi_\mu A(\phi_\nu\cdot)$ differs from that of $\phi_\mu \mathcal{A}(\phi_\nu\cdot)$ by an infinitely often continuously differentiable function. Hence, by the above considerations for a closed surface, $\phi_\mu A(\phi_\nu\varphi)$ is an element of $H^{s+1}_Q(\Gamma_j)$. Here we also make use of the special property of the partition of unity required above which makes a periodic extension of this function possible. Thus, the proof is complete. ■

Theorem 4.23 *Let assumption 4.21 hold. Then the operator* $T_j^+ - T_j^-$ *maps* $H^s_Q(\Gamma_j)$ *continuously into* $H^{s+1}_Q(\Gamma_j)$ *for all* $s \in \mathbb{R}$ *such that* $-m+1 \leq s \leq m-1$.

Proof: For a closed surface Γ of class $C^{m,\alpha}$, the difference of the hypersingular operator for Laplace's equation and the Hemholtz equation maps $H^s(\Gamma)$ to $H^{s+1}(\Gamma)$ for the asserted range for s [41, Theorem 2.20 (b)]. Two applications of this result yield the same mapping properties for the difference of the hypersingular operators for two Helmholtz equations with different wave numbers.

Making use of Theorem 3.8, we can extend this result to the difference $T_j^+ - T_j^-$ by the approach used in the proof of Theorem 4.22. ■

The previous two theorems immediately result in the following regularity result for solutions to the systems of boundary integral equations under consideration.

Corollary 4.24 *Let Assumption 4.21 hold and that* $(\boldsymbol{\varphi}, \boldsymbol{\psi})$ *is a solution to one of the matrix equations* (4.11), (4.7) *or* (4.9)*, respectively. Then each entry in the vector* $(\boldsymbol{\varphi}, \boldsymbol{\psi})$ *is an element of* $H^{m-1}_Q(\Gamma_j)$ *for the correct choice of* $j \in \{0, \dots, N\}$.

Proof: This is a direct application of Theorems 4.22 and 4.23 to the three systems of the second kind, noting that by the smoothness of the interfaces, the relevant right hand sides are also elements of the corresponding spaces $H^{m-1}_Q(\Gamma_j)$. ■

With smoothing properties established, solvability of the systems of boundary integral equations is now a straight-forward consequence of Sobolev's imbedding theorem and of the Fredholm alternative.

Theorem 4.25 *Let Assumption 4.21 hold.*

(a) Assume that $b_j^{(1)} \in H_Q^m(\Gamma_j)$*,* $j = 0, \dots, N$*,* $b_j^{(2)} \in H_Q^{m-1}(\Gamma_j)$*,* $j = 1, \dots, N$ *and that the conditions of Theorem 4.20 are satisfied. Then the system* (4.7) *posseses a unique solution* $(\boldsymbol{\psi}, \boldsymbol{\varphi})$ *where* $\psi_j \in H_Q^m(\Gamma_j)$*,* $j = 0, \dots, N$*, and* $\varphi_j \in H_Q^{m-1}(\Gamma_j)$*,* $j = 1, \dots, N$*.*

(b) Assume that $b_j^{(1)} \in H_Q^m(\Gamma_j)$*,* $j = 1, \dots, N$*,* $b_j^{(2)} \in H_Q^{m-1}(\Gamma_j)$*,* $j = 0, \dots, N$ *and that the conditions of Theorem 4.17 or of Theorem 4.16 are satisfied, respectively. Then the system* (4.9) *posseses a unique solution* $(\boldsymbol{\psi}, \boldsymbol{\varphi})$ *where* $\psi_j \in H_Q^m(\Gamma_j)$*,* $j = 1, \dots, N$*, and* $\varphi_j \in H_Q^{m-1}(\Gamma_j)$*,* $j = 0, \dots, N$*.*

(c) Assume that $b_j^{(l)} \in H_Q^{m-l+1}(\Gamma_j)$*,* $l = 1, 2$*,* $j = 0, \dots, N$ *and that the conditions of Theorem 2.40 are satisfied. Then the system* (4.11) *posseses a unique solution* $(\boldsymbol{\psi}, \boldsymbol{\varphi})$ *where* $\psi_j \in H_Q^m(\Gamma_j)$*,* $j = 0, \dots, N$*, and* $\varphi_j \in H_Q^{m-1}(\Gamma_j)$*,* $0 = 1, \dots, N$*.*

Proof: By Theorems 4.22 and 4.23 and Sobolev's imbedding theorem, all operators occuring in the relevant matrix operator are either identity operators multiplied by a scalar λ with $\arg \lambda \in [0, \pi/2)$ or compact. Hence the matrix operator is a compact perturbation of a coercive operator and thus a Fredholm operator of index 0. By applying either Theorem 4.13, Theorem 4.20, Theorem 4.17 or Theorem 4.16, respectively, it follows that the matrix operator is bijective in $[L^2(Q)]^l$ with dimension l according to the problem. The regularity of the solution is obtained by isolating the identity operators on the left hand side of the equations and applying Theorems 4.22 and 4.23 iteratively. ∎

Chapter 5

Nyström Methods for a Class of Q-Periodic Integral Equations

In Chapter 4 we have derived systems of integral equations for the scattering and transmission problems defined in Chapter 2. The integral operators all involve the Q-quasi-periodic Green's function. The question to be addressed in the last two chapters of this work is the numerical solution of such systems of equations by methods exploiting the regularity of the scattering surfaces through high convergence rates.

In the present chapter, we will consider integral equations with slightly less complicated singularities than those arising from the scattering and transmission problems: we will assume that the function $|\tilde{x}-\tilde{y}|/|x-y|$, present in the representations of Theorems 3.10 and 3.12 is replaced by a smooth function. Such integral equations can be stated equivalently as equations on the unit cell Q of the periodic lattice.

For such integral equations we will discuss a Nyström method obtained using interpolatory quadrature rules with uniformly spaced quadrature points. We will establish stability and high-order convergence rates, leading to super-algebraic convergence if the non-singular terms in the kernel are infinitely often differentiable. As a related method, we will also discuss a collocation method using trigonometic polynomials.

As a further simplification, we will consider only a single integral equation of the second kind. This simplification is carried out for purely presentational reasons, the methods discussed can easily be generalized to systems of equation.

As the kernel of the integral operators under consideration in this chapter is smoother than that in the scattering problem – except for flat surfaces – the method, although of interest in itself, is not directly applicable to the problems introduced in Chapter 2. However, the directional singularity can be replaced by a smooth function, leading to a regularization. We will discuss this approach briefly in Section 5.4.

5.1 Trigonometric Interpolation

The trigonometric monomials will play a central role throughout this chapter. To simplify notation, we will set

$$T^{(\nu)}(\tilde{x}) := \exp(iq^{(\nu)} \cdot \tilde{x}), \qquad \tilde{x} \in Q.$$

We will consider certain finite dimensional subspaces of $L^2(Q)$ obtained as the span of linear combinations of these monomials, setting

$$\mathcal{T}_{\mathcal{N}} := \operatorname{span}\{T^{(\nu)} : -N_1 < \nu_1 \le N_1, -N_2 < \nu_2 \le N_2\}, \qquad \mathcal{N} := (N_1, N_2)^\top \in \mathbb{N}^2,$$

which has dimension $4N_1N_2$.

We next define a linear operator $P_{\mathcal{N}}$ from $L^2(Q)$ to $\mathcal{T}_{\mathcal{N}}$. For $\rho \in \mathbb{Z}^2$, there exist unique pairs ν, $\kappa \in \mathbb{Z}^2$ with $-N_1 < \nu_1 \le N_1$, $-N_2 < \nu_2 \le N_2$ such that

$$\rho = 2\operatorname{diag}(\kappa)\mathcal{N} + \nu. \tag{5.1}$$

Consider now a function $v \in L^2(Q)$, such that v can be written as a Fourier series

$$v = \sum_{\rho \in \mathbb{Z}^2} v_\rho \, T^{(\rho)}.$$

Then we set

$$P_{\mathcal{N}} v := \sum_{\substack{-N_1 < \nu_1 \le N_1 \\ -N_2 < \nu_2 \le N_2}} \left(\sum_{\kappa \in \mathbb{Z}^2} v_{2\operatorname{diag}(\kappa)\mathcal{N}+\nu} \right) T^{(\nu)},$$

whenever all coefficient series

$$\left(\sum_{\kappa \in \mathbb{Z}^2} v_{2\operatorname{diag}(\kappa)\mathcal{N}+\nu} \right), \qquad -N_1 < \nu_1 \le N_1, -N_2 < \nu_2 \le N_2,$$

converge. In particular, the images of the trigonometric monomials under $P_{\mathcal{N}}$ are well defined and given by

$$P_{\mathcal{N}} T^{(\rho)} = T^{(\nu)},$$

and hence we are dealing with a projection onto $T_{\mathcal{N}}$. The next lemma will characterise subspaces of $L^2(Q)$ such that $P_{\mathcal{N}}$ is a bounded operator. For the definition of H^s_Q and its norm $|||\cdot|||_{Q,s}$, refer to page 14.

Lemma 5.1 *Suppose that $s > 1$ and $0 \le \sigma \le s$. Then $P_{\mathcal{N}} : H^s_Q \to H^\sigma_Q$ is bounded and*

$$|||P_{\mathcal{N}}v - v|||_{Q,\sigma} \le C \, \frac{(\max\{N_1, N_2\})^\sigma}{(\min\{N_1, N_2\})^s} \, |||v|||_{Q,s},$$

where C is constant depending on σ and s.

Proof: For $v \in H^s_Q$, the square of the norm on the left hand side of the bound can be written as

$$|||P_{\mathcal{N}}v - v|||^2_{Q,\sigma} = \sum_{\nu \in \mathbb{Z}^2} (1 + |\nu|^2)^\sigma \, |v_\nu - (P_{\mathcal{N}}v)_\nu|^2,$$

where v_ν denotes the Fourier coefficient of v and $(P_{\mathcal{N}}v)_\nu$ the corresponding Fourier coefficient of $P_{\mathcal{N}}v$. Define

$$\mathbb{Z}^2_{\mathcal{N}} = \{\nu \in \mathbb{Z}^2 : -N_1 < \nu_1 \le N_1, -N_2 < \nu_2 \le N_2\}.$$

From the definition of $P_{\mathcal{N}}$ we obtain

$$|||P_{\mathcal{N}}v - v|||^2_{Q,\sigma} \le \sum_{\nu \notin \mathbb{Z}^2_{\mathcal{N}}} (1 + |\nu|^2)^\sigma \, |v_\nu|^2 + \sum_{\nu \in \mathbb{Z}^2_{\mathcal{N}}} (1 + |\nu|^2)^\sigma \left| \sum_{\kappa \in \mathbb{Z}^2 \setminus \{0\}} v_{2\mathrm{diag}(\kappa)\mathcal{N} + \nu} \right|^2$$

For the first sum, we obtain

$$\begin{aligned} \sum_{\nu \notin \mathbb{Z}^2_{\mathcal{N}}} (1 + |\nu|^2)^\sigma \, |v_\nu|^2 &= \sum_{\nu \notin \mathbb{Z}^2_{\mathcal{N}}} (1 + |\nu|^2)^{\sigma - s} (1 + |\nu|^2)^s \, |v_\nu|^2 \\ &\le c \, (1 + |\mathcal{N}|^2)^{\sigma - s} \sum_{\nu \notin \mathbb{Z}^2_{\mathcal{N}}} (1 + |\nu|^2)^s \, |v_\nu|^2 \le \frac{c}{|\mathcal{N}|^{2(s-\sigma)}} \, |||v|||^2_{Q,s}. \end{aligned} \tag{5.2}$$

We furthermore have the estimate

$$\begin{aligned} &\left| \sum_{\kappa \in \mathbb{Z}^2 \setminus \{0\}} v_{2\mathrm{diag}(\kappa)\mathcal{N} + \nu} \right|^2 \le \left(\sum_{\kappa \in \mathbb{Z}^2 \setminus \{0\}} \frac{|2\mathrm{diag}(\kappa)\mathcal{N} + \nu|^s}{|2\mathrm{diag}(\kappa)\mathcal{N} + \nu|^s} \, |v_{2\mathrm{diag}(\kappa)\mathcal{N} + \nu}| \right)^2 \\ &\le \left[\sum_{\kappa \in \mathbb{Z}^2 \setminus \{0\}} \frac{1}{|2\mathrm{diag}(\kappa)\mathcal{N} + \nu|^{2s}} \right] \left[\sum_{\kappa \in \mathbb{Z}^2 \setminus \{0\}} |2\mathrm{diag}(\kappa)\mathcal{N} + \nu|^{2s} |v_{2\mathrm{diag}(\kappa)\mathcal{N} + \nu}|^2 \right] \\ &\qquad \le \frac{c}{(\min\{N_1, N_2\})^{2s}} \sum_{\kappa \in \mathbb{Z}^2 \setminus \{0\}} |2\mathrm{diag}(\kappa)\mathcal{N} + \nu|^{2s} |v_{2\mathrm{diag}(\kappa)\mathcal{N} + \nu}|^2, \end{aligned}$$

where the assumption $s > 1$ is essential. It follows that

$$\sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}} (1+|\nu|^2)^\sigma \left| \sum_{\kappa\in\mathbb{Z}^2\setminus\{0\}} v_{2\mathrm{diag}(\kappa)\mathcal{N}+\nu} \right|^2 \leq c \sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}} \frac{(1+|\nu|^2)^\sigma}{(\min\{N_1,N_2\})^{2s}} \sum_{\kappa\in\mathbb{Z}^2\setminus\{0\}} |2\mathrm{diag}(\kappa)\mathcal{N}+\nu|^{2s} |v_{2\mathrm{diag}(\kappa)\mathcal{N}+\nu}|^2 .$$

For $\nu \in \mathbb{Z}^2$ such that $|\nu| \leq |\mathcal{N}|$, we furthermore have the estimate

$$\frac{(1+|\nu|^2)^\sigma}{(\min\{N_1,N_2\})^{2s}} \leq 2^\sigma \frac{(\max\{N_1,N_2\})^{2\sigma}}{(\min\{N_1,N_2\})^{2s}} .$$

Hence, we obtain that

$$\sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}} (1+|\nu|^2)^\sigma \left| \sum_{\kappa\in\mathbb{Z}^2\setminus\{0\}} v_{2\mathrm{diag}(\kappa)\mathcal{N}+\nu} \right|^2 \leq c \frac{(\max\{N_1,N_2\})^{2\sigma}}{(\min\{N_1,N_2\})^{2s}} \sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}} \sum_{\kappa\in\mathbb{Z}^2} |2\mathrm{diag}(\kappa)\mathcal{N}+\nu|^{2s} |v_{2\mathrm{diag}(\kappa)\mathcal{N}+\nu}|^2 \leq c \frac{(\max\{N_1,N_2\})^{2\sigma}}{(\min\{N_1,N_2\})^{2s}} |||v|||^2_{Q,s} .$$

Combining this estimate with (5.2) completes the proof. ■

In particular, Lemma 5.1 implies that $P_{\mathcal{N}} v \to v$ in any Q-periodic Sobolev space H^σ_Q, $s > \sigma \geq 0$, provided $v \in H^s_Q$ and that $\max\{N_1, N_2\} = O(\min\{N_1, N_2\})$ as $|\mathcal{N}| \to \infty$. If we suppose that v is analytic, we obtain super-algebraic convergence in $H^\sigma : Q$ for every fixed $\sigma \geq 0$.

The spaces H^s_Q, $s > 1$, for which we show boundedness of $P_{\mathcal{N}}$ in Lemma 5.1, by Sobolev's imbedding theorem contain only continuous functions. Hence a pointwise evaluation of functions in these spaces is possible. In fact, the operator $P_{\mathcal{N}}$ is nothing else than an interpolation operator in disguise, for interpolation by Q-periodic trigonometric polynomials on the uniform grid $\mathcal{M}_{\mathcal{N}}$ consisting of the grid points

$$\tilde{x}_\mu := \left(\frac{\mu_1 L_1}{2N_1}, \frac{\mu_2 L_2}{2N_2} \right)^\top , \qquad \mu \in \mathbb{Z}^2_{\mathcal{N}} .$$

To see this, observe that for any $\rho \in \mathbb{Z}^2$, with the representation (5.1),

$$T^{(\rho)}(\tilde{x}_\mu) = \exp(i\, q^{(2\mathrm{diag}(\kappa)\mathcal{N}+\nu)} \cdot \tilde{x}_\mu) = \exp(i\, q^{(2\mathrm{diag}(\kappa)\mathcal{N})} \cdot \tilde{x}_\mu)\, T^{(\nu)}(\tilde{x}_\mu) = \exp\left(2\pi i \left(\frac{2\kappa_1 N_1}{L_1} \cdot \frac{\mu_1 L_1}{2N_1} + \frac{2\kappa_2 N_2}{L_2} \cdot \frac{\mu_2 L_2}{2N_2} \right) \right) T^{(\nu)}(\tilde{x}_\mu) = T^{(\nu)}(\tilde{x}_\mu).$$

Hence

$$P_{\mathcal{N}} v(\tilde{x}_\mu) = v(\tilde{x}_\mu), \qquad \text{for} \quad v \in H_Q^s,\ s > 1,$$

follows directly from the definition of the operator.

The Lagrange basis for this interpolation consists of the functions

$$L_{\mathcal{N}}^{(\mu)}(\tilde{x}) = \frac{1}{4N_1N_2} \sum_{\nu \in \mathbb{Z}_{\mathcal{N}}^2} T^{(\nu)}(\tilde{x} - \tilde{x}_\mu), \qquad \mu \in \mathbb{Z}_{\mathcal{N}}^2.$$

These can be directly obtained as tensor products of the corresponding one-dimensional Lagrange basis functions. Obviously $L_{\mathcal{N}}^{(\mu)}(\tilde{x}_\mu) = 1$ by definition. To see that $L_{\mathcal{N}}^{(\mu)}(\tilde{x}_\nu) = 0$ for $\mu \neq \nu$, we observe as in [43, section 11.3],

$$\sum_{-N_j < \nu_j \leq N_1} \exp\left(\frac{2\pi\nu_j}{L_j}(x_j - x_{\mu,j})\right)$$
$$= \sin\left(\frac{2\pi N_j}{L_j}(x_j - x_{\mu,j})\right)\left[\cot\left(\frac{\pi}{L_j}(x_j - x_{\mu,j})\right) + i\right], \qquad j = 1, 2,$$

for $x_j \neq x_{\mu,j}$. The sine function vanishes for $x_j = x_{\nu,j}$, $-N_1 < \nu \leq N_1$, $\nu \neq \mu$. Of course, there then holds

$$P_{\mathcal{N}} v(\tilde{x}) = \sum_{\tilde{x}_\mu \in \mathcal{M}_{\mathcal{N}}} v(\tilde{x}_\mu)\, L_{\mathcal{N}}^{(\mu)}(\tilde{x}), \qquad v \in H_Q^s, \quad \tilde{x} \in Q, \tag{5.3}$$

provided $s > 1$.

We finish this section with an additional result on the Lagrange basis.

Lemma 5.2 *For every $\mathcal{N} \in \mathbb{N}^2$, the Lagrange basis $\{L_{\mathcal{N}}^{(\mu)} : \mu \in \mathbb{Z}_{\mathcal{N}}^2\}$ is orthogonal in $L^2(Q)$, each function satisfying*

$$\left\| L_{\mathcal{N}}^{(\mu)} \right\|_{L^2(Q)}^2 = \frac{|Q|}{4N_1N_2}, \qquad \mu \in \mathbb{Z}_{\mathcal{N}}^2.$$

Proof: For μ, $\nu \in \mathbb{Z}_{\mathcal{N}}^2$, we compute

$$\int_Q L_{\mathcal{N}}^{(\mu)}(\tilde{x})\, \overline{L_{\mathcal{N}}^{(\nu)}(\tilde{x})}\, d\tilde{x} = \frac{1}{16N_1^2N_2^2} \sum_{\iota,\kappa \in \mathbb{Z}_{\mathcal{N}}^2} \int_Q T^{(\iota)}(\tilde{x} - \tilde{x}_\mu)\, \overline{T^{(\kappa)}(\tilde{x} - \tilde{x}_\nu)}\, d\tilde{x}$$
$$= \frac{|Q|}{16N_1^2N_2^2} \sum_{\iota \in \mathbb{Z}_{\mathcal{N}}^2} T^{(\iota)}(\tilde{x}_\nu - \tilde{x}_\mu) = \frac{|Q|}{4N_1N_2} L_{\mathcal{N}}^{(\mu)}(\tilde{x}_\nu) = \frac{|Q|}{4N_1N_2}\, \delta_{\mu,\nu}.$$

■

5.2 Operator Approximation

Using trigonometric interpolation we can obtain approximations to the integral operators under consideration. These are integral operators defined for Q-periodic functions involving an integration over the unit cell Q of the periodic lattice.

Operators in $\mathbf{H^s_Q}$. We define several integral operators for densities in H^s_Q, related to the kernels of the single- and the double-layer potential operators on Γ, where Γ denotes one of the surfaces Γ_j; $j = 0, \ldots, N$. These are the operators

$$I^{(1)}\varphi(\tilde{x}) := \int_Q F^{(1)}(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y},$$
$$I^{(2)}\varphi(\tilde{x}) := \int_Q \exp(i\tilde{\alpha}\cdot(\tilde{y}-\tilde{x}))\,G_k(\tilde{x},\tilde{y})\,F^{(2)}(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y},$$
$$I^{(3)}_{jl}\varphi(\tilde{x}) := \int_Q \exp(i\tilde{\alpha}\cdot(\tilde{y}-\tilde{x}))\,\frac{\partial G_k(\tilde{x},\tilde{y})}{\partial y_j}\,\sin\left(\frac{2\pi}{L_l}\,(x_l-y_l)\right)F^{(3)}_{jl}(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y},$$
$$j,l = 1,2.$$

Precise assumption on the functions $F^{(1)}$, $F^{(2)}$ and $F^{(3)}_{jl}$ shall be given in the assumptions of the individual theorems stating stability and convergence results. However, let us remark now that for the application to scattering and transmission problems discussed in Section 5.4, we can expect $F^{(1)}$, $F^{(2)} \in C^{m-1}(\mathbb{R}^2\times\mathbb{R}^2)$, $F^{(3)}_{jl} \in C^{m-2}(\mathbb{R}^2\times\mathbb{R}^2)$, where m is the regularity of the function defining Γ, and that all functions are Q-periodic with respect to both arguments.

