BOUNDARY INTEGRAL EQUATIONS
METHODS FOR ELECTROMAGNETIC
SCATTERING BY PERIODIC ARRAYS

THOMAS STRAUSZER-CAUSSADE

Thesis submitted to the Office of Research and Graduate Studies
in partial fulfillment of the requirements for the degree of
Master of Science in Engineering

Advisors:
MANUEL SÁNCHEZ
CARLOS PÉREZ-ARANCIBIA

Santiago de Chile, January 2023

© MMXXII, THOMAS STRAUSZER-CAUSSADE
BOUNDARY INTEGRAL EQUATIONS
METHODS FOR ELECTROMAGNETIC
SCATTERING BY PERIODIC ARRAYS

THOMAS STRAUSZER-CAUSSADE

Members of the Committee:
MANUEL SÁNCHEZ
CARLOS PÉREZ-ARANCIBIA
EDUARDO CERPA
LUIZ FARIA
CÉSAR SAEZ

Thesis submitted to the Office of Research and Graduate Studies
in partial fulfillment of the requirements for the degree of
Master of Science in Engineering

Santiago de Chile, January 2023

© MMXXII, THOMAS STRAUSZER-CAUSSADE
I would like to dedicate this work to my family, friends and professors who pushed me to never let down and persevere toward my goals.
ACKNOWLEDGEMENTS

To my advisor, Carlos Pérez-Arancibia, for his support and guidance during both my undergraduate and graduate studies. I will be forever grateful to him for introducing me to research and applied mathematics and encouraging me to tackle challenging problems. I am looking forward to pursuing a Ph.D. in a related area, and hope to collaborate with him in the future, on some another wild and laborious question requiring a disruptive solution. To Luiz Faria, for his supervision during the “The Bridge” exchange program, especially for the fruitful discussions about mathematics or future possibilities. To all the members at UMA in ENSTA-Paris, who made my internship an amusing research environment. To Eduardo Cerpa, for his unequivocal support over the last year of this master, and to the neurostimulation group at Millenium Nucleus ACIP, for motivating and proposing to me different and interesting research topics in mathematical biology. To Manuel Sánchez, for his enlightening teaching in many courses, and also for introducing me to many key topics in applied mathematics and numerical analysis.

To my friends, who have been there when I needed help in these tough years of study, and unexpected changes.

Finally, to my mother, Nicole, for her unconditional love and total support during all these years, and to my grandparents, Pedro and Estela, for their backing. Thank you for believing in me, so I could carry on this far.

This work has been financially supported by the Fondo Nacional de Desarrollo Científico y tecnológico (FONDECYT), Chile Grant Number 11181032; and by the research exchange program “The Bridge”, funded by the Institut National de Recherche en Informatique et Automatique (INRIA), and the School of Engineering at Pontificia Universidad Católica de Chile (PUC).
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>iv</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>vii</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>xi</td>
</tr>
<tr>
<td>RESUMEN</td>
<td>xii</td>
</tr>
<tr>
<td>PUBLICATIONS FROM THIS WORK</td>
<td>xiii</td>
</tr>
</tbody>
</table>

## 1. INTRODUCTION

1.1. Motivation

1.2. Background

1.2.1. Time-harmonic waves

1.2.2. Electromagnetic waves

1.3. Boundary integral equation methods

1.3.1. Free-space Green function

1.3.2. Nyström methods

1.4. Contributions

1.5. Outline of this thesis

## 2. WAVE SCATTERING BY PERIODIC LINE ARRAYS OF 2D OBSTACLES

2.1. Previous work

2.2. Preliminaries

2.3. Green’s representation formulae

2.4. Parametrized integral operators

2.5. Boundary integral equation formulation

2.6. Windowed Green function method

2.7. An illustrative numerical example

2.8. Corrected windowed integral equation
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.8.1.</td>
<td>Windowed Green function approximation of the scattered field</td>
<td>48</td>
</tr>
<tr>
<td>2.8.2.</td>
<td>Corrected windowed integral equation at Rayleigh-Wood anomalies</td>
<td>52</td>
</tr>
<tr>
<td>2.8.3.</td>
<td>Fredholm property</td>
<td>54</td>
</tr>
<tr>
<td>2.9.</td>
<td>Numerical examples</td>
<td>55</td>
</tr>
<tr>
<td>2.9.1.</td>
<td>Validation examples</td>
<td>55</td>
</tr>
<tr>
<td>2.9.2.</td>
<td>Photonic crystal slab</td>
<td>59</td>
</tr>
<tr>
<td>3.</td>
<td>EXTENSION TO PERIODIC ARRAYS OF 3D OBSTACLES</td>
<td>62</td>
</tr>
<tr>
<td>3.1.</td>
<td>Periodic line arrays of 3D obstacles</td>
<td>62</td>
</tr>
<tr>
<td>3.1.1.</td>
<td>Boundary integral formulation</td>
<td>62</td>
</tr>
<tr>
<td>3.1.2.</td>
<td>Numerical results</td>
<td>64</td>
</tr>
<tr>
<td>3.2.</td>
<td>Bi-periodic surface arrays of 3D obstacles</td>
<td>66</td>
</tr>
<tr>
<td>3.2.1.</td>
<td>Scattered field representation</td>
<td>66</td>
</tr>
<tr>
<td>3.2.2.</td>
<td>Boundary integral equation formulation</td>
<td>70</td>
</tr>
<tr>
<td>3.2.3.</td>
<td>Modified boundary integral equations</td>
<td>72</td>
</tr>
<tr>
<td>3.2.4.</td>
<td>Validation examples</td>
<td>78</td>
</tr>
<tr>
<td>4.</td>
<td>CONCLUSIONS AND FUTURE WORK</td>
<td>83</td>
</tr>
<tr>
<td>REFERENCES</td>
<td></td>
<td>85</td>
</tr>
<tr>
<td>APPENDIX</td>
<td></td>
<td>93</td>
</tr>
<tr>
<td>A.</td>
<td>SUPER ALGEBRAIC DECAY OF WINDOWED OSCILLATORY INTEGRALS</td>
<td>94</td>
</tr>
</tbody>
</table>
LIST OF FIGURES

1.1 (left) Scanning electron microscope image of an interface. The pattern consists of eight regions, each occupied by one constituent antenna with a fixed shape. (right) Zoom-in view of the center part of the left figure. (Yu et al., 2011) ........................................ 2

2.1 Depiction of the quasi-periodic domain and the curves used in the derivation of the boundary integral equation formulation. ................................................................. 19

2.2 Depiction of the curves involved in the derivation of Green’s representation formula. ........................................... 23

2.3 Depiction of the relevant curve parametrizations and associated scattered-field and total-field traces (2.28) utilized in our BIE formulation. ................................. 29

2.4 Solution of the problem scattering of a planewave at $\theta^{inc} = \frac{\pi}{4}$ by an infinite periodic array of kite-shaped obstacles obtained using the naive windowed BIE (2.53) and the scattered field approximation (2.59) for $k_2 = 20$, $L = 2$, $c = 0.5$ and various window sizes $A$ and wavenumbers $k_1$ at and around a RW-anomaly configuration corresponding to $k_1 = k^* \approx 10.7261$. Energy balance error (2.57) as a function of $A$ in (a) semi-log and (b) log-log scale computed at $h = 1$. (c) Wavenumber sweep of the energy balance error around $k^*$. (d) Real part of the computed total field within the region $[-\frac{L}{2}, \frac{L}{2}] \times [-cA, cA]$ for $k_1 = 10.68$ and $A = 20\lambda$. ................................. 40

2.5 Errors (2.60) in the quasi-periodicity condition of the numerical solution produced by the windowed integral equation (2.53). (a) Depiction of the supercell configuration used to assess the left ($l$) and right ($r$) mismatch errors (2.60). The density functions associated with the $3L$-periodic supercell are obtained from the densities of the middle $L$-periodic cell by multiplying them by $\zeta = e^{i\alpha L}$ and $\zeta^{-1} = e^{-i\alpha L}$ to transfer them from left to right and from right to left, respectively. Errors in semi-log (b) and log-log (c) scale for the exterior wavenumbers $k_1 = 10.68$, $k^*$, and 10.76, and window sizes $A \in [10\lambda, 60\lambda]$. ................................. 42
2.6 Errors (2.61) in the numerical solution obtained from the windowed integral equation (2.53) in the enforcement of the radiation condition (2.11). Three different exterior wavenumbers are considered corresponding to \( k_1 = 10.68 \) in (a), \( k_1 = k^* \) in (b), and \( k_1 = 10.76 \) in (c). The modes \( n \in C_{3k_1/4} \) used in these examples correspond to the smallest \( \beta_n \) values arising in each case, which include \( \beta_1 \) that vanishes in the RW-tanomaly case \( k_1 = k^* \) in (b).

2.7 Energy balance errors (2.57) in the numerical solution of the test problem of Section 2.7 obtained using the corrected windowed integral equation (2.79) for \( c = 0.5 \) (top row) and \( c = 0.1 \) (bottom row) and various window sizes \( A > 0 \). Three different exterior wavenumbers are considered corresponding to (a)-(d) \( k_1 = 10.68 \), (c)-(f) \( k_1 = 10.76 \), and (b)-(e) \( k_1 = k^* \approx 10.7261 \), that corresponds to a RW-anomaly frequency. The fixed parameter value \( \delta = 3k_1/4 \), which yields a four-element set \( C_\delta \) of correcting terms, is used in all these examples.

2.8 Energy balance error (2.57) sweeps for \( k_1 \in [k^* - 0.1, k^{**} + 0.1] \), where \( k^* \) and \( k^{**} \) are two consecutive RW frequencies, in the solution of the test problem of Section 2.7 produced by the corrected windowed BIE (2.79) using the parameter values \( \delta \in \{k_1/2, 3k_1/4, k_1\} \) and (a) \( A = 10\lambda \), (b) \( A = 30\lambda \), and (c) \( A = 50\lambda \).

2.9 Reflectance and transmittance spectra of a finite-thickness photonic crystal slab in TE and TM polarizations at normal planewave incidence. (a) Depiction of the lattice geometry and the curves involved the numerical solution of the problem by the proposed windowed Green function method. Computed reflectance \( (R) \) and transmittance \( (T) \) for various frequencies \( \lambda^{-1} = k_1/(2\pi) \) in TE (a) and TM (b) polarization. The first stop band, from 17783 cm\(^{-1}\) to 23152 cm\(^{-1}\), is marked in grey, which is the same in both polarizations. The location of RW-anomaly frequencies is marked by the vertical dashed lines.

2.10 Solution of the problem of scattering of planewave at normal incidence by the finite-thickness photonic crystal of Figure 2.9(a). Top row: real part of the \( z \)-component total electric field at the lowest RW-anomaly frequency (left) and at
the lowest stop-band frequency (right). Bottom row: real part of the z-component of the total magnetic field at the lowest RW-anomaly frequency (left) and at the lowest stop-band frequency (right).

3.1 Depiction of the quasi-periodic boundary and the curves to integrate and evaluate the boundary integral equations of line arrays in 3D. In the bottom-left a small depiction of the cylindrical coordinates reference.

3.2 Results using $k_1 = 9$, $k_2 = 15$ and $L = 1$ (a) Energy balance criterion (error$_{enf}$) enforcement in semi-log scale using (3.3) and a patch-based representation of the obstacle. (b) Real part of the total field with window parameters $(c, A) = (0.8, 5.5\lambda)$.

3.3 Depiction of the single unit-cell quasi-periodic domain and the curves used in the derivation of the boundary integral equation formulation in three dimensions. Here the vertical cell boundaries surfaces extend infinitely in the $\pm z$ directions.

3.4 Top view depiction of the extended nine-cell unitary domain used for the modified operator’s definition and the modified scattered field representation. Note the center cell in green corresponds to the single-cell unit domain accounted for in the previous section 3.2.2. The z-axis is pointing outside the page.

3.5 Errors of the quasi-periodicity condition of the numerical solution produced by the windowed integral equation. (a) Depiction of the sample points to assess the mismatch errors. The sample point $r_2^\pm$ and its respective translations are highlighted in orange, together with the associated quasiperiodic constants in (3.8). Errors in semi-log (b) and log-log (c) scale for window sizes $A \in [3\lambda, 12\lambda]$ for different DIM interpolation orders $p \in \{2, 3, 4\}$ (blue, red, green respectively).

3.6 Self-convergence pointwise errors in semi-log (a) and log-log (b) scale of the scattered field evaluated at $r_0 = (0, 0, h)$ with $h = L/2$ for window sizes $A \in [3\lambda, 12\lambda]$ for different integration orders $p \in \{2, 3, 4\}$ (blue, red, green respectively). (c) Horizontal planes above and below the obstacle are used to compute Rayleigh’s coefficients.
3.7 Real part of the total field over 121 cells in TE polarization mode using window parameters \((c, A) = (0.3, 5\lambda)\) with different setups. In both scenarios we use \(k_1 = 8.8, k_2 = 14\), but the incidence angle \(\theta^{\text{inc}}\) and spatial periods \(L\) differ. (a) \(\theta^{\text{inc}} = (\pi/6, \pi/4), L = (0.5, 0.5)\). (b) \(\theta^{\text{inc}} = (\pi/6, \pi/6), L = (0.5, 1.0)\).

4.1 Scattered field with \(k_1 = 10.72, k_2 = 20, \theta = \pi/4, L = 2\) and window parameters \((c, A) = (0.5, 20\lambda)\). (a) Real-part of the total solution using the corrected operator \(\tilde{\mathbf{M}}\) (2.83). (b) Pointwise difference between corrected and non-corrected scattered fields (logscale).
ABSTRACT

This thesis introduces a novel boundary integral equation (BIE) method for the numerical solution of problems of planewave scattering by periodic line arrays of two- and three-dimensional and biperiodic surface arrays of three-dimensional penetrable obstacles.

The approach is built upon a direct BIE formulation that leverages the simplicity of the free-space Green function but in turn entails evaluation of integrals over the unit-cell boundaries. Such integrals are here treated via the window Green function method. The windowing approximation together with a finite-rank operator correction—used to properly impose the Rayleigh radiation condition—yield a robust secondkind BIE that produces super-algebraically convergent solutions throughout the spectrum, including at the challenging Rayleigh-Wood anomalies.

The corrected windowed BIE can be discretized by means of off-the-shelf Nyström and boundary element methods, and it leads to linear systems suitable for iterative linear-algebra solvers as well as standard fast matrix-vector product algorithms.

A variety of numerical examples demonstrate the accuracy and robustness of the proposed methodology.

**Keywords:** Periodic scattering problem, Wood anomaly, boundary-integral equations, diffraction gratings, quasi-periodic Green function.
RESUMEN

Esta tesis introduce un nuevo método de ecuaciones integrales de frontera (BIE) para la solución numérica de problemas de dispersión de ondas planas por conjuntos de ordenamientos periódicos de obstáculos penetrables bi- y tri-dimensionales y biperiódicos tri-dimensionales penetrables. El enfoque se basa en una formulación BIE directa que aprovecha la simplicidad de la función de Green en el espacio libre, pero que a su vez implica evaluación de integrales sobre los límites de la celda unitaria. Estas integrales se tratan aquí mediante el método de la función ventana de Green. La aproximación por ventanas, junto con una corrección basada en un operador de rango finito es utilizado para imponer correctamente la condición de radiación de Rayleigh, obteniendo una BIE robusta de segunda clase que produce soluciones super-algebraicamente convergentes en todo el espectro, incluso en las desafiantes anomalías de Rayleigh-Wood. El BIE corregido con ventanas puede discretizarse mediante los métodos habituales de Nyström y y métodos de elementos de frontera, y conduce a sistemas lineales adecuados para los solucionadores iterativos de álgebra lineal, así como para los algoritmos rápidos de productos matriciales y vectoriales. Una serie de ejemplos numéricos demuestran la precisión y robustez de la metodología propuesta.

Palabras Claves: Problemas periódicos de difracción, anomalía de Wood, ecuaciones integrales de frontera, difracción de enrejados, función de Green cuasi-periódica.
PUBLICATIONS FROM THIS WORK

Journal papers


Conferences

1. INTRODUCTION

“The first principle is that you must not fool yourself and you are the easiest person to fool.”
- Richard Feynman

1.1. Motivation

The law of refraction, also known as Snell-Descartes’ law, describes the relationship between the incident and refracted angles of light across a material interface. The latter corresponds to the boundary at two different media where each one is characterized by a refractive index. In engineering optics, often the goal is to design the interface’s shape and choose the material properties so as to guide the propagation of light along a prescribed optical path. Until recently, this has been partially achieved by means of simple mathematical models that exploit Snell-Descartes’ law. Classical optics, for instance, rely on conventional lenses whose particular shape enables focusing or defocusing light rays but they can hardly achieve complex light control, such as perfect wave reflection, wave-guiding, and light confinement, among many other capabilities that lay at the core of modern optic technology. Indeed, traditional devices typically fall short when it comes to advanced applications for pulsating lasers (Claire Gmachl et al., 2001), holograms (Genevet & Capasso, 2015), optical transistors (Achouri et al., 2015), etc.

A novel theoretical framework that extends the above-mentioned paradigm is the so-called generalized Snell’s law (GSL) (Yu et al., 2011). It does so by accounting for the possibility of local interface variations on the overall refracted and reflected wave fields as they interact with the interface. The GSL has opened up new design capabilities for the control of light by enabling engineering such interface variations at the nanoscale. A physical realization of the GSL is found in optical meta-surfaces (Kildishev et al., 2013; Yu & Capasso, 2014), which are made of ultrathin optical components that are placed at
the interface of two media to effect abrupt changes in phase, amplitude, and/or polarization to both reflected and transmitted wave fields. Figure 1.1 shows a microscope image of a metasurface structure where a pattern of optical components at the interface is created by an assembly of anisotropic metallic scatterers (the spacing between obstacles and the dimension of the scatterers is comparable to incident wavelength). This particular metasurface example is designed in such a manner that it produces phase shifts. In order to achieve complex optical capabilities, inverse design methods are needed (Li et al., 2022). The inverse design of metasurfaces, however, in principle requires solving the full Maxwell equations system that governs the propagation of light. Given the massive scale of the problem at hand, brute-force computations are often unfeasible due to memory and processing power constraints. A computational framework that lies in between the GSL and the full-wave solution, in terms of computational complexity and accuracy, is the locally periodic approximation (Pestourie et al., 2018). This model reduction approach recasts the problem of scattering by a general aperiodic surface, consisting of different scatterers placed in fixed-size and shape cells, as a finite number of periodic problems. This is done based on the observation that the scattered/reflected field above and below a given metasurface cell (containing one or a few scatterers) is “close” to the corresponding field obtained by solving the same problem but by an infinite periodic surface obtained by

Figure 1.1. (left) Scanning electron microscope image of an interface. The pattern consists of eight regions, each occupied by one constituent antenna with a fixed shape. (right) Zoom-in view of the center part of the left figure. (Yu et al., 2011)
replicating the given cell. This way, solutions to the full-Maxwell equations system can be approximated as the superposition of solutions of several periodic problems that can be efficiently solved in a parallel fashion.

Yet another type of optical structure that benefits from the accurate and efficient solution of problems of scattering by infinite periodic media are the so-called photonic crystals (Joannopoulos, 2008). These consist of piece-wise homogeneous media exhibiting intrinsic spatial periodicity in one, two, or three dimensions. The shape and dimension of the crystal can be tuned to prohibit the propagation of waves at a certain range of frequencies, which are known as band gaps. Given the large size of these structures, compared to the wavelength and the unit cell size, computational methods for the photonic crystal simulations typically assume the structure to be infinite and periodic in the relevant dimensions. While most interest has been put on computing band gaps by solving suitable eigenvalue problems (Dobson, 1999; Johnson & Joannopoulos, 2001), more realistic models aim at solving problems of scattering by these structures for certain ranges of frequencies.


In the following section, we briefly describe the physics and mathematics background of the problems tackled in this thesis.
1.2. Background

This section presents the basic physical and mathematical background of wave phenomena that will be utilized in the following chapters of this thesis. In particular, we focus on scalar time-harmonic waves and their relation with Maxwell’s equations.

1.2.1. Time-harmonic waves

The concept of “wave” is somewhat vague, but one accepted definition is a dynamic and propagative disturbance of one or more physical quantities, sometimes described by the wave equation. In this thesis we consider linear scalar waves governed by the famous scalar wave equation (Griffiths et al., 1999; Strauss, 2007) is

\[ \Delta p = \frac{1}{c^2} \frac{\partial^2 p}{\partial t^2}, \]  

(1.1)

where \( c > 0 \) is the wave propagation’s speed and the sought function \( p = p(r, t) \) is defined in a certain domain \( \Omega \times \mathbb{R}_+ \), where \( \Omega \subset \mathbb{R}^d \) \((d = 2, 3)\) is the spatial domain. We further focus on time-harmonic solutions of the wave equation (1.1), which take the form

\[ p(r, t) = \text{Re} \left( u(r) e^{-i\omega t} \right) \]  

(1.2)

where \( \omega > 0 \) is the angular frequency. Using (1.2), the wave equation can be reduced to find the amplitude function \( u = u(r) \) defined over \( \Omega \), which satisfies the Helmholtz equation

\[ \Delta u + k^2 u = 0 \quad \text{in} \: \Omega \subset \mathbb{R}^d, \]  

(1.3)

where \( k = \omega/c \) is the wavenumber, that is related to the wavelength \( \lambda > 0 \) through

\[ \lambda = \frac{2\pi}{k}. \]  

(1.4)

The case of interest for us is when the wavenumber \( k \) is piecewise constant over \( \Omega = \mathbb{R}^d \). For simplicity, we assume that \( \Omega \) is given by the union of two disjoint subdomains \( \Omega_j \subset \Omega, j = 1, 2 \), where the wavenumber is given by \( k = k_j \) with \( k_1 \neq k_2 \). As such, the
complex amplitude function, $u$, satisfies the Helmholtz equation (1.3) with wavenumber $k_j$ over each subdomain $\Omega_j$ and suitable transmission conditions need to be prescribed at the common interface $\Gamma$ between the two domains. In what follows we refer to $\Omega_2$ as the \textit{interior domain} (according to the direction of the unit normal $n$ to its boundary $\Gamma$ that points toward $\Omega_2$) and to $\Omega_1 = \mathbb{R}^d \setminus \overline{\Omega}_2$ as the \textit{exterior domain}, which is assumed unbounded.

In this thesis, we are interested in solving problems of scattering. In particular, the problems we consider concern the scattering of planewaves:

$$u^{\text{inc}}(r) = e^{ik \cdot r}, \quad k \in \mathbb{R}^d, \quad |k| = k_1$$

that impinge on $\Gamma$ generating a scattered field $u^s : \Omega_1 \to \mathbb{C}$ that propagates to infinity, and a transmitted field $u^t : \Omega_2 \to \mathbb{C}$ that is confined to $\Omega_2$. Additional conditions at infinity are needed to be imposed on $u^s$ to ensure the problem’s wellposedness (Nédélec, 2001; D. Colton & Kress, 2012). Intuitively, this condition ensures that the scattered field $u^s$ is an outgoing wave propagating to infinity from the interface $\Gamma$ between the two media. Such a condition is known as \textit{radiation condition}. Helmholtz equation solutions that satisfy the radiation condition are called \textit{radiative} solutions. The most common radiation condition, suitable for $\Omega_2$ bounded, is the Sommerfeld radiation condition which states that:

$$\lim_{|r| \to \infty} |r|^{-\frac{d-1}{2}} \left( \frac{\partial}{\partial |r|} - ik_1 \right) u^s(r) = 0$$

uniformly in all directions $r/|r|$. Periodic problems like the ones considered in this thesis that involve an unbounded $\Omega_2$, however, require a different radiation condition that we discuss in detail in Section 2.2.
To summarize, the sought time-harmonic total field \( u \), which equals \( u = u^s + u^{inc} \) in \( \Omega_1 \) and \( u = u^t \) in \( \Omega_2 \), satisfies

\[
\begin{cases}
\Delta u + k_j^2 u = 0 & \text{in } \Omega_j, (j = 1, 2) \\
\text{+ transmission conditions at } \Gamma = \partial \Omega_1 = \partial \Omega_2, \\
\text{+ radiation condition at infinity.}
\end{cases}
\]  

(1.5)

where the radiation condition applies to \( u^s \) and the transmission conditions — that are specified below in the case of electromagnetic waves — give rise to boundary sources expressed in terms of the known incidence planewave \( u^{inc} \) and its normal derivative on \( \Gamma \).

### 1.2.2. Electromagnetic waves

As mentioned above, in Section 1.1, the main motivation of this thesis is the solution to problems of scattering of time-harmonic electromagnetic waves. The propagation of electromagnetic fields is governed by Maxwell’s equations (Griffiths et al., 1999; Nédélec, 2001; Müller, 2013). In the case of a homogeneous medium with electric permittivity \( \varepsilon \) and magnetic permeability \( \mu \) and in absence of free charges and current sources, Maxwell’s equations become

\[
\begin{cases}
\varepsilon \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H}, \\
\mu \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}, \\
\nabla \cdot \mathbf{E} = 0, \\
\nabla \cdot \mathbf{H} = 0,
\end{cases}
\]

(1.6)

where \( \mathbf{E}(\mathbf{r}, t) \) and \( \mathbf{H}(\mathbf{r}, t) \) denote the time-dependent electric and magnetic fields respectively, for \( (\mathbf{r}, t) \in D \times [0, \infty), \) \( D \subset \mathbb{R}^3 \). Using the vector Laplacian identity \( \Delta \mathbf{A} = \nabla (\nabla \cdot \mathbf{A}) - \nabla \times \nabla \times \mathbf{A} \), where \( \mathbf{A} \) is a sufficiently smooth vector field, it can be easily verified that both the electromagnetic field \( (\mathbf{E}, \mathbf{H}) \) satisfies the wave equation (1.1):

\[
\frac{\partial^2 \mathbf{E}}{\partial t^2} - c^2 \Delta \mathbf{E} = 0 \quad \text{and} \quad \frac{\partial^2 \mathbf{H}}{\partial t^2} - c^2 \Delta \mathbf{H} = 0,
\]

(1.7)
where \( c = 1 / \sqrt{\varepsilon \mu} \) corresponds to the speed of light of the medium. It is worth mentioning here that electromagnetic media are often characterized by the refractive index

\[
n := \frac{c_0}{c} = \sqrt{\frac{\varepsilon \mu}{\varepsilon_0 \mu_0}},
\]

where \( c_0 = 1 / \sqrt{\varepsilon_0 \mu_0} \) is the speed of light in the vacuum.

