ANALYSIS OF A PML METHOD APPLIED TO COMPUTATION OF RESONANCES IN OPEN SYSTEMS AND ACOUSTIC SCATTERING PROBLEMS

A Dissertation

by

SEUNGIL KIM

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

August 2009

Major Subject: Mathematics

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Approved by:

Chair of Committee,	Joseph E. Pasciak
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ABSTRACT

Analysis of a PML Method Applied to Computation of Resonances in Open Systems and Acoustic Scattering Problems. (August 2009)

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M.S., Seoul National University
Chair of Advisory Committee: Dr. Joseph E. Pasciak

We consider computation of resonances in open systems and acoustic scattering problems. These problems are posed on an unbounded domain and domain truncation is required for the numerical computation. In this paper, a perfectly matched layer (PML) technique is proposed for computation of solutions to the unbounded domain problems.

For resonance problems, resonance functions are characterized as improper eigenfunction (non-zero solutions of the eigenvalue problem which are not square integrable) of the Helmholtz equation on an unbounded domain. We shall see that the application of the spherical PML converts the resonance problem to a standard eigenvalue problem on the infinite domain. Then, the goal will be to approximate the eigenvalues first by replacing the infinite domain by a finite computational domain with a convenient boundary condition and second by applying finite elements to the truncated problem. As approximation of eigenvalues of problems on a bounded domain is classical [12], we will focus on the convergence of eigenvalues of the (continuous) PML truncated problem to those of the infinite PML problem. Also, it will be shown that the domain truncation does not produce spurious eigenvalues provided that the size of computational domain is sufficiently large.

The spherical PML technique has been successfully applied for approximation of scattered waves [13]. We develop an analysis for the case of a Cartesian PML

application to the acoustic scattering problem, i.e., solvability of infinite and truncated Cartesian PML scattering problems and convergence of the truncated Cartesian PML problem to the solution of the original solution in the physical region as the size of computational domain increases.

To my family

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER I

INTRODUCTION

Wave phenomena in many applications take place in unbounded domains. For the numerical study of the wave propagation it is required to truncate the unbounded domain to a finite region of computational interest. For this purpose many numerical techniques have been proposed, and over the last decay a fictitious layer technique, so-called a perfectly matched layer (PML), has attracted attention of mathematicians, physicists and engineers and has been successfully applied to many wave propagation problems.

In this dissertation, we investigate the application of PML techniques to compute resonances in open systems and solve acoustic scattering problems. Resonance problems in open systems are important since they arise in many applications, for example, the modeling of slat and flap noise from an airplane wing, designing photonic band gap devices for wave guides and quantum mechanical systems. Scattering theory is a framework to study and understand the acoustic properties of objects and shape recognition from scattered fields.

These problems are set on an unbounded domain and, in case of resonances, have solutions which grow exponentially at infinity. For approximation of solutions to problems posed on an unbounded domain, domain truncation is required. For this purpose many numerical methods have been designed, including boundary element methods [17, 33, 39], infinite element methods [11, 28] and artificial boundary condition approaches [8, 25, 26, 32, 42].

The original PML technique was introduced by Bérenger in the seminal papers

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The dissertation model is SIAM Journal on Numerical Analysis.

[9, 10]. PML is a domain truncation approach which involves the use of a fictitious absorbing layer outside of the region of computational interest. A properly defined PML method absorbs waves propagating into it without producing spurious reflections and results in an exponentially decaying solution. Because of this exponential decay it is natural to truncate the problem to a bounded domain with a convenient outer boundary condition, e.g., a homogeneous Dirichlet boundary condition. The PML technique has been applied to approximation of solutions to Maxwell's equations [9, 10, 13, 14, 20], elasticity problems [15, 34] and acoustic resonances [35, 36] as well as acoustic scattering problems [13, 43].

PMLs are classified according to shapes of the layers, e.g., spherical/cylindrical PML, Cartesian PML or elliptical PML. Initially, the PML technique was introduced by Bérenger for electromagnetic scattering problems on unbounded domains in Cartesian coordinates [9, 10]. Subsequently, Chew and Weedon [18] interpreted it using a complex coordinate stretching for each component in Cartesian coordinates. In [20, 43] a coordinate stretching viewpoint for PMLs was extended to a curvilinear coordinate system. A more general PML with a convex geometry was developed in [44].

First, we consider application of a spherical/cylindrical PML to resonance problems in three dimensional space. The model operators of resonance problems are a perturbation of the negative Laplacian, i.e.,

$$L = -\Delta + L_1$$

where L_1 is symmetric and supported in a compact set in $\mathbb{R}^3$. *Resonance functions* are characterized as non-zero solutions ψ to

$$L\psi = k^2\psi$$

with an outgoing condition at infinity, and their k in the problem are called *resonances*. A resonance value k corresponds to an improper eigenvalue problem, and the corresponding eigenvector (resonance function) grows exponentially.

There are two difficulties in computing resonances. One is that the problem is posed on the infinite domain, and the other is that resonance functions grows rapidly at infinity. In order to circumvent these difficulties the PML technique is utilized. In time dependent wave propagation problems one introduces a wave number dependent PML stretching which results in wave number independent decay. In contrast, for resonance problems we define a PML stretching which is independent of wave numbers, yielding wave number dependent decay. For this reason, the wave number independent PML stretching provides certain resonance functions with stronger exponential decay than their exponential growth. This stronger exponential decay changes the resonance functions of the original problem to eigenfunctions of the PML problem (on the infinite domain). In other words, the application of PML converts the resonance problem to a standard eigenvalue problem (on the infinite domain). The exponential decay of PML eigenfunctions enables us to truncate the problem to a finite domain, and impose a convenient boundary condition on the artificial boundary, which reduces the eigenvalue problem on the infinite domain to one on a finite domain.

The numerical approximation of resonance values consists of two steps: the first step is domain truncation which converts the infinite domain eigenvalue problem to one on truncated domains and the second is the finite element approximation on the truncated domain. As the convergence of the eigenvalues associated with the finite element approximation to those of the PML problem on the truncated domain is standard (See, e.g., [12]), we will focus on the convergence of eigenvalues of the truncated PML problem to those of the infinite PML problem as the truncated domain is increasing.

The second part of this dissertation introduces the analysis of a Cartesian PML approximation of acoustic scattering problems in $\mathbb{R}^2$

$$\begin{aligned} -\Delta u - k^2 u = 0 \ \text{ in } \ \bar{\Omega}^c, \\ u = g \ \text{ on } \ \partial\Omega, \\ \lim_{r\to\infty} r^{1/2}\left|\frac{\partial u}{\partial r} - iku\right| = 0. \end{aligned}$$

Here k is real and positive and Ω is a bounded domain with a Lipschitz continuous boundary contained in the square[†] $[-a, a]^2$ for some positive a.

The application of spherical/cylindrical PML to the acoustic scattering problem is well understood [13, 43], but unfortunately the compact perturbation argument [47, 54], that was used in [13], is not applicable to the problem reformulated in terms of a Cartesian PML. We need to follow a significantly different approach to establish well-posedness of the Cartesian PML problem.

The first important ingredient for the analysis is the construction of solutions to the PML equation in terms of integrals. In the case of the Helmholtz equation with a real and positive wave number k, these results are classical. These results are alluded to for the PML Helmholtz equation based on a smooth convex geometry by Lassas and Somersalo [44]. Such results are needed for proving uniqueness and exponential decay of solutions to the PML problem on the infinite domain.

Another critical component for the analysis is examination of the essential spectrum of the Cartesian PML operator. By identifying the essential spectrum of the Cartesian PML operator, we will show that any point on the real axis excluding the origin is either in the resolvent set or is in the discrete spectrum (i.e., an isolated point of spectrum of finite algebraic multiplicity). Once uniqueness of solutions is

[†]We consider a domain in $\mathbb{R}^2$ for convenience. The extension to domains in $\mathbb{R}^3$ is completely analogous.

established for all real $k \neq 0$, we conclude stability of the PML scattering problem on the infinite domain. This is one of the main ingredients in the subsequent analysis of the truncated Cartesian PML problem.

Finally, the outline of this dissertation follows. In Chapter II we introduce Sobolev spaces, traces and regularity results. From Chapter III through Chapter VI we study an application of spherical PML to compute resonances in open systems. Chapter III introduces the Helmholtz equation and an outgoing condition, and finds two important representations of solutions to the Helmholtz equation with the outgoing condition. In Chapter IV we define a perfectly matched layer in terms of a complex coordinate stretching in spherical geometry and reformulate the original resonance problem into a weak form in the spherical PML framework. Also, we establish a one-to-one correspondence between some of resonance values of the original problem and eigenvalues of the spherical PML problem (on the infinite domain), and verify exponential decay of generalized eigenfunctions of the spherical PML problem. Chapter V shows that the truncated PML problem does not produce spurious eigenvalues provided that the truncated domain is large enough, and that its generalized eigenfunctions decay exponentially. In Chapter VI, as the main result, we prove that the eigenvalues of truncated problems converges to those of the infinite PML problem as the size of the computational domain increases. The numerical results illustrating the theory will be provided here.

From Chapter VII through Chapter IX we study an analysis of a Cartesian PML approximation to acoustic scattering problems in $\mathbb{R}^2$. In Chapter VII we reformulate a model problem with a Cartesian PML and find a fundamental solution of a Cartesian PML Helmholtz equation and its exponential decay. Chapter VIII examines the essential spectrum of the Cartesian PML associated with the scattering problem. As the main result, Chapter IX shows the solvability of the Cartesian PML problem in both of infinite and truncated domains. Here we prove that exponential convergence of solutions to truncated problems to those of the infinite domain problem as the thickness of PML increases. This chapter concludes with the numerical experiments that illustrate the convergence of finite element PML approximations

CHAPTER II

PRELIMINARIES

In this chapter, we recall the definition and properties of Sobolev spaces, trace theorems and regularity for second-order elliptic problems to be used throughout this dissertation. We shall start with defining Sobolev spaces and introduce a Sobolev embedding theorem. A trace theorem and interior and global regularity theorem will be stated here. The results quoted can be found in [2, 19, 27, 29, 31].

A. Sobolev spaces

Let Ω be an open subset of $\mathbb{R}^N$ and $\partial\Omega$ denote the boundary of Ω. Here N is the space dimension. $C^k(\Omega)$ is denoted by the set of functions defined on Ω which have continuous k-th order derivatives. For $1 \le p < \infty$, the $L^p(\Omega)$ space is a Banach space of the functions on Ω with the norm

$$\|u\|_{L^p(\Omega)} := \left(\int_\Omega |u(x)|^p \, \mathrm{d}x \right)^{1/p}.$$

We define a multi-index $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_N)$ where α_i is a non-negative integer for $i = 1, 2, \ldots, N$. The length of α is defined by $|\alpha| = \sum_{i=1}^N \alpha_i$. With this multi-index let

$$D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \cdots \partial x_N^{\alpha_N}}$$

denote the weak derivatives.

Definition II.1. Let Ω be an open subset of $\mathbb{R}^N$. For a non-negative integer k and $1 \le p < \infty$, the Sobolev space $W^{k,p}(\Omega)$ consists of functions u such that for each multi-index α with $|\alpha| \le k$, $D^\alpha u$ exists in the weak sense and belongs to $L^p(\Omega)$.

The Sobolev space $W^{k,p}(\Omega)$ is equipped with the norm

$$\|u\|_{W^{k,p}(\Omega)} := \left(\sum_{|\alpha| \le k} \int_\Omega |D^\alpha u|^p \, \mathrm{d}x \right)^{1/p}.$$

$W^{k,p}(\Omega)$ is a Banach space with the norm defined above. If $p = 2$, in particular, then $W^{k,2}(\Omega)$ is commonly written as $H^k(\Omega)$ for $k = 0, 1, \ldots$. In this case, $H^k(\Omega)$ is a Hilbert space with the corresponding inner product

$$(u, v)_{H^k(\Omega)} = \sum_{|\alpha| \le k} \int_\Omega D^\alpha u D^\alpha v \, \mathrm{d}x.$$

We define $W_0^{k,p}(\Omega)$ to be the closure of $C_0^\infty(\Omega)$, the space of infinitely differentiable functions on Ω whose support is compact, in $W^{k,p}(\Omega)$. In case of $p = 2$, we write $H_0^k(\Omega) = W_0^{k,2}(\Omega)$ for $k = 0, 1, \ldots$.

For a non-integer $k = m + s$ with m being a non-negative integer and $0 < s < 1$, the Sobolev space $W^{k,p}(\Omega)$ is defined as the set of functions u which are bounded with respect to the Sobolev norm

$$\|u\|_{W^{k,p}(\Omega)} := \left(\|u\|^p_{W^{m,p}(\Omega)} + \sum_{|\alpha| = m} \int_\Omega \int_\Omega \frac{|D^\alpha u(x) - D^\alpha u(y)|^p}{|x - y|^{N+sp}} \, \mathrm{d}x\mathrm{d}y \right)^{1/p}.$$

See [2, 19, 27, 29] for properties of Sobolev spaces. Here, we recall a Sobolev embedding theorem that describes continuous inclusions between certain Sobolev spaces. We assume that the boundary of the domain Ω under consideration is regular in the following sense: (It is taken from [31])

Definition II.2. Let Ω be an open subset of $\mathbb{R}^N$. We say that its boundary Γ is Lipschitz-continuous (m times continuously differentiable or C^m) if for every $x \in \Gamma$ there exists a neighborhood $\mathcal{O}$ of x in $\mathbb{R}^N$ and new orthogonal coordinates $\{y_1, \ldots, y_N\}$ such that

(a) $\mathcal{O}$ is an hypercube in the new coordinates:

$$\mathcal{O} = \{ \ (y_1, \ldots, y_N) \mid \ - a_j < y_j < a_j, \ 1 \leq j \leq N\},$$

(b) there exists a Lipschitz-continuous (m times continuously differentiable or C^m) function φ, defined in

$$\mathcal{O}' = \{ \ (y_1, y_2, \ldots, y_{N-1}) \mid \ - a_j < y_j < a_j, \ 1 \leq j \leq N - 1\}$$

and such that

$$\begin{aligned} |\varphi(y')| \ &\leq \ a_N/2 \ \text{ for every } y' = (y_1, y_2, \ldots, y_{N-1}) \in \mathcal{O}', \\ \Omega \cap \mathcal{O} \ &= \ \{ \ y = (y', y_N) \in \mathcal{O} \mid y_N < \varphi(y')\}, \\ \Gamma \cap \mathcal{O} \ &= \ \{ \ y = (y', y_N) \in \mathcal{O} \mid y_N = \varphi(y')\}. \end{aligned}$$

In other words, a Lipschitz-continuous boundary is thought as locally being a graph of a Lipschitz-continuous function. We shall that Ω is Lipschitz-continuous when it has a Lipschitz-continuous boundary.

Finally, we need Hölder spaces to state the Sobolev embedding theorem. For any non-negative integer k and $0 < \gamma \leq 1$, $C^{k,\gamma}(\bar{\Omega})$ denotes the space of all functions in $C^k(\bar{\Omega})$ whose k-th derivatives satisfy a Hölder's condition with exponent γ: there is a non-negative constant C such that for $x, y \in \Omega$ and $|\alpha| = k$,

$$|D^\alpha u(x) - D^\alpha u(y)| \leq C|x - y|^\gamma.$$

The space $C^{k,\gamma}(\bar{\Omega})$ is a Banach space with the norm

$$\|u\|_{C^{k,\gamma}(\bar{\Omega})} := \sum_{|\alpha| \leq k} \sup_{x \in \Omega} |u(x)| + \sum_{|\alpha| = k} \sup_{\substack{x,y \in \Omega \\ x \neq y}} \left\{ \frac{|D^\alpha u(x) - D^\alpha u(y)|}{|x - y|^\gamma} \right\}.$$

Theorem II.3. *Let Ω be a Lipschitz-continuous and bounded domain in $\mathbb{R}^N$. For all* *integer $k \geq 0$ and all $1 \leq p < \infty$, the following inclusion holds:*

$$W^{k,p}(\Omega) \subset \begin{cases} L^{p^*}(\Omega) & \textit{with } \frac{1}{p^*} = \frac{1}{p} - \frac{k}{N}, & \textit{if } \; k < \frac{N}{p}, \\ L^q(\Omega) & \textit{for all } \; q \in [1,\infty), & \textit{if } \; k = \frac{N}{p}, \\ C^{0,k-N/p}(\bar{\Omega}), & & \textit{if } \; \frac{N}{p} < k < \frac{N}{p}+1, \\ C^{0,\gamma}(\bar{\Omega}) & \textit{for all } \; 0 < \gamma < 1, & \textit{if } \; k = \frac{N}{p}+1, \\ C^{0,1}(\bar{\Omega}), & & \textit{if } \; \frac{N}{p}+1 < k. \end{cases}$$

This embedding theorem implies that in $\mathbb{R}^1$ the functions in $H^1(\Omega)$ are continuous, whereas in $\mathbb{R}^2$ or $\mathbb{R}^3$ this may not hold. If $N = 2$ or 3 then functions in $H^2(\Omega)$ are continuous.

B. Trace theorems

Functions on Lipschitz-continuous boundaries will play an important role throughout this dissertation . In this section, we define Sobolev spaces on a Lipschitz-continuous boundary and discuss the boundary values of functions defined on Lipschitz-continuous bounded domains.

Definition II.4. Assume that Ω be a Lipschitz-continuous bounded domain of $\mathbb{R}^N$ with a boundary Γ. Let Φ be a function defined on $\mathcal{O}'$ by

$$\Phi(y') = (y', \varphi(y'))$$

with φ given in Definition II.2. A function u on Γ belongs to $W^{k,p}(\Gamma)$ for $0 \leq k \leq 1$ if $u \circ \Phi$ belongs to $W^{k,p}(\mathcal{O}' \cap \Phi^{-1}(\Gamma \cap \mathcal{O}))$ for all possible $\mathcal{O}$ and φ fulfilling the assumption of Definition II.2.