In order to derive mapping properties of these operators, we will employ simpler ones that correspond to boundary integral operators in the case of a flat surface. These are the operators

$$S\varphi(\tilde{x}) := \int_Q \exp(i\tilde{\alpha}\cdot(\tilde{y}-\tilde{x}))\,G_k(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y},$$
$$V_{jl}\varphi(\tilde{x}) := \int_Q \exp(i\tilde{\alpha}\cdot(\tilde{y}-\tilde{x}))\,\frac{\partial G_k(\tilde{x},\tilde{y})}{\partial y_j}\,\sin\left(\frac{2\pi}{L_l}\,(x_l-y_l)\right)\varphi(\tilde{y})\,d\tilde{y}, \quad j,l = 1,2.$$

Lemma 5.3 *The operators S and V_{jl}, j, $l = 1, 2$, are bounded operators from H^s_Q to H^{s+1}_Q for every $s \in \mathbb{R}$. The trigonometric monomials are eigenfunctions of all these operators, specifically*

$$ST^{(\nu)} = \frac{i}{2\,k\rho^{(\nu)}}\,T^{(\nu)},$$
$$V_{jl}T^{(\nu)} = \frac{1}{4i}\left[\frac{d_j^{(\nu-e_l)}}{\rho^{(\nu-e_l)}} - \frac{d_j^{(\nu+e_l)}}{\rho^{(\nu+e_l)}}\right]T^{(\nu)}, \qquad j,l = 1,2,$$

where e_l denotes the l-th unit coordinate vector.

Proof: Note that

$$\exp\left(i\,\tilde\alpha\cdot\tilde y\right)\,T^{(\nu)}(\tilde y) = \exp\left(ik\,d^{(\nu)}\cdot\tilde y\right).$$

Then from Theorem 3.13, we directly obtain

$$\begin{aligned}
ST^{(\nu)}(\tilde x) &= \exp\left(-i\,\tilde\alpha\cdot\tilde x\right)\int_Q G_k(\tilde x,\tilde y)\,\exp(ik\,d^{(\nu)}\cdot\tilde y)\,d\tilde y\\
&= \frac{i}{2\,k\rho^{(\nu)}}\,\exp\left(-i\,\tilde\alpha\cdot\tilde x\right)\exp(ik\,d^{(\nu)}\cdot\tilde x) = \frac{i}{2\,k\rho^{(\nu)}}\,T^{(\nu)}(\tilde x).
\end{aligned}$$

Now we can estimate the norm of $ST^{(\nu)}$ by

$$|||ST^{(\nu)}|||^2_{Q,s+1} = \frac{(1+|\nu|^2)^{s+1}}{4\,|k\rho^{(\nu)}|^2} \le \frac{(1+|\nu|^2)^s}{4\,k^2\,c_1} = \frac{1}{4\,k^2\,c_1}|||T^{(\nu)}|||^2_{Q,s},$$

where c_1 is the constant from Remark 2.9. As the trigonmetric monomials form a complete orthonormal system in H^s_Q, we have established the mapping properties of S.

Noting

$$\begin{aligned}
\sin\left(\frac{2\pi}{L_l}\,(x_l-y_l)\right)\,T^{(\nu)}(\tilde y) = \frac{1}{2i}\Bigg[&\exp\left(\frac{2\pi i}{L_l}\,x_l\right)\,T^{(\nu-e_l)}(\tilde y)\\
&-\exp\left(-\frac{2\pi i}{L_l}\,x_l\right)\,T^{(\nu+e_l)}(\tilde y)\Bigg],
\end{aligned}$$

for V_{jl} we write

$$\begin{aligned}
V_{jl}T^{(\nu)}(\tilde x) = \frac{1}{2i}\Bigg[&\exp\left(-i\,\left(\tilde\alpha-\frac{2\pi e_l}{L_l}\right)\cdot\tilde x\right)\int_Q \frac{\partial G_k(\tilde x,\tilde y)}{\partial y_j}\,\exp(ik\,d^{(\nu-e_l)}\cdot\tilde y)\,d\tilde y\\
&-\exp\left(-i\,\left(\tilde\alpha+\frac{2\pi e_l}{L_l}\right)\cdot\tilde x\right)\int_Q \frac{\partial G_k(\tilde x,\tilde y)}{\partial y_j}\,\exp(ik\,d^{(\nu+e_l)}\cdot\tilde y)\,d\tilde y\Bigg].
\end{aligned}$$

Here we can apply Theorem 3.14 to obtain

$$\begin{aligned}
V_{jl}T^{(\nu)}(\tilde x) &= \frac{1}{2i}\Bigg[\exp\left(-i\,\left(\tilde\alpha-\frac{2\pi e_l}{L_l}\right)\cdot\tilde x\right)\frac{d_j^{(\nu-e_l)}}{2\,\rho^{(\nu-e_l)}}\,\exp(ik\,d^{(\nu-e_l)}\cdot\tilde x)\\
&\qquad -\exp\left(-i\,\left(\tilde\alpha+\frac{2\pi e_l}{L_l}\right)\cdot\tilde x\right)\frac{d_j^{(\nu+e_l)}}{2\,\rho^{(\nu+e_l)}}\,\exp(ik\,d^{(\nu+e_l)}\cdot\tilde x)\Bigg]\\
&= \frac{1}{4i}\left[\frac{d_j^{(\nu-e_l)}}{\rho^{(\nu-e_l)}}-\frac{d_j^{(\nu+e_l)}}{\rho^{(\nu+e_l)}}\right]T^{(\nu)}(\tilde x).
\end{aligned}$$

It remains to analyse the decay rate of these eigenvalues as $|\nu| \to \infty$ and this is entirely elementary. We assume $|\nu|$ to be large enough such that either $|d_1^{(\nu - t\, e_l)}|^2 > 1$ or $|d_2^{(\nu - t\, e_l)}|^2 > 1$ for all $t \in [-1,1]$, and set

$$g_{jl}(t) = \frac{d_j^{(\nu - t\, e_l)}}{\rho^{(\nu - t\, e_l)}} = \begin{cases} \frac{a_1 t + a_2}{\sqrt{(a_1 t + a_2)^2 + a_3^2 - 1}}, & j = l, \\ \frac{a_3}{\sqrt{(a_1 t + a_2)^2 + a_3^2 - 1}}, & j \neq l, \end{cases} \qquad j, l = 1, 2,$$

with certain coefficients a_1, a_2 and a_3 where all coefficients depend on k, L_1, L_2 and α. The coefficients a_2 and a_3 also depend on ν, but not a_1. By the mean value theorem we obtain

$$\left| \frac{d_j^{(\nu - e_l)}}{\rho^{(\nu - e_l)}} - \frac{d_j^{(\nu + e_l)}}{\rho^{(\nu + e_l)}} \right| \leq 2 \max_{t \in [-1,1]} \left| g'_{jl}(t) \right| .$$

In the case $j = l$ we have

$$g'_{jj}(t) = \frac{a_1}{\sqrt{(a_1 t + a_2)^2 + a_3^2 - 1}} - \frac{a_1\,(a_1 t + a_2)^2}{((a_1 t + a_2)^2 + a_3^2 - 1)^{3/2}} = \frac{a_1\,(a_3^2 - 1)}{((a_1 t + a_2)^2 + a_3^2 - 1)^{3/2}} .$$

Thus, for $a_3^2 \leq 1$,

$$|g'_{jj}(t)| \leq \frac{|a_1|}{((a_1 t + a_2)^2 + a_3^2 - 1)^{3/2}},$$

and for $a_3^2 > 1$,

$$|g'_{jj}(t)| \leq \frac{|a_1|\,(a_3^2 - 1)}{(a_3^2 - 1)((a_1 t + a_2)^2 + a_3^2 - 1)^{1/2}} = \frac{|a_1|}{((a_1 t + a_2)^2 + a_3^2 - 1)^{1/2}} .$$

Finally, in the case $j \neq l$,

$$g'_{jl}(t) = -\frac{a_1\, a_3\,(a_1 t + a_2)}{((a_1 t + a_2)^2 + a_3^2 - 1)^{3/2}} .$$

By assumption we have that either $|a_1 t + a_2| > 1$ or $|a_3| > 1$. If both conditions hold, we conclude

$$|g'_{jl}(t)| \leq \frac{|a_1|\,|a_3|\,|a_1 t + a_2|}{|a_1 t + a_2|\,|a_3|\,((a_1 t + a_2)^2 + a_3^2 - 1)^{1/2}} = \frac{|a_1|}{((a_1 t + a_2)^2 + a_3^2 - 1)^{1/2}} .$$

If $|a_1 t + a_2| \leq 1$ for some $t \in [-1,1]$,

$$|g'_{jl}(t)| \leq \frac{|a_3|}{a_3^2 - 1} \, \frac{|a_1|}{((a_1 t + a_2)^2 + a_3^2 - 1)^{1/2}} .$$

However, there are only finitely many values of ν_l such that this case occurs, hence the first factor in this estimate is bounded. The argument is similar for $|a_3| \leq 1$.

Noting that the assumption $|d_1^{(\nu - t\, e_l)}|^2 > 1$ or $|d_2^{(\nu - t\, e_l)}|^2 > 1$ for all $t \in [-1, 1]$ is only violated for a finite number of $\nu \in \mathbb{Z}^2$, we have proved the existence of a constant C such that

$$\left| \frac{d_j^{(\nu - e_l)}}{\rho^{(\nu - e_l)}} - \frac{d_j^{(\nu + e_l)}}{\rho^{(\nu + e_l)}} \right| \leq \frac{C}{|\rho^{(\nu)}|} \qquad \text{for all } \nu \in \mathbb{Z}\,.$$

The boundedness of $V_{jl} : H_Q^s \to H_Q^{s+1}$ now follows as in the proof for S. ■

Remark 5.4 Noting that S is equal to the operator S_0^+ in the case of a flat surface, the assertion of the Lemma for this operator is in fact already stated in Theorem 4.22. However, for V_{jl} we cannot argue in this way and the proof for S given here nicely complements that for V_{jl}. □

In order to prove corresponding mapping properties of the integral operators $I^{(1)}$, $I^{(2)}$ and $I_{jl}^{(3)}$ we will express them through S and V_{jl} by expanding the smooth part of the kernel as a Fourier series. The next lemma is the main tool used in this argument.

Lemma 5.5 *Suppose $m \in \mathbb{N}$ and that $F \in C^m(\mathbb{R}^2 \times \mathbb{R}^2)$ is Q-periodic. Then*

$$F(\tilde{x}, \tilde{y}) = \sum_{\nu \in \mathbb{Z}^2} F^{(\nu)}(\tilde{x})\, T^{\nu}(\tilde{y}), \qquad \tilde{x}, \tilde{y} \in \mathbb{R}^2$$

where $F^{(\nu)} \in C^m(\mathbb{R}^2)$ and

$$\sup_{\nu \in \mathbb{Z}^2} \sup_{\tilde{x} \in \mathbb{R}^2} |\nu|^{m - |\beta| + 1}\, |D^{\beta} F^{(\nu)}(\tilde{x})| < \infty$$

for any partial derivative $D^{\beta} F^{(\nu)}$ with $|\beta| \leq m$.

Proof: By expanding F into a Fourier series with respect to the second argument, we obtain the series representation in the lemma with

$$F^{(\nu)}(\tilde{x}) = \frac{1}{|Q|} \int_Q F(\tilde{x}, \tilde{y})\, T^{(-\nu)}(\tilde{y})\, d\tilde{y}.$$

Note that it follows from the theory of integral operators with continuously differentiable kernels that $F^{(\nu)} \in C^m(\mathbb{R}^2)$ and that the sets $\{D^{\beta} F^{(\nu)}\}$ are equicontinuous for $|\beta| \leq m$.

Now, let G denote any partial derivative of order $m - |\beta|$ of F with respect to the second argument. We similarly expand

$$G(\tilde{x}, \tilde{y}) = \sum_{\nu \in \mathbb{Z}^2} G^{(\nu)}(\tilde{x})\, T^{\nu}(\tilde{y}).$$

Then it follows from standard results on Fourier series that $(G^{(\nu)}(\tilde{x})) \in \ell^2$. However, by performing integration by parts on the integral

$$\int_Q G(\tilde{x}, \tilde{y})\, T^{(-\nu)}(\tilde{y})\, d\tilde{y}$$

and combining results for various partial derivatives G using the binomial theorem, we obtain

$$\left(|\nu|^{m-|\beta|}\, D^{\beta} F^{(\nu)}(\tilde{x})\right) \in \ell^2$$

for every $\tilde{x} \in \mathbb{R}^2$. It follows that $D^{\beta} F^{(\nu)}(\tilde{x}) = o(|\nu|^{m-|\beta|+1})$ as $|\nu| \to \infty$.

It remains to show this asymptotic behaviour is uniform in $\tilde{x}$. However, this follows directly from the equicontinuity of the set $\{F^{(\nu)}\}$. The same arguments can be repeated for any partial derivative of $F^{(\nu)}$ with respect to $\tilde{x}$ up to order m. ■

Two more technical results are required to establish the mapping properties. The next Lemma is well-known and stated for reference in the notation used here.

Lemma 5.6 *Suppose $\varphi \in H^s_Q$ and $\psi \in C^{\sigma}_Q(\overline{Q})$, $\sigma \in \mathbb{N}_{\geq s}$. Then $\psi\varphi \in H^s_Q$ and*

$$|||\psi\varphi|||_{Q,s} \leq C\, \|\psi\|_{\infty;\sigma}\, |||\varphi|||_{Q,s},$$

where the constant C is independent of φ and ψ and

$$\|\psi\|_{\infty;\sigma} := \sup_{\tilde{x} \in \overline{Q}} |\psi(\tilde{x})| + \max_{|\beta|=\sigma} \sup_{\tilde{x} \in \overline{Q}} |D^{\beta}\psi(\tilde{x})|.$$

Proof: The result follows from the equivalence of the norm $||| \cdot |||_{Q,s}$ with a Sobelev-Slobodeckiĭ norm. ■

We also require an estimate on the supremum norm of trigonometric monomials and their derivatives.

Lemma 5.7 *For $\nu \in \mathbb{Z}^2$ and $\sigma \in \mathbb{N}$, and set*

$$B_{\sigma} := \max\left\{1\,,\, \left(\frac{2\pi}{\min\limits_{j=1,2} L_j}\right)^{\sigma}\right\}.$$

Then for some constant $C > 0$, independent of ν and σ, there holds

$$\left\|T^{(\nu)}\right\|_{\infty;\sigma} \leq C\, B_{\sigma}\, (1 + |\nu|^{\sigma}).$$

Proof: Let $|\beta| = \sigma$. Then

$$D^\beta T^{(\nu)}(\tilde{x}) = \frac{\partial^\sigma}{\partial x_1^{\beta_1}\, \partial x_2^{\beta_2}} \exp(iq^{(\nu)} \cdot \tilde{x}) = (i)^\sigma\, (q_1^{(\nu)})_1^\beta\, (q_2^{(\nu)})_2^\beta \exp(iq^{(\nu)} \cdot \tilde{x}),$$

and hence

$$\left\| T^{(\nu)} \right\|_{\infty;\sigma} = 1 + \max_{|\beta|=\sigma} |q_1^{(\nu)}|^{\beta_1}\, |q_2^{(\nu)}|^{\beta_2} \leq 1 + \left(\frac{2\pi}{\min\limits_{j=1,2} L_j} \right)^\sigma |\nu|_\infty^\sigma.$$

From this estimate the assertion follows immediately. ■

Together, the previous three lemmas allow us to establish the mapping properties of the operators $I^{(1)}$, $I^{(2)}$ and $I_{jl}^{(3)}$ which we state next.

Theorem 5.8 *Suppose that for some* $m \geq 5$, $F^{(1)}$, $F^{(2)}$ *and* $F_{jl}^{(3)}$, $j,\ l = 1,\ 2$ *are* m *times continuously differentiable and that* $0 \leq s < m/2 - 2$. *Then*

$$I^{(1)},\ I^{(2)},\ I_{jl}^{(3)} : H_Q^s \to H_Q^{s+1} \qquad j, l = 1, 2$$

are well-defined bounded linear operators.

Proof: Let $\sigma := \text{floor}(s)$. Using the Fourier expansion of $F^{(1)}$ with respect to its second argument, we obtain the representation

$$I^{(1)}\varphi(\tilde{x}) = \sum_{\nu \in \mathbb{Z}^2} F^{(1,\nu)}(\tilde{x}) \int_Q T^{(\nu)}(\tilde{y})\, \varphi(\tilde{y})\, d\tilde{y},$$

For the integral in the representation of $I^{(1)}$, we use the Cauchy-Schwarz inequality and Lemma 5.6 to obtain

$$\left| \int_Q T^{(\nu)}(\tilde{y})\, \varphi(\tilde{y})\, d\tilde{y} \right| \leq |Q|^{1/2} \left\| T^{(\nu)}\varphi \right\|_{L^2(Q)} \leq |Q|^{1/2}\, |||T^{(\nu)}\varphi|||_{Q,s}$$
$$\leq C \left\| T^{(\nu)} \right\|_{\infty;\sigma+1} |||\varphi|||_{Q,s}.$$

Hence, using again Lemma 5.6 for the product $1 \cdot F^{(\nu)}$,

$$|||I^{(1)}\varphi|||_{Q,s+1} \leq \sum_{\nu \in \mathbb{Z}^2} \left| \int_Q T^{(\nu)}(\tilde{y})\, \varphi(\tilde{y})\, d\tilde{y} \right| |||F^{(1,\nu)}|||_{Q,s+1}$$
$$\leq C\, |||\varphi|||_{Q,s} \sum_{\nu \in \mathbb{Z}^2} \left\| T^{(\nu)} \right\|_{\infty;\sigma+1} \left\| F^{(1,\nu)} \right\|_{\infty;\sigma+2}.$$

By Lemma 5.7, we conclude

$$|||I^{(1)}\varphi|||_{Q,s+1} \le C\,|Q|^{1/2}\,B_{\sigma+1}\,|||\varphi|||_{Q,s} \sum_{\nu\in\mathbb{Z}^2} (1+|\nu|^{\sigma+1})\,\left\|F^{(1,\nu)}\right\|_{\infty;\sigma+2},$$

and the series converges as for some $\varepsilon > 0$ we have $2\sigma + 5 + \varepsilon \le m+1$ and hence Lemma 5.5 implies that $|\nu|^{\sigma+3+\varepsilon}\left\|F^{(1,\nu)}\right\|_{\infty;\sigma+2}$ is bounded.

For the operator $I^{(2)}$, using the operator S, we obtain the formal representation

$$I^{(2)}\varphi = \sum_{\nu\in\mathbb{Z}^2} F^{(2,\nu)} S(T^{(\nu)}\varphi).$$

Hence

$$\begin{aligned} |||I^{(2)}\varphi|||_{Q,s+1} &\le \sum_{\nu\in\mathbb{Z}^2} |||F^{(2,\nu)} S(T^{(\nu)}\varphi)|||_{Q,s+1} \\ &\le C \sum_{\nu\in\mathbb{Z}^2} \left\|F^{(2,\nu)}\right\|_{\infty;\sigma+2} |||S(T^{(\nu)}\varphi)|||_{Q,s+1} \end{aligned}$$

by Lemma 5.6 if the series converges. Noting

$$|||S(T^{(\nu)}\varphi)|||_{Q,s+1} \le C\,|||T^{(\nu)}\varphi|||_{Q,s} \le C\,\left\|T^{(\nu)}\right\|_{\infty;\sigma+1}\,|||\varphi|||_{Q,s}$$

again by Lemma 5.6, the assertion now follows as in the proof for $I^{(1)}$.

The proof for $I^{(3)}_{jl}$ is the same as for $I^{(2)}$. ∎

Approximation by Interpolation. We now approximate the integral operators studied above by finite dimensional approximations which we obtain through trigonometric interpolation. Formally, we set for $\mathcal{N} \in \mathbb{N}^2$

$$\begin{aligned} I^{(1)}_{\mathcal{N}}\psi(\tilde{x}) &:= \int_Q P_{\mathcal{N}}[F^{(1)}(\tilde{x},\cdot)\psi](\tilde{y})\,d\tilde{y}\,, \\ I^{(2)}_{\mathcal{N}}\psi(\tilde{x}) &:= \int_Q G_k(\tilde{x},\tilde{y})\,P_{\mathcal{N}}[F^{(2)}(\tilde{x},\cdot)\psi](\tilde{y})\,d\tilde{y}\,, \\ I^{(3)}_{jl,\mathcal{N}}\psi(\tilde{x}) &:= \int_Q \frac{\partial}{\partial y_j} G_k(\tilde{x},\tilde{y})\,\sin\left(\frac{2\pi}{L_l}(x_l-y_l)\right) P_{\mathcal{N}}[F^{(3)}_{jl}(\tilde{x},\cdot)\psi](\tilde{y})\,d\tilde{y} \\ & \qquad j,l = 1,2. \end{aligned}$$

We will proceed by establishing mapping properties and estimates for the approximation of the continuous operators by the discrete ones.

Theorem 5.9 *Suppose that for some $m \geq 6$, $F^{(1)}$, $F^{(2)}$ and $F^{(3)}_{jl}$, j, $l = 1$, 2 are m times continuously differentiable and that $1 < s \leq (m-3)/2$. Let A denote one of the operators $I^{(1)}$, $I^{(2)}$, $I^{(3)}_{jl}$ and $A_{\mathcal{N}}$ the corresponding discretized operator. Then for all $t \in [0, s]$,*

$$A_{\mathcal{N}} : H^s_Q \to H^{t+1}_Q$$

is a well-defined operator for all $\mathcal{N} \in \mathbb{N}^2$ and

$$|||(A - A_{\mathcal{N}})\varphi|||_{Q,t+1} \leq C \, \frac{(\max\{N_1, N_2\})^t}{(\min\{N_1, N_2\})^s} \, |||\varphi|||_{Q,s}$$

for all $\varphi \in H^s_Q$ and $\mathcal{N} \in \mathbb{N}^2$, where C is a constant dependent on t, s and on $F^{(1)}$, $F^{(2)}$ or $F^{(3)}_{jl}$, respectively.