Our case of interest assumes Maxwell’s equations are time-harmonic. We hence seek electromagnetic fields of the form

\[
\mathbf{E}(\mathbf{r}, t) = \text{Re} \left( \mathbf{\hat{E}}(\mathbf{r}) e^{-i \omega t} \right) \quad \text{and} \quad \mathbf{H}(\mathbf{r}, t) = \text{Re} \left( \mathbf{\hat{H}}(\mathbf{r}) e^{-i \omega t} \right).
\]

(1.9)

By replacing (1.9) in (1.6), the Maxwell’s equation system becomes

\[
\begin{aligned}
\left\{ \begin{array}{c}
  i \omega \varepsilon \mathbf{\hat{E}} = \nabla \times \mathbf{\hat{H}}, \\
  \nabla \cdot \mathbf{\hat{E}} = 0,
\end{array} \right.
\end{aligned}
\]

\[
\begin{aligned}
\left\{ \begin{array}{c}
  i \omega \mu \mathbf{\hat{H}} = -\nabla \times \mathbf{\hat{E}}, \\
  \nabla \cdot \mathbf{\hat{H}} = 0.
\end{array} \right.
\]

(1.10)

Even though the time-harmonic Maxwell’s equation system (1.10) is vectorial and three-dimensional, in an important case of interest it can be reduced to the scalar Helmholtz equation (1.3). Indeed, when dealing with (cylindrical) domains that exhibit invariance along one axis, the system (1.10) reduces to solving just two scalar Helmholtz equations for the transverse electric (TE) and transverse magnetic (TM) fields (Nédélec, 2001). In short, assuming invariance along along the \( z \)-axis, i.e., that \( D = \Omega \times \mathbb{R}, \Omega \subset \mathbb{R}^2 \), and that both \( \mathbf{E} \) and \( \mathbf{H} \) are independent of \( z \), (1.10) reduces to find \( E_z, H_z : \Omega \to \mathbb{C} \) such that

\[
\Delta \mathbf{\hat{E}}_z + k^2 \mathbf{\hat{E}}_z = 0 \quad \text{and} \quad \Delta \mathbf{\hat{H}}_z + k^2 \mathbf{\hat{H}}_z = 0,
\]

(1.11)

where \( k = \omega \sqrt{\varepsilon \mu} \), with \( \mathbf{\hat{E}}_z \) (resp. \( \mathbf{\hat{H}}_z \)) corresponding to the \( z \)-component of \( \mathbf{\hat{E}} \) (resp. \( \mathbf{\hat{H}} \)) in TE (resp. TM) polarization. The entire electromagnetic field can then be retrieved from
As explained above in Section 1.2.1, in the case of problems of scattering by a medium with piecewise constant material properties, i.e., piecewise constant $\varepsilon$ and $\mu$, we decompose $D = \mathbb{R}^3$ into two subdomains, $D_1 = \Omega_1 \times \mathbb{R}$ and $D_2 = \Omega_2 \times \mathbb{R}$, where the wavenumber is constant and equal to $k_j = \omega \sqrt{\varepsilon_j \mu_j}$ in $D_j$, $j = 1, 2$. This approach entails the use of transmission conditions for the electromagnetic field across the common boundary $\Gamma \times \mathbb{R}$ between $D_1$ and $D_2$. As is well known (Griffiths et al., 1999), such conditions correspond to the continuity of the tangential components of the total electric and magnetic fields across the material interface. In view of (1.12), these conditions lead to the continuity of the Dirichlet and Neumann traces of the total transverse fields $E_z$ and $H_z$ across $\Gamma$, which are presented in detail in equation (2.2c) in the next chapter. The resulting transmission problem for $E_z$ and $H_z$, are completely uncoupled from each other and both take the form (1.5).

The next section describes, in a nutshell, the solution of problems of scattering via boundary integral formulations.

### 1.3. Boundary integral equation methods

This section briefly describes the main ideas behind boundary integral equation (BIE) methods for the numerical solution of the Helmholtz equation.

#### 1.3.1. Free-space Green function

At the core of BIE methods lies the concept of the Green function (D. L. Colton & Kress, 1983; McLean, 2000; Nédélec, 2001; D. Colton & Kress, 2012). In the case of
Helmholtz equation, such a function $G(r, r')$, satisfies

$$\Delta_r G(r, r') + k^2 G(r, r') = -\delta(r - r'), \quad r, r' \in \mathbb{R}^d$$  \hspace{1cm} (1.13)

in the distributional sense (Salsa, 2016), where $\delta$ denotes the Dirac’s delta distribution. Looking for a radiative solutions of (1.13) (in the sense of Sommerfeld (Nédélec, 2001)), we find that

$$G(r, r') = \begin{cases} 
  \frac{i}{4} H_0^{(1)}(k|r - r'|), & \text{if } d = 2; \\
  \exp(ik|r - r'|) \frac{4}{4\pi |r - r'|}, & \text{if } d = 3.
\end{cases}$$  \hspace{1cm} (1.14)

The function defined above is known as the free-space Green function for the Helmholtz equation in $\mathbb{R}^d$.

In order to illustrate how the Green function (1.14) can be utilized to solve a problem of scattering, consider the following exterior Dirichlet boundary value problem:

$$\begin{cases} 
  \Delta u + k^2 u = 0 & \text{in } \mathbb{R}^d \setminus \Omega, \\
  u = f & \text{on } \Gamma = \partial \Omega, \\
  \lim_{|r| \to \infty} |r|^{d-1} \left( \frac{\partial}{\partial |r|} - ik \right) u(r) = 0,
\end{cases}$$  \hspace{1cm} (1.15)

where we assume $\Gamma$ is of class $C^2$ and $f \in H^{1/2}(\Gamma)$.

To solve this problem, one can consider an indirect BIE formulation based on the double-layer potential (D. L. Colton & Kress, 1983; McLean, 2000). In detail, we consider the following solution ansatz:

$$u(r) = \int_{\Gamma} \frac{\partial G(r, r')}{\partial n(r')} \varphi(r') \, ds(r'), \quad r \in \mathbb{R}^d \setminus \overline{\Omega}$$  \hspace{1cm} (1.16)

where $\varphi : \Gamma \to \mathbb{C}$, $\varphi \in L^2(\Gamma)$ is an unknown density function. It can be verified that $u$ in (1.16) satisfies both $\Delta u + k^2 u = 0$ in all of $\mathbb{R}^d \setminus \Omega$ and the Sommerfeld radiation condition. Imposing the boundary condition $u = f$ on $\Gamma$ and using the jump condition for the double-layer potential (D. L. Colton & Kress, 1983), one finds that the unknown
density \( \varphi \) must satisfy the following BIE:

\[
\frac{\varphi(r)}{2} + \int_{\Gamma} \frac{\partial G(r, r')}{\partial n(r')} \varphi(r') \, ds(r') = f(r), \quad r \in \Gamma.
\]  

(1.17)

The boundary integral operator in (1.17), known as the double-layer operator, can be proven to be compact on \( L^2(\Gamma) \) making the BIE (1.17) Fredholm of the second-kind. This fact provides a theoretical framework, known as Fredholm’s alternative (Salsa, 2016), to establish the existence and uniqueness of the solution to (1.17).

This formulation allows the exterior boundary value problem (1.15) to be recast as a BIE posed on the boundary of the obstacle \( \Gamma \), which can be efficiently solved numerically. Once an approximation of \( \varphi \) is obtained, an approximate solution to (1.15) everywhere in \( \mathbb{R}^d \setminus \overline{\Omega} \) can be produced via numerical evaluation of the smooth integral in (1.16). In this thesis, we exploit this idea to develop an efficient and high-order BIE method for problems of scattering (1.5) by infinite period arrays of penetrable scatterers.

It is clear from its definition that the Green’s function (1.14) and its normal derivative, used in (1.16) and (1.17), exhibit a problematic \( O(\log |r - r'|) \) (resp. \( O(|r - r'|^{-1}) \)) singularity as \( r \) approaches the source location \( r' \) in \( \mathbb{R}^2 \) (resp. \( \mathbb{R}^3 \)). Indeed, \( G \), for instance, becomes undefined if evaluated exactly at the singularity, i.e., when \( r = r' \). This fact leads to numerous issues when designing BIE methods, which require the numerical integration of this function over curves/surfaces.

In the next section, we discuss a class of numerical methods for solving BIEs akin to (1.17).

1.3.2. Nyström methods

In order to describe Nyström methods, we consider second-kind Fredholm BIEs like the one presented above, which can be put in abstract form as

\[
(I - A)[\varphi](r) = f(r), \quad r \in \Gamma,
\]  

(1.18)
where $A : L^2(\Gamma) \to L^2(\Gamma)$ is a compact operator, $I$ is the identity operator in $L^2(\Gamma)$, $f \in L^2(\Gamma)$ is known, and the unknown density is $\varphi \in L^2(\Gamma)$. For the time being, we assume that the continuous integral kernel $K : \Gamma \times \Gamma \to \mathbb{C}$ defines the operator

$$A[\varphi](\mathbf{r}) := \int_{\Gamma} K(\mathbf{r}, \mathbf{r}') \varphi(\mathbf{r}') \, d\mathbf{s}(\mathbf{r}'), \quad \mathbf{r} \in \Gamma.$$  

(1.19)

To numerically discretize the BIE (1.18) we can employ an $n$-points rule with quadrature nodes $\{\mathbf{r}_k\}_{k=1}^n$ and quadrature weights $\{\alpha_k\}_{k=1}^n$. Then, an approximation of the operator $A$ can be computed as

$$\tilde{A}[\varphi](\mathbf{r}) := \sum_{k=1}^n \alpha_k K(\mathbf{r}, \mathbf{r}_k) \varphi(\mathbf{r}_k), \quad \mathbf{r} \in \Gamma.$$  

(1.20)

Evaluating $\tilde{A}[\varphi]$ at the same quadrature nodes $\{\mathbf{r}_j\}_{j=1}^n$, the continuous equation (1.18) can be reworked as a finite-dimensional discrete system given by

$$\left( I_n - \tilde{A} \right) [\tilde{\varphi}](\mathbf{r}_j) = f(\mathbf{r}_j), \quad j = 1 \ldots n,$$  

(1.21)

where $I_n \in \mathbb{C}^{n \times n}$ is the identity matrix, $\tilde{A}$ is the discrete operator defined in (1.20) and $\tilde{\varphi}$ is an approximation of $\varphi$ such that $\tilde{\varphi}_j = \tilde{\varphi}(\mathbf{r}_j)$ where $\tilde{\varphi}_j$ are the entries of the vector solution of the linear

$$\tilde{\varphi}_j - \sum_{k=1}^n \alpha_k K(\mathbf{r}_j, \mathbf{r}_k) \tilde{\varphi}_k = f(\mathbf{r}_j), \quad j = 1 \ldots n.$$  

(1.22)

Since we have so far assumed a continuous kernel $K$, its evaluations at the quadrature nodes can be performed using standard quadrature rules, e.g., the trapezoidal rule or Féjer quadratures. However, in (1.17) as well in BIEs considered below in this thesis, the integral kernel (1.14) is singular, preventing the direct evaluation at every pair of points. Particularly, this thesis deals with weakly-singular kernels, for which the operator $A$ in (1.18) can be expressed as

$$A[\varphi](\mathbf{r}) := \int_{\Gamma} w(|\mathbf{r} - \mathbf{r}'|) \kappa(\mathbf{r}, \mathbf{r}') \varphi(\mathbf{r}') \, d\mathbf{s}(\mathbf{r}'), \quad \mathbf{r} \in \Gamma,$$  

(1.23)
where the function $w$ captures the weak singularity of the kernel, i.e., $w(t)$ is smooth for $t > 0$ and is absolutely integrable in the Lebesgue sense within any sufficiently small neighborhood of the origin. The function $\kappa : \Gamma \times \Gamma \rightarrow \mathbb{C}$, on the other hand, is assumed to be continuous. If the integral operator (1.23) is evaluated directly by means of any standard quadrature rules, to obtain a linear system similar to equation (1.22), we encounter a problem whenever $r_j = r_k$ because $w$ is often unbounded at the origin. Therefore, some kind of regularization strategy or specialized quadrature is required at accurately evaluate the boundary integral. In this work, we employ two different strategies, namely, Martensen-Kussmaul (MK) method for problems in $\mathbb{R}^2$ and the density interpolation method (DIM) for problems in both $\mathbb{R}^2$ and $\mathbb{R}^3$.

MK method (Kress, 2014; D. Colton & Kress, 2012) assumes the boundary $\Gamma \subset \mathbb{R}^2$ is smooth and has an analytic $2\pi$-periodic parametrization. By rewriting the kernel in a parametric form, it is split into two terms: one exhibiting an explicit (weak) logarithmic singularity and a smooth part. Constructing a specialized quadrature rule that integrates exact products of the logarithm and trigonometric polynomials, this method effectively evaluates the singular boundary integral with errors that decay exponentially fast as the number of quadrature nodes increases. As stated in (D. Colton & Kress, 2012), the resulting Nyström method using this integration technique is the most efficient for the numerical BIE-solution of the Helmholtz equation in two dimensions. Unfortunately, these ideas do not carry over directly to non-smooth boundaries and to three dimensions.

DIMs (Pérez-Arancibia, Turc, & Faria, 2019b; Faria et al., 2021; Pérez-Arancibia, Turc, & Faria, 2019a), on the other hand, produce accurate BIE-solutions of the Helmholtz equation in both two and three dimensions. In brief, these methods rely on the construction of a family of functions that interpolate the density function up to the desired order. The interpolant functions are combined with Green’s representation formula (Nédélec, 2001) to recast the singular integral operator in terms of boundary integrals with bounded or smoother integrands. Once this regularization is effected, the resulting boundary integrals can be numerically evaluated with high precision by means of standard quadrature rules.
1.4. Contributions

The main objective of this thesis is the development of a novel numerical method to solve electromagnetic wave-scattering problems by periodic arrays of obstacles, that is accurate and robust at all frequencies. The specific objectives of this thesis are the following:

(i) Derive a well-posed formulation to ensure the methodology’s accuracy and robustness, even at the challenging Rayleigh-Wood anomalies.
(ii) Implement efficient and high-order domain truncation techniques to effectively reduce the computational problem’s size.
(iii) Develop open-source software, relying on the efficient general-purpose DIM for numerical computations.

The computer code produced as a result of this thesis is written in Julia and is freely available at

https://github.com/tstrauszer/PeriodicMedia_WP

1.5. Outline of this thesis

This thesis is organized as follows. Chapter 2 describes the main contribution of this thesis and corresponds to our published paper; it presents the methodology for the scattering-transmission problem of line arrays in two spatial dimensions and a variety of numerical examples, first validating the expected results and then applying it to real-case situations. Chapter 3 extends the methodology to line and surface periodic arrays of 3D obstacles, starting from the results of the previous chapter; additional considerations to avoid ill-conditioning issues and numerical experiments are provided. Chapter 4 presents the conclusions and future work.
2. WAVE SCATTERING BY PERIODIC LINE ARRAYS OF 2D OBSTACLES

The following chapter was published as a scientific paper, under the title “Windowed Green function method for wave scattering by periodic arrays of 2D obstacles” in Studies for Applied Mathematics, Wiley Online Library (Strauszer-Caussade et al., 2022)

2.1. Previous work

This work presents a novel windowed Green function boundary integral equation (BIE) method for the numerical solution of problems of time-harmonic electromagnetic planewave scattering by infinite periodic arrays of penetrable obstacles in two spatial dimensions (although the proposed methodology can also be applied to acoustics). Problems of this type often arise in a number of application areas that greatly benefit from accurate and efficient numerical computations such as, for instance, photonic crystal modeling (Joannopoulos, 2008) and inverse design of metasurfaces (Yu & Capasso, 2014; Xie et al., 2014) whereby the so-called locally periodic approximation is used to deal with scattering by large aperiodic structures by decomposing it in a finite number of unit-cell periodic problems (Pestourie et al., 2018; Pérez-Arancibia et al., 2018; Lin et al., 2019).

Classical BIE formulations for scattering by periodic media rely on the quasi-periodic Green function (C. Linton, 1998). As is well known, standard spatial and spectral representations of the quasi-periodic Green function give rise to infinite series that (a) converge slowly depending on the relative location of the source and target points and, in addition, (b) cease to exist at the so-called Rayleigh-Wood (RW) anomalies (i.e., when at least one scattered/transmitted mode propagates in the direction parallel to the array axis). Several analytical techniques have been proposed to tackle the former problem including most notably Ewald’s method (see (C. M. Linton, 2010; C. Linton, 1998) for a thorough review on the subject). A strikingly simple method that also addresses the aforementioned slow convergence issue is developed in (Monro Jr, 2008; O. P. Bruno et al., 2016), which relies on a smooth windowed sum approximation of the spatial series representation of the Green
function. Away from RW anomalies, this approach achieves super-algebraically fast convergence as the truncation radius increases. In view of the fact that the quasi-periodic Green function itself does not exist at RW anomalies, all the aforementioned approaches simply break down at these singular configurations (although, as shown in (O. P. Bruno & Fernandez-Lado, 2020, Fig. 1.3), Ewald’s method produces accurate solutions at almost machine precision “distance” from RW anomalies).

Improving on the windowed summation approach, (O. P. Bruno & Delourme, 2014) and subsequent related work (O. P. Bruno & Fernandez-Lado, 2017; O. P. Bruno, Shipman, et al., 2017) introduce the quasi-periodic shifted Green function. BIE solvers that leverage this modified Green function (O. Bruno & Maas, 2018; Nicholls et al., 2020; Pérez-Arancibia, Shipman, et al., 2019) exhibit super-algebraic convergence away from RW anomalies and algebraic but arbitrarily high-order convergence at and around RW anomalies, at the cost of \( n \)-tupling the number of function evaluations where \( n \) is the numbers of “shifts” utilized in the approximation. Recent developments in this direction (O. P. Bruno & Fernandez-Lado, 2020; Fernandez-Lado, 2016) present a general methodology based on hybrid spatial/spectral Green function representations and the Woodbury-Sherman-Morrison formula that makes classical approaches such as Laplace-type integral and Ewald’s methods, as well as the shifted Green function approach, applicable and robust at and around RW-anomaly configurations.

Yet another class of BIE methods aims at bypassing the use of the problematic quasi-periodic Green function. To the best of the authors’ knowledge, the first method in this class was introduced in (Wu & Lu, 2009). There and in subsequent related contributions (Wu & Lu, 2011; Lu & Lu, 2012), Neumann-to-Dirichlet operators are combined with the quasi-periodic boundary conditions on the unit-cell walls to reduce the problem to a BIE expressed in terms of free-space Green function kernels. No explicit mention of issues associated with RW anomalies are reported in these works. A different approach is adopted in (Barnett & Greengard, 2011) (see also (Gillman & Barnett, 2013)) where the quasi-periodic problem is recast as a formally second-kind indirect BIE formulation.
involving free-space Green function kernels and integrals along the infinite boundaries of the (unbounded) unit cell domain. Leveraging the exponential decay of the boundary integrands in spectral form, the resulting BIE system is effectively reduced to a bounded hybrid spatial-spectral computational domain where standard Nyström discretizations can be applied for its numerical solution. Although this method does not make use of the quasi-periodic Green function, it involves evaluation of cumbersome Sommerfeld-type integrals that need to be painstakingly modified in the presence of RW anomalies (when a pole at origin on the Sommerfeld integration contour needs to be accounted for by suitably deforming the contour and adding the corresponding residue contribution). Building up on this work, a periodizing scheme akin to the method of fundamental solutions is developed in (Cho & Barnett, 2015) and subsequent contributions (Lai et al., 2015). This approach only entails evaluations of free-space Green function kernels in spatial form and it appears immune to the presence of RW anomalies. However, the so-called proxy (equivalent) sources employed by this scheme to enforce the quasi-periodicity condition, give rise to relatively small but ill-conditioned subsystems that are treated by Schur complements and direct linear algebra solvers, hence hindering the straightforward applicability of GMRES and fast algorithms to perform matrix-vector product operations (such as the fast multipole method (Rokhlin, 1990), for instance).

Here, we present a method that falls under the latter class of BIE methods. Our approach amounts to an extension of the windowed Green function (WGF) method for layer media scattering and waveguide problems (O. Bruno et al., 2016; Pérez-Arancibia, 2017; O. P. Bruno & Pérez-Arancibia, 2017; O. P. Bruno, Garza, & Pérez-Arancibia, 2017), to quasi-periodic scattering problems. Inspired by (O. Bruno et al., 2016) we pursue a direct BIE formulation derived from a Green’s representation formula of the scattered field within the unbounded unit-cell domain, which uses the free-space Green function instead of the problem-specific (quasi-periodic) Green function. The quasi-periodicity condition is then readily incorporated into our formulation by exploiting the direct linear relationship between the scattered-field traces on the left- and right-hand side unit-cell walls. Unlike quasi-periodic Green function-based BIE methods, these traces become additional
unknowns that we need to solve for in our formulation. The transmission conditions on
the penetrable boundaries of the obstacles are imposed through Kress-Roach/Müller’s ap-
proach (Kress & Roach, 1978; Müller, 2013) which leads to weakly-singular integral op-
erators. As in (Barnett & Greengard, 2011), we hence obtain a formally second-kind BIE
system given in terms of free-space Green function kernels and boundary integrals over
the unbounded unit-cell boundaries. Indeed, prior to truncation, both formulations entail
evaluation of the same weakly-singular integral operators. The main difference between
the two approaches lies in the truncation strategy. Instead of resorting to spatial-spectral
representations of the integral operators, we work with integral operators in pure spatial
form hence enabling the use of off-the-shelf BIE methods and fast algorithms. We do so
by truncating the oscillatory integrals over the unbounded unit-cell walls using a smooth
window function that multiplies the free-space Green function kernels. When applied to
the traces of the (radiative) scattered field, the resulting windowed BIE operators spawn
small errors that decay super-algebraically fast as the support of the window function in-
creases. As it turns out, however, at certain frequency ranges which include RW-anomaly
configurations, the naive windowing approximation of the BIE operators leads to a BIE
system that fails to account for the radiation condition. In order to properly enforce it, we
then propose a corrected windowed BIE that produces accurate solutions throughout the
entire spectrum, including at and around the challenging RW-anomaly configurations. (In-
terestingly, a somewhat similar correction procedure has been recently proposed in (Zhou
& Wu, 2018) to address the failure of the perfectly matched layer technique at absorbing
RW modes in the context of finite element discretizations.) The corrected windowed BIE
is Fredholm of the second-kind and upon discretization it leads to systems of equations
that can be efficiently solved by iterative linear algebra solvers (i.e., GMRES) which can
be further accelerated by means of fast methods. The proposed methodology exhibits
super-algebraic convergence as the window size increases.

The chapter is organized as follows. Section 2.2 describes the problem under consid-
eration and summarizes some important facts of the problem that will be utilized in the
following sections. Section 2.3 presents the derivation of the non-standard Green’s representation formula on which our direct BIE formulation is based on. Section 2.4 introduces the notation as well as the main properties of the layer potentials and BIE operators. The direct BIE formulation of the problem is derived in Section 2.5 while the naive windowed BIE is motivated and presented in Section 2.6. A series of numerical experiments designed to examine the accuracy of the naive windowed BIE at and around a RW-anomaly configurations is shown in Section 2.7. The corrected windowed BIE formulation is then developed in Section 2.8. A variety of the numerical examples are presented in Section 2.9.

2.2. Preliminaries

This work deals with problems of time-harmonic electromagnetic scattering by infinite periodic arrays of penetrable obstacles in two dimensions for which we adopt the time convention $e^{-i\omega t}$ where $t > 0$ is time and $\omega > 0$ is the angular frequency. In detail, letting $\theta_{\text{inc}} \in [-\pi/2, \pi/2]$ denote the angle of incidence measured with respect to the negative y-axis, we consider the scattering and transmission of a planewave

$$u^{\text{inc}}(x, y) = e^{i \alpha x - i \beta y}, \quad \alpha = k_1 \sin \theta_{\text{inc}}, \quad \beta = k_1 \cos \theta_{\text{inc}} \quad (2.1)$$

by an $L$-periodic array of the form $D_2 = \bigcup_{n \in \mathbb{Z}} \{(x, y) \in \mathbb{R}^2 : (x - nL, y) \in \Omega_2\}$ where $\Omega_2 \subset \mathbb{R}^2$ is an open and bounded domain of class $C^2$. Here, $k_1 = \omega \sqrt{\varepsilon_1 \mu_1} > 0$ is the wavenumber of the exterior domain $D_1 = \mathbb{R}^2 \setminus \overline{D_2}$ with permittivity $\varepsilon_1 > 0$ and permeability $\mu_1 > 0$. Inside the penetrable array $D_2$, on the other hand, the wavenumber is given by $k_2 = \omega \sqrt{\varepsilon_2 \mu_2}$ in terms of $\mu_2 > 0$ and $\varepsilon_2$ which is allowed to be a complex number satisfying $\text{Im} \varepsilon_2 \geq 0$.

The sought total field $u : \mathbb{R}^2 \rightarrow \mathbb{C}$, $u \in (C^2(D_1) \cap C^1(\overline{D_1})) \cup (C^2(D_2) \cap C^1(\overline{D_2}))$, is the transverse component of the total electric field in TE polarization (reps. magnetic field in TM polarization) which satisfies

$$\Delta u + k_1^2 u = 0 \quad \text{in} \quad D_1 \quad \text{and} \quad \Delta u + k_2^2 u = 0 \quad \text{in} \quad D_2. \quad (2.2a)$$
Additionally, the total field satisfies the quasi-periodicity condition
\[ u(x + L, y) = \zeta u(x, y), \quad \zeta := e^{i\alpha L}, \quad (x, y) \in \mathbb{R}^2, \]  
(2.2b)

and the transmission conditions
\[ \gamma_{D,S}^+ u = \gamma_{D,S}^- u \quad \text{and} \quad \gamma_{N,S}^+ u = \gamma_{N,S}^- u \quad \text{on} \quad S := \partial D_2, \]  
(2.2c)

where \( \eta := \mu_1/\mu_2 \) in TE polarization and \( \eta := \varepsilon_1/\varepsilon_2 \) in TM polarization, and where the Dirichlet and Neumann traces are respectively defined as
\[ (\gamma_{D,\Gamma}^\pm u)(r) = \lim_{\delta \to 0^+} u(r \pm \delta n(r)) \quad \text{and} \quad (\gamma_{N,\Gamma}^\pm u)(r) = \lim_{\delta \to 0^+} \nabla u(r \pm \delta n(r)) \cdot n(r), \quad r \in \Gamma, \]  
(2.3)

for a given curve \( \Gamma \) with unit normal \( n \). (Note that the traces are defined with respect to the fixed orientation of the unit normal \( n \) to the curve \( \Gamma \). The precise orientation of \( n \) along the relevant curves employed in this work is displayed in Figure 2.1.)

As usual, the total field is expressed as
\[ u = \begin{cases} u^s + u^{\text{inc}} & \text{in} \ D_1 \\ u^t & \text{in} \ D_2 \end{cases} \]  
(2.4)
in terms of the incident \((u^{\text{inc}})\), transmitted \((u^t)\), and scattered \((u^s)\) fields, with the latter satisfying the Rayleigh expansion

\[
\begin{align*}
u^s(x, y) &= \begin{cases} 
\sum_{n \in \mathbb{Z}} B_n^+ e^{i(\alpha_n x + \beta_n y)} & \text{for } y > h^+ := \sup_{(x,y) \in \Omega_2} y \\
\sum_{n \in \mathbb{Z}} B_n^- e^{i(\alpha_n x - \beta_n y)} & \text{for } y < h^- := \inf_{(x,y) \in \Omega_2} y
\end{cases} \tag{2.5a}
\end{align*}
\]

above \((y > h^+)\) and below \((y < h^-)\) the infinite array \(D_2\), where

\[
\alpha_n := \alpha + n \frac{2\pi}{L} \quad \text{and} \quad \beta_n := \begin{cases} 
\sqrt{k_1^2 - \alpha_n^2} & \text{if } \alpha_n^2 \leq k_1^2 \\
i\sqrt{\alpha_n^2 - k_1^2} & \text{if } \alpha_n^2 > k_1^2.
\end{cases} \tag{2.5b}
\]

As it turns out it is convenient to distinguish the following three integer sets:

\[
\begin{align*}
\mathcal{P} &= \{n \in \mathbb{Z} : \alpha_n^2 < k_1^2\} \tag{2.6a} \\
\mathcal{E} &= \{n \in \mathbb{Z} : \alpha_n^2 > k_1^2\} \tag{2.6b} \\
\mathcal{S} &= \{n \in \mathbb{Z} : \alpha_n^2 = k_1^2\}. \tag{2.6c}
\end{align*}
\]

According to our time convention, it holds that for \(n \in \mathcal{P}\) the modes

\[
u^+_n(x, y) := e^{i\alpha_n x + i\beta_n y} \quad \text{and} \quad \nu^-_n(x, y) := e^{i\alpha_n x - i\beta_n y} \tag{2.7}
\]

in (2.5a) are upgoing and downgoing propagative planewaves, respectively. For \(n \in \mathcal{E}\), in turn, \(u^+_n\) (resp. \(u^-_n\)) correspond to evanescent planewaves; they decay exponentially when \(y \to +\infty\) (resp. \(y \to -\infty\)) while they grow exponentially as \(y \to -\infty\) (resp. \(y \to +\infty\)).