Let $(\mathcal{O}_j, \Phi_j)_{1 \leq j \leq J}$ be any atlas of Γ such that each $(\mathcal{O}_j, \Phi_j)$ satisfies the assumptions of Definition II.4. One possible Banach norm on $W^{k,p}(\Gamma)$ is

$$u \mapsto \left(\sum_{j=1}^{J} \|u \circ \Phi_j\|^p_{W^{k,p}(\mathcal{O}'_j \cap \Phi^{-1}(\Gamma \cap \mathcal{O}'_j))} \right)^{1/p} . \tag{II.1}$$

In case when $0 < k < 1$, the norm defined in (II.1) is equivalent to

$$u \mapsto \left(\int_\Gamma |u|^p \,\mathrm{d}S + \int_\Gamma \int_\Gamma \frac{|u(x) - u(y)|^p}{|x - y|^{N-1+kp}} \,\mathrm{d}S_x \mathrm{d}S_y \right)^{1/p} ,$$

where $\mathrm{d}S$ denotes the surface measure of Γ [31].

Theorem II.5. *Let $1 \leq p < \infty$ and Ω be a Lipschitz-continuous bounded domain with a boundary Γ. Let q denote the number such that $1/p + 1/q = 1$. Then there exists a linear operator*

$$\gamma_0 : W^{1,p}(\Omega) \to W^{1/q,p}(\Gamma)$$

such that

(i) γ_0 *is surjective,*

(ii) $\|\gamma_0(u)\|_{W^{1/q,p}(\Gamma)} \leq C\|u\|_{W^{1,p}(\Omega)}$,

(iii) $\gamma_0(u) = u|_\Gamma$ *if* $u \in W^{1,p}(\Omega) \cap C^1(\bar{\Omega})$,

(iv) The kernel of γ_0 *is* $W_0^{1,p}(\Omega)$.

The constant C in (ii) depends only on p and Ω.

If $p = 2$, we set $H^{1/2}(\Gamma) = W^{1/2,2}(\Gamma)$. Every function in $H^{1/2}(\Gamma)$ is a trace of a function in $H^1(\Omega)$. In addition, the subjectivity of the trace operator and the open mapping theorem implies the following corollary.

Corollary II.6. *Let $1 \leq p < \infty$ and Ω be a Lipschitz-continuous bounded domain with a boundary Γ. Let q denote the number such that $1/p + 1/q = 1$. Then there* *exists a constant C such that for $f \in W^{1/q,p}(\Gamma)$ there exists $u_f \in W^{1,p}(\Omega)$ satisfying*

$$\gamma_0(u_f) = f \quad \textit{and} \quad \|u_f\|_{W^{1,p}(\Omega)} \leq C\|f\|_{W^{1/q,p}(\Gamma)}.$$

C. Regularity

In this section, we shall introduce the interior and global regularity results of uniformly elliptic operators of the form

$$L(u) = -\sum_{i,j=1}^{N} \frac{\partial}{\partial x_i}(a^{ij}(x)\frac{\partial}{\partial x_j}u) + \sum_{i=1}^{N} b^i(x)\frac{\partial}{\partial x_i}u + c(x)u,$$

with

$$\sum_{i,j=1}^{N} a^{ij}(x)\xi_i\xi_j \geq \lambda|\xi|^2, \qquad \text{for all } \ x \in \Omega,\ \xi \in \mathbb{R}^N. \tag{II.2}$$

We will state the regularity results. See e.g., [27, 29] for detail.

Theorem II.7. *Let Ω be an open subset of $\mathbb{R}^N$. Let $u \in H^1(\Omega)$ be a weak solution of the equation $Lu = f$ in Ω where L is strictly elliptic in Ω, the coefficients a^{ij} for $i, j = 1, \ldots, N$ are uniformly Lipschitz continuous in Ω, the coefficients b^i, c for $i = 1, \ldots, N$ are essentially bounded in Ω and the function f is in $L^2(\Omega)$. Then for any subdomain $\Omega' \subset\subset \Omega$ (strictly contained in Ω), we have $u \in H^2(\Omega')$ and*

$$\|u\|_{H^2(\Omega')} \leq C(\|u\|_{H^1(\Omega)} + \|f\|_{L^2(\Omega)}) \tag{II.3}$$

for $C = C(N, \lambda, K, l)$, where λ is given by (II.2),

$$K = \max\{\|a^{i,j}\|_{C^{0,1}(\bar{\Omega})}, \|b^i\|_{L^\infty(\Omega)}, \|c\|_{L^\infty(\Omega)}\} \quad \textit{and} \quad l = dist(\Omega', \partial\Omega).$$

Furthermore, u satisfies the equation

$$Lu = -\sum_{i,j=1}^{N} \left(a^{ij}\frac{\partial^2}{\partial x_i \partial x_j}u + \left(\frac{\partial}{\partial x_i}a^{ij}\right)\frac{\partial}{\partial x_j}u \right) + \sum_{i=1}^{N} b^i\frac{\partial}{\partial x_i}u + cu = f$$

almost everywhere in Ω.

We note that in the estimate (II.3), $\|u\|_{H^1(\Omega)}$ may be replaced by $\|u\|_{L^2(\Omega)}$. Under an appropriate smoothness condition on the boundary Γ of Ω the preceding interior regularity result can be extended to all of Ω.

Theorem II.8. *Let us assume, in addition to the hypothesis of Theorem II.7, that* Γ *is of class* C^2 *and that there exists a function* $\phi \in H^2(\Omega)$ *for which* $u - \phi \in H_0^1(\Omega)$. *Then we have also* $u \in H^2(\Omega)$ *and*

$$\|u\|_{H^2(\Omega)} \leq C(\|u\|_{L^2(\Omega)} + \|f\|_{L^2(\Omega)} + \|\phi\|_{H^2(\Omega)})$$

where $C = C(N, \lambda, K, \partial\Omega)$.

In case when we assume Ω to be convex without the assumption of smoothness of the domain, we again obtain the regularity of the solution to the Poisson problem. See e.g., [31, 40]

Theorem II.9. *Let* Ω *be a convex, bounded and open subset of* $\mathbb{R}^N$. *Then for each* $f \in L^2(\Omega)$, *there exists a unique* $u \in H^2(\Omega)$ *satisfying*

$$\Delta u = f \quad in \quad \Omega,$$
$$u = 0 \quad on \quad \Gamma.$$

Moreover, there exists a constant $C = C(\Omega)$ *such that*

$$\|u\|_{H^2(\Omega)} \leq C\|f\|_{L^2(\Omega)}.$$

CHAPTER III

THE HELMHOLTZ EQUATION AND OUTGOING RADIATION CONDITION

In this chapter we introduce the Helmholtz equation and define an outgoing radiation condition. As model problems under consideration reduce to the Helmholtz equation on the outside of a bounded domain, understanding solutions to the Helmholtz equation is important. We introduce two ways to describe solutions to the Helmholtz equation. One is a series representation using spherical Hankel functions and spherical harmonics. The other is an integral formula using the fundamental solution to the Helmholtz equation. These representation formulae will be used to develop the computational technique based on PML. In addition to the Helmholtz equation, resonance functions satisfy a certain *outgoing radiation condition* at infinity. This is also discussed in this chapter.

A. The Helmholtz equation and model problems

Consider the wave equation

$$\Delta U(x,t) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}U(x,t).$$

Here c is the speed of a wave such as light or sound. U is a velocity potential and has a relation with the velocity field v and pressure p as follows:

$$v = \frac{1}{\rho_0}\nabla U, \quad p = -\frac{\partial U}{\partial t} \tag{III.1}$$

with the density ρ_0 at a steady state. If we assume that solutions of the wave equation are time-harmonic, then solutions are of the form $U(x,t) = u(x)e^{\pm i\omega t}$ with frequency ω. There are two choices of a time dependence of $e^{\pm i\omega t}$. The choice is arbitrary as long as it is used consistently. Substituting $U(x,t)$ with $u(x)e^{\pm i\omega t}$ produces the Helmholtz equation

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

where $k = \omega/c$ is called the *wave number*.

As a model problem, we shall consider a resonance problem in three dimensional space which results from a compactly supported perturbation of the negative Laplacian, i.e.,

$$Lu = -\Delta u + L_1 u,$$

where L_1 is symmetric and lives on a bounded domain $\Omega \subset \mathbb{R}^3$. A *resonance* value is defined as k such that there are non-trivial functions ψ satisfying

$$L\psi = k^2\psi \tag{III.2}$$

and an *outgoing radiation condition* corresponding to the wave number k. In Section C we will discuss the outgoing radiation condition to be imposed on the model problem. We note that the equation reduces to the Helmholtz equation outside of Ω. General solutions to the Helmholtz equation are examined in the following sections.

The model problem has only the essential spectrum on $[0, \infty)$ and has no eigenvalues. It has resonance values instead of eigenvalues. We will see that resonance functions of the model problem grow exponentially and hence can be thought as "improper eigenfunctions".

A simple example of the model problem is the problem that stems from classical scattering theory such as the time-harmonic acoustic waves by a penetrable bounded inhomogeneous medium and by a bounded impenetrable obstacle. In case of a penetrable bounded inhomogeneous medium, the problem is to find non-trivial solutions ψ and k such that

$$\Delta\psi + k^2 a(x)\psi = 0 \quad \text{in} \quad \mathbb{R}^3$$

and ψ satisfies an outgoing radiation condition. Here a is the refractive index defined by the ratio of the square of the phase velocity of a wave in a host medium to the square of the phase velocity in the inhomogeneous medium, i.e., if c denotes the phase velocity function on $\mathbb{R}^3$ such that c is a constant c_0 on the host medium, then $a = c_0^2/c^2$. The continuity of the pressure and of the normal velocity across the interface leads to *transmission conditions* at the interface of two media:

- continuity of ψ (that is obtained from the continuity of pressure in (III.1)),
- continuity of $c^2\dfrac{\partial\psi}{\partial n}$ (that is obtained from the continuity of the normal velocity across the interface in (III.1) and the fact that ρ_0 is proportional to $1/c^2$).

A similar situation occurs in the study of a photonic crystal membrane resonator. In this case the continuity of u and its normal derivative at the interface is required. Due to variable dielectric constants in each medium this structure produces resonances.

In case of an impenetrable Lipschitz continuous obstacle Ω, the problem is to find non-trivial solutions ψ and k such that

$$\Delta\psi + k^2\psi = 0 \quad \text{in} \quad \mathbb{R}^3 \setminus \bar{\Omega},$$
$$\frac{\partial\psi}{\partial n} = 0 \quad \text{on} \quad \partial\Omega,$$

and ψ satisfies an outgoing radiation condition. This problem arises from, for example, the study on aerodynamic noise such as slat and flap noise from an airplane wing.

On the other hand, resonance phenomenon occurs in quantum mechanics as well, for instance, resonance values of a Schrödinger equation

$$-\Delta\psi + V\psi = k^2\psi \quad \text{in} \quad \mathbb{R}^3$$

with a compactly supported potential V. These resonances are identified as eigenvalues of a spectrally deformed Schrödinger operator and they are interpreted as states with finite lifetimes of unstable atoms or molecules.

B. Series representation for solutions to the Helmholtz equation

We shall find a general solution to the Helmholtz equation in the exterior of a sphere in $\mathbb{R}^3$. To do this, we first deliver a short description for spherical harmonics and spherical Bessel functions.

Definition III.1. A *spherical harmonic* of order n is the restriction of a homogeneous harmonic polynomial of degree n to the unit sphere.

Recall that in terms of spherical coordinates

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \Delta_{S^2},$$

where Δ_{S^2} is the Laplace-Beltrami operator on the sphere or spherical Laplacian defined by

$$\Delta_{S^2} = \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

(here θ represents the polar angle from z-axis and ϕ the azimuthal angle in xy-plane). Every homogeneous polynomial of degree n is of the form $H_n = r^n Y_n(\theta,\phi)$. If H_n is harmonic, i.e., $\Delta H_n = 0$, then it satisfies

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y_n}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y_n}{\partial\phi^2} = -n(n+1)Y_n.$$

In other words, the spherical harmonic Y_n is an eigenfunction of the spherical Laplacian Δ_{S^2} on the unit sphere associated with the eigenvalue $-n(n+1)$. Some important properties of spherical harmonics are given in the following theorem (See, for instance, [21]):

Theorem III.2. *Let S^2 be the unit sphere in $\mathbb{R}^3$.*

1. *There exist exactly* $2n+1$ *linearly independent spherical harmonics of order* n*, which are denoted by* Y_n^m *for* $-n \le m \le n$*.*
2. *Suitably normalized spherical harmonics* Y_n^m *for* $n = 0, 1, 2, \ldots,$ *and* $|m| \le n$ *form an orthonormal basis in* $L^2(S^2)$*.*

We look for solutions to the Helmholtz equation of the form

$$u(x) = f(k|x|)Y_n(\hat{x}),$$

where Y_n is a spherical harmonic of order n and $\hat{x} = x/|x|$ for $x \neq 0$. u solves the Helmholtz equation provided that f satisfies the *spherical Bessel differential equation*

$$r^2 f''(r) + 2rf'(r) + (r^2 - n(n+1))f(r) = 0.$$

There are two linearly independent solutions j_n and y_n to the spherical Bessel differential equation, which are called *spherical Bessel functions* of order n. j_n and y_n are defined recursively by the formula: for $f_n = j_n$ or $f_n = y_n$ and for $n = 1, 2, \ldots$,

$$f_{n-1}(r) + f_{n+1}(r) = (2n+1)r^{-1}f_n(r)$$

with

$$\begin{aligned} j_0(r) &= \frac{\sin r}{r}, \qquad & j_1(r) &= \frac{\sin r}{r^2} - \frac{\cos r}{r} \\ y_0(r) &= -\frac{\cos r}{r}, \qquad & y_1(r) &= -\frac{\cos r}{r^2} - \frac{\sin r}{r}. \end{aligned}$$

The linear combinations

$$h_n^1 = j_n + iy_n, \qquad h_n^2 = j_n - iy_n$$

are called *spherical Hankel functions* of the first kind and second kind of order n, respectively. See e.g., [1, 21] for properties of the spherical Hankel functions.

We give a brief description of properties that are required to develop our theory.

The spherical Hankel functions are of the form

$$h_n^1(r) = (-i)^n \frac{e^{ir}}{ir} \left\{ 1 + \sum_{p=1}^{n} \frac{a_{pn}}{r^p} \right\}, \quad h_n^2(r) = i^n \frac{e^{-ir}}{-ir} \left\{ 1 + \sum_{p=1}^{n} \frac{\bar{a}_{pn}}{r^p} \right\} \tag{III.3}$$

with complex coefficients $a_{1n}, \ldots, a_{nn}$. The recursive formula for the spherical Bessel functions implies

$$h_{2n}^2(-r) = h_{2n}^1(r) \text{ and } h_{2n-1}^2(-r) = -h_{2n-1}^1(r) \tag{III.4}$$

for $n = 0, 1, 2, \ldots$. From (III.3) the asymptotic behavior of the spherical Hankel functions for large argument is obtained:

$$h_n^l(r) = \frac{1}{r} e^{\pm i(r - \frac{n\pi}{2} - \frac{\pi}{2})} \left\{ 1 + O\left(\frac{1}{r}\right) \right\}, \quad r \to \infty, \tag{III.5}$$

$$h_n^{l\,\prime}(r) = \frac{1}{r} e^{\pm i(r - \frac{n\pi}{2})} \left\{ 1 + O\left(\frac{1}{r}\right) \right\}, \quad r \to \infty \tag{III.6}$$

with $l = 1, 2$. $l = 1$ is attached to the upper sign in the double signs and the lower sign for $l = 2$.

We shall be interested in C^2 solutions to the Helmholtz equation on domains away from the origin. It is enough to find solutions on an annulus $A_{r_0,r_1} = \{x \in \mathbb{R}^3 : r_0 < |x| < r_1\}$ with any two positive numbers $r_0 < r_1$. From here on, r denotes the distance from the origin to x, and $\hat{x} = x/|x|$ for $x \neq 0$.

Theorem III.3. *Let k be a complex number in $\mathbb{C} \setminus \mathbb{R}^-$. Suppose that $u \in C^2(\bar{A}_{r_0,r_1})$. If u satisfies the Helmholtz equation in A_{r_0,r_1}, then u is of the form*

$$u(x) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (a_{n,m} h_n^1(k|x|) + b_{n,m} h_n^2(k|x|)) Y_n^m(\hat{x}). \tag{III.7}$$

The series converges in L^2 sense on $|x| = r$ with $r_0 \leq r \leq r_1$ and in $L^2(A_{r_0,r_1})$.

Proof. Since the spherical harmonics comprise an complete orthonormal system, u

can be written as

$$u(x) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} f_{n,m}(r) Y_n^m(\hat{x})$$

with

$$f_{n,m}(r) = \int_{S^2} u(r\hat{x}) \overline{Y_n^m}(\hat{x}) \, \mathrm{d}\hat{x}.$$

Here the series converges in L^2 sense on each $|x| = r$ with $r_0 \leq r \leq r_1$ and $\mathrm{d}\hat{x}$ is the surface element on the unit sphere. Since the integrand in the integral above is $C^2(A_{r_0,r_1})$, $f_{n,m}$ is in $C^2((r_0, r_1))$. Moreover, $f_{n,m}$ satisfies

$$r^2 f''_{n,m}(r) + 2r f'_{n,m}(r) + (r^2 k^2 - n(n+1)) f_{n,m}(r) = 0. \tag{III.8}$$

Indeed, consider $\chi \in C_0^\infty((r_0, r_1))$ and define $\tilde{\chi}(x) = \chi(|x|) Y_n^m(\hat{x}) \in C_0^\infty(A_{r_0,r_1})$. Using the integration by parts with respect to r and the orthonormality of the spherical harmonics,

$$\begin{aligned}
0 &= \int_{A_{r_0,r_1}} (\Delta u + k^2 u) \, \overline{\tilde{\chi}} \, \mathrm{d}x \\
&= \int_{S^2} \int_{r_0}^{r_1} u(r\hat{x}) \left[\frac{\mathrm{d}}{\mathrm{d}r} \left(r^2 \frac{\mathrm{d}\overline{\chi}}{\mathrm{d}r}(r) \right) \overline{Y_n^m}(\hat{x}) - n(n+1) \overline{\chi}(r) \overline{Y_n^m}(\hat{x}) + r^2 k^2 \overline{\chi}(r) \overline{Y_n^m}(\hat{x}) \right] \mathrm{d}r \mathrm{d}\hat{x} \\
&= \int_{r_0}^{r_1} f_{n,m}(r) \left[\frac{\mathrm{d}}{\mathrm{d}r} \left(r^2 \frac{\mathrm{d}\overline{\chi}}{\mathrm{d}r}(r) \right) - n(n+1) \overline{\chi}(r) + r^2 k^2 \overline{\chi}(r) \right] \mathrm{d}r \\
&= \int_{r_0}^{r_1} \left[r^2 \frac{\mathrm{d}^2 f_{n,m}}{\mathrm{d}r^2}(r) + 2r \frac{\mathrm{d} f_{n,m}}{\mathrm{d}r}(r) + \left(r^2 k^2 - n(n+1) \right) f_{n,m}(r) \right] \overline{\chi}(r) \, \mathrm{d}r.
\end{aligned} \tag{III.9}$$

Since (III.9) holds for any $\chi \in C_0^\infty((r_0, r_1))$, we obtain (III.8).