Proof: We prove the estimates for the differences between corresponding continuous and discrete operators. The mapping properties for the discrete operators then follow directly. Set $\sigma = \text{floor}(t)$. Using the expansion in trigonometric polynomials of the smooth parts of the kernels with notation as in the proof of Theorem 5.8, for $\varphi \in H^s_Q$, $j, l = 1$, 2, we can estimate

$$\begin{aligned}
&|||I^{(1)}\varphi - I^{(1)}_{\mathcal{N}}\varphi|||_{Q,t+1} \\
&\leq \sum_{\nu\in\mathbb{Z}^2} \left| \int_Q \left(T^{(\nu)}(\tilde{y})\varphi(\tilde{y}) - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right](\tilde{y})\right) d\tilde{y} \right| |||F^{(1,\nu)}|||_{Q,t+1} \\
&\leq |Q|^{1/2} \sum_{\nu\in\mathbb{Z}^2} |||T^{(\nu)}\varphi - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right]|||_{Q,t} \, |||F^{(1,\nu)}|||_{Q,t+1}, \\
&|||I^{(2)}\varphi - I^{(2)}_{\mathcal{N}}\varphi|||_{Q,t+1} \\
&\leq \sum_{\nu\in\mathbb{Z}^2} |||F^{(2,\nu)}S(T^{(\nu)}\varphi - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right])|||_{Q,t+1} \\
&\leq C \sum_{\nu\in\mathbb{Z}^2} \left\|F^{(2,\nu)}\right\|_{\infty;\sigma+2} |||S(T^{(\nu)}\varphi - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right])|||_{Q,t+1} \\
&\leq C \sum_{\nu\in\mathbb{Z}^2} \left\|F^{(2,\nu)}\right\|_{\infty;\sigma+2} |||T^{(\nu)}\varphi - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right]|||_{Q,t}, \\
&|||I^{(3)}_{jl}\varphi - I^{(3)}_{jl,\mathcal{N}}\varphi|||_{Q,t+1} \\
&\leq \sum_{\nu\in\mathbb{Z}^2} |||F^{(3,\nu)}V_{jl}(T^{(\nu)}\varphi - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right])|||_{Q,t+1} \\
&\leq C \sum_{\nu\in\mathbb{Z}^2} \left\|F^{(3,\nu)}\right\|_{\infty;\sigma+2} |||V_{jl}(T^{(\nu)}\varphi - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right])|||_{Q,t+1} \\
&\leq C \sum_{\nu\in\mathbb{Z}^2} \left\|F^{(3,\nu)}\right\|_{\infty;\sigma+2} |||T^{(\nu)}\varphi - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right]|||_{Q,t}.
\end{aligned}$$

In all three instances, using Lemma 5.1, we can further estimate

$$|||T^{(\nu)}\varphi - P_{\mathcal{N}}\left[T^{(\nu)}\varphi\right]|||_{Q,t} \leq C\,\frac{(\max\{N_1,N_2\})^t}{(\min\{N_1,N_2\})^s}\,|||T^{(\nu)}\varphi|||_{Q,s}.$$

The rest of the proof is now exactly the same as the corresponding arguments in the proof of Theorem 5.8. ■

5.3 The Nyström Method for Q-Periodic Integral Equations

We here consider an integral equation of the form

$$\left(I + I^{(1)} + I^{(2)} + \sum_{j,l=1}^{2} I^{(3)}_{jl}\right)\varphi = \psi, \tag{5.4}$$

where the functions $F^{(1)}$, $F^{(2)}$ and $F^{(3)}$ used in the definition of the integral operators are supposed to be in $C^m(\mathbb{R}^2\times\mathbb{R}^2)$ for $m\geq 7$ and we assume $\psi\in H^\sigma_Q$ for some $\sigma>1$. For ease of notation, we set

$$A = I^{(1)} + I^{(2)} + \sum_{j,l=1}^{2} I^{(3)}_{jl}\,.$$

From Theorem 5.8, we know that $A : H^s_Q \to H^s_Q$ is bounded for $0\leq s < m/2-2$.

We approximate A by $A_{\mathcal{N}}$, $\mathcal{N}\in\mathbb{N}^2$, defined by

$$A_{\mathcal{N}} = I^{(1)}_{\mathcal{N}} + I^{(2)}_{\mathcal{N}} + \sum_{j,l=1}^{2} I^{(3)}_{jl,\mathcal{N}}\,.$$

As $A_{\mathcal{N}}$ is obtained via trigonometric interpolation, this operator is tied to a grid $\mathcal{M}_{\mathcal{N}}$ of interpolation points. To evaluate $A_{\mathcal{N}}\varphi_{\mathcal{N}}$, it suffices to know the values of $\varphi_{\mathcal{N}}$ on $\mathcal{M}_{\mathcal{N}}$. Setting $\boldsymbol{\varphi}_{\mathcal{N}} = (\varphi_{\mathcal{N}}(\tilde{x}_\nu))_{\nu\in\mathbb{Z}^2_{\mathcal{N}}}$, we obtain a matrix $\mathbf{A}_{\mathcal{N}}$ by setting

$$(\mathbf{A}_{\mathcal{N}}\boldsymbol{\varphi}_{\mathcal{N}})_\mu = (A_{\mathcal{N}}\varphi_{\mathcal{N}})(\tilde{x}_\mu), \qquad \mu\in\mathbb{Z}^2_{\mathcal{N}}\,.$$

The Nyström method in the first instance consists of solving the linear system of equations

$$\boldsymbol{\varphi}_{\mathcal{N}} + \mathbf{A}_{\mathcal{N}}\boldsymbol{\varphi}_{\mathcal{N}} = (\psi(\tilde{x}_\mu))_{\mu\in\mathbb{Z}^2_{\mathcal{N}}}\,. \tag{5.5}$$

Having solved this linear system, there are two possibilities of obtaining an approximation to the solution φ of (5.4). The first is to compute

$$\varphi_{\mathcal{N}} = \psi - A_{\mathcal{N}} \varphi_{\mathcal{N}}\,,$$

noting that the right hand side is computable from knowledge of $\boldsymbol{\varphi}_{\mathcal{N}}$. This amounts to solving

$$\varphi_{\mathcal{N}} = \left(I + A_{\mathcal{N}}\right)^{-1} \psi,$$

which is the Nyström method in the classical sence, as will be shown in Theorem 5.15.

The second possibility consists of computing the trigonometric interpolation polynomial with values $\boldsymbol{\varphi}_{\mathcal{N}}$ on $\mathcal{M}_{\mathcal{N}}$, i.e. a collocation method in the space of trigonometric polynomials $\mathcal{T}_{\mathcal{N}}$. This can be written as

$$\hat{\varphi}_{\mathcal{N}} = \left(I + P_{\mathcal{N}} A_{\mathcal{N}}\right)^{-1} P_{\mathcal{N}} \psi\,,$$

see again Theorem 5.15. The advantage over the classical Nyström method is that derivatives of $\hat{\varphi}_{\mathcal{N}}$ can easily be computed. In this section, we will first analyse both methods, giving proofs of convergence and stability, and then give details on the implementation.

Convergence and Stability. We will assume throughout this section that given $s > 1$, the operator $I + A : H^t_Q \to H^t_Q$ is boundedly invertible for all $t \in [0, s]$. The approximation results for the individual components of A and $A_{\mathcal{N}}$, respectively, which were derived in the previous section, allow the direct application of a Neumann series argument to establish the invertibility of $I + A_{\mathcal{N}}$ and zjr stability of the operators $(I + A_{\mathcal{N}})^{-1}$. The arguments used here are identical to those used in [43, Section 12.4] in the case of a one-dimensional weakly singular integral equation. We additionally need a constraint ensuring the uniformity of the grid in both directions.

Theorem 5.10 *Suppose that for some $m \geq 6$, $F^{(1)}$, $F^{(2)}$ and $F^{(3)}_{jl}$, $j, l = 1, 2$, are m times continuously differentiable and that $1 < s \leq (m-3)/2$. Further, given $c > 0$, assume that $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ satisfies $\max\{N_1, N_2\} \leq c \min\{N_1, N_2\}$. Then, for $\min\{N_1, N_2\}$ large enough, $I + A_{\mathcal{N}} : H^s_Q \to H^s_Q$ is boundedly invertible and all the inverses are uniformly bounded.*

Proof: An application of Theorem 5.9 with $t = s - 1$ taking into account the uniformity constraint on the grid yields the estimate

$$|||A\varphi - A_{\mathcal{N}}\varphi|||_{Q,s} \leq C \left(\min\{N_1, N_2\}\right)^{-1} |||\varphi|||_{Q,s}, \qquad \varphi \in H^s_Q.$$

Hence we have norm convergence of $I + A_{\mathcal{N}} \to I - A$ in the space of bounded linear operators in H^s_Q. The invertibility and uniform boundedness of $(I + A_{\mathcal{N}})^{-1}$

is now a consequence of a standard Neumann series argument, e.g. [43, Theorem 10.1]. ∎

Convergence follows from examining the difference between the original and the discretized equation.

Theorem 5.11 *Suppose that for some* $m \geq 6$, $F^{(1)}$, $F^{(2)}$ *and* $F^{(3)}_{jl}$, $j, l = 1, 2$, *are* m *times continuously differentiable and that* $1 < s \leq (m-3)/2$. *Further, given* $c > 0$, *assume that* $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ *satisfies* $\max\{N_1, N_2\} \leq c \min\{N_1, N_2\}$. *Given* $N_0 \in \mathbb{N}$, *assume that* $I + A_{\mathcal{N}} : H^s_Q \to H^s_Q$ *is boundedly invertible for* $\min\{N_1, N_2\} \geq N_0$. *Then for* $\psi \in H^s_Q$ *and* φ, $\varphi_{\mathcal{N}}$ *defined by* $(I + A)\varphi = \psi = (I + A_{\mathcal{N}})\varphi_{\mathcal{N}}$, *we have*

$$|||\varphi - \varphi_{\mathcal{N}}|||_{Q,t} \leq C \left(\min\{N_1, N_2\}\right)^{\max\{t-1,0\}-s} |||\varphi|||_{Q,s}\,, \qquad 0 \leq t \leq s.$$

Proof: We write

$$\varphi - \varphi_{\mathcal{N}} = A(\varphi_{\mathcal{N}} - \varphi) + (A_{\mathcal{N}} - A)\varphi_{\mathcal{N}}.$$

Hence

$$\varphi - \varphi_{\mathcal{N}} = (I + A)^{-1}(A_{\mathcal{N}} - A)\varphi_{\mathcal{N}} = (I + A)^{-1}(A_{\mathcal{N}} - A)(I + A_{\mathcal{N}})^{-1}(I + A)\varphi.$$

By assumption, $(I + A)^{-1}$ is bounded in H^t_Q. The assertion now follows by combining the results of Theorems 5.9 and 5.10. ∎

Stability and convergence of the second variant of the Nyström method only needs a few additional considerations. We will treat this case within the next two theorems.

Theorem 5.12 *Suppose that for some* $m \geq 6$, $F^{(1)}$, $F^{(2)}$ *and* $F^{(3)}_{jl}$, $j, l = 1, 2$, *are* m *times continuously differentiable and that* $1 < s \leq (m-3)/2$. *Further, given* $c > 0$, *assume that* $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ *satisfies* $\max\{N_1, N_2\} \leq c \min\{N_1, N_2\}$. *Then, for* $\min\{N_1, N_2\}$ *large enough,* $I + P_{\mathcal{N}} A_{\mathcal{N}} : H^s_Q \to H^s_Q$ *is boundedly invertible and all the inverses are uniformly bounded.*

Proof: We write

$$A - P_{\mathcal{N}} A_{\mathcal{N}} = A - A_{\mathcal{N}} + (I - P_{\mathcal{N}})\, A_{\mathcal{N}}\,.$$

The first difference is bounded as in the proof of Theorem 5.10. As a consequence of Theorems 5.8 and 5.9, the operators $A_{\mathcal{N}} : H^s_Q \to H^s_{Q+1}$ are uniformly bounded. From Theorem 5.1 we see that $I - P_{\mathcal{N}} : H^{s+1}_Q \to H^s_Q$ is bounded with

$$\|I - P_{\mathcal{N}}\| \leq C \left(\min\{N_1, N_2\}\right)^{-1}$$

The assertion now follows as in the proof of Theorem 5.10. ∎

Theorem 5.13 *Suppose that for some $m \geq 6$, $F^{(1)}$, $F^{(2)}$ and $F^{(3)}_{jl}$, $j, l = 1, 2$, are m times continuously differentiable and that $1 < s \leq (m-3)/2$. Further, given $c > 0$, assume that $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ satisfies $\max\{N_1, N_2\} \leq c \min\{N_1, N_2\}$. Given $N_0 \in \mathbb{N}$, assume that $I + P_\mathcal{N} A_\mathcal{N} : H^s_Q \to H^s_Q$ is boundedly invertible for $\min\{N_1, N_2\} \geq N_0$. Then for $\psi \in H^s_Q$, $(I + A)\varphi = \psi$ as well as $(I + P_\mathcal{N} A_\mathcal{N})\hat{\varphi}_\mathcal{N} = P_\mathcal{N}\psi$, we have*

$$|||\varphi - \hat{\varphi}_\mathcal{N}|||_{Q,t} \leq C\ (\min\{N_1, N_2\})^{\max\{t-1,0\}-s}\ |||\varphi|||_{Q,s}\,, \qquad 0 \leq t \leq s.$$

Proof: We start from

$$\hat{\varphi}_\mathcal{N} = P_\mathcal{N}\psi - P_\mathcal{N} A_\mathcal{N} \hat{\varphi}_\mathcal{N} = P_\mathcal{N}\left(\varphi + A\varphi - A_\mathcal{N}\hat{\varphi}_\mathcal{N}\right).$$

Hence

$$\begin{aligned}(I + A)(\varphi - \hat{\varphi}_\mathcal{N}) &= \varphi + A\varphi - A_\mathcal{N}\hat{\varphi}_\mathcal{N} - \hat{\varphi}_\mathcal{N} + (A_\mathcal{N} - A)\hat{\varphi}_\mathcal{N} \\ &= (I - P_\mathcal{N})\left(\varphi + A\varphi - A_\mathcal{N}\hat{\varphi}_\mathcal{N}\right) + (A_\mathcal{N} - A)\hat{\varphi}_\mathcal{N}\,.\end{aligned}$$

The last term can be estimated by Theorem 5.9 to obtain the required convergence rate. The uniform boundedness of $A_\mathcal{N}$ and the stability result from Theorem 5.12 also give

$$|||\varphi + A\varphi - A_\mathcal{N}\hat{\varphi}_\mathcal{N}|||_{Q,s} \leq C\, |||\varphi|||_{Q,s}\,.$$

An application of Lemma 5.1 now yields the desired estimate. ■

The previous results imply that for infinitely smooth functions used in the definition of the integral operators, we achieve a convergence rate only limited by the regularity of the right hand side ψ. In particular, if ψ is also infinitely often continuously differentiable, we achieve super-algebraic convergence rates.

Corollary 5.14 *Suppose that $F^{(1)}$, $F^{(2)}$ and $F^{(3)}_{jl}$, $j, l = 1, 2$, are infinitely often continuously differentiable and that $\psi \in C^\infty(\overline{Q})$ is Q-periodic. Then the solution φ of (5.4) is an element of H^s_Q for any $s \geq 0$.*

Given $c > 0$, assume that $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ satisfies $\max\{N_1, N_2\} \leq c \min\{N_1, N_2\}$. Given any $s > 1$, there exists $N_0 \in \mathbb{N}$, such that $I + A_\mathcal{N}, I + P_\mathcal{N} A_\mathcal{N} : H^s_Q \to H^s_Q$ are boundedly invertible for $\min\{N_1, N_2\} \geq N_0$ and that there exists a constant C dependent on s such that for all $t \in [0, s]$

$$\left.\begin{array}{l} |||\varphi - \varphi_\mathcal{N}|||_{Q,t} \\ |||\varphi - \hat{\varphi}_\mathcal{N}|||_{Q,t} \end{array}\right\} \leq C\ (\min\{N_1, N_2\})^{\max\{t-1,0\}-s}\ |||\varphi|||_{Q,s}\,,$$

where $\varphi_\mathcal{N}$, $\hat{\varphi}_\mathcal{N}$ are the solutions from Theorems 5.11 and 5.13, respectively.

Quadrature Rules and the Linear System. In this section we describe the evaluation of the discretized operators. As we know the action of the simple operators S and V_{jl} on trigonometric polynomials, we can evaluate these operators exactly using finite sums. In fact, these operators represent the application of certain quadrature rules to the integrals representing the continuous operators.

Suppose that $\varphi \in H_Q^s$ for some $s > 1$. Using the representation of $P_{\mathcal{N}}$ by the Lagrange functions (5.3),

$$I_{\mathcal{N}}^{(1)} \varphi(\tilde{x}) = \sum_{\tilde{x}_\mu \in \mathcal{M}_{\mathcal{N}}} F^{(1)}(\tilde{x}, \tilde{x}_\mu)\, \varphi(\tilde{x}_\mu) \int_Q L_{\mathcal{N}}^{(\mu)}(\tilde{y})\, d\tilde{y} = \frac{|Q|}{4N_1 N_2} \sum_{\tilde{x}_\mu \in \mathcal{M}_{\mathcal{N}}} F^{(1)}(\tilde{x}, \tilde{x}_\mu)\, \varphi(\tilde{x}_\mu) \quad (5.6)$$

In fact, this is a tensor product composite trapezoidal (or rectangular, as we are dealing with periodic functions) rule on Q.

From Lemma 5.3 we obtain

$$I_{\mathcal{N}}^{(2)} \varphi(\tilde{x}) = \int_Q \exp(i\alpha \cdot (\tilde{y} - \tilde{x}))\, G_k(\tilde{x}, \tilde{y})\, P_{\mathcal{N}} \left[F^{(2)}(\tilde{x}, \cdot)\, \varphi\right](\tilde{y})\, d\tilde{y}$$
$$= \sum_{\tilde{x}_\mu \in \mathcal{M}_{\mathcal{N}}} F^{(2)}(\tilde{x}, \tilde{x}_\mu)\, \varphi(\tilde{x}_\mu)\, S L_{\mathcal{N}}^{(\mu)}(\tilde{x}) = \sum_{\tilde{x}_\mu \in \mathcal{M}_{\mathcal{N}}} S_{\mathcal{N}}^{(\mu)}(\tilde{x})\, F^{(2)}(\tilde{x}, \tilde{x}_\mu)\, \varphi(\tilde{x}_\mu), \quad (5.7)$$

where the quadrature weights $S_{\mathcal{N}}^{(\mu)}(\tilde{x})$ are given by

$$S_{\mathcal{N}}^{(\mu)}(\tilde{x}) = S L_{\mathcal{N}}^{(\mu)}(\tilde{x}) = \frac{i}{4N_1 N_2} \sum_{\nu \in \mathbb{Z}_{\mathcal{N}}^2} \frac{T^{(\nu)}(\tilde{x} - \tilde{x}_\mu)}{2k\rho^{(\nu)}}. \quad (5.8)$$

Finally, the same argument can by applied for the remaining operators. Here we obtain

$$I_{jl,\mathcal{N}}^{(3)} \varphi(\tilde{x}) = \int_Q \frac{\partial}{\partial y_j} G_k(\tilde{x}, \tilde{y}) \sin\left(\frac{2\pi}{L_l}(x_l - y_l)\right) P_{\mathcal{N}}[F_{jl}^{(3)}(\tilde{x}, \cdot)\psi](\tilde{y})\, d\tilde{y}$$
$$= \sum_{\tilde{x}_\mu \in \mathcal{M}_{\mathcal{N}}} F_{jl}^{(3)}(\tilde{x}, \tilde{x}_\mu)\, \varphi(\tilde{x}_\mu)\, V_{jl} L_{\mathcal{N}}^{(\mu)}(\tilde{x}) = \sum_{\tilde{x}_\mu \in \mathcal{M}_{\mathcal{N}}} V_{jl,\mathcal{N}}^{(\mu)}(\tilde{x})\, F_{jl}^{(3)}(\tilde{x}, \tilde{x}_\mu)\, \varphi(\tilde{x}_\mu), \quad (5.9)$$

for $j, l = 1, 2$, with

$$V_{jl,\mathcal{N}}^{(\mu)}(\tilde{x}) = V_{jl} L_{\mathcal{N}}^{(\mu)}(\tilde{x}) = \frac{1}{16i\, N_1 N_2} \sum_{\nu \in \mathbb{Z}_{\mathcal{N}}^2} \left[\frac{d_j^{(\nu - e_l)}}{\rho^{(\nu - e_l)}} - \frac{d_j^{(\nu + e_l)}}{\rho^{(\nu + e_l)}}\right] \frac{T^{(\nu)}(\tilde{x} - \tilde{x}_\mu)}{2k\rho^{(\nu)}}. \quad (5.10)$$

Having found explicit expressions for the evaluation of all integral operators, we can rewrite the linear system (5.5). Setting, for the moment, $\varphi_\mu = \varphi_\mathcal{N}(\tilde{x}_\mu)$, this reads as

$$\varphi_\mu + \sum_{\nu\in\mathbb{Z}^2_\mathcal{N}} \Bigg[\frac{|Q|}{4N_1N_2} F^{(1)}(\tilde{x}_\mu,\tilde{x}_\nu) + S^{(\nu)}_\mathcal{N}(\tilde{x}_\mu)\, F^{(2)}(\tilde{x}_\mu,\tilde{x}_\nu) + \sum_{j,l=1}^{2} V^{(\nu)}_{jl,\mathcal{N}}(\tilde{x}_\mu)\, F^{(3)}_{jl}(\tilde{x}_\mu,\tilde{x}_\nu)\Bigg]\varphi_\nu = \psi(\tilde{x}_\mu), \qquad \mu\in\mathbb{Z}^2_\mathcal{N}\,. \quad (5.11)$$

The correspondence between solutions of this linear system and the discretized operator equations discussed above is a standard result in the analysis of Nyström methods. We here present the result for both variants of the method together in one theorem.

Theorem 5.15 *Suppose that for some $m\geq 6$, $F^{(1)}$, $F^{(2)}$ and $F^{(3)}_{jl}$, $j,l=1,2$, are m times continuously differentiable and that $1 < s \leq (m-3)/2$. Also suppose $\psi\in H^s_Q$.*

- *If $\varphi_\mathcal{N}\in H^s_Q$ is a solution of $(I+A_\mathcal{N})\,\varphi_\mathcal{N} = \psi$, then $(\varphi_\mu)_{\mu\in\mathbb{Z}^2_\mathcal{N}}$ with $\varphi_\mu = \varphi_\mathcal{N}(\tilde{x}_\mu)$ is a solution of (5.11). Conversely, if the vector $(\varphi_\mu)_{\mu\in\mathbb{Z}^2_\mathcal{N}}$ solves (5.11), then the function $\varphi_\mathcal{N}$ defined by*

$$\varphi_\mathcal{N}(\tilde{x}) = \psi(\tilde{x}) - \sum_{\nu\in\mathbb{Z}^2_\mathcal{N}} \Bigg[\frac{|Q|}{4N_1N_2} F^{(1)}(\tilde{x},\tilde{x}_\nu) + S^{(\nu)}_\mathcal{N}(\tilde{x})\, F^{(2)}(\tilde{x},\tilde{x}_\nu) + \sum_{j,l=1}^{2} V^{(\nu)}_{jl,\mathcal{N}}(\tilde{x})\, F^{(3)}_{jl}(\tilde{x},\tilde{x}_\nu)\Bigg]\varphi_\nu, \qquad \tilde{x}\in Q$$

  is an element of H^s_Q that satisfies $(I+A_\mathcal{N})\,\varphi_\mathcal{N}$.