In turn, the set of integers \(\mathcal{S} = \mathcal{S}(k_1, \alpha, L) = \{n \in \mathbb{Z} : (\alpha + 2\pi n / L)^2 = k_1^2\} = \{n \in \mathbb{Z} : \beta_n = 0\}\), corresponds to the so-called Rayleigh-Wood anomaly configurations (Petit, 1980) (see also (Fernandez-Lado, 2016; O. P. Bruno & Fernandez-Lado, 2017, 2020)). For such \(n\) values it holds that

\[
u_n(x, y) := \nu^+_n(x, y) = \nu^-_n(x, y) = e^{i\alpha_n x} \tag{2.8a}
\]
is a planewave that propagates parallel to the array along the \( x \) axis. As it follows from separation of variables, the additional quasi-periodic homogeneous solution of the Helmholtz equation is given by the degenerated solution

\[
v_n(x, y) := ye^{i\alpha_n x}, \quad n \in S. \tag{2.8b}
\]

Typically, the Rayleigh series (2.5) serves as the radiation condition for the quasi-periodic scattered field \( u^s \). Alternatively, however, such a radiation condition can be expressed in a less direct form by projecting the scattered field onto the non-radiative modes. As it turns out, this latter form of the radiation condition is more suitable for our boundary integral equation formulation. To derive it, we first note that since \( u^s \) solves the homogeneous Helmholtz equation \( \Delta u^s + k^2u^s = 0 \) in \( D_1 \) and is quasi-periodic, it formally admits the general series expansion

\[
u_n(x, \pm h) = \begin{cases} \sum_{n \in \mathcal{P} \cup \mathcal{E}} \{ B_n^+ u_n^+ + C_n^+ u_n^- \} + \sum_{n \in \mathcal{S}} \{ B_n^- u_n^- + C_n^- u_n^+ \} & \text{for } y > h^+ \\ \sum_{n \in \mathcal{P} \cup \mathcal{E}} \{ B_n^- u_n^- + C_n^- u_n^+ \} + \sum_{n \in \mathcal{S}} \{ B_n^+ u_n^+ + C_n^+ u_n^- \} & \text{for } y < h^- \end{cases}
\]

(2.9)

The fact that \( u^s \) is radiative and bounded in the sense of (2.5) then implies that \( C_n^\pm = 0 \) for all \( n \in \mathbb{Z} \). Therefore, computing these coefficients by projecting \( u^s(x, \pm h) \) and \( \partial_y u^s(x, \pm h) \) for \( h > \max\{h^+,-h^-\} \) onto \( e^{i\alpha_n x} \), we obtain the relation

\[
C_n^\pm = \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \{ \partial_y u^s(x, \pm h) \mp i\beta_n u^s(x, \pm h) \} e^{-i\alpha_n x} \, dx \cdot \begin{cases} \frac{1}{2i\beta_n} e^{-i\beta_n h} & \text{if } n \in \mathcal{P} \cup \mathcal{E} \\ 1 & \text{if } n \in \mathcal{S}. \end{cases}
\]

(2.10)

We then conclude from here that the radiation condition (2.5) can be equivalently enforced by requesting \( u^s \) to satisfy (2.9) and

\[
\frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \{ \partial_y u^s(x, \pm h) \mp i\beta_n u^s(x, \pm h) \} e^{-i\alpha_n x} \, dx = 0, \quad n \in \mathbb{Z}. \tag{2.11}
\]
2.3. Green’s representation formulae

Unlike most of previous works, our direct BIE formulation is derived from a boundary integral representation formula of the scattered field $u^s$ that uses the free-space Helmholtz Green function:

$$G_k(r, r') := \frac{i}{4} H^{(1)}_0(k|r - r'|) \quad (r \neq r')$$  \hspace{1cm} (2.12)

with $k = k_1$. This formula is derived by applying Green’s third identity to $u^s$ in $\Omega_1 := U \setminus \overline{\Omega_2}$, where $U$ is the unit cell domain

$$U = \{(x, y) \in \mathbb{R}^2 : y = y_2(t), x_2(t) < x < x_2(t) + L, t \in \mathbb{R}\}$$  \hspace{1cm} (2.13)

that lies between the infinite parallel curves

$$\Gamma_2 := \{r \in \mathbb{R}^2 : r = r_2(t), t \in \mathbb{R}\} \quad \text{and} \quad \Gamma_3 := \{r \in \mathbb{R}^2 : r = r_2(t) + L e_1, t \in \mathbb{R}\}$$  \hspace{1cm} (2.14)

which are parameterized by the smooth function $r_2(t) = (x_2(t), y_2(t))$. These curves are assumed to extend infinitely along the $y$-axis not intercepting the boundary of obstacle $\Omega_2$, which is contained within $U$ (see Figure 2.1). In order to simplify the analysis of the windowed integral operators in Sections 2.6-2.8 and Appendix A and unless stated otherwise we further assume that $y_2(t) = t$ for $|t| > \max\{h^+, -h^-\}$.

On the other hand, the $C^2$ boundary of $\Omega_2$ is assumed given by

$$\Gamma_1 := \{r \in \mathbb{R}^2 : r = r_1(t), t \in [0, 2\pi)\}$$

in terms of a (global) positively oriented twice continuously differentiable $2\pi$-periodic parametrization $r_1 : [0, 2\pi) \to \mathbb{R}^2$. (More general piecewise smooth curves $\Gamma_1$ admitting local (patch-based) curve parametrizations as well as multiply connected obstacles $\Omega_2$ can be easily incorporated in our approach.)

We start off with the derivation of the integral representation formula for scattered field $u^s$ in $\Omega_1$. Let us then consider the bounded domain $\Omega_{1,h} = U_h \cap \Omega_1$ where $U_h = \{(x, y) \in \mathbb{R}^2 : y = y_2(t), x_2(t) < x < x_2(t) + L, t \in [0, 2\pi)\}$
Figure 2.2. Depiction of the curves involved in the derivation of Green’s representation formula.

$U : |y| < h$ and $h > \max\{h^+, -h^-\}$; see Figure 2.2 and (2.5a) for the definition of $h^\pm$.

Applying Green’s third identity we have that for any fixed target point $r = (x, y) \in \Omega_{1,h}$, it holds that

$$\left( \int_{\Gamma_1} + \int_{\Gamma_+^h} + \int_{\Gamma_-^h} \right) \left\{ u^s(r') \frac{\partial G_{k_1}(r, r')}{\partial n(r')} - \partial_n u^s(r') G_{k_1}(r, r') \right\} \, ds(r') =$$

$$\begin{cases} u^s(r) & \text{if } r \in \Omega_{1,h} \\ 0 & \text{if } r \in \Omega_2 \end{cases}$$

where integration is carried out over the multiply connected curve $\partial \Omega_{1,h}$ that comprises $\Gamma_1$, $\Gamma_{2,h}$, $\Gamma_{3,h}$, and the straight horizontal lines $\Gamma_{\pm h} = \{(x, y) \in R : y = \pm h\}$ with normals pointing toward the interior of $\Omega_{1,h}$.

Applying the Cauchy-Schwartz inequality, we have

$$\left| \int_{\Gamma_{\pm h}} u^s(r') \frac{\partial G_{k_1}(r, r')}{\partial n(r')} \, ds(r') \right| \leq \left( \int_{\Gamma_{\pm h}} |u^s|^2 \, ds \right)^{1/2} \left( \int_{\Gamma_{\pm h}} \left| \frac{\partial G_{k_1}(r, r')}{\partial n(r')} \right|^2 \, ds \right)^{1/2},$$

$$\left| \int_{\Gamma_{\pm h}} \partial_n u^s(r') G_{k_1}(r, r') \, ds(r') \right| \leq \left( \int_{\Gamma_{\pm h}} |\partial_n u^s|^2 \, ds \right)^{1/2} \left( \int_{\Gamma_{\pm h}} |G_{k_1}(r, r')|^2 \, ds \right)^{1/2}.$$
Therefore, from the uniform boundedness of \( u^s \) and \( \partial_n u^s \) on \( \Gamma_{\pm h} \) for all \( h > \max\{h^+, -h^-\} \) (which follows from (2.5)), and the large-argument asymptotic expansion of the Hankel functions (see e.g. (Abramowitz et al., 1966)), we obtain

\[
\left| \int_{\Gamma_{\pm h}} \frac{u^s(r') \partial G_{k_1}(r, r')}{\partial n(r')} \, ds(r') \right| \lesssim \frac{1}{\sqrt{h}} \to 0 \quad \text{and} \\
\left| \int_{\Gamma_{\pm h}} \partial_n u^s(r') G_{k_1}(r, r') \, ds(r') \right| \lesssim \frac{1}{\sqrt{h}} \to 0 \quad \text{as} \quad h \to \infty.
\]

Taking then the limit as \( h \to \infty \) in the remaining integrals over \( \Gamma_{2,h} \) and \( \Gamma_{3,h} \) we arrive at the integral representation formula

\[
\left( \int_{\Gamma_1} + \int_{\Gamma_2} - \int_{\Gamma_3} \right) \left\{ u^s(r') \frac{\partial G_{k_1}(r, r')}{\partial n(r')} - \partial_n u^s(r') G_{k_1}(r, r') \right\} \, ds(r') =
\begin{cases} 
  u^s(r) & \text{if } r \in \Omega_1 \\
  0 & \text{if } r \in \Omega_2.
\end{cases}
\] (2.15)

Note that only the boundedness of the scattered field and its gradient was used in these derivations, not the radiation condition. More, precisely, any bounded homogenous solutions of the Helmholtz equation in \( \Omega_1 \) admits the integral representation (2.15). In particular, it can be shown (cf. (DeSanto & Martin, 1998)) that upgoing and downgoing planewaves (2.7) for \( n \in \mathcal{P} \) as well as horizontally propagating modes (2.8b) for \( n \in \mathcal{S} \) satisfy

\[
\left( \int_{\Gamma_2} - \int_{\Gamma_3} \right) \left\{ u^\pm_n(r') \frac{\partial G_{k_1}(r, r')}{\partial n(r')} - \partial_n u^\pm_n(r') G_{k_1}(r, r') \right\} \, ds(r') = u^\pm_n(r), \quad r \in U.
\] (2.16)
Finally, applying the standard Green’s third identity inside $\Omega_2$, we readily obtain the representation formulae

$$ - \int_{\Gamma_1} \left\{ u^{\text{inc}}(r') \frac{\partial G_{k_1}(r,r')}{\partial n(r')} - \partial_n u^{\text{inc}}(r') G_{k_1}(r,r') \right\} \, ds(r') = \begin{cases} 0 & \text{if } r \in \Omega_1 \\ u^{\text{inc}}(r) & \text{if } r \in \Omega_2 \end{cases} \quad (2.17) $$

and

$$ - \int_{\Gamma_1} \left\{ u^t(r') \frac{\partial G_{k_2}(r,r')}{\partial n(r')} - \partial_n u^t(r') G_{k_2}(r,r') \right\} \, ds(r') = \begin{cases} 0 & \text{if } r \in \Omega_1 \\ u^t(r) & \text{if } r \in \Omega_2. \end{cases} \quad (2.18) $$

for the incident and transmitted fields inside $\Omega_2$.

### 2.4. Parametrized integral operators

This section presents the notation and the main properties of the Helmholtz layer potentials and boundary integral operators used in the construction of the direct boundary integral equation in Section 2.5.

For a given wavenumber $k_j$, $j = 1$ or $2$, and a sufficiently regular density function $\varphi : \Gamma_i \to \mathbb{C}$, with $\Gamma_i$ being one of the curves defined above in Section 2.3, we respectively define the Helmholtz single- and double-layer potentials by

$$ (SL^j_i \varphi)(r) := \int_{\Gamma_i} G_{k_j}(r,r')\varphi(r') \, ds(r'), \quad \text{and} $$

$$ (DL^j_i \varphi)(r) := \int_{\Gamma_i} \frac{\partial G_{k_j}(r,r')}{\partial n(r')}\varphi(r') \, ds(r'), \quad r \in \mathbb{R}^2 \setminus \Gamma_i $$

where the integrals associated with unbounded curves $\Gamma_i$, $i = 2, 3$, should be interpreted as improper conditionally convergent integrals.
Formally, these operators are defined as

\[
\begin{align*}
(\gamma^+_{D,\Gamma_i} SL_j^i) \varphi &= V^i_j \varphi, \quad (\gamma^+_{N,\Gamma_i} SL_j^i) \varphi = \mp \delta_{i,\ell} \frac{\varphi}{2} + \tilde{K}^i_{j} \varphi; \\
(\gamma^+_{N,\Gamma_i} DL_j^i) \varphi &= W^i_j \varphi, \\
(\gamma^+_{D,\Gamma_i} DL_j^i) \varphi &= \pm \delta_{i,\ell} \frac{\varphi}{2} + K^i_{j} \varphi, 
\end{align*}
\]

(2.20)

where \( V^i_j, K^i_{j}, \tilde{K}^i_{j} \) and \( W^i_j \) are the single-layer, double-layer, adjoint double-layer, and hypersingular operators with wavenumber \( k_j \), target curve \( \Gamma_\ell \), and source curve \( \Gamma_i \). Formally, these operators are defined as

\[
\begin{align*}
(V^i_j \varphi)(r) &= \int_{\Gamma_i} G_{kj}(r, r') \varphi(r') \, ds(r') \quad (2.21a) \\
(K^i_{j} \varphi)(r) &= \int_{\Gamma_i} \frac{\partial G_{kj}(r, r')}{\partial n(r')} \varphi(r') \, ds(r') \quad (2.21b) \\
(\tilde{K}^i_{j} \varphi)(r) &= \int_{\Gamma_i} \frac{\partial G_{kj}(r, r')}{\partial n(r)} \varphi(r') \, ds(r') \quad (2.21c) \\
(W^i_j \varphi)(r) &= \text{f.p.} \int_{\Gamma_i} \frac{\partial^2 G_{kj}(r, r')}{\partial n(r)\partial n(r')} \varphi(r') \, ds(r'), \quad r \in \Gamma_\ell, \quad (2.21d)
\end{align*}
\]

where “f.p.” indicates that the integral in the definition of the hypersingular operator has to be interpreted as a Hadamard finite part integral. The symbol \( \delta_{i,\ell} \) in (2.20), on the other hand, denotes the Kronecker delta.

In order to deal with the quasi-periodicity condition, it will be convenient to work with the layer potentials (2.19) and the integral operators (2.21) in parametric form. For a sufficiently smooth density function \( \varphi : \Gamma_i \to \mathbb{C} \), we let \( \phi = \varphi \circ r_i : I_1 \to \mathbb{C} \), with \( I_1 = [0, 2\pi] \) and \( I_2 = I_3 = \mathbb{R} \), and define the parametric layer potentials as \((S_j^i \phi)(r) := (SL_j^i \varphi)(r)\) and \((D_j^i \phi)(r) := (DL_j^i \varphi)(r)\), or, more explicitly as

\[
\begin{align*}
(S_j^i \phi)(r) &= \frac{i}{4} \int_{I_1} H_0^{(1)}(k_j |r - r_i(\tau)|) \phi(\tau) |r_i'(\tau)| \, d\tau, \\
(D_j^i \phi)(r) &= \frac{ik_j}{4} \int_{I_1} H_1^{(1)}(k_j |r - r_i(\tau)|) \frac{(r - r_i(\tau)) \cdot n_i(\tau)}{|r - r_i(\tau)|} \phi(\tau) |r_i'(\tau)| \, d\tau, \quad r \in \mathbb{R}^2 \setminus \Gamma_i, \quad (2.22)
\end{align*}
\]

where \( n_i = (y_i', -x_i')/|r_i'| \) denotes the parametrized unit normal vector to the curve \( \Gamma_i \).
Similarly, the parametric boundary integral operators are defined as $V_{j}^{\ell,i}\phi = (V_{j}^{\ell,i}\phi) \circ r_{\ell}$, $K_{j}^{\ell,i}\phi = (K_{j}^{\ell,i}\phi) \circ r_{\ell}$, and $W_{j}^{\ell,i}\phi = (W_{j}^{\ell,i}\phi) \circ r_{\ell}$. For self-containment we write them in extensive as

$$
(\mathbf{V}_{j}^{\ell,i})(t) = \int_{I_{i}} Q_{V,j}^{\ell,i}(t, \tau) \phi(\tau) |r'_{i}(\tau)| \, d\tau,
$$

$$
(K_{j}^{\ell,i})(t) = \int_{I_{i}} Q_{K,j}^{\ell,i}(t, \tau) \phi(\tau) |r'_{i}(\tau)| \, d\tau,
$$

$$
(\mathbf{K}_{j}^{\ell,i})(t) = \int_{I_{i}} Q_{K,j}^{\ell,i}(t, \tau) \phi(\tau) |r'_{i}(\tau)| \, d\tau,
$$

$$
(W_{j}^{\ell,i})(t) = \text{f.p.} \int_{I_{i}} Q_{W,j}^{\ell,i}(t, \tau) \phi(\tau) |r'_{i}(\tau)| \, d\tau
$$

(2.23)

where letting $R_{\ell,i} = r_{\ell}(t) - r_{i}(\tau)$ and $R_{\ell,i} = |r_{\ell}(t) - r_{i}(\tau)|$, the integral kernels can be expressed as

$$
Q_{V,j}^{\ell,i}(t, \tau) := \frac{i}{4} H_{0}^{(1)}(k_{j} R_{\ell,i})
$$

(2.24a)

$$
Q_{K,j}^{\ell,i}(t, \tau) := \frac{ik_{j}}{4} H_{1}^{(1)}(k_{j} R_{\ell,i}) \frac{R_{\ell,i} \cdot n_{i}(\tau)}{R_{\ell,i}}
$$

(2.24b)

$$
Q_{K,j}^{\ell,i}(t, \tau) := -\frac{ik_{j}}{4} H_{1}^{(1)}(k_{j} R_{\ell,i}) \frac{R_{\ell,i} \cdot n_{i}(t)}{R_{\ell,i}}
$$

(2.24c)

$$
Q_{W,j}^{\ell,i}(t, \tau) := \frac{ik_{j}}{4} \left( \frac{H_{1}^{(1)}(k_{j} R_{\ell,i})}{R_{\ell,i}} n_{i}(t) \cdot n_{i}(\tau) + \left\{ k_{j} R_{\ell,i} H_{0}^{(1)}(k_{j} R_{\ell,i}) - 2H_{1}^{(1)}(k_{j} R_{\ell,i}) \right\} \frac{R_{\ell,i} \cdot n_{i}(\tau) R_{\ell,i} \cdot n_{i}(t)}{R_{\ell,i}^{3}} \right)
$$

(2.24d)

for $i, \ell = 1, 2, 3$ and $j = 1, 2$.

The following simple result greatly simplifies the final form of the the BIEs derived in the sequel:

**PROPOSITION 2.1.** The identities

$$
V_{1}^{2,2} = V_{1}^{3,3}, \quad K_{1}^{2,2} = K_{1}^{3,3}, \quad \mathbf{K}_{1}^{2,2} = \mathbf{K}_{1}^{3,3} \quad \text{and} \quad W_{1}^{2,2} = W_{1}^{3,3}
$$

(2.25)

hold for the parametrized integral operators defined in (2.23) associated with the parallel curves $\Gamma_{2}$ and $\Gamma_{3}$ defined in (2.14). Furthermore,

$$
V_{1}^{2,3} = V_{1}^{3,2}, \quad K_{1}^{2,3} = -K_{1}^{3,2}, \quad \mathbf{K}_{1}^{2,3} = -\mathbf{K}_{1}^{3,2} \quad \text{and} \quad W_{1}^{2,3} = W_{1}^{3,2}
$$

(2.26)
in the particular case when $\Gamma_2$ and $\Gamma_3$ are straight vertical lines with constant unit normal $e_1$.

**Proof.** The first part (2.25) follows directly from the fact $r_3(t) = r_2(t) + L e_1$, $t \in \mathbb{R}$ and hence $R_{2,2} = R_{3,3}$, $R_{2,2} = R_{3,3}$ and $n_2 = n_3$ in (2.24). For the second part (2.26) the proof follows from writing the integral kernels (2.24) using the parametrizations $r_2(t) = -\frac{L}{2} e_1 + y_2(t) e_2$ for $\Gamma_2$ and $r_3(t) = \frac{L}{2} e_1 + y_2(t) e_2$ for $\Gamma_3$ that have a constant unit normal $n_2(t) = n_3(t) = e_1$ for all $t \in \mathbb{R}$. Therefore, in view of the fact that $R_{2,3} = \sqrt{L^2 + (y_2(t) - y_2(r))^2} = R_{3,2}$, $R_{2,3} \cdot e_1 = -L = -R_{3,2} \cdot e_1$ and $|r_3'| = |r_3'|$ in this case, the identities in (2.26) readily follow. □ □

### 2.5. Boundary integral equation formulation

A direct BIE formulation for the quasi-periodic transmission problem presented in Section 2.2 is derived in this section. Our strategy lies in recasting the problem as a (formally) second-kind system of boundary integral equations for the interior traces of the total field on $\Gamma_1$ and for the traces of the scattered field on the unbounded curves $\Gamma_2$ and $\Gamma_3$. We follow here the Kress-Roach approach (Kress & Roach, 1978) (also known as Müller’s formulation (Müller, 2013) for its 3D electromagnetic version) which yields two second-kind integral equations from enforcing the transmission conditions (2.2c) on $\Gamma_1$. The remaining two equations, on the other hand, are derived from the representation formula (2.15) that is used to suitably combine the traces of the scattered field on $\Gamma_2$ and $\Gamma_3$, to obtain second-kind equations that account for the quasi-periodicity of the scattered field. One salient advantage of our approach is that the resulting integral operators are expressed in terms weakly-singular and smooth kernels that can integrated with high precision using global trigonometric quadrature rules.

We start off by noting that by virtue of the quasi-periodicity condition (2.2b) the traces $\gamma_{D,\Gamma_3} u^s$ and $\gamma_{N,\Gamma_4} u^s$ can be expressed in terms of $\gamma_{D,\Gamma_2} u^s$ and $\gamma_{N,\Gamma_2} u^s$ (see (2.3) for the definition of the trace operators). Indeed, using the curve parametrizations $r_i : I_i \rightarrow \Gamma_i$ for
the curves \( \Gamma_i, i = 1, 2, 3 \), we have that the scattered field traces on the \( \Gamma_2 \) and \( \Gamma_3 \) satisfy
\[
(\gamma_{D,\Gamma_3}^- u^s) \circ r_3 = \zeta (\gamma_{N,\Gamma_3}^- u^s) \circ r_2 \quad \text{and} \quad (\gamma_{D,\Gamma_3}^+ u^s) \circ r_3 = \zeta (\gamma_{N,\Gamma_3}^+ u^s) \circ r_2 \quad (\zeta = e^{i\alpha L}),
\]
(2.27)
where we have used the facts that \( \Gamma_3 \) is parametrized by \( r_3(t) = r_2(t) + Le_1 \) and that the curves share the same unit normal \( n_2 = n_3 = (y'_2, -x'_2)/|r'_2| \) where \( r_2 = (x_2, y_2) \). It hence follows from (2.27) that only the parametrized traces
\[
\phi_1 := (\gamma_{D,\Gamma_1}^- u^t) \circ r_1 : [0, 2\pi) \to \mathbb{C} \quad \phi_2 := (\gamma_{N,\Gamma_1}^- u^t) \circ r_1 : [0, 2\pi) \to \mathbb{C} \\
\phi_3 := (\gamma_{D,\Gamma_2}^+ u^s) \circ r_2 : \mathbb{R} \to \mathbb{C} \quad \phi_4 := (\gamma_{N,\Gamma_2}^+ u^s) \circ r_2 : \mathbb{R} \to \mathbb{C}
\]
are needed in order to retrieve the fields by means of the representation formulae (2.15), (2.18) and (2.17).

![Figure 2.3. Depiction of the relevant curve parametrizations and associated scattered-field and total-field traces (2.28) utilized in our BIE formulation.](image)

Indeed, by the transmission conditions (2.2c) we have \( \gamma_{D,\Gamma_1}^- u^s = \gamma_{D,\Gamma_1}^- (u^t - u^{inc}) \) and \( \gamma_{N,\Gamma_1}^+ u^s = \gamma_{N,\Gamma_1}^- (\eta \partial_n u^t - u^{inc}) \). Therefore, the representation formulae (2.15) and (2.17) can be combined with (2.27) to obtain the following integral representation of the scattered
field
\[ u^e(r) = (D_1^1 \phi_1)(r) - \eta(S_1^1 \phi_2)(r) + (D_2^2 \phi_3)(r) - (S_1^2 \phi_4)(r) \]
\[-\zeta \left\{ (D_1^3 \phi_3)(r) - (S_1^3 \phi_4)(r) \right\}, \quad r \in \Omega_1 \]  
(2.29)
where we have used the parametrized form of the layer potentials (2.22). Similarly, the transmitted field in (2.18) can be expressed as
\[ u^t(r) = - (D_2^2 \phi_1)(r) + (S_2^2 \phi_2)(r), \quad r \in \Omega_2 \]  
(2.30)
in terms of the unknown densities (2.28).

To fix ideas, we present Figure 2.3 which depicts the curve parametrizations involved in the derivations above together with the parametrized traces (2.28) that are the unknowns of our BIE formulation.