The initial value problem (III.8) with the initial conditions

$$f_{n,m}(r_0) = \int_{S^2} u(r_0\hat{x}) Y_n^m(\hat{x}) \, \mathrm{d}\hat{x} \quad \text{and} \quad f'_{n,m}(r_0) = \int_{S^2} \frac{\partial u}{\partial r}(r_0\hat{x}) Y_n^m(\hat{x}) \, \mathrm{d}\hat{x} \tag{III.10}$$

has a unique solution. It follows that $f_{n,m}$ is of the form

$$f_{n,m}(r) = a_{n,m} h_n^1(kr) + b_{n,m} h_n^2(kr)$$

for some constants $a_{n,m}$ and $b_{n,m}$.

If u_n is a partial sum of the series, then by the Parseval's theorem

$$\|u(r,\cdot) - u_n(r,\cdot)\|^2_{L^2(S^2)} \leq \|u(r,\cdot)\|^2_{L^2(S^2)} \text{ for each } r \in [r_0, r_1].$$

Since the right-hand function $\|u(r,\cdot)\|^2_{L^2(S^2)}$ is integrable over $[r_0, r_1]$, by the dominated convergence theorem

$$\begin{aligned}\lim_{n\to\infty} \int_{A_{r_0,r_1}} |u(x) - u_n(x))|^2 \,\mathrm{d}x &= \lim_{n\to\infty} \int_{r_0}^{r_1} \|u(r,\cdot) - u_n(r,\cdot)\|^2_{L^2(S^2)} r^2 \,\mathrm{d}r \\ &= \int_{r_0}^{r_1} \lim_{n\to\infty} \|u(r,\cdot) - u_n(r,\cdot)\|^2_{L^2(S^2)} r^2 \,\mathrm{d}r \\ &= 0,\end{aligned}$$

which shows the convergence of u_n in $L^2(A_{r_0,r_1})$. □

C. Outgoing radiation condition

For a spherical harmonic Y_n, there are two types of solutions to the Helmholtz equation:

$$u(x) = h_n^1(k|x|)Y_n(\hat{x}) \quad \text{and} \quad v(x) = h_n^2(k|x|)Y_n(\hat{x}).$$

When we determine whether a wave is *incoming* or *outgoing*, we need to go to the time-harmonic solutions to the wave equation. The leading terms of expression (III.3) of h_n^1 and h_n^2 determine the behavior of the waves. The following are the leading terms of the waves corresponding to $h_n^1(kr)e^{-i\omega t}$, $h_n^2(kr)e^{-i\omega t}$, $h_n^1(kr)e^{i\omega t}$ and $h_n^2(kr)e^{i\omega t}$, respectively:

$$\frac{e^{ikr-i\omega t}}{ikr} = \frac{e^{-\mathrm{Im}(k)(r-ct)}}{ikr}\left[\cos(\mathrm{Re}(k)(r-ct)) + i\sin(\mathrm{Re}(k)(r-ct))\right], \tag{III.11}$$

$$\frac{e^{-ikr-i\omega t}}{-ikr} = \frac{e^{\mathrm{Im}(k)(r+ct)}}{-ikr}\left[\cos(\mathrm{Re}(k)(r+ct)) - i\sin(\mathrm{Re}(k)(r+ct))\right], \tag{III.12}$$

$$\frac{e^{ikr+i\omega t}}{ikr} = \frac{e^{-\mathrm{Im}(k)(r+ct)}}{ikr}\left[\cos(\mathrm{Re}(k)(r+ct)) + i\sin(\mathrm{Re}(k)(r+ct))\right], \tag{III.13}$$

$$\frac{e^{-ikr+i\omega t}}{-ikr} = \frac{e^{\mathrm{Im}(k)(r-ct)}}{-ikr}\left[\cos(\mathrm{Re}(k)(r-ct)) - i\sin(\mathrm{Re}(k)(r-ct))\right]. \tag{III.14}$$

Among them, only $h_n^1(kr)e^{-i\omega t}$ and $h_n^2(kr)e^{i\omega t}$ are traveling out from the origin and represent outgoing waves. Therefore, when a series representation (III.7) for solutions is available, the expansion with spherical Hankel functions of the first kind

$$\sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{n,m}h_n^1(kr)Y_n^m(\hat{x}) \tag{III.15}$$

coupled with the time variable function $e^{-i\omega t}$ represents an outgoing wave. On the other hand,

$$\sum_{n=0}^{\infty}\sum_{m=-n}^{n} b_{n,m}h_n^2(kr)Y_n^m(\hat{x}) \tag{III.16}$$

coupled with $e^{i\omega t}$ is outgoing. Since (III.16) with wave number k can be written as (III.15) with wave number $-k$, we will say that a solution to the Helmholtz equation satisfies the *outgoing radiation condition* at infinity if it has a series representation (III.15). This outgoing radiation condition will be imposed to the model problem.

Remark III.4. For $k \in \mathbb{R}$, we have a uniqueness result for (III.2) with the outgoing radiation condition (III.15) by the proof of Theorem IV.4 without an essential change. If $\mathrm{Im}(k) > 0$, then $h_n^1(kr)$ decays exponentially and hence solutions to (III.2) that could be expanded as (III.15) away from the origin are square integrable. Since the model problem has no non-trivial solutions in $L^2(\mathbb{R}^3)$, resonance values must appear in the region of $\text{Im}(k) < 0$. The negative imaginary part of resonance values k makes the waves associated with k grow exponentially at infinity at a fixed time but damped at each point, where the series expansion is available, with time increasing by (III.11).

Remark III.5. If we choose (III.16) for a definition of an outgoing radiation condition, then resonance values will be located in the region of $\text{Im}(k) > 0$. However, the resonance functions pertained to k are identical to ones that are defined with the outgoing radiation condition (III.15) with $-k$. Obviously, k and $-k$ have the same square and the resonance function is the improper eigenfunction to (III.2) associated with k^2. The important role of the definition of an outgoing radiation condition is that functions satisfying an outgoing radiation condition are expanded with only one type of spherical Hankel functions.

D. Green's representation theorem

In this section we discuss an integral formula for solutions to the Helmholtz equation with $\text{Im}(k) \geq 0$. To do this, we first introduce a boundary condition at infinity. For exterior problems, a boundary condition at infinity is required in order to have uniqueness of solutions to the Helmholtz equation.

Definition III.6. Let u be a solution to the Helmholtz equation in the exterior of a bounded domain. u is said to satisfy the *Sommerfeld radiation condition* provided that u fulfills the condition

$$\lim_{r\to\infty} r\left(\frac{\partial u}{\partial r} - iku\right) = 0 \tag{III.17}$$

uniformly in all directions $\hat{x} = x/|x|$.

This condition was proposed by Sommerfeld [53] for a scattering problem for k real and positive.

Assume that $\mathrm{Im}(k) \geq 0$. From (III.5)

$$\begin{aligned}\frac{\mathrm{d}h_n^l(kr)}{\mathrm{d}r} - ikh_n^l(kr) &= kh_n^{l\,\prime}(kr) - ikh_n^l(kr) \\ &= (\mp i)^n k\frac{e^{\pm ikr}}{kr}\left\{1 + O\left(\frac{1}{r}\right)\right\} - (\mp i)^n k\frac{e^{\pm ikr}}{kr}\left\{1 + O\left(\frac{1}{r}\right)\right\} \\ &= (\mp i)^n e^{\pm ikr} O\left(\frac{1}{r^2}\right)\end{aligned}$$

with $l = 1, 2$. It follows that $h_n^1(k|x|)$ satisfies the Sommerfeld radiation condition, but $h_n^2(k|x|)$ does not. This condition gets rid of blowing-up functions $h_n^2(k|x|)$ and takes decaying functions $h_n^1(k|x|)$. For $\mathrm{Im}(k) \geq 0$, the Sommerfeld radiation condition (III.17) is equivalent to the series expansion (III.15) (See, e.g., [21]). In [22], it is shown that the Sommerfeld radiation condition makes solutions decay and ensures uniqueness for solutions to scattering problems.

The Green's integral formula is deduced from the fundamental solution to the Helmholtz equation

$$\Phi(x, y) = \frac{e^{ik|x-y|}}{4\pi|x - y|},$$

that satisfies

$$-\Delta\Phi(x, y) - k^2\Phi(x, y) = \delta(x - y),$$

where $\delta(x)$ is the Dirac delta function. There are two possible fundamental solution to the Helmholtz equation:

$$\frac{e^{ik|x-y|}}{4\pi|x - y|} \quad \text{and} \quad \frac{e^{-ik|x-y|}}{4\pi|x - y|}.$$

Φ is the one satisfying the Sommerfeld radiation condition. Indeed, for a fixed $y \in \mathbb{R}^3$

$$\nabla_x\Phi(x, y) = \left(ik - \frac{1}{|x - y|}\right)\frac{e^{ik|x-y|}}{4\pi|x - y|}\frac{x - y}{|x - y|},$$

and

$$|x-y| = |x| - \hat{x}\cdot y + O\left(\frac{1}{|x|}\right). \tag{III.18}$$

Then

$$\begin{aligned}
&\frac{\partial \Phi}{\partial r_x}(x,y) - ik\Phi(x,y) \\
&\quad = ik\left(\frac{(x-y)\cdot x}{|x-y||x|} - 1\right)\frac{e^{ikr}}{4\pi|x-y|} - \frac{e^{ik|x-y|}}{4\pi|x-y|^2}\frac{(x-y)\cdot x}{|x-y||x|} \\
&\quad = ik\left(\frac{|x|^2 + |x-y|^2 - |y|^2}{|x-y||x|} - 1\right)\frac{e^{ik|x-y|}}{4\pi|x-y|} - \frac{e^{ik|x-y|}}{4\pi|x-y|^2}\frac{(x-y)\cdot x}{|x-y||x|} \\
&\quad = ik\left(\frac{(|x|-|x-y|)^2 - |y|^2}{|x-y||x|}\right)\frac{e^{ik|x-y|}}{4\pi|x-y|} - \frac{e^{ik|x-y|}}{4\pi|x-y|^2}\frac{(x-y)\cdot x}{|x-y||x|} \\
&\quad = O\left(\frac{1}{|x|^2}\right), \quad |x|\to\infty,
\end{aligned}$$

because $(|x|-|x-y|)^2 - |y|^2 = O(1)$ by (III.18) and $|x||x-y| = O(|x|^2)$.

Let Ω be a bounded domain of class C^2 and n denote the unit normal vector to the boundary $\partial\Omega$ directed into the exterior of Ω. Then we have the Green's representation theorem [22].

Theorem III.7. *Let $u \in C^2(\mathbb{R}^3 \setminus \bar{\Omega}) \cap C(\mathbb{R}^3 \setminus \bar{\Omega})$ be a solution to the Helmholtz equation*

$$\Delta u + k^2 u = 0 \quad in \quad \mathbb{R}^3 \setminus \bar{\Omega}$$

with $\mathrm{Im}(k) \geq 0$ *satisfying the Sommerfeld radiation condition* (III.17). *Then*

$$u(x) = \int_{\partial\Omega}\left[u(y)\frac{\partial\Phi(x,y)}{\partial n_y} - \frac{\partial u}{\partial n}(y)\Phi(x,y)\right]\mathrm{d}S_y \quad for \quad x \in \mathbb{R}^3 \setminus \bar{\Omega}.$$

Here $\mathrm{d}S_y$ *is the surface element on* $\partial\Omega$.

CHAPTER IV

PERFECTLY MATCHED LAYER AND RESONANCE PROBLEMS

In this chapter we introduce the basic idea of the perfectly matched layer (PML) method and reformulate the resonance model problem. The perfectly matched layer is an artificial boundary condition technique which can be thought of introducing an artificial absorbing layer. The goal is to create a layer surrounding a bounded scatterer or inhomogeneous medium which damps all waves that strike it without producing reflected waves. Due to the damping property of the PML, some of the resonance functions are converted to exponentially decaying functions. This means that PML transforms the resonance problem into a standard eigenvalue problem.

We will show that the PML problem in the infinite domain gives rise to a well-posed in a variational formulation. The resulting well-defined inverse operator T from $H^1(\mathbb{R}^3)$ to $H^1(\mathbb{R}^3)$ follows. We will show exponential decay of eigenfunctions of the PML problem in the infinite domain, which will play a key role in analyzing the convergence of approximate eigenvalues.

A. Perfectly matched layer

The PML method can be well illustrated by example. Consider a simple one-dimensional scattering problem

$$u'' + k^2 u = 0 \quad \text{on} \quad (0, \infty)$$
$$u(0) = g$$

with the Sommerfeld radiation condition

$$\frac{\mathrm{d}u}{\mathrm{d}r} - iku = 0.$$

Here k is a positive wave number and g is a given Dirichlet data. The general solution to the Helmholtz equation in $\mathbb{R}$ is of the form

$$u(x) = c_1 e^{ikx} + c_2 e^{-ikx}$$

with some constants c_1 and c_2. The Sommerfeld radiation condition takes only the outgoing function so that the analytic solution to the problem is

$$u(x) = g e^{ikx} \quad \text{for} \quad x \in (0, \infty).$$

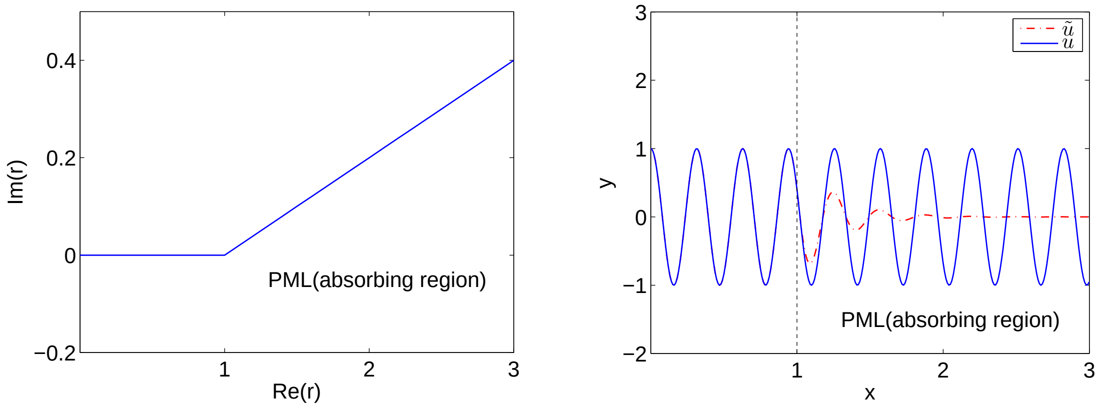
Now we want to approximate the solution in a bounded domain of computational interest, e.g., $\Omega_0 = (0, r_0)$ using finite elements. There are two difficulties in approximating the solution: one is that the domain is infinite and the other is that the real and imaginary part of the solution are oscillating. PML enables us to avoid these difficulties. PML is introduced by using a complex coordinate stretching

$$\tilde{r} = \begin{cases} r & \text{if} \;\; 0 \le r \le r_0, \\ r + i \displaystyle\int_{r_0}^{r} \sigma(s) \, \mathrm{d}s & \text{if} \;\; r_0 < r, \end{cases}$$

where σ is a positive function. A simple example for σ is a constant function σ_0. The plot of $\tilde{r}$ with $r_0 = 1$ and $\sigma_0 = 0.2$ is shown in Figure 1(a). By the definition, $\tilde{r}$ is equal to r for $0 \le r \le r_0$ and complexified for $r > r_0$, and the PML is the region on which r is deformed into the complex plane. We define the PML solution $\tilde{u}(r) := u(\tilde{r})$. Let d denote the derivative of $\tilde{r}$ and so d is defined as

$$d = \begin{cases} 1 & \text{if} \;\; 0 \le r < r_0, \\ 1 + i\sigma_0 & \text{if} \;\; r_0 < r. \end{cases}$$

Then $\tilde{u}$ preserves u in the region of $0 < r < r_0$, and is attenuated inside the PML as in Figure 1(b). The PML acts like an absorbing material without producing reflected



(a) Complex coordinate stretching (b) Graphs of the real part of u and $\tilde{u}$

Fig. 1. Complex stretching and a PML solution

waves. The PML solution $\tilde{u}$ satisfies

$$\frac{1}{d}\left(\frac{1}{d}\tilde{u}'\right)' + k^2\tilde{u} = 0 \quad \text{for} \quad r \in (0, r_0) \cup (r_0, \infty).$$

with the continuity of $\tilde{u}'/d$ across the interface $r = r_0$, which is deduced from the continuity of u' at the interface. Utilizing the continuity of $\tilde{u}'/d$ at the interface, a corresponding weak formulation on the infinite domain is to find $\tilde{u} \in H^1((0,\infty))$ such that $\tilde{u}(0) = g$ and satisfying

$$\int_0^{r_\infty} \frac{1}{d}\tilde{u}'\bar{\phi}'\,\mathrm{d}r - \int_0^{r_\infty} k^2 d\tilde{u}\bar{\phi}\,\mathrm{d}r = 0 \quad \text{for all} \quad \phi \in H_0^1((0,\infty)).$$

Due to the exponential decay of the PML solution $\tilde{u}$, we can truncate the problem to a finite domain $\Omega_\delta = (0, r_\infty)$ with a sufficiently large $r_\infty > r_0$ and impose a convenient boundary condition at the artificial boundary $r = r_\infty$, e.g, the homogeneous Dirichlet boundary condition. Although no longer the exact solution inside, the difference between u and $\tilde{u}_t$ on $(0, r_0)$ is exponentially small. A finite elements method on the truncated domain can gives an approximation for the exact solution u on $(0, r_0)$.