- *If $\hat{\varphi}_\mathcal{N}\in H^s_Q$ is a solution of $(I+P_\mathcal{N}A_\mathcal{N})\,\hat{\varphi}_\mathcal{N} = P_\mathcal{N}\psi$, then $(\varphi_\mu)_{\mu\in\mathbb{Z}^2_\mathcal{N}}$ with $\varphi_\mu = \hat{\varphi}_\mathcal{N}(\tilde{x}_\mu)$ is a solution of (5.11). Conversely, if the vector $(\varphi_\mu)_{\mu\in\mathbb{Z}^2_\mathcal{N}}$ solves (5.11), then the trigonometric polynomial $\hat{\varphi}_\mathcal{N}$ defined by the conditions $\hat{\varphi}_\mathcal{N}(\tilde{x}_\mu) = \varphi_\mu$, $\mu\in\mathbb{Z}^2_\mathcal{N}$ solves $(I+P_\mathcal{N}A_\mathcal{N})\,\hat{\varphi}_\mathcal{N} = P_\mathcal{N}\psi$ if $\mathcal{N}$ is large enough such that this equation admits a unique solution.*

Proof: If $\varphi_\mathcal{N}$ satisfies $(I+A_\mathcal{N})\,\varphi_\mathcal{N}(\tilde{x}) = \psi(\tilde{x})$ for all $\tilde{x}\in Q$, then obviously (5.11) is satisfied by setting $\tilde{x}=\tilde{x}_\mu$, $\mu\in\mathbb{Z}^2_\mathcal{N}$. The same holds for $\hat{\varphi}_\mathcal{N}$ satisfying $(I+P_\mathcal{N}A_\mathcal{N})\,\hat{\varphi}_\mathcal{N}(\tilde{x}) = P_\mathcal{N}\psi(\tilde{x})$ for all $\tilde{x}\in Q$, as $P_\mathcal{N}$ is the operator of interpolation in $\tilde{x}_\mu\in\mathcal{M}_\mathcal{N}$.

Conversely suppose that the vector $(\varphi_\mu)_{\mu\in\mathbb{Z}^2_\mathcal{N}}$ solves (5.11). Then $\varphi_\mathcal{N}$ as defined in the theorem satisfies $\varphi_\mathcal{N}(\tilde{x}_\mu) = \varphi_\mu$, $\mu \in \mathbb{Z}^2_\mathcal{N}$. Hence $(I + A_\mathcal{N})\,\varphi_\mathcal{N} = \psi$. Also $\varphi_\mathcal{N} \in H^s_Q$ because ψ is and all the other functions occuring in the definition are m-times continuously differentiable.

Finally, let $\mathcal{N}$ be large enough such that $(I + P_\mathcal{N} A_\mathcal{N})\,\hat{\varphi}_\mathcal{N} = P_\mathcal{N}\psi$ admits a unique solution $\hat{\varphi}_\mathcal{N}$. Denote by $\varphi^\#_\mathcal{N}$ the trigonometric polynomial defined by $\varphi^\#_\mathcal{N}(\tilde{x}_\mu) = \varphi_\mu$, $\mu \in \mathbb{Z}^2_\mathcal{N}$. Then

$$\varphi^\#_\mathcal{N}(\tilde{x}_\mu) = \varphi_\mu = \psi(\tilde{x}_\mu) - P_\mathcal{N} A_\mathcal{N} \hat{\varphi}_\mathcal{N}(\tilde{x}_\mu), \qquad \tilde{x}_\mu \in \mathcal{M}_\mathcal{N},$$

and hence the functions evaluated on both sides of this equation are trigonometric interpolation polynomials from $\mathcal{T}_\mathcal{N}$ with identical values in all interpolatory points. We conclude that the functions are the same. ■

5.4 Remarks on Application to Scattering and Transmission Problems

We want to end this chapter with a brief discussion of ideas on how to apply these Nyström methods to the (systems of) integral equations arising from scattering by Q-periodic surfaces. Thes boundary integral equations contain more complicated singularities than the ones the Nyström methods are applicable to.

Making use of Theorems 3.10 and 3.12, the boundary integral operators S_0^+ and K_0^+ can be represented by integral operators defined on Q. In addition to the operators discussed above, these take the form

$$\int_Q \left(\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\right)^r F(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y},$$

$$\int_Q \exp(i\tilde{\alpha}\cdot(\tilde{y}-\tilde{x}))\,G_k(\tilde{x},\tilde{y})\left(\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\right)^r F(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y}$$

or

$$\int_Q \exp(i\tilde{\alpha}\cdot(\tilde{y}-\tilde{x}))\,\frac{\partial G_k(\tilde{x},\tilde{y})}{\partial y_j}\left(\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\right)^r \sin\left(\frac{2\pi}{L_l}(x_l-y_l)\right) F(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y},$$

with $r = 1, 3$ and appropriate functions F.

A possible approach for the application of the Nyström methods to scattering by a Q-periodic surfaces is to replace the terms $|\tilde{x}-\tilde{y}|/|x-y|$ by a smooth approximation. We will briefly discuss one such possible approximation.

Representing the surface Γ_0 as the graph of a function f, we can write

$$\frac{|\tilde{x}-\tilde{y}|}{|x-y|} = \left(1 + \frac{|f(\tilde{x}) - f(\tilde{y})|^2}{|\tilde{x}-\tilde{y}|^2}\right)^{-1/2} .$$

From this representation we see that the limit of this function for $\tilde{y} \to \tilde{x}$ can take any value between 1 and $(1 + |\nabla f(\tilde{x})|^2)^{-1/2}$, dependent on the direction in which $\tilde{y}$ approaches $\tilde{x}$. Given a function $\chi \in C_0^\infty(\mathbb{R}^2)$ with values in $[0,1]$ and $\chi(0) = 1$, and $\delta > 0$, we approximate

$$\frac{|\tilde{x}-\tilde{y}|}{|x-y|} \approx \left(1 - \chi\left(\frac{|\tilde{x}-\tilde{y}|}{\delta}\right)\right) \frac{|\tilde{x}-\tilde{y}|}{|x-y|} + \chi\left(\frac{|\tilde{x}-\tilde{y}|}{\delta}\right) \left(\frac{1}{2} + \frac{1}{2}\left(1 + |\nabla f(\tilde{x})|^2\right)^{-1/2}\right) .$$

The first term on the right hand side is zero in a neighborhood of $\tilde{x}$ and hence will give rise to an operator of the form of $I^{(1)}$ if the approximation is inserted in the above 3 operators. The second term is smooth and hence will give rise to operators of the form $I^{(1)}$, $I^{(2)}$ and $I^{(3)}_{jl}$, respectively.

For $\delta \to 0$, the approximation converges pointwise to $|\tilde{x}-\tilde{y}|/|x-y|$ except at $\tilde{x}$. However, derivatives of the functions $F^{(1)}$, $F^{(2)}$ and $F^{(3)}_{jl}$ will increase as $\delta \to 0$ and this will effect the constants in the error estimates of Theorems 5.11 and 5.13. Thus, an analysis of this approach will need to clarify this dependence and tie the choice of δ to that of $\mathcal{N}$, in order to establish an overall convergence rate.

A similar approach has been discussed by Beale in [9] for the boundary integral equation arising from a potential problem in a bounded smooth domain in $\mathbb{R}^3$. An overall convergence rate of $O(|\mathcal{N}|^{-4})$ is established. However, the approximation of the kernel is different in [9] and several results specific to potential problems are used. Hence it remains an open question how such results may be generalized to scattering problems.

Chapter 6

A Quasi-Collocation Method for Boundary Integral Equations

In this chapter we will present and analyse a numerical method for solving the boundary integral equations arising from scattering by bi-periodic surfaces based on ideas presented by Bruno and Kunyanski [13, 14]. The method presented by these authors was introduced for scattering by general bounded obstacles and consists of several separate components of which we consider only one: the transformation of integrals containing weak singularities in polar coordinates around these singularities. This removes the singularity and the remaining integral can be efficiently calculated by a composite trapezoidal rule.

Although conceptionally simple, the analysis of the method is not straightforward. The transformation to polar coordinates introduces a non-linearity in the operator which makes the direct application of results from linear operator approximation difficult. Through a suitable modification of the original idea, we are able to prove that the discretized operator retains the smoothing properties of the continuous one. This is the key to proving stability and convergence of the method.

As the solution of the discretized equation is sought in the space of trigonometric polynomials and obtained by solving in the interpolation points, the method is quite similar to a collocation method. However, in addition to projection by interpolation, an additional approximation of the operator is used. Thus, we have added the word *quasi* to the method's name.

As in Chapter 5, for simplicity of presentation, we will only consider single integral equation on Q arising from scattering of an incident field by a single sound-soft surface. The corresponding integral equation, as derived in Chapter 4, is

$$\frac{1}{2}\,\psi + K_0^{+}\psi - iS_0^{+}\psi = -M_{-\alpha}u^{i}\,.$$

6.1 Approximating Weakly Singular Integrals

In this section we will consider two types of integral operators associated with single and double layer operators on a Q-periodic surface Γ given as the graph of an m-times continuously differentiable function f. Using a parametrization of a periodic cell of Γ over Q, leads to integral operators of the forms

$$J^{(1)}\varphi(\tilde{x}) = \int_Q \frac{1}{|x-y|}\, F^{(1)}(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y}\,,$$
$$J^{(2)}\varphi(\tilde{x}) = \int_Q \frac{n(y)\cdot(x-y)}{|x-y|^3}\, F^{(2)}(\tilde{x},\tilde{y})\,\varphi(\tilde{y})\,d\tilde{y}\,,$$

where $x = (\tilde{x}, f(\tilde{x}))^\top$, $y = (\tilde{y}, f(\tilde{y}))^\top$ and $F^{(j)}$, $j = 1, 2$, are assumed to be $m-1$ times continuously differentiable on $\mathbb{R}^2 \times \mathbb{R}^2$ and Q-periodic with respect to both arguments. We further assume that there exists some $\rho > 0$ such that

$$F^{(j)}(\tilde{x},\tilde{y}) = 0, \qquad |\tilde{x}-\tilde{y}| \geq \rho\,.$$

Expressions in Polar Coordinates. We will establish mapping properties of $J^{(1)}$, $J^{(2)}$ and also of discrete approximations to these operators by a shift to polar coordinates. We first rewrite the singularity and then perform a change of coordinates $\tilde{y} = \tilde{x} + \tilde{z}$. In case of the operator $J^{(1)}$, this leads to

$$J^{(1)}\varphi(\tilde{x}) = \int_Q \frac{1}{|\tilde{z}|}\left(1 + \frac{(f(\tilde{x}) - f(\tilde{x}+\tilde{z}))^2}{|\tilde{z}|^2}\right)^{-1/2} F^{(1)}(\tilde{x},\tilde{x}+\tilde{z})\,\varphi(\tilde{x}+\tilde{z})\,d\tilde{z}\,.$$

For the operator $J^{(2)}$ the expression for the singularity is more complicated. In the first part of the proof of Theorem 3.12 we have proved the expression

$$\frac{n(y)\cdot(x-y)}{|x-y|^3} = \frac{1}{|\tilde{x}-\tilde{y}|}\left(\frac{|\tilde{x}-\tilde{y}|}{|x-y|}\right)^3 \frac{(\tilde{x}-\tilde{y})\cdot[V(\tilde{x},\tilde{y})(\tilde{x}-\tilde{y})]}{|\tilde{x}-\tilde{y}|^2}\,(1+|\nabla f(\tilde{y})|^2)^{-1/2}\,,$$

where V is defined in the proof of Theorem 3.12. Hence

$$J^{(2)}\varphi(\tilde{x}) = \int_Q \frac{1}{|\tilde{z}|}\left(1 + \frac{(f(\tilde{x}) - f(\tilde{x}+\tilde{z}))^2}{|\tilde{z}|^2}\right)^{-3/2} \frac{\tilde{z}\cdot[V(\tilde{x},\tilde{x}+\tilde{z})\tilde{z}]}{|\tilde{z}|^2}$$
$$\times\,(1+|\nabla f(\tilde{x}+\tilde{z})|^2)^{-1/2}\,F^{(2)}(\tilde{x},\tilde{x}+\tilde{z})\,\varphi(\tilde{x}+\tilde{z})\,d\tilde{z}\,.$$

We can now conveniently express both operators in polar coordinates $(r,\theta) \in R = (-\rho,\rho)\times(-\pi,\pi)$. By using the interval $(-\rho,\rho)$ in the radial variable we obtain twice the integrals over Q. For ease of notation $\hat{\theta} = (\cos\theta, \sin\theta)^\top$. Thus

$$J^{(1)}\varphi(\tilde{x}) = \int_R \left(1 + \frac{(f(\tilde{x}) - f(\tilde{x} + r\hat{\theta}))^2}{r^2}\right)^{-1/2} F^{(1)}(\tilde{x}, \tilde{x} + r\hat{\theta})\, \varphi(\tilde{x} + r\hat{\theta})\, d(r, \theta),$$

$$J^{(2)}\varphi(\tilde{x}) = \int_R \left(1 + \frac{(f(\tilde{x}) - f(\tilde{x} + r\hat{\theta}))^2}{r^2}\right)^{-3/2} \hat{\theta} \cdot [V(\tilde{x}, \tilde{x} + r\hat{\theta})\hat{\theta}]$$
$$\times\, (1 + |\nabla f(\tilde{x} + r\hat{\theta})|^2)^{-1/2}\, F^{(2)}(\tilde{x}, \tilde{x} + r\hat{\theta})\, \varphi(\tilde{x} + r\hat{\theta})\, d(r, \theta)\,.$$

The only remaining potentially singular termes are the first factors in the integrands which we analyze next.

Lemma 6.1 *Suppose $f \in C^m(\mathbb{R}^2)$. Then g, defined by*

$$g(\tilde{x}, (r, \theta)) = \frac{(f(\tilde{x}) - f(\tilde{x} + r\hat{\theta}))^2}{r^2} \qquad \tilde{x} \in Q,\ (r, \theta)^\top \in R,$$

is an element of $C^{m-1}(Q \times R)$.

Proof: $g(\tilde{x}, (r, \theta))$ is simply the square of the differential quotient of f associated with the directional derivative of f in $\tilde{x}$ in the direction $\hat{\theta}$. Applying Lemma 3.11 yields the assertion. ■

In the proof of Theorem 3.12 it was already remarked that $V(\tilde{x}, \tilde{x} + r\hat{\theta})\hat{\theta}$ is of class C^{m-1}. Hence, we obtain that both $J^{(1)}\varphi(\tilde{x})$ and $J^{(2)}\varphi(\tilde{x})$ can be expressed as a concatenation of operators $K \circ \mathbf{T}_{\tilde{x}}$, where $\mathbf{T}_{\tilde{x}}$ denotes a translation by $-\tilde{x}$ and K is an integral operator with an $m-1$-times continuously differentiable kernel.

The idea due to Bruno and Kunyanski [13, 14] is to approximate these operators by interpolating the integrand with trigonometric polynomials in R. We hence introduce

$$T_R^{(\mu)}(r, \theta) = \exp(i(\pi\mu_1 r/\rho + \mu_2\theta)), \qquad (r, \theta)^\top \in R, \quad \mu \in \mathbb{Z}^2,$$

and to improve readability, we set $T_Q^{(\nu)} = T^{(\nu)}$ for the trigonometric monomials with respect to $\tilde{x} \in Q$.

The trigonometric monomials $T_R^{(\mu)}$ span the discrete space on which we will interpolate. However, the dependence of $\mathbf{T}_{\tilde{x}}$ on $\tilde{x}$ makes a direct application of results from Chapter 5 difficult. To carry out the analysis, we will require some results on asymptotic estimates for certain integrals.

Asymptotic Estimates. The results in this section are in prinicipal well known from the theory of asymptotic expansions of integrals (see e.g. [10]). However, we here require estimates including an explicit dependence on certain parameters in the integrals, not just the leading order behaviour. This requires a more detailed analysis than is usually carried out.

Lemma 6.2 *Suppose $q \geq q_0 > 0$, and $g \in C^2(\mathbb{R}^2)$ R-periodic. Then*

$$\left| \int_R \exp(i\, q\, r \cos(\theta))\, g(r,\theta)\, d(r,\theta) \right| \leq C\, \frac{\|g\|_{\infty;2}}{q},$$

where C is a constant only depending on q_0.

Proof: As is well known, the asymptotic behaviour of the integral depends on stationary points of

$$\phi(r,\theta) = r\cos(\theta), \qquad (r,\theta)^\top \in R\,.$$

Such points are located at $(0, \pm\pi/2)^\top$.

As a first step we examine the stationary point $(0, \pi/2)^\top$. As the Hession of ϕ is

$$\phi''(r,\theta) = \begin{pmatrix} 0 & -\sin(\theta) \\ -\sin(\theta) & -r\cos(\theta) \end{pmatrix}, \qquad (r,\theta)^\top \in R\,,$$

$\phi''(0,\pi/2)$ has the two eigenvalues ± 1. It follows that in a neighborhood of this stationary point there exist orthogonal coordinates z such that $\psi(z) = \phi(r(z), \theta(z))$ has a Taylor expansion of the form

$$\psi(z) = \frac{1}{2}\left(z_1^2 - z_2^2\right) + \sum_{|\nu|=3}^{\infty} \frac{1}{\nu!}\, D^\nu \psi(0)\, z^\nu\,.$$

Here and in all remaining arguments in this proof, ν denotes a multi-index.

We further set

$$M_1 = \{\nu : |\nu| \geq 3,\ \nu_1 \geq \nu_2\}, \qquad M_2 = \{\nu : |\nu| \geq 3,\ \nu_1 < \nu_2\}\,.$$

and define

$$\xi_1 = z_1 \sqrt{1 + \sum_{\nu \in M_1} \frac{1}{\nu!}\, D^\nu \psi(0)\, z_1^{-2} z^\nu}\,, \qquad \xi_2 = z_2 \sqrt{1 - \sum_{\nu \in M_2} \frac{1}{\nu!}\, D^\nu \psi(0)\, z_2^{-2} z^\nu}\,.$$

These functions are well-defined in a neighborhood of $z = 0$ as both series under the square roots are power series vanishing in 0. Furthermore

$$\psi(z) = \frac{1}{2}\left(\xi_1(z)^2 - \xi_2(z)^2\right).$$

Finally,

$$\frac{\partial \xi}{\partial z}(0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Hence there is a neighborhood of $z = 0$ in which the map $z \mapsto \xi(z)$ has non-vanishing Jacobian and thus is one-to-one. Noting that $(r, \theta)^\top \mapsto z$ is obtained by a bijective affine transform, we conclude that there exists a neighborhood $U \subseteq R$ of $(0, \pi/2)^\top$ and $\hat{U} \subseteq \mathbb{R}^2$ of 0 such that the map

$$X : \begin{cases} \hat{U} \to U \\ \xi \mapsto (r(z(\xi)), \theta(z(\xi))^\top \end{cases}$$

is one-to-one with Jacobian

$$D(\xi) = \left|\det \frac{\partial X}{\partial \xi}(\xi)\right| \neq 0, \quad \xi \in \hat{U}\,, \qquad \text{and} \qquad D(0) = 1\,.$$

Denote by χ an infinitely often differentiable function with support contained in U and $\chi \equiv 1$ in a neighborhood of $(0, \pi/2)^\top$. Then, under the above transformation,

$$\int_U \chi(r, \theta)\, \exp(i\, q\, r \cos(\theta))\, g(r, \theta)\, d(r, \theta) \\ = \int_{\hat{U}} \chi(X(\xi))\, \exp\left(\frac{i\, q}{2}\, (\xi_1^2 - \xi_2^2)\right)\, g(X(\xi))\, D(\xi)\, d\xi\,.$$

As g is twice continuously differentiable, there exists $h \in C^1(\hat{U})$ such that

$$g(X(\xi))\, D(\xi) = g(0, \pi/2) + \begin{pmatrix} \xi_1 \\ -\xi_2 \end{pmatrix} \cdot h(\xi)\,.$$

Thus

$$\int_U \chi(r, \theta)\, \exp(i\, q\, r \cos(\theta))\, g(r, \theta)\, d(r, \theta) \\ = g(0, \pi/2) \int_{\hat{U}} \chi(X(\xi))\, \exp\left(\frac{i\, q}{2}\, (\xi_1^2 - \xi_2^2)\right)\, d\xi \\ + \int_{\hat{U}} \begin{pmatrix} \xi_1 \\ -\xi_2 \end{pmatrix} \cdot h(\xi)\, \chi(X(\xi))\, \exp\left(\frac{i\, q}{2}\, (\xi_1^2 - \xi_2^2)\right)\, d\xi\,. \quad (6.1)$$

Using Fubini's theorem and the standard asymptotic expansion for one dimensional Fourier-type integrals we obtain the estimate

$$\left|\int_{\hat{U}} \chi(X(\xi))\, \exp\left(\frac{i\, q}{2}\, (\xi_1^2 - \xi_2^2)\right)\, d\xi\right| \leq \frac{C}{q}$$

for $q \geq q_0$. Here, and in the remainder of the proof, C denotes a generic constant which may have a different value in each occurence.

The second integral in (6.1) can be rewritten as

$$\int_{\hat{U}} \begin{pmatrix} \xi_1 \\ -\xi_2 \end{pmatrix} \cdot h(\xi)\, \chi(X(\xi))\, \exp\left(\frac{i\,q}{2}\,(\xi_1^2 - \xi_2^2)\right)\, d\xi$$
$$= \int_{\hat{U}} \nabla \cdot \left[\frac{-i}{q}\, h(\xi)\, \chi(X(\xi))\, \exp\left(\frac{i\,q}{2}\,(\xi_1^2 - \xi_2^2)\right)\right] d\xi$$
$$+ \frac{i}{q} \int_{\hat{U}} (\chi(X(\xi))\, \nabla \cdot h(\xi) + h(\xi) \cdot \nabla\chi(X(\xi)))\, \exp\left(\frac{i\,q}{2}\,(\xi_1^2 - \xi_2^2)\right) d\xi\,.$$

The first integral on the right-hand side is seen to vanish by the divergence theorem as $\chi(X(\xi)) = 0$ for $\xi \in \partial\hat{U}$. We can furthermore estimate

$$\left| \int_{\hat{U}} \chi(X(\xi))\, \nabla \cdot h(\xi)\, \exp\left(\frac{i\,q}{2}\,(\xi_1^2 - \xi_2^2)\right) d\xi \right| \leq C\, \|\nabla \cdot h\|_\infty \leq C\, \|g\|_{\infty;2}\,.$$

The remaining integral will be treated in moment.

