Perfect absorbing layers for wave scattering problems and related topics

Gao, Yang

2020

Gao, Y. (2020). Perfect absorbing layers for wave scattering problems and related topics.
Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/137391>

<https://doi.org/10.32657/10356/137391>

This work is licensed under a Creative Commons Attribution-NonCommercial 4.0
International License (CC BY-NC 4.0).

Downloaded on 26 Apr 2023 09:03:57 SGT

**NANYANG
TECHNOLOGICAL
UNIVERSITY**

SINGAPORE

Perfect Absorbing Layers for Wave Scattering Problems and Related Topics

Gao Yang

Division of Mathematical Sciences

School of Physical and Mathematical Sciences

Nanyang Technological University

2020

Perfect Absorbing Layers for Wave Scattering Problems and Related Topics

Gao Yang

Division of Mathematical Sciences
School of Physical and Mathematical Sciences

A thesis submitted to the Nanyang Technological
University in partial fulfilment of the requirement for the
degree of *Doctor of Philosophy*

2020

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research done by me except where otherwise stated in this thesis. The thesis work has not been submitted for a degree or professional qualification to any other university or institution. I declare that this thesis is written by myself and is free of plagiarism and of sufficient grammatical clarity to be examined. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

20/08/2019
.....
Date

GAO YANG
.....
Gao Yang

Supervisor Declaration Statement

I have reviewed the content and presentation style of this thesis and declare it of sufficient grammatical clarity to be examined. To the best of my knowledge, the thesis is free of plagiarism and the research and writing are those of the candidate's except as acknowledged in the Author Attribution Statement. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

Aug. 21, 2018
.....
Date

Li-Lian Wang
.....
Li-Lian Wang

Authorship Attribution Statement

This thesis **does not** contain any materials from papers published in peer-reviewed journals or from papers accepted at conferences in which I am listed as an author.

20/08/2019

Date

GAO YANG

Gao Yang

Acknowledgement

First and foremost, I would like to thank my supervisor Prof. Li-Lian Wang for the guidance and providing me the privilege of working in this interesting research area. Without his invaluable supervision, encouragement, and wisdom over these years, this thesis could not have reached its present form.

I am grateful to Nanyang Technological University for awarding me the Research Scholarship. I am also benefited from the young, energetic and productive environment of the School of Physical and Mathematical Sciences. In particular, I appreciate the management and leadership of Prof. Chan Song Heng, Prof. Ku Chew Yeaw, and Prof. Oggier, Frdrique Elise. I am appreciative of the help from the IT and Admin. staff.

I would like to express my appreciation to Prof. Hoang Viet Ha, Prof. Peyrin, Thomas, Prof. Tong Ping, Prof. Xia Kelin, and Prof. Xing Chaoping, for the lectures and supervising. I am also indebted to the former members in our group including Dr. Zhiguo Yang, Dr. Ying Gu, Dr. Wenjie Liu and Dr. Bo Wang for their friendship and help.

Last but not least, I wish to thank my parents, my dearest husband Jiayu Ye for their love and support.

Contents

Acknowledgement	8
List of Figures	17
Abstract	19
1 Introduction	21
1.1 Existing techniques for domain reduction	21
1.2 Perfect absorbing layer	24
1.3 Wavenumber explicit analysis of the circular PAL	26
1.4 Time-domain PAL	27
1.5 Multiple scattering problems	28
1.6 Main contributions and outline	30
2 Perfect Absorbing Layer & Star-shaped Domain Truncation	33
2.1 PAL for a waveguide problem in a semi-infinite channel	34
2.1.1 The PML technique and its error analysis	35
2.1.2 The new PAL technique	40
2.2 Star-shaped domain truncation	42
2.3 Some new perspectives of circular PAL	45
2.3.1 Bérenger's equations and PML techniques	46

2.3.2	Equivalence of Bérenger's problem and PAL equation . . .	49
2.4	PAL for star-shaped domain truncation	52
2.4.1	Design of the PAL-equation	53
2.4.2	Substitution and implementation	56
2.5	Numerical results and comparisons	63
2.5.1	Waveguide problems	63
2.5.2	Some star-shaped PALs	65
3	Wavenumber-explicit Analysis	67
3.1	The PAL-equation	68
3.2	L^2 -stability analysis	70
3.3	Fourier & spectral-element method and its error analysis	83
3.3.1	The scheme	83
3.3.2	Error estimate	84
4	Time-Domain PAL	99
4.1	Time-domain PAL for one-way wave equation	99
4.2	Time-domain PAL for two-way wave equation	103
4.3	Time-domain PAL using substitution	107
5	Time Harmonic Multiple Acoustic Wave Scattering	115
5.1	Statement of the problem	115
5.1.1	General setup	116
5.1.2	Multiple circular DtN boundary conditions of circular scatterers	117
5.2	Variation problem and spectral discretization	124
5.2.1	Spectral-Galerkin approximation	124
5.3	Numerical iteration method for two scatterers	126
5.3.1	Iteration method	127
5.3.2	Numerical examples	128

Contents	13
-----------------	-----------

6 Conclusion and Future Works	135
--------------------------------------	------------

6.1 Conclusion	135
--------------------------	-----

6.2 Future works	136
----------------------------	-----

Conclusion and Future Works	135
------------------------------------	------------

Appendix	138
-----------------	------------

Bibliography	145
---------------------	------------

List of Figures

1.1	Sketch of a typical setting of wave scattering	22
1.2	Domain reduction by DtN, PML or PAL	23
1.3	Illustration of inside-out invisibility cloaking [97] and the perfect absorbing layer [89].	25
1.4	Bottom: Outgoing plane wave propagates in radial direction (a, ∞) scattered from a circular scatterer. Top: compressed wave in (a, b) has infinite oscillations near $r = b$	26
2.1	A schematic diagram of x -aligned semi-infinite waveguide (left), and the domain reduction by an artificial layer using the PML or PAL technique (right).	35
2.2	Profiles of the error function $ \mathcal{E}_p(x, y) $ of the solution (2.20) with $k =$ $9.99, L = 1, d = 0.1$, and $\sigma_0 = 10, 100$ using PML_2 and PML_∞ . Left: the error curve $ \mathcal{E}_p(L/2, y) $ for $y \in (0, \pi)$; Right: the error curve: $ \mathcal{E}_p(L, y) $ for $y \in (0, \pi)$	39

2.3	Profiles of the PML solution U_p with regular function (2.14) ($\sigma_0 = 1$, $n = 2$) and singular function (2.15) vs PAL solution U_a in Ω and V_a in Ω_d with $k = 99.99$, $(L, d) = (1, 0.2)$ along the x -axis at $y = \pi/2$. Left: real part solution; Right: imaginary part solution.	42
2.4	Left: illustration of the circular PAL from radial direction. Middle: schematic illustration of the rectangular PAL Ω_d with four trapezoidal patches. Right: illustration of the elliptic PAL under elliptic coordinate.	45
2.5	Left: errors against various N for different layers (width $d = 0.1$) with boundary condition $g(y) = \sin(5y) - \sin(30y)$; Right: errors against various N for different layers (width $d = 0.5$) with boundary condition $g(y) = \sin(5y) - \sin(30y)$	64
2.6	In (b)-(c), $\partial D := \{(x, y) = \zeta(\cosh\xi \cos\theta, \sinh\xi \sin\theta), \theta \in [0, 2\pi)\}$ with $(\zeta, \xi) = (0.8, 0.5)$ and $\sigma_0 = 1.5, \sigma_1 = 2$	65
2.7	Left: real part of the electric field with $\mathbf{N} = (60, 20)$. Right: corresponding errors for the approximation in Ω_f for $N = [15 : 5 : 60]$ and $N = 20$ in the layer.	66
3.1	Illustration of circular PAL.	69
3.2	Sketch of $F_1(T)$ and $F_2(T)$, when $T_1 \geq T_0$	80
4.1	Error of PAL methods and PML methods against N with the input wave $g(t) = \sin^p(kt)$ on boundary $x = 0$, $(T, dt) = (2, 10^{-4})$, $(L, d) = (1, 0.5)$, $(k, p) = (20, 5)$	107
4.2	Errors of PAL methods, PML methods and PAL method with substitution against N	113
4.3	Left: Sketches of point-source wave by using PAL method with substitution; Right: Error of PAL methods with substitution of point-source wave against N	113
5.1	Illustration of 2D multiple scatterers.	116
5.2	Local polar coordinates of scatterer i and j	118

5.3	Scattering fields of two cylindrical scatters with $k = 20$, $\theta_0 = \pi/2$	129
5.4	Error compared with T -matrix method $k = 20$, $\theta_0 = \pi/2$	129
5.5	Scattering fields of two cylindrical scatters with $k = 50$, $\theta_0 = 4\pi/3$. . .	130
5.6	Error compared with T -matrix method $k = 50$, $\theta_0 = 4\pi/3$	130
5.7	Scattering fields of two cylindrical scatters with $k = 50$, $\theta_0 = 4\pi/3$. . .	131
5.8	Error compared with T -matrix method $k = 50$, $\theta_0 = 4\pi/3$	131
5.9	Scattering fields of five cylindrical scatters with $k = 30$, $\theta_0 = \pi/2$	132
5.10	Scattering fields of ten cylindrical scatters with $k = 30$, $\theta_0 = \pi/2$	133

Abstract

The main objective of this thesis is to design a truly exact and optimal perfect absorbing layer (PAL) method for domain truncation of the two-dimensional Helmholtz equation in an unbounded domain with bounded scatterers. This PAL is based on a complex compression coordinate transformation and a judicious substitution of the unknown field in the artificial layer. Compared with existing perfectly matched layer (PML) methods, the distinctive features of this technique lie in that (i) it is truly exact in the sense that the PAL-solution is identical to the original solution in the bounded domain enclosed by the truncation layer; (ii) with the substitution, the PAL-equation is free of singularity and the substituted unknown field is essentially non-oscillatory in the layer; and (iii) using the polar coordinates, the construction is valid for general star-shaped domain truncation. By formulating the final variational formulation in Cartesian coordinates, the implementation of this technique using standard spectral-element or finite-element methods can be made easy as a usual coding exercise. We provide ample numerical examples to demonstrate that this method is highly accurate, parameter-free and robust for very high wavenumber and thin layer. It outperforms the classical PML and the recently advocated PML using unbounded absorbing functions. Moreover, it can fix some flaws of the PML approach.

To have more insights into the new PAL technique, we conduct the wavenumber explicit analysis of the associated PAL equation, and estimate the error of the spectral schemes with the characterisation of the convergence order on the wavenumber.

We also extend the frequency domain PALs to the time domain, and show its difference and advantages over the time-domain PML methods, where we concentrate on the one-way and two-way wave equations. Finally, we propose the spectral approximation of multiple scattering problems, where through the Dirichlet-to-Neumann (DtN) artificial boundary conditions and an appropriate iterative solver, the multiple scattering can be decoupled into single scattering problems.

Introduction

In this chapter, we elaborate on the motivations and background of this study, and highlight the main contributions of this dissertation.

1.1 Existing techniques for domain reduction

Many physical and engineering processes involving wave propagations (e.g., acoustic, electromagnetic and elastic waves) are naturally set in unbounded domains. Accurate simulation of such problems becomes exceedingly important in a variety of applications. Typically, the first step is to reduce the unbounded domain to a bounded domain so that most of finite-domain solvers can be applied. The reduced problem should be well-posed, and the underlying solution must be as close as possible to the original solution in the truncated domain. As such, the development of efficient and robust domain truncation techniques has become a research topic of longstanding interest.

For example, we consider the time-harmonic wave scattering governed by the Helmholtz equation

$$\begin{aligned} \nabla \cdot (\mathbf{C}(\mathbf{x}) \nabla u(\mathbf{x})) + k^2 n(\mathbf{x}) u(\mathbf{x}) &= f(\mathbf{x}) \quad \text{in } \Omega_\infty := \mathbb{R}^d \setminus \bar{D} \\ u|_{\Gamma_D} &= g = -u^i, \quad \partial_r u^s - \mathrm{i}k u^s = o(r^{-(d-1)/2}), \quad d = 2, 3, \end{aligned} \tag{1.1}$$

where the total field $u = u^i + u^s$ with u^i (resp. u^s) being the incident (resp. scattering) wave, D is the scatterer. Here, we assume that the inhomogeneity of $\mathbf{C}, n$ and support of f is confined in a disk/ball $B_a = \{r = |\mathbf{x}| \leq a\}$. In other words, $\mathbf{C}, n$ are constant exterior to B_a .

Figure 1.1: Sketch of a typical setting of wave scattering

Several notable techniques have been intensively studied in literature, which particularly includes the artificial boundary conditions (ABCs) (see, e.g., [9, 34, 35, 45, 52, 72, 53, 38]), and the artificial absorbing (or sponge) layers (see, e.g., [10, 23, 11, 12, 25, 86]).

In regards to the former approach, the local ABCs are easy to implement, but they can only provide low order accuracy with undesirable reflections at times. Alternatively, domain truncation based on the Dirichlet-to-Neumann (DtN) map, gives rise to an equivalent boundary-value problem (BVP), so it is transparent (or equivalently non-reflecting). However, such an ABC is nonlocal in both space and time, which brings about substantial complexity in implementation. Moreover, it is only available for special artificial boundaries/surfaces (e.g., circle and sphere). For example, significant effort is needed to seamlessly integrate DtN ABC with curvilinear spectral elements in two dimensions (cf. [39, 93, 94]), but the extension to three dimensions is highly non-trivial (cf. [88]). It is also noteworthy that with a good tradeoff between accuracy and efficiency, the high order ABCs without

high-order derivatives become appealing [46].

Figure 1.2: Domain reduction by DtN, PML or PAL

Pertinent to the latter approach, the perfectly matched layer (PML) first proposed by Berenger [10, 11, 12] essentially builds upon surrounding bounded scatterers by an artificial layer of finite width. The artificial layer is filled with fictitious absorbing media that can attenuate the outgoing waves inside. Since this pioneering work of Berenger, the PML technique has become a widespread tool for various wave simulations; undergone in-depth analysis of its mathematical ground (see, e.g., [62, 19, 20, 18] and the references cited therein); and been populated into major softwares such as the COMSOL Multiphysics. In the past decade, this subject area continues to inspire new developments, just to name a few: [13, 14, 36, 29, 85, 27]. The critical issue here is how to derive the PML-equation in the artificial layer.

Remarkably, the essential idea of constructing PML [10] can be interpreted as a complex coordinate stretching (or transformation) [23, 25]. Consider for example the circular PML in polar coordinates for the two-dimensional Helmholtz problem [25, 19], where the domain of interest is truncated and surrounded by an artificial annulus of width d , with the assumption that the inhomogeneity of the media and scatterers are enclosed by a circle C_R of radius R . The corresponding (radial) complex coordinate transformation that generates the anisotropic media inside the annular layer is of the form

$$\tilde{r} = r + \sigma_0 \int_R^r \sigma(s) ds, \quad R < r < R + d, \quad (1.2)$$

where $\sigma(s) > 0$ is called the *absorbing function* (ABF), and σ_0 is a tuning parameter. Note that the Helmholtz problem inside C_R remains unchanged, i.e., $\tilde{r} = r$. One typical choice of the ABF is

$$\sigma(s) = (s - R)^n / d^n, \quad n = 0, 1, \dots \quad (1.3)$$

The PML truncates domain at a finite distance and attenuates the wave (i.e., the original solution) in the annular layer by enforcing homogeneous Dirichlet boundary condition at the outer boundary $r = R$, where some artificial reflections are usually induced if the width of the layer is thin. In theory, the reflection can be a less important issue based on the fundamental analysis (see, e.g., [62, 25, 19]). Lassas and Somersalo [62] showed that the PML-solution converges to the exact solution exponentially when the thickness of the layer tends to infinity. As pointed out by Collino and Monk [25], it is important to optimally choose the parameters to reduce the potentially increasing error in the discretisation. The use of adaptive techniques can significantly enhance the performance of PML as advocated by Chen and Liu [19]. It is noteworthy that the complex coordinate transformation (1.2)-(1.3) is also used in developing the uniaxial PML in Cartesian coordinates along each coordinate direction [84, 18, 22]. However, Singer and Turkel [84] demonstrated that such a transformation can magnify the evanescent waves in the waveguide setting. Recently, Zhu and Wu [98] proposed a mixed PML and (few-mode) DtN truncation (to deal with the evanescent modes) for the waveguide related to diffraction grating problems. Moreover, as reported in [60, 65, 36], the PML has flaws and failures at times.

1.2 Perfect absorbing layer

One of the main objectives of this thesis is to propose and analyze a new absorbing layer, dubbed as perfect absorbing layer (PAL), for wave scattering problems, which significantly outperform PML and overcome the aforementioned shortcomings of the PML techniques. As reported in the conference proceeding [89], the

[illegible]

However, the invisibility cloaking in [97] was far from perfect, as the material parameters therein were highly singular and the approximation of the solution suffered from *the curse of infinite oscillation* [61]. Indeed, as illustrated in Figure 1.4, the profile of a plane outgoing wave propagating in the open space $\rho > a$ along the radial direction is depicted. The compression of the wave by the real mapping

is plotted at the bottom of Figure 1.4.

In Chapter 2, we shall consider the truncation of the unbounded domain by general star-shaped absorbing layer including circular, elliptic and polygonal layers as special cases. We focus on the two-dimensional setting, but the idea of construction can be extended to three dimensions. Roughly speaking, the

Figure 1.4: Bottom: Outgoing plane wave propagates in radial direction (a, ∞) scattered from a circular scatterer. Top: compressed wave in (a, b) has infinite oscillations near $r = b$.

construction of PAL consists of two essential components:

- (i) Complex compression coordinate transformation (C^3T);
- (ii) Variable substitution.

This leads to a transformed problem in the absorbing layer with the remarkable features: (i) it's truly exact in the sense that the PAL-solution interior to the layer is identical to the original solution in the same domain; (ii) its solution has no oscillation; and (iii) it is nearly definite for arbitrary high wavenumber, as opposite to the strong indefiniteness of the Helmholtz and Maxwell's equations. We shall elaborate on the construction, and justify these advantages in Chapter 2.

1.3 Wavenumber explicit analysis of the circular PAL

The second purpose is to conduct wavenumber explicit analysis of the PAL technique. There has been longstanding research interest in wavenumber explicit estimates for the Helmholtz and Maxwell's problems. In particular, much effort has been devoted to the Helmholtz equations (see, e.g., [58, 7, 81, 31, 57, 28, 4, 26, 82, 54, 16, 70] as a partial list of literature) with exact or approximate artificial boundary conditions. Most of the analysis is essentially based on Rellich

identities [68, 26] (also see, e.g., [54, 16, 70]), which applies only to star-shaped domains (or the bounded scatterer is of star-shape, see [16]). For Maxwell's equations, Hiptmair et al. [55] (and independently by [37]) derived for the first time the wavenumber explicit estimates for the time-harmonic Maxwell's equations but with an approximate boundary condition: $(\nabla \times \mathbf{E}) \times \mathbf{e}_r - ik\mathbf{E}_T = \mathbf{h}$. Ma et al. [66] considered the exact DtN boundary conditions for Maxwell's system in the spherical geometry.

However, there exists very limited works on the wavenumber explicit analysis of Helmholtz equations of the PML techniques (see, e.g., [64] for an up-to-date summary of analysis in different aspects of PML). The main purpose of Chapter 3 is to conduct wavenumber explicit analysis for the PAL technique. As the objective is to understand the performance of the outgoing waves in the artificial layer, we shall focus on the analysis of the circular layer. As we shall see, the argument will be different from the usual argument by using the Rellich identities and taking two different functions.

1.4 Time-domain PAL

It is important to remark that the PML techniques have been widely used in the time-domain scattering problems simulations. In fact, the original Berenger's PML method is based on the splitting of the electromagnetic fields, which is only weakly well-posed (cf. [10]) and might be unstable in practice. To remedy this, the strongly well-posed unsplit-field PMLs, including the uniaxial PML methods for the Maxwell's equations (see, e.g., [79, 96, 43]) and for wave equations (cf. [49]). In the curvilinear coordinates, the split-field PML method is introduced in [25] and the unsplit-field PML methods are introduced in [75] and [87] for Maxwell's equations. For the time-domain PML method, the planar PML method in one space direction is considered in Hagstrom [52] for the wave equation. In de Hoop, van den Berg, and Remis [56] and Diaz and Joly [30], the PML system

with a point source is analyzed based on the Cagniard-de Hoop method. In [17], the convergence of the time-domain PML method with a circular layer is proved by using the exponential decay estimate of the modified Bessel functions. In [17, 21], the long-time stability and convergence of the uniaxial PML are carefully analysed. We also refer to Chen and Zheng [22] for the recent development of PML for two-layer media.

The new PAL techniques in Chapters 2-3 have significant advantages over the PML (using various absorbing functions) in the frequency domain. A natural question to ask is if they have similar outperformance in the time-domain. We intend to answer this question in Chapter 4, where to fix the idea, we shall concentrate on the one-way and two-way wave equations.

1.5 Multiple scattering problems

The acquaintance of many physical phenomena and engineering processes can be significantly enhanced by accurately simulating the multiple scattering problems. It is known that analytic solutions for wave scattering problems from multiple arbitrary shaped obstacles embedded in inhomogeneous media are not available. Partially for this reason, many early works are mostly restricted to cylindrical and spherical obstacles embedded in homogeneous media, where the modal expansions of the scattered field play an essential role (cf. [95, 78, 33, 40, 5]). We highlight that the reader-friendly monograph by Martin [67] was largely concerned with time-harmonic waves with multiple obstacles and with exact methods including separation of variables, integral equations and T -matrices, but only the last chapter discussed some numerics.

In analogue with solving general single scattering problems, one can reduce the unbounded domain by a proper domain truncation technique, before applying a finite-domain solver, e.g., the finite element or spectral element method. Grote and Kirsch [48] proposed the non-reflecting boundary conditions (NRBC) based

on Dirichlet-to-Neumann operators for truncating multiple time-harmonic acoustic scattering problems with well-separated scatterers in two dimensions, where each scatterer is surrounded by an NRBC. The framework therein is well-suited for numerical discretization, but it requires to solve coupled systems. Indeed, Acosta and Villamizar [2, 3] discussed the multiple acoustic scattering from scatterers of complex shapes using coupling of Dirichlet-to-Neumann boundary condition and the finite difference method. In practice, the iterative method is more desirable. Based on the decomposition of the scattering wave into purely outgoing waves, Neumann iterative method was proposed in [8]. At each iteration, only single scattering problems need to be solved. This iterative technique has been further developed for high-frequency problems with a large number of scatterers, see [32, 6, 41, 44, 42] and references therein. Recently, a block Gauss-Seidel iterative method is derived from finite element discretization (cf. [63, 59, 91]). Error estimates between the iterative scheme at a continuous level and its finite element discretization were analyzed in [59].

In Chapter 5, we shall discuss the spectral-element discretisation of the time-harmonic acoustic multiple scattering problems. Here, we follow the framework of Grote and Kirsch [48] by reducing the unbounded domains by using NRBC. The coupling of different scatterers is along the artificial boundaries through the propagation and transport operators that count for the interactions of the scatterers. We study the decoupling of the multiple scatterers into singular scatterers by iteration methods, and the spectral algorithms will be used to solve singular scattering problems in each iteration. In fact, this investigation aims to shed light on the use of new PAL for domain truncation which is expected to be more flexible for spectral element methods and general geometries of the scatterers. In fact, the PML technique for multiple scattering problems is studied in [59]. As shown in the singular scattering problem, the new PAL should be more advantageous.

1.6 Main contributions and outline

The main contents and contributions of this dissertation are highlighted as follows.

- In Chapter 2, we design a truly exact and optimal perfect absorbing layer (PAL) method for domain truncation of the Helmholtz equation in an unbounded domain with bounded scatterers. The idea stems from the design of inside-out (or inverse) invisibility cloak by using the compression coordinate transforms. Differently, we construct the PAL-equation by using the complex coordinate transformation, which can damp the waves in the artificial layer. To deal with the singularity and oscillations caused by the compression from infinity to finite, we introduce a suitable substitution of the unknown field. As a result, in PAL layer, the field to be approximated has no oscillation and is well-behaved. Indeed, we can rigorously show that for arbitrary high wavenumber, as opposed to the strong indefiniteness of the Helmholtz equation, the PAL-equation is nearly definite. We demonstrate that this artificial layer can be star-shaped in general (including, e.g., circular, elliptical and polygonal layers as special cases), and has significant advantages over the PML methods.
- In Chapter 3, we conduct the wavenumber explicit analysis of the Helmholtz equation reduced by the PAL technique. The Helmholtz problem with high wavenumber is highly indefinite. It is challenging but important to characterise the dependence of the solution and its approximation on the wavenumber. In fact, there exist very limited works on the wavenumber explicit analysis of the Helmholtz equations even with the PML technique. In this chapter, we shall analyze the circular PAL with a compactly supported source term, and derive the stability and error estimate of PAL problem. This provides more insights into the newly developed PAL techniques.
- In Chapter 4, we consider the extensions of the perfectly matched layer in

the frequency domain to the time domain, and demonstrate its difference and advantages over the PML methods through the one-way and two-way wave equations. The study along this line will pave the way for the more complicated situations including the multi-dimensional wave equations and Maxwell's equations.

- In Chapter 5, we solve time-harmonic multiple scattering problems, where the main challenge is how to effectively decouple the scatterers and minimise the interaction between different scatterers. Here, we enclose each scatterer by using the exact DtN artificial boundary conditions for multiple scatterers, and decouple the communications between scatterers by using an iterative method. As a result, we only need to solve single scattering problems using e.g, spectral solvers. The study will shed light on the use of PAL for multiple scattering problems in both frequency and time domains.
- The last chapter is for some concluding remarks and future works.

Star-shaped Perfect Absorbing Layer for Time-harmonic Acoustic Wave Scattering Problems

In this chapter, we design a truly exact and optimal perfect absorbing layer (PAL) method for domain truncation of the two-dimensional Helmholtz equation in an unbounded domain with bounded scatterers. This artificial layer can be star-shaped in general (including, e.g., circular, elliptical and polygonal layers as special cases). This PAL is based on a complex compression coordinate transformation in polar coordinates, and a judicious substitution of the unknown field in the artificial layer. Compared with existing perfectly matched layer (PML) methods, the distinctive features of this technique lie in that (i) it is truly exact in the sense that the PAL-solution is identical to the original solution in the bounded domain enclosed by the truncation layer; (ii) with the substitution, the PAL-equation is free of singularity and the substituted unknown field is essentially non-oscillatory in the layer; and (iii) using the polar coordinates, the construction is valid for general star-shaped domain truncation. By formulating the final variational formulation in Cartesian coordinates, the implementation of this technique using standard spectral-element or finite-element methods can be

made easy as a usual coding exercise. We provide ample numerical examples to demonstrate that this method is highly accurate, parameter-free and robust for very high wavenumber and thin layer. It outperforms the classical PML and the recently advocated PML using unbounded absorbing functions. Moreover, it can fix some flaws in the PML approach.

2.1 PAL for a waveguide problem in a semi-infinite channel

In this section, we elaborate on the essential idea of the new PAL, and compare it with the classical PML techniques (cf. [10, 23, 25, 84]), and the “exact” and “optimal” PML methods using unbounded absorbing functions (cf. Bermúdez et al. [13, 14]) in the waveguide setting. Indeed, such a relatively simpler context enables us to conduct a precise error analysis, and better understand the differences between these approaches.

We consider the semi-infinite x -aligned waveguide from $x = 0$ to $x = \infty$ (see Figure 2.1 (left)), governed by the Helmholtz equation in a semi-infinite strip (cf. [84, 76]):

$$\mathcal{L}[U] := \Delta U + k^2 U = 0 \quad \text{in } \Omega_\infty := \{0 < x < \infty, 0 < y < \pi\}; \quad (2.1a)$$

$$U(x, 0) = U(x, \pi) = 0, \quad x \in [0, \infty); \quad U(0, y) = g(y), \quad y \in [0, \pi], \quad (2.1b)$$

and U is outgoing at infinity, and $g \in L^2(0, \pi)$. Here, $k > 0$ is the wavenumber, and we refer to Goldstein [47] for the outgoing radiation condition:

$$\frac{\partial U}{\partial x} - \sum_{l=1}^{\infty} i\hat{k}_l \hat{c}_l e^{i\hat{k}_l x} \sin(l y) = 0 \quad \text{with} \quad U(x, y) = \sum_{l=1}^{\infty} \hat{c}_l e^{i\hat{k}_l x} \sin(l y), \quad (2.2)$$

for any $x \geq x_1$ ($x_1 > 0$ is an artificial boundary on x -axis), where $\hat{k}_l := \sqrt{k^2 - l^2}$, and $\{\hat{c}_l\}$ can be determined by given Dirichlet data (e.g., at $x = x_1$). Using the Fourier sine expansion in y -direction, we find readily that the problem (2.1)-(2.2)

admits the series solution:

$$U(x, y) = \sum_{l=1}^{\infty} \hat{g}_l e^{i\hat{k}_l x} \sin(l y) \quad \text{with} \quad \hat{g}_l = \frac{2}{\pi} \int_0^{\pi} g(y) \sin(l y) dy. \quad (2.3)$$

Figure 2.1: A schematic diagram of x -aligned semi-infinite waveguide (left), and the domain reduction by an artificial layer using the PML or PAL technique (right).

2.1.1 The PML technique and its error analysis

To numerically solve (2.1), we adopt the PML technique that reduces the semi-infinite strip Ω_∞ in (2.1) to a rectangular domain $\Omega := (0, L) \times (0, \pi)$ by appending an artificial layer $\Omega_d := (L, L + d) \times (0, \pi)$ with a finite thickness d (see Figure 2.1 (right)). The artificial layer Ω_d is filled with fictitious absorbing (or lossy) media that can attenuate the waves propagating into the layer. In practice, one would wish the layer can diminish the pollution of the original solution (due to the reflection) in the “physical domain” Ω , and be as thin as possible.

The PML-equation can be obtained from the Helmholtz equation: $(\Delta + k^2)U = 0$ in $(\tilde{x}, \tilde{y})$ -coordinates through the complex coordinate stretching (see, e.g., [25, 84]). In general, we introduce the complex coordinate transformation:

$$\begin{cases} \tilde{x} = S(x), & \tilde{y} = y, & \forall (x, y) \in \Omega \cup \Omega_d \quad \text{such that} \\ S(x) = x, & \forall x \in (0, L); \\ \Re\{S'(x)\} > 0, & \Im\{S'(x)\} > 0, & \forall x \in (L, L + d), \end{cases} \quad (2.4)$$

where $S(x)$ is a differentiable complex-valued function. Typically, one takes

$$S(x) = x + \frac{i}{k} \int_0^x \sigma(t) dt, \quad \forall x \in (0, L + d), \quad (2.5)$$

where $\sigma(\cdot) \geq 0$ is known as the *absorbing function* (ABF). A simple substitution

$$\frac{\partial}{\partial x} \rightarrow \frac{\partial}{\partial \tilde{x}} = \frac{dx}{d\tilde{x}} \frac{\partial}{\partial x} = \frac{1}{S'(x)} \frac{\partial}{\partial x}, \quad (2.6)$$

leads to the PML-equation (see, e.g., [84, (5)]):

$$\frac{\partial}{\partial x} \left(\frac{1}{S'(x)} \frac{\partial U_p}{\partial x} \right) + \frac{\partial}{\partial y} \left(S'(x) \frac{\partial U_p}{\partial y} \right) + k^2 S'(x) U_p = 0, \quad \forall (x, y) \in \Omega \cup \Omega_d, \quad (2.7)$$

which is supplemented with the transmission conditions at the interface $x = L$:

$$U_p|_{\Omega} = U_p|_{\Omega_d}, \quad \frac{\partial U_p}{\partial x}|_{\Omega} = \frac{1}{S'(x)} \frac{\partial U_p}{\partial x}|_{\Omega_d}, \quad (2.8)$$

together with the boundary conditions:

$$\begin{aligned} U_p(x, 0) = U_p(x, \pi) = 0, \quad x \in (0, L + d); \\ U_p(0, y) = g(y), \quad U_p(L + d, y) = 0, \quad y \in (0, \pi). \end{aligned} \quad (2.9)$$

It is noteworthy that the PML-solution is assumed to decay sufficiently fast in the artificial layer, so the homogeneous Dirichlet boundary condition is imposed at $x = L + d$.

Singer and Turkel [84] conducted error analysis of the PML with usual bounded absorbing functions. Here, we provide a much more precise description of the error between the original solution U and the PML-solution U_p in the physical domain Ω . To avoid distraction from the main results, we postpone the proof of the following theorem to Appendix A.1.

Theorem 2.1. *Let U be the solution of (2.1) given by (2.3), and let U_p be the PML-solution of (2.7)-(2.9). If $k > 0$ is not an integer, then for any $(x, y) \in \Omega$,*

$$U(x, y) = U_p(x, y) + \sum_{l=1}^{\infty} \hat{g}_l R_l(x) e^{i\hat{k}_l x} \sin(ly), \quad R_l(x) := \frac{1 - e^{-2i\hat{k}_l x}}{1 - e^{-2i\hat{k}_l S_d}}. \quad (2.10)$$

If $k > 0$ is an integer, then $R_l(x)$ for the mode $l = k$ in (2.10) should be replaced by

$$R_l(x) = -\frac{S(x)}{S_d}, \quad \forall x \in (0, L). \quad (2.11)$$

Moreover, we have the following bounds:

(i) for $0 \leq l < k$,

$$\frac{2|\sin(\hat{k}_l x)|}{e^{2\hat{k}_l \Im\{S_d\}} + 1} \leq |R_l(x)| \leq \frac{2|\sin(\hat{k}_l x)|}{e^{2\hat{k}_l \Im\{S_d\}} - 1}, \quad \forall x \in (0, L); \quad (2.12)$$

(ii) for $l > k$,

$$\frac{e^{2|\hat{k}_l|x} - 1}{e^{2|\hat{k}_l|\Re\{S_d\}} + 1} \leq |R_l(x)| \leq \frac{e^{2|\hat{k}_l|x} - 1}{e^{2|\hat{k}_l|\Re\{S_d\}} - 1}, \quad \forall x \in (0, L). \quad (2.13)$$

Here, $\hat{k}_l := \sqrt{k^2 - l^2}$, $S_d := S(L + d)$ and $S(x)$ is given by (2.4)-(2.5).

We see that for fixed k, l , the decay of $R_l(x)$ is completely determined by the values of $\Re\{S_d\}$ and $\Im\{S_d\}$, i.e., the choice of absorbing function $\sigma(\cdot)$. We now apply Theorem 2.1 to access the performance of some typical ABFs:

$$\text{PML}_n : \quad \sigma(x) = \begin{cases} 0, & \text{if } x \in (0, L), \\ \sigma_0 \left(\frac{x - L}{d} \right)^n, & \text{if } x \in (L, L + d), \end{cases} \quad (2.14)$$

and

$$\text{PML}_\infty : \quad \sigma(x) = \begin{cases} 0, & \text{if } x \in (0, L), \\ \frac{\sigma_0 d}{L + d - x}, & \text{if } x \in (L, L + d), \end{cases} \quad (2.15)$$

where $\sigma_0 > 0$ is a tuneable constant. The absorbing function of PML_n with integer $n \geq 0$, is commonly-used in the design of the PML (see, e.g., [25, 84, 19]). The unbounded absorbing function PML_∞ was first introduced by Bermúdez et al. [13, 14], which was advocated for its being “optimal”, “exact” and “parameter-free” in various settings (see, e.g., [13, 14, 76, 71, 77]). Clearly, for the PML_n and $x \in (L, L + d)$,

$$S(x) = x + \frac{i}{k} \frac{d \sigma_0}{n + 1} \left(\frac{x - L}{d} \right)^{n+1}, \quad \Re\{S_d\} = L + d, \quad \Im\{S_d\} = \frac{\sigma_0 d}{(n + 1)k}, \quad (2.16)$$

while for PML_∞ and $x \in (L, L + d)$,

$$S(x) = x + \frac{i d \sigma_0}{k} \ln \left(\frac{d}{L + d - x} \right), \quad \Re\{S_d\} = L + d, \quad \Im\{S_d\} \rightarrow \infty. \quad (2.17)$$

In both cases, $\Re\{S_d\}$ does not depend on the choice of $\sigma(\cdot)$, so for the evanescent waves, $l > k$, we have

$$|R_l(x)| \sim e^{-2\sqrt{l^2 - k^2}(L + d - x)}, \quad \forall x \in (0, L). \quad (2.18)$$

As a result, the only possibility to reduce the error is to increase the width d . For the waves, $l < k$, the PML_∞ can make the error vanish as $R_l(x) = 0$, but for the PML_n ,

$$|R_l(x)| \sim 2 \left| \sin \left(\sqrt{k^2 - l^2} x \right) \right| e^{-2\sqrt{k^2 - l^2} \sigma_0 d / ((n+1)k)}, \quad \forall x \in (0, L), \quad (2.19)$$

so one has to enlarge the thickness d of the layer or choose large $\sigma_0 d$ to reduce the error.

To illustrate the error behaviour, we consider the exact solution of (2.1) with $\{\hat{g}_l = i^l J_l(k)\}$ (in order to mimic the plane wave expansion):

$$U(x, y) = \sum_{l=1}^{\infty} i^l J_l(k) e^{i\sqrt{k^2 - l^2} x} \sin(l y), \quad (2.20)$$

where $J_l(\cdot)$ is the Bessel function of the first kind of order l . Define the error function, for $\forall (x, y) \in \Omega$:

$$\mathcal{E}_p(x, y) = U(x, y) - U_p(x, y) = \sum_{l=1}^{\infty} i^l J_l(k) R_l(x) e^{i\sqrt{k^2 - l^2} x} \sin(l y). \quad (2.21)$$

Here, we take $k = 9.99$, $L = 1$, $d = 0.1$, and truncate the infinite series for $l \leq 100$ so that the truncation error is negligible. The error curves $|\mathcal{E}_p(x, y)|$ with fixed $x = L/2, L$ and $y \in (0, \pi)$ in Figure 2.2 with PML_2 and PML_∞ in (2.14)-(2.15).

Observe that the errors of the PML_2 become slightly smaller as σ_0 increases, but they are still large. The PML_∞ using unbounded absorbing functions performs relatively better, but does not significantly improve the classical PML.

Figure 2.2: Profiles of the error function $|\mathcal{E}_p(x, y)|$ of the solution (2.20) with $k = 9.99, L = 1, d = 0.1$, and $\sigma_0 = 10, 100$ using PML_2 and PML_∞ . Left: the error curve $|\mathcal{E}_p(L/2, y)|$ for $y \in (0, \pi)$; Right: the error curve: $|\mathcal{E}_p(L, y)|$ for $y \in (0, \pi)$.

Remark 2.1. As shown in [13], the PML_∞ can completely damp the planar waves of the form: $e^{ik_x x + ik_y y}$ with $k_x = k \cos \theta_0, k_y = k \sin \theta_0$, where θ_0 is the incident angle at the left boundary $x = 0$ of the half-plane waveguide: $\Delta u + k^2 u = 0, x > 0, -\infty < y < \infty$. We also refer to [77] for some other successful situations. However, it fails to be “exact” and “optimal” in this setting.