We then proceed to derive a system of BIEs for (2.28). Letting
\[ f = (\gamma^-_{D, \Gamma_1} u^{inc}) \circ r_1 \quad \text{and} \quad g = (\gamma^-_{N, \Gamma_1} u^{inc}) \circ r_1 \]  
(2.31)
we have that a direct application of the jump conditions (2.20) to evaluate (2.29) and its normal derivative on \( \Gamma_1 \), yields the equations
\[- f + \frac{\phi_1}{2} = K^{1,1}_1 \phi_1 - \eta V^{1,1}_1 \phi_2 + (K^{1,2}_1 - \zeta K^{1,3}_1) \phi_3 - (V^{1,2}_1 - \zeta V^{1,3}_1) \phi_4 \]  
(2.32a)
\[- g + \frac{\eta}{2} \phi_2 = W^{1,1}_1 \phi_1 - \eta \tilde{K}^{1,1}_1 \phi_2 + (W^{1,2}_1 - \zeta W^{1,3}_1) \phi_3 - (\tilde{K}^{1,2}_1 - \zeta \tilde{K}^{1,3}_1) \phi_4 \]  
(2.32b)
which hold in \([0, 2\pi]\). Similarly, using (2.20) to evaluate the transmitted field (2.30) and its normal derivative on \( \Gamma_1 \), we obtain
\[ \frac{\phi_1}{2} = - K^{1,1}_2 \phi_1 + V^{1,1}_2 \phi_2 \]  
(2.33a)
\[ \frac{\phi_2}{2} = - W^{1,1}_2 \phi_1 + \tilde{K}^{1,1}_2 \phi_2 \]  
(2.33b)
which hold in \([0, 2\pi]\).
Therefore, adding (2.33a) to (2.32a) and adding (2.33b) to (2.32b) we arrive at the following integral equations

\[
\phi_1 + \sum_{q=1}^{4} M_{1,q} \phi_q = f \quad \text{and} \quad \left(\frac{1 + \eta}{2}\right) \phi_2 + \sum_{q=1}^{4} M_{2,q} \phi_q = g \quad \text{in} \quad [0, 2\pi) \quad (2.34)
\]

where

\[
M_{1,1} := \mathcal{K}_1^{1,1} - \mathcal{K}_1^{1,1}, \quad M_{1,2} := \eta \mathcal{V}_1^{1,1} - \mathcal{V}_2^{1,1},
\]
\[
M_{1,3} := \zeta \mathcal{K}_1^{1,3} - \mathcal{K}_1^{1,2}, \quad M_{1,4} := \mathcal{V}_1^{1,2} - \zeta \mathcal{V}_1^{1,3},
\]
\[
M_{2,1} := \mathcal{W}_2^{1,1} - \mathcal{W}_1^{1,1}, \quad M_{2,2} := \eta \tilde{\mathcal{K}}_1^{1,1} - \tilde{\mathcal{K}}_2^{1,1},
\]
\[
M_{2,3} := \zeta \mathcal{W}_1^{1,3} - \mathcal{W}_1^{1,2}, \quad M_{2,4} := \tilde{\mathcal{K}}_1^{1,2} - \zeta \tilde{\mathcal{K}}_1^{1,3}.
\]

**Remark 2.1.** As mentioned above, all the integral operators in (2.35) are weakly singular. Indeed, for instance, the seemingly hypersingular operator \(M_{2,1} = \mathcal{W}_2^{1,1} - \mathcal{W}_1^{1,1}\) is weakly singular by virtue of the fact that hypersingular parametric kernel, defined in (2.24d), can be expressed as

\[
Q_{W_1}^{1,1}(t, \tau) = \frac{n_1(t) \cdot n_1(\tau)}{2\pi R_1^2} + a_j(t, \tau) \log(|t - \tau|) + b_j(t, \tau), \quad t, \tau \in [0, 2\pi),
\]

where \(a_j, b_j : [0, 2\pi)^2 \to \mathbb{C}\) are smooth \(2\pi\)-periodic functions in both arguments (Kress, 1995). Therefore, since the hypersingular static terms \(\frac{n_1(t) \cdot n_1(\tau)}{2\pi R_1^2}\) cancels when we take the difference \(Q_{W_2}^{1,1} - Q_{W_1}^{1,1}\), the integral kernel of \(M_{2,1}\) features only a logarithmic singularity as \(t \to \tau\). \(\square\)

In order to find the two additional integral equations, we take the Dirichlet and Neumann traces (2.3) of (2.29) on \(\Gamma_2\) and \(\Gamma_3\) using the jump relations (2.20), to obtain

\[
\frac{\phi_3}{2} = \mathcal{K}_1^{1,1} \phi_1 - \eta \mathcal{V}_1^{1,1} \phi_2 + (\mathcal{K}_1^{2,2} - \zeta \mathcal{K}_1^{2,3}) \phi_3 - (\mathcal{V}_1^{2,2} - \zeta \mathcal{V}_1^{2,3}) \phi_4 \quad (2.36a)
\]
\[
\frac{\phi_4}{2} = \mathcal{W}_1^{2,1} \phi_1 - \eta \tilde{\mathcal{K}}_1^{2,1} \phi_2 + (\mathcal{W}_1^{2,2} - \zeta \mathcal{W}_1^{2,3}) \phi_3 - (\mathcal{K}_1^{2,2} - \zeta \mathcal{K}_1^{2,3}) \phi_4 \quad (2.36b)
\]
\[
\zeta \frac{\phi_3}{2} = \mathcal{K}_1^{3,1} \phi_1 - \eta \mathcal{V}_1^{3,1} \phi_2 + (\mathcal{K}_1^{3,2} - \zeta \mathcal{K}_1^{3,3}) \phi_3 - (\mathcal{V}_1^{3,2} - \zeta \mathcal{V}_1^{3,3}) \phi_4 \quad (2.36c)
\]
\[
\zeta \frac{\phi_4}{2} = \mathcal{W}_1^{3,1} \phi_1 - \eta \tilde{\mathcal{K}}_1^{3,1} \phi_2 + (\mathcal{W}_1^{3,2} - \zeta \mathcal{W}_1^{3,3}) \phi_3 - (\mathcal{K}_1^{3,2} - \zeta \mathcal{K}_1^{3,3}) \phi_4 \quad (2.36d)
\]
which hold in \( \mathbb{R} \). We then combine these equations to cancel all the weakly-singular \((V_{i,i}^{1,1}, K_{i,i}^{1,1}, i = 2, 3)\) and hypersingular \((W_{i,i}^{1,1}, i = 2, 3)\) operators. In detail, multiplying (2.36a) by \( \zeta \) and adding it to (2.36c), and multiplying (2.36b) by \( \zeta \) and adding it to (2.36d), while using the identities in (2.25), we arrive at

\[
\zeta \phi_3 + \sum_{q=1}^{4} M_{3,q} \phi_q = 0 \quad \text{and} \quad \zeta \phi_4 + \sum_{q=1}^{4} M_{4,q} \phi_q = 0 \quad \text{in} \quad \mathbb{R} \tag{2.37}
\]

where

\[
M_{3,1} := -\zeta K_{1,1}^{2,1} - K_{1,1}^{3,1}, \quad M_{3,2} = \eta(\zeta V_{1,1}^{2,1} + V_{1,1}^{3,1}), \\
M_{3,3} := \zeta^2 K_{1,1}^{2,3} - K_{1,1}^{3,2}, \quad M_{3,4} = V_{1,1}^{3,2} - \zeta^2 V_{1,1}^{2,3}, \\
M_{4,1} := -\zeta W_{1,1}^{2,1} - W_{1,1}^{3,1}, \quad M_{4,2} = \eta(\zeta K_{1,1}^{2,1} + K_{1,1}^{3,1}), \\
M_{4,3} := \zeta^2 W_{1,1}^{2,3} - W_{1,1}^{3,2}, \quad M_{4,4} = \tilde{K}_{1,1}^{3,2} - \zeta^2 \tilde{K}_{1,1}^{2,3}. \tag{2.38}
\]

Clearly, the operators (2.38) have smooth kernels, by virtue of the fact that integration and evaluation are carried out over different well-separated curves.

Finally, lumping the unknown density functions (2.28) in a single vector \( \phi = [\phi_1, \phi_2, \phi_3, \phi_4]^T \) and combining the equations (2.34) and (2.37) we obtain the system

\[
E \phi + M \phi = \phi^{inc} \tag{2.39}
\]

where \( M \) is the \( 4 \times 4 \) block matrix integral operator \( [M]_{i,j} := M_{i,j}, i, j = 1, \ldots, 4 \),

\[
E := \begin{bmatrix} 1 & \frac{1+n}{2} & \zeta & \zeta \\ \zeta & \zeta & \frac{f}{g} & 0 \\ \end{bmatrix} \quad \text{and} \quad \phi^{inc} := \begin{bmatrix} f \\ g \\ 0 \\ 0 \\ \end{bmatrix} \tag{2.40}
\]

Two observations about the system (2.39) are in order. The first one is that the last two equations in (2.39), which account for the quasi-periodicity of the scattered field, need to be satisfied in all of \( \mathbb{R} \). Being these equations as well as the associated density functions \( \phi_3 \) and \( \phi_4 \) defined in an unbounded interval, they need to be effectively truncated in order for them to be suitable to Nyström or boundary element discretizations. We do so in the
next section by means of the WGF method. Secondly, note that the integral equation system (2.39) does not properly account for the radiation condition. Indeed, only the boundedness and the quasi-periodicity of the scattered field were used in its derivation. This important issue is also address in the next section.

REMARK 2.2. In light of Proposition 2.1, half of the operators (2.38) can be significantly simplified in the case when \( \Gamma_2 \) and \( \Gamma_3 \) are parallel vertical lines. In fact, in such case we have

\[
\begin{align*}
M_{3,3} &= -(1 + \zeta^2)K_1^{3,2}, \\
M_{3,4} &= (1 - \zeta^2)V_1^{3,2}, \\
M_{4,3} &= -(1 - \zeta^2)W_1^{2,3}, \\
M_{4,4} &= (1 + \zeta^2)\bar{K}_1^{3,2}.
\end{align*}
\]  
(2.41)

REMARK 2.3. Note that other direct formulations can be used to account for the transmission conditions on \( \Gamma_1 \). For instance, Kress-Roach equations (2.34) can be replaced by the ones resulting from the well-known Costabel-Stephan formulation (Costabel & Stephan, 1985), that can be easily derived by combining (2.32) and (2.33) so as to eliminate \( \phi_1 \) and \( \phi_2 \) from the left-hand side of the equations. In this case we obtain

\[
\sum_{q=1}^{4} \tilde{M}_{1,q}\phi_q = f \quad \text{and} \quad \sum_{q=1}^{4} \tilde{M}_{2,q}\phi_q = g \quad \text{in} \quad [0, 2\pi),
\]

where

\[
\begin{align*}
\tilde{M}_{1,1} &= -K_2^{1,1} - K_1^{1,1}, \\
\tilde{M}_{1,2} &= \eta V_1^{1,1} + V_2^{1,1}, \\
\tilde{M}_{1,3} &= M_{1,3}, \\
\tilde{M}_{1,4} &= M_{1,4}, \\
\tilde{M}_{2,1} &= -\eta W_2^{1,1} - W_1^{1,1}, \\
\tilde{M}_{2,2} &= \eta \bar{K}_1^{1,1} + \eta K_2^{1,1}, \\
\tilde{M}_{2,3} &= M_{2,3}, \\
\tilde{M}_{2,4} &= M_{2,4}.
\end{align*}
\]

Unlike the advocated Kress-Roach approach, this formulation involves the (non-compact) hypersingular operator \( \tilde{M}_{2,1} \) that negatively affect the conditioning of the discretized integral equation system, hindering the use of GMRES (Saad & Schultz, 1986) and standard acceleration techniques based on fast matrix-vector products (Rokhlin, 1990).  \( \square \)
2.6. Windowed Green function method

In view of the definitions in (2.38), it is clear that several of the operators making up $M$ involve integration and evaluation over the unbounded curves $\Gamma_2$ or $\Gamma_3$. In order to reduce the BIE system (2.39) to a finite-size computational domain where standard BIE solvers can be applied, the domain of integration of the boundary integral operators over $\Gamma_2$ and $\Gamma_3$ has to be effectively truncated. We address this issue here by means of the WGF method (O. Bruno et al., 2016).

The WGF method relies on the use of a slow-rise window function $\chi(\cdot, cA, A) \in C_0^\infty(\mathbb{R})$, $c \in (0, 1)$, $A > 0$, which following (O. Bruno et al., 2016) is selected as

$$
\chi(y, y_0, y_1) := \begin{cases} 
1 & \text{if } |y| \leq y_0 \\
\exp\left(\frac{2e^{-1/u}}{u - 1}\right) & \text{if } y_0 < |y| < y_1, u = \frac{|y| - y_0}{y_1 - y_0} \\
0 & \text{if } |y| > y_1.
\end{cases}
$$

Note that $\chi(\cdot, cA, A)$ vanishes together with all its derivatives in $\mathbb{R} \setminus [-A, A]$ and it equals one within $[-cA, cA]$. In what follows we assume that $cA > \max\{h^+, -h^\}$ so that the periodic array $D_2$ lies within the strip $\mathbb{R} \times [-cA, cA]$.

Next, letting

$$
w_A := \chi(\cdot, cA, A) \circ y_2 \quad \text{and} \quad w_c^c := 1 - w_A, \quad t \in \mathbb{R},
$$

and replacing the split density

$$
\phi_j = w_A \phi_j + w_c^c \phi_j \quad \text{for } j = 3, 4
$$
in (2.34)-(2.37), we obtain

\[
\phi_1(t) + \sum_{q=1}^{2} M_{1,q}[\phi_q](t) + \sum_{q=3}^{4} M_{1,q}[w_A \phi_q](t) = f(t) - \psi_1(t), \quad t \in [0, 2\pi),
\]

(2.44a)

\[
\left(1 + \frac{\eta}{2}\right) \phi_2(t) + \sum_{q=1}^{2} M_{2,q}[\phi_q](t) + \sum_{q=3}^{4} M_{2,q}[w_A \phi_q](t) = g(t) - \psi_2(t), \quad t \in [0, 2\pi),
\]

(2.44b)

\[
\zeta \phi_3(t) + \sum_{q=1}^{2} M_{3,q}[\phi_q](t) + \sum_{q=3}^{4} M_{3,q}[w_A \phi_q](t) = -\psi_3(t), \quad t \in \mathbb{R},
\]

(2.44c)

\[
\zeta \phi_4(t) + \sum_{q=1}^{2} M_{4,q}[\phi_q](t) + \sum_{q=3}^{4} M_{4,q}[w_A \phi_q](t) = -\psi_4(t), \quad t \in \mathbb{R},
\]

(2.44d)

where the terms that were moved to the right-hand side in (2.44) are the tail integrals

\[
\psi_p = M_{p,3}[w_c^e \phi_3] + M_{p,4}[w_c^e \phi_4], \quad p = 1, \ldots, 4.
\]

(2.45)

Our boundary integral equation formulation relies on constructing suitable approximations of \(\psi_p, p = 1, \ldots, 4\), taking into account the radiation condition (2.11) and the super-algebraic decay as \(A \to \infty\) of certain oscillatory windowed integrals. Upon replacing \(\psi_p, p = 1, \ldots, 4\), by their respective approximations in (2.44) and restricting the integral equations (2.44c) and (2.44d) to the bounded interval \([-A, A]\), we obtain a windowed integral equation suitable to be discretize by standard Nyström or boundary element methods.

We then proceed to construct suitable approximations for the tail integrals \(\psi_p, p = 1, \ldots, 4\). For the sake of presentation simplicity and without loss of generality in the remainder of this section we assume that \(r_2(t) = -\frac{i}{2}e_1 + te_2\) (i.e., \(y_2(t) = t\) ) for \(t > |cA|\). From the general quasi-periodic expansion (2.9) of the scattered field it follows that within \(\text{supp}(w_c^e) = \{t \in \mathbb{R} : |t| \geq cA\}\) the parametrized traces \(\phi_3\) and \(\phi_4\) (2.28) associated with
the unbounded curves \( \Gamma_2 \), can be expressed as
\[
\phi_3(t) = \sum_{n \in P \cup E} e^{i \alpha_n \frac{t}{2}} \left\{ B_n^+ e^{i \beta_n t} + C_n^+ e^{i \beta_n t} \right\} + \sum_{n \in S} e^{-i \alpha_n \frac{t}{2}} \left\{ B_n^- + C_n^- \right\},
\]
\[
\phi_4(t) = \sum_{n \in P \cup E} i \alpha_n e^{-i \alpha_n \frac{t}{2}} \left\{ B_n^+ e^{i \beta_n t} + C_n^+ e^{i \beta_n t} \right\} + \sum_{n \in S} i \alpha_n e^{-i \alpha_n \frac{t}{2}} \left\{ B_n^- + C_n^- \right\}
\]
(2.46)
for \( \pm t > cA \). Splitting \( w_A^\epsilon = 1 - w_A \) as \( w_A^c = \chi_A^- + \chi_A^+ \) where
\[
\chi_A^- = 1_{(-\infty,0)} w_A^\epsilon \quad \text{and} \quad \chi_A^+ = 1_{(0,\infty)} w_A^\epsilon,
\]
(2.47)
and replacing (2.46) in (2.45), we arrive at
\[
\psi_p = \psi_p^{(B)} + \psi_p^{(C)}, \quad p = 1, \ldots, 4,
\]
(2.48)
where
\[
\psi_p^{(B)} = \sum_{n \in \mathbb{Z}} e^{i \alpha_n \frac{t}{2}} B_n^\epsilon \left\{ M_{p,3} \left[ \chi_A^+ e^{i \beta_n |\epsilon|} \right] + i \alpha_n M_{p,4} \left[ \chi_A^+ e^{i \beta_n |\epsilon|} \right] \right\} + \sum_{n \in \mathbb{Z}} e^{i \alpha_n \frac{t}{2}} B_n^- \left\{ M_{p,3} \left[ \chi_A^- e^{i \beta_n |\epsilon|} \right] + i \alpha_n M_{p,4} \left[ \chi_A^- e^{i \beta_n |\epsilon|} \right] \right\}
\]
(2.49)
and
\[
\psi_p^{(C)} = \sum_{n \in P \cup E} e^{-i \alpha_n \frac{t}{2}} C_n^+ \left\{ M_{p,3} \left[ \chi_A^+ e^{-i \beta_n |\epsilon|} \right] + i \alpha_n M_{p,4} \left[ \chi_A^+ e^{-i \beta_n |\epsilon|} \right] \right\} + \sum_{n \in P \cup E} e^{-i \alpha_n \frac{t}{2}} C_n^- \left\{ M_{p,3} \left[ \chi_A^- e^{-i \beta_n |\epsilon|} \right] + i \alpha_n M_{p,4} \left[ \chi_A^- e^{-i \beta_n |\epsilon|} \right] \right\} + \sum_{n \in S} e^{-i \alpha_n \frac{t}{2}} C_n^+ \left\{ M_{p,3} \left[ \chi_A^+ e^{\cdot} \right] + i \alpha_n M_{p,4} \left[ \chi_A^+ e^{\cdot} \right] \right\} + \sum_{n \in S} e^{-i \alpha_n \frac{t}{2}} C_n^- \left\{ M_{p,3} \left[ \chi_A^- e^{\cdot} \right] + i \alpha_n M_{p,4} \left[ \chi_A^- e^{\cdot} \right] \right\},
\]
(2.50)
Let us first examine the term \( \psi_p^{(B)}, \ p = 1, \ldots, 4 \). In view of the boundedness of the Rayleigh coefficients \( B_n^\pm \) in (2.49) and the exponential decay as \(|t| \to \infty\) of the functions
e^{i\beta_n|t|} for \( \beta_n \in i\mathbb{R}_{>0} \) (i.e., \( n \in \mathcal{E} \)), we have that the approximation

\[
\psi^{(B)}_p \approx \sum_{n \in \mathcal{P} \cup \mathcal{S}} e^{i\alpha_n \frac{t}{A}} B_n^+ \left\{ M_{p,3} \left[ \chi_A^+ e^{i\beta_n|t|} \right] + i\alpha_n M_{p,4} \left[ \chi_A^+ e^{i\beta_n|t|} \right] \right\} +
\sum_{n \in \mathcal{P} \cup \mathcal{S}} e^{i\alpha_n \frac{t}{A}} B_n^- \left\{ M_{p,3} \left[ \chi_A^- e^{i\beta_n|t|} \right] + i\alpha_n M_{p,4} \left[ \chi_A^- e^{i\beta_n|t|} \right] \right\}
\]

(2.51)

introduces errors that decrease exponentially fast as \( A \to \infty \).

Next, for \( \beta_n \in \mathbb{R}_{\geq 0} \) (i.e., \( n \in \mathcal{P} \cup \mathcal{S} \)), we note that \( M_{p,q} \left[ \chi_A^\pm e^{i\beta_n|t|} \right] \) for \( p = 1, 2 \), \( t \in [0, 2\pi) \), and for \( p = 3, 4 \), \( t \in [-cA, cA] \), decays super-algebraically fast as \( A \to \infty \) (i.e., faster than \( O((k_1 + \beta_n)A^{-m}) \) for all \( m \in \mathbb{N} \)) (O. Bruno et al., 2016; O. P. Bruno & Pérez-Arancibia, 2017; Pérez-Arancibia, 2017). We refer the reader to Appendix A for a detailed justification of this estimate. Given then the fast convergence of these windowed integrals as \( A \to \infty \), we adopt the approximation

\[
\psi^{(B)}_p \approx 0, \quad p = 1, \ldots, 4,
\]

(2.52)

Let us now look into the terms \( \psi^{(C)}_p \), \( p = 1, \ldots, 4 \). In principle, the radiation condition (2.11) requires all the coefficients \( C_n^\pm \) in (2.50) to vanish. These conditions can be easily incorporated in our formulation by simply setting \( \psi^{(C)}_p = 0 \). This together with (2.52)—which amount to simply ignore the tail integrals (2.45)—yield the following windowed integral equation:

\[
E\phi_A + M W_A \phi_A = \phi^{inc}
\]

(2.53)

where

\[
W_A(t) := \begin{bmatrix}
1 \\
1 \\
1 \\
w_A(t)
\end{bmatrix}, \quad t \in \mathbb{R}.
\]

(2.54)

Here, the first two equations of the system (2.53), associated with the curve \( \Gamma_1 \), correspond to the parameter \( t \in [0, 2\pi) \), while the last two, associated with the truncated curve \( \Gamma_{2,A} = \{ \mathbf{r} \in \mathbb{R}^2 : \mathbf{r} = \mathbf{r}_2(t), |t| \leq A \} \), correspond to \( t \in \text{supp}(w_A) = [-A, A] \). Consequently,
the entries $\phi_{j,A}$, $j = 1, \ldots, 4$, of the solution vector $\phi_A$ are considered functions $\phi_{j,A} : [0, 2\pi] \to \mathbb{C}$ for $j = 1, 2$ and $\phi_{j,A} : [-A, A] \to \mathbb{C}$ for $j = 3, 4$.

2.7. An illustrative numerical example

In this section we consider a series of numerical experiments aimed at assessing the accuracy of the quasi-periodic problem solutions produced by the windowed integral equation (2.53). In all such experiments we consider the diffraction and transmission of a planewave (2.1) in TE polarization ($\eta = 1$) that impinges at an angle $\theta_{\text{inc}} = \frac{\pi}{4}$ on an infinite array of period $L = 2$ consisting of penetrable kite-shaped obstacles (see Figure 2.4(d)) parametrized by

$$r_1(t) = \left\{ \frac{1}{2} \cos t + \frac{13}{40} \cos 2t - \frac{13}{40} \right\} e_1 + \frac{3}{4} \sin t e_2, \quad t \in [0, 2\pi).$$

(2.55)

For clarity of exposition the left ($\Gamma_2$) and right ($\Gamma_3$) hand side boundaries of the unit cell are selected as straight vertical lines parametrized by

$$r_2(t) = -\frac{L}{2} e_1 + t e_2 \quad \text{and} \quad r_3(t) = \frac{L}{2} e_1 + t e_2, \quad t \in \mathbb{R},$$

(2.56)

respectively.

In our first experiment the error in the numerical solution is assessed by means of the energy balance relation (Fernandez-Lado, 2016). We define the energy balance error as how much numerical solutions deviate from conserving energy, or more precisely, as

$$\text{error}_{eb} := \left| 2\text{Re} \left( \tilde{B}_0^- \right) + \sum_{n \in P} \frac{\beta_n}{\beta} \left\{ |\tilde{B}_n^-|^2 + |\tilde{B}_n^+|^2 \right\} \right|$$

(2.57)

where the coefficients in (2.57) are computed via (Fernandez-Lado, 2016)

$$\tilde{B}_n^\pm := e^{\pm i \beta_n h} \frac{L}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} u_A^s(x, \pm h) e^{-i \alpha_n x} \, dx$$

(2.58)
using the WGF approximation of the scattered field given by

\[ u^s_A(r) = (D_1^1 \phi_{A,1})(r) - \eta(S_1^1 \phi_{A,2})(r) + (D_1^2 - \zeta D_1^3)[w_A \phi_{A,3}](r) - (S_1^2 - \zeta S_1^3)[w_A \phi_{A,4}](r) \]  

(2.59)

for \( r = (x, y) \in \Omega_1 \) with \( \phi_{A,j}, j = 1, \ldots, 4 \), denoting the components of the vector density \( \phi_A \) solution of (2.53). Note that, as in the approximations that led to the windowed BIE system (2.53), the errors produced by the windowed integrals in (2.59) decay super-algebraically fast as \( A \to \infty \) for \( r \in \Omega_{1,A} := \{(x, y) \in \Omega_1 : \chi(y, cA, A) = 1\} \) when the exact scattered field traces, \( \phi_j, j = 1, \ldots, 4 \) defined in (2.28), are used.

Highly accurate numerical approximations of \( \phi_A \) are used in all the examples presented in this section. These are obtained by numerically solving (2.53) by means of the spectrally accurate Martensen–Kussmaul (MK) Nyström method (D. Colton & Kress, 2012, sec. 3.5) employing a large number of discretization points (roughly, 8 points per wavelength on each of the relevant curves). The finite-domain integrals in (2.58), on the other hand, are computed using the trapezoidal quadrature rule which, by virtue of the fact that \( u_A^s(\cdot, \pm h) e^{-i\alpha n \cdot} \) is smooth and approximately \( L \)-periodic (see Figure 2.5), it is expected to converge fast as the number of quadrature nodes increases. This choice of discretization methods and parameter values ensure that the dominant part of the energy balance error (2.57) stems solely from the WGF approximation employed in (2.53) and (2.59). In what follows of this section we consider fixed parameter values \( k_2 = 20, c = 0.5, \) and \( h = 1 \).

Figures 2.4(a)-(b) display the energy balance error (2.57) in semi-log and log-log scale, respectively, as a function of the window size \( A \) (measured in wavelengths \( \lambda = 2\pi/k_1 \)) for three different informative \( k_1 \) values at and around a RW-anomaly configuration corresponding to \( k_1 = k^* = 2\pi/(L(1 - \sin \theta_{inc})) \approx 10.7261 \) (\( \beta_1 = 0 \) in this case). At \( k_1 = 10.68 \) to the left of \( k^* \) when \( \beta_1 \in i\mathbb{R}_{>0} \) the expected super-algebraic convergence is achieved, as it can be seen in the blue nearly constant-slope curve plotted in semi-log scale in Figure 2.4(a). Figure 2.4(d) displays the real part of the total field within the
Figure 2.4. Solution of the problem scattering of a planewave at $\theta^{\text{inc}} = \frac{\pi}{4}$ by an infinite periodic array of kite-shaped obstacles obtained using the naive windowed BIE (2.53) and the scattered field approximation (2.59) for $k_2 = 20$, $L = 2$, $c = 0.5$ and various window sizes $A$ and wavenumbers $k_1$ at and around a RW-anomaly configuration corresponding to $k_1 = k^* \approx 10.7261$. Energy balance error (2.57) as a function of $A$ in (a) semi-log and (b) log-log scale computed at $h = 1$. (c) Wavenumber sweep of the energy balance error around $k^*$. (d) Real part of the computed total field within the region $[-\frac{L}{2}, \frac{L}{2}] \times [-cA, cA]$ for $k_1 = 10.68$ and $A = 20\lambda$. 

region $[-\frac{L}{2}, \frac{L}{2}] \times [-cA, cA] = \Omega_{1,A} \cup \Omega_{2}$ for $A = 20\lambda$, produced by the numerical evaluation of formulae (2.59) and (2.18). At $k_1 = k^*$ when $\beta_1 = 0$, in turn, slow (algebraic) convergence is observed while at $k = 10.76$—to the right of $k^*$ when $\beta_1 \in \mathbb{R}_{>0}$—no convergence at all is observed. To examine this issue in more detail, a wider range of $k_1$ values is considered in Figure 2.4(c), which shows a sweep of the error over the interval $[k^* - 0.1, k^* + 0.1]$. Clearly, significant accuracy deterioration occurs at and around the RW-anomaly configuration for all the window sizes considered in this experiment.
There are two main factors that could explain the accuracy deterioration seen in Figure 2.4(c). On the one hand we have the radiation condition, which is indirectly incorporated in our formulation by neglecting all the tail integrals $\psi_j^{(C)}$, $j = 1, \ldots, 4$, in (2.44), and on the other hand, the quasi-periodicity condition (2.2b) which is enforced through the equations (2.44c) and (2.44d) restricted to the interval $[-A, A]$.