This concludes the analysis for the stationary point $(0, \pi/2)^\top$. Estimates for the stationary point $(0, -\pi/2)^\top$ are obtained similarly. What remains to be estimated is an integral of the form

$$\int_R \chi(r,\theta)\, \exp(i\,q\,\phi(r,\theta))\, g(r,\theta)\, d(r,\theta)\,,$$

where χ now denotes an infinitely differentiable function vanishing in the neighborhood of all stationary points of ϕ. Note that this includes the integral left out above, as the cut-off function used for $\hat{U}$ was chosen to be identical to one in a neighborhood of the critical point and thus its gradient vanishes there.

We rewrite

$$\int_R \chi(r,\theta)\, \exp(i\,q\,\phi(r,\theta))\, g(r,\theta)\, d(r,\theta)$$
$$= \int_R \nabla \cdot \left[\frac{-i}{q}\, \chi(r,\theta)\, g(r,\theta)\, \frac{\nabla\phi(r,\theta)}{|\nabla\phi(r,\theta)|^2}\, \exp(i\,q\,\phi(r,\theta))\right] d(r,\theta)$$
$$+ \frac{i}{q} \int_R \nabla \cdot \left[\chi(r,\theta)\, g(r,\theta)\, \frac{\nabla\phi(r,\theta)}{|\nabla\phi(r,\theta)|^2}\right] \exp(i\,q\,\phi(r,\theta))\, d(r,\theta)$$

The first integral can be transformed into a boundary integral using the divergence theorem. Then a constant C is easily found such that both integrals are bounded by $C\, \|g\|_{\infty;1}/q$. This concludes the proof. ■

The purpose of this lemma is to be able to estimate certain integrals occuring in the representations of the operators $J^{(1)}$ and $J^{(2)}$. The following corollary gives this specific result.

Corollary 6.3 *Denote by* $\chi \in C^\infty(\mathbb{R})$ *a function such that* $\operatorname{supp}\chi \subseteq (-\rho,\rho)$ *and* $\chi \equiv 1$ *in a neighborhood of* 0. *Then there is some* $C > 0$ *such that for all* μ, $\nu \in \mathbb{Z}^2$

$$\left| \int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,T_Q^{(\nu)}(r\hat{\theta})\,d(r,\theta) \right| \le C\,\frac{1+|\mu|^2}{(1+|\nu|^2)^{1/2}}\,.$$

Proof: Writing $q^{(\nu)} = |q^{(\nu)}|\,(\cos\theta_0, -\sin\theta_0)^\top$ for some $\theta_0 \in (-\pi,\pi]$, we have

$$T_Q^{(\nu)}(r\hat{\theta}) = \exp(i\,|q^{(\nu)}|\,r\cos(\theta-\theta_0))\,.$$

A simple translation and the 2π-periodicity with respect to θ of all functions in the integrand yields,

$$\int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,T_Q^{(\nu)}(r\hat{\theta})\,d(r,\theta)$$
$$= \exp(i\mu_2\theta_0)\int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,\exp(i\,|q^{(\nu)}|\,r\cos(\theta))\,d(r,\theta)\,.$$

Applying Lemma 6.2 gives the estimate

$$\left| \int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,T_Q^{(\nu)}(r\hat{\theta})\,d(r,\theta) \right| \le C\,\frac{\left\| T_R^{(\mu)}\,\chi \right\|_{\infty;2}}{|q^{(\nu)}|}$$

which obviously implies the assertion. ■

Mapping Properties. Both operators $J^{(1)}$ and $J^{(2)}$ can be written in the form

$$J\varphi(\tilde{x}) = \int_R F(\tilde{x},(r,\theta))\,\chi(r)\,\varphi(x+r\hat{\theta})\,d(r,\theta),$$

where F is $m-1$ times continuously differentiable, Q-periodic with respect to the first and R-periodic with respect to the second argument. By χ we denote a function satisfying the conditions of Corollary 6.3, i.e. infintely often differentiable with $\overline{\operatorname{supp}\chi} \subseteq (-\rho,\rho)$ which is identical to 1 in a neighborhood of 0. This function is needed in the proofs below and forms part of the functions $F^{(j)}$ in the expressions for $J^{(j)}$, $j = 1,2$, above.

Theorem 6.4 *Suppose that for some* $m \ge 7$, F *is* $m-1$ *times continuously differentiable and that* $0 \le s < m-6$. *Then*

$$J : H_Q^s \to H_Q^{s+1}$$

is a well-defined bounded linear operator.

Proof: That J is linear follows from performing the transformation to cartesian coordinates in the integral. It remains to show boundedness.

Set $\sigma = \mathrm{floor}(s)$. Writing F as a Fourier series with respect to $(r,\theta)^\top$,

$$F(\tilde{x},(r,\theta)) = \sum_{\mu\in\mathbb{Z}^2} F^{(\mu)}(\tilde{x})\, T_R^{(\mu)}(r,\theta), \qquad \tilde{x}\in Q, \quad (r,\theta)^\top \in R,$$

we obtain

$$\begin{aligned} |||J\varphi|||_{Q,s+1} &\le \sum_{\mu\in\mathbb{Z}^2} |||F^{(\mu)} \int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,\varphi(\cdot + r\hat{\theta})\,d(r,\theta)|||_{Q,s+1} \\ &\le \sum_{\mu\in\mathbb{Z}^2} \left\|F^{(\mu)}\right\|_{\infty,\sigma+2} ||| \int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,\varphi(\cdot + r\hat{\theta})\,d(r,\theta)|||_{Q,s+1}\,, \end{aligned}$$

assuming for the moment that the series indeed converges. Expanding φ in a Fourier series with respect to $\tilde{x}$ and denoting its Fourier coefficients by (φ_ν) yields

$$\int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,\varphi(\cdot{+}r\hat{\theta})\,d(r,\theta) = \sum_{\nu\in\mathbb{Z}^2}\varphi_\nu \int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,T_Q^{(\nu)}(r\hat{\theta})\,d(r,\theta)\; T_Q^{(\nu)}(\tilde{x}).$$

Hence, applying Corollary 6.3 gives

$$\begin{aligned} &||| \int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,\varphi(\cdot + r\hat{\theta})\,d(r,\theta)|||_{Q,s+1}^2 \\ &\quad = \sum_{\nu\in\mathbb{Z}^2}(1+|\nu|^2)^{s+1} \left| \int_R T_R^{(\mu)}(r,\theta)\,\chi(r)\,T_Q^{(\nu)}(r\hat{\theta})\,d(r,\theta)\right|^2 |\varphi_\nu|^2 \\ &\quad\quad \le C\,(1+|\mu|^2)^2 \sum_{\nu\in\mathbb{Z}^2}(1+|\nu|^2)^s|\varphi_\nu|^2 = C\,(1+|\mu|^2)^2\,|||\varphi|||_{Q,s}^2\,. \end{aligned}$$

Thus,

$$|||J\varphi|||_{Q,s+1} \le C\,|||\varphi|||_{Q,s} \sum_{\mu\in\mathbb{Z}^2}(1+|\mu|^2)\,\left\|F^{(\mu)}\right\|_{\infty,\sigma+2}\,.$$

For $s < m-6$, there is some $\varepsilon > 0$ such that $4+2\varepsilon \le m-s-2 \le m-\sigma-2$. Hence,

$$(1+|\mu|^2)^{2+\varepsilon}\,\left\|F^{(\mu)}\right\|_{\infty,\sigma+2}$$

is bounded by Lemma 5.5, so the series on the right hand side of the last the estimate indeed converges. ■

In the numerical method proposed below, we will use different approximations by trigonometric polynomials both on Q and on R. Hence, we will continue the convention of including the respective rectangle as an index in the associated notations. Thus, $P_{R,\mathcal{N}}$ denotes the trigonometric interpolation operator defined in Section 5.1, but taken with respect to R. The corresponding mesh and Lagrange basis functions will be denoted by $\mathcal{M}_{R,\mathcal{N}}$ and $L^{(\mu)}_{R,\mathcal{N}}$, respectively. Mostly, we will write the polar coordinates $(r,\theta)^\top$ explicitely, but in some instances it will simplify notation to use the transform $\Pi(r,\theta) = r\hat{\theta}$ instead.

An additional approximation method we make use of is the L^2-orthogonal projection $O_{R,\mathcal{N}}$ onto the space of trigonometric polynomials $\mathcal{T}_{\mathcal{N}}$ on R. From Lemma 5.2 we obtain

$$O_{R,\mathcal{N}} v = \sum_{\mu \in \mathbb{Z}^2_{\mathcal{N}}} \frac{4N_1N_2}{|R|} \int_R v(r,\theta)\, L^{(\mu)}_{R,\mathcal{N}}(r,\theta)\, d(r,\theta)\, L^{(\mu)}_{R,\mathcal{N}} . \tag{6.2}$$

The approximation of J includes both an orthogonal projection and an interpolation,

$$J_{\mathcal{N}}\varphi(\tilde{x}) = \int_R P_{R,\mathcal{N}} \left[F(x,\cdot)\, O_{R,\mathcal{N}} \left[\chi\, \varphi(\tilde{x} + \Pi(\cdot))\right]\right](r,\theta)\, d(r,\theta), \qquad \mathcal{N} \in \mathbb{N}^2 .$$

Theorem 6.5 *Suppose that for some $m \geq 9$, F is $m-1$ times continuously differentiable and that $0 \leq s \leq m-8$. Then for all $t \in [0,s]$ and all $\mathcal{N} \in \mathbb{N}^2$,*

$$J_{\mathcal{N}} : H^s_Q \to H^{t+1}_Q$$

is a well-defined bounded linear operator and there is some $\tau > 0$ such that

$$|||(J - J_{\mathcal{N}})\varphi|||_{Q,t+1} \leq C\, \frac{(\max\{N_1,N_2\})^\tau}{(\min\{N_1,N_2\})^{s-t+\tau}}\, |||\varphi|||_{Q,s}$$

for all $\varphi \in H^s_Q$ and $\mathcal{N} \in \mathbb{N}^2$, where C is a constant dependent on t, s and on F.

Proof: We start with an observation regarding the orthogonal projection. Denote by $v(r,\theta) = \chi(r)\, T^{(\nu)}_Q(r\hat{\theta})$, $(r,\theta)^\top \in R$. Then

$$\begin{aligned}
&\int_R P_{R,\mathcal{N}} \left[T^{(\mu)}_R\, O_{R,\mathcal{N}} v\right](r,\theta)\, d(r,\theta) \\
&= \sum_{(r_\iota,\theta_\iota) \in \mathcal{M}_{R,\mathcal{N}}} T^{(\mu)}_R(r_\iota,\theta_\iota)\, O_{R,\mathcal{N}} v(r_\iota,\theta_\iota) \int_R L^{(\iota)}_{R,\mathcal{N}}(r,\theta)\, d(r,\theta) \\
&= \sum_{(r_\iota,\theta_\iota) \in \mathcal{M}_{R,\mathcal{N}}} T^{(\mu)}_R(r_\iota,\theta_\iota)\, \frac{|R|}{4N_1N_2}\, O_{R,\mathcal{N}} v(r_\iota,\theta_\iota) \\
&= \sum_{(r_\iota,\theta_\iota) \in \mathcal{M}_{R,\mathcal{N}}} T^{(\mu)}_R(r_\iota,\theta_\iota) \int_R L^{(\iota)}_{R,\mathcal{N}}(r,\theta)\, v(r,\theta)\, d(r,\theta) \\
&= \int_R v(r,\theta)\, P_{R,\mathcal{N}} T^{(\mu)}_R(r,\theta)\, d(r,\theta) .
\end{aligned}$$

Consequently, by Lemma 6.2 and arguments similar to those used in the proof of Corollary 6.3,

$$\left|\int_R \left(T_R^{(\mu)}(r,\theta)\, v(r,\theta) - P_{R,\mathcal{N}}\left[T_R^{(\mu)}\, O_{R,\mathcal{N}} v\right](r,\theta)\right) d(r,\theta)\right|$$
$$= \left|\int_R v(r,\theta)\, \left(T_R^{(\mu)}(r,\theta) - P_{R,\mathcal{N}} T_R^{(\mu)}(r,\theta)\right) d(r,\theta)\right| \le C\, \frac{\left\|T_R^{(\mu)} - P_{R,\mathcal{N}} T_R^{(\mu)}\right\|_{\infty;2}}{(1+|\nu|^2)^{1/2}} .$$

Let now $\varepsilon \in (0, 1/3)$ and define

$$\tau = 3+\varepsilon, \qquad \omega = m-4-t-2\varepsilon .$$

As a consequence

$$\omega = m-4-t-2\varepsilon = m-7-t+\tau-3\varepsilon > m-8-t+\tau \ge s-t+\tau .$$

By Sobolev's Imbedding Theorem, the space H_R^τ is continuously imbedded in the space of twice continuously differentiable R-periodic functions. Hence, by Lemma 5.1,

$$\left\|T_R^{(\mu)} - P_{R,\mathcal{N}} T_R^{(\mu)}\right\|_{\infty;2} \le C\, |||T_R^{(\mu)} - P_{R,\mathcal{N}} T_R^{(\mu)}|||_{R;\tau}$$
$$\le C\, \frac{(\max\{N_1,N_2\})^\tau}{(\min\{N_1,N_2\})^\omega}\, |||T_R^{(\mu)}|||_{R,\omega} \le C\, \frac{(\max\{N_1,N_2\})^\tau}{(\min\{N_1,N_2\})^{s-t+\tau}}\, (1+|\mu|^2)^{\omega/2} .$$

Setting $\sigma = \text{floor}(t)$, we argue similarly as in the proof of Theorem 6.4 to obtain

$$|||(J-J_{\mathcal{N}})\varphi|||_{Q,t+1}$$
$$\le C\, \frac{(\max\{N_1,N_2\})^\tau}{(\min\{N_1,N_2\})^{s-t+\tau}}\, |||\varphi|||_{Q,s} \sum_{\mu\in\mathbb{Z}^2} \left\|F^{(\mu)}\right\|_{\infty,\sigma+2} (1+|\mu|^2)^{\omega/2} .$$

We have

$$\omega + 2 + 2\varepsilon = m-t-2 \le m-\sigma-2 .$$

Hence, by Lemma 5.5

$$(1+|\mu|^2)^{\omega/2+1+\varepsilon}\, \left\|F^{(\mu)}\right\|_{\infty,\sigma+2} < \infty$$

and thus the series on the right hand side of the last estimate converges. This finishes the proof. ■

6.2 The Quasi-Collocation Method

We now consider an integral equation of the form

$$\left(I + J + I^{(1)}\right)\varphi = \psi, \tag{6.3}$$

where $I^{(1)}$ denotes the integral operator analysed in Chapter 5.3 and the functions F in the definition of J and $F^{(1)}$ in the definition of $I^{(1)}$ are supposed to be in $C^{m-1}(\mathbb{R}^2 \times \mathbb{R}^2)$ for $m \geq 9$ and we assume $\psi \in H_Q^\sigma$ for some $\sigma > 1$. As in Section 5.3, we set

$$A = J + I^{(1)}\,.$$

From Theorems 5.8 and 6.4, we know that $A : H_Q^s \to H_Q^s$ is bounded for $0 \leq s < \min\{m/2 - 2, m - 6\}$.

We wish to approximate the solution of (6.3) by the solution of a discretized equation which is obtained by an approach similar to a collocation method. The difference is that we include an additional approximation in the discretized operator. For $\mathcal{N} \in \mathbb{N}^2$, consider the equation

$$(I + A_\mathcal{N})\,\varphi_\mathcal{N} = P_\mathcal{N}\psi, \tag{6.4}$$

with

$$A_\mathcal{N} = P_\mathcal{N}\left(J_\mathcal{N} + I_\mathcal{N}^{(1)}\right).$$

Note that any solution of (6.4) is necessarily an element of $\mathcal{T}_\mathcal{N}$.

Stability and Convergence. We will assume as in Section 5.3 that given $s > 1$, the operator $I + A : H_Q^t \to H_Q^t$ is boundedly invertible for all $t \in [0, s]$. We proceed by proving stability and convergence of the proposed numerical scheme.

Theorem 6.6 *Suppose that for some $m \geq 9$, F and $F^{(1)}$ are $m-1$ times continuously differentiable and that $1 < s \leq \min\{(m-3)/2, m-8\}$. Furter, given $c > 0$, assume that $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ satisfies $\max\{N_1, N_2\} \leq c \min\{N_1, N_2\}$. Then, for $\min\{N_1, N_2\}$ large enough, $I + A_\mathcal{N} : H_Q^s \to H_Q^s$ is boundedly invertible and all the inverses are uniformly bounded.*

Proof: The proof is a combination of arguments already used in the proofs of Theorems 5.10 and 5.12. We observe

$$A - A_\mathcal{N} = J - J_\mathcal{N} + I^{(1)} - I_\mathcal{N}^{(1)} + (I - P_\mathcal{N})\, I_\mathcal{N}^{(1)}\,.$$

We apply Theorems 5.9 and 6.5 with $t = s-1$ and take into account the uniformity constraint on the grid. This yields the estimate

$$|||(J - J_\mathcal{N} + I^{(1)} - I_\mathcal{N}^{(1)})\varphi|||_{Q,s} \leq C\,(\min\{N_1, N_2\})^{-1}\; |||\varphi|||_{Q,s}, \qquad \varphi \in H_Q^s.$$

As a consequence of Theorems 5.8 and 5.9, $I_{\mathcal{N}}^{(1)} : H_Q^s \to H_Q^{s+1}$ is uniformly bounded for all $\mathcal{N} \in \mathbb{N}^2$. From Theorem 5.1 we have that $I - P_{\mathcal{N}} : H_Q^{s+1} \to H_Q^s$ is bounded with

$$\|I - P_{\mathcal{N}}\| \le C \left(\min\{N_1, N_2\}\right)^{-1}$$

Hence we have norm convergence of $I + A_{\mathcal{N}} \to I - A$ in the space of bounded linear operators in H_Q^s. The assertion now follows from [43, Theorem 10.1]. ■

Theorem 6.7 *Suppose that for some $m \ge 9$, F and $F^{(1)}$ are $m-1$ times continuously differentiable and that $1 < s \le \min\{(m-3)/2, m-8\}$. Furter, given $c > 0$, assume that $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ satisfies $\max\{N_1, N_2\} \le c \min\{N_1, N_2\}$.*

Given $N_0 \in \mathbb{N}$, assume that $I + A_{\mathcal{N}} : H_Q^s \to H_Q^s$ is boundedly invertible for $\min\{N_1, N_2\} \ge N_0$. Then for $\psi \in H_Q^s$, $(I+A)\varphi = \psi$ as well as $(I+A_{\mathcal{N}})\varphi_{\mathcal{N}} = P_{\mathcal{N}}\psi$, we have

$$|||\varphi - \varphi_{\mathcal{N}}|||_{Q,t} \le C \ \left(\min\{N_1, N_2\}\right)^{\max\{t-1,0\}-s} \ |||\varphi|||_{Q,s}\,,$$

for $0 \le t \le s$ and $\min\{N_1, N_2\} \ge N_0$.

Proof: The proof is a repetition of the proof of Theorem 5.13. ■

The important application we have in mind is of course the case where F and $F^{(1)}$ are infinitely often differentiable functions. In this case, we achieve super-algebraic convergence rates.

Corollary 6.8 *Suppose that F and are infinitely often continuously differentiable and that $\psi \in C^\infty(\overline{Q})$ is Q-periodic. Then the solution φ of* (6.3) *is an element of H_Q^s for any $s \ge 0$.*

Furter, given $c > 0$, assume that $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ satisfies $\max\{N_1, N_2\} \le c \min\{N_1, N_2\}$. Given any $s > 1$, there exists $N_0 \in \mathbb{N}$, such that $I + A_{\mathcal{N}} : H_Q^s \to H_Q^s$ is boundedly invertible for $\min\{N_1, N_2\} \ge N_0$ and there exists a constant C dependent on s such that for all $t \in [0, s]$

$$|||\varphi - \varphi_{\mathcal{N}}|||_{Q,t} \le C \ \left(\min\{N_1, N_2\}\right)^{\max\{t-1,0\}-s} \ |||\varphi|||_{Q,s}\,,$$

where $\varphi_{\mathcal{N}}$ is the solution from Theorem 6.7.

Implementation. As in the case of a Nyström method, there is an equivalence between solving the approximate equation (6.4) and solving a certain linear system. In order to keep the notation for vectors and matrices close to the notation used for functions, we will denote by $\mathbb{C}^{\mathcal{N}}$ the vector space of complex vectors of dimension $4N_1N_2$. Vectors in $\mathbb{C}^{\mathcal{N}}$ will be denoted in bold face, i.e. $\boldsymbol{\varphi} \in \mathbb{C}^{\mathcal{N}}$, and we will denote their coefficients by using indeces from $\mathbb{Z}_{\mathcal{N}}^2$, i.e. $\boldsymbol{\varphi} = (\boldsymbol{\varphi}_\mu)_{\mu \in \mathbb{Z}_{\mathcal{N}}^2}$. Likewise, matrices in $\mathbb{C}^{\mathcal{N}\times\mathcal{N}} = \mathbb{C}^{4N_1N_2\times 4N_1N_2}$ will be denoted by capital bold face letters, and their coefficents denoted by pairs of indeces from $\mathbb{Z}^2_{\mathcal{N}}$, i.e. $\mathbf{B} = (b_{\mu,\nu})_{\mu,\nu\in\mathbb{Z}^2_{\mathcal{N}}}$.