Remark 2.2. Note from (2.17) that for the PML_∞ , $S'(x) = 1 + i\sigma(x)/k \rightarrow \infty$ as $x \rightarrow L + d$, so the coefficients in (2.7) are singular at the outer boundary $x = L + d$. In [13, 14], the use of e.g, Gauss quadrature to avoid sampling the unbounded endpoints was suggested for evaluating the matrices of the linear system in finite-element discretisation. However, for large wavenumber k and very thin layer, much care is needed to deal with the singularity to achieve high order. Moreover, in more complex situations, e.g., the circular/spherical PML, $S(x)$ also appears in the PML-equation, so the logarithmic singularity poses even more challenges in numerical discretisation.

Remark 2.3. To overcome the failure of PML for the evanescent waves, Zhu and Wu [98] proposed a mixed PML and (few-mode) DtN truncation (to deal with the evanescent modes) for the waveguide related to diffraction grating problems.

2.1.2 The new PAL technique

As reported in [89], the new PAL was inspired by the design of the “inside-out” invisibility cloak [97] using the notion of transformation optics [74]. In fact, the idea in [97] was also applied to create absorbing non-reflecting media as matching layers in numerical simulations of time-harmonic wave propagations. Consider for example the waveguide problem (2.1). In [97], the real rational transformation was introduced to obtain the media and design the layer:

$$\rho = \rho(x) = L + \frac{d(x-L)}{L+d-x}, \quad x \in (L, L+d), \quad \rho \in (L, \infty), \quad (2.22)$$

which compresses the outgoing waves in the infinite strip: $\rho > L$ to that into the finite layer: $(L, L+d)$. However, it is known that any attempt of using a real compression coordinate transform fails to work for Helmholtz and Maxwell’s equations. Indeed, according to [60], “any real coordinate mapping from an infinite to a finite domain will result in solutions that oscillate infinitely fast as the boundary is approached – such fast oscillations cannot be represented by any finite-resolution grid, and will instead effectively form a reflecting hard wall.”

In light of the idea in [89], we propose the complex compression coordinate transformation (C³T), that is, $S(x) = x$ for $x \in (0, L)$, and

$$S(x) = S_R(x) + i S_I(x), \quad x \in (L, L+d), \quad (2.23)$$

where the real part: $S_R(x) = \sigma_1 \rho(x)$ and the imaginary part: $S_I(x) = \sigma_0(\rho(x) - L)/k$. Like (2.15), $S_I(x)$ involves an unbounded absorbing function:

$$S_I(x) = \frac{1}{k} \int_L^x \sigma(t) dt, \quad \sigma(x) = \sigma_0 \left(\frac{d}{L+d-x} \right)^2, \quad x \in (L, L+d). \quad (2.24)$$

For clarity, we denote the PAL-solution by U_a . Thanks to (2.6), we obtain the PAL-equation as the counterpart of (2.7)-(2.9):

$$\begin{aligned} \frac{\partial}{\partial x} \left(\frac{1}{S'(x)} \frac{\partial U_a}{\partial x} \right) + \frac{\partial}{\partial y} \left(S'(x) \frac{\partial U_a}{\partial y} \right) + k^2 S'(x) U_a &= 0, \quad (x, y) \in \Omega \cup \Omega_d, \\ U_a|_{\Omega} &= U_a|_{\Omega_d}, \quad \frac{\partial U_a}{\partial x} \Big|_{\Omega} = \frac{1}{S'(x)} \frac{\partial U_a}{\partial x} \Big|_{\Omega_d} \quad \text{at } x = L, \end{aligned} \quad (2.25)$$

$$U_a(x, 0) = U_a(x, \pi) = 0; \quad U_a(0, y) = g(y), \quad U_a(L+d, y) = 0.$$

We can show that the new PAL is truly exact and non-reflecting.

Theorem 2.2. *Let U be the solution of (2.1), and U_a be the solution of (2.25). Then we have*

$$U_a(x, y) \equiv U(x, y), \quad \forall (x, y) \in \Omega. \quad (2.26)$$

Proof. Note that the error formula in Theorem 2.1 is valid for general $S(x)$. It is evident that by (2.23), we have $\Re\{S(L+d)\} = \infty$ and $\Im\{S(L+d)\} = \infty$. Thus, it follows immediately from (2.12)-(2.13) that $R_l(x) = 0$ uniformly for all l and $x \in (0, L)$, which implies $U_a(x, y) \equiv U(x, y)$ in Ω . $\square$

We see that the PAL is perfect at continuous level, but the compression coordinate transformation induces singular coefficients at $x = L+d$ in the PAL-equation (2.25), which causes some numerical difficulties in discretization. To overcome this, we introduce the following substitution of the unknown:

$$U_a(x, y) = w(x)V_a(x, y), \quad w(x) = \frac{L+d-x}{d}, \quad x \in (L, L+d), \quad (2.27)$$

with $w(x) = 1$ for $x \in (0, L)$. In fact, we can show that the problem of V_a is free of singularity. As with the circular PAL in [89], we find it's more convenient to work with the variational form. Denote

$$\mathbb{U} := \{u = wv : v \in H^1(\Omega \cup \Omega_d), v(x, 0) = v(x, \pi) = 0, \quad x \in (0, L+d)\},$$

and introduce the sesquilinear form on $\mathbb{U} \times \mathbb{U}$:

$$\mathcal{B}(U_a, \Psi) = (\mathbf{C} \nabla U_a, \nabla \Psi) - k^2(S' U_a, \Psi), \quad (2.28)$$

where $\mathbf{C} = \text{diag}(1/S'(x), S'(x))$, and $(\cdot, \cdot)$ is the inner product of $L^2(\Omega \cup \Omega_d)$.

In view of (2.24), a direct calculation leads to $w^2(x)S'(x) = \alpha = \sigma_1 + i\sigma_0/k$. Then, substituting $U_a = wV_a$ and $\Psi = w\Phi$ into (2.28), we obtain from a direct calculation that

$$\tilde{\mathcal{B}}_{\Omega_d}(V_a, \Phi) = \mathcal{B}_{\Omega_d}(wV_a, w\Phi) = (\tilde{\mathbf{C}} \tilde{\nabla} V_a, \tilde{\nabla} \Phi)_{\Omega_d} - \alpha k^2(V_a, \Phi)_{\Omega_d}, \quad (2.29)$$

where $(\cdot, \cdot)_{\Omega_d}$ is the inner product on the artificial layer Ω_d , and

$$\widetilde{\mathcal{C}} = \text{diag}(w^2(x)/\alpha, \alpha), \quad \widetilde{\nabla} = (w(x)\partial_x - 1/d, \partial_y). \quad (2.30)$$

It is seen that the substitution can absorb the singular coefficients. In the implementation, one can easily incorporate the substitution into the basis functions and directly approximate U_a .

Figure 2.3: Profiles of the PML solution U_p with regular function (2.14) ($\sigma_0 = 1$, $n = 2$) and singular function (2.15) vs PAL solution U_a in Ω and V_a in Ω_d with $k = 99.99$, $(L, d) = (1, 0.2)$ along the x -axis at $y = \pi/2$. Left: real part solution; Right: imaginary part solution.

2.2 Star-shaped domain truncation

In this section, we design a PAL with a general star-shaped domain truncation for solving the two-dimensional time-harmonic acoustic wave scattering problem with perfectly conducting boundary in an exterior domain:

$$\mathcal{L}[U] := \Delta U + k^2 U = f \quad \text{in } \Omega_e := \mathbb{R}^2 \setminus \bar{D}; \quad (2.31a)$$

$$U = g \quad \text{on } \partial D; \quad \left| \frac{\partial U}{\partial r} - ikU \right| \leq \frac{c}{r} \quad \text{for } r =: |\mathbf{x}| \gg 1. \quad (2.31b)$$

Here, $D \subset \mathbb{R}^2$ is a bounded scatterer with Lipschitz boundary $\Gamma_D = \partial D$, and $g \in H^{1/2}(\Gamma_D)$. We assume that the source f is compactly supported in a disk

$B(\supset D)$. The far-field condition in (2.31b) is known as the Sommerfeld radiation boundary condition. We point out that the PAL technique to be introduced is applicable to the Helmholtz problems with other types of boundary conditions such as Dirichlet or impedance boundary condition on Γ_D , and also to solve acoustic wave propagation in inhomogeneous media in a bounded domain.

As illustrated in Figure 2.4, we enclose $B(\supset \bar{D})$ by a star-shaped domain Ω_s with respect to the origin. Assume that the boundary of Ω_s is piecewise smooth with the parametric form in the polar coordinates, viz.,

$$\Gamma_{R_1} := \partial\Omega_s = \{(r, \theta) : r = R_1(\theta), \theta \in [0, 2\pi)\}, \quad (2.32)$$

or equivalently, Γ_{R_1} has the parametric form in Cartesian coordinates:

$$\Gamma_{R_1} = \{\mathbf{x} = (x, y) : x = R_1(\theta) \cos \theta, y = R_1(\theta) \sin \theta, \theta \in [0, 2\pi)\}. \quad (2.33)$$

Then the artificial layer is formed by surrounding Ω_s with

$$\Omega_\varrho^{\text{PAL}} := \{(r, \theta) : R_1(\theta) < r < R_2(\theta) := \varrho R_1(\theta), \theta \in [0, 2\pi)\}, \quad (2.34)$$

where the constant $\varrho > 1$ can tune the “thickness” of the layer. The layer $\Omega_\varrho^{\text{PAL}}$ provides a star-shaped truncation of the unbounded domain Ω_e . We further denote the domain of interest and the real computational domain, respectively, by

$$\Omega := \Omega_s \setminus \bar{D}, \quad \Omega_c := \Omega_\varrho^{\text{PAL}} \cup \Omega \cup \Gamma_{R_1}, \quad (2.35)$$

where we need to approximate the original solution in Ω , but have to couple the original equation in Ω with the artificial equation in $\Omega_\varrho^{\text{PAL}}$ in real computation. Since the choice of the truncated domains is *a priori* arbitrary, it could be an advantage to choose non-classical shapes to offer more flexibility to deal with non-standard geometry of the scatterer and inhomogeneity of the media.

It is important to note that the configuration of the artificial layer is solely determined by the parametric form of $R_1(\theta)$ and the tuning “thickness” parameter ϱ . We list below some typical examples of such star-shaped domain truncation.

- (i) In the circular case, the artificial layer is an annulus, i.e.,

$$\Omega_\varrho^{\text{PAL}} = \{R_1 < r < R_2 = \varrho R_1, 0 \leq \theta < 2\pi\}, \quad (2.36)$$

where R_1 is independent of θ . As a variant, the “perturbed” annular layer takes the form:

$$\Omega_\varrho^{\text{PAL}} = \{R_1(\theta) = a + b \sin \theta < r < R_2(\theta) = \varrho R_1(\theta), 0 \leq \theta < 2\pi\}, \quad (2.37)$$

where $a, b > 0$ are some given constants.

- (ii) In the rectangular case, we take for instance the boundary Γ_{R_1} as a square with four vertices: $(a, b), (-a, b), (-a, -b), (a, -b)$ with $a, b > 0$. Then we have

$$R_1(\theta) = \begin{cases} a \sec \theta, & \theta \in [0, \theta_0) \cup [2\pi - \theta_0, 2\pi), \\ b \csc \theta, & \theta \in [\theta_0, \pi - \theta_0), \\ -a \sec \theta, & \theta \in [\pi - \theta_0, \pi + \theta_0), \\ -b \csc \theta, & \theta \in [\pi + \theta_0, 2\pi - \theta_0), \end{cases} \quad (2.38)$$

where $\theta_0 = \arctan \frac{b}{a}$. Similarly, we can consider a general rectangular domain truncation.

- (iii) If we choose Γ_{R_1} to be an ellipse: $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$ with $a > b > 0$, then we have

$$R_1(\theta) = \frac{ab}{\sqrt{b^2 + (a^2 - b^2) \sin^2 \theta}}, \quad \theta \in [0, 2\pi). \quad (2.39)$$

Now, the key issue is how to construct the governing equation in the artificial layer. In practice, one would wish (i) the solution of the resulted coupled problem in Ω_c can approximate the original solution $U|_\Omega$ as accurate as possible to avoid the pollution of the truncation, but (ii) the layer $\Omega_\varrho^{\text{PAL}}$ should be as thin as possible to save computational cost. To show the essence of designing the PAL-equation for the above general star-shaped truncated domain, [89] first recap on the circular PAL, but explore this technique from a very different viewpoint.

Figure 2.4: Left: illustration of the circular PAL from radial direction. Middle: schematic illustration of the rectangular PAL Ω_d with four trapezoidal patches. Right: illustration of the elliptic PAL under elliptic coordinate.

2.3 Some new perspectives of circular PAL

In what follows, we shall reveal that the governing equation (in the annular layer: $r \in (R_1, R_2)$) in [89] can be obtained from the Benenger equation (in the unbounded domain $\rho > R_1$, see Collino and Monk [25]) by a real compression transformation. As a result, we can claim the exactness of the PAL technique – the PAL-solution for $r < R_1$ coincides with the original solution $U|_{r < R_1}$. This should be in contrast with the PML technique [25, 19], where the governing equation in the layer is obtained by naively truncating the Benenger equation in unbounded domain at $r = R_2$, and then impose the homogeneous Dirichlet boundary condition.

Similar to (2.22), Zharova et al. [97] introduced the real compression transformation

$$\rho := \rho(r) = R_1 + (R_2 - R_1) \frac{r - R_1}{R_2 - r} \quad \text{or} \quad r = R_2 - \frac{(R_2 - R_1)^2}{\rho + R_2 - 2R_1}, \quad (2.40)$$

for $\rho \in (R_1, \infty)$ and $r \in (R_1, R_2)$, to design the inside-out (or inverse) invisibility cloak and also a matched layer. In principle, it compresses all the infinite space: $R_1 < \rho < \infty$ into the finite annulus: $R_1 < r < R_2$, where ideally the wave propagation is expected to be equivalent to the wave propagation in the infinite space. However, such a technique fails to work, as the numerical approximation of the waves within the layer suffers from *the curse of infinite oscillation* [61].

Following [89], we propose to fill the cloaking layer with lossy media (i.e., complex material parameters), and deal with the singular media by using a suitable substitution of unknowns. More precisely, we introduce the compression complex coordinate transformation in polar coordinates: as $\tilde{\theta} = \theta$, $\theta \in [0, 2\pi)$,

$$\tilde{r} = S(r) = \begin{cases} r, & r < R_1, \\ R_1 + \sigma_1 T(r) + i\sigma_0 T(r), & R_1 < r < R_2, \end{cases} \quad (2.41)$$

where $\sigma_0, \sigma_1 > 0$ are tuning parameters, and

$$T(r) = \frac{r - R_1}{R_2 - r} = (R_2 - R_1) \int_{R_1}^r \frac{dt}{(R_2 - t)^2}, \quad r \in (R_1, R_2). \quad (2.42)$$

It is important to remark that (i) the real part $\Re\{\tilde{r}\}$ with $\sigma_1 = R_2 - R_1$ is the compression coordinate transformation (2.40), and $\Im\{\tilde{r}\}$ defines a compression mapping between $(0, \infty)$ and (R_1, R_2) ; and the parameters σ_0, σ_1 can be k -dependent, e.g., a constant multiple of $1/k$.

The PAL-equation can be obtained by applying the complex coordinate transformation (2.41) to the Helmholtz problem (2.31) in $(\tilde{r}, \tilde{\theta})$ -coordinates (see [89]):

$$\begin{cases} \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\beta r}{\alpha} \frac{\partial U_{\text{PAL}}}{\partial r} \right) + \frac{1}{r^2} \frac{\alpha}{\beta} \frac{\partial^2 U_{\text{PAL}}}{\partial \theta^2} + \alpha \beta k^2 U_{\text{PAL}} = f, & \text{in } \Omega \cup \Omega_e^{\text{PAL}}, \\ U_{\text{PAL}} = g & \text{on } \Gamma_D, \quad |U_{\text{PAL}}| \text{ is uniformly bounded as } r \rightarrow R_2, \end{cases} \quad (2.43)$$

together with the usual transmission conditions at $\rho = R_1$. Here, we denoted

$$\alpha = \frac{d\tilde{r}}{dr}, \quad \beta = \frac{\tilde{r}}{r}. \quad (2.44)$$

2.3.1 Bérenger's equations and PML techniques

In [89], we adopted the transformed Sommerfeld radiation boundary condition as $r \rightarrow R_2$. In fact, it is only necessary to impose the uniform boundedness to guarantee the unique solvability and exactness with $U|_{r \leq R_1} = U_p|_{r \leq R_1}$ (see Theorem 2.3 below). To justify this, we next show that the PAL-equation (2.43) can be derived from the Bérenger's equation (in unbounded domain) in [25].

Indeed, using separation of variables, the solution U of the Helmholtz problem (2.31) exterior to the circle: $r = R_2$ can be written as

$$U(\mathbf{x}) = \sum_{|m|=0}^{\infty} a_m \frac{H_m^{(1)}(kr)}{H_m^{(1)}(kR_2)} e^{im\theta}, \quad r \geq R_2, \quad (2.45)$$

where $\mathbf{x} = re^{i\theta}$, $H_m^{(1)}$ is the Hankel function of first kind and order m , and $\{a_m\}$ are the Fourier expansion coefficients of U at $r = R_2$. This series converges uniformly for $r \geq b$ (cf. [72]). According to [25], the Bérenger's idea to design PML in the cylindrical coordinates can be interpreted as stretching the solution (2.45) to the complex domain so that the waves become evanescent. Recall the asymptotic behaviour of the Hankel function (cf. [1]):

$$|H_m^{(1)}(k\tilde{r})| \sim \left| \sqrt{\frac{2}{\pi k \tilde{r}}} e^{i(k\{\Re\{\tilde{r}\} + i\Im\{\tilde{r}\}) - \frac{1}{2}m\pi - \frac{1}{4}\pi)} \right| = \sqrt{\frac{2}{\pi k |\tilde{r}|}} e^{-k\Im\{\tilde{r}\}}, \quad (2.46)$$

for $-\pi < \arg\{\tilde{r}\} < 2\pi$. This implies that the extension should be made in the upper half-plane such that $\Im\{\tilde{r}\} \rightarrow \infty$ as $|\tilde{r}| \rightarrow \infty$. In the PML technique, one uses the complex change of variables:

$$\tilde{r} = \tilde{r}(\rho) = \begin{cases} \rho, & \text{for } \rho < R_1, \\ \rho + i \int_{R_1}^{\rho} \hat{\sigma}(t) dt, & \text{for } R_1 \leq \rho < \infty, \end{cases} \quad (2.47)$$

where in general, the absorbing function $\hat{\sigma}$ satisfies

$$\hat{\sigma} \in C(\mathbb{R}), \quad \hat{\sigma} \geq 0 \quad \text{and} \quad \lim_{r \rightarrow \infty} \int_{R_1}^r \hat{\sigma}(t) dt = \infty. \quad (2.48)$$

Denote $\hat{\alpha} = \tilde{r}'(\rho)$ and $\hat{\beta} = \tilde{r}(\rho)/\rho$. Applying the coordinate transformation (2.47) to the Helmholtz equation exterior to the circle of radius R_1 , we can obtain the Bérenger's problem of computing the Bérenger's solution U_B in the form (cf. [25]):

$$\begin{cases} \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\frac{\hat{\beta} \rho}{\hat{\alpha}} \frac{\partial U_B}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\hat{\alpha}}{\hat{\beta}} \frac{\partial^2 U_B}{\partial \theta^2} + \hat{\alpha} \hat{\beta} k^2 U_B = f & \text{in } \Omega_e = \mathbb{R}^2 \setminus \bar{D}; \\ U_B = g & \text{on } \Gamma_D, \\ |U_B| \text{ is uniformly bounded as } \rho \rightarrow \infty, \end{cases} \quad (2.49)$$

together with the usual transmission conditions at $\rho = R_1$. Note that $\hat{\alpha} = \hat{\beta} = 1$ for $|\mathbf{x}| \leq R_1$. According to [25, Theorem 1], the problem (2.49) admits a unique solution, and for any $|\mathbf{x}| \geq R_1$, the Bérenger's solution takes the form

$$U_B(\mathbf{x}) = \sum_{|m|=0}^{\infty} a_m \frac{H_m^{(1)}(k\tilde{r}(\rho))}{H_m^{(1)}(kR_1)} e^{im\theta}, \quad (2.50)$$

where $\{a_m\}$ are the same as in (2.45). In other words, *the Bérenger's solution coincides with the solution of the original problem (2.31) for $r < R_1$.*

As shown in [25, 19], the PML technique directly truncates (2.49) at $\rho = R_2$, and the homogeneous boundary condition: $U_{\text{PML}} = 0$ at $\rho = R_2$ is then imposed. More precisely, we have the following PML-equation:

$$\begin{cases} \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\hat{\beta} r}{\hat{\alpha}} \frac{\partial U_{\text{PML}}}{\partial r} \right) + \frac{1}{r^2} \frac{\hat{\alpha}}{\hat{\beta}} \frac{\partial^2 U_{\text{PML}}}{\partial \theta^2} + \hat{\alpha} \hat{\beta} k^2 U_{\text{PML}} = f \\ \hspace{15em} \text{in } \Omega_e \cap \{|\mathbf{x}| < R_2\}; \\ U_{\text{PML}}|_{\Gamma_D} = g; \quad U_{\text{PML}}|_{r=R_2} = 0, \end{cases} \quad (2.51)$$

where we set $r = \rho$ as the independent variable for clarity. Like the waveguide setting in (2.14) -(2.15), the following two types of absorbing functions have been used in practice.

- (i) PML_n with bounded (or regular) ABFs (see, e.g., [25, 19]):

$$\hat{\sigma}(t) = \left(\frac{t - R_1}{R_2 - R_1} \right)^n, \quad (2.52)$$

so

$$\tilde{r} = r + i\sigma_0 \frac{R_2 - R_1}{n+1} \left(\frac{r - R_1}{R_2 - R_1} \right)^{n+1}, \quad r \in (R_1, R_2), \quad (2.53)$$

where n is a positive integer. We refer to [19] for the detailed error analysis, and also the very recent work [64] for the insightful wavenumber explicit error estimates.

- (iv) PML_∞ with unbounded (or singular) ABFs (see [13, 14]):

$$\hat{\sigma}(t) = \frac{1}{R_2 - t}, \quad \text{so} \quad \tilde{r} = r + i\sigma_0 \ln \left(\frac{R_2 - R_1}{R_2 - r} \right), \quad r \in (R_1, R_2). \quad (2.54)$$

Compared with the PML_n , the PML_∞ renders the solution decay at an infinite rate near the outer boundary $r = R_2$. It is therefore not surprising it is parameter-free [24]. However, from the above analysis, we infer that the PML-equation (2.51) with unbounded ABFs (2.54) does not really exactly solves the original problem in Ω . In addition, the coefficients: $\hat{\alpha} = \tilde{r}'(r)$ and $\hat{\beta} = \tilde{r}(r)/r$ are singular at $r = R_2$, which brings about numerical difficulties in realisation.

2.3.2 Equivalence of Bérenger's problem and PAL equation

We next show that in contrast to the PML technique, our proposed PAL-equation exactly solves the transformed problem (2.49) by further transforming it to a bounded domain by using a real compression mapping.

Theorem 2.3. *Let $U_B(\rho, \theta)$ be the solution of the Bérenger's problem (2.49) with $\hat{\sigma} = \sigma_0/\sigma_1$ in (2.47), that is, the complex coordinate transformation:*

$$\tilde{r} = \rho + i\frac{\sigma_0}{\sigma_1}(\rho - R_1), \quad \text{for } \rho > R_1. \quad (2.55)$$

Then applying the real compression rational mapping

$$\rho = R_1 + \sigma_1 T(r) = R_1 + \sigma_1 \frac{r - R_1}{R_2 - r}, \quad (2.56)$$

to (2.47), we can derive the circular PAL-equation (2.43). Moreover, the PAL-equation (2.43) admits a unique solution, and

$$U_{\text{PAL}}(r, \theta) = U_B(R_1 + \sigma_1 T(r), \theta), \quad r < R_2; \quad \text{and} \quad U_{\text{PAL}}|_{r < R_1} = U|_{r < R_1}, \quad (2.57)$$

where U is the solution of the original problem (2.31).

Proof. It suffices to consider the transformation for $\rho > R_1$. We find from (2.47) with $\hat{\sigma} = \sigma_0/\sigma_1$ that $\hat{\alpha} = 1 + i\sigma_0/\sigma_1$ and $\hat{\beta} = (\rho + i\sigma_0(\rho - R_1)/\sigma_1)/\rho$. Using the

rational mapping: $\rho = R_1 + \sigma_1 T(r)$, we obtain from (2.44) and the composite transformation (2.55)-(2.56) (i.e., (2.41)) that

$$\begin{aligned}\alpha &= (\sigma_1 + i\sigma_0)T'(r) = \hat{\alpha} \frac{d\rho}{dr}, \\ \beta &= \frac{R_1 + (1 + i\sigma_0)T(r)}{r} = \frac{\rho + i\sigma_0(\rho - R_1)}{\rho} = \hat{\beta} \frac{\rho}{r}.\end{aligned}\tag{2.58}$$

By a simple substitution: $\frac{d}{d\rho} = \frac{dr}{d\rho} \frac{d}{dr}$, we can obtain (2.58) from (2.49) straightforwardly.

The unique solvability follows directly from that of (2.49) (see [25, Theorem 1]). Moreover, the PAL-solution is a compression of the Bnenger solution: $U_p(r, \theta) = U_B(R_1 + \sigma_1 T(r), \theta)$ for $r < R_2$, so it is identical to the original solution for $r < R_1$. Thus, by (2.50), we have

$$U_p(\mathbf{x}) = \sum_{|m|=0}^{\infty} \hat{a}_m \frac{H_m^{(1)}(kS(r))}{H_m^{(1)}(kR_1)} e^{im\theta}, \quad R_1 < r < R_2, \tag{2.59}$$

where $\{\hat{a}_m\}$ are the Fourier coefficients of $U_p(R_1, \theta)$. □

With the above understanding, we can show that the PAL-solution in the artificial layer decays exponentially. In fact, the bound is more precise than the estimate in [89, Theorem 1].

Theorem 2.4. *The solution of the PAL-equation (2.43) satisfies that for all $r \in [R_1, R_2)$,*

$$\begin{aligned}& \int_0^{2\pi} |U_{\text{PAL}}(r, \theta)|^2 d\theta \\ & \leq \exp\left(-\sigma_0 k \frac{\tau}{1-\tau} (1 - h(\tau)(1-\tau)^2)^{1/2}\right) \int_0^{2\pi} |U_{\text{PAL}}(R_1, \theta)|^2 d\theta,\end{aligned}\tag{2.60}$$

where

$$h(\tau) = \frac{R_1^2}{(R_1(1-\tau) + \sigma_1 \tau)^2 + \sigma_0^2 \tau^2}, \quad \tau = \frac{r - R_1}{R_2 - R_1} \in [0, 1).$$

Proof. We now show that the PAL-solution decays exponentially in the PAL layer. For this purpose, we recall the uniform estimate of Hankel functions first

derived in [19, Lemma 2.2]: For any complex z with $\Re\{z\}, \Im\{z\} \geq 0$, and for any real Θ such that $0 < \Theta \leq |z|$, we have

$$|H_\nu^{(1)}(z)| \leq e^{-\Im\{z\}\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}} |H_\nu^{(1)}(\Theta)|, \quad (2.61)$$

which is valid for any real order ν . Note that $S(R_1) = R_1$, and for $r \in [R_1, R_2)$,

$$|S(r)|^2 = (R_1 + \sigma_1 T(r))^2 + \sigma_0 T^2(r) \geq R_1^2, \quad \Im\{S(r)\} = \sigma_0 T(r).$$

Thus, we obtain from (2.61) with $z = kS(r)$ and $\Theta = kR_1$ that for $r \in [R_1, R_2)$,

$$\begin{aligned} \max_{|m| \geq 0} \left| \frac{H_m^{(1)}(kS(r))}{H_m^{(1)}(kR_1)} \right| &\leq \exp \left\{ -k\Im\{S(r)\} \left(1 - \frac{R_1^2}{|S(r)|^2} \right)^{1/2} \right\} \\ &= \exp \left(-\sigma_0 k \frac{\tau}{1-\tau} (1 - h(\tau)(1-\tau)^2)^{1/2} \right), \end{aligned} \quad (2.62)$$

where the last step follows from direct calculation. $\square$

It is seen that the PAL-equation leads to the exact Bérnenger solution, which decays exponentially to zero at a rate: $O(e^{-k\sigma_0/(1-\tau)})$ as $r \rightarrow R_2$ (i.e., as $\tau \rightarrow 1$), where we note that $\sigma_0 \sim k^{-1}$. However, there are two numerical issues to be addressed.

- (i) The coefficients of the PAL-equation (2.51) are singular, which are induced by the compression rational mapping: $\rho = R_1 + \sigma_1 T(r)$. In fact, we have

$$\alpha(r) \sim \frac{C_1}{(R_2 - r)^2}, \quad \beta(r) \sim \frac{C_2}{R_2 - r}. \quad (2.63)$$

- (ii) Observe from (2.46) that the real part of the transformation: $\rho = \Re\{S(r)\} = R_1 + \sigma_1 T(r)$ may increase the oscillation near the inner boundary $r = R_1$.

To resolve these two issues, as in [89] a substitution of the unknown: $U_{\text{PAL}} = w(r)V_p$ by using a suitable factor $w(r)$, so that V_p to be approximated is well-behaved. To have the insights into the choice of w , we study the behaviour of the ratio by using (2.46):

$$\begin{aligned} \frac{H_m^{(1)}(kS(r))}{H_m^{(1)}(kR_1)} &\sim \sqrt{\frac{R_1}{S(r)}} e^{ik(\Re\{S(r)\}-R_1)} e^{-k\Im\{S(r)\}} \\ &= \sqrt{\frac{R_1}{S(r)}} e^{ik\sigma_1 T(r)} e^{-k\Im\{S(r)\}}. \end{aligned} \quad (2.64)$$

It implies the oscillatory part of U_{PAL} can be extracted explicitly: $U_{\text{PAL}}(r, \theta) = e^{ikT(r)} \widetilde{U}_{\text{PAL}}(r, \theta)$, where $\widetilde{U}_{\text{p}}(r, \theta)$ is expected to have no essential oscillation. As a result, the second issue can be resolved effectively. As for the first issue, it is seen from Theorem 2.3 that the singular coefficients are induced by the real transformation: $\rho = R_1 + \sigma_1 T(r)$. In fact, similar singular mapping techniques were used to map elliptic problems with rapid decaying solutions in unbounded domains to problems with singular coefficients in bounded domains (see, e.g., [15, 50, 83, 80] and the references therein), so one can also consider a suitable variational formulation weighted with $\omega(r) = R_2 - r$. Unfortunately, the involved variational formulation is usually non-symmetric, which is therefore less efficient for computation. In fact, as shown in [89], we can absorb the singularity and diminish the oscillation by the substitution:

$$U_{\text{p}}(r, \theta) = w(r) V_{\text{p}}(r, \theta), \quad r < R_2, \quad (2.65)$$

where

$$w(r) = \begin{cases} 1, & \text{for } r < R_1, \\ (R_2 - r)^{3/2} e^{ik\sigma_1 T(r)}, & \text{for } R_1 \leq r < R_2, \end{cases} \quad (2.66)$$

which leads to symmetric linear systems.

It is important to remark that in numerical discretisation, we can build the substitution in the basis functions. More precisely, we approximate U_{PAL} by the nonstandard basis $\{w\phi_k\}$ (where $\{\phi_k\}$ are usual spectral or finite element basis functions) to avoid transforming the PAL-equation into a much complicated problem in V_{p} . In the above, we just show the idea, but refer to [89] and the more general case in Section 2.4 for the implementation details.

2.4 PAL for star-shaped domain truncation

With the previous understanding of the circular case, we are now ready to construct the PAL technique for the general star-shaped truncation with the configuration described in Subsection 2.2. We start with the design of PAL-equation

by using the complex compression coordinate transformation, and study its outstanding performance.

2.4.1 Design of the PAL-equation

The first step is to extend the complex compression coordinate transformation (2.41) for the circular PAL to

$$\begin{aligned} \tilde{r} &= S(r, \theta) \\ &= \begin{cases} r, & \text{in } \Omega, \\ R_1(\theta) + \sigma_1 T(r, \theta) + i\sigma_0 T(r, \theta), & \text{in } \Omega_\varrho^{\text{PAL}}, \end{cases} \quad \tilde{\theta} = \theta, \quad \theta \in [0, 2\pi), \end{aligned} \quad (2.67)$$

where

$$T(r, \theta) = \frac{r - R_1}{R_2 - R_1} = (R_2 - R_1) \int_{R_1}^r \frac{dt}{(R_2 - t)^2}, \quad r \in (R_1, R_2). \quad (2.68)$$

Different from the circular case, R_1 and R_2 are now θ -dependent. Indeed, we notice from (2.32) and (2.34) that $R_1 = R_1(\theta)$ defines the inner boundary of the artificial layer $\Omega_\varrho^{\text{PAL}}$, whose outer boundary is given by $R_2 = \varrho R_1(\theta)$. For any fixed $\theta \in [0, 2\pi)$, $\Re\{\tilde{r}\} = R_1(\theta) + \sigma_1 T(r, \theta)$ compresses the infinite “ray”: $R_1 \rightarrow \infty$ into a “line segment”: $R_1 \rightarrow R_2$ in the radial direction. Accordingly, for all $\theta \in [0, 2\pi)$, it compresses the open space exterior to the star-shaped domain $\{r < R_2\}$ to the artificial layer $\Omega_\varrho^{\text{PAL}}$.

Remark 2.4. *Based on the notion of transformation optics [74], the use of a real singular coordinate transformation to expand the origin into a polygonal or star-shaped domain to design invisibility cloaks, is discussed in e.g., [94, 92]. In contrast, the real part of the transformation (2.67): $R_1(\theta) + \sigma_1 T(r, \theta)$ compresses the infinity to the finite boundary $r = R_2(\theta)$, so the cloaking is an inside-out or inverse cloaking as with [97]. However, to the best of our knowledge, this type of cloaking has not been studied in literature.*

In order to derive the PAL-equation in Cartesian coordinates, it is necessary to commute between different coordinates in the course as shown in the diagram:

$$\boxed{\text{Cartesian: } (\tilde{x}, \tilde{y})} \longleftrightarrow \boxed{\text{Polar: } (\tilde{r}, \tilde{\theta})} \xrightarrow{\text{Transform}} \boxed{\text{Polar: } (r, \theta)} \longleftrightarrow \boxed{\text{PAL: } (x, y)} \quad (2.69)$$

In what follows, the differential operators “ $\nabla, \nabla \cdot$ ” are in (x, y) -coordinates, but the coefficient matrix $\mathbf{C}$ and the reflective index n are expressed in (r, θ) -coordinates. For simplicity, we denote the partial derivatives by $S_r = \partial_r S$ and $S_\theta = \partial_\theta S$, etc..

The most important step is to obtain the formulation of the transformed Helmholtz operator as follows.

Lemma 2.1. *Using the transformation (2.67), the Helmholtz operator*

$$\tilde{\mathcal{H}}[\tilde{U}] := \Delta \tilde{U} + k^2 \tilde{U}, \quad (2.70)$$

in $(\tilde{x}, \tilde{y})$ -coordinates, can be transformed into

$$\mathcal{H}[U_p] := \frac{1}{n} \{ \nabla \cdot (\mathbf{C} \nabla U_p) + k^2 n U_p \}, \quad (2.71)$$

where $U_p(x, y) = \tilde{U}(\tilde{x}, \tilde{y})$, $\mathbf{C} = (C_{ij})$ is a two-by-two symmetric matrix and n is the reflective index given by

$$\mathbf{C} = \mathbf{T} \mathbf{B} \mathbf{T}^t, \quad n = \frac{S S_r}{r}, \quad (2.72)$$

and

$$\mathbf{B} = \begin{pmatrix} \frac{S}{r S_r} \left(1 + \frac{S_\theta^2}{S^2} \right) & -\frac{S_\theta}{S} \\ -\frac{S_\theta}{S} & \frac{r S_r}{S} \end{pmatrix}, \quad \mathbf{T} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}. \quad (2.73)$$

To avoid distraction from the main results, we provide the derivation in Appendix A.2.

With the aid of Lemma 2.1, we directly apply (2.67)-(2.68) to the exterior Helmholtz problem and obtain the PAL-equation for the general star-shaped truncation of the unbounded domain, as summarized below.

Theorem 2.5. *The PAL-equation associated with star-shaped domain truncation of the original Helmholtz problem (2.31) takes the form*

$$\begin{cases} \nabla \cdot (\mathbf{C} \nabla U_{\text{PAL}}) + k^2 n U_{\text{PAL}} = f & \text{in } \Omega \cup \Omega_{\varrho}^{\text{PAL}}, \\ U_{\text{PAL}} = g & \text{on } \Gamma_D, \\ |U_{\text{PAL}}| \text{ is uniformly bounded as } r \rightarrow R_2, \end{cases} \quad (2.74)$$

where $\mathbf{C} = \mathbf{I}$, $n = 1$ in Ω , and $\mathbf{C}, n$ in $\Omega_{\varrho}^{\text{PAL}}$ are the same as in Lemma 2.1 with the transformation S given by (2.67)-(2.68). Here, we impose the usual transmission conditions across any interface $\Gamma_{R_1} : r = R_1$.

As an extension of the circular case, the asymptotic boundary condition at $r = R_2$ is obtained from the transformed Sommerfeld radiation condition and the rapid decaying property of U_p near the outer boundary of $\Omega_{\varrho}^{\text{PAL}}$. We elaborate more on this by following the discussions in the previous section based on [25]. For any fixed $\theta \in [0, 2\pi)$, we can formally express the solution of (2.31) as

$$U(r, \theta) = \sum_{|m|=0}^{\infty} \tilde{a}_m \frac{H_m^{(1)}(kr)}{H_m^{(1)}(kR_1)} e^{im\theta}, \quad r > R_1, \quad (2.75)$$

where $\{\tilde{a}_m\}$ are determined by U at the circle $r = R_1$. Then, we extend (2.55) directly to the θ -dependent situation: $\tilde{r} = \rho$ for $\rho < R_1$, and

$$\tilde{r} = \tilde{r}(\rho, \theta) = \rho + i \frac{\sigma_1}{\sigma_0} (\rho - R_1) \quad \text{for } \rho > R_1. \quad (2.76)$$

Then we can apply Lemma 2.1 to derive the Benenger-type problem in the unbounded domain like (2.49). Its solution for $\rho > R_1$ can be obtained from complex stretching of (2.75):

$$U(\rho, \theta) = \sum_{|m|=0}^{\infty} \tilde{a}_m \frac{H_m^{(1)}(k\tilde{r})}{H_m^{(1)}(kR_1)} e^{im\theta}, \quad \rho > R_1. \quad (2.77)$$

Note that the transformation (2.67) is a composition of (2.76) and the real compression transformation: $\rho = R_1 + \sigma_1 T(r, \theta)$. Thus, the PAL-equation in Theorem 2.5 turns out to be a real compression of the Benenger-type problem.