So far, we discussed the basic idea of the PML method for a scattering problem in

$\mathbb{R}$. The complex stretching function we have chosen in the example does not depend on frequency ω and hence the attenuation rate in the PML varies depending on the wave number. In contrast, Collino and Monk [20] used a complex stretching function depending on frequency such as

$$\tilde{r} = \begin{cases} r & \text{if } \ 0 \le r \le r_0, \\ r + \dfrac{i}{\omega} \displaystyle\int_{r_0}^{r} \sigma(s)\,\mathrm{d}s & \text{if } \ r_0 < r. \end{cases}$$

In this case, the attenuation rate is independent of frequency ω because the PML solution $\tilde{u}$ is of the form

$$Ce^{ikr}e^{-k/\omega \int_{r_0}^{r} \sigma(s)\,\mathrm{d}s} = Ce^{ikr}e^{-1/c \int_{r_0}^{r} \sigma(s)\,\mathrm{d}s}$$

for $r > r_0$, where c is a constant phase velocity of the wave on a host medium.

For PML resonance problems, we will use a complex stretching independent of the wave number as in the example. This results in wave number dependent decay. When this decay is stronger than the exponential growth of the resonance eigenfunction, this eigenfunction is transformed into a proper eigenfunction for the PML equation on the infinite domain.

B. Spherical PML reformulation for the resonance problem

We consider a linear operator

$$L = -\Delta + L_1,$$

where L_1 is a linear operator with support contained in the ball $\bar{\Omega}_0$ centered at the origin of radius r_0. For example, we can consider Schrödinger operators $-\Delta + V$ with a real valued potential V supported in $\bar{\Omega}_0$. We shall concentrate on this example as more general applications are similar.

We consider the Helmholtz problem:

$$Lu - k^2 u = f \quad \text{on} \quad \mathbb{R}^3. \tag{IV.1}$$

Here k is a complex number and the support of f is contained in Ω_0. We need to set a "boundary condition" at infinity. We consider solutions which are outgoing. Since L coincides with $-\Delta$ outside of Ω_0, u can be expanded in terms of spherical Hankel functions and spherical harmonics. Because the solutions are outgoing, this expansion takes the form

$$u(x) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{n,m} h_n^1(kr) Y_n^m(\hat{x}) \quad \text{for} \quad r \geq r_0. \tag{IV.2}$$

We shall be interested in weak solutions of (IV.1) which are, at least, locally in H^1. This means that the series (IV.2) converges in $H^{1/2}(\Gamma_0)$, where Γ_0 is the boundary of Ω_0. It follows that the series converges in H^1 on any annular domain $r_0 < r < R$ (see Theorem IV.2 below).

Remark IV.1. Resonances are solutions of (IV.1) with $f = 0$ satisfying the outgoing condition. For resonances, the resonance value k has a negative imaginary part and so u increases exponentially as r becomes large. Accordingly, the Sommerfeld radiation condition

$$\lim_{r \to \infty} r \left(\frac{\partial u}{\partial r} - iku \right) = 0 \tag{IV.3}$$

is not satisfied in this case. There are no exponentially decreasing eigenfunctions for this equation corresponding to any k with non-zero imaginary part.

We consider using a complex coordinate stretching to define a perfectly matched layer surrounding the support of V. A non-smooth complex stretching was utilized in the previous example in $\mathbb{R}$. In the higher dimensional space we will use a spherical PML such that the complex stretching function is C^2 and the resulting PML equation is reduced to a Helmholtz equation with a complex constant coefficient outside of the ball. The second condition enables us to easily show the rapid decay of eigenfunctions of the PML equation[†].

The PML approach [13] provides a convenient way to deal with (IV.1) with the outgoing radiation condition. Let r_1 be greater than r_0 and Ω_1 denote the open ball of radius r_1 centered at the origin with the boundary Γ_1.

The PML problem is defined in terms of a function $\tilde{\sigma} \in C^2(\mathbb{R}^+)$ satisfying

$$\tilde{\sigma}(r) = \begin{cases} 0 & \text{for } \; 0 \le r < r_0, \\ \text{increasing} & \text{for } \; r_0 \le r < r_1, \\ \sigma_0 & \text{for } \; r_1 \le r. \end{cases} \tag{IV.4}$$

A typical C^2 function in $[r_0, r_1]$ with this property is given by

$$\tilde{\sigma}(x) = \sigma_0 \frac{\displaystyle\int_{r_0}^{x} (t - r_0)^2 (r_1 - t)^2 \, \mathrm{d}t}{\displaystyle\int_{r_0}^{r_1} (t - r_0)^2 (r_1 - t)^2 \, \mathrm{d}t}.$$

The PML approximation can be thought of as a formal complex shift in coordinate system with $\tilde{r} = r(1 + i\tilde{\sigma}(r))$. See Figure 2 for the graph of the imaginary part of $\tilde{r}$ as a function of r. The PML solution is defined by

$$\tilde{u}(x) = \begin{cases} u(x), \quad \text{for } \; |x| \le r_0, \\ \displaystyle\sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{n,m} h_n^1(k\tilde{r}) Y_n^m(\hat{x}), \quad \text{for } \; r = |x| \ge r_0. \end{cases} \tag{IV.5}$$

Here $a_{n,m}$ is coefficients from the series for u.

Clearly, $\tilde{u}$ and u coincide for $|x| \le r_0$. Moreover, $\tilde{u}$ satisfies

$$\widetilde{L}\tilde{u} - k^2 \tilde{u} = f \quad \text{in } \; \mathbb{R}^3, \tag{IV.6}$$

[†]This is not true in the Cartesian case.

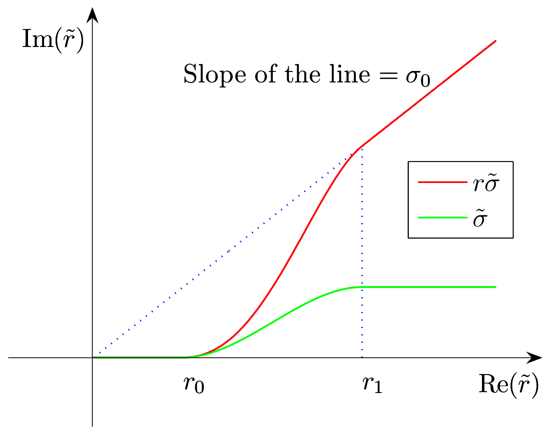


Fig. 2. Complex coordinate stretching

where $\widetilde{L}$ coincides with L for $|x| \leq r_0$ and is given, in spherical coordinates (r, θ, ϕ), by

$$\begin{aligned}\widetilde{L}v = -\Bigg(&\frac{1}{\tilde{d}^2 d r^2}\frac{\partial}{\partial r}\left(\frac{\tilde{d}^2 r^2}{d}\frac{\partial v}{\partial r}\right) + \frac{1}{\tilde{d}^2 r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial v}{\partial \theta}\right) \\ &+ \frac{1}{\tilde{d}^2 r^2 \sin^2\theta}\frac{\partial^2 v}{\partial \phi^2}\Bigg) + Vv.\end{aligned} \tag{IV.7}$$

or, in Cartesian coordinates, by

$$\widetilde{L}v = -\frac{1}{\tilde{d}^2 d}\nabla \cdot \left[\left(\frac{\tilde{d}^2}{d}P(x) + d(I - P(x))\right)\nabla v\right] + Vv.$$

Here $P(x)$ is the orthogonal projection onto the $\hat{x} = x/|x|$-direction, and $\tilde{d} \equiv 1 + i\tilde{\sigma}$ and $d \equiv \tilde{r}' = 1 + i\sigma$ with $\sigma \equiv \tilde{\sigma} + r\tilde{\sigma}'$.

We shall see that (IV.6) has a well-posed variational formulation in $H^1(\mathbb{R}^3)$ when k is real and positive. Let χ be in $C_0^\infty(\mathbb{R}^3)$. Assuming that $\tilde{u}$ is locally in $H^1(\mathbb{R}^3)$, we have

$$A(\tilde{u}, \chi) - k^2 B(\tilde{u}, \chi) = (\tilde{d}^2 f, \chi)_{\mathbb{R}^3}, \tag{IV.8}$$

where

$$A(\tilde{u},\chi) \equiv \left(\frac{\tilde{d}^2}{d}\frac{\partial \tilde{u}}{\partial r}, \frac{\partial}{\partial r}\left(\frac{\chi}{\bar{d}}\right)\right)_{\mathbb{R}^3} + \left(\frac{1}{r^2}\frac{\partial \tilde{u}}{\partial \theta}, \frac{\partial \chi}{\partial \theta}\right)_{\mathbb{R}^3} + \left(\frac{1}{r^2 \sin^2\theta}\frac{\partial \tilde{u}}{\partial \phi}, \frac{\partial \chi}{\partial \phi}\right)_{\mathbb{R}^3} + (V\tilde{u},\chi)_{\Omega_0} \tag{IV.9}$$

and

$$B(\tilde{u},\chi) \equiv (\tilde{d}^2\tilde{u},\chi)_{\mathbb{R}^3}. \tag{IV.10}$$

For an open set $D \subset \mathbb{R}^3$, $(\cdot,\cdot)_D$ denotes the L^2 Hermitian inner-product on D.

The PML problem corresponding to a scattering problem was studied in [13] however the techniques there easily extend to our problem. We consider first the case when k is real and positive. In this case, the Sommerfeld radiation condition can be used as a replacement of the outgoing condition. To obtain a uniqueness result for the PML problem for k real and positive, we introduce the following theorem as in Theorem III.3. Let A_{r_0,r_2} be an annulus bounded by two spheres of radius $r_0 < r_2$.

Theorem IV.2. *Let k be a non-zero complex number not on the negative real axis. Suppose that $u \in H^1(A_{r_0,r_2})$ satisfies $A(u,v) = k^2 B(u,v)$ for all $v \in C_0^\infty(A_{r_0,r_2})$, then*

$$u(x) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(a_{n,m}h_n^1(k\tilde{r}) + b_{n,m}h_n^2(k\tilde{r})\right)Y_n^m(\hat{x}), \tag{IV.11}$$

and the series converges in $H^1(A_{r_0,r_2})$.

Proof. By the orthonormality of Y_n^m, u can be written as

$$u(x) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} f_{n,m}(|x|)Y_n^m(\hat{x}) \tag{IV.12}$$

with

$$f_{n,m}(r) = \int_{S^2} u(r\hat{x})\overline{Y_n^m}(\hat{x})\,\mathrm{d}\hat{x}.$$

The series above converges in the L^2 sense on each sphere $|x| = r$ with $r_0 \le r \le r_1$, and also converges in $L^2(A_{r_0,r_2})$. See the proof of Theorem III.3.

As the first step of the proof, we prove that $f_{n,m}(r)$ is in $H^2((r_0, r_2))$ and of the form $a_{n,m}h_n^1(k\tilde{r}) + b_{n,m}h_n^2(k\tilde{r})$. On $|x| = r \in [r_0, r_2]$ by Parseval's theorem

$$\int_{|x|=r} |u(x)|^2 \,\mathrm{d}S = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} r^2 |f_{n,m}(r)|^2 < \infty,$$

where $\mathrm{d}S$ is the surface element of the sphere of $|x| = r$, i.e., $\mathrm{d}S = r^2 \mathrm{d}\hat{x}$. Then

$$\|u\|^2_{L^2(A_{r_0,r_2})} = \int_{r_0}^{r_2} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} r^2 |f_{n,m}(r)|^2 \,\mathrm{d}r < \infty,$$

which implies

$$\int_{r_0}^{r_2} r^2 |f_{n,m}(r)|^2 \,\mathrm{d}r < \infty \quad \text{for all} \quad |m| \le n, \quad \text{and} \quad n = 0, 1, \dots.$$

Thus $f_{n,m}$ is in $L^2((r_0, r_2))$.

Consider $\chi \in C_0^\infty((r_0, r_2))$ and define $\tilde{\chi}(x) = \chi(|x|)Y_n^m(\hat{x}) \in C_0^\infty(A_{r_0,r_2})$. Thus,

$$\begin{aligned}
\int_{r_0}^{r_2} f_{n,m}(r) \frac{\mathrm{d}\overline{\chi}}{\mathrm{d}r}(r) \,\mathrm{d}r &= \int_{r_0}^{r_2} \left(\int_{S^2} u(r\hat{x}) Y_n^m(\hat{x}) \,\mathrm{d}\hat{x} \right) \frac{\mathrm{d}\overline{\chi}}{\mathrm{d}r}(r) \,\mathrm{d}r \\
&= \int_{S^2} \int_{r_0}^{r_2} u(r\hat{x}) \frac{\partial \overline{\tilde{\chi}}}{\partial r}(r\hat{x}) \,\mathrm{d}r\mathrm{d}\hat{x} \\
&= -\int_{S^2} \int_{r_0}^{r_2} \frac{\partial u}{\partial r}(r\hat{x}) \; \overline{\tilde{\chi}}(r\hat{x}) \,\mathrm{d}r\mathrm{d}\hat{x} \\
&= -\int_{A_{r_0,r_2}} \frac{\partial u}{\partial r}(x) \; \frac{\overline{\tilde{\chi}}}{r^2}(x) \,\mathrm{d}x,
\end{aligned}$$

which implies that

$$\left| \int_{r_0}^{r_2} f_{n,m}(r) \frac{\mathrm{d}\overline{\chi}}{\mathrm{d}r}(r) \,\mathrm{d}r \right| \le C \|u\|_{H^1(A_{r_0,r_2})} \|\chi\|_{L^2((r_0,r_2))}.$$

It follows from the Riesz representation theorem that there exists $g \in L^2((r_0, r_2))$ such that

$$\int_{r_0}^{r_2} g(r) \overline{\chi}(r) \,\mathrm{d}r = -\int_{r_0}^{r_2} f_{n,m}(r) \frac{\mathrm{d}\overline{\chi}}{\mathrm{d}r}(r) \,\mathrm{d}r.$$

Consequently, $\frac{\mathrm{d}f_{n,m}}{\mathrm{d}r}$ exists in the weak sense and it belongs to $L^2((r_0, r_2))$.

We will use the fact that u satisfies $A(u,v) - k^2 B(u,v) = 0$ for all $v \in C_0^\infty(A_{r_0,r_2})$ to show that the second derivative of $f_{n,m}$ is in $L^2((r_0,r_2))$. With $\tilde{\chi}(x)$ as above,

$$\begin{aligned}
0 &= \int_{S^2}\int_{r_0}^{r_2}\left[\frac{r^2\tilde{d}^2}{d}\frac{\partial u}{\partial r}\frac{\partial}{\partial r}\left(\frac{\overline{\tilde{\chi}}}{d}\right) + \frac{\partial u}{\partial\theta}\frac{\partial\overline{\tilde{\chi}}}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial u}{\partial\phi}\frac{\partial\overline{\tilde{\chi}}}{\partial\phi} - k^2r^2\tilde{d}^2u\overline{\tilde{\chi}}\right]\mathrm{d}r\mathrm{d}\hat{x}\\
&= -\int_{S^2}\int_{r_0}^{r_2}\left[u\frac{\partial}{\partial r}\left(\frac{r^2\tilde{d}^2}{d}\frac{\partial}{\partial r}\left(\frac{\overline{\tilde{\chi}}}{d}\right)\right) + ur^2\Delta_{S^2}\overline{\tilde{\chi}} + k^2r^2\tilde{d}^2u\overline{\tilde{\chi}}\right]\mathrm{d}r\mathrm{d}\hat{x}\\
&= -\int_{r_0}^{r_2} f_{n,m}\left[\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{r^2\tilde{d}^2}{d}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{\overline{\chi}}{d}\right)\right) + (k^2r^2\tilde{d}^2 - n(n+1))\overline{\chi}\right]\mathrm{d}r\\
&= \int_{r_0}^{r_2}\left[\frac{r^2\tilde{d}^2}{d}\frac{\mathrm{d}f_{n,m}}{\mathrm{d}r}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{\overline{\chi}}{d}\right) - (k^2r^2\tilde{d}^2 - n(n+1))f_{n,m}\overline{\chi}\right]\mathrm{d}r. \qquad \text{(IV.13)}
\end{aligned}$$

Thus

$$\begin{aligned}
\int_{r_0}^{r_2}\frac{r^2\tilde{d}^2}{d^2}\frac{\mathrm{d}f_{n,m}}{\mathrm{d}r}\frac{\mathrm{d}\overline{\chi}}{\mathrm{d}r}\,\mathrm{d}r &= \int_{r_0}^{r_2}\left[(k^2r^2\tilde{d}^2 - n(n+1))f_{n,m} + \frac{r^2\tilde{d}^2d'}{d^3}\frac{\mathrm{d}f_{n,m}}{\mathrm{d}r}\right]\overline{\chi}\,\mathrm{d}r\\
&= -\int_{r_0}^{r_2} h\overline{\chi}\,\mathrm{d}r
\end{aligned}$$

for some $h \in L^2((r_0,r_2))$. It follows that $\frac{r^2\tilde{d}^2}{d^2}\frac{\mathrm{d}f_{n,m}}{\mathrm{d}r}$ is in $H^1((r_0,r_2))$. Since $\frac{r^2\tilde{d}^2}{d^2}$ is in C^1, $\frac{\mathrm{d}f_{n,m}}{\mathrm{d}r}$ belongs to $H^1((r_0,r_2))$ and hence $f_{n,m}$ is in $H^2((r_0,r_2))$.