In order to verify the quasi-periodicity condition (2.2b), we consider the following experiment. First, the windowed integral equation (2.53) is solved using the MK method to obtain the approximate densities on $\Gamma_1$ and on the truncated vertical curves $\Gamma_{2,A}$ parametrized by $r_2$ in (2.56) with $t$ restricted to $[-A, A]$. Then, assuming that the quasi-periodicity condition holds, we “transfer” the densities to the boundaries of a 3L-period supercell. Referencing to Figure 2.5(a), we have that the supercell consists of the original obstacle’s boundary $\Gamma_1 \subset U$, the shifted obstacles’ boundaries $\Gamma_1 - Le_1$ and $\Gamma_1 + Le_1$, and the truncated parts $\Gamma_{2,A} - Le_1$ and $\Gamma_{3,A} + Le_1$ of the shifted vertical lines $\Gamma_2 - Le_1$ and $\Gamma_3 + Le_1$ which are parametrized by $r_2(\cdot) - Le_1$ and $r_3(\cdot) + Le_1$, respectively. Assuming that the quasi-periodicity condition holds, the densities associated with the supercell boundaries are: $\{\zeta^{-1}\phi_{A,1}, \zeta^{-1}\phi_{A,2}\}$ on $\Gamma_1 - Le_1$, $\{\phi_{A,1}, \phi_{A,2}\}$ on $\Gamma_1 + Le_1$, $\{\zeta^{-1}\phi_{A,3}, \zeta^{-1}\phi_{A,4}\}$ on $\Gamma_{2,A} - Le_1$, and $\{\zeta^2\phi_{A,3}, \zeta^2\phi_{A,4}\}$ on $\Gamma_{3,A} + Le_1$. We then approximate the scattered field within the supercell as $u_A^s$ in (2.59) but integrating on each of the relevant boundaries of the supercell using the aforementioned densities. To verify the quasi-periodicity condition we then introduce the right and left mismatch errors defined as

$$\text{error}^{(r)}_{qp} := \frac{\max_{p=1,\ldots,4} \left| u_A^s(r_p) - \zeta^{-1} u_A^s(r_p + Le_1) \right|}{\max_{p=1,\ldots,4} \left| u_A^s(r_p) \right|}$$

and

$$\text{error}^{(l)}_{qp} := \frac{\max_{p=1,\ldots,4} \left| u_A^s(r_p) - \zeta u_A^s(r_p - Le_1) \right|}{\max_{p=1,\ldots,4} \left| u_A^s(r_p) \right|},$$

respectively, where the sample points are $r_1 = (-0.5, -1)$, $r_2 = (0.5, -1)$, $r_3 = (-0.5, 1)$, and $r_4 = (0.5, 1)$ (they are depicted in Figure 2.5(a) in red). The errors (2.60) corresponding to $k_1 = 10.68$, $k^*$ and 10.76 are displayed in Figures 2.5(b)-(c) in semi-log and log-log scales, respectively, for various window sizes $A \in [10\lambda, 60\lambda]$. These results demonstrate
that, although the enforcement of the quasi-periodicity condition deteriorates as \( k_1 \) approaches the RW-anomaly configuration, the mismatch errors still converge to zero super-algebraically fast as \( A \) increases.

Figure 2.5. Errors (2.60) in the quasi-periodicity condition of the numerical solution produced by the windowed integral equation (2.53). (a) Depiction of the supercell configuration used to assess the left \((l)\) and right \((r)\) mismatch errors (2.60). The density functions associated with the \(3L\)-periodic supercell are obtained from the densities of the middle \(L\)-periodic cell by multiplying them by \( \zeta = e^{i\alpha L} \) and \( \zeta^{-1} = e^{-i\alpha L} \) to transfer them from left to right and from right to left, respectively. Errors in semi-log (b) and log-log (c) scale for the exterior wavenumbers \( k_1 = 10.68, k^* \), and 10.76, and window sizes \( A \in [10\lambda, 60\lambda] \).

Since the quasi-periodicity condition does not seem to be the main factor that explains the poor convergence and the complete lack of it for certain wavenumbers \( k_1 \), we are left
Figure 2.6. Errors (2.61) in the numerical solution obtained from the windowed integral equation (2.53) in the enforcement of the radiation condition (2.11). Three different exterior wavenumbers are considered corresponding to $k_1 = 10.68$ in (a), $k_1 = k^*$ in (b), and $k_1 = 10.76$ in (c). The modes $n \in C_{3k_1/4}$ used in these examples correspond to the smallest $\beta_n$ values arising in each case, which include $\beta_1$ that vanishes in the RW-tanomaly case $k_1 = k^*$ in (b).

Figures 2.6 displays the errors (2.61) for $A \in [10 \lambda, 60 \lambda]$, for the three representative wavenumbers $k_1 = 10.68, k^*$, and 10.76, and for four modes $n \in C_{3k_1/4} = \{-6, -5, 0, 1\}$, where

$$C_\delta := \{n \in \mathbb{Z} : |\beta_n| \leq \delta\}.$$  

This set, which plays an important role below in Section 2.8, consists of the modes which are the closest to horizontally traveling waves. In the case $k_1 = 10.68$, which is considered in Figure 2.6(a) and where $\beta_{-6} \approx 3.6844i$, $\beta_{-5} \approx 6.8950$, $\beta_0 \approx 7.5519$ and
$\beta_1 \approx 0.5370i$, all the corresponding errors (2.61) exhibit superalgebraic convergence as $A$ increases. In turn, in the RW-anomaly case $k_1 = k^*$, considered in Figure 2.6(b) and where $\beta_{-6} \approx 3.4429i$, $\beta_{-5} \approx 7.0041$, $\beta_0 \approx 7.5845$ and $\beta_1 = 0$, slow convergence of $\text{error}_{r_c}^{(\pm,1)}$ is observed. Finally, in the case $k_1 = 10.76$, considered in Figure 2.6(c) and where $\beta_{-6} \approx 3.2534i$, $\beta_{-5} \approx 7.0835$, $\beta_0 \approx 7.6085$ and $\beta_1 \approx 0.4624$, we note that $\text{error}_{r_c}^{(\pm,1)}$ does not seem to converge at the all. These observations are consistent with the results displayed in Figures 2.4(a)-(b), that consider the overall energy balance error, and suggest that in practice the windowed BIE (2.53) on its own does not properly enforce the radiation condition of the problem. Indeed, the non-propagative modes corresponding to the smallest $\beta_n$ values, which are contained in $C_\delta$, seem to be polluting the numerical solution.

As it turns out, there is a subtle issue that explains the remarkable failure of the naive windowed BIE (2.53) for certain frequencies. In light of the estimates derived in Appendix A, not only the tail integrals $M_{p,q} \left[ \chi_A^\pm e^{i\beta_n |\cdot|} \right]$ for $\beta_n \in \mathbb{R}_{>0}$ decay super-algebraically fast as $A$ increases, but also $M_{p,q} \left[ \chi_A^\pm e^{-i\beta_n |\cdot|} \right]$ in (2.50) as long as $\beta_n \in \mathbb{R}_{>0}$ and $\beta_n \neq k_1$. Indeed, these tend to zero faster than $O(((k_1 - \beta_n)A)^{-m})$ for all $m \geq 1$ as $A \to \infty$. For a fixed $A > 0$, this fact renders $C_n^{\pm}M_{p,q} \left[ \chi_A^\pm e^{-i\beta_n |\cdot|} \right]$ for $\beta_n \in \mathbb{R}_{>0}$, $\beta_n \neq k_1$, in (2.50) “small” regardless of the actual value of the coefficient $C_n^{\pm}$, thus making the conditions $\psi_p^{(C)} = 0$, $p = 1, \ldots, 4$, used in the derivation of (2.53), insufficient to enforce the desired (radiation) condition $C_n^{\pm} = 0$. In other words, the equations $\psi_p^{(C)}(t) = 0$, $t \in [-A, A]$, $p = 1, \ldots, 4$, for the vanishing coefficients $C_n^{\pm}$, become in practice ill-conditioned allowing the presence of non-radiative modes that pollute the approximate solution of (2.53). As it turns out, this is not much of an issue for the $n$ values for which $M_{p,q} \left[ \chi_A^\pm e^{-i\beta_n |\cdot|} \right]$ converges slowly, i.e., when $\beta_n \approx k_1$, but it certainly is for those for which $M_{p,q} \left[ \chi_A^\pm e^{-i\beta_n |\cdot|} \right]$ converges fast, i.e., around a RW-anomaly configuration when $\beta_n \approx 0$. Indeed, this phenomenon explains why $\text{error}_{r_c}^{(\pm,1)} = \mp 2i\beta_1 e^{i\beta_1 h}C_1^{\pm}$ in Figure 2.6(c), when $\beta_1 \approx 0.4624$, does not seem to converge as $A$ increases, while in turn $\text{error}_{r_c}^{(\pm,0)}$ when $\beta_0 \approx 7.6085$, exhibits fast convergence. Interestingly, this phenomenon is present even in connection with the divergent tail integrals in (2.50) corresponding to $M_{p,q} \left[ \chi_A^\pm \cdot \right]$ for $\beta_n = 0$ and
for $\beta_n \in i\mathbb{R}_{>0}$ and $\beta_n \approx 0$, due to the slow divergence of the complementary integrals along the bounded interval $[-A, A]$. This is for instance observed in Figure 2.6(b) which shows the slow convergence of $\text{error}_{rc}^{(+,1)} = C_1^{+}$.

2.8. Corrected windowed integral equation

This section presents a corrected windowed integral equation that leads to accurate numerical solutions for all frequencies and planewave incidences. We first consider the non-anomalous configurations, for which $S = \emptyset$ (i.e., $\beta_n \neq 0$ for all $n \in \mathbb{Z}$), and address the RW-anomaly configurations, for which $S \neq \emptyset$, in Section 2.8.2 below.

Our approach to tackle the issues encountered in the previous section lies in retaining certain critical coefficients $C_n^{\pm}$ in (2.9) and (2.50) as unknowns, instead of setting them to zero a priori. Guided by the numerical experiments of the previous section, we focus on the coefficients $C_n^{\pm}$ for $n \in C_\delta$, where the set $C_\delta$ is defined in (2.62) in terms of the parameter $\delta > 0$. The necessary conditions $C_n^{\pm} = 0$ for $n \in C_\delta$, which stem from the Rayleigh series (2.5) and (2.9), are then indirectly enforced through the integral form of the radiation condition (2.11). Following this approach, the tail integrals (2.50) become

$$\psi_p^{(C)} \approx \sum_{n \in C_\delta} \{C_n^+ \Psi_{n,p}^+ + C_n^- \Psi_{n,p}^-\}, \quad p = 1, \ldots, 4,$$

(2.63)

where the functions $\Psi_{n,p}^{\pm}$ are (formally) defined as

$$\Psi_{n,p}^{\pm} = e^{-i\alpha_n \frac{T}{2}} \left\{ M_{p,3} \left[ \chi_A^\pm e^{\mp i\beta_n |\cdot|} \right] + i\alpha_n M_{p,4} \left[ \chi_A^\pm e^{\mp i\beta_n |\cdot|} \right] \right\}, \quad n \in C_\delta.$$

(2.64)

In view of the definition of the functions $\chi_A^{\pm}$ introduced in (2.47), the two terms in (2.64) involve evaluation of improper integrals over the unbounded intervals $(-\infty, -cA]$ and $[cA, \infty)$, associated with the ‘−’ and ‘+’ case, respectively, that either cannot be evaluated in closed form or simply diverge. To produce computable approximations of $\Psi_{n,p}^{\pm}$ in (2.64) we then resort to Green’s representation formula (2.16). To achieve that, suitably
approximations of the complementary integrals

\[
M_{p,3} \left[ \chi_A^+ e^{\mp i\beta_n |x|} \right] + i\alpha_n M_{p,4} \left[ \chi_A^- e^{\mp i\beta_n |x|} \right], \quad n \in \mathbb{Z},
\]

(2.65)

are needed. As it turns out, the complementary tail integrals (2.65) tend to zero either super-algebraically (for \( n \in \mathcal{P} \)) or exponentially (for \( n \in \mathcal{E} \)) fast as \( A \) increases (see Appendix A), so they can simply be neglected. In the sequel we derive the aforementioned computable approximations of (2.64)

Let us first consider the case \( n \in \mathcal{P} \cup \{ m \in \mathbb{Z} : \beta_m \neq k_1 \} \) (\( \beta_n \in \mathbb{R}_{>0}, \beta_n \neq k_1 \)) for which (2.64) are well-defined conditionally convergent integrals. (Note that the condition \( \beta_n \neq k_1 \) is required for the integrals \( M_{p,3} \left[ \chi_A^+ e^{-i\beta_n |x|} \right], M_{p,3} \left[ \chi_A^- e^{i\beta_n |x|} \right], M_{p,4} \left[ \chi_A^+ e^{-i\beta_n |x|} \right], \) and \( M_{p,4} \left[ \chi_A^- e^{i\beta_n |x|} \right] \) in (2.64) to be conditionally convergent, otherwise \( e^{-ik_1 |y|} \) cancels the oscillations of the Helmholtz kernels rendering these integrals divergent). Approximations of \( \Psi_{n,p}^{\pm} \) for the remaining \( \beta_n \) values are obtained by simply considering the analytical extension of the resulting expressions that depend smoothly on \( \beta_n \).

Using then the fact that (2.65) becomes negligible for large \( A \) values, we can add it to \( \Psi_{n,p}^{\pm} \) in (2.64) to form

\[
\Psi_{n,p}^{\pm} \approx e^{-i\alpha_n \pm} \left\{ M_{p,3} \left[ w_A^c e^{\mp i\beta_n |x|} \right] + i\alpha_n M_{p,4} \left[ w_A^c e^{\mp i\beta_n |x|} \right] \right\},
\]

where we used the identities \( w_A^c = 1 - w_A = \chi_A^+ + \chi_A^- \). Then, introducing the notation

\[
\begin{align*}
\phi_{n,1}^{\pm} &= (\gamma_{d,p_1} u_n^\pm) \circ \mathbf{r}_1 = e^{i\alpha_n x_1 \pm i\beta_n y_1}, \\
\phi_{n,2}^{\pm} &= (\gamma_{n,p_1} u_n^\pm) \circ \mathbf{r}_1 = e^{i\alpha_n x_1 \pm i\beta_n y_1}, \\
\phi_{n,3}^{\pm} &= (\gamma_{d,p_2} u_n^\pm) \circ \mathbf{r}_2 = e^{i\alpha_n x_2 \pm i\beta_n y_2}, \\
\phi_{n,4}^{\pm} &= (\gamma_{n,p_2} u_n^\pm) \circ \mathbf{r}_2 = e^{i\alpha_n x_2 \pm i\beta_n y_2},
\end{align*}
\]

(2.66)
for the parametrized traces of the Rayleigh modes (2.7), and exploiting the linearity of the integral operators $M_{p,q}$, we arrive at

$$
\Psi_{n,p}^\pm \approx M_{p,3} \left[(1 - w_A)\phi_{n,3}^\mp\right] + M_{p,4} \left[(1 - w_A)\phi_{n,4}^\mp\right] = \Phi_{n,p}^\pm - \left\{ M_{p,3} \left[w_A\phi_{n,3}^\mp\right] + M_{p,4} \left[w_A\phi_{n,4}^\mp\right] \right\}
$$

(2.67)

where closed-form expressions for the functions

$$
\Phi_{n,p}^\pm = -M_{p,3}\phi_{n,3}^\mp - M_{p,4}\phi_{n,4}^\mp
$$

can be obtained from Green’s representation formula. Indeed, from the definition of the operators $M_{p,q}$, $p = 1, \ldots, 4$ and $q = 2, 3$, in (2.35) and (2.38), and Green’s representation formula (2.16), we find that

$$
\Phi_{n,p}^\pm = -\begin{cases} 
(\zeta K_{1,1} - K_{1,2})\phi_{n,3}^\mp - (\zeta V_{1,1}^\mp - V_{1,2}^\mp)\phi_{n,4}^\mp & p = 1 \\
(\zeta W_{1,1}^\mp - W_{1,2}^\mp)\phi_{n,3}^\mp - (\zeta K_{1,3} - K_{1,2})\phi_{n,4}^\mp & p = 2 \\
(\zeta^2 K_{1,1}^2 - K_{1,2}^2)\phi_{n,3}^\mp - (\zeta^2 V_{1,1}^\mp - V_{1,2}^\mp)\phi_{n,4}^\mp & p = 3 \\
(\zeta^2 W_{1,1}^\mp - W_{1,2}^\mp)\phi_{n,3}^\mp - (\zeta^2 K_{1,3} - K_{1,2})\phi_{n,4}^\mp & p = 4 
\end{cases}
$$

(2.68)

For $n \in P \cup \{ m \in \mathbb{Z} : \beta_m \neq k_1 \}$ we have hence produced a computable approximation (2.67) of the modal integrals $\Psi_{n,p}^\pm$ (2.64) with errors that decay super-algebraically fast as the window size $A$ increases. Such an approximation consists of the closed-form expression (2.68) and the finite-domain windowed integrals in (2.67) that can be evaluated numerically. Corresponding computable expressions for $\Psi_{n,p}^\pm$ in the case $n \in E \cup \{ m \in \mathbb{Z} : \beta_m = k_1 \}$ are obtained by analytically extending the formula on the right-hand side of (2.67) to $\beta_n$ values.

47
We are now in position to write the corrected windowed BIE in the case \( S = \emptyset \). Letting

\[
\Psi_n^\pm = - \begin{bmatrix}
\phi_{n,1}^\pm \\
\phi_{n,2}^\pm \\
\zeta \phi_{n,3}^\pm \\
\zeta \phi_{n,4}^\pm 
\end{bmatrix}
- \text{MW}_A \begin{bmatrix}
0 \\
0 \\
\phi_{n,3}^\pm \\
\phi_{n,4}^\pm 
\end{bmatrix}
\tag{2.69}
\]

and using (2.67) we obtain that the BIE can be expressed in vector form as

\[
E \phi_A + \text{MW}_A \phi_A + \sum_{n \in C_\delta} \left\{ C_n^+ \Psi_n^+ + C_n^- \Psi_n^- \right\} = \phi^{\text{inc}}
\tag{2.70}
\]

where again the first two equations hold in the interval \([0, 2\pi]\) while the last two hold in \([-A, A]\). The additional equations needed to relate the coefficients \( C_n^\pm \) with the vector density \( \phi_A \) follow from enforcing the radiation condition, which in view of (2.10) and (2.11), yields

\[
C_n^\pm = \frac{e^{i\beta_n h}}{2i\beta_n L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \left\{ \partial_y u_A^s(x, \pm h) \mp i\beta_n u_A^s(x, \pm h) \right\} e^{-i\alpha_n x} \, dx = 0, \quad n \in C_\delta.
\tag{2.71}
\]

Note that \( h > 0 \) above has to satisfy the condition \( \max\{h^+, -h^-\} < h < cA \). Finally, expressing \( u_A^s \) in (2.71) in terms of both \( \phi_A \) and \( C_n^\pm, \ n \in C_\delta \), we can form a system of equations from where the unknowns \( \phi_A \) and \( C_n^\pm, \ n \in C_\delta \), can be computed. We do so in the next section by developing a suitable WGF approximation of \( u_A^s \).

### 2.8.1. Windowed Green function approximation of the scattered field

As the matrix integral operator in (2.39), the representation formula (2.29) of the scattered field involves the computation of layer potentials along the unbounded curve \( \Gamma_2 \). In view of the discussion of the previous section we proceed to utilize the following approximation of the \( \Gamma_2 \) traces of \( u_A^s \):

\[
\phi_j \approx w_A \phi_{A,j} + \sum_{n \in C_\delta} \left\{ C_n^+ \chi_n^+ \phi_{n,j}^- + C_n^- \chi_n^- \phi_{n,j}^+ \right\}, \quad j = 3, 4.
\tag{2.72}
\]
where \( \phi_{A,j}, j = 1, \ldots, 4 \), denote the entries of the vector density \( \phi_A \) in (2.53) and \( \phi_{n,j}^+, j = 1, \ldots, 4 \) denote the traces of the (non-radiative) modes introduced in (2.66). The presence of such modes in (2.72) accounts for the fact that the integral equation (2.53) as well as the integral representation of the scattered field (2.59) used in Section 2.7 do not properly account for the radiation condition.

Replacing (2.72) in the integral representation of the scattered field (2.29) we obtain

\[
\begin{align*}
\psi(r) & \approx (D_1^1 \phi_A, 1)(r) - \eta(S_1^1 \phi_A, 2)(r) + \\
& (D_1^2 - \zeta D_1^3)[w_A \phi_A, 3](r) - (S_1^2 - \zeta S_1^3)[w_A \phi_A, 4](r) + \\
& \sum_{n \in \mathcal{C}_3} C_n^+ \left\{ (D_1^2 - \zeta D_1^3)[\chi_A^+ \phi_{n,3}^+](r) - (S_1^2 - \zeta S_1^3)[\chi_A^+ \phi_{n,4}^+](r) \right\} + \\
& \sum_{n \in \mathcal{C}_3} C_n^- \left\{ (D_1^2 - \zeta D_1^3)[\chi_A^- \phi_{n,3}^+](r) - (S_1^2 - \zeta S_1^3)[\chi_A^- \phi_{n,4}^+](r) \right\}, \quad r \in \Omega_1
\end{align*}
\]

(2.73)

where the layer potentials are defined in (2.22).

To produce a computable approximation of the modal terms in (2.73) we resort to the above mentioned properties of the windowed oscillatory integrals to note that, for a target point \( r \in \Omega_{1,A} = \{ r = (x, y) \in \Omega_1 : \chi(y, c_A, A) = 1 \} \), the integrals

\[
(D_1^2 - \zeta D_1^3)[\chi_A^+ \phi_{n,3}^+](r) - (S_1^2 - \zeta S_1^3)[\chi_A^+ \phi_{n,4}^+](r)
\]

(2.74)

can be effectively approximated by

\[
(D_1^2 - \zeta D_1^3)[w_A^c \phi_{n,3}^+](r) - (S_1^2 - \zeta S_1^3)[w_A^c \phi_{n,4}^+](r)
\]

with errors

\[
(D_1^2 - \zeta D_1^3)[\chi_A^+ \phi_{n,3}^+](r) - (S_1^2 - \zeta S_1^3)[\chi_A^+ \phi_{n,4}^+](r)
\]

that converge to zero either super-algebraically fast for \( n \in \mathcal{P} \) (i.e., \( \beta_n \in \mathbb{R}_{>0} \)) or exponentially fast for \( n \in \mathcal{E} \) (i.e., \( \beta_n \in i\mathbb{R}_{>0} \)) as \( A \to \infty \).
Therefore, letting \( \tilde{\phi}_{A,j} \), \( j = 1, \ldots, 4 \), denote the entries of the corrected vector density

\[
\tilde{\phi}_A = \phi_A - \sum_{n \in C_\delta} \left\{ C_n^+ \begin{bmatrix} 0 \\ 0 \\ \phi_{n,3}^- \\ \phi_{n,4}^- \end{bmatrix} + C_n^- \begin{bmatrix} 0 \\ 0 \\ \phi_{n,3}^+ \\ \phi_{n,4}^+ \end{bmatrix} \right\}
\]

(2.75)

we define our WGF approximation of the scattered field as

\[
u_A^s(r) = (D_1^1 \tilde{\phi}_{A,1})(r) - \eta(S_1^1 \tilde{\phi}_{A,2})(r) + (D_2^2 - \zeta D_1^3)[w_A \tilde{\phi}_{A,3}](r) - \]

\[
(S_1^2 - \zeta S_1^3)[w_A \tilde{\phi}_{A,4}](r) + \sum_{n \in C_\delta} \left\{ C_n^+ u_n^-(r) + C_n^- u_n^+(r) \right\}
\]

(2.76)

for \( r \in \Omega_{1,A} \) where the last two terms were obtained by direct application of Green’s representation formula (2.16).

With this expression at hand, we can now easily incorporate the conditions (2.71) into the integral equation system. In order to do so we define the functionals:

\[
L_n^\pm \phi = \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \left[ (\partial_y D_1^1 \mp i \beta_n D_1^1) \phi_1 - \eta(\partial_y S_1^1 \mp i \beta_n S_1^1) \phi_2 + \right.
\]

\[
\left\{ \partial_y D_2^2 \mp i \beta_n D_2^2 - \zeta(\partial_y D_1^3 \mp i \beta_n D_1^3) \right\} \phi_3 - \]

\[
\left\{ \partial_y S_1^2 \mp i \beta_n S_1^2 - \zeta(\partial_y S_1^3 \mp i \beta_n S_1^3) \right\} \phi_4 \right] (r_{\pm h}(t)) e^{-i \alpha n t} \, dt
\]

(2.77)

where \( r_{\pm h}(t) = \pm h e_2 + t e_1 \), with which conditions (2.71) using (2.76) can be readily expressed as

\[
C_n^+ = \frac{e^{i \beta_n h}}{2 i \beta_n} L_n^+ \left[ W_A \tilde{\phi}_A \right] \quad \text{and} \quad C_n^- = - \frac{e^{i \beta_n h}}{2 i \beta_n} L_n^- \left[ W_A \tilde{\phi}_A \right], \quad n \in C_\delta
\]

(2.78)

(note that we are still assuming that \( \beta_n \neq 0 \) for all \( n \in C_\delta \), i.e., \( S = \emptyset \)).

Therefore, both (2.70) and (2.71) can be recast as a single corrected windowed BIE system:

\[
E \tilde{\phi}_A + \tilde{M} W_A \tilde{\phi}_A = \phi^{inc}
\]

(2.79)
for the corrected vector density $\tilde{\phi}_A$ defined in (2.75), where letting $\Phi^\pm_n = \begin{bmatrix} \phi_{n,1}^+ \\ \phi_{n,2}^+ \\ 0 \\ 0 \end{bmatrix}$ the corrected matrix operator is given by

$$\tilde{M} = M + \sum_{n \in \mathbb{C}_\delta} \frac{\exp(i \beta_n h)}{2i \beta_n} \left\{ \Phi_n^- L_n^- - \Phi_n^+ L_n^+ \right\}$$

(2.80)

in the case $\mathcal{S} = \emptyset$.

**Remark 2.4.** Note that the functionals $L_n^\pm$ defined in (2.77) entail evaluation of singular integrals. This is so because the layer potentials $\mathcal{D}_i$ and $\mathcal{S}_i$ involve integration along the unit-cell boundaries $\Gamma_i$, $i = 2, 3$, which are intersected by the horizontal line segments parametrized by $r^\pm_h$.