2.4.2 Substitution and implementation

A key to the success of the PAL technique is to make a substitution of the unknown that can deal with the singular coefficients at $r = R_2$ (note: the PAL-solution is not singular), and diminish the oscillation near $r = R_1$.

We find it is more convenient to work with the weak formulation of (2.74). In what follows, we assume that $g = 0$, and define the space

$$H_{0,\Gamma}^1(\Omega_c) = \{\phi \in H^1(\Omega_c) : \phi|_{\Gamma} = 0\}, \quad \Omega_c := \Omega \cup \Omega_{\rho}^{\text{PAL}}, \quad \Gamma := \partial D. \quad (2.78)$$

A weak form of (2.74) is to find $u = wv$ with $v \in H_{0,\Gamma}^1(\Omega_c)$ such that

$$\mathcal{B}(u, \psi) = (\mathbf{C} \nabla u, \nabla \psi)_{\Omega_c} - k^2(nu, \psi)_{\Omega_c} = (f, \psi)_{\Omega_c}, \quad (2.79)$$

for all $\psi = w\phi$ with $\phi \in H_{0,\Gamma}^1(\Omega_c)$, where

$$w|_{\Omega} = 1, \quad w|_{\Omega_{\rho}^{\text{PAL}}} = t^{3/2} e^{ik\sigma_1 T(r,\theta)}, \quad t := \frac{R_1}{\Re\{S\}} = \frac{R_1}{R_1 + \sigma_1 T}. \quad (2.80)$$

In view of (2.64) and (2.77), we can extract the oscillatory factor as above. As we shall see, the power $3/2$ is the smallest to absorb all the singular coefficients. On the other hand, in numerical approximation, we approximate v by standard spectral-element and finite element methods, so it is necessary to compute the associated “stiffness” matrix: $\mathcal{B}(wv, w\phi)$ with v, ϕ being in the basis set.

We next provide the detailed representation of the transformed sesquilinear form for the convenience of both the computation and also the analysis of the problem in v . For clarity, we reformulate (2.79) as: find $v \in H_{0,\Gamma}^1(\Omega_c)$ (and set $u = wv$) such that

$$\begin{aligned} \check{\mathcal{B}}(v, \phi) &:= \mathcal{B}(wv, w\phi) \\ &= (\mathbf{C} \nabla(wv), \nabla(w\phi))_{\Omega_c} - k^2(n|w|^2 v, \phi)_{\Omega_c} = (f, w\phi)_{\Omega_c}, \end{aligned} \quad (2.81)$$

for all $\phi \in H_{0,\Gamma}^1(\Omega_c)$.

The following formulation holds for any generic differentiable w .

Lemma 2.2. *The sesquilinear form $\check{\mathcal{B}}(v, \phi)$ in (2.81) can be rewritten as*

$$\begin{aligned}\check{\mathcal{B}}(v, \phi) &= (|w|^2 \mathbf{B} \check{\nabla} v, \check{\nabla} \phi)_{\Omega_c} + (w \mathbf{B} \check{\nabla} w^* \cdot \check{\nabla} v, \phi)_{\Omega_c} \\ &\quad + (w^* \mathbf{B} \check{\nabla} w v, \check{\nabla} \phi)_{\Omega_c} + (\check{n} v, \phi)_{\Omega_c} \\ &= (\check{\mathbf{B}} \check{\nabla} v, \check{\nabla} \phi)_{\Omega_c} + (\mathbf{p} \cdot \check{\nabla} v, \phi)_{\Omega_c} + (v, \mathbf{q}^* \cdot \check{\nabla} \phi)_{\Omega_c} + (\check{n} v, \phi)_{\Omega_c}\end{aligned}\tag{2.82}$$

where $\check{\nabla} = (\partial_r, \partial_\theta/r)^t$, and

$$\begin{aligned}\check{\mathbf{B}} &:= |w|^2 \mathbf{B}, \quad \mathbf{p} := w \mathbf{B} \check{\nabla} w^*, \\ \mathbf{q} &:= w^* \mathbf{B} \check{\nabla} w, \quad \check{n} := (\check{\nabla} w^*)^t \mathbf{B} \check{\nabla} w - k^2 |w|^2 n,\end{aligned}\tag{2.83}$$

with $\mathbf{B}$ and n defined in (2.73). In (2.82), $\mathbf{B} = \check{\mathbf{B}} = \mathbf{I}$, $\mathbf{p} = \mathbf{q} = \mathbf{0}$ and $n = -k^2$ in Ω .

Proof. One verifies readily that

$$\nabla = (\partial_x, \partial_y)^t = \mathbf{T}(\partial_r, \partial_\theta/r)^t = \mathbf{T} \check{\nabla}, \tag{2.84}$$

For clarity, we denote $\xi = wv$ and $\eta = (w\phi)^*$. From (2.84), we immediately derive

$$(\nabla \eta)^t \mathbf{C} \nabla \xi = (\mathbf{T} \check{\nabla} \eta)^t \mathbf{C} (\mathbf{T} \check{\nabla} \xi) = (\check{\nabla} \eta)^t (\mathbf{T}^t \mathbf{C} \mathbf{T}) \check{\nabla} \xi = \check{\nabla}^t \eta \mathbf{B} \check{\nabla} \xi, \tag{2.85}$$

where we used the fact: $\mathbf{B} = \mathbf{T}^t \mathbf{C} \mathbf{T}$, due to (2.72) and the property: $\mathbf{T}^{-1} = \mathbf{T}^t$. Since

$$\check{\nabla} \xi = (\check{\nabla} w)v + w \check{\nabla} v, \quad \check{\nabla}^t \eta = (\check{\nabla}^t w^*)\phi^* + w^* \check{\nabla}^t \phi^*, \tag{2.86}$$

we have

$$\begin{aligned}(\mathbf{C} \nabla(wv), \nabla(w\phi))_{\Omega_c} &= (|w|^2 \mathbf{B} \check{\nabla} v, \check{\nabla} \phi)_{\Omega_c} + (w \mathbf{B} \check{\nabla} v, (\check{\nabla} w)\phi)_{\Omega_c} \\ &\quad + (\mathbf{B} \check{\nabla} w v, w \check{\nabla} \phi)_{\Omega_c} + ((\check{\nabla} w^*)^t \mathbf{B} \check{\nabla} w v, \phi)_{\Omega_c}.\end{aligned}\tag{2.87}$$

Thus, the representation (2.82) follows from (2.81) and (2.87). $\square$

We next evaluate the terms involving $\mathbf{B}$, n , and w . The key is to show that the singular coefficients in (2.83) can be fully absorbed by w . Although the derivation appears a bit lengthy and tedious, we strive to present the formulation in an

accessible manner, which depends only on the configuration of the layer: $R_1(\theta)$, ϱ , and the coordinate transformation: T and σ_0, σ_1 . However, to make the derivation relatively concise, we shall arrange the powers of

$$t = \frac{R_1}{R_1 + T} = \frac{R_1(R_2 - r)}{R_1(R_2 - r) + (r - R_1)} \in (0, 1], \quad (2.88)$$

and use following regular functions in r :

$$\begin{aligned} \alpha &= \sigma_1 + i\sigma_0, \quad \beta := tS = R_1 + (\alpha - 1)\tau, \\ \tau &:= tT = \frac{R_1(r - R_1)}{R_1(R_2 - r) + (r - R_1)}, \\ \gamma_1 &:= t^2 T_r = \frac{(\varrho - 1)R_1^3}{(R_1(R_2 - r) + (r - R_1))^2}, \\ \gamma_2 &:= t^2 T_\theta = \frac{(1 - \varrho)R_1^2 R_1' r}{(R_1(R_2 - r) + (r - R_1))^2}, \end{aligned} \quad (2.89)$$

where we used

$$T_r = \frac{(\varrho - 1)R_1}{(R_2 - r)^2}, \quad T_\theta = \frac{(R_1 - R_2)'r + (R_1 R_2' - R_1' R_2)}{(R_2 - r)^2} = \frac{(1 - \varrho)R_1' r}{(R_2 - r)^2}. \quad (2.90)$$

With the following formulation in Cartesian coordinates at our disposal, the implementation of PAL technique using the spectral and finite elements becomes a normal coding exercise.

Theorem 2.6. *The sesquilinear form $\check{\mathcal{B}}(v, \phi)$ takes the form*

$$\check{\mathcal{B}}(v, \phi) = (\mathbf{T} \check{\mathbf{B}} \mathbf{T}^t \nabla v, \nabla \phi)_{\Omega_c} + (\mathbf{T} \mathbf{p} \cdot \nabla v, \phi)_{\Omega_c} + (v, \mathbf{T} \mathbf{q}^* \cdot \nabla \phi)_{\Omega_c} + (\check{n} v, \phi)_{\Omega_c}, \quad (2.91)$$

where the matrix $\mathbf{T}$ is given in (2.73). In Ω , we have $\check{\mathbf{B}} = \mathbf{I}$, $\mathbf{p} = \mathbf{q} = \mathbf{0}$ and $n = -k^2$, while in $\Omega_\varrho^{\text{PAL}}$, the scalar function $\check{n}$, and the entries of the matrix $\check{\mathbf{B}}$, and the vectors $\mathbf{p}, \mathbf{q}$ in (2.83) can be evaluated by the following expressions:

$$\check{n} = k^2 \left(\frac{\beta \sigma_1^2}{\alpha} - \alpha \beta + \frac{\sigma_1^2 R_1'^2 t^2}{\alpha \beta} \right) \frac{\gamma_1}{r} + \frac{9\gamma_1 t^2}{4r R_1^2} \left(\frac{\beta}{\alpha} + \frac{R_1'^2}{\alpha \beta R_1^2} (R_1 t + \alpha \tau)^2 \right). \quad (2.92)$$

$$\begin{aligned} \check{B}_{11} &= \frac{\beta t^2}{\alpha \gamma_1 r} (t^2 + (R_1' t^2 + \alpha \gamma_2)^2 \beta^{-2}), \\ \check{B}_{12} &= - (R_1' t^2 + \alpha \gamma_2) \frac{t^2}{\beta}, \quad \check{B}_{22} = \frac{\alpha \gamma_1 r}{\beta} t^2, \end{aligned} \quad (2.93)$$

$$p_1 = -\frac{\beta}{\alpha r} \left(\frac{3t}{2R_1} + ik\sigma_1 \right) t^2 - \left\{ \frac{3R'_1}{2rR_1\alpha\beta} \left(t + \frac{\alpha\tau}{R_1} \right) + \frac{ik\sigma_1 R'_1}{r\alpha\beta} \right\} (R'_1 t^2 + \alpha\gamma_2) t^2, \quad (2.94)$$

$$p_2 = \frac{3R'_1\gamma_1}{2R_1\beta} \left(t + \frac{\alpha\tau}{R_1} \right) t^2 + ik\sigma_1 \frac{R'_1\gamma_1}{\beta} t^2, \quad (2.95)$$

and the elements of $\mathbf{q}$ can be obtained by changing the signs in front of ik in p_1 and p_2 , i.e., $-ik$ in place of ik in (2.94).

Proof. Using (2.84) and the property: $\mathbf{T}^{-1} = \mathbf{T}$, we have $\check{\nabla} = \mathbf{T}^t \nabla$. Accordingly, we can rewrite the formulation of $\check{\mathcal{B}}(v, \phi)$ in Lemma 2.2 as

$$\begin{aligned} \check{\mathcal{B}}(v, \phi) &= (\check{\mathbf{B}} \check{\nabla} v, \check{\nabla} \phi)_{\Omega_c} + (\mathbf{p} \cdot \check{\nabla} v, \phi)_{\Omega_c} + (v, \mathbf{q}^* \cdot \check{\nabla} \phi)_{\Omega_c} + (\check{n} v, \phi)_{\Omega_c} \\ &= (\mathbf{T} \check{\mathbf{B}} \mathbf{T}^t \nabla v, \nabla \phi)_{\Omega_c} + (\mathbf{T} \mathbf{p} \cdot \nabla v, \phi)_{\Omega_c} + (v, \mathbf{T} \mathbf{q}^* \cdot \nabla \phi)_{\Omega_c} \\ &\quad + (\check{n} v, \phi)_{\Omega_c}. \end{aligned} \quad (2.96)$$

Now, the main task is to derive the representations in (2.92)-(2.94). For clarity, we deal with them separately in three cases below.

(i) We first derive (2.92) from the expression in (2.83). By direct calculation, we find

$$\begin{aligned} (\check{\nabla} w^*)^t \mathbf{B} \check{\nabla} w &= (w_r^*, w_\theta^*/r) \begin{pmatrix} B_{11} & B_{12} \\ B_{12} & B_{22} \end{pmatrix} \begin{pmatrix} w_r \\ w_\theta/r \end{pmatrix} \\ &= B_{11}|w_r|^2 + \frac{B_{22}}{r^2}|w_\theta|^2 + \frac{B_{12}}{r}(w_r^* w_\theta + w_\theta^* w_r) \\ &= B_{11}|w_r|^2 + \frac{B_{22}}{r^2}|w_\theta|^2 + \frac{2B_{12}}{r} \Re\{w_r^* w_\theta\}. \end{aligned} \quad (2.97)$$

Denote $A = t^{3/2}$, so $w = Ae^{ik\sigma_1 T}$ and $A = |w|$. Then, we find readily that

$$w_r = (A_r + ik\sigma_1 T_r A) e^{ik\sigma_1 T} = \left(\frac{A_r}{A} + ik\sigma_1 T_r \right) w, \quad w_\theta = \left(\frac{A_\theta}{A} + ik\sigma_1 T_\theta \right) w, \quad (2.98)$$

so we have

$$\begin{aligned} |w_r|^2 &= \left| \frac{A_r}{A} + ik\sigma_1 T_r \right|^2 |w|^2 = A_r^2 + k^2 \sigma_1^2 T_r^2 A^2, \quad |w_\theta|^2 = A_\theta^2 + k^2 \sigma_1^2 T_\theta^2 A^2, \\ \Re\{w_r^* w_\theta\} &= A_r A_\theta + k^2 \sigma_1^2 T_r T_\theta A^2, \\ w_r^* w &= A A_r - ik\sigma_1 T_r A^2, \quad w_\theta^* w = A A_\theta - ik\sigma_1 T_\theta A^2. \end{aligned} \quad (2.99)$$

Recall from (2.73) that

$$B_{11} = \frac{S}{rS_r} \left(1 + \frac{S_\theta^2}{S^2}\right), \quad B_{12} = -\frac{S_\theta}{S}, \quad B_{22} = \frac{rS_r}{S}, \quad n = \frac{SS_r}{r}. \quad (2.100)$$

Then inserting (2.99)-(2.100) into (2.97), we derive

$$\begin{aligned} (\check{\nabla} w^*)^t \mathbf{B} \check{\nabla} w &= (A_r^2 + k^2 \sigma_1^2 T_r^2 A^2) \left(\frac{S}{rS_r} + \frac{S_\theta^2}{rSS_r} \right) \\ &\quad + \frac{S_r}{rS} (AA_\theta + ik\sigma_1 T_\theta A^2) - \frac{2S_\theta}{rS} (A_r A_\theta + k^2 \sigma_1^2 T_r T_\theta A^2) \\ &= \frac{S}{rS_r} (A_r^2 + k^2 \sigma_1^2 T_r^2 A^2) + \frac{1}{rSS_r} (A_r S_\theta - A_\theta S_r)^2 \\ &\quad + \frac{k^2 \sigma_1^2 A^2}{rSS_r} (T_r^2 S_\theta^2 + T_\theta^2 S_r^2 - 2S_r S_\theta T_r T_\theta) \\ &= \frac{S}{rS_r} (A_r^2 + k^2 \sigma_1^2 T_r^2 A^2) + \frac{1}{rSS_r} (A_r S_\theta - A_\theta S_r)^2 \\ &\quad + \frac{k^2 \sigma_1^2 A^2}{rSS_r} (T_r S_\theta - T_\theta S_r)^2. \end{aligned} \quad (2.101)$$

By (2.83) and (2.100)-(2.101),

$$\begin{aligned} \check{n} &= (\check{\nabla} w^*)^t \mathbf{B} \check{\nabla} w - k^2 |w|^2 n = A_r^2 \frac{S}{rS_r} + k^2 A^2 \left(\sigma_1^2 T_r^2 \frac{S}{rS_r} - \frac{SS_r}{r} \right) \\ &\quad + \frac{1}{rSS_r} (A_r S_\theta - A_\theta S_r)^2 + k^2 \sigma_1^2 \frac{A^2}{rSS_r} (T_r S_\theta - T_\theta S_r)^2. \end{aligned} \quad (2.102)$$

We have from (2.67)-(2.68) that in Ω_ρ^{PAL} , $S = R_1 + \alpha T$, $R_2 = \rho R_1$, and

$$T = \frac{r - R_1}{R_2 - r}, \quad S_r = \alpha T_r, \quad S_\theta = R'_1 + \alpha T_\theta. \quad (2.103)$$

Moreover, from the expression of t in (2.88), we find immediately that

$$A_r = \frac{3}{2} t^{\frac{1}{2}} t_r = -\frac{3}{2R_1} t^{\frac{5}{2}} T_r, \quad A_\theta = \frac{3}{2} t^{\frac{1}{2}} t_\theta = \frac{3t^{\frac{5}{2}}}{2R_1} \left(\frac{R'_1}{R_1} T - T_\theta \right). \quad (2.104)$$

Then by (2.103)-(2.104),

$$\begin{aligned} A_r S_\theta - A_\theta S_r &= -\frac{3}{2R_1} t^{\frac{5}{2}} T_r (R'_1 + \alpha T_\theta) - \frac{3t^{\frac{5}{2}}}{2R_1} \left(\frac{R'_1}{R_1} T - T_\theta \right) \alpha T_r \\ &= -\frac{3R'_1}{2R_1} t^{\frac{5}{2}} T_r \left(1 + \alpha \frac{T}{R_1} \right), \end{aligned} \quad (2.105)$$

and

$$T_r S_\theta - T_\theta S_r = T_r(R'_1 + \alpha T_\theta) - T_\theta(\alpha T_r) = R'_1 T_r. \quad (2.106)$$

We now express $\check{n}$ in terms of the regular functions $t, \beta, \tau, \gamma_1, \gamma_2$ in (2.88)-(2.89) as follows:

$$\begin{aligned} \check{n} &= A_r^2 \frac{S}{r S_r} + k^2 A^2 \left(\sigma_1^2 T_r^2 \frac{S}{r S_r} - \frac{S S_r}{r} \right) \\ &\quad + \frac{1}{r S S_r} \frac{9 R_1'^2}{4 R_1^2} t^5 T_r^2 \left(1 + \alpha \frac{T}{R_1} \right)^2 + k^2 \sigma_1^2 \frac{A^2}{r S S_r} R_1'^2 T_r^2 \\ &= \frac{9 \gamma_1 t^2}{4 r R_1^2} \frac{\beta}{\alpha} + \frac{k^2 \gamma_1}{r} \left(\sigma_1 \frac{\beta}{\alpha} - \alpha \beta \right) + \frac{9 \gamma_1 R_1'^2 t^2}{4 r R_1^2 \alpha \beta} \left(t + \frac{\alpha \tau}{R_1} \right)^2 + k^2 \sigma_1^2 \frac{R_1'^2 \gamma_1 t^2}{r \alpha \beta}. \end{aligned} \quad (2.107)$$

We obtain the identity (2.92) immediately by regrouping the terms.

(ii) Now, we calculate the elements of the vectors $\mathbf{p}$ and $\mathbf{q}$ in (2.82), that is,

$$\begin{aligned} \mathbf{p} &= (p_1, p_2)^t := w \mathbf{B} \check{\nabla} w^* = \mathbf{B} (\check{\nabla} w^* w) \\ &= (B_{11} w_r^* w + B_{12} w_\theta^* w / r, B_{12} w_r^* w + B_{22} w_\theta^* w / r)^t. \end{aligned} \quad (2.108)$$

Then by (2.88)-(2.89), (2.99)-(2.100) and (2.105) -(2.106),

$$\begin{aligned} p_1 &= B_{11} w_r^* w + \frac{B_{12}}{r} w_\theta^* w \\ &= \frac{S}{r S_r} \left(1 + \frac{S_\theta^2}{S^2} \right) (A A_r - i k \sigma_1 T_r A^2) - \frac{S_\theta}{r S} (A A_\theta - i k \sigma_1 T_\theta A^2) \\ &= \frac{S}{r S_r} (A A_r - i k \sigma_1 T_r A^2) + \frac{S_\theta A}{r S S_r} (A_r S_\theta - A_\theta S_r) \\ &\quad - i k \sigma_1 \frac{S_\theta A^2}{r S S_r} (T_r S_\theta - T_\theta S_r) \\ &= -\frac{\beta}{\alpha r} \left(\frac{3t}{2R_1} + i k \sigma_1 \right) t^2 - \frac{3R_1'}{2r R_1 \alpha \beta} \left(t + \frac{\alpha \tau}{R_1} \right) (R_1' t^2 + \alpha \gamma_2) t^2 \\ &\quad - \frac{i k \sigma_1 R_1'}{r \alpha \beta} (R_1' t^2 + \alpha \gamma_2) t^2 \\ &= -\frac{\beta}{\alpha r} \left(\frac{3t}{2R_1} + i k \sigma_1 \right) t^2 - \left(\frac{3R_1'}{2r R_1 \alpha \beta} \left(t + \frac{\alpha \tau}{R_1} \right) + \frac{i k \sigma_1 R_1'}{r \alpha \beta} \right) \\ &\quad \cdot (R_1' t^2 + \alpha \gamma_2) t^2, \end{aligned} \quad (2.109)$$

and

$$\begin{aligned}
p_2 &= B_{12}w_rw^* + \frac{B_{22}}{r}w_\theta w^* \\
&= -\frac{S_\theta}{S}(AA_r - ik\sigma_1 T_r A^2) + \frac{S_r}{S}(AA_\theta - ik\sigma_1 T_\theta A^2) \\
&= \frac{A}{S}(A_\theta S_r - A_r S_\theta) + ik\sigma_1 \frac{A^2}{S}(T_r S_\theta - T_\theta S_r) \\
&= \frac{3R'_1\gamma_1}{2R_1\beta}\left(t + \frac{\alpha\tau}{R_1}\right)t^2 + ik\sigma_1 \frac{R'_1\gamma_1}{\beta}t^2.
\end{aligned} \tag{2.110}$$

Thus, we obtain (2.94).

We now turn to the elements of the vector $\mathbf{q}$. Note that

$$\begin{aligned}
\mathbf{q} &= (q_1, q_2)^t := w^* \mathbf{B} \check{\nabla} w \\
&= (B_{11}w_rw^* + B_{12}w_\theta w^*/r, B_{12}w_rw^* + B_{22}w_\theta w^*/r)^t.
\end{aligned} \tag{2.111}$$

Following the same lines as in (2.109)-(2.110), we find that (q_1, q_2) are identical to (p_1, p_2) with a change of ik therein to $-ik$.

(iii) Finally, we deal with the matrix $\check{\mathbf{B}}$, that is,

$$\check{\mathbf{B}} = |w|^2 \mathbf{B} = \begin{pmatrix} \frac{t^3 S}{r S_r} \left(1 + \frac{S_\theta^2}{S^2}\right) & -\frac{t^3 S_\theta}{S} \\ -\frac{t^3 S_\theta}{S} & \frac{rt^3 S_r}{S} \end{pmatrix} := \begin{pmatrix} \check{B}_{11} & \check{B}_{12} \\ \check{B}_{12} & \check{B}_{22} \end{pmatrix}. \tag{2.112}$$

Using the notation in (2.89) and the properties in (2.103), we can derive the entries of $\check{\mathbf{B}}$ in (2.93) straightforwardly. $\square$

Remark 2.5. *In the circular case, the artificial layer is an annulus, i.e.,*

$$\Omega_\varrho^{\text{PAL}} = \{R_1 < r < R_2 = \varrho R_1, 0 \leq \theta < 2\pi\},$$

where R_1 is independent of θ . Thus, R'_1 and γ_2 in (2.89) reduce to 0. Consequently, several terms in (2.92)-(2.94) vanish and the variables involved in the sesquilinear

form $\check{\mathcal{B}}(v, \phi)$ in (2.91) are reduced to

$$\begin{aligned} \check{B}_{11} &= \frac{\beta}{\alpha\gamma_1 r} t^4, \quad \check{B}_{12} = 0, \quad \check{B}_{22} = \frac{\alpha\gamma_1 r}{\beta} t^2, \\ \check{n} &= k^2 \left(\frac{\beta\sigma_1^2}{\alpha} - \alpha\beta \right) \frac{\gamma_1}{r} + \frac{9\gamma_1}{4rR_1^2} \frac{\beta}{\alpha}, \quad p_1 = -\frac{\beta}{\alpha r} \left(\frac{3t}{2R_1} + ik\sigma_1 \right) t^2, \\ p_2 &= 0, \quad q_1 = -\frac{\beta}{\alpha r} \left(\frac{3t}{2R_1} - ik\sigma_1 \right) t^2, \quad q_2 = 0. \end{aligned} \quad (2.113)$$

2.5 Numerical results and comparisons

In this section, we shall provide ample numerical results and comparisons to demonstrate the advantages of the new PAL techniques than the PML methods using different absorbing functions.

2.5.1 Waveguide problems

To solve the waveguide problem (2.25), we use the Fourier sine expansion in y -direction:

$$U(x, y) = \sum_{m=0}^{\infty} \hat{u}_m(x) \sin(my) \quad \text{with} \quad \hat{u}_m(x) = \frac{2}{\pi} \int_0^{\pi} U(x, y) \sin(my) dy.$$

We also expand the boundary data $g(y)$ in (2.25) as

$$g(y) = \sum_{m=0}^{\infty} \hat{g}_m \sin(my) \quad \text{with} \quad \hat{g}_m = \frac{2}{\pi} \int_0^{\pi} g(y) \sin(my) dy.$$

As $\hat{u}_m(0) = \hat{g}_m$, we introduce

$$\tilde{u}_m(x) = \hat{u}_m(x) + \left(\frac{x}{L} - 1 \right) \hat{g}_m,$$

to reduce it to a problem with homogeneous boundary condition at $x = 0$.

Let $\mathbf{N} = (N_1, N)$ be the number of points in x -direction on $I := [0, L]$ and $I_d := (L, L_d]$. Define

$$\mathbb{X}_{\mathbf{N}} := \{v \in C(I) : v|_I \in \mathbb{P}_{N_1}, v|_{I_d} \in \mathbb{P}_N, v(0) = 0\},$$

and

$$\widehat{\mathbb{X}}_N := \{u = w(x)v, \quad \forall v \in \mathbb{X}_N\},$$

where $w(x)$ is the substitution in (2.27). Here, we drop the subscript m , and

$$\begin{cases} \text{Find } u_N(x) \in \widehat{\mathbb{X}}_N, \text{ such that} \\ a_m(u_N, \phi) = \mathcal{F}(\phi), \quad \forall \phi(x) \in \widehat{\mathbb{X}}_N, \end{cases} \quad (2.114)$$

where

$$\begin{aligned} a_m(u_N, \phi) := & -(u'_N, \phi')_I + (k^2 - m^2)(u_N, \phi)_I \\ & - \left(\frac{1}{S'} u'_N, \phi' \right)_{I_d} + (k^2 - m^2)(S' u_N, \phi)_{I_d}, \end{aligned}$$

and

$$\mathcal{F}(\phi) := \left(\left(\frac{x}{L} - 1 \right) \hat{g}_m, \phi \right)_I - \frac{\hat{g}_m}{L} \phi(L).$$

Figure 2.5: Left: errors against various N for different layers (width $d = 0.1$) with boundary condition $g(y) = \sin(5y) - \sin(30y)$; Right: errors against various N for different layers (width $d = 0.5$) with boundary condition $g(y) = \sin(5y) - \sin(30y)$.

In Figure 2.5, we take the wave number to be $k = 29.9$, and compare the PAL ($\sigma_0 = 0.5$) with singular PML (PML_∞ , $\sigma_0 = 10$), and regular PML (PML_n , $n = 1$, $\sigma_0 = 10$). Here, we set the width of the layer d to be 0.1 or 0.5. We choose $g(y) = \sin(5y) - \sin(30y)$. We truncate the infinite series in y direction with a sufficiently large cut off number, so that the induced error in y can be ignored. Indeed, we see that the PML technique with two types of absorbing

functions fails to produce acceptable reduction of the domain. In other words, this technique causes observable reflecting waves that pollute the numerical solution in the physical domain.

2.5.2 Some star-shaped PALs

We now test the performance of the PAL with the star-shaped layer, e.g., annular, rectangular and triangular layers. In the conference report [89], some tests and comparisons with circular PMLs have been conducted, so here, we focus on more general shapes of the artificial layer.

Consider the exterior problem

$$\begin{aligned} \Delta u + k^2 u &= 0, \quad \Omega_\infty := \mathbb{R}^2 \setminus \bar{D}; \\ u|_{\partial D} &= g; \quad \partial_r u - iku = o(r^{-1/2}), \end{aligned} \quad (2.115)$$

where we take

$$g = -\exp(ika_0 \cos(\theta - \theta_0)) \quad (2.116)$$

with the incident angle θ_0 . We reduce the problem by PAL that encloses the physical domain Ω_f exterior to D by the layer Ω_{ab} . Here, the computational domain is $\Omega = \Omega_f \cup \Omega_{ab}$.

Figure 2.6: In (b)-(c), $\partial D := \{(x, y) = \zeta(\cosh \xi \cos \theta, \sinh \xi \sin \theta), \theta \in [0, 2\pi)\}$ with $(\zeta, \xi) = (0.8, 0.5)$ and $\sigma_0 = 1.5, \sigma_1 = 2$.

We first consider the rectangular PAL with an elliptical scatterer D . Here, we enclose the elliptical scatterer by a rectangular layer with $(L_1, L_2) = (1, 0.8)$ and

Figure 2.7: Left: real part of the electric field with $\mathbf{N} = (60, 20)$. Right: corresponding errors for the approximation in Ω_f for $N = [15 : 5 : 60]$ and $N = 20$ in the layer.

$(d_1, d_2) = (0.1, 0.08)$ (see Figure 2.6 (a)). We partition the computational domain: $\Omega = \{\Omega_f^{(i)}\}_{i=1}^8 \cup \{\Omega_{ab}^{(i)}\}_{i=1}^8$ into 16 non-overlapping quadrilateral elements as shown in Figure 2.6 (b). Note that the spectral-element scheme can be implemented by incorporating the substitution into the usual basis. Let $u_{\mathbf{N}}$ be the spectral-element approximation to the solution in the physical domain Ω_f , and $V_{\mathbf{N}}$ be the field in the artificial layer Ω_{ab} , which involves the substitution. Let $\theta_0 = 0$, $k = 50$, $\sigma_0 = 1.5$ and $\sigma_1 = 2$, we plot $\text{Re}(u_{\mathbf{N}})|_{\Omega_f}$ and $\text{Re}(v_{\mathbf{N}})|_{\Omega_{ab}}$ with $(N_1, N) = (60, 30)$ in Figure 2.6 (b). We plot the maximum error in Ω_f with fixed $N_1 = 60$ and $N = 3, 6, \dots, 30$ in Figure 2.6 (c). Here, we choose $N = 100$ as reference solutions.

We observe from Figure 2.6 (c) that the error decays exponentially as N increases. Moreover, the approximation in the layer has no oscillation and is well-behaved.

We next consider the triangular PAL to reduce the scattering problem (2.115) with the scatterer D being a disk shown in Figure 2.7 (left). Here, we partition the computational domain by the spectral elements (see the dashed line in the figure). The incident wave and the parameters are chosen as with the rectangular case. Indeed, the plots indicate again the field in the layer is well-behaved, so spectral-element approximation converges very fast.

Chapter 3

Wavenumber Explicit Analysis of the Circular PAL

In this chapter, we conduct the wavenumber explicit analysis of the Helmholtz equation reduced by the PAL technique introduced in the previous chapter. It is known that the Helmholtz problem with high wave number is highly indefinite, and it has been a longstanding issue to characterise the dependence of the solution and its approximation on the wavenumber. As already mentioned in Chapter 1, significant efforts have been devoted to the wavenumber explicit analysis for the Helmholtz equations with lower-order absorbing boundary conditions or exact Dirichlet-to-Neumann (DtN) transparent boundary conditions. We refer to the introductory sections of the recent papers [66, 64] for review of many existing works along this line. However, such an analysis for the PML technique is very limited. Very recently, Li and Wu [64] analysed the finite-element method for the Helmholtz problem truncated by the circular PML.

In this chapter, we shall analyse the circular PAL with a compactly supported source term and a setting very similar to [64]. More precisely, we consider the

time harmonic acoustic scattering problem in $\mathbb{R}^d$ ($d = 1, 2, 3$) :

$$\begin{cases} -\Delta u - k^2 u = f & \text{in } \mathbb{R}^d, \\ \frac{\partial u}{\partial r} - iku = o(r^{\frac{1-d}{2}}) & \text{as } r \rightarrow \infty, \end{cases} \quad (3.1)$$

where $r = |\mathbf{x}|$ with $\mathbf{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$, and the source term f is compactly supported in a disk/ball $\mathbb{B}_{R_1}$ centred at the origin and of radius R_1 . Here, we assume the wavenumber $k \gg 1$. Note that for $d = 1$, the far-field Sommerfeld radiation condition can be understood as: $\frac{du}{dr} - iku = 0$ for $r \gg 1$.

The main objective is to understand the behaviour of the outgoing waves in the artificial layer. The restriction to the above relatively simpler setting does not actually lose any generality. In practice, we can consider the Helmholtz problem with a bounded scatterer D confined in $\mathbb{B}_{R_1}$, but the waves entering into the layer take the same form as this simple setting, i.e., in series of Hankel functions in a radial direction and Fourier/spherical harmonic expansions in angular direction(s).

3.1 The PAL-equation

For clarity of presentation, we quickly review the derivation of the PAL-equation by the complex compression coordinate transformation (C³T). We first reduce the unbounded domain by an artificial layer (i.e., annulus in 2D and spherical shell in 3D), which is formed by enclosing $\mathbb{B}_{R_1}$ with a concentric disk/ball $\mathbb{B}_{R_2}$ of radius $R_2 > R_1$. Denote $\varrho = R_2 - R_1$ (see Figure 3.1).

The PAL-equation in $\mathbb{B}_{R_2}$ is obtained by applying the complex compression coordinate transformation (C³T) to the Helmholtz problem (3.1) in the polar coordinates $(\tilde{r}, \tilde{\theta})$ (in the “virtual” space) to the polar coordinate (r, θ) (in the “physical” space). The C³T takes the form

$$\tilde{r} = S(r) = \begin{cases} r, & r < R_1, \\ R_1 + \sigma_1 T(r) + i\sigma_0 T(r), & R_1 < r < R_2, \end{cases} \quad \tilde{\theta} = \theta \in [0, 2\pi), \quad (3.2)$$

Figure 3.1: Illustration of circular PAL.

where $\sigma_0, \sigma_1 > 0$ are tuning parameters, and

$$T(r) = \frac{r - R_1}{R_2 - r} = (R_2 - R_1) \int_{R_1}^r \frac{dt}{(R_2 - t)^2}, \quad r \in (R_1, R_2). \quad (3.3)$$

Note that $T(r)$ is a one-to-one mapping from $[R_1, R_2)$ to $[0, \infty)$, and also we impose $S(R_1) = R_1$ to ensure the continuity at the interface.

In the polar coordinates $(\tilde{r}, \tilde{\theta})$, the first equation of (3.1) takes this form

$$-\frac{1}{\tilde{r}} \frac{\partial}{\partial \tilde{r}} \left(\tilde{r} \frac{\partial \tilde{u}}{\partial \tilde{r}} \right) - \frac{1}{\tilde{r}^2} \frac{\partial^2 \tilde{u}}{\partial \tilde{\theta}^2} - k^2 \tilde{u} = f. \quad (3.4)$$

Let $\alpha = \beta = 1$ for $r < R_1$, and

$$\alpha = \frac{d\tilde{r}}{dr} = (\sigma_1 + i\sigma_0)T'(r), \quad \beta = \frac{\tilde{r}}{r} = \frac{R_1 + \sigma_1 T(r) + i\sigma_0 T(r)}{r}, \quad (3.5)$$

for $r \in (R_1, R_2)$. Setting $u(r, \theta) = \tilde{u}(\tilde{r}, \tilde{\theta})$ and noting that $\tilde{r} = r\beta$ and $\partial_{\tilde{r}} = \alpha \partial_r$, we can obtain the PAL-equation from (3.4) immediately as follows:

$$-\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\beta r}{\alpha} \frac{\partial u}{\partial r} \right) - \frac{1}{r^2} \frac{\alpha}{\beta} \frac{\partial^2 u}{\partial \theta^2} - \alpha \beta k^2 u = f \quad (3.6)$$

in $\mathcal{D} := \mathbb{B}_{R_1} \cup \Omega_\varrho^{\text{PAL}}$. Here, $\Omega_\varrho^{\text{PAL}} = \mathbb{B}_{R_2} \setminus \bar{\mathbb{B}}_{R_1}$ and $\varrho > 1$ can tune the "thickness" of the layer.

For clarity, we denote the PAL-solution by U_{PAL} . The PAL-equation reads

$$\begin{cases} -\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\beta r}{\alpha} \frac{\partial U_{\text{PAL}}}{\partial r} \right) - \frac{1}{r^2} \frac{\alpha}{\beta} \frac{\partial^2 U_{\text{PAL}}}{\partial \theta^2} - \alpha \beta k^2 U_{\text{PAL}} = f, & \text{in } \mathcal{D}, \\ |U_{\text{PAL}}| \text{ is uniformly bounded as } r \rightarrow R_2, \end{cases} \quad (3.7)$$

which satisfies the usual “pole” conditions at $r = 0$, and the transmission conditions at $r = R_1$.

We find from (3.3) and (3.5) that

$$\begin{aligned}\frac{\beta r}{\alpha} &= \frac{R_1 + (\sigma_1 + i\sigma_0)T(r)}{(\sigma_1 + i\sigma_0)T'(r)} \sim (R_2 - r)^2, \\ \frac{\alpha}{\beta r} &= \frac{(\sigma_1 + i\sigma_0)T'(r)}{R_1 + (\sigma_1 + i\sigma_0)T(r)} \sim \frac{1}{R_2 - r}, \\ \alpha\beta r &= (\sigma_1 + i\sigma_0)(R_1 + (\sigma_1 + i\sigma_0)T(r))T'(r) \sim \frac{1}{(R_2 - r)^3}.\end{aligned}\tag{3.8}$$

Note that the coefficients of the PAL-equation (3.7) are singular at $r = R_2$. As shown in Chapter 2, we have to make the substitution of the unknown

$$U_{\text{PAL}}(r, \theta) = w(r)V_{\text{PAL}}(r, \theta), \quad 0 < r < R_2, \quad \theta \in [0, 2\pi), \tag{3.9}$$

where

$$w(r) = \begin{cases} 1, & \text{for } r < R_1, \\ (R_2 - r)^{3/2}e^{ik\sigma_1 T(r)}, & \text{for } R_1 \leq r < R_2. \end{cases} \tag{3.10}$$

In the computation, we actually approximate V_{PAL} (rather than U_{PAL}), which is well-behaved.