From (IV.13) we have

$$\int_{r_0}^{r_2}\left(\frac{1}{d}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{\tilde{d}^2r^2}{d}\frac{\mathrm{d}f_{n,m}}{\mathrm{d}r}\right) + \left(k^2\tilde{d}^2r^2 - n(n+1)\right)f_{n,m}\right)\overline{\chi}\,\mathrm{d}r = 0$$

for all $\chi \in C_0^\infty(A_{r_0,r_2})$. Thus $f_{n,m}$ satisfies the differential equation

$$\frac{1}{r^2\tilde{d}^2d}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{r^2\tilde{d}^2}{d}\frac{\mathrm{d}f_{n,m}}{\mathrm{d}r}\right) + \left(k^2 - \frac{n(n+1)}{r^2\tilde{d}^2}\right)f_{n,m} = 0. \qquad \text{(IV.14)}$$

It is easy to show that (IV.14) has two linearly independent solutions $h_n^1(k\tilde{r})$ and $h_n^2(k\tilde{r})$. With the initial conditions $f_{n,m}(r_0)$ and $f'_{n,m}(r_0)$ it follows that $f_{n,m}$ is of the form

$$f_{n,m}(r) = a_{n,m}h_n^1(k\tilde{r}) + b_{n,m}h_n^2(k\tilde{r})$$

for some constants $a_{n,m}$ and $b_{n,m}$.

Next, we will see the series (IV.11) converges in $H^1(A_{r_0,r_2})$. Using the L^2-orthogonality of $\{Y_n^m\}$, it is not hard to see that a function $g \in L^2(\Gamma_j)$ is in $H^1(\Gamma_j)$ for $j = 0, 2$ if and only if the series

$$\sum_{n=0}^{\infty} \sum_{m=-n}^{n} (1 + n(n+1))|(g, Y_n^m)_{\Gamma_j}|^2 \equiv \|g\|^2_{H^1(\Gamma_j)}$$

is finite. By interpolation [16], g is in $H^{1/2}(\Gamma_j)$ if and only if the series

$$\sum_{n=0}^{\infty} \sum_{m=-n}^{n} (1 + n(n+1))^{1/2}|(g, Y_n^m)_{\Gamma_j}|^2 \equiv \|g\|^2_{H^{1/2}(\Gamma_j)}$$

is finite. This shows that the series (IV.12) at r_0 and r_2 converge in $H^{1/2}(\Gamma_0)$ and $H^{1/2}(\Gamma_2)$ respectively. Let $\tilde{u}$ denote a partial sum in the series (IV.11) and $\tilde{g}_j$ denote its trace to Γ_j, for $j = 0, 2$. We note that $\tilde{u} \in H^1(A_{r_0,r_2})$ satisfies the variational problem,

$$\begin{aligned} A(\tilde{u}, \bar{d}\phi) = k^2 B(\tilde{u}, \bar{d}\phi) \ \text{ for all } \ \phi \in H_0^1(A_{r_0,r_2}), \\ \tilde{u} = \tilde{g}_0 \ \text{ on } \ \Gamma_0, \\ \tilde{u} = \tilde{g}_2 \ \text{ on } \ \Gamma_2. \end{aligned}$$

Examining the coefficients appearing in the form on the left hand side above, we see that this is a well-posed variational problem since the real parts of $\tilde{d}^2/d$ and d are positive and uniformly (as r varies) bounded away from zero. It follows that

$$\|\tilde{u}\|_{H^1(A_{r_0,r_2})} \leq C(\|\tilde{u}\|_{L^2(A_{r_0,r_2})} + \|\tilde{g}_0\|_{H^{1/2}(\Gamma_0)} + \|\tilde{g}_2\|_{H^{1/2}(\Gamma_2)}),$$

which implies convergence of (IV.11) in $H^1(A_{r_0,r_2})$.

□

The uniqueness of solutions to the PML problem (IV.8) now follows from the above theorem and the proof of [20, Theorem 1]. For completeness we present the proof here. For this, the following unique continuation result (see e.g., [46, Lemma 4.15]) is required.

Lemma IV.3. *Let Ω be a connected domain in $\mathbb{R}^3$ and suppose that $v \in H^1(\Omega)$ is a real-valued function that satisfies*

$$|\Delta v| \leq C(|\nabla v| + |v|)$$

almost everywhere in Ω, where C is a constant. If v vanishes identically in a neighborhood of a point $x \in \Omega$, then v is identically zero in Ω.

Theorem IV.4. *The PML problem* (IV.8) *has at most one solution in $H^1(\mathbb{R}^3)$ when k is real and positive.*

Proof. Assume that $f = 0$ and u is a solution to (IV.8) with $u \in H^1(\mathbb{R}^3)$. Then u satisfies

$$-\Delta u + Vu = k^2 u \quad \text{on} \quad \Omega_0.$$

By the second Green's identity

$$\int_{\Gamma_0} \left(u\frac{\partial \bar{u}}{\partial n} - \bar{u}\frac{\partial u}{\partial n} \right) \,\mathrm{d}\hat{x} = \int_{\Omega_0} (u\Delta\bar{u} - \bar{u}\Delta u) \,\mathrm{d}x = 0. \tag{IV.15}$$

It follows from Theorem IV.2 that u has a series representation (IV.11) for $r > r_0$. Since $h_n^2(k\tilde{r})$ grows exponentially as $r \to \infty$, we must have $b_{n,m} = 0$ and hence u is of the form

$$u(x) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{n,m} h_n^1(k\tilde{r}) Y_n^m(\hat{x}). \tag{IV.16}$$

Using (IV.16) and the orthonormality of the spherical harmonics (note that $\tilde{d} = 1$ on Γ_0), we find that the left hand side of (IV.15) is

$$k \sum_{n=0}^{\infty} \sum_{m=-n}^{n} |a_{n,m}|^2 (h_n^1(kr_0) h_n^{2\prime}(kr_0) - h_n^2(kr_0) h_n^{1\prime}(kr_0)) = 0.$$

Since the Wronskian of the spherical Hankel functions of the first and second kind is

$$h_n^1(z)h_n^{2\prime}(z) - h_n^2(z)h_n^{1\prime}(z) = -2iz^{-2},$$

we conclude $a_{n,m} = 0$ for all $n = 0, 1, \ldots,$ and $|m| \leq n$. Therefore $u = 0$ in $\mathbb{R}^3 \setminus \bar{\Omega}_0$. Now the unique continuation principle Lemma IV.3 shows that $u = 0$ in $\mathbb{R}^3$, which completes the proof. □

To prove the well-posedness of the variational problem (IV.8) we require the following theorem which follows from the Peetre-Tartar lemma (See, e.g., [30, Theorem 2.1],[47, 54]).

Theorem IV.5. *Let $A(\cdot,\cdot)$ be a bounded sesquilinear form on a complex Hilbert space V with norm $\|\cdot\|_V$. Let W be another Hilbert space with norm $\|\cdot\|_W$ and T a compact operator from V to W. Suppose that the only solution of*

$$A(u, v) = 0 \quad \textit{for all} \quad v \in V$$

is $u = 0$ and that

$$\|u\|_V \leq C_1 \left(\sup_{v \in V} \frac{|A(u,v)|}{\|v\|_V} + \|Tu\|_W \right) \quad \textit{for all} \quad u \in V.$$

Then there exists $C_2 > 0$ such that for all $u \in V$,

$$\|u\|_V \leq C_2 \sup_{v \in V} \frac{|A(u,v)|}{\|v\|_V}.$$

The proof of the well-posedness theorem follows [13, Theorem 3.1].

Theorem IV.6. *Let $A_k(\cdot,\cdot) \equiv A(\cdot,\cdot) - k^2 B(\cdot,\cdot)$ and k is real and positive. Then for $f \in L^2(\mathbb{R}^3)$, the problem*

$$A_k(u, v) = B(f, v) \quad \textit{for all} \quad v \in H^1(\mathbb{R}^3) \tag{IV.17}$$

has a unique solution u satisfying

$$\|u\|_{H^1(\mathbb{R}^3)} \leq C\|f\|_{L^2(\mathbb{R}^3)}.$$

Proof. Using Theorem IV.5, we will show an inf-sup condition for $A_k(\cdot,\cdot)$. The uniqueness of solutions to (IV.17) follows from Theorem IV.4. We break the form $A_k(\cdot,\cdot)$ into two parts:

$$A_k(u,v) = \widetilde{A}(u,v) + I(u,v)$$

where

$$\begin{aligned}\widetilde{A}(u,v) = &\left(\frac{\tilde{d}^2}{d^2}\frac{\partial u}{\partial r}, \frac{\partial v}{\partial r}\right)_{\mathbb{R}^3} + \left(\frac{1}{r^2}\frac{\partial u}{\partial \theta}, \frac{\partial v}{\partial \theta}\right)_{\mathbb{R}^3} \\ &+ \left(\frac{1}{r^2 \sin^2\theta}\frac{\partial u}{\partial \phi}, \frac{\partial v}{\partial \phi}\right)_{\mathbb{R}^3} - d_0^2 k^2 (u,v)_{\mathbb{R}^3}\end{aligned} \tag{IV.18}$$

and

$$I(u,v) = k^2((d_0^2 - \tilde{d}^2)u, v)_{\Omega_1} - \left(\frac{\tilde{d}^2 d'}{d^3}\frac{\partial u}{\partial r}, v\right)_{\Omega_1} + (Vu,v)_{\Omega_1}.$$

Since $\widetilde{A}(\cdot,\cdot)$ is coercive and $A_k(\cdot,\cdot)$ is a low order perturbation of $\widetilde{A}(\cdot,\cdot)$ on a bounded domain, the inf-sup condition,

$$\|u\|_{H^1(\mathbb{R}^3)} \leq C_k \sup_{\phi \in H^1(\mathbb{R}^3)} \frac{|A_k(u,\phi)|}{\|\phi\|_{H^1(\mathbb{R}^3)}} \quad \text{for all} \quad u \in H^1(\mathbb{R}^3) \tag{IV.19}$$

follows from Theorem IV.5 (see [13] for details). The analogous inf-sup condition for the adjoint operator holds as well:

$$\|\phi\|_{H^1(\mathbb{R}^3)} \leq C_k \sup_{u \in H^1(\mathbb{R}^3)} \frac{|A_k(u,\phi)|}{\|u\|_{H^1(\mathbb{R}^3)}} \quad \text{for all} \quad \phi \in H^1(\mathbb{R}^3). \tag{IV.20}$$

This easily follows from

$$A_k(u,\phi) = A_k(\bar{\phi}/d, \bar{d}\bar{u}). \tag{IV.21}$$

By the generalized Lax-Milgram Lemma, there exists a unique $u \in H^1(\mathbb{R}^3)$ satisfying (IV.17) and $\|u\|_{H^1(\mathbb{R}^3)} \leq C\|f\|_{L^2(\mathbb{R}^3)}$. □

Fix $k = 1$ above. We define $T : L^2(\mathbb{R}^3) \to H^1(\mathbb{R}^3)$ of $\widetilde{L} - k^2$ as follows. For $f \in L^2(\mathbb{R}^3)$ we define $T(f) = w$ where w is the unique solution of

$$A_1(w, \phi) = B(f, \phi) \quad \text{for all} \quad \phi \in H^1(\mathbb{R}^3).$$

It follows from Theorem IV.6 that

$$\|T(f)\|_{H^1(\mathbb{R}^3)} \leq C\|f\|_{L^2(\mathbb{R}^3)}.$$

We can clearly restrict T to an operator on $H^1(\mathbb{R}^3)$ and so its resolvent and spectrum are well-defined.

The complex stretching that we introduced is a special case of general stretching, i.e., exterior dilations, given by the Aguilar-Balslev-Combes-Simon (ABCS) Theorem [3, 5, 38, 52, 48]. The deformed operator using an exterior dilation is defined as follows. Let $h : \mathbb{R}^3 \to \mathbb{R}^3$ be a C^2 function such that $h(x) = 0$ for $|x| < r_0$ and $h(x) = x$ for $|x| \geq r_1$ with $0 < r_0 < r_1$. An exterior dilation is a C^2 function φ_η with a parameter $\eta \in \mathbb{R}$, which is defined by $\varphi_\eta(x) = x + \eta h(x)$. Let J_η denote the Jacobian determinant of φ_η. For sufficiently small $\eta \in \mathbb{R}$, U_η defined by $U_\eta(f(x)) = J_\eta^{1/2} f(\varphi_\eta(x))$ is an unitary operator in $L^2(\mathbb{R}^3)$. Then the deformed operator L_η is defined by

$$L_\eta \equiv U_\eta L U_\eta^{-1}.$$

Since U_η is unitary for small $\eta \in \mathbb{R}$, the spectrum of L_η is the same as that of L for such η. On the other hand, according to the ABCS theory when L_η is continued analytically to a small neighborhood of the origin, some of resonance values of L become isolated eigenvalues of L_η. We produce this results using PML, and discuss now how PML can be used for computing resonance values.

In order to see the relation of the PML operator $\widetilde{L}$ and the spectrally deformed operator L_η, when $\varphi_\eta(x) \equiv \tilde{d}x = (1+\eta\tilde{\sigma}(r))x$ is the exterior dilation, we will first compute the Jacobian matrix J of φ_η for real $\eta > -1/(2\sigma_M)$ where $\sigma_M \equiv \max_{r\geq 0}\{\sigma(r)\}$. Since $\varphi_{\eta,i}(x) = (1+\eta\tilde{\sigma}(r))x_i$,

$$\begin{aligned} J_{ij} &= \frac{\partial \varphi_{\eta,i}}{\partial x_j} = \tilde{d}\delta_{ij} + \frac{\partial r}{\partial x_j}\tilde{d}' x_i \\ &= \tilde{d}\delta_{ij} + \frac{x_j}{r}\frac{d-\tilde{d}}{r}x_i. \end{aligned}$$

In the last equality we have used $d = (r\tilde{d})' = \tilde{d} + r\tilde{d}'$. Finally, we have

$$J = \tilde{d}(I-P) + dP.$$

Thus the Jacobian determinant J_η is $d\tilde{d}^2$. Note that for real $\eta > -1/(2\sigma_M)$, J_η is positive. In addition, $0 \leq \arg(J_\eta) < 3\pi/2$ for η with $\mathrm{Re}(\eta) > 1/(2\sigma_M)$, and hence there is a branch cut for $J_\eta^{1/2}$ for such η.

Let $\tilde{J}_\eta$ be the Jacobian determinant of φ_η^{-1}. For $f, g \in C_0^\infty(\mathbb{R}^3)$ and real η with $\eta > -1/(2\sigma_M)$

$$\begin{aligned} I(\eta) \equiv \int_{\mathbb{R}^3} -U_\eta \Delta U_\eta^{-1} f(x) g(x)\,\mathrm{d}x &= \int_{\mathbb{R}^3} -\Delta(U_\eta^{-1}f)(x)(U_\eta^{-1}g)(x)\,\mathrm{d}x \\ &= \int_{\mathbb{R}^3} \nabla(U_\eta^{-1}f)(x)\cdot\nabla(U_\eta^{-1}g)(x)\,\mathrm{d}x \\ &= \int_{\mathbb{R}^3} \nabla\tilde{J}_\eta^{1/2}(x) f(\varphi_\eta^{-1}(x))\cdot\nabla\tilde{J}_\eta^{1/2}(x) g(\varphi_\eta^{-1}(x))\,\mathrm{d}x. \end{aligned}$$

Using the change of variables $x = \varphi_\eta(y)$ gives

$$\begin{aligned} I(\eta) &= \int_{\mathbb{R}^3} J^{-t}(y)\nabla(J_\eta^{-1/2}(y)f(y))\cdot J^{-t}(y)\nabla(J_\eta^{-1/2}(y)g(y))d\tilde{d}^2\,\mathrm{d}y \\ &= \int_{\mathbb{R}^3} d\tilde{d}^2\left[d^{-2}P + \tilde{d}^{-2}(I-P)\right]\nabla J_\eta^{-1/2}f\cdot\nabla J_\eta^{-1/2}g\,\mathrm{d}y \\ &= \int_{\mathbb{R}^3} -J_\eta^{-1/2}\left[\nabla\cdot\left(\frac{\tilde{d}^2}{d}P + d(I-P)\right)\nabla J_\eta^{-1/2}f\right] g\,\mathrm{d}y. \end{aligned}$$

As will be seen later, $I(\eta)$ is an analytic function of η on $\{z \in \mathbb{C} \,:\, \mathrm{Re}(z) > -1/(2\sigma_M)\}$

and

$$\Delta_\eta = J_\eta^{-1/2}\left[\nabla\cdot\left(\frac{\tilde{d}^2}{d}P + d(I-P)\right)\nabla\right]J_\eta^{-1/2}$$
$$= J_\eta^{1/2}\widetilde{\Delta}J_\eta^{-1/2}.$$

It is easy to show that the resolvent sets of the PML operator and the spectrally deformed operator are the same and hence these two operators have the same spectrum.

Although the ABCS theory provides a one-to-one correspondence between resonance values of the original operator and eigenvalues of the spectrally deformed operator, we present a simple proof which works when the solutions of the PML problem are available in the explicit form (IV.5).

Given a solution of (IV.1), we defined the PML solution $\tilde{u}$ by (IV.5) and noting that $\tilde{u}$ satisfied (IV.6). Conversely, given a function $\tilde{u}$ satisfying (IV.5), we can define $u(\tilde{u})$ by

$$u(\tilde{u})(x) = \begin{cases} \tilde{u}(x) & \text{for } \; 0 \le r \le r_0, \\ \displaystyle\sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{n,m}h_n^1(kr)Y_n^m(\hat{x}) & \text{for } \; r_0 < r, \end{cases}$$

where $a_{n,m}$ are coefficients from the series for $\tilde{u}$. The following theorem connects the resonance values with the eigenvalues of the PML operator T.