To avoid this issue altogether we leverage the quasi-periodicity condition satisfied by the scattered field and express it by means of Green’s representation formula applied within a three-period wide cell, like the one employed in the numerical examples of Figure 2.5. The scattered field is then produced through integration on the super-cell walls $\Gamma_2 - Le_1$ and $\Gamma_3 + Le_1$, which are parametrized by $r_2(\cdot) - Le_1$ and $r_2(\cdot) + 2Le_1$, respectively, as well as on the annexed left and right obstacle boundaries $\Gamma_1 - Le_1$ and $\Gamma_1 + Le_1$, which are parametrized by $r_1(\cdot) - Le_1$ and $r_1(\cdot) + Le_1$, respectively. The densities on the new curves are given by multiplying the original densities by $\zeta^{-1}$ and $\zeta$ depending on whether the new curve corresponds to left or right $L$-translation of the original curve,
respectively. Doing so the functionals can be recast as

\[
L_n^c \phi = \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \left[ \{ \partial_y (D_1^1 + \zeta^{-1}D_1^{1-L} + \zeta D_1^{1+L}) \mp i \beta_n (D_1^1 + \zeta^{-1}D_1^{1-L} + \zeta D_1^{1+L}) \} \phi_1 - \right.
\]

\[
\eta \left\{ (\partial_y (S_1^1 + \zeta^{-1}S_1^{1-L} + \zeta S_1^{1+L}) \mp i \beta_n (S_1^1 + \zeta^{-1}S_1^{1-L} + \zeta S_1^{1+L}) \} \phi_2 + \right.
\]

\[
\{ \zeta^{-1}(\partial_y D_1^{2-L} \mp i \beta_n D_1^{2-L}) - \zeta^2(\partial_y D_1^{3+L} \mp i \beta_n D_1^{3+L}) \} \phi_3 - \right.
\]

\[
\{ \zeta^{-1}(\partial_y S_1^{2-L} \mp i \beta_n S_1^{2-L}) - \zeta^2(\partial_y S_1^{3+L} \mp i \beta_n S_1^{3+L}) \} \phi_4 \right) (r_{\pm h}(t)) e^{-i \alpha_n t} \, dt
\]

(2.81)

in terms of the layer potentials: \( D_1^{1+L} \) and \( S_1^{1+L} \) associated with \( \Gamma_1 + Le_1 \); \( D_1^{1-L} \) and \( S_1^{1-L} \) associated with \( \Gamma_1-L \); \( D_1^{2-L} \) and \( S_1^{2-L} \) associated with \( \Gamma_2 - Le_1 \); and, \( D_1^{3+L} \) and \( S_1^{3+L} \) associated with \( \Gamma_3 + Le_1 \).

\[\square\]

### 2.8.2. Corrected windowed integral equation at Rayleigh-Wood anomalies

In order to extend (2.79) to the challenging RW-anomaly case, i.e., when \( \beta_n = 0 \) for some \( n \in C_\delta \) (\( S \neq \emptyset \)), we resort to L’Hôpital’s rule. In detail, we evaluate the correcting terms in (2.80) associated with \( n \in S \) as the limit

\[
\lim_{\beta_n \to 0} \frac{e^{i \beta_n h}}{\beta_n} \left\{ \Phi_n L_n^c - \Phi_n^+ L_n^c \right\} = \partial_{\beta_n} \left\{ \Phi_n L_n^c - \Phi_n^+ L_n^c \right\} \bigg|_{\beta_n=0} = \left\{ \partial_{\beta_n} \Phi_n^c|_{\beta_n=0} L_n^c|_{\beta_n=0} + \Phi_n^-|_{\beta_n=0} \partial_{\beta_n} L_n^-|_{\beta_n=0} \right\} - \left\{ \partial_{\beta_n} \Phi_n^+|_{\beta_n=0} L_n^+|_{\beta_n=0} + \Phi_n^+|_{\beta_n=0} \partial_{\beta_n} L_n^-|_{\beta_n=0} \right\}.
\]

(2.82)

Doing so the general expression for the corrected matrix operator in (2.80) becomes

\[
\tilde{M} := M + \frac{1}{2l} \sum_{n \in C_\delta \setminus S} \frac{e^{i \beta_n h}}{\beta_n} \left\{ \Phi_n L_n^c - \Phi_n^+ L_n^c \right\} + \frac{1}{2l} \sum_{n \in S} \left\{ \Phi_n \partial_{\beta_n} (L_n^c - L_n^c) + \partial_{\beta_n} \Phi_n (L_n^c + L_n^c) \right\}
\]

(2.83)
where we have introduced the vectors $\Phi_n := \Phi_n^\pm$ and

$$\partial_{\beta_n} \Phi_n = \begin{bmatrix} iy_1 \\ n_1 \cdot (-y_1\alpha, i) \\ 0 \\ 0 \end{bmatrix} e^{i\alpha_n x}$$

for $n \in S$, which correspond to the $\Gamma_1$ traces of the Raleigh modes $u_n$ and $iv_n$ defined in (2.8). The $\beta_n$-derivative of the functionals $L_n^\pm$ are given by

$$\partial_{\beta_n} L_n^\pm \Phi = \mp i \int_{-\frac{L}{2}}^{\frac{L}{2}} [D_1^1 \phi_1 - \eta S_1^1 \phi_2 + \zeta D_1^{1+L} \phi_1 - \zeta \eta S_1^{1+L} \phi_2 +$$

$$\zeta^{-1} D_1^{1-L} \phi_1 - \zeta^{-1} \eta S_1^{1-L} \phi_2 + \zeta^{-1} D_1^{2-L} \phi_3 - \zeta^2 D_1^{3+L} \phi_3 -$$

$$\zeta^{-1} S_1^{2-L} \phi_4 + \zeta^2 S_1^{3+L} \phi_4] (r^\pm(t)) e^{-i\alpha_n t} dt.$$  \hspace{1cm} (2.84)

Similarly, the expression for the corrected approximate scattered field reads as

$$u_s^A(r) = (D_1^1 \tilde{\phi}_{A,1})(r) - \eta (S_1^1 \tilde{\phi}_{A,2})(r) + (D_1^2 - \zeta D_1^3) [w_A \tilde{\phi}_{A,3}](r) -$$

$$(S_1^2 - \zeta S_1^3) [w_A \tilde{\phi}_{A,4}](r) +$$

$$\frac{1}{2i} \sum_{n \in \mathbb{C} \setminus \mathbb{N}} \frac{e^{i\beta_n h}}{\beta_n} \left\{ u_n^-(r) L^+_n [W_A \tilde{\phi}_A] - u_n^+(r) L^-_n [W_A \tilde{\phi}_A] \right\} +$$

$$\frac{1}{2i} \sum_{n \in \mathbb{S}} \partial_{\beta_n} \left\{ u_n^-(r) L^+_n [W_A \tilde{\phi}_A] - u_n^+(r) L^-_n [W_A \tilde{\phi}_A] \right\}, \quad r \in \Omega_1 A.$$  \hspace{1cm} (2.85)

Finally, it is worth to mention that when $\beta_n$ is small but not zero, round-off errors can in practice make both expressions (2.80) and (2.83) of the corrected operator $\tilde{M}$, not suitable to achieve a desired accuracy. In such case, a suitable approximation of $\tilde{M}$ can be obtained by means of higher-order Taylor series expansions of the expressions in (2.82) about $\beta_n = 0$.
2.8.3. Fredholm property

Assuming that $\Gamma_1$ and $\Gamma_2$ are sufficiently smooth, say, with twice continuously differentiable parametrizations $r_1$ and $r_2$, respectively, it is easy to show that the corrected windowed BIE (2.79) is Fredholm of the second kind.

For the sake of presentation simplicity we prove Fredholmness of the corrected windowed BIE (2.79) in the product space $X := [L^2(0, 2\pi)]^2 \times [L^2(-A, A)]^2$ for which we first write it as

$$(\operatorname{Id}_X E + \tilde{M} \circ \operatorname{Id}_X W_A) \tilde{\phi}_A = \phi_{\text{inc}}$$

(2.86)

where $\phi_{\text{inc}} \in X$ and the solution $\tilde{\phi}_A$ is sought in that same space. Here, $\operatorname{Id}_X$ denotes the identity mapping of $X$ and, slightly abusing the notation, $\tilde{M}$ is considered as an operator acting on $X$, i.e., all the integrals over $\mathbb{R}$ in the definition of $\tilde{M}$ are truncated to the finite interval $[-A, A]$.

Using then the fact that the sub-block operators $M_{p,q}$, $p, q = 1, \ldots, 4$, defined in (2.35) and (2.38), are of the Hilbert-Schmidt type (because the associated kernels belong to $L^2([0, 2\pi] \times [0, 2\pi])$ for $p = q = 1, 2$, $L^2([0, 2\pi] \times [-A, A])$ for $p = 1, 2, q = 3, 4$, $L^2([-A, A] \times [-A, A])$ for $p = q = 3, 4$, and $L^2([-A, A] \times [0, 2\pi])$ for $p = 3, 4, q = 1, 2$) it follows from classical arguments (Atkinson, 1997) that $\tilde{M} : X \to X$ is compact. On the other hand, since the functionals $L_n^{\pm}, \partial_{\beta_n} L_n^{\pm} : X \to \mathbb{C}$ are bounded (because all the integrands involved in their definition (2.81) are $L^2$-integrable) and $\Phi_n^{\pm}, \Phi_n, \partial_{\beta_n} \Phi_n^{\pm} \in X$, we have that the finite-rank operators $\Phi_n^{\pm} L_n^{\pm}, \Phi_n \partial_{\beta_n} L_n^{\pm}, \partial_{\beta_n} \Phi_n L_n^{\pm} : X \to X$ are also compact, and so it is the finite linear combination of them that appears in the definition of $\tilde{M}$ in (2.83). This shows that $\tilde{M} : X \to X$ is compact.

Therefore, being $\tilde{M} \circ \operatorname{Id}_X W_A$ the composition of $\tilde{M}$, which is compact, and $\operatorname{Id}_X W_A : X \to X$, which is bounded, we conclude that $\tilde{M} \circ \operatorname{Id}_X W_A : X \to X$ is itself compact. The Fredholm property of (2.86) hence follows directly from the invertibility of the operator $\operatorname{Id}_X E : X \to X$. 

54
Having established the Fredholm property of the system (2.79), we can conclude from the Fredholm alternative that existence of solutions in the function space $X$ is implied by uniqueness. We found, however, the uniqueness property difficult to prove since standard arguments based on the unique solvability of associated PDEs (e.g. (Bonnet-Bendhia & Starling, 1994)) does not directly apply in this case due to the presence of the windowed integral kernels. Nevertheless, extensive numerical experimentation supports the conjecture that the corrected windowed BIE system (2.79) does not suffer from uniqueness issues, which typically manifests at the discrete level as severely ill-conditioned linear systems at certain countable frequencies. A similar analysis can be carried out in higher-order Sobolev spaces by relying on the well-established mapping properties (McLean, 2000) of the integral operators (2.21).

Finally, we mention that the results presented in this section rely heavily on the fact that $A$ is finite. Unfortunately, at this point we do not have a theory to study the Fredholm property of the corresponding limit equation as $A \to \infty$. The main difficulty here is that the space $[L^2(0, 2\pi)]^2 \times [L^2(\mathbb{R})]^2$, does not contain the traces of the scattered field, which do not necessary decay on the unbounded curves $\Gamma_2$ and $\Gamma_3$.

2.9. Numerical examples

This section presents a variety of numerical examples that demonstrate the accuracy and robustness of the proposed WGF methodology.

2.9.1. Validation examples

We start off by applying the proposed windowed BIE approach to the kite-shaped array test problem of Section 2.7, where the naive windowed BIE formulation failed to produce accurate solutions at and around RW-anomaly configurations.

Figure 2.7 displays the energy balance errors (2.57) for the problem of scattering by the 2-periodic array of penetrable kite-shaped obstacle (2.55) for $k_1 \in \{10.68, k^* , 10.76\}$.
Figure 2.7. Energy balance errors (2.57) in the numerical solution of the test problem of Section 2.7 obtained using the corrected windowed integral equation (2.79) for \( c = 0.5 \) (top row) and \( c = 0.1 \) (bottom row) and various window sizes \( A > 0 \). Three different exterior wavenumbers are considered corresponding to (a)-(d) \( k_1 = 10.68 \), (c)-(f) \( k_1 = 10.76 \), and (b)-(e) \( k_1 = k^* \approx 10.7261 \), that corresponds to a RW-anomaly frequency. The fixed parameter value \( \delta = 3k_1/4 \), which yields a four-element set \( C_\delta \) of correcting terms, is used in all these examples.

and \( A \in [10\lambda, 70\lambda] \) produced by the naive (blue curves) and corrected (red curves) BIE formulations. The same high-order Nyström discretization scheme was employed to numerically solve both BIEs. The additional parameter \( \delta > 0 \) that enters the corrected BIE (2.79) through the set \( C_\delta \) in (2.62), which selects the modes to be used in the correcting terms in (2.83) and (2.85), is chosen as \( \delta = 3k_1/4 \) in these examples. Two different values of the parameter \( c > 0 \), which controls the smoothness of the window function \( w_A \), are used. As can be observed in Figure 2.7, the upper envelopes to the red error
curves corresponding to the corrected windowed BIE formulation, exhibit super-algebraic convergence as the window size $A$ increases, for all three wavenumbers considered including the challenging RW-anomaly configuration at $k_1 = k^*$. Significantly smoother error curves and higher accuracies are achieved for $c = 0.1$ than for $c = 0.5$. This may have to do with the smoothness of the window function $w_A$ defined (2.43) which becomes discontinuous in the limit when $c \rightarrow 1$. Indeed, smoother window functions are numerically integrated with higher accuracy along the curves $\Gamma_{2,A}$ and $\Gamma_{3,A}$ using a fixed discretization, hence partially explaining the smaller errors obtained for $c = 0.1$. These results suggest that $c = 0$ is the optimal value of this parameter. It is however important to keep in mind that there is a trade-off when selecting the windows function parameters $A$ and $c$. This is that the smaller $c$ is, the smaller is the area of the region where the WGF method produces accurate solutions (i.e., the region where $\{ (x, y) \in \mathbb{R}^2 : w_A(y) = 1 \} = \mathbb{R} \times [-cA, cA]$).

Therefore, the constrain $cA > r$, where $r > 0$ is obstacle diameter, needs to be considered to obtain accurate solutions inside and around the obstacle $\Omega_2$.

Figure 2.8. Energy balance error (2.57) sweeps for $k_1 \in [k^* - 0.1, k^{**} + 0.1]$, where $k^*$ and $k^{**}$ are two consecutive RW frequencies, in the solution of the test problem of Section 2.7 produced by the corrected windowed BIE (2.79) using the parameter values $\delta \in \{ k_1/2, 3k_1/4, k_1 \}$ and (a) $A = 10\lambda$, (b) $A = 30\lambda$, and (c) $A = 50\lambda$.

Next, Figure 2.8 displays wavenumber sweeps of the energy balance error (2.57) obtained using the naive and the corrected BIE formulations for three window sizes $A \in$
\( \{10\lambda, 30\lambda, 50\lambda\} \) and \( \delta = \{3k_1/4, k_1/4, k_1\} \). The \( k_1 \)-wavenumber range \([k^*-0.1, k^{**}+0.1]\) considered in these examples includes two RW-anomaly frequencies at \( k^* \approx 10.7261 \) and \( k^{**} \approx 11.0418 \) where \( \beta_1 = 0 \) and \( \beta_{-6} = 0 \), respectively. Unlike the results produced by the naive windowed BIE (blue curves) the corrected approach does not break down at and around RW-anomaly frequencies. Indeed, despite the proximity to the RW frequencies, no extreme accuracy variations are observed as \( k_1 \) changes while maintaining the main parameters \( A \) and \( \delta \) fixed. These results demonstrate the robustness of the proposed methodology. Moreover, these results show that the parameter value \( \delta = 3k_1/4 \) (red curves) is good enough to achieve highly accurate solutions throughout the spectrum as no significant improvement is achieved using \( \delta = k_1 \) (purple curves).

Figure 2.9. Reflectance and transmittance spectra of a finite-thickness photonic crystal slab in TE and TM polarizations at normal planewave incidence. (a) Depiction of the lattice geometry and the curves involved the numerical solution of the problem by the proposed windowed Green function method. Computed reflectance \( (R) \) and transmittance \( (T) \) for various frequencies \( \lambda^{-1} = k_1/(2\pi) \) in TE (a) and TM (b) polarization. The first stop band, from 17783 cm\(^{-1}\) to 23152 cm\(^{-1}\), is marked in grey, which is the same in both polarizations. The location of RW-anomaly frequencies is marked by the vertical dashed lines.
2.9.2. Photonic crystal slab

In our next and final example we apply the proposed BIE method to the solution of a problem of scattering by a finite-thickness photonic crystal slab. As shown in Figure 2.9(a) and following the experimental setup of (Huisman et al., 2012), we examine a 2D photonic crystal with a centered rectangular lattice of width $a_1 = 693$ nm and height $a_2 = 488$ nm. The refractive index inside the crystal— which is assumed to occupy the exterior domain $\Omega_1$—is taken equal to $n = k_1/k_2 = 2.6$. The boundaries of the 21 pores encompassed by our computational domain (which make up a non-connected curve $\Gamma_1$) are circles of radius $r = 155$ nm centered at

$$a_l = \frac{(-1)^{l-1}a_1}{4}e_1 + \frac{(11-l)a_2}{2}e_2, \quad l = 1, \ldots 21.$$

Non-straight unit-cell boundaries $\Gamma_2$ and $\Gamma_3$ parametrized by properly scaled sine functions are used in this example. Note that non-straight curves $\Gamma_2$ and $\Gamma_3$ are necessary in this case to avoid them to intercept the pores ($\Gamma_1$). All the curves involved in the computations are displayed in Figure 2.9(a) together the lattice geometry. Both TE and TM polarization cases are considered under normal planewave incidence ($\theta_{\text{inc}} = 0$) and the spectrally accurate MK Nyström method is employed in the numerical solution of the corrected windowed BIE (2.86).

The computed reflectance ($R$) and transmittance ($T$), which are given by

$$R := \sum_{n \in P} \frac{\beta_n}{\beta} |B_n^+|^2 \quad \text{and} \quad T := 1 + 2\Re(\beta_0) + \sum_{n \in P} \frac{\beta_n}{\beta} |B_n^-|^2,$$

are displayed in Figures 2.9(b)-(c) for TE and TM polarizations, respectively, as functions of the frequency $\lambda^{-1} = k_1/(2\pi)$ in the range from 4000 cm$^{-1}$ to 38000 cm$^{-1}$. Both $R$ and $T$ are here computed using (2.58) to approximate the Rayleigh coefficients $B_n^\pm$ and (2.85) to evaluate the scattered field $u_s^\pm$ on the horizontal lines $y = \pm(5a_2+2r)$ where coefficients are computed. The quantity $R + T$, which is also displayed in those figures, deviates less than 0.01% from its theoretical value of one in all the frequencies considered in this example where we used the parameter values $c = 0.5$, $A = 20\lambda$, $\delta = 3k_1/4$ and $h = cA$.  

59
as well as sufficiently refined discretizations of the curves involved. The resulting linear systems, whose sizes remain almost constant around $4920 \times 4920$, were solved by means of GMRES with a tolerance of $10^{-6}$. The observed numbers of GMRES iterations needed to achieve the prescribed tolerance grew with the frequency from 33 (resp. 44) iterations at $4000 \text{ cm}^{-1}$ to 348 (resp. 470) iterations at $38000 \text{ cm}^{-1}$ in TE (resp. TM) polarization. The preconditioned system $(\text{Id}_X + \text{Id}_X E^{-1} \circ M_c \circ \text{Id}_X W_A) \tilde{\phi}_A = \text{Id}_X E^{-1} \phi_{\text{inc}}$ was used in the latter case, as it yields smaller number of iterations.

As expected, band structures form in the reflectance and transmittance spectra displayed in Figures 2.9(b)-(c). The lowest frequency band structure occurs at roughly the same frequency range in both polarizations between $17783 \text{ cm}^{-1}$ and $23152 \text{ cm}^{-1}$ at which $R \approx 1$ in both cases. These results differ slightly from (Huisman et al., 2012) that places the first stop band for TE-polarized incidence between $4700n = 12220 \text{ cm}^{-1}$ and $7300n = 18980 \text{ cm}^{-1}$.

Finally, Figure 2.10 shows the real part of the total field solution of the problem of scattering by the photonic crystal slab in TE (top row) and TM (bottom row) polarizations for two different frequencies. The left column plots correspond to the RW-anomaly frequency that is marked by the left dashed vertical line in Figures 2.9(b)-(c). The reflectance $R$ equals $1.5 \times 10^{-2}$ and $7.2 \times 10^{-4}$ in TE and TM polarization, respectively, at this frequency. The right column plots, on the other hand, correspond to the frequency at the beginning of the stop-band where $R \approx 1$ in both polarizations.
Figure 2.10. Solution of the problem of scattering of planewave at normal incidence by the finite-thickness photonic crystal of Figure 2.9(a). Top row: real part of the $z$-component total electric field at the lowest RW-anomaly frequency (left) and at the lowest stop-band frequency (right). Bottom row: real part of the $z$-component of the total magnetic field at the lowest RW-anomaly frequency (left) and at the lowest stop-band frequency (right).
3. EXTENSION TO PERIODIC ARRAYS OF 3D OBSTACLES

In the conclusion section of our published work (Strauszer-Caussade et al., 2022), it is stated as future work that the windowed Green function methodology applies to Helmholtz scattering problems by line and surface arrays of three-dimensional obstacles. In this chapter, we present the modifications of the 2D setup to extend our methodology to three dimensions and we offer some preliminary numerical results.

3.1. Periodic line arrays of 3D obstacles

This section extends the methodology to scattering problems by periodic line arrays of 3D obstacles. We here consider an incident planewave given by

\[ u^{\text{inc}}(x, y, z) = \exp(i\alpha x - i\beta_1 y - i\beta_2 z) \quad \text{with} \quad (\theta_1, \theta_2) \in \left[\frac{-\pi}{2}, \frac{\pi}{2}\right] \times [0, 2\pi), \quad (3.1) \]

where \( \alpha = k_1 \sin \theta_1 \cos \theta_2, \beta_1 = k_1 \sin \theta_1 \sin \theta_2 \) and \( \beta_2 = k_1 \cos \theta_2 \).

The incident planewave (3.1) is assumed to impinge on an infinite line array of three-dimensional obstacles, such as the one depicted in Figure 3.1. The array has periodicity \( L > 0 \) along the \( x \)-axis. This structure is a direct generalization of the two-dimensional domain used in the previous chapter (see Figure 2.1). As in the two-dimensional case, the unit normal vectors to the two unbounded parallel surfaces that make up the boundary of the unit cell point along the \( x \)-axis.

3.1.1. Boundary integral formulation

To generalize the proposed methodology to this three-dimensional setting we simply replace in the field representation formulae (2.15), (2.16), (2.17), (2.18), the two-dimensional free-space Green function—given by the Hankel function—by the corresponding three-dimensional Green function. The integrals over \( \Gamma_1, \Gamma_2, \) and \( \Gamma_3 \) in the resulting formulae must be now understood as surface integrals rather than line integrals.
Combining the representation formulae in the same way as in the two-dimensional case, we arrive at a BIE system analogous to (2.39), but given in terms of boundary integral operators involving surface integrals.

In order to truncate the surface integral over the infinite surfaces $\Gamma_2$ and $\Gamma_3$, we introduce a two-dimensional window function. To properly define such a window function, we need to introduce a parametrization of the surfaces $\Gamma_2$ and $\Gamma_3$. In detail, we let $\Gamma_2$ be given in parametric form as

$$\Gamma_2 = \{(x, y, z) \in \mathbb{R}^3 : x = x_2(t_1, t_2), y = y_2(t_1, t_2), z = z_2(t_1, t_2), (t_1, t_2) \in \mathbb{R}^2\}.$$  

The surface $\Gamma_3$, on the other hand, is defined as a horizontal translation of $\Gamma_2$, i.e., $\Gamma_3 = \Gamma_2 + Le_1$. The window function is then straightforwardly defined in the parameter space by the tensor product;

$$w_A := (\chi(\cdot, cA, A) \circ y_2) \cdot (\chi(\cdot, cA, A) \circ z_2)$$

Figure 3.1. Depiction of the quasi-periodic boundary and the curves to integrate and evaluate the boundary integral equations of line arrays in 3D. In the bottom-left a small depiction of the cylindrical coordinates reference.
where \( \chi \) is defined in (2.42).

The resulting windowed BIE system takes then the form of (2.53) but is given in terms of windowed surface integrals that involve the window function (3.2).

The derivation of the finite-rank correction operator needed to deal with RW anomalies is in this case difficult to evaluate numerically due to the lack of closed-form expressions to approximate the resulting slowly-decaying oscillatory integral over \( \Gamma_2 \) and \( \Gamma_3 \). This is so, mainly, because, unlike the (planewave) Rayleigh modes utilized in the two-dimensional problem, the Hankel functions that define the correction operator in this case, are not entire functions. Nevertheless, the resulting naive windowed BIE system yields relatively good convergence results provided the configuration formed by the wavenumbers, the array period, and the incidence angles, are sufficiently far from RW-anomaly configurations. In what follows we present these numerical results.

### 3.1.2. Numerical results

We consider the problem of scattering by a one-dimensional infinite array of period \( L = 1 \) of identical spheres of radius \( \rho = L/4 \). The wavenumbers are \( k_1 = 9 \) and \( k_2 = 15 \), and the incident planewave propagates along \((\sqrt{2}/2, 0, \sqrt{2}/2)\). Figure 3.2 presents the numerical errors measured using the energy balance relation. In detail, the energy balance error (Fernandez-Lado, 2016) is defined in this case as

\[
\text{error}_{eb} \approx \left| \sum_{n \in \mathcal{P}} \left( \sum_{|\ell| \leq \ell_T} \left| \tilde{B}^{(n)}_{\ell} \right|^2 \right) + \operatorname{Im} \left( \sum_{|\ell| \leq \ell_T} e^{i(\tilde{\theta} - \pi/2)} \tilde{B}^{(0)}_{\ell} \right) \right|, \tag{3.3}
\]

where the angle \( \tilde{\theta} \) is such that \((\beta_2, \beta_1) = |(\beta_2, \beta_1)|(\cos \tilde{\theta}, \sin \tilde{\theta})\), \( \ell_T > 0 \) is a truncation parameter, and the coefficients \( \tilde{B}^{(n)}_{\ell} \approx B^{(n)}_{\ell} \) correspond to the approximated coefficients in the Rayleigh series expansion of the scattered field, which in cylindrical coordinates \((x, r, \theta)\), is given by:

\[
u^n(x, r, \theta) = \sum_{n \in \mathbb{Z}} \left( \sum_{\ell \in \mathbb{Z}} B^{(n)}_{\ell} H_\ell^{(1)}(\beta_n r e^{i\theta}) e^{i\alpha_n x} \right), \tag{3.4}
\]
where $\beta_n = \sqrt{k_1^2 - \alpha_n^2}$, with $\alpha_n = \alpha + 2\pi n/L$, defined in the same manner as before (see (2.5b)). Even though the series (3.4) entails an infinite number of coefficients for $n, \ell \in \mathbb{Z}$, to assess the energy balance error we only need to consider the propagative modes, i.e., the coefficients corresponding to $n \in \mathcal{P}$ where $\mathcal{P}$ is defined in (2.6), and $|\ell| \leq \ell_T$, as shown in (3.3). Due to the exponential decay of the Fourier series coefficients of analytic functions over periodic domains, the latter approximation requires just a few terms to be accurately computed.

Figure 3.2. Results using $k_1 = 9$, $k_2 = 15$ and $L = 1$ (a) Energy balance criterion (error$_{eb}$) enforcement in semi-log scale using (3.3) and a patch-based representation of the obstacle. (b) Real part of the total field with window parameters $(c, A) = (0.8, 5.5\lambda)$.

To numerically compute the Rayleigh coefficients in (3.3), we introduce a cylindrical envelope surface $\Gamma_c$ of radius $\rho_0 > \rho$,

$$\Gamma_c := \{(x, r, \theta) \in \mathbb{R}^3 : x \in [-L/2, L/2], \ \theta \in [0, 2\pi), \ r = \rho_0\}$$

which is large enough to contain the obstacle. Then, letting $b_{\ell}^{(n)} = (\alpha_n, 0, \ell)$, the approximate coefficients are retrieved as

$$\tilde{B}_{\ell}^{(n)} := \frac{1}{2\pi H_{\ell}^{(1)}(\beta_n \rho_0)} \int_{\Gamma_c} u^s(r) e^{-ir \cdot b_{\ell}^{(n)}} ds(r), \quad n \in \mathcal{P}, \ |\ell| < \ell_T, \quad (3.5)$$
using the WGF approximation of $u^s$, as in (2.59).