Remark 3.1. *As proven in the previous chapter, the PAL technique leads to an exact reduction of the unbounded domain.*

3.2 L^2 -stability analysis

In what follows, we estimate the L^2 -stability of the solution, and explicitly characterise its dependence of k . The result plays a fundamental role in the wavenumber explicit error analysis. As we shall see, the argument is based on the choice of the standard test function, which is very different from that in [68, 26] (where a second test function related to the derivative information of the solution). The analysis in [64] sheds light on our analysis hereafter.

We start with the expansions

$$\{U_{\text{PAL}}, f\}(r, \theta) = \sum_{|m|=0}^{\infty} \{\hat{u}_m, \hat{f}_m\}(r) e^{im\theta}.$$

For notational convenience, we introduce

$$a_m(\hat{u}_m, \hat{u}_m) := \int_0^{R_2} \left\{ \frac{\beta r}{\alpha} |\hat{u}'_m(r)|^2 + \left(\frac{\alpha m^2}{\beta r} - k^2 \alpha \beta r \right) |\hat{u}_m(r)|^2 \right\} dr. \quad (3.11)$$

In the analysis, we shall frequently use the following identities derived from (3.3), (3.8) and direct calculation:

$$\begin{aligned} \Re \left\{ \frac{\beta r}{\alpha} \right\} &= \frac{(\sigma_1^2 + \sigma_0^2)T(r) + \sigma_1 R_1}{(\sigma_1^2 + \sigma_0^2)T'(r)}, \\ \Re \left\{ \frac{\alpha}{\beta r} \right\} &= \frac{(\sigma_1^2 + \sigma_0^2)T(r) + \sigma_1 R_1}{(\sigma_1 T(r) + R_1)^2 + \sigma_0^2 T^2(r)} T'(r), \\ \Re \{\alpha \beta r\} &= ((\sigma_1^2 - \sigma_0^2)T(r) + \sigma_1 R_1) T'(r), \end{aligned} \quad (3.12)$$

and

$$\begin{aligned} \Im \left\{ \frac{\beta r}{\alpha} \right\} &= -\frac{\sigma_0 R_1}{(\sigma_0^2 + \sigma_1^2)T'(r)}, \\ \Im \left\{ \frac{\alpha}{\beta r} \right\} &= \frac{\sigma_0 R_1}{(\sigma_1 T(r) + R_1)^2 + \sigma_0^2 T^2(r)} T'(r), \\ \Im \{\alpha \beta r\} &= \sigma_0 (2\sigma_1 T(r) + R_1) T'(r). \end{aligned} \quad (3.13)$$

The following constants will be used in Theorem 3.1 and its proof:

$$\begin{aligned} C_1 &= \frac{\sigma_0 R_1}{(\sigma_1^2 + \sigma_0^2)(R_2 - R_1)}, \quad \tau = \frac{\sqrt{C_1(R_2 - R_1)}(R_2 - R_1)}{2\sqrt{\sigma_0 \sigma_1 k} + \sqrt{C_1(R_2 - R_1)}}, \\ \hat{\tau} &= \frac{\sqrt{C_1(R_2 - R_1)}(R_2 - R_1)}{2\sqrt{\sigma_0 \sigma_1 k}}, \quad \lambda = \frac{C_1(R_2 - R_1 - 3\hat{\tau})^4}{4\hat{\tau} k \sigma_0 R_1 (R_2 - R_1)^2}, \\ \varepsilon_T &= \frac{\lambda R_2 (\sigma_0^2 - \sigma_1^2 + \sigma_1 R_1)}{k(R_2 - R_1)^2 (\sigma_0^2 - \sigma_1^2)^2 - \lambda R_2 (\sigma_0^2 - \sigma_1^2)}. \end{aligned} \quad (3.14)$$

Throughout this chapter, C is used to denote a generic positive constant, which is independent of the solution, data, k and discretization parameters. We also use the shorthand notations $A \gtrsim B$ and $A \lesssim B$ for the inequalities $A \geq CB$ and $A \leq CB$.

Theorem 3.1. *Assume that*

$$\sigma_0 > (1 + \sqrt{2})\sigma_1, \quad \sigma_0^2 - \sigma_1^2 \geq \sigma_1 R_1, \quad (3.15)$$

and

$$k > k_0 := \frac{\lambda R_2}{(R_2 - R_1)^2(\sigma_0^2 - \sigma_1^2)}.$$

Then, we have the following estimates:

(i) If $m^2 \leq k^2 R_1^2 + \lambda k R_1^2$, then

$$\begin{aligned} -\Im\{a_m(\hat{u}_m, \hat{u}_m)\} &\gtrsim \int_{R_1}^{R_2} (R_2 - r)^2 r |\hat{u}'_m(r)|^2 dr \\ &\quad + \int_{R_1}^{R_2} \frac{\lambda k r}{(R_2 - r)^3} |\hat{u}_m(r)|^2 dr. \end{aligned} \quad (3.16)$$

(ii) If $m^2 > k^2 R_1^2 + \lambda k R_1^2$, then

$$\begin{aligned} \Re\{a_m(\hat{u}_m, \hat{u}_m)\} &\gtrsim \int_0^{R_2} (R_2 - r) r |\hat{u}'_m(r)|^2 \\ &\quad + \int_0^{R_2} \frac{\lambda k r}{(R_2 - r)^3} |\hat{u}_m(r)|^2 dr. \end{aligned} \quad (3.17)$$

Proof. Step 1: We first deal with the imaginary part in (3.11). From (3.13), we obtain

$$\begin{aligned} -\Im\{a_m(\hat{u}_m, \hat{u}_m)\} &= - \int_0^{R_2} \left\{ \Im\left\{\frac{\beta r}{\alpha}\right\} |\hat{u}'_m(r)|^2 + \left[k^2 \Im\{\alpha \beta r\} \right. \right. \\ &\quad \left. \left. - m^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right] |\hat{u}_m(r)|^2 \right\} dr. \end{aligned} \quad (3.18)$$

It is clear that by (3.3) and (3.13),

$$-\Im\left\{\frac{\beta r}{\alpha}\right\} = \frac{\sigma_0 R_1}{(\sigma_1^2 + \sigma_0^2)T'} = C_1 (R_2 - r)^2 \geq 0, \quad (3.19)$$

where C_1 is given in (3.14), and

$$\left\{ k^2 \Im\{\alpha \beta r\} - m^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right\} \Big|_{r=R_1} = k^2 \sigma_0 R_1 - m^2 \frac{\sigma_0}{R_1}, \quad (3.20)$$

which might be negative, if $m > kR_1$.

To make the lower bound positive, we resort to the first term in the interval $(R_1, R_1 + \tau)$ for some small $0 < \tau < R_2 - R_1$ to be determined. For this purpose, we first prove the inequality:

$$\begin{aligned} \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr \\ \geq \frac{1}{\tau} \int_{R_1}^{R_1+\tau} (-3r + 2R_1 + R_2) |\hat{u}_m(r)|^2 dr - 2 \int_{R_1+\tau}^{R_2} |\hat{u}_m(r)|^2 dr. \end{aligned} \quad (3.21)$$

Indeed, for $r \in (R_1, R_2)$, we have

$$\begin{aligned} (R_2 - r) |\hat{u}_m(r)|^2 &= - \int_r^{R_2} [(R_2 - t) |\hat{u}_m(t)|^2]' dt \\ &= \int_r^{R_2} |\hat{u}_m(t)|^2 dt - 2\Re \int_r^{R_2} (R_2 - t) \hat{u}'_m(t) \bar{\hat{u}}_m(t) dt \\ &\leq 2 \int_r^{R_2} |\hat{u}_m(t)|^2 dt + \int_{R_1}^{R_2} (R_2 - t)^2 |\hat{u}'_m(t)|^2 dt. \end{aligned} \quad (3.22)$$

Integrating (3.22) on both sides and using integration by parts, we obtain

$$\begin{aligned} \int_{R_1}^{R_1+\tau} (R_2 - r) |\hat{u}_m(r)|^2 dr &\leq 2 \int_{R_1}^{R_1+\tau} \int_r^{R_2} |\hat{u}_m(t)|^2 dt dr + \tau \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr \\ &= \left\{ 2r \int_r^{R_2} |\hat{u}_m(t)|^2 dt \right\} \Big|_{r=R_1}^{r=R_1+\tau} + 2 \int_{R_1}^{R_1+\tau} r |\hat{u}_m(r)|^2 dr \\ &\quad + \tau \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr \\ &= 2(R_1 + \tau) \int_{R_1+\tau}^{R_2} |\hat{u}_m(r)|^2 dr - 2R_1 \int_{R_1}^{R_2} |\hat{u}_m(r)|^2 dr \\ &\quad + 2 \int_{R_1}^{R_1+\tau} r |\hat{u}_m(r)|^2 dr + \tau \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr, \end{aligned}$$

which implies

$$\begin{aligned} \int_{R_1}^{R_1+\tau} (R_2 - r) |\hat{u}_m(r)|^2 dr &\leq 2 \int_{R_1}^{R_1+\tau} (r - R_1) |\hat{u}_m(r)|^2 dr + 2\tau \int_{R_1+\tau}^{R_2} |\hat{u}_m(r)|^2 dr \\ &\quad + \tau \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr. \end{aligned}$$

The desired inequality (3.21) follows from the above immediately.

With the aid of (3.21), we can estimate (3.18) as

$$\begin{aligned}
-\Im\{a_m(\hat{u}_m, \hat{u}_m)\} &\geq \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr \\
&\quad + \frac{C_1}{2\tau} \int_{R_1}^{R_1+\tau} (-3r + 2R_1 + R_2) |\hat{u}_m(r)|^2 dr \\
&\quad - C_1 \int_{R_1+\tau}^{R_2} |\hat{u}_m(r)|^2 dr + \int_{R_1}^{R_2} \left[k^2 \Im\{\alpha\beta r\} \right. \\
&\quad \left. - m^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right] |\hat{u}_m(r)|^2 dr.
\end{aligned} \tag{3.23}$$

We next show that there exists a positive constant λ , such that for $m^2 \leq k^2 R_1^2 + \lambda k R_1^2$, we have the lower bound (3.16). To determine λ , we eliminate m in the last term and obtain from (3.13) that

$$\begin{aligned}
k^2 \Im\{\alpha\beta r\} - m^2 \Im\left\{\frac{\alpha}{\beta r}\right\} &\geq k^2 \Im\{\alpha\beta r\} - (k^2 R_1^2 + \lambda k R_1^2) \Im\left\{\frac{\alpha}{\beta r}\right\} \\
&= 2k^2 \sigma_1 \sigma_0 T T' + k^2 \left\{ \sigma_0 R_1 T' - R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right\} - \lambda k R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \\
&\geq 2k^2 \sigma_1 \sigma_0 T T' - \lambda k R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\},
\end{aligned} \tag{3.24}$$

where we used the property derived from (3.3) and (3.23) as follows:

$$\sigma_0 R_1 T' - R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} = \frac{\sigma_0 R_1 (R_1 - R_2)}{(R_2 - r)^2} + \frac{\sigma_0 R_1^3 (R_2 - r)^2}{(\sigma_0^2 + \sigma_1^2)(R_2 - R_1)} > 0. \tag{3.25}$$

Here, we drop this term as it is not dominated. One also finds readily from (3.3) and (3.23) that $T T' > 0$, so we have

$$2k^2 \sigma_1 \sigma_0 \int_{R_1}^{R_2} T T' |\hat{u}_m(r)|^2 dr \geq 2k^2 \sigma_1 \sigma_0 \int_{R_1+\tau}^{R_2} T T' |\hat{u}_m(r)|^2 dr. \tag{3.26}$$

In a nutshell, from the above derivations, we have

$$\begin{aligned}
&-\Im\{a_m(\hat{u}_m, \hat{u}_m)\} \\
&\geq \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr + \frac{C_1}{2\tau} \int_{R_1}^{R_1+\tau} (-3r + 2R_1 + R_2) |\hat{u}_m(r)|^2 dr \\
&\quad + \int_{R_1+\tau}^{R_2} (2k^2 \sigma_1 \sigma_0 T T' - C_1) |\hat{u}_m(r)|^2 dr - \lambda k R_1^2 \int_{R_1}^{R_2} \Im\left\{\frac{\alpha}{\beta r}\right\} |\hat{u}_m(r)|^2 dr \\
&= \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr + \int_{R_1}^{R_1+\tau} H_1(r) \frac{|\hat{u}_m(r)|^2}{(R_2 - r)^3} dr \\
&\quad + \int_{R_1+\tau}^{R_2} H_2(r) \frac{|\hat{u}_m(r)|^2}{(R_2 - r)^3} dr - \lambda k R_1^2 \int_{R_1}^{R_2} \Im\left\{\frac{\alpha}{\beta r}\right\} |\hat{u}_m(r)|^2 dr,
\end{aligned}$$

where for clarity, we denoted

$$H_1(r) := \frac{C_1}{2\tau}(-3r + 2R_1 + R_2)(R_2 - r)^3, \quad r \in (R_1, R_1 + \tau), \quad (3.27a)$$

$$H_2(r) := (2k^2\sigma_1\sigma_0TT' - C_1)(R_2 - r)^3, \quad r \in [R_1 + \tau, R_2]. \quad (3.27b)$$

It is clear that if $\tau \leq \frac{R_2 - R_1}{2}$, we have

$$H_1'(r) = -\frac{3C_1}{2\tau}(R_2 - r)^2(R_1 + R_2 - 2r) \leq 0, \quad r \in (R_1, R_1 + \tau), \quad (3.28)$$

which implies when $r \in (R_1, R_1 + \tau)$,

$$H_1(r) \geq H_1(R_1 + \tau) = \frac{C_1}{2\tau}(R_2 - R_1 - \tau)^3(R_2 - R_1 - 3\tau). \quad (3.29)$$

Similarly, we have

$$H_2'(r) = 2k^2\sigma_0\sigma_1(R_2 - R_1) + 3C_1(R_2 - r)^2 > 0, \quad r \in [R_1 + \tau, R_2],$$

so it has the lower bound:

$$\begin{aligned} H_2(r) &\geq H_2(R_1 + \tau) = 2k^2\sigma_0\sigma_1\tau(R_2 - R_1) - C_1(R_2 - R_1 - \tau)^3 \\ &\geq 2k^2\sigma_0\sigma_1\tau(R_2 - R_1 - \tau) - \frac{3C_1}{2}(R_2 - R_1 - \tau)^3. \end{aligned} \quad (3.30)$$

Now, we equate the lower bounds in (3.29) and (3.30), we can readily find the root of the resulted equation:

$$\tau = \frac{\sqrt{C_1(R_2 - R_1)}(R_2 - R_1)}{2\sqrt{\sigma_0\sigma_1}k + \sqrt{C_1(R_2 - R_1)}} \sim \frac{1}{k}. \quad (3.31)$$

Therefore, we have that in their respective domain,

$$H_1(r), H_2(r) \geq \frac{C_1}{2\tau}(R_2 - R_1 - \tau)^3(R_2 - R_1 - 3\tau).$$

With this, we can obtain

$$\begin{aligned} -\Im\{a_m(\hat{u}_m, \hat{u}_m)\} &\geq \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}_m'(r)|^2 dr \\ &\quad + \frac{C_1}{2\tau} (R_2 - R_1 - \tau)^3 (R_2 - R_1 - 3\tau) \int_{R_1}^{R_2} \frac{|\hat{u}_m(r)|^2}{(R_2 - r)^3} dr \\ &\quad - \lambda k R_1^2 \int_{R_1}^{R_2} \Im\left\{\frac{\alpha}{\beta r}\right\} |\hat{u}_m(r)|^2 dr, \end{aligned} \quad (3.32)$$

where τ is given by (3.31).

Now, we are in position of deriving the condition of λ in (3.16). For clarity, we combine the last two terms and rewrite (3.32) as

$$-\Im\{a_m(\hat{u}_m, \hat{u}_m)\} \geq \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |\hat{u}'_m(r)|^2 dr + \int_{R_1}^{R_2} Q(\tau, r) \frac{|\hat{u}_m(r)|^2}{(R_2 - r)^3} dr.$$

where by (3.3) and (3.13), the coefficient reads

$$Q(\tau, r) := \frac{C_1}{2\tau} (R_2 - R_1 - \tau)^3 (R_2 - R_1 - 3\tau) - \frac{\lambda k \sigma_0 R_1^3 (R_2 - R_1) (R_2 - r)^3}{[R_1(R_2 - r) + \sigma_1(r - R_1)]^2 + \sigma_0^2(r - R_1)^2}. \quad (3.33)$$

Here, we determine λ by requiring

$$Q(\tau, r) \geq \lambda k r, \quad r \in (R_1, R_2).$$

Note that $Q(\tau, r)$ is decreasing with respect to τ if $\tau < \frac{R_2 - R_1}{\sqrt{10} - 1}$, since

$$\begin{aligned} \partial_\tau Q(\tau, r) &= -\frac{C_1}{2} \frac{6\tau(R_2 - R_1 - \tau)^2(R_2 - R_1 - 2\tau) + (R_2 - R_1 - \tau)^3(R_2 - R_1 - 3\tau)}{\tau^2} \\ &= -\frac{C_1}{2} \frac{(R_2 - R_1 - \tau)^2[(R_2 - R_1 + \tau)^2 - 10\tau^2]}{\tau^2} < 0. \end{aligned}$$

To simplify the calculation, we introduce

$$\hat{\tau} := \frac{\sqrt{C_1(R_2 - R_1)(R_2 - R_1)}}{2\sqrt{\sigma_0\sigma_1}k} > \tau \quad (3.34)$$

and require that $Q(\hat{\tau}, r) \geq \lambda k R_2$, as

$$Q(\tau, r) \geq Q(\hat{\tau}, r) \geq \lambda k R_2 \geq \lambda k r. \quad (3.35)$$

Direct calculation from $Q(\hat{\tau}, r) \geq \lambda k R_2$, we find λ should satisfy

$$\lambda \max_{r \in [R_1, R_2]} \{P(r)\} \leq \frac{C_1}{2\hat{\tau}k} (R_2 - R_1 - 3\hat{\tau})^4, \quad (3.36)$$

where

$$\begin{aligned} P(r) &:= R_2 + R_1^2(R_2 - r)^3 \Im\left\{\frac{\alpha}{\beta r}\right\} \\ &= R_2 + \frac{\sigma_0 R_1^3 (R_2 - R_1) (R_2 - r)^3}{[R_1(R_2 - r) + \sigma_1(r - R_1)]^2 + \sigma_0^2(r - R_1)^2}. \end{aligned} \quad (3.37)$$

In fact, we can show that $P(r)$ is decreasing, as

$$P'(r) = - \frac{\sigma_0 R_1^4 (R_1 + 2\sigma_1)(R_2 - r)^4 + 2\sigma_0 \sigma_1 R_1^3 (2R_1 + \sigma_1 + \sigma_0^2)(R_2 - r)^3 (r - R_1)}{[(R_1(R_2 - r) + \sigma_1(r - R_1))^2 + \sigma_0^2(r - R_1)^2]^2} \\ - \frac{3\sigma_0 R_1^3 (R_2 - R_1)(\sigma_1^2 + \sigma_0^2)(R_2 - r)^2 (r - R_1)^2}{[(R_1(R_2 - r) + \sigma_1(r - R_1))^2 + \sigma_0^2(r - R_1)^2]^2} < 0.$$

As a result, the constant λ should satisfy

$$\lambda P(R_1) = \lambda \sigma_0 R_1 (R_2 - R_1)^2 \leq \frac{C_1}{2\hat{\tau}k} (R_2 - R_1 - 3\hat{\tau})^4.$$

Therefore, we choose

$$\lambda = \frac{C_1 (R_2 - R_1 - 3\hat{\tau})^4}{4\hat{\tau}k\sigma_0 R_1 (R_2 - R_1)^2}, \quad (3.38)$$

where $\hat{\tau}$ is given in (3.34). We complete the proof of (3.16).

Step 2: With λ given by (3.38), we now deal with the real part:

$$\Re\{a_m(\hat{u}_m, \hat{u}_m)\} = \int_0^{R_2} \Re\left\{\frac{\beta r}{\alpha}\right\} |\hat{u}_m'(r)|^2 + \left[m^2 \Re\left\{\frac{\alpha}{\beta r}\right\} - k^2 \Re\{\alpha\beta r\}\right] |\hat{u}_m(r)|^2 dr, \quad (3.39)$$

for all $m^2 > k^2 R_1^2 + \lambda k R_1^2$. Recall that $\alpha = \beta = 1$ for $r \in (0, R_1)$, and clearly,

$$\frac{m^2}{r} - k^2 r > \frac{m^2}{R_1} - k^2 R_1 > \lambda k R_1 \geq \lambda k r.$$

Thus we have

$$\int_0^{R_1} r |\hat{u}_m'(r)|^2 + \left(\frac{m^2}{r} - k^2 r\right) |\hat{u}_m(r)|^2 dr \geq \int_0^{R_1} r |\hat{u}_m'(r)|^2 dr \\ + \lambda k \int_0^{R_1} r |\hat{u}_m(r)|^2 dr. \quad (3.40)$$

We now turn to the integrals in (3.39) for $r \in (R_1, R_2)$. Assuming that

$$\sigma_1^2 + \sigma_0^2 \geq \sigma_1 R_1, \quad (3.41)$$

we obtain from (3.3) that

$$\Re\left\{\frac{\beta r}{\alpha}\right\} = \frac{(\sigma_1^2 + \sigma_0^2)(r - R_1) + \sigma_1 R_1 (R_2 - r)}{(\sigma_1^2 + \sigma_0^2)(R_2 - R_1)} (R_2 - r) \\ \geq \frac{\sigma_1 R_1}{\sigma_1^2 + \sigma_0^2} (R_2 - r), \quad r \in [R_1, R_2].$$

We now estimate the last term in (3.39), and the rest of the proof is to show that for $r \in (R_1, R_2)$, we have

$$m^2 \Re\left\{\frac{\alpha}{\beta r}\right\} - k^2 \Re\{\alpha \beta r\} \geq \lambda k \frac{r}{(R_2 - r)^3}. \quad (3.42)$$

Indeed, if this is true, substituting (3.42) into (3.39), we shall obtain (3.17) from (3.40) immediately.

As $m^2 > kR_1^2 + \lambda kR_1^2$, (3.39) becomes

$$(k^2 + \lambda k)F_1(T) + k^2 F_2(T) \geq \lambda k \frac{r}{R_2 - r}, \quad (3.43)$$

where by (3.12),

$$F_1(T) := R_1^2 (R_2 - r)^2 \Re\left\{\frac{\alpha}{\beta r}\right\} = (R_2 - R_1) R_1^2 \frac{(\sigma_1^2 + \sigma_0^2)T + \sigma_1 R_1}{(\sigma_1 T + R_1)^2 + \sigma_0^2 T^2}, \quad (3.44)$$

$$F_2(T) := -(R_2 - r)^2 \Re\{\alpha \beta r\} = -(R_2 - R_1)[(\sigma_1^2 - \sigma_0^2)T + \sigma_1 R_1].$$

Here, we view them as functions of $T \in (0, \infty)$ (with $r \in (R_1, R_2)$) for the convenience of computation. Observe that $F_1(T) > 0$, but $F_2(T)$ changes sign from negative to positive in $T \in (0, \infty)$. Direct calculation from (3.44) leads to

$$F_1'(T) = (R_2 - R_1) R_1^2 \frac{-(\sigma_1^2 + \sigma_0^2)^2 T^2 - 2\sigma_1 R_1 (\sigma_1^2 + \sigma_0^2)T + (\sigma_0^2 - \sigma_1^2) R_1^2}{[(\sigma_1 T + R_1)^2 + \sigma_0^2 T^2]^2},$$

so the extreme point of $F_1(T)$ is:

$$F_1'(T_1) = 0 \quad \Rightarrow \quad T_1 = \frac{(\sigma_0 - \sigma_1) R_1}{\sigma_1^2 + \sigma_0^2}. \quad (3.45)$$

We find that if

$$\sigma_0^2 - \sigma_1^2 \geq \sigma_1 R_1, \quad (3.46)$$

then

$$F_1'(T_1) > 0, \quad T < T_1; \quad F_1'(T_1) < 0, \quad T > T_1. \quad (3.47)$$

Simple calculation from $F_2(T)$ in (3.44) leads to

$$F_2'(T) = (R_2 - R_1)(\sigma_0^2 - \sigma_1^2) > 0, \quad (3.48)$$

so F_2 is increasing, and changes the sign at the zero T_0 :

$$F_2(T_0) = 0, \quad \text{where} \quad T_0 := \frac{\sigma_1 R_1}{\sigma_0^2 - \sigma_1^2}. \quad (3.49)$$

Note from (3.44) that

$$F_1(T) \sim R_2 - r, \quad F_2(T) \sim (R_2 - r)^{-1}, \quad \text{as } r \rightarrow R_2.$$

This implies when $T \rightarrow 0$ (i.e., $r \rightarrow R_1$), $F_1(T)$ is the leading term; whereas when $T \rightarrow \infty$ (i.e., $r \rightarrow R_2$), $F_2(T)$ is dominant. Therefore, we proceed with splitting the interval $T \in (0, \infty)$ into two subintervals $T \in (0, T_0 + \varepsilon_T)$ and $T \in [T_0 + \varepsilon_T, \infty)$, where ε_T given in (3.14), which is of order k^{-1} , will be derived later on. We find

$$\begin{aligned} T(R_0) &= T_0, \quad \text{where} \quad R_0 := R_1 \frac{\sigma_0^2 - \sigma_1^2 + \sigma_1 R_2}{\sigma_0^2 - \sigma_1^2 + \sigma_1 R_1}; \\ T(R_\varepsilon) &= T_0 + \varepsilon_T, \quad \text{where} \quad R_\varepsilon := \frac{(T_0 + \varepsilon_T)R_2 + R_1}{T_0 + \varepsilon_T + 1}. \end{aligned} \quad (3.50)$$

(i) To prove (3.43), we first show that for $T \in (0, T_0 + \varepsilon_T)$,

$$\begin{aligned} (k^2 + \lambda k)F_1(T) + k^2 F_2(T) &\geq k^2(F_1(0) + F_2(0)) + \lambda k F_1(0) \\ &= \lambda k(R_2 - R_1)\sigma_1 R_1. \end{aligned} \quad (3.51)$$

It is clear that if

$$\sigma_0 \geq (1 + \sqrt{2})\sigma_1 \Rightarrow T_1 \geq T_0, \quad (3.52)$$

Note that both $F_1(T)$ and $F_2(T)$ are increasing on this interval $T \in (0, T_0 + \varepsilon_T)$ (see Figure 3.2 for an illustration). Then (3.51) follows, so does (3.43) in Case (i).

(ii) Now, we turn to the proof (3.43) with $T \in [T_0 + \varepsilon_T, \infty)$. As $F_1(T) \geq 0$ on this interval, the left-hand side of (3.43) has the lower bound:

$$(k^2 + \lambda k)F_1(T) + k^2 F_2(T) \geq k^2 F_2(T). \quad (3.53)$$

Hence, it is equivalent to proving

$$F_2(T) \geq \frac{\lambda}{k} \frac{r}{R_2 - r}, \quad T \in [T_0 + \varepsilon_T, \infty). \quad (3.54)$$

Figure 3.2: Sketch of $F_1(T)$ and $F_2(T)$, when $T_1 \geq T_0$.

By (3.44), we can rewrite it as

$$(\sigma_0^2 - \sigma_1^2)(r - R_1) - \sigma_1 R_1(R_2 - r) \geq \frac{\lambda R_2}{k(R_2 - R_1)}, \quad r \in [R_\varepsilon, R_2], \quad (3.55)$$

where R_ε is given in (3.50). Under the condition (3.46), the left-hand side of (3.55) is decreasing with respect to r . Therefore, it suffices to justify the existence of ε_T such that

$$(\sigma_0^2 - \sigma_1^2)(R_\varepsilon - R_1) - \sigma_1 R_1(R_2 - R_\varepsilon) \geq \frac{\lambda R_2}{k(R_2 - R_1)}. \quad (3.56)$$

Taking the equality and using (3.50), we solve out ε_T :

$$\varepsilon_T = \frac{\lambda R_2(\sigma_0^2 - \sigma_1^2 + \sigma_1 R_1)}{k(R_2 - R_1)^2(\sigma_0^2 - \sigma_1^2)^2 - \lambda R_2(\sigma_0^2 - \sigma_1^2)}. \quad (3.57)$$

It is positive and of order k^{-1} , under the conditions:

$$k > k_0 := \frac{\lambda R_2}{(R_2 - R_1)^2(\sigma_0^2 - \sigma_1^2)}. \quad (3.58)$$

We finally combining the conditions and completes the proof of the real part. $\square$

With the bounds in Theorem 3.1, we can obtain the following main result on the L^2 -estimate with explicit wavenumber dependence.

Theorem 3.2. *Under the same conditions as in Theorem 3.1, we have the a priori estimate of the PAL-solution of (3.7):*

$$\|U_{\text{PAL}}\|_{L^2_{\omega^{-3,0}}(\mathcal{D})} \lesssim \frac{1}{k} \|f\|_{L^2(\mathcal{D})}, \quad (3.59)$$

where the weight function: $\omega^{-3,0}(r) = (R_2 - r)^{-3}$. With the substitution in (3.9), we have

$$\|V_{\text{PAL}}\|_{L^2(\mathcal{D})} \lesssim \frac{1}{k} \|f\|_{L^2(\mathcal{D})}, \quad (3.60)$$

where $\mathcal{D} = \mathbb{B}_{R_1} \cup \Omega_\rho^{\text{PAL}}$ as before.

Proof. To prove (3.59), it suffices to prove that

$$\int_0^{R_2} r(R_2 - r)^{-3} |\hat{u}_m(r)|^2 dr \lesssim \frac{1}{k^2} \int_0^{R_1} r |\hat{f}_m(r)|^2 dr, \quad m \in \mathbb{Z}.$$

CASE 1 : $m^2 > k^2 R_1^2 + \lambda k R_1^2$. We know that $\hat{u}_m$ satisfies the following variational formulation:

$$a_m(\hat{u}_m, \hat{u}_m) = \int_0^{R_2} r \hat{f}_m \bar{\hat{u}}_m(r) dr.$$

Combining with conclusion (3.17) of Theorem 3.1,

$$\lambda k \int_0^{R_2} r(R_2 - r)^{-3} |\hat{u}_m(r)|^2 dr \lesssim \Re(a_m(\hat{u}_m, \hat{u}_m)) \lesssim \left| \int_0^{R_2} r \hat{f}_m \bar{\hat{u}}_m(r) dr \right|,$$

which means we have

$$\lambda k \int_0^{R_2} r(R_2 - r)^{-3} |\hat{u}_m(r)|^2 dr \lesssim \left(\frac{1}{\lambda k} \int_0^{R_1} r |\hat{f}_m|^2 dr \right)^{\frac{1}{2}} \left(\lambda k \int_0^{R_2} r(R_2 - r)^{-3} |\hat{u}_m(r)|^2 dr \right)^{\frac{1}{2}}.$$

Thus,

$$\int_0^{R_2} r(R_2 - r)^{-3} |\hat{u}_m(r)|^2 dr \lesssim \frac{1}{\lambda^2 k^2} \int_0^{R_1} r |\hat{f}_m|^2 dr.$$

CASE 2 : $m^2 \leq k^2 R_1^2 + \lambda k R_1^2$. Similar to CASE 1, by (3.16),

$$\int_0^{R_2} r(R_2 - r)^{-3} |\hat{u}_m(r)|^2 dr \lesssim \frac{1}{\lambda^2 k^2} \int_0^{R_1} r |\hat{f}_m|^2 dr + \int_0^{R_1} r |\hat{u}_m(r)|^2 dr. \quad (3.61)$$

Next, we estimate the last term in (3.61). Recall that the PAL-solution in the physical domain coincides with the original solution of the Helmholtz problem in the same domain. Then, by expanding

$$\{U_{\text{PAL}}, f\}(r, \theta) = \sum_{|m|=0}^{\infty} \{\hat{u}_m(r), \hat{f}_m(r)\} e^{\text{im}\theta},$$

we can solve (3.6) by using separation of variables or a direct verification: for $0 < r < R_1$,

$$\begin{aligned} \hat{u}_m(r) = & \frac{\pi k i}{2} J_m(kr) \int_r^{R_1} t H_m^{(1)}(kt) \hat{f}_m(t) dt \\ & + \frac{\pi k i}{2} H_m^{(1)}(kr) \int_0^r t J_m(kt) \hat{f}_m(t) dt, 0 < r < R_1. \end{aligned} \quad (3.62)$$

It is clear that $\hat{u}_m e^{im\theta}$ is the exact solution to the Helmholtz problem (3.1). Then, by using the following lemma proved in [69]:

$$k^{-1} \|u\|_{H^2(\mathbb{B}_{R_1})} + \|u\|_{H^1(\mathbb{B}_{R_1})} + k \|u\|_{L^2(\mathbb{B}_{R_1})} \leq C \|f\|_{L^2(\mathbb{B}_{R_1})},$$

where C is a positive constant. Therefore, as a consequence of the above lemma, we have

$$\int_0^{R_1} r |\hat{u}_m(r)|^2 dr \lesssim \frac{1}{k^2} \int_0^{R_1} r |\hat{f}_m(r)|^2 dr,$$

which means

$$\int_0^{R_1} r |\hat{u}_m(r)|^2 dr \lesssim \frac{1}{\lambda^2 k^2} \int_0^{R_1} r |\hat{f}_m(r)|^2 dr. \quad (3.63)$$

Also, by inserting (3.63) into (3.61), we can derive that

$$\int_0^{R_2} r (R_2 - r)^{-3} |\hat{u}_m(r)|^2 dr \lesssim \frac{1}{\lambda^2 k^2} \int_0^{R_1} r |\hat{f}_m|^2 dr.$$

We can obtain the estimate of $\|U_{\text{PAL}}\|_{L^2_{\omega-3,0}(\mathcal{D})}$:

$$\|U_{\text{PAL}}\|_{L^2_{\omega-3,0}(\mathcal{D})} \lesssim \frac{1}{k} \|f\|_{L^2(\mathcal{D})}.$$

Moreover, using the substitution in (3.9), the estimate of $\|V_{\text{PAL}}\|_{L^2(\mathcal{D})}$ can be derived as:

$$\|V_{\text{PAL}}\|_{L^2(\mathcal{D})} \lesssim \frac{1}{k} \|f\|_{L^2(\mathcal{D})}.$$

This completes the proof. $\square$

Remark 3.2. *With the L^2 -stability wavenumber explicit estimate in Theorem 3.2, we can obtain the H^1 -estimate by following a standard procedure.*

3.3 Fourier & spectral-element method and its error analysis

We find it is more convenient to work with the weak formulation of (3.7). In what follows, we assume that $g = 0$, and define the space

$$H_{0,\Gamma}^1(\mathcal{D}) = \{\phi \in H^1(\mathcal{D}) : \phi|_{\Gamma} = 0\}, \quad \mathcal{D} := \Omega \cup \Omega_{\varrho}^{\text{PAL}}, \quad \Gamma := \partial D.$$

A weak form of (3.7) is to find $U_{\text{PAL}} := w(r)V_{\text{PAL}}$ with $V_{\text{PAL}} \in H_{0,\Gamma}^1(\mathcal{D})$ such that

$$\mathcal{B}(U_{\text{PAL}}, \phi) = (\mathbf{C} \nabla U_{\text{PAL}}, \nabla \phi)_{\mathcal{D}} - k^2(n U_{\text{PAL}}, \phi)_{\mathcal{D}} = (f, \phi)_{\mathcal{D}}, \quad (3.64)$$

where $\mathbf{C} = \mathbf{I}$, $n = 1$ in Ω , and $\mathbf{C}, n$ in $\Omega_{\varrho}^{\text{PAL}}$ are the same as in Lemma 2.1 with the transformation S given by (2.67)-(2.68). For all $\phi = w(r)\psi$ with $\psi \in H_{0,\Gamma}^1(\mathcal{D})$, where $w(r)$ proposed in (3.10).

Then, after Fourier series transformation, the weak formulation (3.64) will be reduced to:

$$\mathcal{B}_m(\hat{u}_m, \hat{\phi}_m) := \left(\frac{\beta r}{\alpha} \hat{u}'_m, \hat{\phi}'_m \right)_I + \left(\left(\frac{\alpha m^2}{\beta r} - k^2 \alpha \beta r \right) \hat{u}_m, \hat{\phi}_m \right)_I. \quad (3.65)$$

3.3.1 The scheme

For the numerical scheme, we define the spaces first. As $I_1 = (0, R_1)$ and $I_2 = (R_1, R_2)$, define

$$\mathbb{X}_N^m := \{\hat{v}_m \in C(I) : \hat{v}_m|_{I_1} \in \mathbb{P}_N, \hat{v}_m|_{I_2} \in \mathbb{P}_N, \hat{v}_m|_{I_1}(0) = 0, m > 0\},$$

and

$$\mathbb{X}_N^0 := \{\hat{v}_0 \in C(I) : \hat{v}_0|_{I_1} \in \mathbb{P}_N, \hat{v}_0|_{I_2} \in \mathbb{P}_N\}.$$

Denote $\mathbb{X}_N := \mathbb{X}_N^m \cup \mathbb{X}_N^0$, and

$$\widehat{\mathbb{X}}_N := \{u = w(r)v, \text{ where } v \in \mathbb{X}_N\},$$

Also, for the θ -direction, we have the space

$$\mathbb{Y}_M = \text{span}\{e^{im\theta} : -M \leq m \leq M\}.$$

The numerical reduced problem is as following: Find $U_{MN} \in \mathcal{V}_{MN} := \widehat{\mathbb{X}}_N \times \mathbb{Y}_M$, such that

$$\mathcal{B}(U_{MN}, \Phi_{MN}) = (f, \Phi_{MN})_I,$$

for $\forall \Phi_{MN} \in \mathcal{V}_{MN}$, where $\mathcal{B}(\cdot, \cdot)$ mentioned in (3.64). Expanding the numerical solution and test function as

$$(U_{MN}, \Phi_{MN}) = \sum_{|m|=0}^M (\hat{u}_m^N(r), \hat{\phi}_m^N(r)) e^{im\theta},$$

requires $u_N = \hat{u}_m^N(r)$ and $\phi_N = \hat{\phi}_m^N(r)$.