We have already seen in equation (5.6) that for $\tilde{x} \in Q$,

$$I^{(1)}_{\mathcal{N}}\varphi(\tilde{x}) = \frac{|Q|}{4N_1N_2}\sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}} F^{(1)}(\tilde{x},\tilde{x}_\nu)\,\varphi(\tilde{x}_\nu)\,.$$

Consequently, we define the matrix $\mathbf{C} = (c_{\mu\nu}) \in \mathbb{C}^{\mathcal{N}\times\mathcal{N}}$ by

$$c_{\mu\nu} = \frac{|Q|}{4N_1N_2}F^{(1)}(\tilde{x}_\mu,\tilde{x}_\nu)\,, \qquad \mu,\nu\in\mathbb{Z}^2_{\mathcal{N}}.$$

Similarly, we have

$$J_{\mathcal{N}}\varphi(\tilde{x}) = \frac{|R|}{4N_1N_2}\sum_{\iota\in\mathbb{Z}^2_{\mathcal{N}}} F(\tilde{x},(r_\iota,\theta_\iota))\,O_{R,\mathcal{N}}\left[\chi\,\varphi(\tilde{x}+\Pi(\cdot))\right](r_\iota,\theta_\iota)\,.$$

Recalling (6.2), we have for $\varphi = \sum\limits_{\nu\in\mathbb{Z}^2_{\mathcal{N}}}\varphi_\nu T^{(\nu)}_Q \in \mathcal{T}_{\mathcal{N}}$,

$$\begin{aligned} O_{R,\mathcal{N}}\left[\chi\,\varphi(\tilde{x}+\Pi(\cdot))\right](r_\iota,\theta_\iota) &= \frac{4N_1N_2}{|R|}\int_R \chi(r)\,\varphi(\tilde{x}+r\hat{\theta})\,L^{(\iota)}_{R,\mathcal{N}}(r,\theta)\,d(r,\theta)\\ &= \frac{4N_1N_2}{|R|}\sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}}\int_R \chi(r)\,T^{(\nu)}_Q(r\hat{\theta})\,L^{(\iota)}_{R,\mathcal{N}}(r,\theta)\,d(r,\theta)\,\varphi_\nu\,T^{(\nu)}_Q(\tilde{x})\,. \end{aligned}$$

Hence

$$J_{\mathcal{N}}\varphi(\tilde{x}) = \sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}}\left[\sum_{\iota\in\mathbb{Z}^2_{\mathcal{N}}}\int_R \chi(r)\,T^{(\nu)}_Q(r\hat{\theta})\,L^{(\iota)}_{R,\mathcal{N}}(r,\theta)\,d(r,\theta)\,F(\tilde{x},(r_\iota,\theta_\iota))\right]T^{(\nu)}_Q(\tilde{x})\,\varphi_\nu\,.$$

Here we define the matrix $\mathbf{B} = (b_{\mu\nu}) \in \mathbb{C}^{\mathcal{N}\times\mathcal{N}}$ by

$$b_{\mu\nu} = \sum_{\iota\in\mathbb{Z}^2_{\mathcal{N}}}\int_R \chi(r)\,T^{(\nu)}_Q(r\hat{\theta})\,L^{(\iota)}_{R,\mathcal{N}}(r,\theta)\,d(r,\theta)\,F(\tilde{x}_\mu,(r_\iota,\theta_\iota))\,T^{(\nu)}_Q(\tilde{x}_\mu) \tag{6.5}$$

for $\mu,\nu\in\mathbb{Z}^2_{\mathcal{N}}$.

We also denote by $\mathbf{D}$ the matrix in $\mathbb{C}^{\mathcal{N}\times\mathcal{N}}$ that maps the function values $(\varphi(\tilde{x}_\mu))_{\mu\in\mathbb{Z}^2_{\mathcal{N}}}$ onto the vector of coefficients of the corresponding trigonometric interpolation polynomial $P_{\mathcal{N}}\varphi$. This is nothing else than the Discrete Fourier Transform. Furthermore, by $\mathbf{I}$ we denote the identity matrix in $\mathbb{C}^{\mathcal{N}\times\mathcal{N}}$.

Now, abbreviating $\boldsymbol{\varphi}_\mu = \varphi_\mathcal{N}(\tilde{x}_\mu)$, posing equation (6.4) in each of the points $\tilde{x}_\mu$, $\mu \in \mathbb{Z}^2_\mathcal{N}$, is equivalent to the linear system

$$(\mathbf{I} + \mathbf{BD} + \mathbf{C})\boldsymbol{\varphi} = \boldsymbol{\psi} \tag{6.6}$$

for some right hand side vector $\boldsymbol{\psi} \in \mathbb{C}^\mathcal{N}$.

Theorem 6.9 *Suppose that for some $m \geq 9$, F and $F^{(1)}$ are $m-1$ times continuously differentiable and that $1 < s \leq \min\{(m-3)/2, m-8\}$. Also suppose $\psi \in H^s_Q$. If $\varphi_\mathcal{N} \in H^s_Q$ is a solution of (6.4) then $\boldsymbol{\varphi} \in \mathbb{C}^\mathcal{N}$ with $\boldsymbol{\varphi}_\mu = \varphi_\mathcal{N}(\tilde{x}_\mu)$ is a solution of (6.6). Conversely, if the vector $\boldsymbol{\varphi} \in \mathbb{C}^\mathcal{N}$ solves (6.6), then the trigonometric polynomial $\varphi_\mathcal{N}$ defined by the conditions $\varphi_\mathcal{N}(\tilde{x}_\mu) = \boldsymbol{\varphi}_\mu$, $\mu \in \mathbb{Z}^2_\mathcal{N}$, solves (6.4) if $\mathcal{N}$ is such that this equation admits a unique solution.*

Proof: The proof is identical to arguments used in the proof of Theorem 5.15. ■

Remark 6.10 Introducing the norm

$$|\boldsymbol{\varphi}|_s = \left(\sum_{\nu \in \mathbb{Z}^2_\mathcal{N}} (1 + |\nu|^2)^s \, |(\mathbf{D}\boldsymbol{\varphi})_\nu|^2 \right)^{1/2} \qquad \boldsymbol{\varphi} \in \mathbb{C}^\mathcal{N} ,$$

Theorem 6.6 yields the uniform boundedness with respect to $\mathcal{N}$ of the inverses $(\mathbf{I}+\mathbf{BD}+\mathbf{C})^{-1}$ from $(\mathbb{C}^{\mathcal{N}\times\mathcal{N}}, |\cdot|_s)$ to $(\mathbb{C}^{\mathcal{N}\times\mathcal{N}}, |\cdot|_s)$. Similarly, Theorem 6.7 carries over to the discrete case with norms $|\cdot|_t$ and $|\cdot|_s$, where $0 \leq t \leq s$. □

We wish to stress that the method described so far is only semidescrete in the sense that the assembly of the matrix $\mathbf{B}$ requires the evaluation of the integrals

$$\int_R \chi(r)\, T^{(\nu)}_Q(r\hat{\theta})\, L^{(\iota)}_{R,\mathcal{N}}(r,\theta)\, d(r,\theta), \qquad \iota, \nu \in \mathbb{Z}^2_\mathcal{N} .$$

We will approximately evaluate this integral by

$$\int_R P_\ell \left[\chi\, T^{(\nu)}_Q(\Pi(\cdot))\, L^{(\iota)}_{R,\mathcal{N}} \right] (r,\theta)\, d(r,\theta), \qquad \iota, \nu \in \mathbb{Z}^2_\mathcal{N} .$$

with an appropriately chosen number $\ell \in \mathbb{N}$ for each matrix coefficent. The approximate matrix assembled in this way will be denoted by $\tilde{\mathbf{B}}$.

Lemma 6.11 *Given $c > 0$, denote $N = \min\{N_1, N_2\}$ for $\mathcal{N} = (N_1, N_2)^\top \in \mathbb{N}^2$ and assume $\max\{N_1, N_2\} \leq c\,N$. Denote by t_0 some real number larger than 1. Suppose that for some C, $\varepsilon > 0$, ℓ is chosen such that*

$$\ell \geq \left(C\, |||\chi\, T^{(\nu)}_Q(\Pi(\cdot))\, L^{(\iota)}_{R,\mathcal{N}}|||_{R,t}\, N^{4+\varepsilon} \right)^{1/t}$$

for some $t \geq t_0$. Then the matrix $\mathbf{I} + \tilde{\mathbf{B}}\mathbf{D} + \mathbf{C}$ is invertible for N large enough.

Proof: From standard results on the invertibility of perturbed matrices we see that it suffices to estimate the matrix norm of $(\mathbf{B}-\tilde{\mathbf{B}})\mathbf{D}$ from $(\mathbb{C}^{\mathcal{N}\times\mathcal{N}}, |\cdot|_s)$ to $(\mathbb{C}^{\mathcal{N}\times\mathcal{N}}, |\cdot|_s)$, proving that it will converge to 0 as $N := \min\{N_1, N_2\} \to \infty$.

We define for ν, $\iota \in \mathbb{Z}^2_{\mathcal{N}}$,

$$f_{\iota\nu} = \int_R \chi(r)\, T_Q^{(\nu)}(r\hat{\theta})\, L_{R,\mathcal{N}}^{(\iota)}(r,\theta)\, d(r,\theta)\,,$$
$$\tilde{f}_{\iota\nu} = \int_R P_\ell \left[\chi\, T_Q^{(\nu)}(\Pi(\cdot))\, L_{R,\mathcal{N}}^{(\iota)}\right](r,\theta)\, d(r,\theta)\,.$$

For $\boldsymbol{\varphi} \in \mathbb{C}^{\mathcal{N}}$,

$$|\mathbf{BD}\boldsymbol{\varphi}|_s^2 = \sum_{\mu\in\mathbb{Z}^2_{\mathcal{N}}} (1+|\mu|^2)^s |(\mathbf{DBD}\boldsymbol{\varphi})_\mu|^2\,.$$

The vector $\mathbf{DBD}\boldsymbol{\varphi}$ is composed of the Fourier coefficients of the trigonmetric interpolation polynomial φ where $\varphi(\tilde{x}_\mu) = (\mathbf{BD}\boldsymbol{\varphi})_\mu$, $\mu \in \mathbb{Z}^2_{\mathcal{N}}$. Using the Lagrange basis,

$$\begin{aligned}\varphi(\tilde{x}) &= \sum_{\mu,\nu,\iota\in\mathbb{Z}^2_{\mathcal{N}}} f_{\iota\nu}\, F(\tilde{x}_\mu, (r_\iota,\theta_\iota))\, T_Q^{(\nu)}(\tilde{x}_\mu)(\mathbf{D}\boldsymbol{\varphi})_\nu\, L_{Q,\mathcal{N}}^{(\mu)}(\tilde{x})\\ &= \frac{1}{4N_1N_2} \sum_{\mu,\nu,\iota,\kappa\in\mathbb{Z}^2_{\mathcal{N}}} f_{\iota\nu}\, F(\tilde{x}_\mu, (r_\iota,\theta_\iota))\, T_Q^{(\nu)}(\tilde{x}_\mu)(\mathbf{D}\boldsymbol{\varphi})_\nu\, T_Q^{(\kappa)}(\tilde{x}-\tilde{x}_\mu)\,,\end{aligned}$$

and hence

$$(\mathbf{DBD}\boldsymbol{\varphi})_\kappa = \frac{1}{4N_1N_2} \sum_{\mu,\nu,\iota\in\mathbb{Z}^2_{\mathcal{N}}} f_{\iota\nu}\, F(\tilde{x}_\mu, (r_\iota,\theta_\iota))\, T_Q^{(\nu-\kappa)}(\tilde{x}_\mu)(\mathbf{D}\boldsymbol{\varphi})_\nu\,, \qquad \kappa \in \mathbb{Z}^2_{\mathcal{N}}\,.$$

We obtain the same expression with $f_{\iota\nu}$ replaced by $\tilde{f}_{\iota\nu}$ for $(\mathbf{D}\tilde{\mathbf{B}}\mathbf{D}\boldsymbol{\varphi})_\kappa$. Thus,

$$\begin{aligned}&|(\mathbf{BD}-\tilde{\mathbf{B}}\mathbf{D})\,\boldsymbol{\varphi}|_s^2\\ &= \frac{1}{(4N_1N_2)^2} \sum_{\kappa\in\mathbb{Z}^2_{\mathcal{N}}} (1+|\kappa|^2)^s \left| \sum_{\mu,\nu,\iota\in\mathbb{Z}^2_{\mathcal{N}}} (f_{\iota\nu}-\tilde{f}_{\iota\nu})\, F(\tilde{x}_\mu, (r_\iota,\theta_\iota))\, T_Q^{(\nu-\kappa)}(\tilde{x}_\mu)(\mathbf{D}\boldsymbol{\varphi})_\nu \right|^2\\ &\le \left(\frac{\|F\|_\infty^2}{(4N_1N_2)^2} \sum_{\kappa,\nu\in\mathbb{Z}^2_{\mathcal{N}}} \frac{(1+|\kappa|^2)^s}{(1+|\nu|^2)^s} \left(\sum_{\mu,\iota\in\mathbb{Z}^2_{\mathcal{N}}} |f_{\iota\nu}-\tilde{f}_{\iota\nu}| \right)^2 \right)\\ &\qquad\qquad \times \left(\sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}} (1+|\nu|^2)^s\, |(\mathbf{D}\boldsymbol{\varphi})_\nu|^2 \right)\end{aligned}$$

$$\leq 4N_1 N_2\, c^s\, \|F\|_\infty^2 \sum_{\nu\in\mathbb{Z}^2_{\mathcal{N}}} \left(\sum_{\iota\in\mathbb{Z}^2_{\mathcal{N}}} |f_{\iota\nu} - \tilde{f}_{\iota\nu}| \right)^2 |\boldsymbol{\varphi}|_s^2$$
$$\leq 16N_1^2 N_2^2\, c^s\, \|F\|_\infty^2 \sum_{\iota,\nu\in\mathbb{Z}^2_{\mathcal{N}}} |f_{\iota\nu} - \tilde{f}_{\iota\nu}|^2\, |\boldsymbol{\varphi}|_s^2 \,.$$

From this analysis we see that ℓ has to be chosen large enough such that, for some C, $\varepsilon > 0$,

$$|f_{\iota\nu} - \tilde{f}_{\iota\nu}| \overset{!}{\leq} C\, N^{-4-\varepsilon} \,. \tag{6.7}$$

Set $g(r,\theta) = \chi(r)\, T_Q^{(\nu)}(r\hat{\theta})\, L^{(\iota)}_{R,\mathcal{N}}(r,\theta)$, $(r,\theta)^\top \in R$ and denote its Fourier coefficients by $(g_\nu)_{\nu\in\mathbb{Z}^2}$. Then $g \in C^\infty(R)$ and R-periodic. So, as in the proof of Lemma 5.1, for any $t_0 > 1$ and every $t \geq t_0 > 1$,

$$\left| \int_R (g(r,\theta) - P_{R,\ell\mathcal{N}}\, g(r,\theta))\, d(r,\theta) \right| = \left| \sum_{\kappa\in\mathbb{Z}^2\setminus\{0\}} g_{2\mathrm{diag}(\kappa)\ell} \right| \leq \frac{c_2}{\ell^t}\, |||g|||_{R,t} \,.$$

Note that it follows from the proof of Lemma 5.1 that c_2 depends on t_0 but not on t. Thus, if ℓ is chosen according to the rule in the lemma, (6.7) is satisfied. ■

Remark 6.12 Unfortunately, it is technically difficult to prove explicit bounds on the norm $|||\chi\, T_Q^{(\nu)}(\Pi(\cdot))\, L^{(\iota)}_{R,\mathcal{N}}|||_{R,t}$ to cast the assumptions of the lemma in a more concrete form. This remains true also for a specific choice of χ. Using Lemma 5.6, for integer t we can immediately conclude

$$|||\chi\, T_Q^{(\nu)}(\Pi(\cdot))\, L^{(\iota)}_{R,\mathcal{N}}|||_{R,t} \leq C\, t^p \left\| \chi\, T_Q^{(\nu)}(\Pi(\cdot)) \right\|_{\infty,t} |\iota|$$

for some C, $p > 0$. In order to estimate the remaining norm, we have numerically computed values for the derivatives of $T_Q^{(\nu)}(\Pi(\cdot))$ and of a typical choice for χ. The results, some of which are displayed in Figure 6.1 suggest that

$$|||\chi\, T_Q^{(\nu)}(\Pi(\cdot))\, L^{(\iota)}_{R,\mathcal{N}}|||_{R,t} \leq \left(C\, |\nu|\, |\iota|\, t^3 \right)^t \,.$$

This, in turn, means that a lower bound

$$\ell \geq C\, |\nu|\, |\iota|\, t^3\, N^{(4+\varepsilon)/t}$$

is sufficient to satisfy the assumptions of Lemma 6.11. The minimum of the right-hand side as a function of t can be computed exactly, giving

$$\ell \geq C\, |\nu|\, |\iota|\, (\log N)^3 \,.$$

□

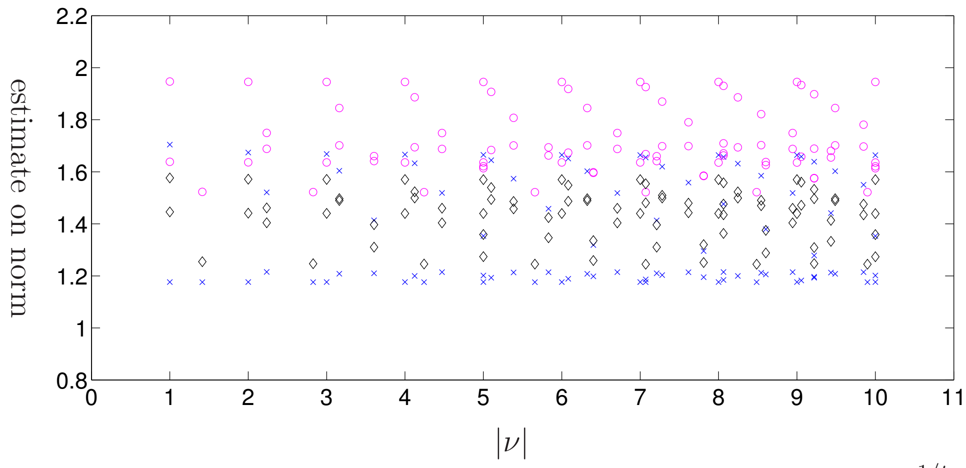


Figure 6.1: Numerical evaluations of $\left(\left\|\chi^{(t)}\right\|_\infty \max_{|\beta=t|}\left\|D^\beta T_Q^{(\nu)}(\Pi(\cdot))\right\|_\infty\right)^{1/t}/(|\nu|\,t^3)$ against $|\nu|$. Each symbol corresponds to a certain choice of ν for $t=2$ ($\times$), $t=4$ ($\circ$) and $t=8$ ($\diamond$)

.

Remark 6.13 It would be particularly attractive to choose $\ell = N$ for all entries of the matrix $\tilde{\mathbf{B}}$. Because of the definition of the $L^{(\iota)}_{R,\mathcal{N}}$ as the Lagrange basis functions for trigonometric interpolation on the grid $\mathcal{M}_{R,\mathcal{N}}$, this means just one evaluation of the integrand is required for the computation of the quadrature formula. Retracting the steps in the derivation of the expression for $\mathbf{B}$, it is easy to see that this strategy amounts to replacing $J_\mathcal{N}$ by the operator $\tilde{J}_\mathcal{N}$ defined by

$$\tilde{J}_\mathcal{N}\varphi(\tilde{x}) = \int_R P_{R,\mathcal{N}}\left[F(\tilde{x},\cdot)\,\chi\,\varphi(\tilde{x}+\Pi(\cdot))\right](r,\theta)\,d(r,\theta), \qquad \varphi \in H^s_Q\,.$$

This, modulo some further technical sophistications, is the approach taken by Bruno and Kunyanski in [13, 14]. The invertibility of the system matrix is an open question in this case. However, provided the inverse exists, the norm of the inverse is bounded by N^p for some integer p and the right hand side of the linear system is given by an infinitely often differentiable function, arguments similar to those in the proof of Lemma 6.11 prove super-algebraic convergence of the method. □

Complexity Analysis. We will in this section set $N = \min\{N_1, N_2\}$ and assume throughout all arguments that there is some $c > 0$ such that $\max\{N_1, N_2\} \le c\,N$. We will start by considering the case where (6.6) is solved using a direct solver. The cost for solving the linear system is then $O(N^6)$ operations.

The cost for assembling the matrices is of a slightly higher complexity. Indeed, assembling $\mathbf{C}$ and $\mathbf{D}$ only takes $O(N^4)$ operations, computing the product $\tilde{\mathbf{B}}\mathbf{D}$ is more costly with $O(N^6)$ operations. The assembly of $\tilde{\mathbf{B}}$ can be estimated using Lemma 6.11 if the heuristic arguments of Remark 6.12 are applied.

Lemma 6.14 *Assume that $\ell \in \mathbb{N}$ is chosen as an integer multiple of N according to the rules*

$$\begin{aligned} C\,|\iota|\,|\nu|\,(\log N)^3 < \ell \le 2C\,|\iota|\,|\nu|\,(\log N)^3\,, &\qquad \text{if } C\,|\iota|\,|\nu|\,(\log N)^3 \ge N\,,\\ \ell = 1, &\qquad \text{otherwise.} \end{aligned}$$

Here C is the constant obtained at the end of Remark 6.12. Then the assembly of $\tilde{\mathbf{B}}$ requires $O((N\log(N))^6)$ operations.

Proof: We start by calculating the number of operations to compute the quantities $\tilde{f}_{\iota\nu}$, ι, $\nu \in \mathbb{Z}^2_{\mathcal{N}}$, in the notation used in the proof of Lemma 6.11. Recall Remark 6.13: In the case $\ell = N$ just one evaluation of the integrand is required for each evaluation of an integral. We calculate the required evaluations of the integrand:

$$\begin{aligned} \sum_{\iota,\nu\in\mathbb{Z}^2_{\mathcal{N}}} \ell^2 &\le \max\{1, 4C^2\log(N)^6\} \sum_{\iota,\nu\in\mathbb{Z}^2_{\mathcal{N}}} (1 + |\iota|^2|\nu|^2)\\ &\le \max\{1, 4C^2\log(N)^6\} \left(16N^4 + \left(2\sum_{M=1}^{N} 8M^2\right)^2\right)\\ &\le \max\{1, 4C^2\log(N)^6\} \left(16N^4 + \frac{64}{9}N^2(N+1)^2(2N+1)^2\right) . \end{aligned}$$

The number of additions and multiplications is proportional to the number of evaluations of the integrand. Hence, computing the $\tilde{f}_{\iota\nu}$, ι, $\nu \in \mathbb{Z}^2_{\mathcal{N}}$, requires $O((N\log(N))^6)$ operations.

The evaluation of the other terms in (6.5) also requires $O(N^4)$ operations. Then, the computation of each $b_{\mu\nu}$, μ, $\nu \in \mathbb{Z}^2_{\mathcal{N}}$ requires $O(N^2)$ multiplications and additions. Hence the assembly of $\tilde{\mathbf{B}}$ requires $O((N\log(N))^6)$ operations. ∎

The storage requirement is $O(N^4)$ storage locations for all matrices that need to be computed. We conclude that the application of our quasi-collocation method to solving a Q-periodic integral equation requires the same memory but has a slightly higher complexity as the direct solution of a linear system of equations.

Of course, the operation count for matrix assembly is prohibitive in the case that an iterative solver is used to solve the linear system. It is an open problem to derive an approximate scheme based on the one presented here that preserves the superalgebraic convergence rate with a reduced computational complexity.