The convergence of the method is demonstrated in Figure 3.2a, by computing energy balance errors corresponding to the scattered field computation using the WGF method with $c = 0.8$ and taking different window size values $A \in [2.5\lambda, 5.5\lambda]$. The real part of the total field is displayed in Figure 3.2b. The expected super-algebraic rate of convergence is observed in this simple example which involves only one propagative mode. The convergence of the method, however, deteriorates significantly when more propagative modes contribute to the scattered field expansions and does not converge at all for configurations close to an RW anomaly. In order to retrieve the high-order convergence in these more challenging cases, a finite-rank correction operator is needed.

Nonetheless, a more relevant case of interest is the computation of scattered fields by arrays exhibiting spatial periodicity in two directions, which is addressed in the next section.

### 3.2. Bi-periodic surface arrays of 3D obstacles

This section extends the time-harmonic scattering by infinite periodic surface arrays in two dimensions of penetrable obstacles in three dimensions. Most of the important computations and theoretical results are very similar to the ones presented in Chapter 2 so, for the sake of conciseness, we refer to that chapter when needed.

#### 3.2.1. Scattered field representation

This section presents the WGF methodology for an incident planewave, with incidence angle $(\theta_1, \theta_2) \in [-\frac{\pi}{2}, \frac{\pi}{2}] \times [0, 2\pi)$, is given by

$$u^\text{inc}(x, y, z) = e^{i\alpha \cdot (x, y) - i\beta z}, \quad \alpha = k_1 (\sin \theta_1 \cos \theta_2, \sin \theta_1 \sin \theta_2), \quad \beta = k_1 \cos \theta_2 \quad (3.6)$$
where \( \alpha = (\alpha_1, \alpha_2) \), which impinges on an \( L \)-periodic surface arrays of obstacles in three dimensions, with spatial periods \( L = (L_1, L_2) \), which is given by

\[
D_2 = \bigcup_{m \in \mathbb{Z}^2} \left\{ \mathbf{r} \in \mathbb{R}^3 : (\mathbf{r} - m \cdot \mathbf{L}) \in \Omega_2, \, m \in \mathbb{Z}^2 \right\},
\]

(3.7)

where \( \Omega_2 \subset \mathbb{R}^3 \) is an open and bounded domain and denotes the multi-index \( m = (m_1, m_2) \). For simplicity, the array extends on \( XY \)-plane and is assumed orthogonal to the \( z \)-axis.

The sought scattered field satisfies the Helmholtz equation in \( \mathbb{R}^3 \) and the same transmission conditions as in (2.2c). Furthermore, the fields satisfy the quasi-periodicity condition

\[
u(x + m_1 L_1, y + m_2 L_2, z) = (\zeta_1, \zeta_2)^m u(x, y, z), \quad \zeta_j = e^{i \alpha_j L_j}, \ j = 1, 2,
\]

(3.8)
and admits a Rayleigh series expansion (Fernandez-Lado, 2016)

\[
\begin{align*}
\quad u_s(x, y, z) &= \begin{cases} 
\sum_{m \in \mathbb{Z}^2} B_m e^{i \alpha_m \cdot (x, y) + i \beta_m z} & \text{for } z > h^+ := \sup_{(x, y, z) \in \Omega_2} z, \\
\sum_{m \in \mathbb{Z}^2} B_m e^{i \alpha_m \cdot (x, y) - i \beta_m z} & \text{for } z < h^- := \inf_{(x, y, z) \in \Omega_2} z,
\end{cases}
\end{align*}
\]

(3.9)

above \((z > h^+)\) and below \((z < h^-)\) the infinite surface array \(D_2\), where

\[
\alpha_m = \alpha + 2\pi \left( \frac{m_1}{L_1}, \frac{m_2}{L_2} \right) \quad \text{and} \quad \beta_m = \sqrt{k_1^2 - |\alpha_m|^2}.
\]

(3.10)

Unlike the line array setup of the previous section, now we need additional vertical boundaries to enclose a single scatterer (see Figure 3.3). Henceforth, we restrict the exterior domain \(D_1 = \mathbb{R}^3 \setminus D_2\) and \(D_2\) to a single unit-cell \(U\) given by

\[
U = \{(x, y, z) \in \mathbb{R}^3 : x_2(t_1, t_2) < x < x_2(t_1, t_2) + L_1, \ y_4(t_1, t_2) < y < y_4(t_1, t_2) + L_2, \ z = z_\ell(t_1, t_2), \ (t_1, t_2) \in \mathbb{R}^2 \},
\]

(3.11)

lying in between the vertical surfaces

\[
\Gamma_2 = \{ \mathbf{r} \in \mathbb{R}^3 : \mathbf{r} = \mathbf{r}_2(t_1, t_2), \ (t_1, t_2) \in I_1 \times \mathbb{R} \},
\]

\[
\Gamma_4 = \{ \mathbf{r} \in \mathbb{R}^3 : \mathbf{r} = \mathbf{r}_4(t_1, t_2), \ (t_1, t_2) \in I_2 \times \mathbb{R} \},
\]

and the translations of \(\Gamma_2\) and \(\Gamma_4\), defined as \(\Gamma_3 := \Gamma_2 + L_1 \mathbf{e}_1\) and \(\Gamma_5 := \Gamma_4 + L_2 \mathbf{e}_2\) respectively. In particular, the surfaces are unbounded only along the \(z\)–direction, so we consider the bounded parametric domains \(I_j = [-L_j/2, L_j/2] \) \((j = 1, 2\) accordingly), together with a smooth function \(r_\ell : I_j \times \mathbb{R} \rightarrow \mathbb{R}^3\) parametrizing \(\Gamma_\ell\), such that \(r_\ell := r_\ell(t_1, t_2) = (x_\ell(t_1, t_2), y_\ell(t_1, t_2), z_\ell(t_1, t_2))\), for \(\ell = 2 \ldots 5\). The surfaces \(\Gamma_\ell\) are displayed in Figure 3.3. The unit normal vectors on \(\Gamma_2\) and \(\Gamma_3\) point in the \(x\)–direction while on \(\Gamma_4\) and \(\Gamma_5\) they point in the \(y\)–direction.

On the other hand, the obstacle’s boundary \(\Gamma_1 = \partial \Omega_2\) is assumed of class \(C^2\) and is given by

\[
\Gamma_1 := \{ \mathbf{r} \in \mathbb{R}^3 : \mathbf{r} = \mathbf{r}_1(t_1, t_2), \ (t_1, t_2) \in [0, 2\pi) \times [-\pi, \pi] \}.
\]
in terms of a parametrization \( \mathbf{r}_1 : [0, 2\pi) \times [-\pi, \pi] \to \mathbb{R}^3 \). Without loss of generality, we have assumed that \( \Gamma_1 \) is parametrized by a single function, but this can be easily relaxed by utilizing a multiple coordinate patches representation.

Now we are in a position to present the integral representation formulae for the scattered field \( u^s \) by relying on the free-space Green function (1.14) in \( \mathbb{R}^3 \). The exterior domain \( \Omega_1 := U \setminus \Omega_2 \) of the unit cell is truncated as \( \Omega_{1,h} := U_h \cap \Omega_1 \), where \( U_h = \{(x, y, z) \in U : |z| < h\} \) and \( h > \max\{h^+, h^-\} \).

Using Green’s third identity, we have that for any fixed target point \( \mathbf{r} \in \Omega_{1,h} \) it holds that

\[
\left( \int_{\Gamma_1} \int_{\Gamma_2} - \int_{\Gamma_3} - \int_{\Gamma_4} + \int_{\Gamma_5} + \int_{\Gamma_6} \right) \left\{ \frac{\partial u^s (\mathbf{r}')}{\partial n(\mathbf{r}')} G_1 (\mathbf{r}, \mathbf{r}') \right\} ds(\mathbf{r}') = \begin{cases} u^s(\mathbf{r}), & \mathbf{r} \in \Omega_{1,h} \\ 0, & \mathbf{r} \in \Omega_2 \end{cases}
\]

(3.12)

where integration is carried over the multiply connected surfaces \( \partial \Omega_{1,h} \) that comprises the obstacle’s boundary \( \Gamma_1 \), the truncated vertical boundaries \( \Gamma^h_\ell := \Gamma_\ell \cup \Omega^h_{\ell} (\ell = 2 \ldots 5) \), and the horizontal planes

\[
\Gamma^h_\pm = \{(x, y, z) \in U : z = \pm h\}
\]

(3.13)

with unit normal pointing towards the interior of \( \Omega_{1,h} \).

Applying the Cauchy-Schwarz inequality over the horizontal surfaces we have

\[
\left| \int_{\Gamma^h_\pm} u^s (\mathbf{r}') \frac{\partial G_1 (\mathbf{r}, \mathbf{r}')}{\partial n(\mathbf{r}')} ds(\mathbf{r}') \right| \leq \left( \int_{\Gamma^h_\pm} |u^s|^2 ds \right)^{1/2} \left( \int_{\Gamma^h_\pm} \left| \frac{\partial G_1 (\mathbf{r}, \mathbf{r}')}{\partial n(\mathbf{r}')} \right| ds(\mathbf{r}') \right)^{1/2}
\]

\[
\left| \int_{\Gamma^h_\pm} \frac{\partial u^s (\mathbf{r}')}{\partial n(\mathbf{r}')} G_1 (\mathbf{r}, \mathbf{r}') ds(\mathbf{r}') \right| \leq \left( \int_{\Gamma^h_\pm} \left| \frac{\partial u^s (\mathbf{r}')}{\partial n(\mathbf{r}')} \right|^2 ds \right)^{1/2} \left( \int_{\Gamma^h_\pm} |G_1 (\mathbf{r}, \mathbf{r}')}| ds(\mathbf{r}') \right)^{1/2}
\]
Therefore, using the fact that $u^s$ and $\partial_n u^s$ are uniformly bounded on $\Gamma^h_{\pm}$ for all $h > \max\{h^+, h^-\}$ due to Rayleigh series, and the kernels decay, we obtain

\[
\left| \int_{\Gamma^h_{\pm}} u^s(r') \frac{\partial G_1(r, r')}{\partial n(r')} \, ds(r') \right| \leq \frac{1}{h} \to 0 \quad \text{and} \\
\left| \int_{\Gamma^h_{\pm}} \frac{\partial u^s(r')}{\partial n(r')} G_1(r, r') \, ds(r') \right| \leq \frac{1}{h} \to 0 \quad \text{as} \quad h \to \infty
\]

Taking $h \to \infty$ for the remaining integrals over $\Gamma^h_1$, we arrive to the integral representation formula

\[
\left\{ \int_{\Gamma_1} + \int_{\Gamma_2} - \int_{\Gamma_3} + \int_{\Gamma_4} - \int_{\Gamma_5} \left( \frac{\partial G(r, r')}{\partial n(r')} u^s(r') - G(r, r') \frac{\partial u^s(r')}{\partial n(r')} \right) \, dS(r') \right\} =
\begin{cases} 
  u^s(r), & r \in \Omega_1 \\
  0, & r \in \Omega_2
\end{cases}
\]

(3.14)

The previous steps are derived by means of a boundary integral representation over a unit cell containing a single scatterer. Yet, it can be directly proved that (3.14) also holds for unit cells containing more than one scatterer, by taking $\Gamma_1$ as the union of each scatterer’s boundary, and the vertical surfaces as the outer boundaries of the unit cell. In the following section, a BIE formulation is proposed by reproducing the results in Chapter 2.

3.2.2. Boundary integral equation formulation

Here we present the straightforward attempt to extend the integral formulation derived in section 2.5. Unlike the two-dimensional setup of Chapter 2, there are non-empty intersections between the vertical domains, which hinders the smoothness of the integral kernels that need to be numerically integrated. In the following, we detail the occurrence and severity of this issue.
To begin, we define the parametrized traces in the same manner as usual,

\[
\begin{align*}
\phi_1 &= (\gamma_{D_1} u^t) \circ r_1 : [0, 2\pi) \times [-\pi, \pi] \to \mathbb{C}, \\
\phi_2 &= (\gamma_{N_1} u^t) \circ r_1 : [0, 2\pi) \times [-\pi, \pi] \to \mathbb{C}, \\
\phi_3 &= (\gamma_{D_2} u^s) \circ r_2 : [-L_2/2, L_2/2] \times \mathbb{R} \to \mathbb{C}, \\
\phi_4 &= (\gamma_{N_2} u^s) \circ r_2 : [-L_2/2, L_2/2] \times \mathbb{R} \to \mathbb{C}, \\
\phi_5 &= (\gamma_{D_4} u^s) \circ r_4 : [-L_1/2, L_1/2] \times \mathbb{R} \to \mathbb{C}, \\
\phi_6 &= (\gamma_{N_4} u^s) \circ r_4 : [-L_1/2, L_1/2] \times \mathbb{R} \to \mathbb{C}.
\end{align*}
\] (3.15)

Likewise, using the representation formula obtained in equation (3.14), we impose both the transmission and the quasiperiodicity conditions to obtain the scattered representation in terms of the layer potentials, defined in the same manner as in (2.22),

\[
\begin{align*}
0 &= \mathcal{D}_1^1 \phi_1 + \eta \mathcal{S}_1^1 \phi_2 + \left(\mathcal{D}_1^2 - \zeta_1 \mathcal{D}_1^3\right) \phi_3 + \left(\mathcal{S}_1^2 - \zeta_1 \mathcal{S}_1^3\right) \phi_4 \\
&\quad + \left(\mathcal{D}_1^4 - \zeta_2 \mathcal{D}_1^5\right) \phi_5 + \left(\mathcal{S}_1^4 - \zeta_2 \mathcal{S}_1^5\right) \phi_6.
\end{align*}
\] (3.16)

Similarly, as in (2.18), we obtain the following representation for the transmitted field:

\[
\begin{align*}
u^t(r) &= -\mathcal{D}_2^1 \phi_1(r) + \mathcal{S}_2^1 \phi_2(r). \\
\end{align*}
\] (3.17)

Again, take the Dirichlet and Neumann parametric traces \(f\) and \(g\) respectively of the incident field over the obstacle’s boundary \(\Gamma_1\) (recall eq. (2.31)), to enforce the transmission conditions. Executing similar steps as in equations (2.32)-(2.33), we arrive at

\[
\begin{align*}
\phi_1 + \sum_{q=1}^{6} M_{1,q} \phi_q &= f, \\
\left(\frac{\eta + 1}{2}\right) \phi_2 + \sum_{q=1}^{6} M_{2,q} \phi_q &= g,
\end{align*}
\] (3.18)

where the \(M_{p,q}\) operators for \(q = 1 \ldots 6\) are defined by

\[
\begin{align*}
M_{p,1} &= \mathcal{H}_{2,p}^{1,1} - \mathcal{H}_{1,p}^{1,1}, \\
M_{p,2} &= \eta \mathcal{J}_{2,p}^{1,1} - \mathcal{J}_{2,p}^{1,1}, \\
M_{p,3} &= \zeta_1 \mathcal{H}_{1,p}^{1,3} - \mathcal{H}_{1,p}^{1,2}, \\
M_{p,4} &= \mathcal{J}_{1,p}^{1,2} - \zeta_1 \mathcal{J}_{1,p}^{1,3}, \\
M_{p,5} &= \zeta_2 \mathcal{H}_{1,p}^{1,5} - \mathcal{H}_{1,p}^{1,4}, \\
M_{p,6} &= \mathcal{J}_{1,p}^{1,4} - \zeta_2 \mathcal{J}_{1,p}^{1,5}.
\end{align*}
\] (3.19)
where

\[ J_{j,p}^{\ell,i} = V_{j}^{\ell,i} \quad \text{and} \quad H_{j,p}^{\ell,i} = K_{j}^{\ell,i} \quad \text{if} \quad p = 1 \quad \text{and} \quad (3.20) \]

\[ J_{j,p}^{\ell,i} = \tilde{K}_{j}^{\ell,i} \quad \text{and} \quad H_{j,p}^{\ell,i} = W_{j}^{\ell,i} \quad \text{if} \quad p = 2. \quad (3.21) \]

Still, four more equations are needed, which are obtained by evaluating the potential representations along the vertical surfaces, and that’s when the problem occurs. Basically, imposing the quasiperiodic conditions entails nearly-singular expressions. For example, following the steps in (2.36) to enforce the quasi-periodicity along the \( x \)-axis brings the term \( M_{4,5}[\phi_5] \), which explicitly defined as

\[ M_{4,5}[\phi_5] = (\zeta_1 W_1^{2,4} - \zeta_2 W_1^{2,5} + W_1^{3,4} - \zeta_2 W_1^{3,5}) [\phi_5]. \quad (3.22) \]

In this equation, the integration is carried along \( \Gamma_4 \) and \( \Gamma_5 \), while the evaluation is over \( \Gamma_2 \) and \( \Gamma_4 \). As it can be observed in Figure 3.3, \( \Gamma_2 \cap \Gamma_4 \), \( \Gamma_2 \cap \Gamma_5 \), \( \Gamma_3 \cap \Gamma_4 \) and \( \Gamma_2 \cap \Gamma_4 \) are non-empty sets. For instance,

\[ \Gamma_2 \cap \Gamma_4 = \{ (-L_1/2, -L_2/2, t) \in \mathbb{R}^3 : t \in \mathbb{R} \}, \quad (3.23) \]

defines an infinite vertical curve. The fact that the intersection is not empty leads to nearly singular terms that appear when evaluating numerically \( W_1^{2,4} \). In fact, this issue occurs for all four integral operators when considering all the linear combinations, and certainly, it does for the challenging hyper-singular operators. The next section proposes a novel approach that bypasses the need to deal with kernel singularities while retaining the use of the free-space Green function and smooth kernels.

### 3.2.3. Modified boundary integral equations

As the naive extension produces inaccurate numerical BIE solutions, here we propose a modified BIE formulation that relies on an extended unit containing nine scatterers, as displayed in Figure 3.4, instead of a single-scatterer cell. To do so, we heavily rely on the quasiperiodicty (3.8) to stay away from nearly-singular computations...
Figure 3.4. Top view depiction of the extended nine-cell unitary domain used for the modified operator’s definition and the modified scattered field representation. Note the center cell in green corresponds to the single-cell unit domain accounted for in the previous section 3.2.2. The z-axis is pointing outside the page.

To start with, we define the extended unit-cell sub-boundaries as the translations of the original single scatterer cell. On the one hand,

$$\Gamma_{(1,m)} := \Gamma_1 + m_1L_1e_1 + m_2L_2e_2$$

for the obstacles’ boundaries, and remark that $\Gamma_{(1,(0,0))} = \Gamma_1$ is the same boundary from the single unit-cell domain; and on the other hand, the vertical surfaces become

$$\Gamma_{(2,m)} := \Gamma_2 - L_1e_1 + mL_2e_2,$$

$$\Gamma_{(3,m)} := \Gamma_2 + 2L_1e_1 + mL_2e_2,$$

$$\Gamma_{(4,m)} := \Gamma_4 - L_2e_2 + mL_1e_1,$$

$$\Gamma_{(5,m)} := \Gamma_4 + 2L_2e_2 + mL_1e_1.$$
So, the modified cell boundaries $\tilde{\Gamma}_\ell$ are defined as the union of the sub-boundaries, letting the set of indexes $\mathcal{I}_m = \{-1, 0, 1\}^2$, as

$$\tilde{\Gamma}_1 = \bigcup_{m \in \mathcal{I}_m} \Gamma_{(1,m)} \quad \text{and} \quad \tilde{\Gamma}_\ell = \bigcup_{m=-1}^1 \Gamma_{(\ell,m)}, \quad \ell = 2 \ldots 5.$$  \hspace{1cm} (3.24)

Essentially, the evaluation of exterior vertical boundaries is now only needed at the middle surface $\Gamma_{(\ell,0)}$ of each face $\tilde{\Gamma}_\ell$, by means of the quasiperiodicity, because it allows recovering the integration over its adjacent sub-boundaries. In what follows we show this fact.

Indeed, the traces over each sub-boundary $\Gamma_{(\ell,j)}$, for $j = \pm 1$, are connected to their respective centered boundary $\Gamma_{(\ell,0)}$, for $2 \leq \ell \leq 5$, as

$$\begin{aligned}
(\gamma_{D,\Gamma_{(2,\pm 1)}}^- u^s) &= \varsigma^\pm_2 \left( \gamma_{D,\Gamma_{(2,0)}}^- u^s \right) \quad \text{and} \quad (\gamma_{N,\Gamma_{(2,\pm 1)}}^- u^s) = \varsigma^\pm_2 \left( \gamma_{N,\Gamma_{(2,0)}}^- u^s \right), \\
(\gamma_{D,\Gamma_{(3,\pm 1)}}^- u^s) &= \varsigma^\pm_2 \left( \gamma_{D,\Gamma_{(3,0)}}^- u^s \right) \quad \text{and} \quad (\gamma_{N,\Gamma_{(3,\pm 1)}}^- u^s) = \varsigma^\pm_2 \left( \gamma_{N,\Gamma_{(3,0)}}^- u^s \right), \\
(\gamma_{D,\Gamma_{(4,\pm 1)}}^- u^s) &= \varsigma^\pm_1 \left( \gamma_{D,\Gamma_{(4,0)}}^- u^s \right) \quad \text{and} \quad (\gamma_{N,\Gamma_{(4,\pm 1)}}^- u^s) = \varsigma^\pm_1 \left( \gamma_{N,\Gamma_{(4,0)}}^- u^s \right), \\
(\gamma_{D,\Gamma_{(5,\pm 1)}}^- u^s) &= \varsigma^\pm_1 \left( \gamma_{D,\Gamma_{(5,0)}}^- u^s \right) \quad \text{and} \quad (\gamma_{N,\Gamma_{(5,\pm 1)}}^- u^s) = \varsigma^\pm_1 \left( \gamma_{N,\Gamma_{(5,0)}}^- u^s \right). \\
\end{aligned}$$  \hspace{1cm} (3.25)

Furthermore, the middle outer boundaries’ densities are mapped to the densities of the original single-unit cell domain $U$, using the multiplication by the quasiperiodic constants, as displayed in Figure 3.4.

$$\begin{aligned}
(\gamma_{D,\Gamma_{(2,0)}}^+ u^s) &= \varsigma^{-1}_1 \left( \gamma_{D,\Gamma_{(2,0)}}^+ u^s \right), \quad (\gamma_{N,\Gamma_{(2,0)}}^+ u^s) = \varsigma^{-1}_1 \left( \gamma_{N,\Gamma_{(2,0)}}^+ u^s \right), \\
(\gamma_{D,\Gamma_{(3,0)}}^+ u^s) &= \varsigma^{-1}_2 \left( \gamma_{D,\Gamma_{(3,0)}}^+ u^s \right), \quad (\gamma_{N,\Gamma_{(3,0)}}^+ u^s) = \varsigma^{-1}_2 \left( \gamma_{N,\Gamma_{(3,0)}}^+ u^s \right), \\
(\gamma_{D,\Gamma_{(4,0)}}^+ u^s) &= \varsigma^{-2}_1 \left( \gamma_{D,\Gamma_{(4,0)}}^+ u^s \right), \quad (\gamma_{N,\Gamma_{(4,0)}}^+ u^s) = \varsigma^{-2}_1 \left( \gamma_{N,\Gamma_{(4,0)}}^+ u^s \right), \\
(\gamma_{D,\Gamma_{(5,0)}}^+ u^s) &= \varsigma^{-2}_2 \left( \gamma_{D,\Gamma_{(5,0)}}^+ u^s \right), \quad (\gamma_{N,\Gamma_{(5,0)}}^+ u^s) = \varsigma^{-2}_2 \left( \gamma_{N,\Gamma_{(5,0)}}^+ u^s \right). \\
\end{aligned}$$  \hspace{1cm} (3.26)

Overall, in this manner, the Dirichlet and Neumann traces over all the extended cell’s boundaries are referred to as the original single-scatterer cell densities, defined in (3.15). Using the representation formula (3.14), the densities, and the quasiperiodic relations
In (3.25)-(3.26), the scattered field \( u^s = u^s(r) \) is expressed as

\[
  u^s = \sum_{m \in I_m} (\zeta_1, \zeta_2)^m \left( D_1^{(1,m)}[\phi_1] - \eta S_1^{(1,m)}[\phi_2] \right)
  + \zeta_1^{-1} \left\{ \left( \zeta_2 D_1^{(2,1)} + D_1^{(2,0)} + \zeta_2^{-1} D_1^{(2,-1)} \right)[\phi_3] - \left( \zeta_2 S_1^{(2,1)} + S_1^{(2,0)} + \zeta_2^{-1} S_1^{(2,-1)} \right)[\phi_4] \right\}
  - \zeta_1^2 \left\{ \left( \zeta_2 D_1^{(3,1)} + D_1^{(3,0)} + \zeta_2^{-1} D_1^{(3,-1)} \right)[\phi_3] - \left( \zeta_2 S_1^{(3,1)} + S_1^{(3,0)} + \zeta_2^{-1} S_1^{(3,-1)} \right)[\phi_4] \right\}
  + \zeta_2^{-1} \left\{ \left( \zeta_1 D_1^{(4,1)} + D_1^{(4,0)} + \zeta_1^{-1} D_1^{(4,-1)} \right)[\phi_5] - \left( \zeta_1 S_1^{(4,1)} + S_1^{(4,0)} + \zeta_1^{-1} S_1^{(4,-1)} \right)[\phi_6] \right\}
  - \zeta_2^2 \left\{ \left( \zeta_1 D_1^{(5,1)} + D_1^{(5,0)} + \zeta_1^{-1} D_1^{(5,-1)} \right)[\phi_5] - \left( \zeta_1 S_1^{(5,1)} + S_1^{(5,0)} + \zeta_1^{-1} S_1^{(5,-1)} \right)[\phi_6] \right\}.
\]

(3.27)

In order to obtain the modified BIE, we introduce operators \( O_{\zeta}^{\ell,i} \), that map the integration over each sub-domain of the extended surfaces \( \bar{\Gamma}_i \) to the single-unit cell boundaries \( \Gamma_i \). Here we use the symbol \( O \) to refer to any of the operators \( \{ V, K, \bar{K}, W \} \). In detail, the new operators are defined as

\[
  O_{\zeta}^{\ell,i} = \sum_{m \in I_m} (\zeta_1, \zeta_2)^m O_1^{\ell,m}, \quad i = 1 \tag{3.28}
\]

\[
  O_{\zeta}^{\ell,i} = \zeta^{-1} O_1^{\ell,(i,-1)} + O_1^{\ell,(i,0)} + \zeta O_1^{\ell,(i,1)}, \quad i = 2 \ldots 5
\]

It can be verified by linearity that proposition (2.1) also holds for the modified operators (3.28). To further simplify the notation, we introduce

\[
  \mathcal{J}_{\zeta,p}^{\ell,i} = V_{\zeta}^{\ell,i} \quad \text{and} \quad \mathcal{H}_{\zeta,p}^{\ell,i} = K_{\zeta}^{\ell,i}, \quad \text{if} \quad p = 3, 5; \tag{3.29}
\]

\[
  \mathcal{J}_{\zeta,p}^{\ell,i} = \bar{K}_{\zeta}^{\ell,i} \quad \text{and} \quad \mathcal{H}_{\zeta,p}^{\ell,i} = W_{\zeta}^{\ell,i}, \quad \text{if} \quad p = 4, 6. \tag{3.30}
\]