Then, after Fourier series transformation, the reduced numerical problem is as following: Find $u_N \in \widehat{\mathbb{X}}_N$,

$$\mathcal{B}_m(u_N, \phi_N) = (f, \phi_N)_I, \quad \forall \phi_N \in \widehat{\mathbb{X}}_N, \quad (3.66)$$

where $\mathcal{B}_m(\cdot, \cdot)$ mentioned in (3.65).

3.3.2 Error estimate

For convenience, we estimate the error between analytic solution $\hat{u}_m$ of (3.65) and the numerical solution u_N of (3.66). Denote the first two parts of (3.65) as

$$\widetilde{\mathcal{B}}_m(u, \phi) := \int_I \frac{\beta r}{\alpha} u'(r) \overline{\phi}'(r) dr + \int_I \frac{\alpha m^2}{\beta r} u(r) \overline{\phi}(r) dr, \quad (3.67)$$

where $I = I_1 \cup I_2$. In order to carry out the error analysis, we define the orthogonal projection $\pi_N^1: \mathbb{X} \rightarrow \mathbb{X}_N$ by

$$\widetilde{\mathcal{B}}_m(\hat{u}_m - \pi_N^1 u, \phi) = 0, \quad (3.68)$$

where $I = I_1 \cup I_2$ and $w(r)$ mentioned in (3.10). Let $\tilde{e}_N = \hat{u}_m - \pi_N^1 u$, and $e_N = u_N - \pi_N^1 u$,

Before deriving the error estimates, we first define some useful notations in this section. For the norm $\|\cdot\|_*$:

$$\|\cdot\|_* = \|\cdot\|_{1,0,1,0,-1}^{I_1} + \|\cdot\|_{1,4,0,0,0}^{I_2,m,k}, \quad (3.69)$$

where

$$\|\cdot\|_{1,0,1,0,-1}^{I_1} := \|\cdot\|_{1,\omega^{0,1}}^{I_1} + \|\cdot\|_{\omega^{0,-1}}^{I_1}, \quad \|\cdot\|_{1,4,0,0,0}^{I_2,m,k} := \|\cdot\|_{1,\omega^{4,0}}^{I_2} + \sqrt{m^2 + k^2} \|\cdot\|_{\omega^{0,0}}^{I_2}.$$

Denote

$$X := \{\hat{u}_m \in H_{\omega^{0,1}}^1(I_1) : \hat{u}_m \in L_{\omega^{0,-1}}^2(I_1); \hat{u}_m(0) = 0, \text{ with } m > 0\},$$

where $H_{\omega^{0,1}}^1(I_1)$ is the weighted Sobolev space on I_1 with weight $(L-x)$, $L_{\omega^{0,-1}}^2(I_1)$ is the weighted L_2 -space with weight $(L-x)^{-1}$. For $s \in \mathbb{N}$ and $s \geq 1$,

$$\widetilde{H}^s(I_1) := \{u \in L_{\omega^{0,1}}^2(I_1), \quad [r(R_1 - r)]^{(\tilde{s}-1)/2} \partial_r^{\tilde{s}} u \in L_{\omega^{0,1}}^2(I_1), \quad 1 \leq \tilde{s} \leq s\}.$$

Then, the weighted sobolev space will be

$$B_{4,0,0,0}^1(I_2) = \{u \mid u \text{ is measurable and } \|u\|_{1,4,0,0,0}^{m,k} < \infty\},$$

and $B_{\omega^{4,0},*}^s(I_2)$, $s \geq 1$, is the space with following weighted norm and semi-norm:

$$\|u\|_{s,\omega^{4,0},*} := \left(\sum_{\tilde{s}=0}^{s-1} \|\partial_r^{\tilde{s}+1} u\|_{\omega^{\tilde{s}+4,\tilde{s}}}^2 \right)^{\frac{1}{2}}, \quad |u|_{s,\omega^{4,0},*} := \|\partial_r^s u\|_{\omega^{s+3,s-1}}.$$

From above, we denote

$$B_*^s(I) := \{v : v|_{I_1} \in X \cap \widetilde{H}^s(I_1), \quad v|_{I_2} \in B_{4,0,0,0}^1(I_2) \cap B_{\omega^{4,0},*}^s(I_2)\},$$

so that we have

$$\|\hat{u}_m - u_N\|_* \leq \|\tilde{e}_N\|_* + \|e_N\|_*,$$

which means after substitution, we have

$$\|\hat{v}_m - v_N\|_* \leq \|(R_2 - r)^3 \tilde{e}_N\|_* + \|(R_2 - r)^3 e_N\|_*,$$

First, let us figure out the upper bound of $\|(R_2 - r)^3 \tilde{e}_N\|_*$, by using the following lemma:

Lemma 3.3. As $\widetilde{\mathcal{B}}_m(u, \phi)$ denoted in (3.67), and $\hat{u}_m = w(r)\hat{v}_m$, $w(r)$ mentioned in (3.10), the following equivalence relation of $\Re\{\widetilde{\mathcal{B}}_m(\hat{u}_m, \hat{u}_m)\}$ can be derived: when $r \in I_2$,

$$\Re\{\widetilde{\mathcal{B}}_m(\hat{u}_m, \hat{u}_m)\} \simeq (\|\hat{v}_m\|_{1,4,0,0}^{m,k})^2. \quad (3.70)$$

Here, $A \simeq B$ is a notation for the statement $A \lesssim B$ and $A \gtrsim B$.

Proof. When $r \in I_2$, to derive the equivalence from (3.67), we only need to consider its real part as following

$$\Re\{\widetilde{\mathcal{B}}_m(\hat{u}_m, \phi)\} := \int_{R_1}^{R_2} \Re\left\{\frac{\beta r}{\alpha}\right\} |\hat{u}'_m(r)|^2 dr + m^2 \int_{R_1}^{R_2} \Re\left\{\frac{\alpha}{\beta r}\right\} |\hat{u}_m(r)|^2 dr. \quad (3.71)$$

Then, we need to find its upper and lower bounds. From (3.12), it is obvious to derive:

$$(R_2 - r) \geq \Re\left\{\frac{\beta r}{\alpha}\right\} \geq \frac{\sigma_1 R_1}{\sigma_1^2 + \sigma_0^2} (R_2 - r),$$

which means

$$\Re\left\{\frac{\beta r}{\alpha}\right\} \simeq (R_2 - r).$$

For $\Re\left\{\frac{\alpha}{\beta r}\right\}$ shown in (3.12), after substituting $T(r)$ shown in (3.3),

$$\Re\left\{\frac{\alpha}{\beta r}\right\} = \frac{(\sigma_1^2 + \sigma_0^2)(r - R_1) + \sigma_1 R_1 (R_2 - r)}{[\sigma_1(r - R_1) + R_1(R_2 - r)]^2 + \sigma_0^2(r - R_1)^2} \frac{R_2 - R_1}{R_2 - r}. \quad (3.72)$$

Following the conditions (3.1) about σ_1 and σ_0 , we can derive that

$$\begin{aligned} \{(\sigma_1^2 + \sigma_0^2)(r - R_1) + \sigma_1 R_1 (R_2 - r)\}' &\geq 0 \\ \{[\sigma_1(r - R_1) + R_1(R_2 - r)]^2 + \sigma_0^2(r - R_1)^2\}' &> 0. \end{aligned}$$

Then, to derive the lower bound of (3.72), we have

$$\begin{aligned} \Re\left\{\frac{\alpha}{\beta r}\right\} &\geq \frac{\min_{r \in (R_1, R_2)} \{(\sigma_1^2 + \sigma_0^2)(r - R_1) + \sigma_1 R_1 (R_2 - r)\}}{\max_{r \in (R_1, R_2)} \{[\sigma_1(r - R_1) + R_1(R_2 - r)]^2 + \sigma_0^2(r - R_1)^2\}} \frac{R_2 - R_1}{R_2 - r} \\ &= \frac{\sigma_1 R_1}{\sigma_1^2 + \sigma_0^2} \frac{1}{R_2 - r}. \end{aligned}$$

To derive the upper bound of (3.72), we have

$$\begin{aligned}\Re\left\{\frac{\alpha}{\beta r}\right\} &\leq \frac{\max_{r \in (R_1, R_2)} \{(\sigma_1^2 + \sigma_0^2)(r - R_1) + \sigma_1 R_1(R_2 - r)\}}{\min_{r \in (R_1, R_2)} \{[\sigma_1(r - R_1) + R_1(R_2 - r)]^2 + \sigma_0^2(r - R_1)^2\}} \frac{R_2 - R_1}{R_2 - r} \\ &= \frac{\sigma_1^2 + \sigma_0^2}{R_1^2} \frac{1}{R_2 - r}.\end{aligned}$$

After that, we have

$$\Re\left\{\frac{\alpha}{\beta r}\right\} \simeq (R_2 - r)^{-1}.$$

Above all, when $r \in I_2$,

$$\Re\{\widetilde{\mathcal{B}}_m(\hat{u}_m, \hat{u}_m)\} \simeq \int_{I_2} (R_2 - r) |\hat{u}'_m(r)|^2 dr + m^2 \int_{I_2} (R_2 - r)^{-1} |\hat{u}_m(r)|^2 dr. \quad (3.73)$$

Then, we want to derive the equivalence about $\hat{u}_m(r)$. As $\hat{u}_m(r) = w(r)\hat{v}_m(r)$, $w(r)$ first proposed in (3.10), we know that

$$\begin{aligned}w(r) &= (R_2 - r)^{3/2} e^{ik\sigma_1 T}, \\ w'(r) &= \left(ik\sigma_1 \frac{R_2 - R_1}{R_2 - r} - \frac{3}{2}\right) (R_2 - r)^{1/2} e^{ik\sigma_1 T}.\end{aligned}$$

It can be derived that

$$w(r)\overline{w}(r) = (R_2 - r)^3, \quad w'(r)\overline{w'}(r) = \frac{9}{4}(R_2 - r) + k^2\sigma_1^2 \frac{(R_2 - R_1)^2}{R_2 - r}, \quad (3.74)$$

and

$$w(r)\overline{w'}(r) + w'(r)\overline{w}(r) = -3(R_2 - r)^2. \quad (3.75)$$

So that, we have

$$|\hat{u}_m(r)|^2 = (R_2 - r)^3 |\hat{v}_m(r)|^2,$$

and

$$\begin{aligned}|\hat{u}'_m(r)|^2 &= |\hat{v}'_m(r)w(r) + \hat{v}_m(r)w'(r)|^2 \\ &\leq |\hat{v}'_m(r)|^2 |w(r)|^2 + |\hat{v}_m(r)|^2 |w'(r)|^2 \\ &\leq (R_2 - r)^3 |\hat{v}'_m(r)|^2 + \frac{9}{4}(R_2 - r) |\hat{v}_m(r)|^2 + k^2 \frac{\sigma_1^2 (R_2 - R_1)^2}{R_2 - r} |\hat{v}_m(r)|^2,\end{aligned}$$

which means

$$\begin{aligned} \Re\{\widetilde{\mathcal{B}}_m(\hat{u}_m, \hat{u}_m)\} &\lesssim \int_{I_2} (R_2 - r)^4 |\hat{v}'_m(r)|^2 dr \\ &\quad + \int_{I_2} \left[\left(m^2 + \frac{9}{4} \right) (R_2 - r)^2 + k^2 \sigma_1^2 (R_2 - R_1)^2 \right] |\hat{v}_m(r)|^2 dr. \end{aligned}$$

To find out the lower bound of $\Re\{\widetilde{\mathcal{B}}_m(\hat{u}_m, \hat{u}_m)\}$ on I_2 , after variable substitution of $u(r)$ in (3.73), we have

$$\begin{aligned} \Re\{\widetilde{\mathcal{B}}_m(\hat{u}_m, \hat{u}_m)\} &\gtrsim \int_{I_2} (R_2 - r) [|w(r)|^2 |\hat{v}'_m(r)|^2 + |w'(r)|^2 |\hat{v}_m(r)|^2 \\ &\quad + (w(r)\overline{w'}(r) + w'(r)\overline{w}(r)) \Re\{\hat{v}_m(r)\} \Re\{\hat{v}'_m(r)\}] dr \quad (3.76) \\ &\quad + m^2 \int_{I_2} (R_2 - r)^{-1} |w(r)|^2 |\hat{v}_m(r)|^2 dr. \end{aligned}$$

From (3.75), by taking integration by parts,

$$\begin{aligned} &\int_{I_2} (R_2 - r) [(w(r)\overline{w'}(r) + w'(r)\overline{w}(r)) \Re\{\hat{v}_m(r)\} \Re\{\hat{v}'_m(r)\}] dr \\ &= -3 \int_{I_2} (R_2 - r)^3 \Re\{\hat{v}_m(r)\} \Re\{\hat{v}'_m(r)\} dr \\ &= \frac{3}{2} \left(\Re\{\hat{v}_m(R_1)\} \right)^2 (R_2 - R_1)^2 - \frac{9}{2} \int_{I_2} (R_2 - r)^2 \left(\Re\{\hat{v}_m(r)\} \right)^2 dr \\ &\geq -\frac{9}{2} \int_{I_2} (R_2 - r)^2 \left(\Re\{\hat{v}_m(r)\} \right)^2 dr. \end{aligned}$$

So that, the inequality (3.76) becomes

$$\begin{aligned} \Re\{\widetilde{\mathcal{B}}_m(\hat{u}_m, \hat{u}_m)\} &\geq \int_{I_2} (R_2 - r)^4 |\hat{v}'_m(r)|^2 dr + \int_{I_2} \left(m^2 - \frac{9}{2} \right) (R_2 - r)^2 |\hat{v}_m(r)|^2 \\ &\quad + k^2 \sigma_1^2 (R_2 - R_1)^2 |\hat{v}_m(r)|^2 dr, \end{aligned}$$

which derives (3.70). □

With the aid of Lemma 3.3, we propose the following lemma, to find the upper bound of $\|(R_2 - r)^3 \tilde{e}_N\|_*$:

Lemma 3.4. *If $\hat{v}_m \in B_*^s(I)$, then for $s \geq 1$, $s \in \mathbb{N}$,*

$$\begin{aligned} \|\hat{v}_m - \pi_N^1 v\|_* &\lesssim (1 + mN^{-1}) N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s-1, s-1}, I_1} \\ &\quad + (1 + \sqrt{k^2 + m^2} N^{-1}) N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s+1, s-1}, I_2}, \end{aligned}$$

where $\|\cdot\|_*$ denoted in (3.69) before.

Proof. From (3.70), we can see, when $r \in I_1$,

$$\widetilde{\mathcal{B}}_m(\hat{u}_m, \phi) = (r\hat{u}'_m, \phi')_{I_1} + m^2 \left(\frac{1}{r} \hat{u}_m, \phi \right)_{I_1}.$$

From Lemma 3.5 in [81], when $\hat{u}_m \in X \cap \widetilde{H}^s(I_1)$,

$$\|r(\hat{u}_m - \pi_N^1 u)'\| + m \left\| \frac{1}{r} (\hat{u}_m - \pi_N^1 u) \right\| \lesssim (1 + mN^{-1})N^{1-s} \|\partial_r^s \hat{u}_m\|_{\omega^{s-1, s-1, I_1}}. \quad (3.77)$$

When $r \in I_2$, after taking substitution (3.9), and by projection theorem,

$$\begin{aligned} & \int_{I_2} (R_2 - r)^4 |(\hat{v}_m(r) - \pi_N^1 v(r))'|^2 dr + \int_{I_2} [k^2 + m^2(R_2 - r)^2] |\hat{v}_m(r) - \pi_N^1 v(r)|^2 dr \\ &= \inf_{\psi \in \mathbb{X}_N} \|\hat{v}_m - \psi\|^2 \\ &\leq \|\hat{v}_m - \hat{\pi}_N^1 v\|_{1, \omega^{2,0}} + \sqrt{k^2 + m^2} \|\hat{v}_m - \hat{\pi}_N^1 v\|_{\omega^{0,0}}, \end{aligned}$$

where $\hat{\pi}_N^1 v$ is defined by $\widehat{\mathcal{B}}_m(\hat{v}_m - \hat{\pi}_N^1 v, \psi) = 0$, $\forall \psi \in \mathbb{X}_N$, and

$$\widehat{\mathcal{B}}_m(v, \psi) := (\hat{v}'_m, \psi')_{I_2, \omega^{2,0}} + (k^2 + m^2)(\hat{v}_m, \psi)_{I_2}.$$

Then, from Theorem 3.1 in [51]. If $\hat{v}_m \in B_{4,0,0,0}^1(I_2) \cap B_{\omega^{4,0,*}}^s(I_2)$, the following inequality can be derived:

$$\begin{aligned} & \int_{I_2} (R_2 - r)^4 |(\hat{v}_m(r) - \pi_N^1 v(r))'|^2 dr + \int_{I_2} [k^2 + m^2(R_2 - r)^2] |\hat{v}_m(r) - \pi_N^1 v(r)|^2 dr \\ &\lesssim (1 + \sqrt{k^2 + m^2}N^{-1})N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s+1, s-1, I_2}}. \end{aligned}$$

Above all,

$$\begin{aligned} \|\hat{v}_m - \pi_N^1 v\|_* &\lesssim (1 + mN^{-1})N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s-1, s-1, I_1}} \\ &\quad + (1 + \sqrt{k^2 + m^2}N^{-1})N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s+1, s-1, I_2}}, \end{aligned}$$

then this proof completes. $\square$

Next step, let us figure out the upper bound of $\|(R_2 - r)^3 e_N\|_*$. By (3.65) and (3.66), we have

$$\mathcal{B}_m(\hat{u}_m - u_N, \phi) = 0, \quad \forall \phi \in \widehat{\mathbb{X}}_N. \quad (3.78)$$

Then we derive from (3.11), (3.68), and (3.78) that for any $v_N \in \mathbb{X}_N$,

$$\mathcal{B}_m(e_N, \phi) = \mathcal{B}_m(\tilde{e}_N, \phi) = -k^2(\alpha\beta r \tilde{e}_N, \phi)_I.$$

Then, set $\phi = e_N$ in this weak formulation, and comparing the forms of $a_m(\cdot, \cdot)$ and $\mathcal{B}_m(\cdot, \cdot)$ in (3.11) and (3.65), we have

$$\mathcal{B}_m(e_N, e_N) = a_m(e_N, e_N) = -k^2(\alpha\beta r \tilde{e}_N, e_N)_I, \quad (3.79)$$

From (3.13) and (3.12), we can derive that

$$\Im\{\alpha\beta r\} = \sigma_0(2\sigma_1 T + R_1)T' > 0,$$

and from previous derivation (3.50),

$$\Re\{\alpha\beta r\} = ((\sigma_1^2 - \sigma_0^2)T + \sigma_1 R_1)T'$$

is negative, when $r \in I_a := (R_1, R_0)$; is positive, when $r \in I_b := (R_0, R_2)$. We already knew

$$R_0 = R_1 \frac{\sigma_0^2 - \sigma_1^2 + \sigma_1 R_2}{\sigma_0^2 - \sigma_1^2 + \sigma_1 R_1}.$$

After that, for a small enough positive constant ξ , we can derive from (3.79),

$$\begin{aligned} \Im\{a_m(e_N, e_N)\} &\leq \xi k^2(\Im\{\alpha\beta r\} e_N, e_N)_I + \frac{k^2}{\xi}(\Im\{\alpha\beta r\} \tilde{e}_N, \tilde{e}_N)_I, \\ \Re\{a_m(e_N, e_N)\} &\leq \xi k^2(e_N, e_N)_{I_1} + \frac{k^2}{\xi}(\tilde{e}_N, \tilde{e}_N)_{I_1} \\ &\quad - \xi k^2(\Re\{\alpha\beta r\} e_N, e_N)_{I_a} - \frac{k^2}{\xi}(\Re\{\alpha\beta r\} \tilde{e}_N, \tilde{e}_N)_{I_a} \\ &\quad + \xi k^2(\Re\{\alpha\beta r\} e_N, e_N)_{I_b} + \frac{k^2}{\xi}(\Re\{\alpha\beta r\} \tilde{e}_N, \tilde{e}_N)_{I_b}, \end{aligned}$$

as $I_1 = (0, R_1)$ mentioned before.

Then, we will propose the following theorem for analysing error estimate, and its proof follows the one of Theorem 3.1 in stability analysis. Before that, we first denote a new bilinear form $b_m(e_N, e_N) = (f_0, e_N)$ as following:

$$\begin{aligned} \Im\{b_m(e_N, e_N)\} &:= \Im\{a_m(e_N, e_N)\} - \xi k^2(\Im\{\alpha\beta r\} e_N, e_N)_I, \\ \Re\{b_m(e_N, e_N)\} &:= \Re\{a_m(e_N, e_N)\} - \xi k^2(e_N, e_N)_{I_1} \\ &\quad + \xi k^2(\Re\{\alpha\beta r\} e_N, e_N)_{I_a} - \xi k^2(\Re\{\alpha\beta r\} e_N, e_N)_{I_b}, \end{aligned} \quad (3.80)$$

and

$$\begin{aligned}\Im\{(f_0, e_N)\} &:= \frac{k^2}{\xi} (\Im\{\alpha\beta r\} \tilde{e}_N, \tilde{e}_N)_I, \\ \Re\{(f_0, e_N)\} &:= \frac{k^2}{\xi} (\tilde{e}_N, \tilde{e}_N)_{I_1} - \frac{k^2}{\xi} (\Re\{\alpha\beta r\} \tilde{e}_N, \tilde{e}_N)_{I_a} \\ &\quad + \frac{k^2}{\xi} (\Re\{\alpha\beta r\} \tilde{e}_N, \tilde{e}_N)_{I_b}.\end{aligned}\tag{3.81}$$

Theorem 3.3. *Assume*

$$\begin{aligned}\xi &\leq \frac{\sigma_1(R_2 - R_1 - \tau)\tau}{R_1^3(R_2 - R_1)^2} - \frac{3C_1(R_2 - R_1 - \tau)^3}{4k^2R_1^3\sigma_0(R_2 - R_1)^2}, \\ \sigma_0^3 &\geq \frac{3R_1C_1(R_2 - R_1 - \tau)^2}{4k^2},\end{aligned}\tag{3.82}$$

and under the conditions (3.15) of Theorem 3.1. For any $e_N \in \widehat{\mathbb{X}}_N$, there exists positive constants shown in (3.14), such that the following holds:

A. If $m^2 \leq (1 + \xi)k^2R_1^2 + \lambda kR_1^2$, then

$$-\Im\{b_m(e_N, e_N)\} \gtrsim \int_{R_1}^{R_2} (R_2 - r)^2 r |e'_N(r)|^2 dr + \int_{R_1}^{R_2} \frac{\lambda k r}{(R_2 - r)^3} |e_N(r)|^2 dr; \tag{3.83}$$

B. If $m^2 > (1 + \xi)k^2R_1^2 + \lambda kR_1^2$, then

$$\Re\{b_m(e_N, e_N)\} \gtrsim \int_0^{R_2} (R_2 - r) r |e'_N(r)|^2 dr + \int_0^{R_2} \frac{\lambda k r}{(R_2 - r)^3} |e_N(r)|^2 dr. \tag{3.84}$$

Proof. Step 1 : We first deal with the imaginary part. From $\Im\{b_m(e_N, e_N)\}$ in (3.80),

$$\begin{aligned}-\Im\{b_m(e_N, e_N)\} &= -\Im\{a_m(e_N, e_N)\} + \xi k^2 \int_0^{R_2} \Im\{\alpha\beta r\} dr \\ &\geq -\Im\{a_m(e_N, e_N)\},\end{aligned}$$

to prove (3.83), it remains to prove when $m^2 \leq (1 + \xi)k^2R_1^2 + \lambda kR_1^2$,

$$-\Im\{a_m(e_N, e_N)\} \gtrsim \int_{R_1}^{R_2} (R_2 - r)^2 r |e'_N(r)|^2 + \lambda k \frac{r}{(R_2 - r)^3} |e_N(r)|^2 dr, \tag{3.85}$$

where the form of $-\Im\{a_m(e_N, e_N)\}$ has been shown in (3.18) before.

Next, to derive (3.85), similar with (3.23), we have the following inequality with λ and C_1 determined in (3.38) and (3.19), respectively: when $m^2 \leq (1 + \xi)k^2 R_1^2 + \lambda k R_1^2$,

$$\begin{aligned} -\Im\{a_m(e_N, e_N)\} &\geq \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |e'_N(r)|^2 dr - C_1 \int_{R_1+\tau}^{R_2} |e_N(r)|^2 dr \\ &\quad + \frac{C_1}{2\tau} \int_{R_1}^{R_1+\tau} (-3r + 2R_1 + R_2) |e_N(r)|^2 dr \\ &\quad + \int_{R_1}^{R_2} \left[k^2 \Im\{\alpha \beta r\} - m^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right] |e_N(r)|^2 dr. \end{aligned} \quad (3.86)$$

We next show that the constant λ , for $m^2 \leq (1 + \xi)k^2 R_1^2 + \lambda k R_1^2$, we have the lower bound (3.85). Then, we eliminate m in the last term and obtain from (3.13) that

$$\begin{aligned} &k^2 \Im\{\alpha \beta r\} - m^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \\ &\geq k^2 \Im\{\alpha \beta r\} - [(1 + \xi)k^2 R_1^2 + \lambda k R_1^2] \Im\left\{\frac{\alpha}{\beta r}\right\} \\ &= 2k^2 \sigma_1 \sigma_0 T T' - \xi k^2 R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} + k^2 \left[\sigma_0 R_1 T' - R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right] - \lambda k R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \\ &\geq 2k^2 \sigma_1 \sigma_0 T T' - \xi k^2 R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} - \lambda k R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\}, \end{aligned}$$

from (3.25)

$$\sigma_0 R_1 T' - R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} > 0.$$

After similar step in (3.26),

$$2k^2 \sigma_1 \sigma_0 \int_{R_1}^{R_2} T T' |e_N(r)|^2 dr \geq 2k^2 \sigma_1 \sigma_0 \int_{R_1+\tau}^{R_2} T T' |e_N(r)|^2 dr.$$

we have

$$\begin{aligned}
-\Im\{a_m(e_N, e_N)\} &\geq \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |e'_N(r)|^2 dr \\
&\quad + \int_{R_1}^{R_1+\tau} \left[\frac{C_1}{2\tau} (-3r + 2R_1 + R_2) - \xi k^2 R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right] |e_N(r)|^2 dr \\
&\quad + \int_{R_1+\tau}^{R_2} \left[2k^2 \sigma_1 \sigma_0 T T' - C_1 - \xi k^2 R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right] |e_N(r)|^2 dr \\
&\quad - \lambda k R_1^2 \int_{R_1}^{R_2} \Im\left\{\frac{\alpha}{\beta r}\right\} |e_N(r)|^2 dr \\
&= \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |e'_N(r)|^2 dr + \int_{R_1}^{R_1+\tau} \widetilde{H}_1(r) \frac{|e_N(r)|^2}{(R_2 - r)^3} dr \\
&\quad + \int_{R_1+\tau}^{R_2} \widetilde{H}_2(r) \frac{|e_N(r)|^2}{(R_2 - r)^3} dr - \lambda k R_1^2 \int_{R_1}^{R_2} \Im\left\{\frac{\alpha}{\beta r}\right\} |e_N(r)|^2 dr,
\end{aligned}$$

where for clarity, we denote

$$\begin{aligned}
\widetilde{H}_1(r) &:= \left[\frac{C_1}{2\tau} (-3r + 2R_1 + R_2) - \xi k^2 R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right] (R_2 - r)^3, \quad r \in (R_1, R_1 + \tau), \\
\widetilde{H}_2(r) &:= \left[2k^2 \sigma_1 \sigma_0 T T' - C_1 - \xi k^2 R_1^2 \Im\left\{\frac{\alpha}{\beta r}\right\} \right] (R_2 - r)^3, \quad r \in [R_1 + \tau, R_2].
\end{aligned}$$

For $\widetilde{H}_1(r)$, as $H_1(r)$ shown in (3.27a) and $P(r)$ shown in (3.37),

$$\widetilde{H}_1(r) = H_1(r) - \xi k^2 (P(r) - R_2), \quad r \in (R_1, R_1 + \tau).$$

From the lower bounds shown in (3.29) and $P'(r) < 0$ proved before, as $r \in (R_1, R_1 + \tau)$, we have

$$\begin{aligned}
\widetilde{H}_1(r) &\geq H_1(R_1 + \tau) - \xi k^2 (P(R_1) - R_2) \\
&= \frac{C_1}{2\tau} (R_2 - R_1 - \tau)^3 (R_2 - R_1 - 3\tau) - \xi \sigma_0 R_1 (R_2 - R_1)^2 k^2,
\end{aligned} \tag{3.87}$$

as $H'_1(r) \leq 0$, $P'(r) < 0$.

Then consider $\widetilde{H}_2(r)$, as $H_2(r)$ shown in (3.27b) and $P(r)$ shown in (3.37),

$$\widetilde{H}_2(r) = H_2(r) - \xi k^2 (P(r) - R_2), \quad r \in [R_1 + \tau, R_2].$$

From the lower bounds shown in (3.30) and $P'(r) < 0$ proved before, as $r \in$

$[R_1 + \tau, R_2)$, we have

$$\begin{aligned}\widetilde{H}_2(r) &\geq H_2(R_1 + \tau) - \xi k^2 (P(R_1 + \tau) - R_2) \\ &= 2k^2 \sigma_0 \sigma_1 \tau (R_2 - R_1 - \tau) - \frac{3C_1}{2} (R_2 - R_1 - \tau)^3 \\ &\quad - \xi \sigma_0 R_1 (R_2 - R_1)^2 k^2,\end{aligned}\tag{3.88}$$

as $H'_2(r) > 0$, $P'(r) < 0$.

Now, we consider the lower bounds in (3.87) and (3.88), as τ shown in (3.31), we can readily find out:

$$\widetilde{H}_1(r), \widetilde{H}_2(r) \geq \frac{C_1}{2\tau} (R_2 - R_1 - \tau)^3 (R_2 - R_1 - 3\tau) - \xi \sigma_0 R_1 (R_2 - R_1)^2 k^2.$$

From condition (3.82), we can derive

$$H_2(R_1 + \tau) \geq 2\xi k^2 \sigma_0 R_1^3 (R_2 - R_1)^2.$$

which means

$$\begin{aligned}\widetilde{H}_1(r) &\geq H_1(R_1 + \tau) - \xi \sigma_0 R_1 (R_2 - R_1)^2 k^2 \\ &\geq \frac{H_1(R_1 + \tau)}{2} \\ &= \frac{C_1}{4\tau} (R_2 - R_1 - \tau)^3 (R_2 - R_1 - 3\tau),\end{aligned}$$

and the same with $\widetilde{H}_2(r)$:

$$\widetilde{H}_2(r) \geq \frac{C_1}{4\tau} (R_2 - R_1 - \tau)^3 (R_2 - R_1 - 3\tau).$$

With this, we can obtain

$$\begin{aligned}-\Im\{a_m(e_N, e_N)\} &\geq \frac{C_1}{2} \int_{R_1}^{R_2} (R_2 - r)^2 |e'_N(r)|^2 dr \\ &\quad + \frac{C_1}{4\tau} (R_2 - R_1 - \tau)^3 (R_2 - R_1 - 3\tau) \int_{R_1}^{R_2} \frac{|e_N(r)|^2}{(R_2 - r)^3} dr \\ &\quad - \lambda k R_1^2 \int_{R_1}^{R_2} \Im\left\{\frac{\alpha}{\beta r}\right\} |e_N(r)|^2 dr,\end{aligned}$$

where τ is given by (3.31).

To prove (3.85), it means to prove, when $r \in [R_1, R_2]$,

$$Q(\tau, r) - \frac{\lambda k \sigma_0 R_1^3 (R_2 - R_1)(R_2 - r)^3}{[R_1(R_2 - r) + \sigma_1(r - R_1)]^2 + \sigma_0^2(r - R_1)^2} \geq 2\lambda k r,$$

where $Q(\tau, r)$ first introduced in (3.33).

Following the derivation in the proof of Lemma 3.1, we can derive

$$\lambda \leq \frac{C_1(R_2 - R_1 - 3\hat{\tau})^4}{4\hat{\tau}k\sigma_0 R_1(R_2 - R_1)^2}, \quad (3.89)$$

where $\hat{\tau}$ is given in (3.34). Here, λ shown in (3.38), satisfied (3.89).

Step 2 : For real part ($m^2 > (1 + \xi)k^2 R_1^2 + \lambda k R_1^2$): With λ given by (3.38), we now deal with the real part $\Re\{b_m(e_N, e_N)\}$ from (3.80):

$$\begin{aligned} \Re\{b_m(e_N, e_N)\} &:= \Re\{a_m(e_N, e_N)\} - \xi k^2 (e_N, e_N)_{I_1} \\ &\quad + \xi k^2 (\Re\{\alpha \beta r\} e_N, e_N)_{I_a} - \xi k^2 (\Re\{\alpha \beta r\} e_N, e_N)_{I_b}, \end{aligned} \quad (3.90)$$

for all $m^2 > (1 + \xi)k^2 R_1^2 + \lambda k R_1^2$. Recall that $\alpha = \beta = 1$ for $r \in (0, R_1)$. It is evident that we have

$$\frac{m^2}{r} - (1 + \xi)k^2 r > \frac{m^2}{R_1} - (1 + \xi)k^2 R_1 > \lambda k R_1 \geq \lambda k r.$$

Thus we have

$$\begin{aligned} &\int_0^{R_1} r |e'_N(r)|^2 + \left(\frac{m^2}{r} - k^2 r\right) |e_N(r)|^2 dr \\ &\geq \int_0^{R_1} r |e'_N(r)|^2 dr + \lambda k \int_0^{R_1} r |e_N(r)|^2 dr. \end{aligned} \quad (3.91)$$

We now turn to the integrals for $r \in [R_1, R_2]$. Under the condition $\sigma_1^2 + \sigma_0^2 \geq \sigma_1 R_1$, we obtain from (3.3) that

$$\begin{aligned} \Re\left\{\frac{\beta r}{\alpha}\right\} &= \frac{(\sigma_1^2 + \sigma_0^2)(r - R_1) + \sigma_1 R_1(R_2 - r)}{(\sigma_1^2 + \sigma_0^2)(R_2 - R_1)}(R_2 - r) \\ &\geq \frac{\sigma_1 R_1}{\sigma_1^2 + \sigma_0^2}(R_2 - r). \end{aligned}$$

We now estimate the last term in (3.90). Under the conditions (3.15) of Theorem 3.1, similar as proof of Theorem 3.1, we can derive

(1) When $T \in (0, T_0 + \varepsilon_T)$, i.e., $r \in I_a$, following proof of (3.51), we have

$$[(1 + \xi)k^2 + \lambda k]F_1(T) + (1 - \xi)k^2F_2(T) \geq \lambda kF_1(0) \geq \lambda k \frac{r}{R_2 - r},$$

as $F_1(T)$ and $F_2(T)$ proposed in (3.44).

(2) When $T \in [T_0 + \varepsilon_T, \infty)$, following proof of (3.54), as $F_1(T) \geq 0$ on this interval, we have

$$(1 + \xi)F_2(T) > F_2(T) \geq \frac{\lambda}{k} \frac{r}{R_2 - r},$$

which can prove (3.84). $\square$

With the aid of Theorem 3.1 and Theorem 3.4, we are able to obtain the following error estimates.

Theorem 3.4. *If $\hat{v}_m(r) \in B_*^s(I)$, for $s \geq 1$ and $s \in \mathbb{N}$,*

$$\begin{aligned} \left(\int_I r |\hat{v}_m(r) - v_N(r)|^2 dr \right)^{\frac{1}{2}} &\lesssim \|\hat{v}_m - \pi_N^1 v\|_* + \|v_N - \pi_N^1 v\|_* \\ &\lesssim (1 + mN^{-1})k^{\frac{1}{2}}N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s-1, s-1, I_1}} \\ &\quad + (1 + \sqrt{k^2 + m^2}N^{-1})k^{\frac{1}{2}}N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s+1, s-1, I_2}}. \end{aligned}$$

What is more, as $\hat{u}_m(r) = w(r)\hat{v}_m(r)$, we have

$$\|\hat{u}_m - u_N\| \leq \left(\int_I r |\hat{v}_m(r) - v_N(r)|^2 dr \right)^{\frac{1}{2}}.$$

Proof.

$$\begin{aligned} \Re\{(f_0, e_N)\} &:= \frac{k^2}{\xi} (\tilde{e}_N, \tilde{e}_N)_{I_1} - \frac{k^2}{\xi} (\Re\{\alpha\beta r\} \tilde{e}_N, \tilde{e}_N)_{I_a} \\ &\quad + \frac{k^2}{\xi} (\Re\{\alpha\beta r\} \tilde{e}_N, \tilde{e}_N)_{I_b}. \end{aligned} \tag{3.92}$$

From (3.81), it shows that

$$\begin{aligned} \Im\{f_0\} &= \frac{k^2}{\xi} \Im\{\alpha\beta r\} \\ &\lesssim k^2(R_2 - r)^{-3}. \end{aligned} \tag{3.93}$$

Then, for $\Re\{f_0\}$,

$$\Re\{f_0\} \lesssim \begin{cases} rk^2, & r \in I_1, \\ k^2(R_2 - r)^{-3}, & r \in I_2. \end{cases} \quad (3.94)$$

After that, we also prove it by separating in imaginary and real parts.