Theorem IV.7. *Let* $\mathrm{Im}(d_0k)$ *be greater than zero and set* $\lambda = 1/(k^2-1)$*. If there is a non-zero outgoing solution* u *(locally in* H^1*) satisfying* (IV.1) *with* $f=0$*, then* $\tilde{u}$ *given by* (IV.5) *is an eigenfunction for* T *with an eigenvalue* λ*. Conversely, if* $\tilde{u}$ *is an eigenfunction for* T *with an eigenvalue* λ*, then* $\tilde{u}$ *is of the form* (IV.5) *for* $r \ge r_0$ *and* $u = u(\tilde{u})$ *satisfies the outgoing condition and* (IV.1) *with* $f=0$ *and*

For the proof of the above theorem, we shall require the following proposition.

Proposition IV.8. *Let* β *be a constant with positive imaginary part and* g *be given* *in* $H^{1/2}(\Gamma_1)$*. There is a unique* $w \in H^1(\Omega_1^c)$ *satisfying* $w = g$ *on* Γ_1 *and*

$$\Delta w + \beta^2 w = 0 \quad on \quad \Omega_1^c. \tag{IV.22}$$

Moreover, w *is outgoing (the series representation given by Theorem IV.2 has vanishing* b_k*).*

Proof. Consider the sesquilinear form

$$a(u, v) = (\nabla u, \nabla v)_{\Omega_1^c} - (\beta^2 u, v)_{\Omega_1^c}$$

for $u, v \in H^1(\Omega_1^c)$. Since $\operatorname{Im}(a(u, -1/\bar{\beta}u)) \geq C\|u\|^2_{H^1(\Omega_1^c)}$ with $C = \operatorname{Im}(\beta)\max\{1, 1/|\beta|\}$, it is straightforward to see that there is a unique w in $H^1(\Omega_1^c)$ satisfying

$$\begin{aligned} a(w, v) &= 0 \quad \text{for all} \quad v \in H_0^1(\Omega_1^c), \\ w &= g \quad \text{on} \quad \Gamma_1. \end{aligned} \tag{IV.23}$$

Terms involving $b_{n,m}$ in the series of Theorem IV.2 blow up exponentially at infinity. The presence of any one results in a function not in $H^1(\Omega_1^c)$, i.e., w is outgoing. □

Remark IV.9. It follows from the above proposition and the proof of Theorem IV.2 that an outgoing series (with such β) which coincides with a function in $H^{1/2}(\Gamma_1)$, in fact, converges in $H^1(\Omega_1^c)$.

Proof of Theorem IV.7. Suppose that u is outgoing, locally in H^1 and satisfies (IV.1) with $f = 0$. Then u has a series representation (IV.2). The resulting $\tilde{u}$ defined by (IV.5) converges uniformly on compact sets of Ω_0^c. It follows from the definition of $\widetilde{L}$ and the uniform convergence that $\tilde{u}$ satisfies

$$(\widetilde{L} - k^2)\tilde{u} = 0.$$

Outside of Ω_1, this coincides with (IV.22) with $\beta = d_0 k$. Theorem IV.2 and Remark IV.9 imply that the series for $\tilde{u}$ converges in $H^1(\Omega_1^c)$, i.e., $\tilde{u} \in H^1(\mathbb{R}^3)$. For $\phi \in C_0^\infty(\mathbb{R}^3)$,

$$A(\tilde{u}, \phi) - k^2 B(\tilde{u}, \phi) = 0.$$

This is the same as

$$A_1(\tilde{u}, \phi) = (k^2 - 1) B(\tilde{u}, \phi). \tag{IV.24}$$

Thus, $\tilde{u} = (k^2 - 1) T \tilde{u}$.

Suppose, conversely, that $\tilde{u} \in H^1(\mathbb{R}^3)$ is an eigenfunction for T with eigenvalue λ. Then $\tilde{u}$ satisfies (IV.24). By Theorem IV.2, $\tilde{u}$ can be written as a series (IV.11) for $|x| \geq r_0$. Proposition IV.8 implies that $\tilde{u}$ is outgoing. Then $u = u(\tilde{u})$ satisfies (IV.1) with $f = 0$ and is also outgoing. This completes the proof of the theorem. □

Remark IV.10. It is clear that the PML method is only guaranteed to gives the resonances which satisfy $\mathrm{Im}(d_0 k) > 0$, i.e., those which are in the sector bounded by the positive real axis and the line $\arg(z) = \arg(1/d_0)$. To get the resonances to the left of this line, we need to increase σ_0.

The ABCS theory provides additional information about the spectrum of the PML operator $\widetilde{L}$. Specifically, these results imply that the essential spectrum of $\widetilde{L}$ is

$$\sigma_{ess}(\widetilde{L}) = \{z \mid \arg(z) = -2 \arg(1 + i\sigma_0)\}$$

(cf. Theorem 18.6 [38]). These type of results are also proved in Theorem VIII.20. This implies that the eigenvalues of $\widetilde{L}$ corresponding to resonances are isolated and of finite multiplicity. Note that if z is in $\sigma_{ess}(\widetilde{L})$, then $\mathrm{Im}(d_0 k) = 0$.

C. Exponential decay of eigenfunctions of the spherical PML problem in the infinite domain

We are interested in finding isolated eigenvalues λ of T, which are mapped via the map $\lambda = 1/(k^2 - 1)$ into the sector bounded by the positive real axis and the line $\arg(z) = 2\arg(1/d_0)$. Let λ be an isolated eigenvalue of T that is mapped into this sector and V denote the generalized eigenspace of T associated with λ. Since the multiplicity of λ is finite, V is a finite dimensional subspace of $H^1(\mathbb{R}^3)$. In this section, we shall show that every function in V decays exponentially. We start with the following lemma.

Lemma IV.11. *Suppose that w is in $H^1(\Omega_1^c)$ and satisfies*

$$\Delta w + \beta^2 w = f \quad in \quad \Omega_1^c \tag{IV.25}$$

with $\mathrm{Im}(\beta)$ positive and $f \in L^2(\Omega_1^c)$. If f decays exponentially, i.e., there are positive constants α, C_f and $M > r_1$ such that $|f(x)| \le C_f e^{-\alpha|x|}$ for $|x| > M$, then there are positive constant α_1, C_1 and $M_1 > M$ such that

$$|w(x)| \le C_1 e^{-\alpha_1 |x|} \left(\|w\|_{H^1(\Omega_1^c)} + \|f\|_{L^2(\Omega_1^c)} + C_f \right) \tag{IV.26}$$

and

$$\|w\|_{H^{1/2}(\Gamma_\infty)} \le C_1 e^{-\alpha_1 \delta} \left(\|w\|_{H^1(\Omega_1^c)} + \|f\|_{L^2(\Omega_1^c)} + C_f \right)$$

for $|x|, \delta > M_1$. Here α_1, C_1 and M_1 can be chosen independently of w, f and δ.

Proof. Choose any $\tilde{M}_1 > M$. For $|x| > \tilde{M}_1$ let Ω_M and Ω_R be open balls centered at the origin of radius M and $2|x|$, respectively. Let Γ_M and Γ_R denote their boundaries.

By Green's theorem, we have for $|x| > \tilde{M}_1$

$$w(x) = -\int_{\Gamma_M \cup \Gamma_R} \left[\frac{\partial w}{\partial n}(y)\Phi(x,y) - w(y)\frac{\partial \Phi}{\partial n_y}(x,y) \right] \mathrm{d}S_y + \int_D f(y)\Phi(x,y)\,\mathrm{d}y, \tag{IV.27}$$

where n is the outward normal vector on the boundaries of $D = \Omega_R \setminus \bar{\Omega}_M$ and $\Phi(x,y) = -e^{i\beta|x-y|}/(4\pi|x-y|)$ is the fundamental solution of the Helmholtz equation with wave number β.

Note that for $|x| > \tilde{M}_1$

$$\int_{\Gamma_M} \frac{\mathrm{d}S_y}{|x-y|^2} \leq \int_{\Gamma_M} \frac{\mathrm{d}S_y}{(|x|-M)^2} \leq \frac{4\pi M^2}{(\tilde{M}_1 - M)^2}.$$

By Schwarz's inequality and the properties of Φ,

$$\begin{aligned}\left|\int_{\Gamma_M} \left[\frac{\partial w}{\partial n}(y)\Phi(x,y) - w(y)\frac{\partial \Phi}{\partial n_y}(x,y)\right] \mathrm{d}S_y\right|^2 \\ &\leq Ce^{-2\mathrm{Im}(\beta)|x|}\left(\|\frac{\partial w}{\partial n}\|^2_{L^2(\Gamma_M)} + \|w\|^2_{L^2(\Gamma_M)}\right)\int_{\Gamma_M} \frac{\mathrm{d}S_y}{|x-y|^2} \\ &\leq Ce^{-2\mathrm{Im}(\beta)|x|}(\|w\|^2_{H^1(\Omega_1^c)} + \|f\|^2_{L^2(\Omega_1^c)}).\end{aligned}$$

For the last inequality above, we used an interior regularity estimate, i.e., since w satisfies (IV.25), its H^2-norm in a neighborhood of Γ_M can be bounded by the H^1-norm of w and the L^2-norm of f in a slightly larger neighborhood. The analogous inequality bounding the integral on Γ_R holds and hence

$$\begin{aligned}\left|\int_{\Gamma_M \cup \Gamma_R} \left[\frac{\partial w}{\partial n}(y)\Phi(x,y) - w(y)\frac{\partial \Phi}{\partial n_y}(x,y)\right] \mathrm{d}S_y\right|^2 \\ &\leq Ce^{-2\mathrm{Im}(\beta)|x|}(\|w\|^2_{H^1(\Omega_1^c)} + \|f\|^2_{L^2(\Omega_1^c)}).\end{aligned} \quad \text{(IV.28)}$$

For the volume integral in (IV.27), let $\tilde{\alpha} = \min\{\alpha, \mathrm{Im}(\beta)\}$. Then

$$\begin{aligned}\left|\int_D f(y)\Phi(x,y)\,\mathrm{d}y\right| &\leq CC_f \int_D e^{-\alpha|y|}\frac{e^{-\mathrm{Im}(\beta)|x-y|}}{|x-y|}\,\mathrm{d}y \\ &\leq CC_f e^{-\tilde{\alpha}|x|}\int_D \frac{1}{|x-y|}\,\mathrm{d}y \\ &\leq CC_f|x|^2 e^{-\tilde{\alpha}|x|} \leq CC_f e^{-\alpha_1|x|}\end{aligned} \quad \text{(IV.29)}$$

for $|x| > \tilde{M}_2$ and $0 < \alpha_1 < \tilde{\alpha}$. The first inequality of Lemma IV.11 now follows from inequalities (IV.28) and (IV.29).

For the second inequality, let $D_1 \subset S_\gamma$ be open sets such that S_γ is a γ-neighborhood of Γ_∞ with γ independent of δ and $\bar{D}_1 \subset S_\gamma$. Using an interior regularity estimate and integrating (IV.26) over S_γ gives

$$\begin{aligned} \|w\|_{H^{1/2}(\Gamma_\infty)} &\leq C\|w\|_{H^2(D_1)} \leq C\|w\|_{L^2(S_\gamma)} \\ &\leq Ce^{-\alpha_1 \delta} \left(\|w\|_{H^1(\Omega_1^c)} + \|f\|_{L^2(\Omega_1^c)} + C_f \right), \end{aligned}$$

which completes the proof. □

The following lemma shows the pointwise exponential decay of the generalized eigenfunctions of T. An important remark is that the decay rate depends only the eigenvalue of interest and its algebraic multiplicity. This rapid decay of the eigenfunctions gives a motivation to truncate the infinite domain to approximate the resonance values.

Lemma IV.12. *Let V be as above. Then there are constants α, C and $M > r_1$ such that for all $\psi \in V$,*

$$|\psi(x)| \leq Ce^{-\alpha|x|}\|\psi\|_{H^1(\mathbb{R}^3)} \quad \text{for} \quad |x| > M. \tag{IV.30}$$

Proof. Let m be the (algebraic) multiplicity of λ. For any non-zero $\psi \in V$,

$$(T - \lambda I)^m \psi = 0.$$

There exists a positive integer $n \leq m$, such that

$$(T - \lambda I)^{n-1}\psi \neq 0 \quad \text{and} \quad (T - \lambda I)^n \psi = 0. \tag{IV.31}$$

We will show that there exist constants α, C and M depending only on λ, T and n such that ψ satisfies (IV.30) with these constants. The proof is by induction on n.

The case of $n = 1$ corresponds to an eigenfunction ψ and immediately follows from Lemma IV.11 since ψ satisfies

$$\Delta\psi(x) + (d_0 k(\lambda))^2 \psi(x) = 0, \quad \text{for} \quad |x| > r_1.$$

Let ψ satisfy (IV.31) with $2 \leq n \leq m$ and denote $\psi_j = (T - \lambda I)^{n-j}\psi$ for $j = 1, \ldots, n$. Assume that (IV.30) holds for ψ_j for $j = 1, \ldots, n-1$ with constants depending only on λ, T, and j. We need to estimate the decay of ψ_n. Then $(T - \lambda I)\psi_n = \psi_{n-1}$ so outside of Ω_1,

$$d_0^2 \psi_n + \lambda(\Delta\psi_n + d_0^2 \psi_n) = -(\Delta\psi_{n-1} + d_0^2 \psi_{n-1}).$$

A straightforward computation gives

$$\Delta\psi_n + (d_0 k(\lambda))^2 \psi_n = d_0^2 \sum_{j=1}^{n-1} \frac{(-1)^{j+1}}{\lambda^{j+1}} \psi_{n-j}. \tag{IV.32}$$

Since the function on the right of (IV.32) decays exponentially by the inductive assumption, by Lemma IV.11 there exist $\alpha = \alpha(T, \lambda, n), C = C(T, \lambda, n)$ and $M = M(T, \lambda, n)$ such that ψ_n satisfies

$$|\psi_n(x)| \leq C e^{-\alpha|x|} \sum_{j=1}^{n} \|\psi_j\|_{H^1(\mathbb{R}^n)} \tag{IV.33}$$

for $|x| > M$. In addition, from the continuity of $T - \lambda I$ and the definition of ψ_j there is a constant $C = C(T, \lambda, n)$ such that

$$\|\psi_j\|_{H^1(\mathbb{R}^3)} \leq C \|\psi_n\|_{H^1(\mathbb{R}^3)}$$

for $j = 1, \ldots, n-1$. Thus, from (IV.33), there exist $\alpha = \alpha(T, \lambda, n), C = C(T, \lambda, n)$, and $M = M(T, \lambda, n)$ such that $|\psi_n(x)| \leq C e^{-\alpha|x|} \|\psi_n\|_{H^1(\mathbb{R}^3)}$ for $|x| > M$. $\square$

CHAPTER V

TRUNCATED PML PROBLEM

In this chapter we analyze the PML problem in a truncated domain. As indicated by Lemma IV.12, the generalized PML eigenfunctions decay exponentially. It is then natural to approximate them on a bounded computational domain with a convenient boundary condition, for example, the homogeneous Dirichlet boundary condition. To this end, we introduce a bounded (computational) domain Ω_δ whose boundary is denoted by Γ_δ.

We will prove the theorems for the PML problem in the truncated domain that are analogous to those for the PML problem in the infinite domain in the previous chapter. We will show that the PML problem in a truncated domain Ω_δ has a well-posed variational formulation. The well-posedness of the PML problem in Ω_δ leads to a well-defined inverse operator T_δ. We will consider its restriction to $H^1(\mathbb{R}^3)$, $T_\delta : H^1(\mathbb{R}^3) \to H^1_0(\Omega_\delta) \subset H^1(\mathbb{R}^3)$, for eigenvalues. Our goal will be to study convergence of eigenvalues of T_δ to those of T. As the first result, we will prove that the resolvent set for T_δ approaches that of T as the domain Ω_δ becomes large. Exponential decay of the generalized eigenfunctions of T_δ will be covered here.

A. Well-posedness of the spherical PML problem in a truncated domain

We shall always assume that the transition layer is in Ω_δ, i.e., $\Omega_1 \subset \Omega_\delta$. We assume that the outer boundary of Ω_δ is given by dilation of a fixed boundary by a parameter δ, e.g., Ω_δ is a cube of side length 2δ.

The following theorem is the well-posedness result for the truncated PML problem for δ large enough. Its proof was given in [13]. We provide a proof for completeness.

Theorem V.1. *There exists $\delta_0 > 0$ such that if $\delta \geq \delta_0$, then for $f \in L^2(\Omega_\delta)$ the problem*

$$A_1(u, v) = B(f, v) \text{ for all } v \in H_0^1(\Omega_\delta) \tag{V.1}$$

has a unique solution $u \in H_0^1(\Omega_\delta)$ satisfying

$$\|u\|_{H^1(\Omega_\delta)} \leq C\|f\|_{L^2(\Omega_\delta)},$$

where C does not depend on δ.

Proof. We will show that the sesquilinear form $A_1(\cdot, \cdot)$ still satisfies an inf-sup condition on $H_0^1(\Omega_\delta)$ provided that $\delta \geq \delta_0$ and δ_0 is sufficiently large, i.e., for $u \in H_0^1(\Omega_\delta)$,

$$\|u\|_{H^1(\Omega_\delta)} \leq C \sup_{\phi \in H_0^1(\Omega_\delta)} \frac{|A_1(u, \phi)|}{\|\phi\|_{H^1(\Omega_\delta)}}. \tag{V.2}$$

Here and in the remainder of this paper, C is independent of δ once δ is sufficiently large. Once we have the inf-sup condition, by (IV.21) the inf-sup condition for the adjoint operator holds as well: for $\phi \in H_0^1(\Omega_\delta)$

$$\|\phi\|_{H^1(\Omega_\delta)} \leq C \sup_{u \in H_0^1(\Omega_\delta)} \frac{|A_1(u, \phi)|}{\|u\|_{H^1(\Omega_\delta)}}. \tag{V.3}$$

Then the generalized Lax-Milgram theorem completes the proof.