We are now ready to derive a singularity-free BIE over the vertical boundaries. To enforce the quasiperiodic condition along the \( x \)-axis, we evaluate along the middle surfaces \( \Gamma_{(2,0)} \) and \( \Gamma_{(3,0)} \), of \( \bar{\Gamma}_2 \) and \( \bar{\Gamma}_3 \) respectively, and then follow the steps in (2.36) to arrive at

\[
  \zeta_1^2 \phi_p + \sum_{q=1}^{6} M_{p,q} \phi_q = 0, \quad p = 3, 4, \tag{3.31}
\]

75
where the entries \( M_{p,q} \) are

\[
\begin{align*}
M_{p,1} &= -\zeta_1 \left( \zeta_1^3 \mathcal{H}_{\xi_2,p}^{(2,0),1} + \mathcal{H}_{\xi_2,p}^{(3,0),1} \right), \\
M_{p,2} &= \zeta_1 \eta \left( \zeta_1^3 \mathcal{J}_{\xi_2,p}^{(2,0),1} + \mathcal{J}_{\xi_2,p}^{(3,0),1} \right), \\
M_{p,3} &= \zeta_1^6 \mathcal{H}_{\xi_2,p}^{(2,0),3} - \mathcal{H}_{\xi_2,p}^{(3,0),2}, \\
M_{p,4} &= \mathcal{J}_{\xi_2,p}^{(3,0),2} - \zeta_1^6 \mathcal{J}_{\xi_2,p}^{(2,0),3}, \\
M_{p,5} &= -\zeta_1 \zeta_2^{-1} \left( \left[ \zeta_1^3 \mathcal{H}_{\xi_1,p}^{(2,0),4} + \mathcal{H}_{\xi_1,p}^{(3,0),4} \right] - \zeta_1^3 \left[ \zeta_1^3 \mathcal{H}_{\xi_1,p}^{(2,0),5} + \mathcal{H}_{\xi_1,p}^{(3,0),5} \right] \right), \\
M_{p,6} &= \zeta_1 \zeta_2^{-1} \left( \left[ \zeta_1^3 \mathcal{J}_{\xi_1,p}^{(2,0),4} + \mathcal{J}_{\xi_1,p}^{(3,0),4} \right] - \zeta_1^3 \left[ \zeta_1^3 \mathcal{J}_{\xi_1,p}^{(2,0),5} + \mathcal{J}_{\xi_1,p}^{(3,0),5} \right] \right).
\end{align*}
\]

(3.32)

In a similar fashion, to enforce the quasiperiodicity along the \( y \)-axis, we evaluate the traces over \( \Gamma_{(4,0)} \) and \( \Gamma_{(5,0)} \), and apply the steps described in (2.36), to obtain

\[
\zeta_2^3 \phi_p + \sum_{q=1}^{6} M_{p,q} \phi_q = 0 \quad p = 5, 6
\]

(3.33)

where

\[
\begin{align*}
M_{p,1} &= -\zeta_2 \left( \zeta_2^3 \mathcal{H}_{\xi_2,p}^{(4,0),1} + \mathcal{H}_{\xi_2,p}^{(5,0),1} \right), \\
M_{p,2} &= \zeta_2 \eta \left( \zeta_2^3 \mathcal{J}_{\xi_2,p}^{(4,0),1} + \mathcal{J}_{\xi_2,p}^{(5,0),1} \right), \\
M_{p,3} &= -\zeta_2 \zeta_1^{-1} \left( \left[ \zeta_2^3 \mathcal{H}_{\xi_2,p}^{(4,0),2} + \mathcal{H}_{\xi_2,p}^{(5,0),2} \right] - \zeta_1^3 \left[ \zeta_1^3 \mathcal{H}_{\xi_2,p}^{(4,0),3} + \mathcal{H}_{\xi_2,p}^{(5,0),3} \right] \right), \\
M_{p,4} &= \zeta_2 \zeta_1^{-1} \left( \left[ \zeta_2^3 \mathcal{J}_{\xi_2,p}^{(4,0),2} + \mathcal{J}_{\xi_2,p}^{(5,0),2} \right] - \zeta_1^3 \left[ \zeta_1^3 \mathcal{J}_{\xi_2,p}^{(4,0),3} + \mathcal{J}_{\xi_2,p}^{(5,0),3} \right] \right), \\
M_{p,5} &= \zeta_2^6 \mathcal{H}_{\xi_1,p}^{(4,0),5} - \mathcal{H}_{\xi_1,p}^{(5,0),4}, \\
M_{p,6} &= \mathcal{J}_{\xi_1,p}^{(5,0),4} - \zeta_2^6 \mathcal{J}_{\xi_1,p}^{(4,0),5}.
\end{align*}
\]

(3.34)

Combining (3.18), which correspond to the transmission conditions, with (3.31) and (3.33), which account for the quasiperiodicity over the extended cell, we arrive at the following BIE system for the unknown vector of densities \( \phi \) with entries \( \{ \phi \}_j = \phi_j \):

\[
\mathbf{E}\phi + \mathbf{M}\phi = \phi^{\text{inc}}
\]

(3.35)
where \( M \) is the \( 6 \times 6 \) block matrix integral operator with entries \([M]_{p,q} = M_{p,q}\), defined in (3.19), (3.32) and (3.34),

\[
E = \begin{bmatrix}
1 & \frac{1+\eta}{2} & \zeta_1^3 & \zeta_1^3 & \zeta_1^3 & \zeta_1^3 \\
\frac{1+\eta}{2} & \frac{1+\eta}{2} & \zeta_1^3 & \zeta_2^3 & \zeta_2^3 & \zeta_2^3 \\
\zeta_1^3 & \zeta_1^3 & \frac{1+\eta}{2} & \zeta_1^3 & \zeta_1^3 & \zeta_1^3 \\
\zeta_1^3 & \zeta_1^3 & \zeta_1^3 & \frac{1+\eta}{2} & \zeta_1^3 & \zeta_1^3 \\
\zeta_1^3 & \zeta_1^3 & \zeta_1^3 & \zeta_1^3 & \frac{1+\eta}{2} & \zeta_1^3 \\
\zeta_1^3 & \zeta_1^3 & \zeta_1^3 & \zeta_1^3 & \zeta_1^3 & \frac{1+\eta}{2}
\end{bmatrix}
\quad \text{and} \quad
\phi^\text{inc} = \begin{bmatrix} f \\ g \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \quad (3.36)
\]

In order to truncate the surface integrals over \( \tilde{\Gamma}_2, \tilde{\Gamma}_3, \tilde{\Gamma}_4 \) and \( \tilde{\Gamma}_5 \), we resort again to the WGF method. To extend the ideas in section 2.6, we use the same window function \( \chi(\cdot, cA, A) \) defined in (2.42). We then let

\[
w_{A,1}(t_1, t_2) := \chi(\cdot, cA, A) \circ z_2(t_1, t_2) \quad w_{A,2}(t_1, t_2) := \chi(\cdot, cA, A) \circ z_4(t_1, t_2)
\]

with their respective complements \( w_{cA,j} = 1 - w_{A,j} \), and split the density as

\[
\phi_j = w_{A,1}\phi_j + w_{cA,1}\phi_j, \quad j = 3, 4 \quad \text{and} \quad \phi_j = w_{A,2}\phi_j + w_{cA,2}\phi_j, \quad j = 5, 6.
\]

As illustrated in section 2.7, neglecting the complementary tails does not guarantee the method’s expected convergence. Although, the derivation of adequate corrections for the bi-periodic setup has proven itself a major challenge. Due to time constraints, this thesis is limited to the “naive” windowing, previously used to obtain (2.54). That is to say, simply taking

\[
w_{cA,1}\phi_j \approx 0 \quad \text{and} \quad w_{cA,2}\phi_j \approx 0,
\]

leading to the windowed integral equation system

\[
E\phi_A + M W_A\phi_A = \phi^\text{inc}, \quad (3.37)
\]

where \( W_A = \text{diag}(1, 1, w_{A,1}, w_{A,1}, w_{A,2}, w_{A,2}) \).
The following section presents various numerical experiments to assess the modified methodology’s convergence.

3.2.4. Validation examples

This section presents a variety of numerical experiments, aimed at assessing the accuracy of the quasiperiodic solutions produced by the windowed integral equation (3.37). We consider the diffraction and transmission problem of a planewave, using $\eta = 1$, on an infinite bi-periodic array with $L = L_1 = L_2 = 0.5$ consisting of penetrable spheres of ratio $L/4$. The exterior and interior wavenumbers were fixed to $k_1 = 8.8$ and $k_2 = 14$ accordingly.

The scattered field was computed using (3.27), employing the solution of the windowed system (3.37). The errors produced by the windowed integrals are expected to decay super-algebraically fast as $A \to \infty$. Moreover, as suggested by figure 2.7, the oscillations in the error curve are related to the choice of the window parameter $c$. In the following, it is fixed at $c = 0.3$.

The meshes were constructed using 7 points per wavelength on each relevant surface, and numerical integration is performed using a composite quadrature rule based on Chebyshev’s polynomials of degree $p \in \{2, 3, 4\}$. To deal with the singular terms, we employ the general-purpose DIM\(^1\) (Faria et al., 2021). Afterward, the resulting linear system is solved iteratively using the GMRES with a prescribed tolerance of $10^{-6}$. All the simulations were run within a single core of an Intel(R) Xeon(R) Gold 6240R CPU of 2.40GHz in a remote server with 503Gb of RAM.

To verify the quasi-periodicity condition enforcement, we set an incident angle $\theta^{\text{inc}} = (\pi/6, \pi/6)$, and compute the mismatch errors as

$$\text{err}_{qp} = \max_{p=1\ldots9} \left( \max \{ \text{err}_p^+, \text{err}_p^- \} \right) \quad (3.38)$$

\(^1\)WaveProp Julia package, written by Luiz Faria. Available at https://github.com/WaveProp

78
where

$$
er_{p}^{\pm} = \max_{m \in \mathbb{Z}} \left| (\zeta_1, \zeta_2)^m u_A^s(x_p^\pm, y_p^\pm, z_p^\pm) - u_A^s(x_p^\pm + m_1 L_1, y_p^\pm + m_2 L_2, z_p^\pm) \right| \left| u_A^s(x_p^\pm, y_p^\pm, z_p^\pm) \right|$$

(3.39)

for nine test points $r_p^\pm = (x_p^\pm, y_p^\pm, z_p^\pm)$ above, and below the obstacle. Let $h = 0.25$, then fix the sample points as $r_1^\pm = (-5/12, 5/12, \pm h), r_2^\pm = (0, 5/12, \pm h), r_3^\pm = (5/12, 5/12, \pm h), r_4^\pm = (-5/12, 0, \pm h), r_5^\pm = (0, 0, \pm h), r_6^\pm = (5/12, 0, \pm h), r_7^\pm = (-5/12, -5/12, \pm h), r_8^\pm = (0, -5/12, \pm h)$ and $r_9^\pm = (5/12, -5/12, \pm h)$. For illustration, refer to Figure 3.5(a), depicting the $XY$-plane and highlighting in orange $r_2^\pm$. The numerical errors are displayed in 3.5(b)-(c) in semi-log and log-log scale respectively.

Figure 3.5. Errors of the quasi-periodicity condition of the numerical solution produced by the windowed integral equation. (a) Depiction of the sample points to assess the mismatch errors. The sample point $r_2^\pm$ and its respective translations are highlighted in orange, together with the associated quasiperiodic constants in (3.8). Errors in semi-log (b) and log-log (c) scale for window sizes $A \in [3\lambda, 12\lambda]$ for different DIM interpolation orders $p \in \{2, 3, 4\}$ (blue, red, green respectively).

It is observed that for low-order integration orders ($p = 2$), the numerical error is completely dominated by grid errors that explain the plateau of the error curves, thus hiding
the convergence error associated with larger window truncation. Nevertheless, increasing the integration order \((p = 3, 4)\), which leads to lower discretization errors, allowing us to observe the window error decay, setting the plateau at a lower error, which corresponds to grid errors dominating again. This result demonstrates that the enforcement of the quasiperiodic condition converges with super-algebraic high-order as \(A\) increases.

Secondly, to validate the convergence of the method, we perform a self-convergence experiment. Consider a normal incident planewave and compute the scattered field at a single point \(r_0 = (0, 0, L/2)\) with a large window as \(A = 15\lambda\). This defines the reference solution as \(u_0 = u^s_A(r_0)\). Consequently, the point-wise error is reported as

\[
(\text{error}_{sc})_j = |u_0 - u_{A_j}(r_0)|
\]

(3.40)

where \(\{A_j\}_{j=1}^N\) denotes a sequence of \(N\) trial windows, \(A_j \in [3\lambda, 12\lambda]\). The experiment is repeated for different integration orders \(p = 2, 3, 4\), and the results are presented in Figs. 3.6(a)-(b). The reported errors suggest convergence as the window size increases. Still, no improvement is observed for higher integration degrees, suggesting the error is not dominated by the discretization, nor the window truncation.

However, to fully validate the solver, energy balance error convergence is needed. Indeed, the exact solution of the problem satisfies (Fernandez-Lado, 2016)

\[
2\text{Re}(B_{(0,0)}) + \sum_{m \in \mathbb{Z}^2} \frac{\beta_m}{\beta} \left\{ |B_m^-|^2 + |B_m^+|^2 \right\} = 0,
\]

(3.41)

so, the numerical errors can be assessed by evaluating

\[
\text{error}_{eb} = \left| 2\text{Re}(\tilde{B}_{(0,0)}^-) + \sum_{m \in \mathbb{Z}^2} \frac{\beta_m}{\beta} \left\{ |\tilde{B}_m^-|^2 + |\tilde{B}_m^+|^2 \right\} \right|.
\]

(3.42)

Here, the computations of the coefficients \(\tilde{B}_m^\pm\) are carried by projecting the propagating modes onto horizontal planes at heights \(\pm h\) above and below the obstacles, as displayed Figure 3.6(c), so, recalling the definition of \(\Gamma_{h+}^{\pm}\) in (3.13) and performing integration, letting
Figure 3.6. Self-convergence pointwise errors in semi-log (a) and log-log (b) scale of the scattered field evaluated at $r_0 = (0, 0, h)$ with $h = L/2$ for window sizes $A \in [3\lambda, 12\lambda]$ for different integration orders $p \in \{2, 3, 4\}$ (blue, red, green respectively). (c) Horizontal planes above and below the obstacle are used to compute Rayleigh’s coefficients.

\[ \alpha'_m = (\alpha_{m1}, \alpha_{m2}, 0), \]

one computes

\[ \hat{B}_m^\pm = \frac{e^{\mp i \beta_m h}}{\mid \Gamma_{h}^\pm \mid} \int_{\Gamma_{h}^\pm} u(r)e^{-i \alpha'_m \cdot r} ds(r) \quad (3.43) \]

However, no convergence at all was observed when computing the coefficients directly and assessing the energy using (3.42). As suggested in section 2.7, the presence of non-radiative modes that pollute the solution prevents the accurate computation of the desired $B_m^\pm$ coefficients. For no particular set of parameters tested, super-algebraic convergent solutions were obtained, urging the use of a corrective operator, as proposed in 2.8, which is mandatory in all cases.
Nonetheless, both the quasiperiodic and the transmission conditions enforcement are qualitatively validated, which is concluded from the solution continuity from one cell to another, and through the obstacles. As evidence, in Figures 3.7 (a)-(b), the above-stated is verified. In both experiments, the window parameters are set to $c = 0.3$ and $A = 5\lambda$, and the wavenumbers as $k_1 = 8.8$, $k_2 = 14$. However, in (a) the incident angle is fixed at $\theta^{\text{inc}} = (\pi/6, \pi/4)$, and spatial period to $L = (0.5, 0.5)$; while in (b) the parameters are $\theta^{\text{inc}} = (\pi/6, \pi/6)$ and $L = (0.5, 1.0)$. The visual agreement validates qualitative the methodology, yet the expected high-order accuracy is not successfully retrieved. In other words, preliminary positive results were obtained, but the implementation of adequate corrective terms remains an open issue.

Figure 3.7. Real part of the total field over 121 cells in TE polarization mode using window parameters $(c, A) = (0.3, 5\lambda)$ with different setups. In both scenarios we use $k_1 = 8.8$, $k_2 = 14$, but the incidence angle $\theta^{\text{inc}}$ and spatial periods $L$ differ. (a) $\theta^{\text{inc}} = (\pi/6, \pi/4)$, $L = (0.5, 0.5)$. (b) $\theta^{\text{inc}} = (\pi/6, \pi/6)$, $L = (0.5, 1.0)$
4. CONCLUSIONS AND FUTURE WORK

This thesis presented in Chapter 2 a novel BIE method for the numerical solution of problems of planewave scattering by periodic line arrays of penetrable obstacles in two dimensions. Our windowed BIE involves the compact operator $\tilde{M}$ (2.83) that is expressed in terms of free-space Green function kernels. As such, the equation system can be directly discretized and solved by employing various 2D Helmholtz BIE solvers available. We demonstrated through numerical experiments that the combination of our proposed super-algebraically convergent WGF method with the spectrally accurate MK Nyström method yields a high-order frequency-robust BIE solver that does not break down at and around the challenging RW-anomaly configurations.

The methodology is also extended to penetrable 1D and 2D arrays of obstacles in three dimensions in Chapter 3. For line arrays the formulation’s extension is straightforward. In contrast, for two-dimensional arrays, nearly-singular terms arise at the intersection of the vertical surfaces enclosing a single scatterer, thus preventing the reproduction of the same formulation. To avoid this issue, an enlarged unit cell containing nine obstacles is employed, modifying the formulation to ensure the smooth evaluation of kernels at the vertical domains. However, in both setups, the robustness is not ensured, because the finite-rank operator has yet to be properly computed and implemented. For line arrays, the Rayleigh series are not entire functions, thus they cannot be analytically extended to account the RW anomalies. This matter in question actually poses an open problem, since a new strategy will be required. For surface arrays, on the other hand, the construction is expected to be similar to the development in section 2.8, by adding the complementary windows to enforce the non-radiative modes to zero.

As future work, on mathematical aspects, weaker assumptions on the boundaries, or the scattered fields, regularity could be demanded. Preliminary results are presented in
Figure 4.1, using similar parameters as in section 2.7, but adding a (non-smooth) droplet-shaped obstacle. The general-purpose DIM was employed, instead of MK, displaying numerical errors unaffected by the boundary’s regularity.

Figure 4.1. Scattered field with $k_1 = 10.72$, $k_2 = 20$, $\theta = \pi/4$, $L = 2$ and window parameters $(c, A) = (0.5, 20\lambda)$. (a) Real-part of the total solution using the corrected operator $\mathbf{M}$ (2.83). (b) Pointwise difference between corrected and non-corrected scattered fields (logscale).

Other mathematical aspects of the problem’s geometry could be modified, to deal with problems of periodic obstacles embedded in layered media, with defects, etc. Also, we mention the natural extension of these ideas to Maxwell equations. On physical aspects, provided adequate assumptions, wave-scattering in other physics contexts also lead to the Helmholtz equation (Nédélec, 2001), such as time-harmonic acoustics and elastodynamics (seismic waves). For each physical setup, the boundary conditions at each obstacle interface should be dealt with in their own way, in order to modify the windowed BIE system accordingly and to solve the scattered waves.
REFERENCES


Physics) doi: 10.1063/1.523808


A. SUPER ALGEBRAIC DECAY OF WINDOWED OSCILLATORY INTEGRALS

The main argument to establish the super-algebraic convergence as $A \to \infty$ of the terms in (2.51) corresponding to the propagative modes $\beta_n \in \mathbb{R}_{>0}$ is essentially the repeated use of the integration by parts procedure. In order to illustrate this argument, let us consider the single-layer operator $e_A := V_1^{1,2}[\chi_A^+ e^{i\beta_n}]$ which contributes to the term $M_{1,4}[\chi_A^+ e^{i\beta_n}]$ where $M_{1,4}$ is defined in (2.35). In detail, we examine the oscillatory integral

$$e_A(t) = \frac{i}{4} \int_{cA}^{\infty} H^{(1)}_0 \left( k_1 \sqrt{(x_1(t) + \frac{L}{2})^2 + (y_1(t) - \tau)^2} \right) w_A^\xi(\tau) e^{i\beta_n \tau} \, d\tau, \quad t \in [0, 2\pi).$$

In view of the addition theorem (Abramowitz et al., 1966), i.e.,

$$H^{(1)}_0 \left( k_1 \sqrt{(x_1(t) + \frac{L}{2})^2 + (y_1(t) - \tau)^2} \right) = \sum_{\ell=-\infty}^{\infty} H^{(1)}_{\ell}(k_1|\tau|) J_{\ell}(k_1 \varrho(t)) e^{i(\tau_2 - \varrho(t))} \tag{A.1}$$

where $\varrho = \sqrt{(x_1 + \frac{L}{2})^2 + y_1^2}$, $\varrho(t) < cA \leq |\tau|$, it suffices to estimate the convergence of the integrals

$$E^{(n,\ell)}_A := \int_{cA}^{\infty} H^{(1)}_{\ell}(k_1 \tau) w^\xi_A(\tau) e^{i\beta_n \tau} \, d\tau, \quad \ell \geq 0, \tag{A.2}$$

as $A \to \infty$. Performing the change variable $\tau = As$ and letting $\xi(s) = w^\xi_A(sA)$ where $w^\xi_A(As) = 1 - \chi(s, c, 1)$ with $\chi$ defined in (2.42) (note that it does not depend on $A$), $h_{A,\ell}(s) = e^{-ik_1 A s} H^{(1)}_{\ell}(k_1 As)$ and $\kappa_n = \beta_n + k_1 \neq 0$, we arrive at

$$E^{(n,\ell)}_A = A \int_{c}^{\infty} \xi(s) h_{A,\ell}(s) e^{i\kappa_n As} \, ds.$$

Integrating by parts $m > 0$ times, the integral above can be recast as

$$E^{(n,\ell)}_A = \frac{1}{(i\kappa_n)^m A^{m-1}} \int_{c}^{\infty} e^{i\kappa_n As} \left( \frac{d}{ds} \right)^m [\xi(s) h_{A,\ell}(s)] \, ds$$

$$= \frac{1}{(i\kappa_n)^m A^{m-1}} \sum_{p=0}^{m} \binom{m}{p} \int_{c}^{\infty} e^{i\kappa_n As} \xi^{(m-p)}(s) h_{A,\ell}^{(p)}(s) \, ds$$

94
where we have used Leibniz’s rule and the fact that $\xi$ together with its derivatives of any order vanish at $s = c$. We then conclude that

$$
|E_A^{(m,\ell)}| \leq \frac{\|\xi\|_{C^m(\mathbb{R})}}{|\kappa_n|^{m} A^{m-1}} \left\{ \|h_{A,\ell}\|_{L^1(c,1)} + \sum_{p=1}^{m} \left( \frac{m}{p} \right) \|h_{A,\ell}^{(p)}\|_{L^1(c,\infty)} \right\}.
$$

To estimate the $L^1$-norm of $h_{A,\ell}^{(p)}$, $0 \leq p \leq m$, we employ a slight refinement of Lemma 1 in (Demanet & Ying, 2010) which yields

$$
|h_{A,\ell}^{(p)}(s)| = \left| \left( \frac{d}{ds} \right)^p \left[ e^{-ik_1 As} H_{\ell}^{(1)}(k_1 As) \right] \right| \leq \frac{1}{\sqrt{8k_1 A |\Gamma(\ell - \frac{1}{2})|}} 2^\ell P_p(\ell) s^{-(p+\frac{1}{2})}
$$

for $s \geq c$ and $p, \ell \geq 0$, where $P_p$ are positive-coefficient polynomials of degree $p$. It hence follows from these bounds that

$$
\|h_{A,\ell}\|_{L^1(c,1)} \leq \frac{1}{\sqrt{8k_1 A |\Gamma(\ell - \frac{1}{2})|}} 2^\ell P_0(\ell) \int_c^1 s^{-\frac{3}{2}} \, ds \leq \frac{1}{\sqrt{8k_1 A |\Gamma(\ell - \frac{1}{2})|}} \left( P_0(\ell) \frac{1-c^{\frac{1}{2}}}{2} \right)
$$

and

$$
\|h_{A,\ell}^{(p)}\|_{L^1(c,\infty)} \leq \frac{1}{\sqrt{8k_1 A |\Gamma(\ell - \frac{1}{2})|}} 2^\ell P_p(\ell) \int_c^\infty s^{-(p+\frac{1}{2})} \, ds = \frac{1}{\sqrt{8k_1 A |\Gamma(\ell - \frac{1}{2})|}} \left( P_p(\ell) \frac{c^{-(p+\frac{1}{2})}}{p - \frac{1}{2}} \right)
$$

for $p \geq 1$, and, consequently,

$$
|E_A^{(n,\ell)}| \leq \frac{\|\xi\|_{C^m(\mathbb{R})}}{|\kappa_n|^{m} A^{m-1} \sqrt{8k_1 A |\Gamma(\ell - \frac{1}{2})|}} 2^\ell \tilde{P}_m(\ell),
$$

where $\tilde{P}_m$ is the $m$-degree polynomial given by

$$
\tilde{P}_m(\ell) = \left\{ P_0(\ell) \frac{1-c^{\frac{1}{2}}}{2} + \sum_{p=1}^{m} \left( \frac{m}{p} \right) P_p(\ell) \frac{c^{-(p+\frac{1}{2})}}{p - \frac{1}{2}} \right\}.
$$
With the suitable upper bounds (A.3) for $E_{n,\ell}$ we return to the addition theorem (A.1) to obtain

$$
|e_A(t)| = \frac{1}{4} \left| \sum_{\ell = -\infty}^{\infty} J_\ell (k_1 \vartheta(t)) e^{i\ell\left(\frac{\pi}{2} - \vartheta(t)\right)} E_A^{(n,\ell)} \right| \leq \frac{1}{2} \sum_{\ell = 0}^{\infty} |J_\ell (k_1 \vartheta(t))| \left| E_A^{(n,\ell)} \right|
$$

\[ \leq \frac{\|\xi\|_{C^m(\mathbb{R})}}{|\kappa_n| m A^{m-1} \sqrt{32k_1 A}} \sum_{\ell = 0}^{\infty} a_\ell(t) \quad \text{for all} \quad m \geq 1,
\]

where coefficients in the series above are given by $a_\ell(t) = |J_\ell (k_1 \vartheta(t))| \frac{2^{2m} P_m(\ell)}{|\Gamma\left(\frac{\ell}{2}\right)|}$.

Finally, to prove the super-algebraic decay of the function $e_A$ as $A \to \infty$ is suffices to show that the series in (A.4) converges for all $t \in [0, 2\pi)$. In order to do so we resort to the ratio test. From the asymptotic form of the Bessel functions $J_\ell(x)$ for a fixed real number $x$ and large integers $\ell$, and Stirling’s formula (Abramowitz et al., 1966), we readily get that

$$
a_\ell(t) \sim \frac{\widetilde{P}_m(\ell)}{2\pi} \left( \frac{e^2 k_1 \vartheta(t)}{\ell(\ell - \frac{1}{2})} \right)^{\frac{\ell}{2}} \left( \frac{\ell}{e} \right)^{\frac{1}{2}} \quad \text{as} \quad \ell \to \infty.
$$

Therefore,

$$
\lim_{\ell \to \infty} \frac{a_{\ell+1}(t)}{a_\ell(t)} = \lim_{\ell \to \infty} \left\{ \frac{e^2 k_1 \vartheta(t)}{(\ell + 1)(\ell + \frac{1}{2})} \left( \frac{\ell(\ell - \frac{1}{2})}{(\ell + 1)(\ell + \frac{1}{2})} \right)^{\ell} \right\} = 0
$$

and hence the desired result follows.