(1) When $m^2 \leq (1 + \xi)k^2R_1^2 + \lambda kR_1^2$, from (3.79), (3.83) and (3.93), we will have

$$\begin{aligned} \lambda k \int_I r |v_N - \pi_N^1 v|^2 dr &\lesssim -\Im(b_m(e_N, e_N)) \\ &\lesssim k^2 \int_{I_2} |\hat{v}_m(r) - \pi_N^1 v(r)|^2 dr \\ &\lesssim k^2 \|\hat{v}_m(r) - \pi_N^1 v\|_*^2. \end{aligned}$$

Using Lemma 3.4, if $v \in B_*^s(I)$, as $|w(r)(v_N - \pi_N^1 v)|^2 = |e_N|^2$,

$$\left(\int_I r |v_N - \pi_N^1 v|^2 dr \right)^{\frac{1}{2}} \lesssim (1 + \sqrt{k^2 + m^2}N^{-1})k^{\frac{1}{2}}N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s+1, s-1}, I_2}.$$

(2) When $m^2 > (1 + \varepsilon_1)k^2R_1^2 + \lambda kR_1^2$, from (3.79), (3.84) and (3.94), we will have

$$\begin{aligned} \lambda k \int_I r |v_N - \pi_N^1 v|^2 dr &\lesssim \Re(b_m(e_N, e_N)) \\ &\lesssim k^2 \int_{I_1} r |\hat{v}_m(r) - \pi_N^1 v(r)|^2 dr \\ &\quad + k^2 \int_{I_2} |\hat{v}_m(r) - \pi_N^1 v(r)|^2 dr \\ &\lesssim k^2 \|\hat{v}_m(r) - \pi_N^1 v\|_*^2. \end{aligned}$$

Also, using Lemma 3.4, if $v \in B_*^s(I)$,

$$\begin{aligned} \left(\int_I r |v_N - \pi_N^1 v|^2 dr \right)^{\frac{1}{2}} &\lesssim (1 + mN^{-1})k^{\frac{1}{2}}N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s-1, s-1}, I_1} \\ &\quad + (1 + \sqrt{k^2 + m^2}N^{-1})k^{\frac{1}{2}}N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s+1, s-1}, I_2}, \end{aligned}$$

which can derive the conclusion:

$$\begin{aligned} \left(\int_I r |\hat{v}_m(r) - v_N(r)|^2 dr \right)^{\frac{1}{2}} &\lesssim \left(\int_I r |\hat{v}_m(r) - \pi_N^1 v(r)|^2 dr \right)^{\frac{1}{2}} + \left(\int_I r |v_N(r) - \pi_N^1 v(r)|^2 dr \right)^{\frac{1}{2}} \\ &\lesssim (1 + mN^{-1})k^{\frac{1}{2}}N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s-1, s-1}, I_1} \\ &\quad + (1 + \sqrt{k^2 + m^2}N^{-1})k^{\frac{1}{2}}N^{1-s} \|\partial_r^s \hat{v}_m\|_{\omega^{s+1, s-1}, I_2}. \end{aligned}$$

At last, as $\hat{v}_m = w(r)\hat{u}_m$,

$$\begin{aligned} \left(\int_I r |\hat{u}_m(r) - u_N(r)|^2 dr \right)^{\frac{1}{2}} &= \left(\int_I r (R_2 - r)^3 |\hat{v}_m(r) - v_N(r)|^2 dr \right)^{\frac{1}{2}} \\ &\leq \left(\int_I r |\hat{v}_m(r) - v_N(r)|^2 dr \right)^{\frac{1}{2}}. \end{aligned}$$

□

As Theorem 3.4 showing the error between $\hat{v}_m$ and v_N , we also can have the 2D conclusion of the error between V_{PAL} and V_{MN} , which are substituted from U_{PAL} and U_{MN} :

Corollary 3.1. *From Theorem 3.4 we can derive that*

$$\begin{aligned} \left(\int_{\mathcal{D}} r |V_{\text{PAL}} - V_{MN}|^2 dr d\theta \right)^{\frac{1}{2}} &\lesssim k^{\frac{1}{2}} N^{1-s} \|\partial_r^s V_{\text{PAL}}\|_{\omega^{s-1, s-1}, \mathbb{B}_{R_1}} \\ &\quad + k^{\frac{1}{2}} N^{-s} \|\partial_r^s \partial_\theta^2 V_{\text{PAL}}\|_{\omega^{s-1, s-1}, \mathbb{B}_{R_1}} \\ &\quad + k^{\frac{3}{2}} N^{1-s} \|\partial_r^s V_{\text{PAL}}\|_{\omega^{s+1, s-1}, \Omega_\varrho^{\text{PAL}}} \\ &\quad + k^{\frac{1}{2}} N^{-s} \|\partial_r^s \partial_\theta^2 V_{\text{PAL}}\|_{\omega^{s+1, s-1}, \Omega_\varrho^{\text{PAL}}}. \end{aligned}$$

Time-Domain PAL

In this chapter, we consider the extensions of the perfect matched layer in the frequency domain (Chapter 2) to time domain. We primarily solved advection equation and two-way wave problem. Also, we derive some conclusions about waveguide problem, comparing with regular PML [25, 19, 84], and singular PML [13, 14] methods.

4.1 Time-domain PAL for one-way wave equation

To illustrate the idea of the extension of PAL from frequency domain to time domain, we consider one-way wave equation:

$$\begin{aligned}\partial_t U + \partial_x U &= 0, \quad x, t > 0, \\ U(0, t) &= g(t), \quad t \geq 0; \quad U(x, 0) = u_0(x), \quad x \geq 0,\end{aligned}\tag{4.1}$$

where $g(t)$ and $u_0(x)$ are given functions, and $u_0(x)$ is compactly supported in I .

To numerically solve (4.1), we reduce the infinite domain to a bounded domain by appending it with an artificial layer (interval) $I_d := [L, L + d]$ with a finite thickness d . The domain $I := [0, L]$ is the so-called "physical domain", where we intend to compute the solution of (4.1). The interval I_d is filled with fictitious

absorbing media to damp and absorb the wave that propagate into the layer and avoid the reflection as much as possible.

We first recap on the time-domain PML-technique. Based on [25], the PML-problem can be obtained from $(\tilde{x}, \tilde{t})$ -coordinates by using the transformation: $\tilde{t} = t$, and

$$\tilde{x} = S(x) = \begin{cases} x, & 0 \leq x \leq L, \\ S_R(x) + \frac{i}{\omega} \sigma_0 S_I(x), & L \leq x \leq L + L_d, \end{cases} \quad (4.2)$$

where $\sigma_0 > 0$ is a tuneable constant, and

$$S_R(x) = x, \quad S_I(x) = \int_L^x \sigma(\tau) d\tau.$$

Typically, the following two types of $\sigma(x)$ were used in literature:

- Regular function (see, e.g., [25, 19, 84]):

$$\sigma(x) = \left(\frac{x - L}{d} \right)^n, \quad (4.3)$$

where $n \geq 1$ is an integer.

- Singular function (or unbounded absorbing function) (see [13, 14]):

$$\sigma(x) = \frac{1}{L_d - x}, \quad (4.4)$$

where we denote $L_d := L + d$.

For any $\omega > 0 \in \mathbb{R}$, let $\widehat{U}_p = \mathcal{F}(U_p)$ and the vector-valued function $\mathbf{P}_f = (\widehat{P}_1, \widehat{P}_2) = \mathcal{F}(\mathbf{P})$ be respectively the Fourier transform of function U_p and $\mathbf{P}$ in time

$$\widehat{U}_p(x, \omega) = \int_{-\infty}^{\infty} e^{-i\omega t} \overline{U}_p(x, t) dt, \quad \mathbf{P}_f(x, \omega) = \int_{-\infty}^{\infty} e^{-i\omega t} \overline{\mathbf{P}}(x, t) dt,$$

where we have the zero extensions of $U_p(x, t)$ and $\mathbf{P}(x, t)$ as:

$$\overline{U}_p(x, t) = \begin{cases} U_p(x, t) & t \geq 0, \\ 0 & t < 0, \end{cases} \quad \overline{\mathbf{P}}(x, t) = \begin{cases} \mathbf{P}(x, t) & t \geq 0, \\ 0 & t < 0, \end{cases} \quad (4.5)$$

here, $\bar{a}$ means the conjugate of a .

Theorem 4.1. *Using the PML coordinate transformation (4.2) in space domain and $\tilde{t} = t$ in time domain, we derive the PML type equation of (4.1) with operator $\mathcal{L}_{PML}$:*

$$\mathcal{L}_{PML}[U_p] := \partial_t U_p + \partial_x U_p = 0, \quad x \in (0, L); \quad (4.6a)$$

$$\mathcal{L}_{PML}[U_p] := \partial_t U_p + \partial_x U_p + \sigma_0 \sigma(x) U_p = 0, \quad x \in (L, L_d), \quad (4.6b)$$

where $\sigma(x)$ is the same as in (4.2).

Proof. In $(0, L)$, $S(x) = x$ and $\tilde{t} = t$, so

$$\mathcal{L}_{PML}[U_p] = \partial_t U_p + \partial_x U_p.$$

In (L, L_d) , after using Fourier transform on the advection equation, we obtain

$$-i\omega \widehat{U} + \partial_x \widehat{U} = 0,$$

where $\omega \in \mathbb{R}$ such that $\omega > 0$. Then, using the transformation (4.2), we derive

$$-i\omega \widehat{U}_p + \sigma_0 \sigma(x) \widehat{U}_p + \partial_x \widehat{U}_p = 0.$$

Then, taking the inverse Fourier transform, we get

$$\partial_t U_p + \partial_x U_p + \sigma_0 \sigma(x) U_p = 0,$$

which completes the proof. $\square$

Remark 4.1. *It is seen from (4.6) that the additional term $\sigma_0 \sigma(x) U_p$ turns out to be a damping term.*

Following the spirit of the frequency domain PAL, we construct the time-domain PAL based on

- Complex compression coordinate transformation $S(x)$ with unbounded real and imaginary parts;
- Effective treatment of the singularity induced by the singular transformation.

Set

$$\tilde{x} = S(x) = \begin{cases} x, & 0 \leq x \leq L, \\ L + \sigma_1 T(x) + \sigma_0 \frac{i}{\omega} T(x), & L \leq x \leq L + L_d, \end{cases} \quad (4.7)$$

where $\sigma_0, \sigma_1 > 0$ are tuning parameters, and

$$T(x) = \frac{x - L}{L_d - x} = d \int_L^x \frac{dt}{(L_d - t)^2}, \quad T'(x) = \frac{d}{(L_d - x)^2}, \quad x \in (L, L_d), \quad (4.8)$$

with $L_d = L + d$.

Theorem 4.2. *Using the coordinate transformation (4.7) in space domain and in time domain $\tilde{t} = t$, we derive the PAL-equation of (4.1) with the operator $\mathcal{L}_{PAL}$:*

$$\begin{aligned} \mathcal{L}_{PAL}[U_a] &:= \partial_t U_a + \partial_x U_a = 0, \quad x \in (0, L); \\ \mathcal{L}_{PAL}[U_a] &:= \partial_t U_a + \frac{1}{\sigma_1 T'(x)} \partial_x U_a + \frac{\sigma_0}{\sigma_1} U_a = 0, \quad x \in (L, L_d). \end{aligned} \quad (4.9)$$

Proof. For $x \in (0, L)$, we have $S(x) = x$, so

$$\mathcal{L}_{PAL}[U_a] = \partial_t U_a + \partial_x U_a.$$

For $x \in (L, L_d)$, using Fourier transform on the advection equation leads to

$$-i\omega \widehat{U} + \partial_{\tilde{x}} \widehat{U} = 0.$$

Then, by the transformation (4.7), we derive

$$-i\omega \sigma_1 T'(x) \widehat{U}_a + \sigma_0 T'(x) \widehat{U}_a + \partial_x \widehat{U}_a = 0.$$

Then, taking the inverse Fourier transform yields

$$\partial_t U_a + \frac{1}{\sigma_1 T'(x)} \partial_x U_a + \frac{\sigma_0}{\sigma_1} U_a = 0,$$

which ends the proof. $\square$

Remark 4.2. *Compared with (4.6), the PAL-equation in the artificial interval damps the wave in a very different fashion, which we shall provide more details later on.*

4.2 Time-domain PAL for two-way wave equation

Consider the initial boundary value problem for the two-way wave equation

$$\begin{cases} \partial_t^2 U - \partial_x^2 U = 0, & x, t > 0, \\ U|_{t=0} = U_0(x), \quad \partial_t U|_{t=0} = U_1(x), & x \geq 0, \\ U|_{x=0} = g(t), & t \geq 0, \end{cases} \quad (4.10)$$

where $U_0(x)$ and $U_1(x)$ are assumed to be supported in the interior domain $0 \leq x \leq L$, and $g(t)$ is a given function.

Note that by using the standard solution technique, we can find its solution as follows

$$U(x, t) = \begin{cases} \frac{1}{2}[U_0(x+t) + U_0(x-t)] + \frac{1}{2} \int_{x-t}^{x+t} U_1(\xi) d\xi, & x-t \geq 0, \\ g(t-x) + \frac{1}{2}[U_0(x+t) - U_0(t-x)] + \frac{1}{2} \int_{t-x}^{x+t} U_1(\xi) d\xi, & x-t < 0. \end{cases} \quad (4.11)$$

Using the coordinate transformation in space domain and $\tilde{t} = t$ in time domain, we derive the general PML transformed equations of (4.10) with operator $\mathcal{L}_P$:

$$\begin{cases} \mathcal{L}_P[U] := \partial_{\tilde{t}}^2 U - \partial_x^2 U = 0, & x \in I := (0, L); \\ \mathcal{L}_P[U] := \partial_{\tilde{t}}^2 U - \frac{dx}{d\tilde{x}} \partial_x \left(\frac{dx}{d\tilde{x}} \partial_x U \right) = 0, & x \in I_d := (L, L_d); \\ U|_I = U|_{I_d}, \quad \partial_x U|_I = \frac{dx}{d\tilde{x}} \partial_x U|_{I_d}, & \text{at } x = L, \\ U|_{t=0} = U_0, \quad \partial_t U|_{t=0} = U_1, \quad U|_{x=0} = g, \quad U|_{x=L_d} = 0. \end{cases} \quad (4.12)$$

As the one-way wave case, we first examine the PML-technique.

Theorem 4.3. *Using the PML coordinate transformation (4.2), we derive the PML type equation of (4.12) with operator $\mathcal{L}_P$:*

$$\mathcal{L}_P[U_p] = \partial_{\tilde{t}}^2 U_p - \partial_x^2 U_p, \quad \text{on } I; \quad (4.13)$$

and on I_d , we will have the equations:

$$\partial_t U_p + \sigma_0 \sigma(x) U_p = \partial_x P, \quad (4.14a)$$

$$\partial_t P = \partial_x U_p - \sigma_0 \sigma(x) \int_0^t e^{-\sigma_0 \sigma(x)(t-\tau)} \partial_x U_p(x, \tau) d\tau \quad (4.14b)$$

where P is “auxiliary” variable. Moreover, we can derive the second order equation in the PML I_d :

$$\begin{aligned} \mathcal{L}_P[U_p] = & \partial_t^2 U_p + \sigma_0 \sigma(x) \partial_t U_p - \partial_x^2 U_p \\ & + \sigma_0 \partial_x \left\{ \sigma(x) \int_0^t e^{-\sigma_0 \sigma(x)(t-\tau)} \partial_x U_p(x, \tau) d\tau \right\}. \end{aligned} \quad (4.15)$$

Proof. For $x \in I$, we have $S(x) = x$, so

$$\mathcal{L}_P[U_p] = \mathcal{L}[U_p] = \partial_t^2 U_p - \partial_x^2 U_p.$$

For $x \in I_d$, using Fourier transform on the two coupled first-order system, we can derive

$$-i\omega \widehat{U} = \partial_{\tilde{x}} \widehat{P}, \quad -i\omega \widehat{P} = \partial_{\tilde{x}} \widehat{U}.$$

Then by the transformation (4.2), we have

$$-i\omega \widehat{U}_p = \frac{1}{1 + \frac{i}{\omega} \sigma_0 \sigma(x)} \partial_x \widehat{P}, \quad (4.16a)$$

$$-i\omega \widehat{P} = \frac{1}{1 + \frac{i}{\omega} \sigma_0 \sigma(x)} \partial_x \widehat{U}_p. \quad (4.16b)$$

Multiplying (4.16a) by $S'(x) = 1 + \frac{i}{\omega} \sigma_0 \sigma(x)$ leads to

$$-i\omega \widehat{U}_p + \sigma_0 \sigma(x) \widehat{U}_p = \partial_x \widehat{P}, \quad -i\omega \widehat{P} = \frac{1}{1 + \frac{i}{\omega} \sigma_0 \sigma(x)} \partial_x \widehat{U}_p.$$

Then, taking the inverse Fourier transform of the above equations leads to

$$\partial_t U_p + \sigma_0 \sigma(x) U_p = \partial_x P, \quad \partial_t P = \int_0^t e^{-\sigma_0 \sigma(x)(t-\tau)} \partial_{\tau x}^2 U_p(x, \tau) d\tau.$$

Using the integration by parts, we can derive the system:

$$\partial_t U_p + \sigma_0 \sigma(x) U_p = \partial_x P, \quad (4.17a)$$

$$\partial_t P = \partial_x U_p - \sigma_0 \sigma(x) \int_0^t e^{-\sigma_0 \sigma(x)(t-\tau)} \partial_x U_p(x, \tau) d\tau. \quad (4.17b)$$

To derive (4.15), we first find $\partial_{xt}^2 P$ from (4.17a) and (4.17b):

$$\begin{aligned}\partial_{xt}^2 P &= \partial_t^2 U_p + \sigma_0 \sigma(x) \partial_t U_p, \\ \partial_{xt}^2 P &= \partial_x^2 U_p - \sigma_0 \partial_x \left[\sigma(x) \int_0^t e^{-\sigma_0 \sigma(x)(t-\tau)} \partial_x U_p(x, \tau) d\tau \right].\end{aligned}$$

Thus, we obtain

$$\mathcal{L}_P[U_p] = \partial_t^2 U_p + \sigma_0 \sigma(x) \partial_t U_p - \partial_x^2 U_p + \sigma_0 \partial_x \left\{ \sigma(x) \int_0^t e^{-\sigma_0 \sigma(x)(t-\tau)} \partial_x U_p(x, \tau) d\tau \right\},$$

which completes the proof. $\square$

We next show that the time-domain PAL for the two-way wave equation takes a different form as follows.

Theorem 4.4. *Using the PAL coordinate transformation (4.7), we derive the PAL type equation of (4.12) with operator $\mathcal{L}_{PAL}$:*

$$\mathcal{L}_{PAL}[U_a] = \partial_t^2 U_a - \partial_x^2 U_a, \quad \text{on } I; \quad (4.18)$$

and on I_d , we will have the equations:

$$\partial_t U_a + \frac{\sigma_0}{\sigma_1} U_a = \frac{1}{\sigma_1 T'} \partial_x P, \quad \partial_t P + \frac{\sigma_0}{\sigma_1} P = \frac{1}{\sigma_1 T'} \partial_x U_a.$$

where P is “auxiliary” variable. Moreover, we can derive the second-order equation:

$$\mathcal{L}_{PAL}[U_a] = \partial_t^2 U_a + \frac{2\sigma_0}{\sigma_1} \partial_t U_a - \frac{1}{(\sigma_1 T')^2} \partial_x^2 U_a + \frac{T''}{\sigma_1^2 (T')^3} \partial_x U_a + \frac{\sigma_0^2}{\sigma_1^2} U_a. \quad (4.20)$$

Proof. For $x \in I$, we have $S(x) = x$, so

$$\mathcal{L}_{PAL}[U_a] = \mathcal{L}[U_a] = \partial_t^2 U_a - \partial_x^2 U_a.$$

For $x \in I_d$, using the Fourier transform on the two coupled first-order equations, we can derive

$$-i\omega \widehat{U} = \partial_{\bar{x}} \widehat{P}, \quad -i\omega \widehat{P} = \partial_{\bar{x}} \widehat{U},$$

Using the transformation (4.7) leads to

$$-i\omega\widehat{U}_a = \frac{1}{(\sigma_1 + \frac{i}{\omega}\sigma_0)T'}\partial_x\widehat{P}, \quad -i\omega\widehat{P} = \frac{1}{(\sigma_1 + \frac{i}{\omega}\sigma_0)T'}\partial_x\widehat{U}_a. \quad (4.21)$$

Multiplying $\gamma(x) = (\sigma_1 + \frac{i}{\omega}\sigma_0)T'$ on both sides of (4.21) gives

$$-i\omega\sigma_1\widehat{U}_a + \sigma_0\widehat{U}_a = \frac{1}{T'}\partial_x\widehat{P}, \quad -i\omega\sigma_1\widehat{P} + \sigma_0\widehat{P} = \frac{1}{T'}\partial_x\widehat{U}_a.$$

Then, taking the inverse Fourier transform of the above equations, we obtain

$$\partial_t U_a + \frac{\sigma_0}{\sigma_1} U_a = \frac{1}{\sigma_1 T'} \partial_x P, \quad (4.22a)$$

$$\partial_t P + \frac{\sigma_0}{\sigma_1} P = \frac{1}{\sigma_1 T'} \partial_x U_a. \quad (4.22b)$$

In order to derive (4.20), we compute $\partial_{xt}^2 P$ from (4.22b) and $\partial_x P$ from (4.22a) as follows:

$$\begin{aligned} \partial_x P &= \sigma_1 T' (\partial_t U_a + \frac{\sigma_0}{\sigma_1} U_a), \\ \partial_{xt}^2 P &= -\frac{1}{\sigma_1} \frac{T''}{(T')^2} \partial_x U_a + \frac{1}{\sigma_1 T'} \partial_x^2 U_a - \frac{\sigma_0}{\sigma_1} \partial_x P. \end{aligned} \quad (4.23)$$

Furthermore, taking ∂_t on (4.22a), yields

$$\partial_t^2 U_a + \frac{\sigma_0}{\sigma_1} \partial_t U_a = \frac{1}{\sigma_1 T'} \partial_{xt}^2 P. \quad (4.24)$$

Combining (4.23) and (4.24), yields

$$\partial_t^2 U_a + \frac{2\sigma_0}{\sigma_1} \partial_t U_a - \frac{1}{(\sigma_1 T')^2} \partial_x^2 U_a + \frac{T''}{\sigma_1^2 (T')^3} \partial_x U_a + \frac{\sigma_0^2}{\sigma_1^2} U_a = 0.$$

This implies

$$\mathcal{L}_{PAL}[U_a] = \partial_t^2 U_a + \frac{2\sigma_0}{\sigma_1} \partial_t U_a - \frac{1}{(\sigma_1 T')^2} \partial_x^2 U_a + \frac{T''}{\sigma_1^2 (T')^3} \partial_x U_a + \frac{\sigma_0^2}{\sigma_1^2} U_a, \quad (4.25)$$

which completes the proof. $\square$

Remark 4.3. *It is clear that if $\sigma(x)$ in PML equation (4.15) is singular function mentioned in (4.4), the equation becomes singular at the outer boundary $x = L_d$. This brings about some difficulty in numerical solution of it. In [14, 13], they use Gauss quadrature to avoid sampling the endpoints was recommended, but for large and high resolution, we need pay a lot on it. In PAL equation (4.20), we will not have this kind of problem. Moreover, PAL equation does not have time-convolution part. This will simplify the algorithm in time domain.*

4.3 Time-domain PAL using substitution

To motivate the study, we perform a numerical test. Assume that $g(t) = \sin^p(kt)$, where $(k, p) = (25, 5)$ and $u_0(x) = 0$ in the two-way wave equation. We use a spectral method in space and Newmark's scheme (see [73, 90]). We take the time size to be small, so that the main source of the errors should be from the design of the equation in the layer. As shown in Figure 4.1, the performance of both PML and PAL methods is not satisfactory for such an oscillatory input. As with

Figure 4.1: Error of PAL methods and PML methods against N with the input wave $g(t) = \sin^p(kt)$ on boundary $x = 0$, $(T, dt) = (2, 10^{-4})$, $(L, d) = (1, 0.5)$, $(k, p) = (20, 5)$.

the frequency-domain case, we intend to propose a new PAL method to capture the oscillation of U_a , and approximate a better behaved field.

To remove the essential oscillations of U_a , we introduce the following substitution on I_d :

$$\widehat{U}_a(x) = \widehat{V}_a(x)\widehat{W}(x), \quad (4.26)$$

as

$$\widehat{W}(x) = \begin{cases} 1, & x \in (0, L], \\ e^{i\omega\sigma_1 T(x)}, & x \in (L, L_d). \end{cases} \quad (4.27)$$

We could derive the substitution from PAL solution of one-way wave equation (4.1). First take Fourier transform on it:

$$(-i\omega)\widehat{U} + \partial_{\bar{x}}\widehat{U} = 0.$$

With the boundary condition, we will have the Fourier solution:

$$\widehat{U} = e^{i\omega\tilde{x}}\widehat{g}.$$

Then, as

$$\tilde{x} = L + \sigma_1 T(x) + \frac{i}{\omega} \sigma_0 T(x),$$

we have

$$\widehat{U}_a(x) = e^{i\omega(L+\sigma_1 T(x))-\sigma_0 T(x)}\widehat{g}(x). \quad (4.28)$$

After the numerical experiments with inputting an initial value or boundary condition with high oscillation, or long time propagation, the wave in artificial layer will be difficult to simulate. We next focus on removing the oscillation in PAL. From (4.28), the part $e^{-\sigma_0 T(x)}\widehat{g}$ is the well behaved part and decays fast and smoothly. Then we could introduce the following substitution on I_d :

$$\widehat{U}_a(x) = \widehat{V}_a(x)\widehat{W}(x),$$

as

$$\widehat{W}(x) = \begin{cases} 1, & x \in [0, L], \\ e^{i\omega\sigma_1 T(x)}, & x \in (L, L_d], \end{cases}$$

where $T(x)$ showed in (2.68) has the property $T(L) = 0$.

So, the new PAL variable V_a in time domain is

$$V_a(x, t) = \begin{cases} e^{-\sigma_0 T(x)} g(t - L), & t \geq L \\ 0, & t < L. \end{cases} \quad (4.29)$$

From above, we will have the following operator $\mathcal{L}_{subPAL}$. Using the substitution (4.26), we have the new second order equation of (4.20) in I_d :

$$\begin{aligned} \mathcal{L}_{subPAL}[V_a] = & \partial_t V_a + \frac{1}{\sigma_0 T'} \partial_{xt}^2 V_a - \frac{1}{2\sigma_0 \sigma_1 (T')^2} \partial_x^2 V_a + \frac{T''}{2\sigma_0 \sigma_1 (T')^3} \partial_x V_a \\ & + \frac{\sigma_0}{2\sigma_1} V_a. \end{aligned} \quad (4.30)$$

To convert the problem to an equivalent problem with homogeneous boundary condition at $x = 0$, we introduce

$$V(x, t) = U(x, t) + \frac{g(t)}{L}x - g(t),$$

when $x \in I$, so that

$$V(0, t) = 0, \quad V(L, t) = U(L, t). \quad (4.31)$$

Let $L^2(\bar{I})$, $\bar{I} = I \cup I_d$, be a space of integrable functions with the inner product and norm denoted by $(\cdot, \cdot)_{\bar{I}}$ and $\|\cdot\|_{\bar{I}}$ as usual. Formally, we define the bilinear form of space associated with (4.12):

$$\mathbb{B}_{\bar{I}}(U, \phi) := \mathbb{B}_I(U, \phi) + \mathbb{B}_{I_d}(U, \phi),$$

with

$$\mathbb{B}_I(U_a, \phi) := (\partial_t^2 U, \phi)_I + (\partial_x U, \partial_x \phi)_I - \partial_x U \phi \Big|_{x=L} + \partial_x U \phi \Big|_{x=0}, \quad (4.32)$$

and

$$\begin{aligned} \mathbb{B}_{I_d}(U, \phi) := & (\partial_t^2 U, \phi \frac{d\tilde{x}}{dx})_{I_d} + (\partial_x U, \partial_x \phi \frac{dx}{d\tilde{x}})_{I_d} \\ & - \partial_x U \phi \frac{dx}{d\tilde{x}} \Big|_{x=L_d} + \partial_x U \phi \frac{dx}{d\tilde{x}} \Big|_{x=L}, \end{aligned} \quad (4.33)$$

where $\frac{d\tilde{x}}{dx}$ is dependent on the transforms to generate the layer.

Remark 4.4. *Considering the coefficient functions of (4.30) in theorem before:*

$$\begin{aligned} \frac{1}{\sigma_0 T'} &= \frac{(R_2 - r)^2}{\sigma_0 (R_2 - R_1)}, \\ \frac{1}{2\sigma_0 \sigma_1 (T')^2} &= \frac{(R_2 - r)^4}{2\sigma_0 \sigma_1 (R_2 - R_1)^2}, \\ \frac{T''}{2\sigma_0 \sigma_1 (T')^3} &= \frac{(R_2 - r)^3}{\sigma_0 \sigma_1 (R_2 - R_1)^2}, \end{aligned}$$

we can find out that there is no singularity in $\mathcal{L}_{subPAL}[V_a]$.

Theorem 4.5. *The weak scheme of (4.31) is: find*

$$V \in H_0^1(I) := \{v \in H_1(I) : v(0) = 0\}$$

and

$$V_a \in H_1(I_d).$$

Then we have

$$\mathbb{B}_{\bar{I}}(U_a, \phi) = \mathcal{F}(\phi),$$

where

$$\begin{aligned} \mathbb{B}_{\bar{I}}(U_a, \phi) := & \int_0^L \partial_t^2 V \phi_1 dx + \int_0^L \partial_x V \partial_x \phi_1 dx + 2\sigma_0 \int_L^{L_d} \partial_t V_a \phi_2 dx \\ & + 2 \int_L^{L_d} \frac{1}{\hat{\sigma}(x)} \partial_{xt}^2 V_a \phi_2 dx + \int_L^{L_d} \frac{1}{\hat{\sigma}(x)} \left(\frac{1}{\hat{\sigma}(x)} \right)' \partial_x V_a \phi_2 dx \\ & + \int_L^{L_d} \frac{1}{\hat{\sigma}^2(x)} \partial_x V_a \partial_x \phi_2 dx + \sigma_0^2 \int_L^{L_d} V_a \phi_2 dx \\ & + \int_0^t (\sigma_0 \partial_x V_a(L, \tau) + \sigma_0^2 V_a(L, \tau)) e^{-\sigma_0(t-\tau)} d\tau \phi_1(L) \\ & + \partial_t V_a(L, t) \phi_1(L) - \sigma_0 V_a(L, t) \phi_1(L), \end{aligned}$$

and

$$\mathcal{F}(\phi) := \int_0^L \left(\frac{x}{L} - 1 \right) g''(t) \phi_1 dx + \frac{g}{L} \phi_1(L),$$

where $\hat{\sigma}(x) = \left(\frac{d}{L_d - x} \right)^2$, for any $\phi_1 \in L_{\omega,0}^2(I)$, $\phi_2 \in L_{\omega,0}^2(I_d)$.

Proof. From (4.18), then simplify the problem with homogeneous boundary condition, the weak form on I will be

$$\begin{aligned} \mathbb{B}_I(U_a, \phi) = & \int_0^L \partial_t^2 V(x) \phi_1(x) dx + \int_0^L \partial_x V(x) \partial_x \phi_1(x) dx \\ & - \int_0^L \left(\frac{x}{L} - 1 \right) g''(t) \phi_1(x) dx - \partial_x V(L) \phi_1(L). \end{aligned} \quad (4.34)$$

From (4.30), the weak form on I_d will be

$$\begin{aligned} \mathbb{B}_{I_d}(U_a, \phi) = & 2\sigma_0 \int_L^{L_d} \partial_t V_a(x) \phi_2(x) dx + 2 \int_L^{L_d} \frac{1}{T'} \partial_{xt}^2 V_a(x) \phi_2(x) dx \\ & - \frac{1}{\sigma_1} \int_L^{L_d} \frac{1}{(T')^2} \partial_x^2 V_a(x) \phi_2(x) dx + \frac{1}{\sigma_1} \int_L^{L_d} \frac{T''}{(T')^3} \partial_x V_a(x) \phi_2(x) dx \\ & + \frac{\sigma_0^2}{\sigma_1} \int_L^{L_d} V_a(x) \phi_2(x) dx. \end{aligned}$$

After integration by parts, we will have

$$\begin{aligned}
\mathbb{B}_{I_d}(U_a, \phi) = & 2\sigma_0 \int_L^{L_d} \partial_t V_a(x) \phi_2(x) dx + 2 \int_L^{L_d} \frac{1}{T'} \partial_{xt}^2 V_a(x) \phi_2(x) dx \\
& + \frac{1}{\sigma_1} \int_L^{L_d} \partial_x V_a(x) \partial_x \left(\frac{1}{(T')^2} \phi_2(x) \right) dx \\
& + \frac{1}{\sigma_1} \int_L^{L_d} \frac{T''}{(T')^3} \partial_x V_a(x) \phi_2(x) dx \\
& + \frac{\sigma_0^2}{\sigma_1} \int_L^{L_d} V_a(x) \phi_2(x) dx + \frac{1}{\sigma_1} \partial_x V_a(L) \partial_x \phi_2(L).
\end{aligned} \tag{4.35}$$

By flux continuity of interface $x = L$, we could find out

$$-\partial_x U_a \Big|_{x=L} + \partial_x U_a \frac{dx}{d\tilde{x}} \Big|_{x=L} = 0,$$

where $\frac{d\tilde{x}}{dx} = T'(x) \left(\sigma_1 + \frac{i}{\omega} \sigma_0 \right)$ mentioned in (4.7) before. From (4.31), to reduce the problem with homogeneous boundary condition by using

$$V = U_a + \frac{g(t)}{L} - g(t),$$

we could derive the boundary relationship on $x = L$:

$$-\partial_x V \Big|_{x=L} = -\partial_x U_a \frac{dx}{d\tilde{x}} \Big|_{x=L} - \frac{g(t)}{L}.$$

Next, take Fourier transform on it and from the variable substitution (4.26),

$$\begin{aligned}
-\partial_x \widehat{V} \Big|_{x=L} &= -\partial_x (\widehat{V}_a e^{i\omega\sigma_1}) \frac{1}{T'(\sigma_1 + \frac{i}{\omega}\sigma_0)} \Big|_{x=L} - \frac{\hat{g}(t)}{L} \\
&= -\partial_x \widehat{V}_a(L) \frac{-i\omega}{\sigma_0 - i\omega\sigma_1} + \widehat{V}_a(L) \frac{(-i\omega)^2 \sigma_1}{\sigma_0 - i\omega\sigma_1} - \frac{\hat{g}(t)}{L}
\end{aligned}$$

Next step, by inverse Fourier transform,

$$\begin{aligned}
-\partial_x V \Big|_{x=L} &= -\frac{1}{\sigma_1} \int_0^t \partial_{x\tau}^2 V_a(L, \tau) e^{-\frac{\sigma_0}{\sigma_1}(t-\tau)} d\tau + \int_0^t \partial_\tau^2 V_a(L, \tau) e^{-\frac{\sigma_0}{\sigma_1}(t-\tau)} d\tau - \frac{g(t)}{L} \\
&= -\frac{1}{\sigma_1} \partial_x V_a(L, t) + \int_0^t \left(\frac{\sigma_0}{\sigma_1^2} \partial_x V_a(L, \tau) + \frac{\sigma_0^2}{\sigma_1^2} V_a(L, \tau) \right) e^{-\frac{\sigma_0}{\sigma_1}(t-\tau)} d\tau \\
&\quad - \partial_t V_a(L, t) + \frac{\sigma_0}{\sigma_1} V_a(L, t) - \frac{g(t)}{L}.
\end{aligned}$$

Then, combining with (4.34) and (4.35), after moving the items without unknown parts to right parts, we can derive

$$\mathbb{B}_{\bar{I}}(U_a, \phi) = \mathcal{F}(\phi), \quad (4.36)$$

where

$$\begin{aligned} \mathbb{B}_{\bar{I}}(U_a, \phi) = & \int_0^L \partial_t^2 V(x) \phi_1(x) dx + \int_0^L \partial_x V(x) \partial_x \phi_1(x) dx \\ & + 2\sigma_0 \int_L^{L_d} \partial_t V_a(x) \phi_2(x) dx + 2 \int_L^{L_d} \frac{1}{T'} \partial_{xt}^2 V_a(x) \phi_2(x) dx \\ & + \frac{1}{\sigma_1} \int_L^{L_d} \frac{1}{(T')^2} \partial_x V_a(x) \partial_x \phi_2(x) dx - \frac{1}{\sigma_1} \int_L^{L_d} \frac{T''}{(T')^3} \partial_x V_a(x) \phi_2(x) dx \\ & + \frac{\sigma_0^2}{\sigma_1} \int_L^{L_d} V_a(x) \phi_2(x) dx + \int_0^t \left(\frac{\sigma_0}{\sigma_1^2} \partial_x V_a(L, \tau) + \frac{\sigma_0^2}{\sigma_1^2} V_a(L, \tau) \right) e^{-\frac{\sigma_0}{\sigma_1}(t-\tau)} d\tau \phi(L) \\ & - \partial_t V_a(L, t) \phi(L) + \frac{\sigma_0}{\sigma_1} V_a(L, t) \phi(L). \end{aligned}$$

and

$$\mathcal{F}(\phi) = \int_0^L \left(\frac{x}{L} - 1 \right) g''(t) \phi dx + \frac{g}{L} \phi(L), \quad (4.37)$$

which complete the proof. $\square$

Here, we introduce the space

$$\mathbb{X}_0^N := \{v \in C(I \cup I_d) : v|_I \in \mathbb{P}_N, v|_{I_d} \in \mathbb{P}_N, v|_I(0) = 0\}.$$

From (4.36), here is the discrete PAL reduced problem substitution: Find $v_N \in \mathbb{X}_0^N$,

$$\begin{aligned} & (\partial_t^2 v_N, \phi)_I + (\partial_x v_N, \partial_x \phi)_I + 2\sigma_0 (\partial_t v_N, \phi)_{I_d} + 2 \left(\frac{1}{T'} \partial_{xt}^2 v_N, \phi \right)_{I_d} \\ & + \frac{1}{\sigma_1} \left(\frac{1}{(T')^2} \partial_x v_N, \partial_x \phi \right)_{I_d} - \frac{1}{\sigma_1} \left(\frac{T''}{(T')^3} \partial_x v_N, \phi \right)_{I_d} + \frac{\sigma_0^2}{\sigma_1} (v_N, \phi)_{I_d} \\ & + \int_0^t \left(\frac{\sigma_0}{\sigma_1^2} \partial_x v_N(L, \tau) + \frac{\sigma_0^2}{\sigma_1^2} v_N(L, \tau) \right) e^{-\frac{\sigma_0}{\sigma_1}(t-\tau)} d\tau \phi(L) \\ & - \partial_t v_N(L, t) \phi(L) + \frac{\sigma_0}{\sigma_1} v_N(L, t) \phi(L) = \left(\left(\frac{x}{L} - 1 \right) g''(t), \phi \right)_I + \frac{g(t)}{L} \phi(L), \end{aligned} \quad (4.38)$$

In Fig 4.2, it shows errors of PAL methods, PML methods and PAL method with substitution against N with the input wave $g(t) = \sin^p(kt)$ on boundary

$x = 0$, $(T, dt) = (2, 10^{-4})$, $(L, d) = (1, 0.5)$, and $(k, p) = (10, 5)$. We can find out PAL method with substitution has much better behaviour than PML. It uses less nodes (less than 20) to reach 10^{-6} accuracy, as well as PML needs to use around 35 nodes to reach around only 10^{-4} accuracy. Next numerical example, if a point

Figure 4.2: Errors of PAL methods, PML methods and PAL method with substitution against N .

source wave $2 * \exp(-x^2/0.01)$ generate in an infinite waveguide, the left one of Fig 4.3 shows its sketches of different time from $T = 0$ to $T = 1$ by using PAL method with substitution. We can see the movement and shape of this two-way wave. The right one shows its error against N . It is clear that the error decays exponentially and reaches spectral accuracy by using only 60 nodes.

Figure 4.3: Left: Sketches of point-source wave by using PAL method with substitution; Right: Error of PAL methods with substitution of point-source wave against N .