We start with (IV.19) to verify (V.2). The test function ϕ appearing in (IV.19) is decomposed $\phi = \phi_0 + \phi_1$, where ϕ_1 solves

$$\begin{aligned} A_1(\chi, \phi_1) &= 0 \text{ for all } \chi \in H_0^1(\Omega_\infty \setminus \bar{\Omega}_1), \\ \phi_1 &= 0 \text{ on } \Omega_1, \\ \phi_1 &= \phi \text{ on } \Omega_\infty^c. \end{aligned} \tag{V.4}$$

This problem is uniquely solvable. Indeed, let $\chi \in H^1_0(\Omega_\delta \setminus \bar{\Omega}_1)$ and $\gamma = i/d_0$. Then

$$A_1(\gamma\chi, \chi) = \gamma D(\chi, \chi) - d_0^2 \gamma(\chi, \chi).$$

Here $D(\cdot, \cdot)$ denotes the Dirichlet form. Since γ and $-d_0^2\gamma$ have a positive real part,

$$|A_1(\gamma\chi, \chi)| \geq C\|\chi\|^2_{H^1(\Omega_\delta \setminus \bar{\Omega}_1)}.$$

The unique solvability of (V.4) follows and by the stability of (V.4) and Lemma II.5 we have

$$\|\phi_1\|_{H^1(\mathbb{R}^3)} \leq C\|\phi\|_{H^1(\mathbb{R}^3)}. \tag{V.5}$$

Next for $u \in H^1_0(\Omega_\delta)$, we write $u = u_0 + u_1$, where

$$\begin{aligned} A_1(u_1, \chi) &= 0 \quad \text{for all} \quad \chi \in H^1_0(\Omega_\delta \setminus \bar{\Omega}_1), \\ u_1 &= u \quad \text{on} \quad \Omega_1, \\ u_1 &= 0 \quad \text{on} \quad \Omega^c_\delta. \end{aligned} \tag{V.6}$$

As above, this problem is also uniquely solvable and

$$\|u_1\|_{H^1(\mathbb{R}^3)} \leq C\|u\|_{H^1(\Omega_\delta)}.$$

We then have

$$\begin{aligned} A_1(u, \phi) &= A_1(u, \phi_0) + A_1(u_0, \phi_1) + A_1(u_1, \phi_1) \\ &= A_1(u, \phi_0) + A_1(u_1, \phi_1). \end{aligned}$$

Now, let $\tilde{u}_1$ solve

$$\begin{aligned} A_1(\tilde{u}_1, \eta) &= 0 \quad \text{for all} \quad \eta \in H^1_0(\Omega^c_1), \\ \tilde{u}_1 &= u \quad \text{on} \quad \Omega_1. \end{aligned} \tag{V.7}$$

The argument showing unique solvability of (V.4) works as well here.

We then have

$$A_1(u_1, \phi_1) = A_1(u_1 - \tilde{u}_1, \phi_1) + A_1(\tilde{u}_1, \phi_1) = A_1(u_1 - \tilde{u}_1, \phi_1).$$

Now

$$A_1(u_1 - \tilde{u}_1, v) = 0 \ \text{ for all } \ v \in H_0^1(\Omega_\delta \setminus \bar{\Omega}_1) \oplus H_0^1(\Omega_\delta^c),$$

from which it follows that

$$\|u_1 - \tilde{u}_1\|_{H^1(\mathbb{R}^3)} \leq C\|\tilde{u}_1\|_{H^{1/2}(\Gamma_\delta)} \leq Ce^{-\alpha\delta}\|u\|_{H^{1/2}(\Gamma_1)}.$$

We used Lemma IV.11 and the stability of the problem (V.7) for the last inequality above. It then follows from (V.5) and a standard trace estimate that

$$|A_1(u_1, \phi_1)| \leq Ce^{-\alpha\delta}\|u\|_{H^1(\Omega_\delta)}\|\phi\|_{H^1(\mathbb{R}^3)}.$$

Thus,

$$\|u\|_{H^1(\Omega_\delta)} \leq C \sup_{\phi_0 \in H_0^1(\Omega_\delta)} \frac{|A_1(u, \phi_0)|}{\|\phi_0\|_{H^1(\Omega_\delta)}} + Ce^{-\alpha\delta}\|u\|_{H^1(\Omega_\delta)}. \tag{V.8}$$

The inf-sup condition (V.2) follows taking δ_0 large enough so that $Ce^{-\alpha\delta_0} < 1$.

□

B. Convergence of the resolvent sets of the operators in truncated domains

Because of the well-posedness of the PML problem in a truncated domain, we can define the operator $T_\delta : H^1(\mathbb{R}^3) \to H_0^1(\Omega_\delta) \subset H^1(\mathbb{R}^3)$ by $T_\delta f = u$, where $u \in H_0^1(\Omega_\delta)$ is the unique solution to

$$A_1(u, \phi) = B(f, \phi) \ \text{ for all } \ \phi \in H_0^1(\Omega_\delta).$$

The following theorem shows that the resolvent set for T_δ approaches that of T as δ goes to infinity. This means that the truncated problem does not result in spurious eigenvalues in the region of interest, $\mathrm{Im}(d_0 k) > 0$.

Theorem V.2. *Let U be a compact subset of $\rho(T)$, the resolvent set of T, whose image under the map $z \mapsto \sqrt{(1+z)/z} \equiv k(z)$ satisfies $\mathrm{Im}(d_0 k(z)) > 0$ for all $z \in U$. Here we have taken $-\pi < \arg(k(z)) \leq 0$. Then, there exists a δ_0 (depending on U) such that for $\delta > \delta_0$, $U \subset \rho(T_\delta)$.*

We shall need the following proposition for the proof of the above theorem.

Proposition V.3. *Assume that w is in $H^1(\mathbb{R}^3)$ and satisfies (IV.22) in Ω_1^c with $\beta^2 = d_0^2 k(z)^2$ and $z \in U$ as in Theorem V.2. Then there is a positive number α and $\delta_0 > r_1$ such that for $\delta \geq \delta_0$*

$$\|w\|_{H^{1/2}(\Gamma_\delta)} \leq C e^{-\alpha\delta} \|w\|_{H^{1/2}(\Gamma_1)}.$$

The constants C and α can be taken independently of $z \in U$ and $\delta \geq \delta_0$.

Proof. Since U is compact, it follows that α_1 in Lemma IV.11 can be chosen independent of $z \in U$. The proposition follows from Lemma IV.11. □

Proof of Theorem V.2. Let $R_z(T) = (T - zI)^{-1}$ be the resolvent operator and $\|R_z(T)\|_{H^1(\mathbb{R}^3)}$ denote its operator norm. This norm depends continuously for $z \in \rho(T)$ so there is a constant $C = C_U$ such that

$$\|R_z(T)\|_{H^1(\mathbb{R}^3)} \leq C \quad \text{for all} \quad z \in U.$$

For $u \in H^1(\mathbb{R}^3)$, set $\phi = (T - zI)u$. Then for $z \in U$, using (IV.19),

$$\begin{aligned} \|u\|_{H^1(\mathbb{R}^3)} \leq C\|\phi\|_{H^1(\mathbb{R}^3)} &\leq C \sup_{v \in H^1(\mathbb{R}^3)} \frac{|A_1(\phi, v)|}{\|v\|_{H^1(\mathbb{R}^3)}} \\ &= C \sup_{v \in H^1(\mathbb{R}^3)} \frac{|\widetilde{A}_z(u, v)|}{\|v\|_{H^1(\mathbb{R}^3)}}. \end{aligned} \tag{V.9}$$

Here we have set $\widetilde{A}_z(\cdot,\cdot) \equiv B(\cdot,\cdot) - zA_1(\cdot,\cdot)$. The inf-sup condition for the adjoint problem holds as well by similar reasoning.

We will show that the corresponding inf-sup conditions on the truncated domain hold for all $z \in U$ if δ_0 is large enough. Namely, for $u \in H_0^1(\Omega_\infty)$,

$$\|u\|_{H^1(\Omega_\delta)} \leq C \sup_{v \in H_0^1(\Omega_\delta)} \frac{|\widetilde{A}_z(u,v)|}{\|v\|_{H^1(\Omega_\delta)}} \tag{V.10}$$

and

$$\|u\|_{H^1(\Omega_\delta)} \leq C \sup_{v \in H_0^1(\Omega_\delta)} \frac{|\widetilde{A}_z(v,u)|}{\|v\|_{H^1(\Omega_\delta)}}. \tag{V.11}$$

Once we show (V.10) and (V.11), then it follows that the solution $v \in H_0^1(\Omega_\delta)$ to the variational problem

$$\widetilde{A}_z(v,\phi) = A_1(w,\phi) \ \text{ for all } \ \phi \in H_0^1(\Omega_\infty) \tag{V.12}$$

satisfies

$$(T_\delta - zI)v = w.$$

This shows that z is in $\rho(T_\delta)$.

The idea of the proof for (V.10) is essentially the same as one for (V.2). The only modification needed is

- inf-sup condition of $\widetilde{A}_z(\cdot,\cdot)$ on $H^1(\mathbb{R}^3)$,
- coercivity of $\widetilde{A}_z(\cdot,\cdot)$ on $H_0^1(\Omega_\delta \setminus \bar{\Omega}_1)$ and $H_0^1(\Omega_1^c)$,
- exponential decay of solutions to the problem

$$\widetilde{A}_z(u,\phi) = 0 \ \text{ for all } \ \phi \in H_0^1(\Omega_1^c)$$

  with a Dirichlet boundary condition on Γ_1, (that is, exponential decay of solutions to the Helmholtz equation with a complex coefficient $\beta^2 = d_0^2 k(z)^2$ and

$z \in U$ in the sense of Proposition V.3).

Once the above conditions for $\widetilde{A}_z(\cdot,\cdot)$ are verified, then the proof for (V.10) will be completed.

Because of the inf-sup condition (V.9) of $\widetilde{A}_z(\cdot,\cdot)$ on $H^1(\mathbb{R}^3)$ and Proposition V.3, it suffices to show that $\widetilde{A}_z(\cdot,\cdot)$ is coercive on $H_0^1(X)$ where $X = \Omega_\delta \setminus \bar{\Omega}_1$ or Ω_1^c. Now, let $\chi \in H_0^1(X)$ and γ be in $\mathbb{C}$. Then

$$\widetilde{A}_z(\gamma\chi,\chi) = z(\gamma d_0^2 k(z)^2(\chi,\chi) - \gamma D(\chi,\chi)).$$

Since U is compact, there is an ϵ with $0 < \epsilon < \pi$ such that $\epsilon < \arg(d_0^2 k(z)^2) < \pi$ for all $z \in U$. Taking $\gamma = \exp(-i\epsilon/2)$ above implies that both $-\gamma$ and $\gamma d_0^2 k(z)^2$ have a positive imaginary part. It follows that

$$|\widetilde{A}_z(\gamma\chi,\chi)| \geq C\|\chi\|_{H^1(X)}^2,$$

from which the unique solvability is obtained.

The proof of (V.11) is similar. This completes the proof of the theorem. □

C. Exponential decay of eigenfunctions of the spherical PML problem in the truncated domain

As mentioned in Chapter IV, the eigenvalues of T corresponding to resonances are isolated and of finite multiplicity. Let λ be such an eigenvalue. Since λ is isolated, there is a neighborhood of it with all points excluding λ in $\rho(T)$. Let $\eta > 0$ be such that the circle of radius η centered at λ is in this neighborhood. We denote this circle by Γ. By Theorem V.2, $\rho(T_\delta)$ contains Γ for sufficiently large δ. Let V_δ be a subspace of $H_0^1(\Omega_\delta)$ spanned by the generalized eigenfunctions associated with the eigenvalues of T_δ inside Γ.

As T_δ is compact, the generalized eigenspace V_δ has a finite dimension and a basis of the form $\psi_{i,j}$, $i = 1, \ldots, k$, $j = 1, \ldots, m(i)$. Here if λ_i^δ is an eigenvalue of T_δ inside Γ for $i = 1, \ldots, k$, we may take

$$\psi_{i,j} = (T_\delta - \lambda_i^\delta)\psi_{i,j+1} \text{ and } (T_\delta - \lambda_i^\delta)\psi_{i,1} = 0.$$

A priori we do not have a bound on the dimension of V_δ. To deal with this, we consider subspaces of $\widetilde{V}_\delta$ of dimension at most $\dim(V) + 1$. Specifically, let $\widetilde{V}_\delta$ have a basis of the form $\{\psi_{i,j}\}$, $\psi_{i,j}$, $i = 1, \ldots, k$, $j = 1, \ldots, \tilde{m}(i)$ with $\{\psi_{i,j}\}$ as above and $\sum_i \tilde{m}(i) \le \dim(V) + 1$. The space $\widetilde{V}_\delta$ is invariant under T_δ and P_Γ^δ. The following lemma gives a decay estimate for functions in $\widetilde{V}_\delta$. The constant can be taken so that it only depends on the dimension of V provided that δ is large enough. We will first prove the result for the truncated problem analogous to Lemma IV.11.

Lemma V.4. *If $\psi_\delta \in H_0^1(\Omega_\delta \setminus \bar{\Omega}_1)$ satisfies*

$$\Delta\psi_\delta + \beta^2\psi_\delta = f \quad in \quad \Omega_\delta \setminus \bar{\Omega}_1$$

with $\mathrm{Im}(\beta)$ positive, $f \in L^2(\Omega_\delta \setminus \bar{\Omega}_1)$ and there exist positive constants α, C and M such that $|f(x)| \le C_f e^{-\alpha|x|}$ for $|x| > M > r_1$, then there exist positive constants α_1, C_1 and M_1 independent of ψ_δ, f and δ such that

$$|\psi_\delta(x)| \le C_1 e^{-\alpha_1|x|} \left(\|\psi_\delta\|_{H^1(\Omega_\delta \setminus \bar{\Omega}_1)} + \|f\|_{L^2(\Omega_\delta \setminus \bar{\Omega}_1)} + C_f \right) \tag{V.13}$$

for $|x| > M_1$.

Proof. We start by decomposing $\psi_\delta = \psi + w$, where ψ is defined to be equal to ψ_δ in Ω_1 and satisfies

$$\begin{aligned} \Delta\psi + \beta^2\psi &= f \text{ in } \Omega_1^c, \\ \psi &= \psi_\delta \text{ on } \Gamma_1, \end{aligned} \tag{V.14}$$

where f is the zero extension to Ω_∞^c. Then w satisfies the equations

$$\begin{aligned} \Delta w + \beta^2 w &= 0 \quad \text{in} \ \ \Omega_\infty \setminus \bar{\Omega}_1, \\ w &= 0 \quad \text{on} \ \ \Gamma_1, \\ w &= -\psi \ \ \text{on} \ \ \Gamma_\infty. \end{aligned}$$

Note that ψ decays exponentially by Lemma IV.11 and the stability of (V.14) implies

$$|\psi(x)| \leq C_1 e^{-\alpha_1 |x|} \left(\|\psi_\delta\|_{H^1(\Omega_\delta \setminus \bar{\Omega}_1)} + \|f\|_{L^2(\Omega_\delta \setminus \bar{\Omega}_1)} + C_f \right) \tag{V.15}$$

for $|x| > M_1$. So we have only to show exponential decay of w.

We do this by showing that

$$\|w\|_{H^2(\Omega_\delta \setminus \bar{\Omega}_1)} \leq C_\delta \|\psi\|_{H^2(S_\epsilon \cap \Omega_\delta)}, \tag{V.16}$$

where S_ϵ is an ϵ-neighborhood of Γ_δ for $\epsilon > 0$. Here C_δ only grows as a polynomial of δ. Using (V.16) gives (for $\epsilon' > \epsilon$ independent of δ)

$$\begin{aligned} \|w\|_{H^2(\Omega_\delta \setminus \bar{\Omega}_1)} &\leq C_\delta \|\psi\|_{L^2(S_{\epsilon'})} \\ &\leq C_\delta e^{-\alpha_1 \delta} \left(\|\psi\|_{H^1(\Omega_1^c)} + \|f\|_{L^2(\Omega_\delta \setminus \bar{\Omega}_1)} + C_f \right) \\ &\leq C_1 e^{-\alpha_2 |x|} \left(\|\psi_\delta\|_{H^1(\Omega_\delta \setminus \bar{\Omega}_1)} + \|f\|_{L^2(\Omega_\delta \setminus \bar{\Omega}_1)} + C_f \right). \end{aligned} \tag{V.17}$$

Here we absorbed the polynomial growth in C_δ by making $\alpha_2 < \alpha_1$. Combining the above inequalities with a Sobolev embedding theorem proves (V.13).

Finally, to prove (V.16), we decompose $w = \tilde{w} + w_0$, where $\tilde{w} = -\chi\psi$ and χ is a cutoff function which is defined on $\Omega_\delta \setminus \bar{\Omega}_1$, is one in a neighborhood of Γ_δ and vanishes outside of $S_\epsilon \cap (\Omega_\delta \setminus \bar{\Omega}_1)$. We need only show that

$$\|w_0\|_{H^2(\Omega_\delta \setminus \bar{\Omega}_1)} \leq C_\delta \|\psi\|_{H^2(S_\epsilon \cap \Omega_\delta)}.$$

Note that w_0 satisfies

$$\begin{aligned} \Delta w_0 + \beta^2 w_0 &= g \text{ in } \Omega_\delta \setminus \bar{\Omega}_1, \\ w_0 &= 0 \text{ on } \Gamma_1 \cup \Gamma_\delta, \end{aligned} \tag{V.18}$$

where $g = -(\Delta\tilde{w} + \beta^2\tilde{w})$ is in $L^2(S_\epsilon \cap (\Omega_\delta \setminus \bar{\Omega}_1))$. Clearly, $\|w_0\|_{H^1(\Omega_\delta\setminus\bar{\Omega}_1)}$ is bounded by $C\|g\|_{L^2(\Omega_\delta\setminus\bar{\Omega}_1)}$.