Numerical evidence for the existence of such schemes has been presented. Let us briefly outline the approach taken by the authors of [13,14]. As was pointed out in Remark 6.13, they rely on the stability of the scheme when using the approximation

$$\tilde{J}_{\mathcal{N}}\varphi(\tilde{x}) = \int_R P_{R,\mathcal{N}}\left[F(\tilde{x},\cdot)\,\chi\,\varphi(\tilde{x}+\Pi(\cdot))\right](r,\theta)\,d(r,\theta), \qquad \varphi \in H^s_Q\,,$$

to $J_{\mathcal{N}}$. Provided the values of $\varphi(\tilde{x}_\mu + r_\iota\hat{\theta}_\iota)$ can be computed efficiently from knowledge of φ on the grid $\mathcal{M}_{\mathcal{N}}$, the application of $\tilde{J}_{\mathcal{N}}$ can be computed in $O(N^4)$ operations, making this scheme applicable when using an iterative solver. The authors of [13,14] achieve the evalation of $\varphi(\tilde{x}_\mu + r_\iota\hat{\theta}_\iota)$ by combining one-dimensional Fast Fourier Transforms with a modified grid on R and interpolation. However, the interpolation step introduces a limit on the accuracy on the scheme that thus not results in an asymptotically superalgebraically converging method.

However, let us point out here, that there is no requirement to use the same number of $4N_1N_2$ grid points in R as in Q. We have only stuck to this convention in order not to avoid the further technicalities introduced by different number of quadrature points. Using the scheme of [13, 14] with a reduced number of quadrature points, say $(4N_1N_2)^p$ with $p < 1$ and provided the system matrices are invertible, will result in order $O(N^{4/p})$ complexity count for treating the singularity while preserving the superalgebraic convergence rate for smooth right hand sides. Such a scheme may be combined with a matrix compression scheme approximating the operator $I^{(1)}_{\mathcal{N}}$ thus reducing the overall complexity of the solver dramatically.

6.3 Application to the Scattering Problem

In this section we will give explicit expressions for the functions F in the definition of the integral operator J and of $F^{(1)}$ in the definition of the integral operator $I^{(1)}$ in the case of scattering by a bi-periodic, infinitely smooth sound soft surface Γ. The equivalent integral equation to this problem, derived in Chapter 4, is

$$\hat{\varphi} + 2\,K^+_0\hat{\varphi} - 2i\,S^+_0\hat{\varphi} = -2\,M_{-\alpha}u^i$$

For some unknown density $\hat{\varphi} \in H^{1/2}_Q(\Gamma)$. In order to apply the quasi-collocation method, we have to rewrite the boundary operators as operators on Q. Let Γ be given as the graph of the Q-periodic function f, i.e. $x = (\tilde{x}, f(\tilde{x}))^\top$ for $x \in \Gamma$. We subsitute

$$\varphi(\tilde{x}) = \hat{\varphi}(\tilde{x}, f(\tilde{x})), \qquad \text{such that } \varphi \in H^{1/2}_Q\,,$$

and define the right-hand side

$$\psi(\tilde{x}) = -2M_{-\alpha}u^i(\tilde{x}, f(\tilde{x}))\,.$$

Expressions for the kernels of these integral operators are given in Theorem 4.7. These involve the Green's function and its normal derivative, for which, from Theorem 3.8, we have the expressions

$$\begin{aligned} G_k(x,y) &= \frac{\cos(k|x-y|)}{4\pi\,|x-y|} + H_2(x,y)\,, \\ n(y)\cdot\nabla_y G_k(x,y) &= \frac{n(y)\cdot(x-y)\,\cos(k|x-y|)}{4\pi\,|x-y|} \\ &\quad + k\,\frac{n(y)\cdot(x-y)\,\sin(k|x-y|)}{4\pi\,|x-y|^2} + n(y)\cdot\nabla_y H_2(x,y) \end{aligned}$$

for the Green's function and its normal derivative on Γ with respect to y. To cast the kernel functions in the form required for the formulation of the quasi-collocation method, we define for $\tilde{x}$, $\tilde{z}\in Q$, the auxiliary expressions

$$\begin{aligned} R(\tilde{x},\tilde{z}) &= \big[|\tilde{z}|^2 + (f(\tilde{x}) - f(\tilde{x}+\tilde{z}))^2\big]^{1/2} \\ A(\tilde{x},\tilde{z}) &= \nabla f(\tilde{x}+\tilde{z})\cdot\tilde{z} + f(\tilde{x}) - f(\tilde{x}+\tilde{z})\,, \\ B(\tilde{x},\tilde{z}) &= \sqrt{1+|\nabla f(\tilde{x}+\tilde{z})|^2}\,. \end{aligned}$$

We further set

$$\begin{aligned} K_1(\tilde{x},\tilde{z}) &= \exp(i\tilde{\alpha}\cdot\tilde{z})\,\frac{|\tilde{z}|}{|R(\tilde{x},\tilde{z})|}\bigg[\frac{A(\tilde{x},\tilde{z})\cos(kR(\tilde{x},\tilde{z}))}{R(\tilde{x},\tilde{y})^2} + \frac{k\,A(\tilde{x},\tilde{y})\,\sin(kR(\tilde{x},\tilde{z}))}{R(\tilde{x},\tilde{z})} \\ &\qquad - i\,\cos(kR(\tilde{x},\tilde{z}))\,B(\tilde{x},\tilde{z})\bigg], \\ K_2(\tilde{x},\tilde{z}) &= \exp(i\tilde{\alpha}\cdot\tilde{z})\bigg[\big(-\nabla f(\tilde{x}+\tilde{z}),1\big)^\top\cdot\nabla_y H_2\big((\tilde{x},f(\tilde{x})),(\tilde{x}+\tilde{z},f(\tilde{x})+f(\tilde{z}))\big) \\ &\qquad - i\,H_2\big((\tilde{x},f(\tilde{x})),(\tilde{x}+\tilde{z},f(\tilde{x})+f(\tilde{z}))\big)\,B(\tilde{x},\tilde{z})\bigg]. \end{aligned}$$

With all these abbreviations the integral equation takes the form

$$\varphi(\tilde{x}) + \int_Q \left[\frac{1}{2\pi\,|\tilde{x}-\tilde{y}|}\,K_1(\tilde{x},\tilde{y}-\tilde{x}) + K_2(\tilde{x},\tilde{y}-\tilde{x})\right]\varphi(\tilde{y})\,d\tilde{y} = \psi(\tilde{x}), \qquad \tilde{x}\in Q\,.$$

This equation is of the form (6.3), if we furthermore set

$$\begin{aligned} F(\tilde{x},\tilde{z}) &= \frac{\chi(|\tilde{z}|)}{2\pi}\,K_1(\tilde{x},\tilde{z})\,, \\ F^{(1)}(\tilde{x},\tilde{z}) &= \frac{1-\chi(|\tilde{z}|)^2}{2\pi}\,K_1(\tilde{x},\tilde{z}) + K_2(\tilde{x},\tilde{z})\,. \end{aligned}$$

Note that if Γ is given as the graph of a m times continuously differentiable function, both F and $F^{(1)}$ are $m-1$ times continuously differentiable.

We can thus directly apply the quasi-collocation method to solve the integral equation. In particular, we have proved that the method converges if f is a 9-times continuously differentiable function. For an infinitely smooth surface, we obtain super-algebraic convergence.

Appendix A

Evaluation of the Green's Function

When implementing integral equation methods for Q-periodic geometries, many evaluations of the Green's function are necessary. It is therefore highly desirable to compute this function efficiently to a prescribed precision. All the Green's function representations derived in Chapter 3 may be suitable for an efficient evaluation, depending on the choice of the parameters. For example, when $\mathrm{Im}(k) > 0$, (3.8) provides an exponentially convergent representation which only involves standard functions and is relatively simple to evaluate. If $|x_3 - y_3| \geq c > 0$ for some suitably chosen c, the modal representation (3.5) is appropriate. In other cases, Ewald's representation should be used as the basis for numerical evaluation.

In contrast to the other represenations, Ewald's representation involves the additional complexity of choosing the parameter a appropriately. This parameter influences the rate of convergence of both the series representing $G_k^{(1)}$ and $G_k^{(2)}$, respectively: for large values of a, the convergence of $G_k^{(1)}$ will be slow while that of $G_k^{(2)}$ will be quick, and vice versa. However, as will be clarified below, the choice of a also influences the stability of any numerical evaluation scheme.

Although there is significant work in the literature on how to derive expressions similar to those found by us [37, 45, 60], little attention has been paid to making a mathematically sound choice of a. In [47] some arguments are developed, but the heuristic choice proposed there does not appear plausible. Recently, in [15] a more rigorous analysis for the two-dimensional case was carried out using asymptotic expansions. Although sound recommendations for the choice of a are given, no error estimates are provided that give control over the effect of truncating the series representation. Independently of the present work, such estimates are derived in coorperation with Lechleiter, Schmitt and Sandfort in [5] both for two- and three-dimensional quasi-periodic Green's functions. We want to present some results from [5] in this appendix.

The parameter domain of interest is when the wave number is real or has small positive imaginary part and when $|x_3 - y_3|$ is small. In particular, we will investigate for which values of $|x_3 - y_3|$ it is advantageous to use Ewald's representation rather than the modal representation. Other results will include guidelines on the choice of a backed by rigourous estimates on the truncation errors.

Estimating the effect of the truncation. To keep notation as simple as possible, we will write the Green's function as

$$G_k(x,y) = F^{(1)}(x-y) + F^{(2,+)}(x-y) + F^{(2,-)}(x-y), \qquad x-y \neq p^{(\mu)} \text{ for all } \mu \in \mathbb{Z}^2\,,$$

where

$$F^{(1)}(z) = \frac{a}{4\pi^{3/2}} \sum_{\mu\in\mathbb{Z}^2} e^{i\,\alpha\cdot p^{(\mu)}} \sum_{j=0}^{\infty} \frac{1}{j!}\left(\frac{k}{2a}\right)^{2j} \int_1^\infty s^{-j-1/2} e^{-a^2|z-p^{(\mu)}|^2 s}\, ds\,,$$

$$F^{(2,\pm)}(z) = \frac{i}{4\,L_1\,L_2} \sum_{\nu\in\mathbb{Z}^2} \frac{1}{k\rho_\nu}\, e^{ik\,d^{(\nu)}\cdot z}\, e^{\mp i\,k\rho_\nu\, z_3}\, \operatorname{erfc}\left(\pm a\,z_3 - i\,\frac{k\rho_\nu}{2a}\right).$$

The partial sums used for the evaluation will be written in the form

$$F^{(1)}_M(z) = \frac{a}{4\pi^{3/2}} \sum_{m=0}^{M} \sum_{|\mu-\mu_0|_\infty = m} \frac{e^{i\,\alpha\cdot p^{(\mu)}}}{4\pi}\, F_{\text{aux}}\left(a^2|z-p^{(\mu)}|^2, \left(\frac{k}{2a}\right)^2, \frac{1}{2}\right),$$

$$F^{(2,\pm)}_M(z) = \frac{i}{4\,L_1\,L_2} \sum_{m=0}^{M} \sum_{|\nu-\nu_0|_\infty = m} \frac{1}{k\rho_\nu}\, e^{ik\,d^{(\nu)}\cdot z}\, e^{\mp i\,k\rho_\nu\, z_3}\, \operatorname{erfc}\left(\pm a\,z_3 - i\,\frac{k\rho_\nu}{2a}\right),$$

with appropriate choices for μ_0, ν_0 given below and F_{aux} defined by

$$F_{\text{aux}}(R,\kappa,\nu) = \sum_{j=0}^{\infty} \frac{1}{j!}\,\kappa^j \int_1^\infty s^{-j-\nu} e^{-Rs}\, ds.$$

In all later arguments, we will assume that we can evaluate F_{aux} exactly. However, the following lemma gives us some essential properties of this function and control over its evaluation.

Lemma A.1 (Lemma 4.1 from [5]) *For $R > 0$, $arg(\kappa) \in [0, \pi/2)$ and $\nu > 0$ we have*

$$\left|F^{(1)}_{\text{aux}}(R,\kappa,\nu)\right| \leq \frac{\exp(|\kappa| - R)}{R}\,,$$

and additionally for all $M \in \mathbb{N}$,

$$\left|F^{(1)}_{\text{aux}}(R,\kappa,\nu) - \sum_{j=0}^{M} \frac{1}{j!}\,\kappa^j \int_1^\infty s^{-j-\nu} e^{-Rs}\, ds\right| \leq \frac{e^{|\kappa|-R}}{M+\nu}\left(\frac{|\kappa|}{M+1}\right)^{M+1}.$$

Proof: The first estimate is elementary. The estimate for the remainder can be obtained from the observation that the integral in the expression for $F^{(1)}_{\mathrm{aux}}$ is equal to a generalized exponential integral. From [39, page 26] we obtain

$$\frac{e^{-R}}{R+p} < \int_1^\infty s^{-p} e^{-Rs}\, ds \le \frac{e^{-R}}{R+p-1}, \qquad R, p > 0\,.$$

Hence

$$\left| \sum_{j=M+1}^{\infty} \frac{1}{j!} \kappa^j \int_1^\infty s^{-j-\nu} e^{-Rs}\, ds \right| \\ \le \frac{e^{-R}}{R+M+\nu} \sum_{j=M+1}^{\infty} \frac{1}{j!} |\kappa|^j \le \frac{e^{|\kappa|-R}}{M+\nu} \left(\frac{|\kappa|}{M+1} \right)^{M+1}\,.$$

■

A second consideration addresses the complementary error function. The terms involving this function may be expressed with the help of the Faddeeva function w (see [2, Formula 7.1.3]) as

$$e^{\mp i\, k\rho^{(\nu)}\, z_3} \operatorname{erfc}\left(\pm a z_3 - i\, \frac{k\rho^{(\nu)}}{2a} \right) = e^{-a^2 z_3^2 + \left(\frac{k\rho^{(\nu)}}{2a} \right)^2} w\left(\pm i a z_3 + \frac{k\rho^{(\nu)}}{2a} \right). \tag{A.1}$$

However, in the case $\pm a z_3 + \mathrm{Im}(k\rho^{(\nu)}/(2a)) < 0$ a numeric evaluation of the right hand side of (A.1) may not be stable. In this case, we use the elementary formula

$$w(\overline{z}) = \overline{w(-z)} = 2\, e^{-\overline{z}^2} - \overline{w(z)},$$

to obtain

$$e^{-i\, k\rho^{(\nu)}\, z_3} \operatorname{erfc}\left(a z_3 - i\, \frac{k\rho^{(\nu)}}{2a} \right) = 2\, e^{-i\, k\rho^{(\nu)}\, z_3} - e^{-a^2 z_3^2 + \left(\frac{k\rho^{(\nu)}}{2a} \right)^2} \overline{w\left(-i a z_3 + \frac{\overline{k\rho^{(\nu)}}}{2a} \right)}. \tag{A.2}$$

Is is proved in [5, Lemma 3.2] that $|w(z)| \le 1$ for $\mathrm{Im}(z) > 0$ so that either (A.1) or (A.2) can always be used for a stable evaluation of these terms.

A further requirement to estimate the effect of the truncation of the series are estimates from below for the quadratic terms $|z - p^{(\mu)}|^2$ appearing in $F^{(1)}$ and $|k\rho^{(\nu)}|^2$ appearing in $F^{(2,\pm)}$, respectively. For all these estimates we will use the abbreviation

$$L_{\min} = \min\{L_1, L_2\}, \qquad L_{\max} = \max\{L_1, L_2\}\,.$$

Define $\mu_0 \in \mathbb{Z}^2$ by $z - p^{(\mu_0)} \in (-L_1/2, L_1/2] \times (-L_2/2, L_2/2]$. Let $M \in \mathbb{N}$ and $|\mu - \mu_0|_\infty = m \geq M + 1$. Denote by j_0 the index of a component for which $|\mu_{j_0} - \mu_{0,j_0}|_\infty = m$. Then,

$$\begin{aligned}|z - p^{(\mu)}|^2 &\geq (z_{j_0} - \mu_{j_0} L_{j_0})^2 = (z_{j_0} - \mu_{0,j_0} L_{j_0} + (\mu_0 - \mu)_{j_0} L_{j_0})^2 \\ &\geq [(M+1)L_{j_0} - |z_{j_0} - \mu_{0,j_0} L_{j_0}| + (m - (M+1))L_{j_0}]^2 \\ &\geq M^2 L_{\min}^2 + 2M L_{\min}^2 (m - (M+1)) \geq M^2 L_{\min}^2 . \end{aligned} \quad \text{(A.3)}$$

We also have

$$\begin{aligned}|z - p^{(\mu)}|^2 &\geq (z_{j_0} - \mu_{j_0} L_{j_0})^2 \\ &= (\mu_{j_0} - \mu_{0,j_0})^2 \left(L_{j_0} - \frac{z_{j_0} - \mu_{0,j_0} L_{j_0}}{\mu_{j_0} - \mu_{0,j_0}} \right)^2 \geq m^2 \frac{L_{\min}^2}{4} \geq M\, m \frac{L_{\min}^2}{4} . \end{aligned} \quad \text{(A.4)}$$

We furthermore choose $\nu_0 \in \mathbb{Z}^2$ such that $|d^{(\nu_0)}|_\infty \leq |d^{(\nu)}|_\infty$ for all $\nu \in \mathbb{Z}^2$ and set

$$M_0 = \max \left\{ \left| \frac{L_1 \alpha_1}{2\pi} + \nu_{0,1} \right|, \left| \frac{L_2 \alpha_2}{2\pi} + \nu_{0,2} \right| \right\} ,$$

as well as

$$M_1 = M_0 + \begin{cases} \dfrac{L}{2\pi} \sqrt{\mathrm{Re}(k^2)}, & \mathrm{Re}(k^2) \geq 0 \\ 0, & \text{otherwise.} \end{cases}$$

Let $M \geq M_0$ and $|\nu - \nu_0|_\infty = m \geq M + 1$, denoting by j_0 the index of a coordinate in which this maximum is attained. It is then possible to estimate

$$\begin{aligned}|kd^{(\nu)}|^2 &\geq \left(\alpha_{j_0} + \frac{2\pi}{L_{j_0}} \nu_{j_0} \right)^2 = \left(kd^{(\nu_0)}_{j_0} + \frac{2\pi}{L_{j_0}} (\nu_{j_0} - \nu_{0,j_0}) \right)^2 \\ &\geq \left(\frac{2\pi}{L_{j_0}} (m - M_0) - |kd^{(\nu_0)}_{j_0}| + \frac{2\pi}{L_{j_0}} M_0 \right)^2 \geq \frac{4\pi^2}{L_{\max}^2} (m - M_0)^2 \\ &\geq \frac{4\pi^2}{L_{\max}^2} \left[(M - M_0)^2 + 2(M - M_0)(m - M) \right] . \end{aligned} \quad \text{(A.5)}$$

For any $\nu \in \mathbb{Z}^2$ such that $|kd^{(\nu)}|^2 \geq \mathrm{Re}(k^2)$ we have

$$|k\rho^{(\nu)}|^2 = |(k\rho^{(\nu)})^2| \geq |\,\mathrm{Re}((k\rho^{(\nu)})^2)| = |\,\mathrm{Re}(k^2) - |kd^{(\nu)}|^2| = |kd^{(\nu)}|^2 - \mathrm{Re}(k^2) .$$

Thus, for $|\nu - \nu_0|_\infty = |\nu_{j_0} - \nu_{0,j_0}| = m > M \geq M_1$ and if also $|kd^{(\nu)}|^2 \geq \mathrm{Re}(k^2)$, we obtain similarly as above

$$\begin{aligned}|k\rho^{(\nu)}|^2 &\geq \left(\frac{2\pi}{L_{j_0}} (m - M_1) - |kd^{(\nu_0)}_{j_0}| + \frac{2\pi}{L_{j_0}} M_1 \right)^2 - \mathrm{Re}(k^2) \\ &\geq \frac{4\pi^2}{L_{\max}^2} (m - M_1)^2 \geq \frac{4\pi^2}{L_{\max}^2} (m - M)^2 . \end{aligned} \quad \text{(A.6)}$$

Note furthermore that $|kd^{(\nu)}|^2 \geq \mathrm{Re}(k^2)$ if and only if $\mathrm{Re}(k\rho^{(\nu)}) \leq \mathrm{Im}(k\rho^{(\nu)})$.

With these preparations, we are ready to prove the next two theorems.