Time Harmonic Multiple Acoustic Wave Scattering

5.1 Statement of the problem

For the numerical simulation of wave propagations in an infinite domain, a method of choice is to enclose all obstacles, and inhomogeneities (and nonlinearities at times) with an artificial boundary, where a suitable artificial boundary condition (ABC) is then imposed. This leads to a numerical solvable boundary-value problem (BVP) in a finite domain. If the solution to the reduced BVP coincides with the restriction of the solution to the original problem, then the underlying ABC is referred to as a transparent (or nonreflecting) boundary condition (TBC) (or NRBC). Hereafter, we are concerned with the circular/spherical DtN TBCs (cf. [48]) for multiple well-separated bounded scatterers.

5.1.1 General setup

Consider the time-harmonic acoustic multiple scattering problem governed by the Helmholtz equation:

$$\begin{cases} \Delta u + k^2 u = f & \text{in } \mathbb{R}^d \setminus \bar{D}, \quad d = 2, \\ u|_{\partial D} = g, \quad \lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left| \frac{\partial u}{\partial r} - iku \right| = 0, \end{cases} \quad (5.1a)$$

$$(5.1b)$$

where $k > 0$ is the wavenumber, and the far-field Sommerfeld radiation boundary condition the scattered field is purely outgoing. Here, the scatterer D consists of J well-separated, bounded sub-scatterers $\{D_j\}_{j=1}^J$, i.e., $D = \cup_{j=1}^J D_j$. Suppose that the boundary $\partial D = \cup_{j=1}^J \partial D_j$ is of Lipschitz type, and $g \in H^{1/2}(\partial D)$. Since $\{D_j\}_{j=1}^J$ are well separated, we can enclose them by non-intersecting disks/balls $\{B_j\}_{j=1}^J$ centred at $\{c_j\}_{j=1}^J$ with radius $\{R_j\}_{j=1}^J$, respectively. Figure 5.1 is an illustration of four well-separated scatterers and artificial boundaries.

Figure 5.1: Illustration of 2D multiple scatterers.

Denote

$$\begin{aligned}\Omega_j &= B_j \setminus \bar{D}_j, \quad \Omega = \cup_{j=1}^J \Omega_j; \quad \Omega_\infty^j = \mathbb{R}^d \setminus \bar{B}_j; \\ \Omega_\infty &= \cap_{j=1}^J \Omega_\infty^j = \mathbb{R}^d \setminus \bar{B}, \quad B := \cup_{j=1}^J B_j.\end{aligned}\tag{5.2}$$

Note that the finite computational domain Ω is formed by J disconnected subdomains $\{\Omega_j\}_{j=1}^J$; Ω_∞^j is the infinite domain exterior to each B_j ; and $\Omega_\infty (\subset \Omega_\infty^j)$ is the infinite domain outside all $\{B_j\}_{j=1}^J$.

To solve the multiple scattering problem (5.1), we want to derive artificial boundary conditions to surround each scatterer separately. This boundary condition must ensure that the new solution of problem with that condition in Ω must coincide with the restriction of the solution in the original unbounded region Ω_∞ .

Assume that the support of the source term f is confined in Ω . We reduce the problem of interest to find u in Ω and the outgoing fields $\{U_j \text{ along } \partial B_j\}_{j=1}^J$, such that

$$\begin{cases} \Delta u + k^2 u = f & \text{in } \Omega, \end{cases}\tag{5.3a}$$

$$\begin{cases} u = g & \text{on } \partial D, \end{cases}\tag{5.3b}$$

$$\begin{cases} u = \sum_{j=1}^J \mathcal{P}_i[U_j], \quad \frac{\partial u}{\partial \mathbf{n}} = \sum_{j=1}^J \mathcal{T}_i[U_j] & \text{on } \partial B_i, \quad i = 1, 2, \dots, J, \end{cases}\tag{5.3c}$$

where $\mathbf{n}$ is the unit outer normal vector along ∂B , and $\mathcal{P}_i$ and $\mathcal{T}_i$ are the propagation and transfer operators (cf. [48]) associated with the sub-scatterer D_i through B_i , respectively. The boundary condition (5.3c) is the DtN boundary condition for multiple scatterers.

5.1.2 Multiple circular DtN boundary conditions of circular scatterers

Consider the case of circular scatterers D_j centered at point c_j , with radius d_j . In [48], such DtN BC is derived in 2D setting. Below, we follow the spirit therein to sketch the derivation.

Let $\mathbf{r}_j$ be the position vector of a general point P with respect to the origin c_j , and the local polar coordinates: $\mathbf{r}_j = r_j(\cos \theta_j, \sin \theta_j)$ with $r_j = |\mathbf{r}_j|$ and

Figure 5.2: Local polar coordinates of scatterer i and j

$\theta_j \in [0, 2\pi)$ for $j = 1, \dots, J$. As the support of the source term f is confined in Ω . We denote $\{U_j\}$ outgoing fields in $\{\Omega_\infty^j\}_{j=1}^J$, which ignoring the other scatterers. Moreover, confined on ∂B , $\{w_j\}_{j=1}^J = \{U_j \text{ along } \partial B_j\}_{j=1}^J$. For $j = 1, \dots, J$, it is known that the exterior problem:

$$\begin{cases} \Delta U_j + k^2 U_j = 0 & \text{in } \Omega_\infty^j := \mathbb{R}^2 \setminus \bar{B}_j, \\ U_j = w_j & \text{on } \partial B_j, \\ \lim_{r_j \rightarrow \infty} \sqrt{r_j} \left| \frac{\partial U_j}{\partial r_j} - ik U_j \right| = 0, \end{cases} \quad (5.4a)$$

$$(5.4b)$$

$$(5.4c)$$

admits the unique series solution:

$$U_j(\mathbf{r}_j) = \sum_{|n|=0}^{\infty} \hat{w}_n^j \frac{H_n^{(1)}(kr_j)}{H_n^{(1)}(kR_j)} e^{in\theta_j}, \quad \hat{w}_n^j = \frac{1}{2\pi} \int_0^{2\pi} w_j e^{-in\theta_j} d\theta_j, \quad (5.5)$$

for $1 \leq j \leq J$.

The following important decomposition theorem can be shown as [48, Prop. 1].

Proposition 5.1. *Let u be the unique solution to the exterior Dirichlet problem (5.1) with $d = 2$, and impose the matching condition along ∂B :*

$$u = w_1 + \dots + w_J \quad \text{on } \partial B. \quad (5.6)$$

Then we have the unique decomposition of u in the infinite domain Ω_∞ :

$$u \equiv U_1 + \dots + U_J \quad \text{in } \Omega_\infty := \cap_{j=1}^J \Omega_\infty^j, \quad (5.7)$$

where $\{U_j\}$ are the solutions to (5.4) given by (5.5).

In view of the above, we can derive (5.3c) by requiring (5.6) and the continuity of the normal derivative across ∂B . More precisely, we have

$$\begin{aligned} u|_{\partial B_i} &= (U_1 + \cdots + U_J)|_{\partial B_i} = \sum_{j=1}^J \mathcal{P}_i[w_j], \quad \text{so } \mathcal{P}_i[w_j] = w_j(R_i, \theta_i), \\ \partial_{r_i} u|_{\partial B_i} &= \partial_{r_i} (U_1 + \cdots + U_J)|_{\partial B_i} = \sum_{j=1}^J \mathcal{T}_i[w_j], \quad \text{so } \mathcal{T}_i[w_j] = \partial_{r_i} w_j(R_i, \theta_i), \end{aligned} \quad (5.8)$$

for $1 \leq i \leq J$. It is seen from (5.5) that w_j is represented in its local polar coordinates related to B_j , but the DtN BC involves the evaluation of w_j and its derivative value in a different polar coordinates. For this purpose, let O be the origin of the global coordinate system (see, e.g., Figure 5.2), and denote

$$\mathbf{b}_{ji} = \overrightarrow{c_j c_i} = b_{ji}(\cos \beta_{ji}, \sin \beta_{ji}) = -\mathbf{b}_{ij}, \quad b_{ji} = |\mathbf{b}_{ji}| = |\mathbf{b}_{ij}|, \quad (5.9)$$

(note: $b_{ij} = b_{ji}$ and $b_{ii} = 0$), so we have $\mathbf{r}_j = \mathbf{r}_i + \mathbf{b}_{ji}$, or equivalently,

$$r_j \cos \theta_j = r_i \cos \theta_i + b_{ji} \cos \beta_{ji}, \quad r_j \sin \theta_j = r_i \sin \theta_i + b_{ji} \sin \beta_{ji}, \quad (5.10)$$

$$r_j = \sqrt{r_i^2 + 2r_i b_{ji} \cos(\theta_i - \beta_{ji}) + b_{ji}^2}, \quad (5.11)$$

This shows the connection between local coordinates. Moreover, we have the following rules for computing the partial derivatives, to be used in formulating (5.8) in Fourier series.

Proposition 5.2. *For $1 \leq i, j \leq J$ and $i \neq j$, we have*

$$\frac{\partial r_j}{\partial r_i} = \frac{1}{r_j} \{r_i + b_{ji} \cos(\theta_i - \beta_{ji})\}, \quad \frac{\partial \theta_j}{\partial r_i} = \frac{b_{ji}}{r_j^2} \sin(\theta_i - \beta_{ji}). \quad (5.12)$$

Proof. The rule for $\partial r_j / \partial r_i$ is a direct consequence of (5.11). It remains to derive the latter. One verifies readily from (5.10) and the trigonometric identities that

$$r_j \sin(\theta_j - \beta_{ji}) = r_i \sin(\theta_i - \beta_{ji}), \quad r_j \cos(\theta_j - \beta_{ji}) = r_i \cos(\theta_i - \beta_{ji}) + b_{ji}. \quad (5.13)$$

Taking partial derivative with respect to r_i leads to

$$\begin{aligned}\sin(\theta_j - \beta_{ji}) \frac{\partial r_j}{\partial r_i} + r_j \cos(\theta_j - \beta_{ji}) \frac{\partial \theta_j}{\partial r_i} &= \sin(\theta_i - \beta_{ji}), \\ \cos(\theta_j - \beta_{ji}) \frac{\partial r_j}{\partial r_i} - r_j \sin(\theta_j - \beta_{ji}) \frac{\partial \theta_j}{\partial r_i} &= \cos(\theta_i - \beta_{ji}).\end{aligned}$$

Multiplying the first (resp. second) equation by $\cos(\theta_j - \beta_{ji})$ (resp. $-\sin(\theta_j - \beta_{ji})$), and summing up the resulted equations, we obtain from (5.10) that

$$\begin{aligned}r_j \frac{\partial \theta_j}{\partial r_i} &= \sin(\theta_i - \beta_{ji}) \cos(\theta_j - \beta_{ji}) - \cos(\theta_i - \beta_{ji}) \sin(\theta_j - \beta_{ji}) \\ &= \sin(\theta_i - \theta_j) = \sin \theta_i \cos \theta_j - \sin \theta_j \cos \theta_i \\ &= \frac{1}{r_j} \sin \theta_i (r_i \cos \theta_i + b_{ji} \cos \beta_{ji}) - \frac{1}{r_j} \cos \theta_i (r_i \sin \theta_i + b_{ji} \sin \beta_{ji}) \\ \frac{\partial \theta_j}{\partial r_i} &= \frac{b_{ji}}{r_j^2} \sin(\theta_i - \beta_{ji}).\end{aligned}$$

This ends the proof. $\square$

Before derive the formulation of the operator in (5.3c), we first introduce the following addition theorems in 2D.

Theorem 5.1. (Neumann's addition theorem)

$$J_0(kr_j) = \sum_{|n|=0}^{\infty} (-1)^n J_n(kb_{ji}) J_n(kr_i) e^{in(\theta_i - \beta_{ji})}, \text{ for } j \neq i. \quad (5.14)$$

Theorem 5.2. (Graf's addition theorem for $J_m(kr)e^{im\theta}$) For $m = 0, \pm 1, \pm 2, \dots$, and $j \neq i$, we have

$$\begin{aligned}J_m(kr_j) e^{im\theta_j} &= \sum_{|n|=0}^{\infty} J_n(kb_{ji}) e^{in\beta_{ji}} J_{m-n}(kr_i) e^{i(m-n)\theta_i} \\ &= \sum_{|n|=0}^{\infty} J_{m-n}(kb_{ji}) e^{i(m-n)\beta_{ji}} J_n(kr_i) e^{in\theta_i}.\end{aligned} \quad (5.15)$$

This is a special case of an addition theorem published by Graf in 1893. Graf's theorem gives an expansion for $J_\nu(kr_j) e^{i\nu\theta_j}$ with arbitrary complex ν .

Theorem 5.3. (Graf's addition theorem for $H_m^{(1)}(kr)e^{im\theta}$) For $m = 0, \pm 1, \pm 2, \dots$, and $j \neq i$, we have

$$H_m^{(1)}(kr_j)e^{im\theta_j} = \sum_{|n|=0}^{\infty} H_{m-n}^{(1)}(kb_{ji})e^{i(m-n)\beta_{ji}} J_n(kr_i)e^{in\theta_i} \quad (5.16)$$

for $r_i < b_{ji}$, and

$$H_m^{(1)}(kr_j)e^{im\theta_j} = \sum_{|n|=0}^{\infty} J_{m-n}(kb_{ji})e^{i(m-n)\beta_{ji}} H_n^{(1)}(kr_i)e^{in\theta_i} \quad (5.17)$$

for $r_i > b_{ji}$.

Proposition 5.3. The operators in the circular DtN BC (5.3c) are given by

- For $i = 1, \dots, J$,

$$\begin{aligned} \mathcal{P}_i(w_i) &= w_i, \\ \mathcal{T}_i(w_i) &= \sum_{|n|=0}^{\infty} \widehat{w}_n^i \frac{kH_n^{(1)'}(kR_i)}{H_n^{(1)}(kR_i)} e^{in\theta_i}. \end{aligned} \quad (5.18)$$

- For $j = 1, \dots, J$, and $j \neq i$,

$$\begin{aligned} \mathcal{P}_i(w_j) &= \sum_{|n|=0}^{\infty} \widehat{w}_n^j \frac{H_n^{(1)}(kr_j(R_i, \theta_i))}{H_n^{(1)}(kR_j)} e^{in\theta_j} \\ &= \sum_{|n|=0}^{\infty} \sum_{|m|=0}^{\infty} \widehat{w}_m^j \frac{H_{m-n}^{(1)}(kb_{ji})}{H_m^{(1)}(kR_j)} e^{i(n-m)\beta_{ji}} J_n(kR_i)e^{in\theta_i}, \\ \mathcal{T}_i(w_j) &= \sum_{|n|=0}^{\infty} \widehat{w}_n^j \frac{kH_n^{(1)'}(kr_j(R_i, \theta_i))}{H_n^{(1)}(kR_j)} \frac{\partial r_j(R_i, \theta_i)}{\partial r_i} e^{in\theta_j} \\ &\quad + \sum_{|n|=0}^{\infty} \widehat{w}_n^j \frac{inH_n^{(1)}(kr_j(R_i, \theta_i))}{H_n^{(1)}(kR_j)} \frac{\partial \theta_j}{\partial r_i} e^{in\theta_j}, \\ &= k \sum_{|n|=0}^{\infty} \sum_{|m|=0}^{\infty} \widehat{w}_m^j \frac{H_{m-n}^{(1)}(kb_{ji})}{H_m^{(1)}(kR_j)} e^{i(n-m)\beta_{ji}} J'_n(kR_i)e^{in\theta_i} \end{aligned} \quad (5.19)$$

where $\widehat{w}_n^j$ is the extension coefficients of w_j .

Proof. By proposition 5.1, we could decompose u by

$$u = U_1 + \dots + U_J \quad \text{in} \quad \partial B \cup \Omega_\infty \quad (5.20)$$

to solve the Helmholtz equation with Sommerfeld radiation condition at infinity.

As a consequence of the proposition, we can now explicitly determine a DtN map for u by differentiating u as follows, for $i, j = 1, \dots, J, j \neq i$:

$$u = U_i|_{\partial B_i} + U_j|_{\partial B_i}, \quad \partial_{r_i} u = \partial_{r_i} U_i|_{\partial B_i} + \partial_{r_i} U_j|_{\partial B_i}, \quad \text{on } \partial B_i. \quad (5.21)$$

Then, on ∂B_i , we want to putting Graf's additional theorem for $H_n^{(1)}(kr)e^{in\theta}$ on,

$$\begin{aligned} u &= U_i|_{\partial B_i} + U_j|_{\partial B_i} \\ &= \sum_{|n|=0}^{\infty} \widehat{w}_n^i \frac{H_n^{(1)}(kR_i)}{H_n^{(1)}(kR_i)} e^{in\theta_i} + \sum_{|n|=0}^{\infty} \widehat{w}_n^j \frac{H_n^{(1)}(kr_j(R_i, \theta_i))}{H_n^{(1)}(kR_j)} e^{in\theta_j} \\ &= w_i + \sum_{|n|=0}^{\infty} \sum_{|m|=0}^{\infty} \widehat{w}_n^j \frac{H_{n-m}^{(1)}(k\mathbf{b}_{ji})}{H_n^{(1)}(kR_j)} e^{i(m-n)\beta_{ji}} J_m(kR_i) e^{im\theta_i}, \\ \partial_{r_i} u &= \partial_{r_i} U_i|_{\partial B_i} + \partial_{r_i} U_j|_{\partial B_i} \\ &= \sum_{|n|=0}^{\infty} \widehat{w}_n^i \frac{kH_n^{(1)'}(kR_i)}{H_n^{(1)}(kR_i)} e^{in\theta_i} + \sum_{|n|=0}^{\infty} \widehat{w}_n^j \frac{inH_n^{(1)}(kr_j(R_i, \theta_i))}{H_n^{(1)}(kR_j)} \frac{\partial \theta_j}{\partial r_i} e^{in\theta_j} \\ &\quad + \sum_{|n|=0}^{\infty} \widehat{w}_n^j \frac{kH_n^{(1)'}(kr_j(R_i, \theta_i))}{H_n^{(1)}(kR_j)} \frac{\partial r_j(R_i, \theta_i)}{\partial r_i} e^{in\theta_j} \\ &= \sum_{|n|=0}^{\infty} \widehat{w}_n^i \frac{kH_n^{(1)'}(kR_i)}{H_n^{(1)}(kR_i)} e^{in\theta_i} \\ &\quad + \sum_{|n|=0}^{\infty} \sum_{|m|=0}^{\infty} \widehat{w}_n^j \frac{H_{n-m}^{(1)}(k\mathbf{b}_{ji})}{H_n^{(1)}(kR_j)} e^{i(m-n)\beta_{ji}} kJ'_m(kR_i) e^{im\theta_i}. \end{aligned}$$

We define $\mathcal{P}_i(w_i) = U_i|_{\partial B_i}$, $\mathcal{P}_i(w_j) = U_j|_{\partial B_i}$, and $\mathcal{T}_i(w_i) = \partial_{r_i} U_i|_{\partial B_i}$, $\mathcal{T}_i(w_j) = \partial_{r_i} U_j|_{\partial B_i}$. Finally, after changing the order of m, n of the derivative part, we can get the information of the operators. $\square$

After taking Fourier expansion,

$$w(r, \theta) = \sum_{n \in \mathbb{Z}} \widehat{w}_n(r) e^{in\theta} \quad \text{with} \quad \widehat{w}_n(r) \in L^2(\mathbb{R}^2),$$

which

$$\widehat{w}_n(r) = \frac{1}{2\pi} \int_0^{2\pi} w(r, \theta) e^{-in\theta} d\theta.$$

Denote $\mathcal{P}_n$ and $\mathcal{T}_n$ are n -th terms of Fourier expansion of $\mathcal{P}$ and $\mathcal{T}$:

- For $i = 1, \dots, J$,

$$\begin{aligned} \mathcal{P}_n^i(\widehat{w}_n^i) &= \widehat{w}_n^i, \\ \mathcal{T}_n^i(\widehat{w}_n^i) &= \widehat{w}_n^i \frac{k H_n^{(1)'}(kR_i)}{H_n^{(1)}(kR_i)}. \end{aligned} \quad (5.22)$$

- For $j = 1, \dots, J$, and $j \neq i$,

$$\begin{aligned} \mathcal{P}_n^i(\widehat{w}_n^j) &= \sum_{|m|=0}^{\infty} \widehat{w}_m^j \frac{H_{m-n}^{(1)}(k\mathbf{b}_{ji})}{H_m^{(1)}(kR_j)} e^{i(n-m)\beta_{ji}} J_n(kR_i), \\ \mathcal{T}_n^i(\widehat{w}_n^j) &= k \sum_{|m|=0}^{\infty} \widehat{w}_m^j \frac{H_{m-n}^{(1)}(k\mathbf{b}_{ji})}{H_m^{(1)}(kR_j)} e^{i(n-m)\beta_{ji}} J'_n(kR_i). \end{aligned} \quad (5.23)$$

Then, (5.3) will reduce to the following 1D problem in each scatterer i , for $n \in \mathbb{Z}$:

$$\left\{ \begin{aligned} \frac{1}{r} \frac{d}{dr} \left(r \frac{d\widehat{u}_n^i}{dr} \right) + \left(k^2 - \frac{n^2}{r} \right) \widehat{u}_n^i &= \widehat{f}_n \quad r \in I := (d_i, R_i), \end{aligned} \right. \quad (5.24a)$$

$$\widehat{u}_n^i = \widehat{g}_n \quad \text{on } r = d_i, \quad (5.24b)$$

$$\left\{ \begin{aligned} \widehat{u}_n^i &= \sum_{j=1}^J \mathcal{P}_n^i(\widehat{w}_n^j), \quad \frac{\partial \widehat{u}_n^i}{\partial \mathbf{n}} = \sum_{j=1}^J \mathcal{T}_n^i(\widehat{w}_n^j) \quad \text{on } r = R_i, \end{aligned} \right. \quad (5.24c)$$

where $i = 1, 2, \dots, J$, $\widehat{u}_n^i$, $\widehat{g}_n$ and $\widehat{f}_n$ are Fourier expansions of u^i , g and f , respectively.

5.2 Variation problem and spectral discretization

For simplifying the discretization, we rewrite problem (5.24) by denoting $u_n^i = \widehat{u}_n^i - \widehat{g}_n$:

$$\begin{cases} \frac{1}{r} \frac{d}{dr} \left(r \frac{du_n^i}{dr} \right) + \left(k^2 - \frac{n^2}{r} \right) u_n^i = \widehat{f}_n + \left(k^2 - \frac{n^2}{r} \right) \widehat{g}_n & r \in I, \end{cases} \quad (5.25a)$$

$$\begin{cases} u_n^i = 0 & \text{on } r = d_i, \end{cases} \quad (5.25b)$$

$$\begin{cases} u_n^i = \sum_{j=1}^J \mathcal{P}_n^i(\widehat{w}_n^j) - \widehat{g}_n, & \frac{\partial u_n^i}{\partial \mathbf{n}} = \sum_{j=1}^J \mathcal{T}_n^i(\widehat{w}_n^j) & \text{on } r = R_i, \end{cases} \quad (5.25c)$$

where $i = 1, 2, \dots, J$.

In this section, we derive the variational problem of (5.25) and then introduce the spectral element discretization. We introduce the function spaces:

$$\mathcal{V}_0 = \{v \in H^1(I) : v|_{r=d_i, i=1, \dots, J} = 0\}. \quad (5.26)$$

For each scatterer i , find $u_n^i \in \mathcal{V}_0$ and $w_n^i \in \mathbb{R}$,

$$\begin{cases} -\left(r(u_n^i)'\right)_I + \left((k^2 r^2 - n^2) u_n^i\right)_I + R_i^2 \langle \mathcal{T}_n^i(w_n^i), v_n \rangle_{\partial B_i} = \\ -R_i^2 \sum_{j=1, j \neq i}^J \langle \mathcal{T}_n^i(w_n^j), v_n \rangle_{\partial B_i} + (r^2 \widehat{f}_n)_I + \left((k^2 r - n^2) \widehat{g}_n\right)_I, \end{cases} \quad (5.27a)$$

$$\begin{cases} \langle u_n^i, v_{w,n} \rangle_{\partial B_i} - \langle \mathcal{P}_n^i(w_n^i), v_{w,n} \rangle_{\partial B_i} = \sum_{j=1, j \neq i}^J \langle \mathcal{P}_n^i(w_n^j), v_{w,n} \rangle_{\partial B_i} \\ - \langle \widehat{g}_n, v_{w,n} \rangle_{\partial B_i}, & \text{on } \partial B_i, \end{cases} \quad (5.27b)$$

$$\begin{cases} \langle u_n^i, v_n \rangle_{\partial D_i} = 0, & \text{on } \partial D_i, \end{cases} \quad (5.27c)$$

where $i = 1, 2, \dots, J$, for all $v_n \in \mathcal{V}_0$, $v_{w,n} \in \mathbb{R}$.

5.2.1 Spectral-Galerkin approximation

We consider the approximation by using Galerkin method in polynomial space for each scatterer,

$$\mathcal{V}_{N_p} = \{u_{N_p} \in \mathcal{V}_0 : u_{N_p} \in \mathbb{P}_{N_p}(\widehat{I})\}, \quad \mathcal{W}_{N_p} = \{w_{N_p} \in \mathbb{R}\}.$$

Here, $N_p = N_I + 2$, $\mathbb{P}_{N_p}$ is the polynomial basis space of N_I degree and add two liner functions on the boundary points. Also, $\hat{I} = [-1, 1]$ is the normal domain mapped from $r \in [d_i, R_i]$.

The modal basis functions $\{\phi_k\}_{k=0}^{N_p} \subset \mathcal{V}_{N_p}$, and

$$u_n^i = \sum_{k=0}^{N_p} u_{n,k} \phi_k(\xi), \quad \xi \in [-1, 1], \quad \text{as} \quad r = \frac{R_i - d_i}{2} \xi + \frac{R_i + d_i}{2},$$

where $i = 1, 2, \dots, J$,

$$\phi_k(\xi) = \begin{cases} L_k(\xi) - L_{k+2}(\xi), & k = 0, \dots, N_p - 2, \quad \text{in } I_i \\ \frac{1 - \xi}{2}, & k = N_p - 1, \quad \text{on } \partial D_i \\ \frac{1 + \xi}{2}, & k = N_p, \quad \text{on } \partial B_i \end{cases},$$

$L_k(\xi)$ are Legendre polynomials. From the properties of Legendre polynomials in [80], we will have

$$\phi'_k(\xi) = \begin{cases} -(2k+3)L_{k+1}, & k = 0, \dots, N_p - 2, \quad \text{in } I_i \\ -\frac{1}{2}, & k = N_p - 1, \quad \text{on } \partial D_i \\ \frac{1}{2}, & k = N_p, \quad \text{on } \partial B_i \end{cases},$$

where $i = 1, 2, \dots, J$.

We denote by u_I^n the values of the spectral solution on I_i , by $u_{\partial B}^n$ its values on ∂B_i , by $u_{\partial D}^n$ its values on ∂D_i and by w^n the values of w_n^i on ∂B_i , which yields from (5.27) the following linear system of equations

$$\left(\begin{array}{ccc|c} \mathbb{K}^I & K_{12} & K_{13} & 0 \\ 0 & 1 & 0 & 0 \\ K_{31} & K_{32} & K_{33} & \mathbb{T} \\ \hline 0 & 0 & \mathbb{I} & \mathbb{P} \end{array} \right) \begin{pmatrix} u_I^n \\ u_{\partial D}^n \\ u_{\partial B}^n \\ w^n \end{pmatrix} = \begin{pmatrix} \mathbb{F}^I \\ 0 \\ \mathbb{F}^{\partial B} \\ \mathbb{G} \end{pmatrix}. \quad (5.28)$$

To explain each part in this linear System (5.28), first denote $a = \frac{R_i - d_i}{2}$,

$b = \frac{R_i + d_i}{2}$, the entries are given by

$$\begin{aligned}
K_{ij}^I &= -(r(\phi_j)', \phi_i)_I - (r(\phi_j)', r(\phi_i)')_I + ((k^2 r^2 - n^2) \phi_j, \phi_i)_I, \\
&\quad i = 0, \dots, N_p - 2, \quad j = 0, \dots, N_p - 2, \\
K_{12} &= -(r(\phi_{N_p-1}', \phi_i)_I - (r(\phi_{N_p-1}', r(\phi_i)')_I + ((k^2 r^2 - n^2) \phi_{N_p-1}, \phi_i)_I, \\
&\quad i = 0, \dots, N_p - 2, \\
K_{13} &= -(r(\phi_{N_p}', \phi_i)_I - (r(\phi_{N_p}', r(\phi_i)')_I + ((k^2 r^2 - n^2) \phi_{N_p}, \phi_i)_I, \\
&\quad i = 0, \dots, N_p - 2, \\
K_{31} &= -(r(\phi_j)', \phi_{N_p})_I - (r(\phi_j)', r(\phi_{N_p})')_I + ((k^2 r^2 - n^2) \phi_j, \phi_{N_p})_I, \\
&\quad j = 0, \dots, N_p - 2, \\
K_{32} &= -(r(\phi_{N_p-1}', \phi_{N_p})_I - (r(\phi_{N_p-1}', r(\phi_{N_p})')_I + ((k^2 r^2 - n^2) \phi_{N_p-1}, \phi_{N_p})_I, \\
K_{33} &= -(r(\phi_{N_p}', \phi_{N_p})_I - (r(\phi_{N_p}', r(\phi_{N_p})')_I + ((k^2 r^2 - n^2) \phi_{N_p}, \phi_{N_p})_I,
\end{aligned}$$

details about above elements shown in Appendix A.3. What is more,

$$\begin{aligned}
T &= R_i^2 \langle \mathcal{T}_n^i, \phi_{N_p} \rangle_{\partial B_i}, \\
I &= \langle \phi_{N_p}, 1 \rangle_{\partial B_i} \\
P &= -\langle \mathcal{P}_n^i, 1 \rangle_{\partial B_i}, \\
F_i^I &= (r^2 \hat{f}_n, \phi_i)_I + ((k^2 r - n^2) \hat{g}_n, \phi_i)_I, \\
F^{\partial B} &= -R_i^2 \sum_{j=1, j \neq i}^J \mathcal{T}_n^i(w_n^j), \\
G &= \sum_{j=1, j \neq i}^J \mathcal{P}_n^i(w_n^j) - \hat{g}_n.
\end{aligned}$$

5.3 Numerical iteration method for two scatterers

In this section, we give an example of two scatterers ($J = 2$) to introduce the numerical iterative algorithm about multiple scattering problems. The linear system (5.28) requires to solve a large and coupled equation for more than one

scatterers. We present an efficient iterative method, which can decouple the problem, simplify the linear system, and reduce the computation complexity.

5.3.1 Iteration method

Denote $u_n^{j,(t)}$ and $w_n^{j,(t)}$ are the t -th step values of scatterer j in the iterative process. Given the initial guess $w_n^{2,(0)}$, as known information of the following problem. From (5.27), we could have u_n^1 of the first step ($t = 1$) by solving the variational problem

$$\begin{cases} -\left(r(u_n^{1,(1)})', (v_n + rv_n')\right)_I + \left((k^2 r^2 - n^2) u_n^{1,(1)}, v_n\right)_I + R_1^2 \langle \mathcal{T}_n^1(w_n^{1,(1)}), v_n \rangle_{\partial B_1} = \\ \quad -R_1^2 \langle \mathcal{T}_n^1(w_n^{2,(0)}), v_n \rangle_{\partial B_1} + (r^2 \hat{f}_n, v_n)_I + \left((k^2 r - n^2) \hat{g}_n, v_n\right)_I, \\ \langle u_n^{1,(1)}, v_{w,n} \rangle_{\partial B_1} - \langle \mathcal{P}_n^1(w_n^{1,(1)}), v_{w,n} \rangle_{\partial B_1} = \langle \mathcal{P}_n^1(w_n^{2,(0)}), v_{w,n} \rangle_{\partial B_1} - \langle \hat{g}_n, v_{w,n} \rangle_{\partial B_1}, \\ \langle u_n^{1,(1)}, v_n \rangle_{\partial D_1} = 0. \end{cases}$$

Then, after solving this problem by using the linear system (5.28), $w_n^{1,(1)}$ will be the known information for the following variational problem of first step value $u_n^{2,(1)}$ in scatterer 2.

$$\begin{cases} -\left(r(u_n^{2,(1)})', (v_n + rv_n')\right)_I + \left((k^2 r^2 - n^2) u_n^{2,(1)}, v_n\right)_I + R_2^2 \langle \mathcal{T}_n^2(w_n^{2,(1)}), v_n \rangle_{\partial B_2} = \\ \quad -R_2^2 \langle \mathcal{T}_n^2(w_n^{1,(1)}), v_n \rangle_{\partial B_2} + (r^2 \hat{f}_n, v_n)_I + \left((k^2 r - n^2) \hat{g}_n, v_n\right)_I, \\ \langle u_n^{2,(1)}, v_{w,n} \rangle_{\partial B_2} - \langle \mathcal{P}_n^2(w_n^{2,(1)}), v_{w,n} \rangle_{\partial B_2} = \langle \mathcal{P}_n^2(w_n^{1,(1)}), v_{w,n} \rangle_{\partial B_2} - \langle \hat{g}_n, v_{w,n} \rangle_{\partial B_2}, \\ \langle u_n^{2,(1)}, v_n \rangle_{\partial D_2} = 0. \end{cases}$$

Then, we solve the problem and get the 1-st iteration result $u_n^{2,(1)}$ in scatterer 2. Then, set $w_n^{2,(1)}$ as the known condition of next iteration step. Iterate this process to T -th step, since norm $\|w_n^{i,(T)} - w_n^{i,(T-1)}\|$, $i = 1$ or 2 , satisfies condition

$$\|w_n^{i,(T)} - w_n^{i,(T-1)}\| \leq \varepsilon, \quad (5.31)$$

for some decided $\varepsilon > 0$.

5.3.2 Numerical examples

In this section, we use plane wave $\sum_{|n|=0}^{\infty} i^n e^{in(\theta-\theta_0)} J_n(kr)$ as an incident wave, i.e., the data $g = -\sum_{|n|=0}^{\infty} i^n e^{in(\theta-\theta_0)} J_n(kr)$, to test the proposed numerical method. Here θ_0 is the incident angle and k is the given propagation wavenumber.

Compared with T -Matrix method in [88]

The solution of multiple scattering problems consists of combining the T -matrices for each individual scatterer in the ensemble in a large linear system. So, there is no iteration inside this method. However, when J is large, which means there are several scatterers in the domain, linear system in [88] would be expensive to simulate both in time-spending and space-spending. We just use T -Matrix method to compare with ours in two scatterers case. First, denote $N = N_p$.

Example 1 (Two cylindrical scatters) The scatter $D = D_1 \cup D_2$ consists of two cylindrical scatters centered at point $O_1(-1.5, 0)$ and $O_2(1.5, 0)$ of radius $d_1 = d_2 = 0.5$. During the iteration process, set the initial value $w_n^{2,(0)} = 0$ and $\varepsilon = 10^{-14}$ in (5.31), and the iteration number is 16. The scattering fields computed by the proposed numerical method are depicted in Figure 5.3. Error between spectral method and T -matrix method shows in Figure 5.4.

Example 2 (Two cylindrical scatters) The scatter $D = D_1 \cup D_2$ consists of two cylindrical scatters centered at point $O_1(-1.5, -0.5)$ and $O_2(1.5, 0)$ of radius $d_1 = d_2 = 0.5$. During the iteration process, set the initial value $w_n^{2,(0)} = 0$ and $\varepsilon = 10^{-14}$ in (5.31), and the iteration number is 16. The scattering fields computed by the proposed numerical method are depicted in Figure 5.5. Error between spectral method and T -matrix method shows in Figure 5.6.

Example 3 (Two cylindrical scatters) The scatter $D = D_1 \cup D_2$ consists of two cylindrical scatters centered at point $O_1(-1.5, -0.5)$ and $O_2(1.5, 0)$ of radius $d_1 = d_2 = 0.5$. During the iteration process, set the initial value $w_n^{2,(0)} = 0$ and $\varepsilon = 10^{-14}$ in (5.31), and the iteration number is 16. The scattering fields

Figure 5.3: Scattering fields of two cylindrical scatterers with $k = 20$, $\theta_0 = \pi/2$.

Figure 5.4: Error compared with T -matrix method $k = 20$, $\theta_0 = \pi/2$.

computed by the proposed numerical method are depicted in Figure 5.7. Error between spectral method and T -matrix method shows in Figure 5.8.

Example 4 (Two cylindrical scatterers) The scatter $D = D_1 \cup D_2$ consists of two cylindrical scatterers centered at point $O_1(-1.5, 0)$ and $O_2(1.5, 0)$ of radius $d_1 = d_2 = 0.5$. Angle θ_0 of the incident wave is $\pi/2$. During the iteration process, set $\varepsilon = 10^{-14}$ in (5.31). The following table shows that the error and iteration number will not influenced a lot by different initial value $w_n^{2,(0)}$ and wavenumber k . For big enough N , in Table 5.1, E means the L_2 error compared with T -matrix,

Figure 5.5: Scattering fields of two cylindrical scatters with $k = 50$, $\theta_0 = 4\pi/3$.

Figure 5.6: Error compared with T -matrix method $k = 50$, $\theta_0 = 4\pi/3$.

and $\widehat{N}$ denotes the iteration number.

Example 5 (Five cylindrical scatters) The scatter D consists of five cylindrical scatters centered at point $O_1(-4, 1)$, $O_2(3, 0)$, $O_3(6, 4)$, $O_4(0, -3)$ and $O_5(0, 5)$ of radius $d = 0.5$. During the iteration process, set the initial value $w_0 = 0$ and $\varepsilon = 10^{-14}$ in (5.31), and the iteration number is 37. The scattering fields computed by the proposed numerical method are depicted in Figure 5.9.

Example 6 (Ten cylindrical scatters) The scatter D consists of ten cylindrical scatters centered at point $O_1(-4, 1)$, $O_2(3, 0)$, $O_3(6, 4)$, $O_4(0, -3)$, $O_5(0, 5)$,

Figure 5.7: Scattering fields of two cylindrical scatterers with $k = 50$, $\theta_0 = 4\pi/3$.

Figure 5.8: Error compared with T -matrix method $k = 50$, $\theta_0 = 4\pi/3$.

$O_6(0, -7.5)$, $O_7(7, 8)$, $O_8(6, -6)$, $O_9(-5, -5)$, and $O_{10}(-4, 6)$ of radius $d = 0.5$. During the iteration process, set the initial value $w_0 = 0$ and $\varepsilon = 10^{-14}$ in (5.31), and the iteration number is 70. The scattering fields computed by the proposed numerical method are depicted in Figure 5.10.

Table 5.1: L_2 error E compared with T -matrix, and iteration number $\widehat{N}$ in different k and w_0

	$k = 20$		$k = 30$		$k = 40$		$k = 50$		$k = 60$	
$w_0 \backslash$	E	$\widehat{N}$	E	$\widehat{N}$	E	$\widehat{N}$	E	$\widehat{N}$	E	$\widehat{N}$
0	$5.1e - 13$	16	$5.2e - 13$	16	$3.8e - 13$	16	$5.6e - 13$	16	$6.7e - 13$	16
0.1	$5.1e - 13$	16	$5.0e - 13$	16	$3.8e - 13$	16	$6.1e - 13$	15	$6.7e - 13$	16
1	$5.1e - 13$	16	$5.1e - 13$	16	$3.7e - 13$	16	$5.8e - 13$	16	$6.7e - 13$	16
10	$5.1e - 13$	16	$5.0e - 13$	16	$3.8e - 13$	16	$5.7e - 13$	16	$6.6e - 13$	16

Figure 5.9: Scattering fields of five cylindrical scatters with $k = 30$, $\theta_0 = \pi/2$.

Figure 5.10: Scattering fields of ten cylindrical scatters with $k = 30$, $\theta_0 = \pi/2$.

Conclusion and Future Works

We conclude the thesis with a summary of the work done and present some relevant topics for further investigation.

6.1 Conclusion

In this thesis, we developed a new domain reduction technique, called perfect absorbing layer (PAL), as a viable and more advantageous alternative to the usual PML technique for wave scattering problems. We mainly elaborated on the construction in the two-dimensional time-harmonic setting, but the idea can be extended to three dimensions. We conducted the wavenumber explicit analysis for the circular PAL, which provided more insights into this new techniques. We also discussed the extensions to the time domain and multiple scatterers. Below, we give more details on the contributions in each chapter.

- In Chapter 2, we constructed a perfect absorbing layer (PAL), which is shown truly exact and optimal for domain truncation of the exterior Helmholtz problems. This technique integrated two essential components: (i) the complex compression coordinate transformation; and (ii) suitable substitution of the unknown field. The advantages reside in that the field to be approximated is well-behaved in the layer, requiring very few grid points to resolve

even for high wavenumber and thin layer. The geometry of the layer can be general star-shaped so it is flexible to enclose scatterers of general shape.

- In Chapter 3, we conducted the wavenumber explicit analysis for the circular PAL, where the argument is very different from the usual one based on the Rellich's identities using two different test functions. The obtained results have deep insights into the PAL technique.
- In Chapter 4, we extended the PAL in the frequency domain to the time domain using the Fourier transforms and the complex compression coordinate transformation in the Fourier domain. We also incorporate the frequency domain substitution into the construction of time-domain PAL, which appears necessary when the initial input is highly oscillatory.
- In Chapter 5, we discussed the solution of multiple scattering problems, where the emphasis was put on the decoupling of multiple scattering problems into single scattering problems. This was accomplished by the DtN NRBC as in Grote-Kirsch's method, and a suitable iterative solver together with spectral solvers for single scattering problems.

6.2 Future works

The construction of the PAL technique sets a good example to show the integration of numerical and analytic tools can lead to new findings. Indeed, in the polar/spherical coordinates, the outgoing waves have the Fourier/spherical/vector spherical harmonic expressions, so performing the compression coordinate transform (in the radial direction) on the outgoing waves can well separate the oscillatory and singular factors (which is the basis for the substitution used in the PAL). This is the key to the success of this technique. Note that the PML technique is usually constructed in the Cartesian coordinates. The idea and methodology can be further explored at least in the following directions beyond this thesis.

-
- (i) *PAL in three dimensions.* In this thesis, we focused on two-dimensional construction, but the idea can be extended to three dimension in both frequency and time domains. In particular, the study of the Maxwell's equation will be feasible (based on the vector spherical harmonic expansions of the outgoing waves), but much more involved.
 - (ii) *PAL for elastic waves.* There has been much recent interest in the simulation of the elastic waves, where the coupling of wave components will add some difficulty for the PAL construction.
 - (iii) *Multiple scattering with PAL truncation.* The PAL technique has advantages in the adaption to general geometry of the shape of scatterers and the use of very few grid points to resolve the damped waves in the thin layer. Therefore, it is promising to replace the DtN truncation in multiple scattering simulations. However, how to efficiently deal with the interaction of scatterers in this context will be the critical issue to explore.

Appendix

A.1 Proof of Theorem 2.1

For clarity, we first consider (2.1) with $g(y) = \hat{g}_l \sin(l y)$, and then apply the principle of superposition to obtain (2.10). Note that by (2.3), the exact solution of (2.1) is

$$U_l(x, y) = \hat{g}_l e^{i k_l x} \sin(l y), \quad (\text{A.1})$$

and the PML-solution of (2.7)-(2.8) is

$$U_{p,l}(x, y) = \frac{e^{i k_l (S_d - S)} - e^{-i k_l (S_d - S)}}{e^{i k_l S_d} - e^{-i k_l S_d}} \hat{g}_l \sin(l y). \quad (\text{A.2})$$

In fact, one verifies directly that (A.2) satisfies the PML-equation (2.7) and all conditions in (2.9)-(2.8). Since $S(x) = x$ for $x \in (0, L)$, we find

$$U_{p,l}(x, y) = \frac{e^{i k_l (S_d - 2x)} - e^{-i k_l S_d}}{e^{i k_l S_d} - e^{-i k_l S_d}} U_l(x, y) = (1 - R_l(x)) U_l(x, y), \quad (\text{A.3})$$

$\forall (x, y) \in \Omega$, where the representation of $R_l(x)$ in (2.10) can be obtained straightforwardly. Thanks to the identity (A.3), we derive from the principle of superposition, (2.3) and (A.1) that the PML-solution in Ω is given by

$$U_p(x, y) = \sum_{l=1}^{\infty} U_{p,l}(x, y) = U(x, y) - \sum_{l=1}^{\infty} \hat{g}_l R_l(x) e^{i k_l x} \sin(l y), \quad (\text{A.4})$$

which yields (2.10).

It remains to derive the bounds in (2.12). One verifies readily that for $z = \alpha + \beta i$ with $\alpha, \beta \in \mathbb{R}$,

$$|1 - e^\alpha| \leq |1 - e^z| \leq 1 + e^\alpha, \quad |\sin z| = \left| \frac{e^{iz} - e^{-iz}}{2i} \right| = \frac{e^{-\beta}}{2} |1 - e^{-2iz}|. \quad (\text{A.5})$$

Then we have

$$|1 - e^{2\text{Im}\{\hat{k}_l S_d\}}| \leq |1 - e^{-2i\hat{k}_l S_d}| \leq 1 + e^{2\text{Im}\{\hat{k}_l S_d\}}. \quad (\text{A.6})$$

Therefore, (i) for $k > l$ (note $\hat{k}_l = \sqrt{k^2 - l^2}$), we obtain (2.12) from (A.5)-(A.6) immediately.

On the other hand, (ii) for $k < l$ (note $\hat{k}_l = i|\hat{k}_l|$), the lower and upper bounds in (2.13) are a direct consequence of (A.6).

If k is a positive integer, we find that for the mode $l = k$, (A.1) is still valid (i.e., $U_l = \hat{g}_l \sin(ly)$), while (A.2) becomes

$$U_{p,l}(x, y) = \left(1 - \frac{S(x)}{S_d}\right) \hat{g}_l \sin(ly). \quad (\text{A.7})$$

Thus, for the mode $l = k$, $R_l(x)$ should be replaced by $R_l(x) = -S(x)/S_d$ in the identity (2.10).

A.2 Proof of Lemma 2.1

Proof. Without loss of generality, we start with a general nonsingular Cartesian coordinate transformation: $\tilde{x} = X(x, y)$, $\tilde{y} = Y(x, y)$, with Jacobian and Jacobian matrix given by

$$\mathbf{J} = \frac{\partial(x, y)}{\partial(\tilde{x}, \tilde{y})} = \frac{1}{\det(\mathbf{J})} \begin{pmatrix} Y_y & -X_y \\ -Y_x & X_x \end{pmatrix}, \quad \det(\mathbf{J}) = X_x Y_y - X_y Y_x \neq 0. \quad (\text{A.8})$$

It is known that (2.70) can be transformed into

$$\mathcal{H}[U] = \frac{1}{n} \{ \nabla \cdot (\mathbf{C} \nabla U) + k^2 n U \}, \quad (\text{A.9})$$

where $U(x, y) = \tilde{U}(\tilde{x}, \tilde{y})$ and

$$\mathbf{C} = \begin{pmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{pmatrix} = \frac{\mathbf{J} \mathbf{J}^t}{\det(\mathbf{J})}, \quad n = \frac{1}{\det(\mathbf{J})}. \quad (\text{A.10})$$

To represent $\mathbf{J}$ and its determinant in polar coordinates, we rewrite the above nonsingular transformation as $\tilde{r} = R(r, \theta)$, $\tilde{\theta} = \Theta(r, \theta)$. Then by the chain rule, we have

$$\frac{\partial(x, y)}{\partial(\tilde{x}, \tilde{y})} \frac{\partial(\tilde{x}, \tilde{y})}{\partial(x, y)} = \frac{\partial(\tilde{x}, \tilde{y})}{\partial(\tilde{r}, \tilde{\theta})} \frac{\partial(\tilde{r}, \tilde{\theta})}{\partial(x, y)} = \frac{\partial(r, \theta)}{\partial(x, y)} \frac{\partial(x, y)}{\partial(r, \theta)} = \mathbf{I}_2.$$

As a result, the matrix $\mathbf{J}$ can be computed by

$$\begin{aligned}\mathbf{J} &= \frac{\partial(x, y)}{\partial(\tilde{x}, \tilde{y})} = \left(\frac{\partial(\tilde{x}, \tilde{y})}{\partial(x, y)} \right)^{-1} = \left(\frac{\partial(\tilde{x}, \tilde{y})}{\partial(\tilde{r}, \tilde{\theta})} \frac{\partial(\tilde{r}, \tilde{\theta})}{\partial(r, \theta)} \frac{\partial(r, \theta)}{\partial(x, y)} \right)^{-1} \\ &= \frac{\partial(x, y)}{\partial(r, \theta)} \left(\frac{\partial(\tilde{r}, \tilde{\theta})}{\partial(r, \theta)} \right)^{-1} \frac{\partial(\tilde{r}, \tilde{\theta})}{\partial(\tilde{x}, \tilde{y})}.\end{aligned}\quad (\text{A.11})$$

Straightforward calculation leads to

$$\frac{\partial(x, y)}{\partial(r, \theta)} = \mathbf{T}(\theta) \begin{pmatrix} 1 & 0 \\ 0 & r \end{pmatrix}, \quad \frac{\partial(\tilde{r}, \tilde{\theta})}{\partial(\tilde{x}, \tilde{y})} = \begin{pmatrix} 1 & 0 \\ 0 & 1/\tilde{r} \end{pmatrix} \mathbf{T}^t(\tilde{\theta}), \quad (\text{A.12})$$

and

$$\frac{\partial(\tilde{r}, \tilde{\theta})}{\partial(r, \theta)} = \begin{pmatrix} R_r & R_\theta \\ \Theta_r & \Theta_\theta \end{pmatrix}, \quad \left(\frac{\partial(\tilde{r}, \tilde{\theta})}{\partial(r, \theta)} \right)^{-1} = \frac{1}{R_r \Theta_\theta - R_\theta \Theta_r} \begin{pmatrix} \Theta_\theta & -R_\theta \\ -\Theta_r & R_r \end{pmatrix}. \quad (\text{A.13})$$

Inserting (A.12)-(A.13) into (A.11), and using the property: $\det(\mathbf{T}(\theta)) = \det(\mathbf{T}(\tilde{\theta})) = 1$, we find

$$\begin{aligned}\det(\mathbf{J}) &= \frac{r}{R(R_r \Theta_\theta - R_\theta \Theta_r)}, \\ \mathbf{J} &= \det(\mathbf{J}) \mathbf{T}(\theta) \begin{pmatrix} R\Theta_\theta/r & -R_\theta/r \\ -R\Theta_r & R_r \end{pmatrix} \mathbf{T}^t(\Theta).\end{aligned}\quad (\text{A.14})$$

We now apply the above general formulas to (2.67), that is, $\tilde{r} = R = S(r, \theta)$, $\tilde{\theta} = \Theta = \theta$, so $R_r = S_r$, $R_\theta = S_\theta$, $\Theta_r = 0$, $\Theta_\theta = 1$. Then we obtain immediately from (A.14) that

$$\det(\mathbf{J}) = \frac{r}{SS_r}, \quad \mathbf{J} = \mathbf{T}(\theta) \begin{pmatrix} \frac{1}{S_r} & -\frac{S_\theta}{SS_r} \\ 0 & \frac{r}{S} \end{pmatrix} \mathbf{T}^t(\theta). \quad (\text{A.15})$$

Then, $\mathbf{C}$ and n in (2.72) can be derived directly from (A.10) and (A.15). This ends the proof. $\square$

A.3 Formulations of each element in linear system (5.28)

For elements in linear system (5.28), the specific formulations are

$$\begin{aligned}
 K_{12} &= \int_{-1}^1 -\frac{1}{2}(a\xi + b)\phi_i + \frac{1}{2a}(a\xi + b)^2(\phi_i)' \\
 &\quad + ak^2 \frac{(1-\xi)(a\xi + b)^2}{2} \phi_i - an^2 \frac{1-\xi}{2} \phi_i d\xi \\
 &= \begin{cases} -3b + \frac{ak^2}{5}(a^2 - 2ab + b^2) - an^2, & i = 0, \\ -a - ak^2 \left(\frac{1}{7}a^2 - \frac{2}{3}ab + \frac{1}{3}b^2 \right) + \frac{an^2}{3}, & i = 1, \\ \frac{2}{15}a^2k^2(a - 2b), & i = 2, \\ -\frac{2}{35}a^3k^2, & i = 3, \end{cases}
 \end{aligned}$$

and

$$\begin{aligned}
 K_{13} &= \int_{-1}^1 \frac{1}{2}(a\xi + b)\phi_i + \frac{1}{2a}(a\xi + b)^2(\phi_i)' \\
 &\quad + ak^2 \frac{(1+\xi)(a\xi + b)^2}{2} \phi_i - an^2 \frac{1+\xi}{2} \phi_i d\xi \\
 &= \begin{cases} 3b + \frac{ak^2}{5}(a^2 + 2ab + b^2) - an^2, & i = 0, \\ a + ak^2 \left(\frac{1}{7}a^2 + \frac{2}{3}ab + \frac{1}{3}b^2 \right) - \frac{an^2}{3}, & i = 1, \\ \frac{2}{15}a^2k^2(a + 2b), & i = 2, \\ \frac{2}{35}a^3k^2, & i = 3, \end{cases}
 \end{aligned}$$

and

$$\begin{aligned}
K_{31} &= \int_{-1}^1 \frac{(a\xi + b)(1 + \xi)}{2} (\phi_j)' - \frac{1}{2a} (a\xi + b)^2 (\phi_j)' \\
&\quad + ak^2 \frac{(1 + \xi)(a\xi + b)^2}{2} \phi_j - an^2 \frac{1 + \xi}{2} \phi_j d\xi \\
&= \begin{cases} -a + b + \frac{ak^2}{5} (a^2 + 2ab + 2b^2) - an^2, & j = 0, \\ ak^2 \left(\frac{1}{7} a^2 + \frac{2}{3} ab + \frac{1}{3} b^2 \right) - \frac{an^2}{3}, & j = 1, \\ \frac{2}{15} a^2 k^2 (a + 2b), & j = 2, \\ \frac{2}{35} a^3 k^2, & j = 3, \end{cases}
\end{aligned}$$

and

$$\begin{aligned}
K_{32} &= \int_{-1}^1 -\frac{(a\xi + b)(1 + \xi)}{4} + \frac{1}{4a} (a\xi + b)^2 \\
&\quad + ak^2 \frac{(1 - \xi^2)(a\xi + b)^2}{4} - an^2 \frac{1 - \xi^2}{4} d\xi \\
&= -\frac{1}{2}b + \frac{b^2}{2a} + \frac{1}{15}ak^2(a^2 + 5b^2) - \frac{an^2}{3}.
\end{aligned}$$

and

$$\begin{aligned}
K_{33} &= \int_{-1}^1 \frac{(a\xi + b)(1 + \xi)}{4} - \frac{1}{4a} (a\xi + b)^2 \\
&\quad + ak^2 \frac{(1 + \xi)^2 (a\xi + b)^2}{4} - an^2 \frac{(1 + \xi)^2}{4} d\xi \\
&= \frac{1}{2}b - \frac{b^2}{2a} + \frac{2}{15}ak^2(2a^2 + 5ab + 5b^2) - \frac{2}{3}an^2.
\end{aligned}$$

Then, to show the details for K_{ij}^I ,

$$\begin{aligned}
K_{ij}^I &= \int_{-1}^1 -(a\xi + b)(\phi_j)' \phi_i - \frac{1}{a} (a\xi + b)(\phi_j)' (a\xi + b)(\phi_i)' \\
&\quad - an^2 \phi_j \phi_i + ak^2 (a\xi + b)^2 \phi_j \phi_i d\xi \\
&:= K_{ij}^A - K_{ij}^B + K_{ij}^C + K_{ij}^D,
\end{aligned}$$

where

$$K_{ij}^A = \int_{-1}^1 -(a\xi + b)(\phi_j)' \phi_i d\xi$$

$$= \begin{cases} \frac{2a(j+2)}{2j+5} - \frac{2a(j+1)}{2j+1} & j = i, \\ -2b & j = i-1, \\ 2b & j = i+1, \\ -\frac{2a(j+2)}{2j+5} & j = i-2, \\ \frac{2a(j+1)}{2j+1} & j = i+2, \end{cases}$$

and

$$K_{ij}^C = -an^2 \int_{-1}^1 \phi_j \phi_i d\xi = -n^2 \begin{cases} a \left(\frac{2}{2i+1} + \frac{2}{2i+5} \right) & j = i \\ -\frac{2a}{2i+1} & j = i-2 \\ -\frac{2a}{2j+1} & j = i+2, \end{cases}$$

and

$$K_{ij}^B = \frac{1}{a} \int_{-1}^1 (a\xi + b)(\phi_j)' (a\xi + b)(\phi_i)' d\xi$$

$$= \begin{cases} \frac{2a(j+2)^2}{2j+5} + \frac{2a(j+1)^2}{2j+1} + 2b(2j+3) & j = i, \\ 4b(i+1) & j = i-1, \\ 4b(j+1) & j = i+1, \\ \frac{2ai(i+1)}{2i+1} & j = i-2, \\ \frac{2aj(j+1)}{2j+1} & j = i+2, \end{cases}$$

and

$$\begin{aligned}
 K_{ij}^D &= ak^2 \int_{-1}^1 (a\xi + b)^2 \phi_j \phi_i d\xi \\
 &= k^2 \left\{ \begin{aligned}
 &2a^3 \left[\frac{(i+3)^2}{(2i+5)^2(2i+7)} + \frac{2b^2(i+3)}{a^2(2i+1)(2i+5)} + \frac{2i+3}{(2i+1)^2(2i+5)^2} \right. \\
 &\quad \left. + \frac{i^2}{(2i-1)(2i+1)^2} \right], \quad j = i \\
 &a^2 \left[\frac{4bi}{(2i-1)(2i+1)} - \frac{4b(i+1)}{(2i+1)(2i+3)} + \frac{(i+1)^2(i+2)}{(2i+1)(2i+3)(2i+5)} \right], \quad j = i-1 \\
 &a^2 \left[\frac{4bj}{(2i-1)(2j+1)} - \frac{4b(j+1)}{(2j+1)(2j+3)} + \frac{(j+1)^2(j+2)}{(2j+1)(2j+3)(2j+5)} \right], \quad j = i+1 \\
 &3a^3 \left[\frac{(i+1)^2(i+2)}{(2i+1)(2i+3)(2i+5)} - \frac{(i+1)^2}{(2i+1)^2(2i+3)} - \frac{2b}{a(2i+1)} \right. \\
 &\quad \left. + \frac{i(i-1)}{(2i-3)(2i-1)(2i+1)} - \frac{i^2}{(2i-1)(2i+1)^2} \right], \quad j = i-2 \\
 &3a^3 \left[\frac{(j+1)^2(j+2)}{(2j+1)(2j+3)(2j+5)} - \frac{(j+1)^2}{(2j+1)^2(2j+3)} - \frac{2b}{a(2j+1)} \right. \\
 &\quad \left. + \frac{j(j-1)}{(2j-3)(2j-1)(2j+1)} - \frac{j^2}{(2j-1)(2j+1)^2} \right], \quad j = i+2 \\
 &-4a^2b \frac{i}{(2i-1)(2i+1)}, \quad j = i-3 \\
 &-4a^2b \frac{j}{(2j-1)(2j+1)}, \quad j = i+3 \\
 &-2a^3 \frac{i(i-1)}{(2i-3)(2i-1)(2i+1)}, \quad j = i-4 \\
 &-2a^3 \frac{j(j-1)}{(2j-3)(2j-1)(2j+1)}, \quad j = i+4
 \end{aligned} \right\}
 \end{aligned}$$

After that, $K = K^A - K^B + K^C + K^D$, and set $K_{N_p-1, N_p-1} = 1$.

Bibliography

- [1] M. Abramowitz and I. Stegun. *Handbook of Mathematical Functions*. Dover, New York, 1964.
- [2] S. Acosta and V. Villamizar. Coupling of Dirichlet-to-Neumann boundary condition and finite difference methods in curvilinear coordinates for multiple scattering. *J. Comput. Phys.*, 229(15):5498–5517, 2010.
- [3] S. Acosta, V. Villamizar, and B. Malone. The dtn nonreflecting boundary condition for multiple scattering problems in the half-plane. *Comput. Methods Appl. Mech. Engrg.*, 217:1–11, 2012.
- [4] M. Ainsworth. Discrete dispersion relation for hp-version finite element approximation at high wave number. *SIAM J. Numer. Anal.*, 42(2):553–575, 2004.
- [5] F. Amirkulova and A. Norris. Acoustic multiple scattering using recursive algorithms. *J. Comput. Phys.*, 299:787–803, 2015.
- [6] A. Anand, Y. Boubendir, F. Ecevit, and F. Reitich. Analysis of multiple scattering iterations for high-frequency scattering problems. II: The three-dimensional scalar case. *Numer. Math.*, 114(3):373, 2010.
- [7] I. Babuska and S. Sauter. Is the pollution effect of the fem avoidable for the helmholtz equation considering high wave numbers? *SIAM J. Numer. Anal.*, 34(6):2392–2423, 1997.

-
- [8] M. Balabane. Boundary decomposition for Helmholtz and Maxwell equations 1: disjoint sub-scatterers. *Asymp. Anal.*, 38(1):1–10, 2004.
 - [9] A. Bayliss and E. Turkel. Radiation boundary conditions for wave-like equations. *Comm. Pure Appl. Math.*, 33(6):707–725, 1980.
 - [10] J. Berenger. A perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Phys.*, 114(2):185–200, 1994.
 - [11] J. Berenger. Perfectly matched layer for the fdtd solution of wave-structure interaction problems. *IEEE Trans. Antennas and Propagation*, 44(1):110–117, 1996.
 - [12] J. Berenger. Three-dimensional perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Phys.*, 127(2):363–379, 1996.
 - [13] A. Bermúdez, L. Hervella-Nieto, A. Prieto, and R. Rodríguez. An exact bounded perfectly matched layer for time-harmonic scattering problems. *SIAM J. Sci. Comp.*, 30(1):312–338, 2007.
 - [14] A. Bermúdez, L. Hervella-Nieto, A. Prieto, and R. Rodríguez. An optimal perfectly matched layer with unbounded absorbing function for time-harmonic acoustic scattering problems. *J. Comp. Phys.*, 223(2):469–488, 2007.
 - [15] J. Boyd. *Chebyshev and Fourier spectral methods*. Dover Publications Inc., Mineola, NY, second edition, 2001.
 - [16] S. Chandler-Wilde and P. Monk. Wave-number-explicit bounds in time-harmonic scattering. *SIAM J. Math. Anal.*, 39(5):1428–1455, 2008.
 - [17] Z. Chen. Convergence of the time-domain perfectly matched layer method for acoustic scattering problems. *Int. J. Numer. Anal. Model.*, 6(1):124–146, 2009.
 - [18] Z. Chen, T. Cui, and L. Zhang. An adaptive anisotropic perfectly matched layer method for 3-d time harmonic electromagnetic scattering problems. *Numer. Math.*, 125(4):639–677, 2013.
 - [19] Z. Chen and X. Liu. An adaptive perfectly matched layer technique for time-harmonic scattering problems. *SIAM J. Numer. Anal.*, 43(2):645–671, 2005.
 - [20] Z. Chen and X. Wu. An adaptive uniaxial perfectly matched layer method for time-harmonic scattering problems. *Numer. Math. Theor. Meth. Appl.*, 1:113–137, 2008.

-
- [21] Z. Chen and X. Wu. Long-time stability and convergence of the uniaxial perfectly matched layer method for time-domain acoustic scattering problems. *SIAM J. Numer. Anal.*, 50(5):2632–2655, 2012.
- [22] Z. Chen and W. Zheng. PML method for electromagnetic scattering problem in a two-layer medium. *SIAM J. Numer. Anal.*, 55(4):2050–2084, 2017.
- [23] W. Chew and W. Weedon. A 3d perfectly matched medium from modified maxwell’s equations with stretched coordinates. *Microwave and optical technology letters*, 7(13):599–604, 1994.
- [24] R. Cimpanu, A. Martinsson, and M. Heil. A parameter-free perfectly matched layer formulation for the finite-element-based solution of the helmholtz equation. *J. Comput. Phys.*, 296:329–347, 2015.
- [25] F. Collino and P. Monk. The perfectly matched layer in curvilinear coordinates. *SIAM J. Sci. Comput.*, 19(6):2061–2090, 1998.
- [26] P. Cummings and X. Feng. Sharp regularity coefficient estimates for complex-valued acoustic and elastic Helmholtz equations. *Math. Models Methods Appl. Sci.*, 16(1):139–160, 2006.
- [27] A. Darvish, B. Zakeri, and N. Radkani. An optimized hybrid convolutional perfectly matched layer for efficient absorption of electromagnetic waves. *J. Comput. Phys.*, 356:31–45, 2018.
- [28] L. Demkowicz and F. Ihlenburg. Analysis of a coupled finite-infinite element method for exterior helmholtz problems. *Numer. Math.*, 88(1):43–73, 2001.
- [29] C. Deng, M. Luo, M. Yuan, B. Zhao, M. Zhuang, and Q. Liu. The auxiliary differential equations perfectly matched layers based on the hybrid setd and pstd algorithms for acoustic waves. *J. Theor. Comput. Acoust.*, 26(01):1750031, 2018.
- [30] J. Diaz and P. Joly. A time domain analysis of pml models in acoustics. *Comput. Methods Appl. Mech. Engrg.*, 195(29-32):3820–3853, 2006.
- [31] J. Douglas, J. Santos, D. Sheen, and L. Bennethum. Frequency domain treatment of one-dimensional scalar waves. *Math. Models Methods Appl. Sci.*, 3(2):171–194, 1993.

-
- [32] F. Ecevit and F. Reitich. Analysis of multiple scattering iterations for high-frequency scattering problems. I: The two-dimensional case. *Numer. Math.*, 114(2):271–354, 2009.
 - [33] A. Elsherbeni. A comparative study of two-dimensional multiple scattering techniques. *Radio Sci.*, 29(04):1023–1033, 1994.
 - [34] B. Engquist and A. Majda. Absorbing boundary conditions for numerical simulation of waves. *Proc. Nat. Acad. Sci. U.S.A.*, 74(5):1765–1766, 1977.
 - [35] K. Feng. Finite element method and natural boundary reduction. *Proceeding of ICM.*, pages 1439–1453, 1983.
 - [36] N. Feng, Y. Yue, C. Zhu, L. Wan, and Q. Liu. Second-order pml: Optimal choice of n th-order pml for truncating fdtd domains. *Internat. J. Comput. Phys.*, 285, 2015.
 - [37] X. Feng. Wave number-depended a priori estimates for the time-harmonic Maxwell equations. *Private Communication*, 2011.
 - [38] X. Feng, Z. Li, and Z. Qiao. High order compact finite difference schemes for the Helmholtz equation with discontinuous coefficients. *J. Comput. Math.*, 29(3):324–340, 2011.
 - [39] A. Fournier. Exact calculation of Fourier series in nonconforming spectral-element methods. *J. Comput. Phys.*, 215(1):1–5, 2006.
 - [40] P. Gabrielli and M. Mercier-Finidori. Acoustic scattering by two spheres: multiple scattering and symmetry considerations. *J. Sound Vib.*, 241(3):423–439, 2001.
 - [41] M. Ganesh and S. Hawkins. An efficient algorithm for simulating scattering by a large number of two dimensional particles. *ANZIAM J. Electron. Suppl.*, 52((C)):C139–C155, 2010.
 - [42] M. Ganesh and S. Hawkins. An efficient $\mathcal{O}(N)$ algorithm for computing $\mathcal{O}(N^2)$ acoustic wave interactions in large N -obstacle three dimensional configurations. *BIT Numer. Math.*, 55:117–139, 2015.
 - [43] S. Gedney. An anisotropic perfectly matched layer-absorbing medium for the truncation of fdtd lattices. *IEEE Trans. on Antennas and Propagation*, 44(12):1630–1639, 1996.

-
- [44] C. Geuzaine, A. Vion, R. Gaignaire, and P. Dular. An amplitude finite element formulation for multiple-scattering by a collection of convex obstacles. *IEEE Trans. Magnet.*, 46(8):2963–2966, 2010.
- [45] D. Givoli. Non-reflecting boundary conditions. *J. Comput. Phys.*, 94(1):1–29, 1991.
- [46] D. Givoli and B. Neta. High-order non-reflecting boundary scheme for time-dependent waves. *J. Comput. Phys.*, 186(1):24–46, 2003.
- [47] C. Goldstein. A finite element method for solving helmholtz type equations in waveguides and other unbounded domains. *Math. Comp.*, 39(160):309–324, 1982.
- [48] M. Grote and C. Kirsch. Dirichlet-to-Neumann boundary conditions for multiple scattering problems. *J. Comput. Phys.*, 201(2):630–650, 2004.
- [49] M. Grote and I. Sim. Efficient pml for the wave equation. *arXiv preprint arXiv:1001.0319*, 2010.
- [50] B. Guo. Gegenbauer approximation and its applications to differential equations with rough asymptotic behaviors at infinity. *Appl. Numer. Math.*, 38(4):403–425, 2001.
- [51] B. Guo and L. Wang. Jacobi approximations in non-uniformly jacobi-weighted sobolev spaces. *J. Approx. Theory*, 128(1):1–41, 2004.
- [52] T. Hagstrom. Radiation boundary conditions for the numerical simulation of waves. *Acta Numer.*, 8:47–106, 1999.
- [53] T. Hagstrom and S. Lau. Radiation boundary conditions for maxwell’s equations: a review of accurate time-domain formulations. *J. Comput. Math.*, pages 305–336, 2007.
- [54] U. Hetmaniuk. Stability estimates for a class of Helmholtz problems. *Commun. Math. Sci.*, 5(3):665–678, 2007.
- [55] R. Hiptmair, A. Moiola, and I. Perugia. Stability results for the time-harmonic Maxwell equations with impedance boundary conditions. *Math. Mod. Meth. Appl. Sci.*, 21(11):2263–2287, 2011.

-
- [56] T. De Hoop, P. Van den Berg, and R. Remis. Absorbing boundary conditions and perfectly matched layers-an analytic time-domain performance analysis. *IEEE Trans. Magnet.*, 38(2):657–660, 2002.
 - [57] F. Ihlenburg. *Finite element analysis of acoustic scattering*, volume 132 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1998.
 - [58] F. Ihlenburg and I. Babuška. Finite element solution of the Helmholtz equation with high wave number. I. The h -version of the FEM. *Comput. Math. Appl.*, 30(9):9–37, 1995.
 - [59] X. Jiang and W. Zheng. Adaptive perfectly matched layer method for multiple scattering problems. *Comp. Meth. Appl. Mech. Engng.*, 201:42–52, 2012.
 - [60] S. Johnson. Notes on perfectly matched layers (pmls). *Lecture notes, Massachusetts Institute of Technology, Massachusetts*, 29, 2008.
 - [61] S. Johnson. Notes on Perfectly Matched Layers. *Technical Report, Massachusetts Institute of Technology, Cambridge, MA*, 2010.
 - [62] M. Lassas and E. Somersalo. On the existence and convergence of the solution of PML equations. *Computing*, 60(3):229–241, 1998.
 - [63] P. Li and A. Wood. A two-dimensional Helmholtz equation solution for the multiple cavity scattering problem. *J. Comput. Phys.*, 240:100–120, 2013.
 - [64] Y. Li and H. Wu. FEM and CIP-FEM for Helmholtz equation with high wave number and perfectly matched layer truncation. *SIAM J. Numer. Anal.*, 57(1):96–126, 2019.
 - [65] P. Loh, A. Oskooi, M. Ibanescu, M. Skorobogatiy, and S. Johnson. Fundamental relation between phase and group velocity, and application to the failure of perfectly matched layers in backward-wave structures. *Phys. Rev. E*, 79(6):065601, 2009.
 - [66] L. Ma, J. Shen, L. Wang, and Z. Yang. Wavenumber explicit analysis for time-harmonic Maxwell equations in a spherical shell and spectral approximations. *IMA J. Numer. Anal.*, 38(2):810–851, 2018.
 - [67] P. Martin. *Multiple Scattering: Interaction of Time-Harmonic Waves with N Obstacles*. Cambridge University Press, 2006.

-
- [68] J. Melenk. *On Generalized Finite Element Methods*. PhD thesis, University of Maryland, College Park, 1995.
- [69] J. Melenk and S. Sauter. Convergence analysis for finite element discretizations of the helmholtz equation with Dirichlet-to-Neumann boundary conditions. *Math. Comput.*, 79(272):1871–1914, 2010.
- [70] J. Melenk and S. Sauter. Wavenumber explicit convergence analysis for Galerkin discretizations of the Helmholtz equation. *SIAM J. Numer. Anal.*, 49(3):1210–1243, 2011.
- [71] A. Modave, E. Delhez, and C. Geuzaine. Optimizing perfectly matched layers in discrete contexts. *Internat. J. Numer. Methods Engrg.*, 99(6):410–437, 2014.
- [72] J. Nédélec. *Acoustic and electromagnetic equations: integral representations for harmonic problems*. Springer Science & Business Media, 2001.
- [73] N. Newmark. A method of computation for structural dynamics. 1959.
- [74] J. Pendry, D. Schurig, and D. Smith. Controlling electromagnetic fields. *Science*, 312(5781):1780–1782, 2006.
- [75] P. Petropoulos. Reflectionless sponge layers as absorbing boundary conditions for the numerical solution of Maxwell equations in rectangular, cylindrical, and spherical coordinates. *SIAM J. Appl. Math.*, 60(3):1037–1058, 2000.
- [76] D. Rabinovich, D. Givoli, and E. Bécache. Comparison of high-order absorbing boundary conditions and perfectly matched layers in the frequency domain. *Int. J. Numer. Methods Biomed. Eng.*, 26(10):1351–1369, 2010.
- [77] C. Radu, M. Anton, and H. Matthias. A parameter-free perfectly matched layer formulation for the finite-element-based solution of the Helmholtz equation. *J. Comput. Phys.*, 296:329–347, 2015.
- [78] H. Ragheb and M. Hamid. Scattering by N parallel conducting circular cylinders. *Int. J. Electron.*, 59(4):407–421, 1985.
- [79] Z. Sacks, D. Kingsland, R. Lee, and J. Lee. A perfectly matched layer anisotropic absorber for use as an absorbing boundary conditions. *SIAM*, 2012.

-
- [80] J. Shen, T. Tang, and L. Wang. *Spectral methods: algorithms, analysis and applications*, volume 41. Springer Science & Business Media, 2011.
 - [81] J. Shen and L. Wang. Spectral approximation of the helmholtz equation with high wave numbers. *SIAM J. Numer. Anal.*, 43(2):623–644, 2005.
 - [82] J. Shen and L. Wang. Analysis of a spectral-Galerkin approximation to the Helmholtz equation in exterior domains. *SIAM J. Numer. Anal.*, 45:1954–1978, 2007.
 - [83] J. Shen and L. Wang. Some recent advances on spectral methods for unbounded domains. *Commun. Comput. Phys.*, 5(2-4):195–241, 2009.
 - [84] I. Singer and E. Turkel. A perfectly matched layer for the helmholtz equation in a semi-infinite strip. *J. Comp. Phys.*, 201(2):439–465, 2004.
 - [85] Q. Sun, R. Zhang, Q. Zhan, and Q. Liu. A novel coupling algorithm for perfectly matched layer with wave equation-based discontinuous galerkin time-domain method. *IEEE Trans. on Antennas and Propagation*, 66(1):255–261, 2017.
 - [86] A. Taflov and S. Hagness. *Computational electrodynamics: the finite-difference time-domain method*. Artech House, Inc., Boston, MA, 2005.
 - [87] F. Teixeira and W. Chew. *Advances in the theory of perfectly matched layer*. Citeseer, 2001.
 - [88] B. Wang, L. Wang, and Z. Xie. Accurate calculation of spherical and vector spherical harmonic expansions via spectral element grids. *Adv. Comput. Math.*, 44(3):951–985, 2018.
 - [89] L. Wang and Z. Yang. A perfect absorbing layer for high-order simulation of wave scattering problems. In *Spectral and High Order Methods for Partial Differential Equations ICOSAHOM 2016*, pages 81–101. Springer, Cham, 2017.
 - [90] W. Wood. *Practical time-stepping schemes*. Oxford Applied Mathematics and Computing Science Series. The Clarendon Press, Oxford University Press, New York, 1990.
 - [91] X. Wu and W. Zheng. An adaptive perfectly matched layer method for multiple cavity scattering problems. *Commun. Comput. Phys.*, 19(2):534–558, 2016.

-
- [92] W. Yang, J. Li, and Y. Huang. Mathematical analysis and finite element time domain simulation of arbitrary star-shaped electromagnetic cloaks. *SIAM J. Numer. Anal.*, 56(1):136–159, 2018.
- [93] Z. Yang and L. Wang. Accurate simulation of circular and elliptic cylindrical invisibility cloaks. *Commun. Comput. Phys.*, 17(3):822–849, 2015.
- [94] Z. Yang, L. Wang, Z. Rong, B. Wang, and B. Zhang. Seamless integration of global Dirichlet-to-Neumann boundary condition and spectral elements for transformation electromagnetics. *Comput. Methods Appl. Mech. Eng.*, 301:137–163, 2016.
- [95] J. Young and J. Bertrand. Multiple scattering by two cylinders. *J. Acoust. Soc. Am.*, 58(6):1190–1195, 1975.
- [96] L. Zhao and A. Cangellaris. A general approach for the development of unsplit-field time-domain implementations of perfectly matched layers for fdtd grid truncation. *IEEE Microwave and Guided Wave Letters*, 6(5):209–211, 1996.
- [97] N. Zhavorozhina, L. Shadrivov, and Y. Kivshar. Inside-out electromagnetic cloaking. *Opt. Express*, 16(7):4615–4620, 2008.
- [98] W. Zhou and H. Wu. An adaptive finite element method for the diffraction grating problem with pml and few-mode dtn truncations. *SIAM J. Sci. Comput.*, 76(3):1813–1838, 2018.