Theorem A.2 (Theorem 5.1 from [5]) *Define $\mu_0 \in \mathbb{Z}^2$ by the condition $z - p^{(\mu_0)} \in (-L_1/2, L_1/2] \times (-L_2/2, L_2/2]$ and let $M \in \mathbb{N}$. Then*

$$\left|F^{(1)}(z) - F_M^{(1)}(z)\right| \leq \frac{8\, e^{|k|^2/(4a^2) - a^2 z_3^2}}{\pi^{3/2}\, a\, M L_{\min}^2\, (1 - e^{-2a^2 M L_{\min}^2})}\, e^{-(aML_{\min})^2}\,.$$

Proof: From Lemma A.1 we have

$$\left|F^{(1)}(z) - F_M^{(1)}(z)\right| \leq \frac{a\, e^{|k^2|/(4a^2) - a^2 z_3^2}}{4\,\pi^{3/2}} \sum_{m=M+1}^{\infty} \sum_{|\mu|_\infty = m} \frac{e^{-a^2\,|\tilde{z} - p^{(\mu)}|^2}}{a^2\,|z - p^{(\mu)}|^2}\,.$$

Note further that for $m \in \mathbb{N}$ there are 8 different $\mu \in \mathbb{Z}^2$ such that $|\mu|_\infty = m$. Hence using (A.3) and (A.4) we obtain

$$\left|F^{(1)}(z) - F_M^{(1)}(z)\right| \leq \frac{8a\, e^{\frac{|k^2|}{4a^2} - a^2 z_3^2 - a^2 M^2 L_{\min}^2}}{\pi^{3/2}\, a^2 M\, L_{\min}^2} \sum_{m=M+1}^{\infty} e^{-2ML_{\min}^2 a^2\,(m-(M+1))}\,.$$

The assertion now follows using the geometric series. ■

Theorem A.3 (Theorem 5.2 from [5]) *Let ν_0, M_0 and M_1 be defined as above and let $M \geq M_1$ such that also $\mathrm{Im}(k\rho^{(\nu)}) \geq \mathrm{Re}(k\rho^{(\nu)})$ for all $\nu \in \mathbb{Z}^2$ with $|\nu - \nu_0|_\infty > M$. Then*

$$\begin{aligned}\left|F^{(2,\pm)}(z) - F_M^{(2,\pm)}(z)\right| \leq\; & \frac{e^{\left|\frac{k}{2a}\right|^2 - a^2 z_3^2 - \frac{2\pi^2\,(M-M_0)}{a^2 L_{\max}^2}}}{\pi L_{\min}\left(1 - e^{-\frac{2\pi^2\,(M-M_0)}{a^2 L_{\max}^2}}\right)}\, e^{-\frac{\pi^2}{a^2 L_{\max}^2}\,(M-M_0)^2} \\ & + \frac{e^{-\frac{\sqrt{2}\pi\,|z_3|}{L_{\max}}}}{\pi L_{\min}\left(1 - e^{-\frac{\sqrt{2}\pi\,|z_3|}{L_{\max}}}\right)}\, e^{-\frac{\sqrt{2}\pi}{L_{\max}}\,|z_3|\,(M-M_1)}\,.\end{aligned}$$

If additionally $\pm a z_3 + \mathrm{Im}(k\rho^{(\nu)}/(2a)) \geq 0$ for all $\nu \in \mathbb{Z}^2$ with $|\nu - \nu_0|_\infty > M$, then

$$\left|F^{(2,\pm)}(z) - F_M^{(2,\pm)}(z)\right| \leq \frac{(1+M)\, e^{\left|\frac{k}{2a}\right|^2 - a^2 z_3^2 - \frac{2\pi^2\,(M-M_0)}{a^2 L_{\max}^2}}}{\pi L_{\min}\left(1 - e^{-\frac{2\pi^2\,(M-M_0)}{a^2 L_{\max}^2}}\right)}\, e^{-\frac{\pi^2}{a^2 L_{\max}^2}\,(M-M_0)^2}\,.$$

Proof: In the case $\pm a z_3 + \mathrm{Im}(k\rho^{(\nu)}/(2a)) \geq 0$ for $|\nu - \nu_0|_\infty = m > M$, we use (A.1) to estimate

$$
\begin{aligned}
&\left| F^{(2,\pm)}(z) - F^{(2,\pm)}_M(z) \right| \\
&= \frac{1}{4\,L_1\,L_2} \left| \sum_{m=M+1}^{\infty} \sum_{|\nu-\nu_0|_\infty = m} \frac{1}{k\rho^{(\nu)}}\, e^{ik\,d^{(\nu)}\cdot z}\, e^{\mp i\,k\rho^{(\nu)}\,z_3}\, \mathrm{erfc}\left(\pm a\, z_3 - i\,\frac{k\rho^{(\nu)}}{2a} \right) \right| \\
&\leq \frac{e^{\left|\frac{k}{2a}\right|^2 - a^2 z_3^2}}{4\,L_1\,L_2} \sum_{m=M+1}^{\infty} \sum_{|\nu-\nu_0|=m} \frac{1}{|k\rho^{(\nu)}|} \exp\left(-\frac{|kd^{(\nu)}|^2}{4a^2} \right).
\end{aligned}
$$

Hence, using (A.5) and (A.6),

$$
\begin{aligned}
&\left| F^{(2,\pm)}(z) - F^{(2,\pm)}_M(z) \right| \\
&\leq \frac{L_{\max}\, e^{\left|\frac{k}{2a}\right|^2 - a^2 z_3^2 - \frac{\pi^2\,(M-M_0)^2}{a^2 L_{\max}^2}}}{\pi\, L_1\, L_2} \sum_{m=M+1}^{\infty} \frac{m}{m-M}\, e^{-\frac{\pi^2}{a^2 L_{\max}^2}[2(M-M_0)\,(m-M)]} \\
&\leq \frac{(1+M)\, e^{\left|\frac{k}{2a}\right|^2 - a^2 z_3^2 - \frac{\pi^2\,(M-M_0)^2}{a^2 L_{\max}^2}}}{\pi\, L_{\min}} \, \frac{e^{-\frac{2\pi^2\,(M-M_0)}{a^2 L_{\max}^2}}}{1 - e^{-\frac{2\pi^2\,(M-M_0)}{a^2 L_{\max}^2}}}.
\end{aligned}
$$

To treat the general case, (A.2) must be used to estimate certain terms in the series. Additionally, we obtain that for $|\nu - \nu_0|_\infty = m > M$, there holds

$$
\mathrm{Im}(k\rho^{(\nu)}) \geq \frac{\sqrt{2}\pi}{L_{\max}}(m - M_1).
$$

The additional terms introduced by the use of (A.2) can then be estimated from above by an additional series, which we bound from above by

$$
\begin{aligned}
\sum_{m=M+1}^{\infty} \sum_{|\nu-\nu_0|_\infty = m} \frac{e^{-\,\mathrm{Im}(k\rho^{(\nu)})\,|z_3|}}{4\,L_1\,L_2\,|k\rho^{(\nu)}|} &\leq \frac{L_{\max}}{\pi\,L_1\,L_2} \sum_{m=M+1}^{\infty} e^{-\frac{\sqrt{2}\pi}{L}\,(m-M_1)\,|z_3|} \\
&\leq \frac{1}{\pi\,L_{\min}}\, e^{-\frac{\sqrt{2}\pi}{L}\,(M-M_1)\,|z_3|}\, \frac{e^{-\frac{\sqrt{2}\pi\,|z_3|}{L}}}{1 - e^{-\frac{\sqrt{2}\pi\,|z_3|}{L}}}.
\end{aligned}
$$

■

Choosing a. An optimal choice for the parameter a should minimize the cost for the evaluation of the function up to a required accuracy. This goal amounts to an a priori balancing in the number of terms evaluated in the truncated series.

To be able to judge the costs for the evaluation of the series fairly, as a prerequesite to choosing a, the time for an accurate evaluation of each term in the series should be bounded. For the case of $F^{(1)}$, this means bounding the time for an efficient evaluation of F_{aux}. To this end, we fix a value of M and prescribe that given an $\varepsilon > 0$, a should be chosen such that

$$\left(\frac{|k|^2}{4a^2\,(M+1)}\right)^{M+1} \leq \varepsilon\,,$$

which amounts to the lower bound for a,

$$a \geq \frac{|k|}{\sqrt{M+1}\,\varepsilon^{\frac{2}{M+1}}}\,. \tag{A.7}$$

For any a satisfying this lower bound, we obtain from Lemma A.1 that

$$\left| F^{(1)}_{\text{aux}}\left(R, \frac{k^2}{4a^2}, \nu\right) - \sum_{j=0}^{M} \frac{1}{j!}\left(\frac{k^2}{4a^2}\right)^j \int_1^\infty s^{-j-\nu} e^{-Rs}\, ds \right| \leq \frac{e^{(M+1)\,\varepsilon^{1/(M+1)}}\,\varepsilon}{M+\nu}\,. \tag{A.8}$$

A second issue in choosing a is that care has to be taken to avoid instability and cancellation effects. The bounds on the terms in the series all contain a factor $\exp\left(|k|^2/(4a^2) - a^2\,z_3^2\right)$. The control paramter a has to be chosen so that this expression is of the same order as the expected value of the Green's function in order to avoid cancellation effects.

Crude estimates of the order of magnitude of the value of the Green's function can be obtained from (3.8). Choosing μ_0 as in Theorem A.2, one can define

$$G_{\text{est}}(z) = \frac{1}{4\pi} \sum_{|\mu-\mu_0|_\infty \leq p} e^{i\alpha\cdot p^{(\mu)}}\, \frac{e^{ik|z-p^{(\mu)}|}}{|z-p^{(\mu)}|}\,,$$

for some small value of p, i.e. the value of the truncated series of point sources. The condition

$$\exp\left(\frac{|k|^2}{4a^2} - a^2\,z_3^2\right) \leq 10^q\,|G_{\text{est}}(z)| \tag{A.9}$$

can be used for obtaining a lower bound for sensible values of a. Here q is the acceptable number of decimal digits that may be lost in the calculation. If all numbers and standard functions are evaluated to 14 significant digits and G_k is to be computed to 12 significant digits, then $q = 2$.

Assuming $|z_3| > 0$, we obtain

$$a^2 \geq \sqrt{\frac{|k|^2}{4\,z_3^2} + \left(\frac{\log|10^q\,G_{\text{est}}(z)|}{2\,z_3^2}\right)^2} - \frac{\log|10^q\,G_{\text{est}}(z)|}{2\,z_3^2}\,. \tag{A.10}$$

Note however, that (A.9) cannot be satisfied for any value of a if $z_3 = 0$ and $|G_{\text{est}}(z)| < 10^{-q}$. For small values of $|z_3|$ the lower bound (A.10) may also require a value of a far from a value considered optimal for the reasons outlined below. These situations reflect cases in which we can only guarantee an absolute but not a relative error on the value computed for the Green's function, as individual terms in both of the series in Ewald's expression will be larger than its value.

We now return to the question of an optimal choice for a, bearing in mind the necessity to satisfy the lower bounds (A.7) and (A.10). Given the complexity of the error estimates, the exact optimal a for a given parameter set is hard to obtain. However, the dominating factor influenciable by choosing a in Theorem A.2 is $\exp\left(-a^2 L_{\min}^2 M^{(1)^2}\right)$, where $M^{(1)}$ denotes the cut-off index of the series. Similarly, the dominating factor in the second estimate in Theorem A.3 is $\exp\left(-\frac{-\pi^2}{a^2 L_{\max}^2}(M^{(2)} - M_0)^2\right)$. Note that the slower decaying term in the first estimate in Theorem A.3 is independent of a. The costs for evaluating the series grows quadratically in $M^{(l)}$, $l = 1, 2$. Equating the dominating terms to ε, we minimze

$$M^{(1)^2} + M^{(2)^2} = \frac{\log(1/\varepsilon)}{a^2 L_{\min}^2} + \left(\frac{a L_{\max}\sqrt{\log(1/\varepsilon)}}{\pi} + M_0\right)^2 .$$

This leads to

$$a^4 + \frac{M_0 \pi}{L_{\max}\sqrt{\log(1/\varepsilon)}}\, a^3 - \frac{\pi^2}{L_{\min}^2 L_{\max}^2} = 0 . \tag{A.11}$$

The left-hand side is a strictly monotonic function for positive a with a single root which can be easily computed by a few iterations of Newton's method. Possible starting values for the iteration are

$$a_0 = \sqrt{\frac{\pi}{L_{\min} L_{\max}}} \qquad \text{or} \qquad a_0 = \sqrt[3]{\frac{\pi\sqrt{\log(1/\varepsilon)}}{M_0 L_{\min}^2 L_{\max}}}$$

which are both larger than the root and guarantee convergence. We recommend to choose a as the maximum the root of (A.11) and the lower bounds in (A.7) and (A.10).

Numerical examples. We want to present some numerical examples demonstrating that the choice of a recommended in the previous subsection indeed leads to a reliable computation of the Green's function with computation times that are not significantly higher than the optimum.

As a first example, we consider the computation of G_k for the same point $z = x - y$ for different values of a such that the estimates for the series remainders of all three series as given in Theorems A.2 and A.3 are less than 10^{-12}. This test was carried out for various values of z_3 and the periods L_1, L_2. As a first step, the recommended value of a was obtained using the above estimates and $q = 1.8$. Then the value of the Green's function for the recommended value of a was computed 1000 times and the average computation time was determined. This computation was then repeated for various values of a in the interval $[0.1, 1]$.

Some typical results are presented in Figure A.1. In the left column, the differences between the values computed for a and the recommended value are displayed. For reference, the dashed line indicates the prescribed tolerance of 10^{-12} used for the evaluation. The recommended value of a is indicated by the dotted line. In the right column, the computation times are displayed, the time for the recommended value of a is indicated as a red circle. Such computation times of course depend on the hardware being used, so the relative behaviour of these times is of importance here rather than the absolute value.

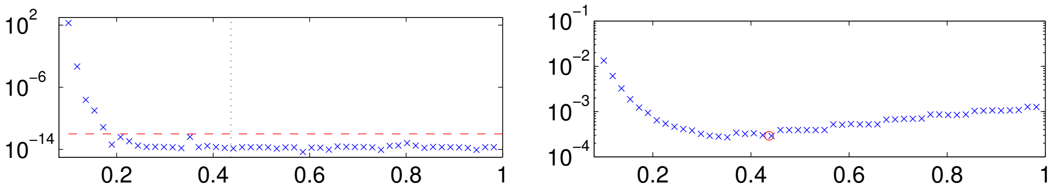
These examples indicate first of all, that the error bounds given by Theorems A.2 and A.3 are relatively sharp. Especially for larger periods, the Green's function is not computed to a significantly higher precision than indicated by the estimates. Secondly, the effect of choosing a too small is clearly visible: Cancellation errors in this case prevent the Green's function from being computed to the precision predicted by the error estimates.

Finally, we indeed recommend a value of a that leads to near minimal computing time. For the examples using the smaller period this is clearer than for the larger period. However, for the larger period, the effect of cancellation is more pronounced leading to a slightly higher choice of a than would be necessary in some cases. Note, that in the example (f), the recommended value of a is exactly at the point where cancellation errors start to be visible.

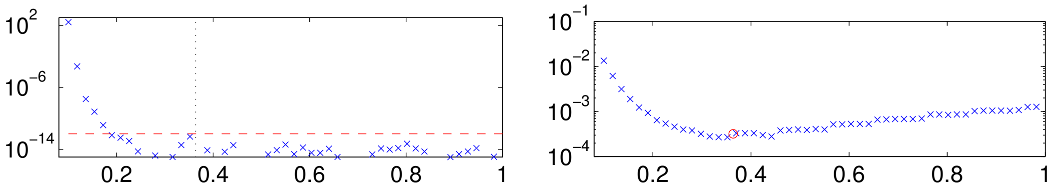
We wish to remark that choosing the recommended value of a was not included in the computation time. However, separate tests have shown that the time used for making this choice is insignificant compared to the computation time for the Green's function evaluation itself.

A second issue is the question of which representation of the Green's function should be used for carrying out evaluations in what parameter regime. Limiting ourselves to the case of real k, the modal representation (3.5) presents itself as an alternative, if $|z_3|$ is larger than 0. This representation uses only exponential functions rather than the special functions present in Ewald's representation which are more costly to evaluate.

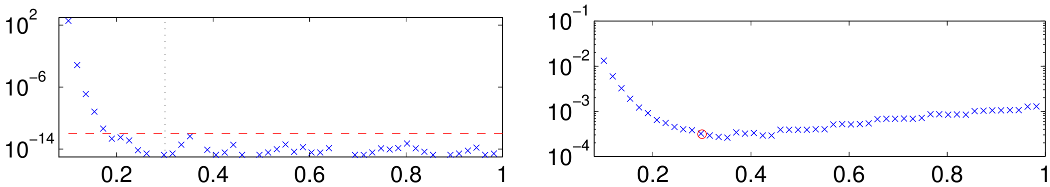
Tests have been carried out for various values of k, L_1, L_2 and z_3 comparing computation times. For each combination of parameters, 1000 (for small values of z_3) or 5000 (for large values of z_3) random pairs of (z_1, z_2) were generated and the Green's function evaluated both using Ewald's representation with the recommended value of a and using (3.5). In the case of Ewald's representation,



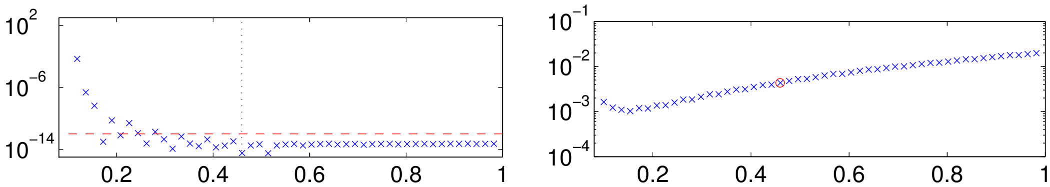
(a) $z_3 = 0.5,\ L_1 = L_2 = 2\pi$



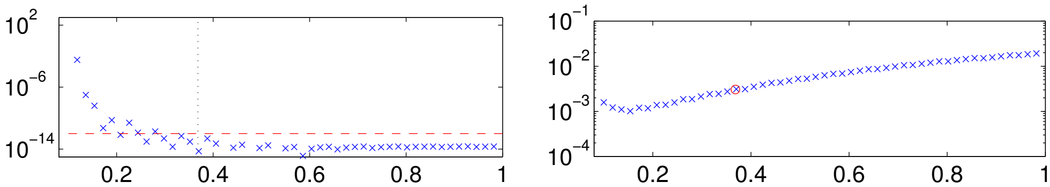
(b) $z_3 = 0.125,\ L_1 = L_2 = 2\pi$



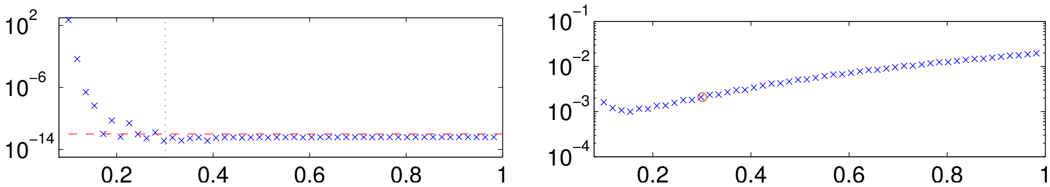
(c) $z_3 = 0,\ L_1 = L_2 = 2\pi$



(d) $z_3 = 0.5,\ L_1 = L_2 = 8\pi$



(e) $z_3 = 0.125,\ L_1 = L_2 = 8\pi$



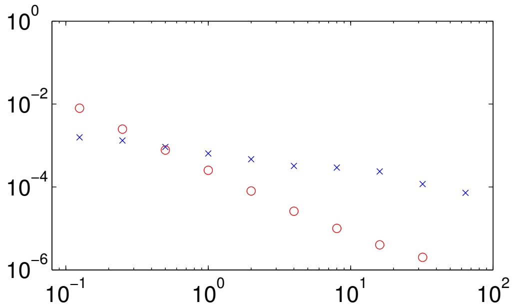
(f) $z_3 = 0,\ L_1 = L_2 = 8\pi$

Figure A.1: Plots of difference to value computed for recommended a against a (left) and computation time per Green's function evaluation against a in seconds (right). All examples use $k = \sqrt{2},\ z_1 = 0,\ z_2 = 0.02,\ \alpha_1 = \alpha_2 = \sqrt{3}/4$.

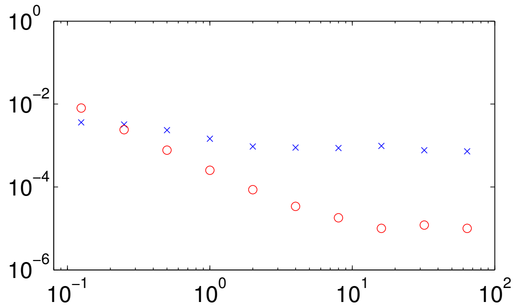
the series were evaluated up to a guaranteed error of 10^{-12} using the bounds in Theorems A.2 and A.3. For the modal representation, the first partial sum having a value within a 10^{-11}-neighborhood of the value computed using Ewald's method was evaluated. This methodology contains a bias towards the modal representation, in that the modal representation is computed to a slightly less accurate level, that no error estimators need to be computed and that there are no influences due to a possibly pessimistic error estimator.

The results are displayed in Figure A.2. Firstly, it appears that the computation times using Ewald's representation remain fairly constant when z_3 is varied. In contrast, for small z_3, the computation time using the modal expansion increases by a factor ranging between 3.0 and 3.5 if z_3 is divided by a factor of 2. This increase is observable in all examples, uniformly for all parameter choices. For large z_3, the computation time using the modal expansion also becomes constant. This behaviour corresponds to the fact that for large z_3 only the plane wave terms form an observable contribution to the Green's function value.

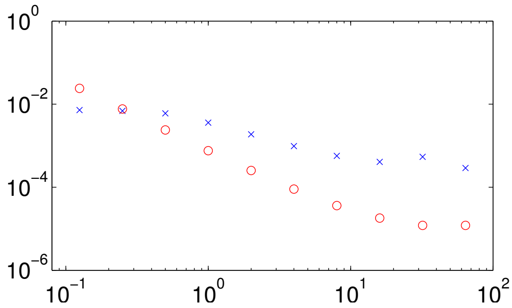
The point where Ewald's method becomes more efficient appears to lie roughly at one tenth of a wave length. As a preliminary recommendation, taking into account the bias towards the modal representation in these examples, it appears reasonable to use the modal expansion for $|z_3| > \lambda/2$ where $\lambda = 2\pi/k$ denotes the wave length. However, more numerical experiments should be carried out to support this recommendation.



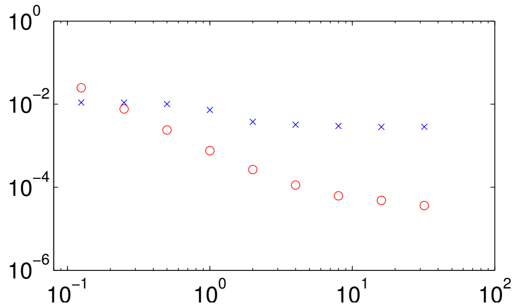
(a) $k = \sqrt{2}$, $L_1 = L_2 = 2\pi$



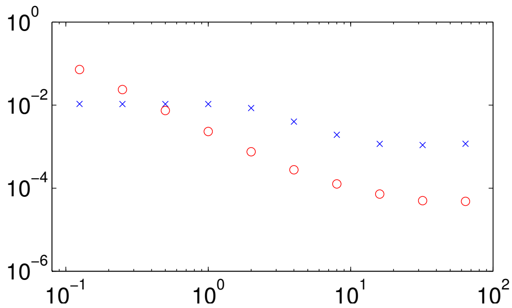
(d) $k = 2\sqrt{2}$, $L_1 = L_2 = 2\pi$



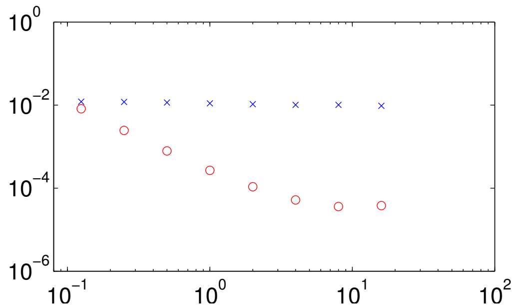
(b) $k = \sqrt{2}$, $L_1 = L_2 = 4\pi$



(e) $k = 2\sqrt{2}$, $L_1 = L_2 = 4\pi$



(c) $k = \sqrt{2}$, $L_1 = L_2 = 8\pi$



(f) $k = 4\sqrt{2}$, $L_1 = L_2 = 2\pi$

Figure A.2: Plots of computation time against z_3 for Ewald's method using the recommended value of a (blue crosses) and for the modal expansion (red circles). Between 1000 and 5000 random values for z_1 and z_2 are used and computation times are averaged. Values using Ewald's expansion are computed up to guaranteed error of 10^{-12}, values using the modal expansion up to a difference of 10^{-11} to the value for Ewald's method. All examples use $\alpha_1 = \alpha_2 = \sqrt{3}/4$.

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