Let Ω_2 be a ball centered at the origin and of radius $r_2 > r_1$, independent of δ, and contained in Ω_δ. Let χ_1 be a cutoff function on $\Omega_\delta \setminus \bar{\Omega}_1$, which is one on $\Omega_\delta \setminus \bar{\Omega}_2$ and vanishes near Γ_1. Then $(1-\chi_1)w_0$ and $\chi_1 w_0$ (extended by zero in Ω_1) satisfy equations similar to (V.18) on domains $\Omega_2 \setminus \bar{\Omega}_1$ and Ω_δ, respectively. The data for these problems involves g above and at most first order derivatives of w_0 and hence is controlled in $L^2(\Omega_\delta \setminus \bar{\Omega}_1)$. It follows from a regularity on the smooth domain $\Omega_2 \setminus \bar{\Omega}_1$ that

$$\|(1-\chi)w_0\|_{H^2(\Omega_\delta\setminus\bar{\Omega}_1)} = \|(1-\chi)w_0\|_{H^2(\Omega_2\setminus\bar{\Omega}_1)} \le C(\|g\|_{L^2(\Omega_2\setminus\bar{\Omega}_1)} + \|w_0\|_{H^1(\Omega_2\setminus\bar{\Omega}_1)}).$$

Finally, by dilation to a fixed sized domain,

$$\|\chi w_0\|_{H^2(\Omega_\delta\setminus\bar{\Omega}_1)} = \|\chi w_0\|_{H^2(\Omega_\delta)} \le C_\delta(\|g\|_{L^2(\Omega_\delta\setminus\bar{\Omega}_1)} + \|w_0\|_{H^1(\Omega_\delta\setminus\bar{\Omega}_1)}).$$

The inequality (V.16) follows combining the above.

□

The same technique as used in the proof of Lemma IV.12 will justify the following lemma.

Lemma V.5. *Let $\widetilde{V}_\delta$ be as above. Then there are constants α, C and $M > r_1$ such that for $\delta > M$ and $\psi_\delta \in \widetilde{V}_\delta$,*

$$|\psi_\delta(x)| \le Ce^{-\alpha|x|}\|\psi_\delta\|_{H^1(\Omega_\infty)} \text{ for all } |x| > M. \tag{V.19}$$

Proof. Let $\tilde{m} = \sum_i \tilde{m}(i)$. For any non-zero $\psi \in \tilde{V}_\delta$,

$$\prod_{i=1}^{k} (T_\delta - \lambda_i^\delta I)^{\tilde{m}(i)} \psi = \prod_{i=1}^{\tilde{m}} (T_\delta - \tilde{\lambda}_i I)\psi = 0,$$

with the obvious definition of $\tilde{\lambda}_i$. There is a positive integer $n \leq \tilde{m}$ such that

$$\prod_{i=1}^{n-1} (T_\delta - \tilde{\lambda}_i I)\psi \neq 0 \quad \text{and} \quad \prod_{i=1}^{n} (T_\delta - \tilde{\lambda}_i I)\psi = 0.$$

Setting $\psi_n = \psi$ and $\psi_j = (T_\delta - \tilde{\lambda}_{n-j} I)\psi_{j+1}$ for $j = 1, \ldots, n-1$, we have

$$\Delta \psi_n + (d_0 k(\lambda_1))^2 \psi_n = d_0^2 \sum_{j=1}^{n-1} \frac{(-1)^{j+1}}{\Pi_{l=1}^{j+1} \tilde{\lambda}_l} \psi_{n-j} \quad \text{in} \quad \Omega_1^c.$$

Recall that the norm of T_δ is bounded by a constant independent of δ from (V.2) and (V.3) and $\tilde{\lambda}_i$, for each i, is inside Γ and so that $\mathrm{Im}(d_0 k(\tilde{\lambda}_i)) > 0$. The induction argument used in the proof of Lemma IV.12 completes the proof.

□

CHAPTER VI

EIGENVALUE CONVERGENCE

In this chapter we will show the eigenvalue convergence as the main result. The eigenvalue convergence consists of two parts. One is the convergence of eigenvalues of T_δ with δ increasing in the continuous level, and the second part is the convergence of eigenvalues of the corresponding discrete operators T_δ^h with a mesh size h converging to zero in the discrete level. Because the second part is standard [12], the first part will be the focus. To develop this result, we will use the exponential decay property of generalized eigenfunctions of T and T_δ that we provided in Chapter IV and Chapter V.

Numerical experiments illustrating these results will also be given. Specifically, we will consider a resonance problem in a penetrable inhomogeneous media of one and two space dimension. Although some experiments appear to have spurious numerical eigenvalues, we will explain how this relates to the theory.

A. Convergence of eigenvalues

In the previous two chapters, we studied the inverse of the operator $\widetilde{L}$ on $L^2(\mathbb{R}^3)$ and $L^2(\Omega_\delta)$, specifically $T : H^1(\mathbb{R}^3) \to H^1(\mathbb{R}^3)$ and $T_\delta : H^1(\mathbb{R}^3) \to H^1_0(\Omega_\delta) \subset H^1(\mathbb{R}^3)$. Our goal is to now show that the eigenvalues of T_δ converge to those of T as δ increases. The typical approach for proving eigenvalue convergence results involves norm convergence (see, e.g., [41]). Unfortunately, this approach is not viable in this case because the approximate operator T_δ is compact while the full operator T is not, which means that T_δ can not converge to T in norm as δ grows. Thus the analysis of the eigenvalue convergence will be developed in a non-standard way based on the exponential decay property of eigenfunctions of the operator T and T_δ. First we will show that T_δ converges to T on a subspace of exponentially decaying functions.

Lemma VI.1. *Suppose that* $u \in H^1(\mathbb{R}^3)$ *satisfies*

$$|u(x)| \leq Ce^{-\alpha|x|}\|u\|_{H^1(\mathbb{R}^3)} \tag{VI.1}$$

for $|x| > M > r_1$. *Then there exist positive constants* α_1, C_1 *and* $M_1 > M$ *such that*

$$\|(T - T_\delta)u\|_{H^1(\mathbb{R}^3)} \leq C_1 e^{-\alpha_1 \delta}\|u\|_{H^1(\mathbb{R}^3)}$$

for $\delta > M_1$.

Proof. The H^1-estimate for $(T - T_\delta)u$ will be computed in two subdomains Ω_∞ and Ω_∞^c. First, note that since Tu is the solution to the problem

$$A_1(Tu, \phi) = B(u, \phi) \ \text{ for } \ \phi \in H^1(\mathbb{R}^3),$$

it satisfies

$$\Delta Tu + d_0^2 Tu = -d_0^2 u \ \text{ in } \ \Omega_1^c. \tag{VI.2}$$

It follows from Lemma IV.11 that

$$\|Tu\|_{H^{1/2}(\Gamma_\infty)} \leq C_1 e^{-\alpha_1 \delta}(\|Tu\|_{H^1(\Omega_1^c)} + \|u\|_{H^1(\Omega_1^c)}) \tag{VI.3}$$

for $\delta > M_1$.

Take $M_1 > \delta_0$ in Theorem V.2. In Ω_∞, $\psi \equiv (T - T_\delta)u$ is the unique solution to the problem

$$\begin{aligned} A_1(\psi, \phi) &= 0 \ \text{ for all } \ \phi \in H_0^1(\Omega_\infty), \\ \psi &= Tu \ \text{ on } \ \Gamma_\infty, \end{aligned}$$

so that by stability and (VI.3),

$$\begin{aligned} \|(T - T_\delta)u\|_{H^1(\Omega_\infty)} &\leq C\|Tu\|_{H^{1/2}(\Gamma_\infty)} \\ &\leq C_1 e^{-\alpha_1 \delta}(\|Tu\|_{H^1(\mathbb{R}^3)} + \|u\|_{H^1(\mathbb{R}^3)}) \end{aligned} \tag{VI.4}$$

for $\delta > M_1$.

In Ω_δ^c, $\psi \equiv (T - T_\delta)u = Tu$ is the unique solution to (VI.2) with the boundary condition Tu on Γ_∞. By stability,

$$\|Tu\|_{H^1(\Omega_\delta^c)} \leq C(\|u\|_{L^2(\Omega_\delta^c)} + \|Tu\|_{H^{1/2}(\Gamma_\infty)}).$$

Integrating the square of (VI.1) over Ω_δ^c and using (VI.3) gives

$$\|Tu\|_{H^1(\Omega_\delta^c)} \leq C_\delta e^{-\alpha_1 \delta}\left(\|u\|_{H^1(\mathbb{R}^3)} + \|Tu\|_{H^1(\mathbb{R}^3)}\right). \tag{VI.5}$$

for $\delta > M_1$ and C_δ a linear function of δ. The δ-dependence in the constant can be removed by making α_1 slightly smaller. The result follows from (VI.4), (VI.5) and the boundedness of T. □

Before stating the main theorem, we shall recall the finite dimensional subspaces V and V_δ in $H^1(\mathbb{R}^3)$ defined in the previous chapters. We are considering λ, an isolated eigenvalue of finite multiplicity of T, and Γ is a circle of radius η centered at λ contained in $\rho(T)$. η is chosen so small enough that all points in the interior of Γ except for λ belong to $\rho(T)$. Furthermore, it is guaranteed that $\Gamma \subset \rho(T_\delta)$ for sufficiently large δ due to Theorem V.2. V is the generalized eigenspace of T associated with λ and V_δ is the space spanned by the generalized eigenfunctions associated with the eigenvalues of T_δ inside Γ. $\widetilde{V}_\delta$ denotes a T_δ-invariant subspace of V_δ of dimension $\leq \dim(V) + 1$ defined in Chapter V. We observe that V is a $R_z(T)$-invariant space for $z \in \Gamma$, since V is finite-dimensional and invariant under the action of the injective operator $T - zI$. For the same reason, $\widetilde{V}_\delta$ is $R_z(T_\delta)$-invariant for $z \in \Gamma$.

We define the Riesz projections P_Γ and P_Γ^δ onto V and V_δ, respectively: For

$u \in H^1(\mathbb{R}^3)$

$$P_\Gamma(u) = \frac{1}{2\pi i}\int_\Gamma R_z(T)u\,\mathrm{d}z \tag{VI.6}$$

and

$$P_\Gamma^\delta(u) = \frac{1}{2\pi i}\int_\Gamma R_z(T_\delta)u\,\mathrm{d}z. \tag{VI.7}$$

Since Γ is contained in $\rho(T_\delta)$ for sufficiently large δ, P_Γ^δ is well-defined for such δ.

We are now in a position to prove the eigenvalue convergence.

Theorem VI.2. *For any η sufficiently small, there is a $\delta_1 > 0$ such that*

$$\dim(V) = \dim(V_\delta)$$

for $\delta > \delta_1$.

Remark VI.3. The above theorem shows that the eigenvalues for the truncated problem converge to those of the full problem since the radius η of Γ is arbitrary small. This convergence respects the eigenvalue multiplicity in the sense that the sum of the multiplicities of the eigenvalues inside the circle of radius η for the truncated problem equals the multiplicity of λ for any η provided that $\delta \geq \delta_1(\eta)$ is sufficiently large.

Proof of Theorem VI.2. We first note that for $z \in \Gamma$,

$$\|R_z(T)\|_{H^1(\mathbb{R}^3)} \leq C.$$

In addition, for $\delta > \delta_0$ in Theorem V.2, (V.10) and (V.11) implies that

$$\|R_z(T_\delta)\|_{H^1(\mathbb{R}^3)} \leq C$$

with C independent of δ. It follows that P_Γ and P_Γ^δ are bounded operators in $H^1(\mathbb{R}^3)$.

Let ψ be in V. Since V is invariant under the action of $R_z(T)$, by Lemma VI.1,

$$\|(T - T_\delta)R_z(T)\psi\|_{H^1(\mathbb{R}^3)} \leq Ce^{-\alpha_1 \delta}\|\psi\|_{H^1(\mathbb{R}^3)}.$$

We also have

$$\begin{aligned}(I - P^\delta_\Gamma)P_\Gamma &= \frac{1}{2\pi i}\int_\Gamma (R_z(T) - R_z(T_\delta))P_\Gamma \,\mathrm{d}z \\ &= -\frac{1}{2\pi i}\int_\Gamma R_z(T_\delta)(T - T_\delta)R_z(T)P_\Gamma \,\mathrm{d}z.\end{aligned}$$

Thus,

$$\begin{aligned}\|(I - P^\delta_\Gamma)\psi\|_{H^1(\mathbb{R}^3)} &= \frac{1}{2\pi}\|\int_\Gamma R_z(T_\delta)(T - T_\delta)R_z(T)\psi \,\mathrm{d}z\|_{H^1(\mathbb{R}^3)} \\ &\leq \frac{1}{2\pi}\int_\Gamma \|R_z(T_\delta)\|_{H^1(\mathbb{R}^3)}\|(T - T_\delta)R_z(T)\psi\|_{H^1(\mathbb{R}^3)} \,\mathrm{d}z \\ &\leq Ce^{-\alpha_1 \delta}\|\psi\|_{H^1(\mathbb{R}^3)}. \qquad \text{(VI.8)}\end{aligned}$$

We choose $\delta_1 \geq \delta_0$ so that $Ce^{-\alpha_1 \delta_1}$ is less than one. For (VI.8) to hold, it is necessary that the rank of P^δ_Γ be greater than or equal to $\dim(V)$, i.e., $\dim(V_\delta) \geq \dim(V)$.

For the other direction, we let ψ be in $\widetilde{V}_\delta$ with $\widetilde{V}_\delta$ as above. An argument similar to that used above (using the invariance of $\widetilde{V}_\delta$ under P^δ_Γ) gives

$$\|(I - P_\Gamma)\psi\|_{H^1(\mathbb{R}^3)} \leq Ce^{-\alpha_1 \delta}\|\psi\|_{H^1(\mathbb{R}^3)}.$$

Choosing $\delta_1 \geq \delta_0$ so that $Ce^{-\alpha_1 \delta_1} < 1$ then leads to $\dim(V) \geq \dim(\widetilde{V}_\delta)$. This implies that there is no subspace $\widetilde{V}_\delta \subseteq V_\delta$ with dimension greater than $\dim(V)$, i.e., $\dim(V_\delta) = \dim(V)$. □

So far, we studied convergence of eigenvalues of T_δ to those of T in the continuous level as δ is increasing. Now we shift our concern to the problem in a discrete level. For a fixed $\delta > \delta_1(\eta)$ in Theorem VI.2 we discretize the system with finite elements. Let h represent the diameters of elements of a triangulation of the domain Ω_δ and

S_h denote a finite dimensional subspace of $H_0^1(\Omega_\delta)$. Then for a given $f \in L^2(\Omega_\delta)$ the problem to find $u_h \in S_h$ such that

$$A_1(u_h, \phi_h) = B(f, \phi_h) \quad \text{for all} \quad \phi_h \in S_h \tag{VI.9}$$

is solvable. The solvability of the problem (VI.9) follows from the Aubin-Nitsche duality argument [50]. In fact, if u_h satisfies (VI.9) with an exact solution u, then by the duality argument there exists $s > 1/2$ such that

$$\|u - u_h\|_{L^2(\Omega_\delta)} \le Ch^s \|u - u_h\|_{H^1(\Omega_\delta)}. \tag{VI.10}$$

Now, from coercivity of $\widetilde{A}(\cdot,\cdot)$ in (IV.18), Galerkin orthogonality, boundedness of $A_1(\cdot,\cdot)$, and (VI.10) we obtain

$$\begin{aligned} \|u - u_h\|_{H^1(\Omega_\delta)} &\le C \frac{|\widetilde{A}(u-u_h, u-u_h)|}{\|u_h\|_{H^1(\Omega_\delta)}} \\ &\le C \frac{|A_1(u, u-u_h)| + \|u-u_h\|_{L^2(\Omega_\delta)} \|u-u_h\|_{H^1(\Omega_\delta)}}{\|u-u_h\|_{H^1(\Omega_\delta)}} \\ &\le C\|u\|_{H^1(\Omega_\delta)} + Ch^s \|u-u_h\|_{H^1(\Omega_\delta)}. \end{aligned} \tag{VI.11}$$

Consequently, for h with $Ch^s < 1$

$$\|u - u_h\|_{H^1(\Omega_\delta)} \le C\|u\|_{H^1(\Omega_\delta)}. \tag{VI.12}$$

Since S_h is finite dimensional, for the solvability of (VI.9), it suffices to show that (VI.9) has a unique solution. To this end, assume that $f = 0$. Then $u = 0$ and it follows from (VI.12) that $u_h = 0$.

Therefore, for $f \in H^1(\mathbb{R}^3)$ we can define $T_\delta^h(f)$ by the unique solution to the problem

$$A_1(T_\delta^h f, \phi_h) = B(f, \phi_h) \quad \text{for all} \quad \phi_h \in S_h.$$

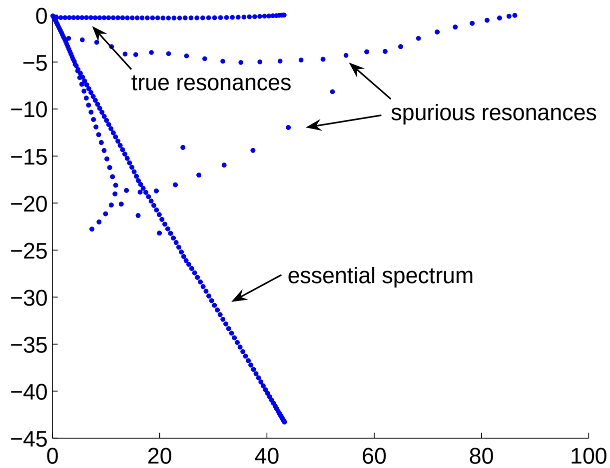


Fig. 3. Spectrum of a one dimensional resonance problem

From (VI.10),

$$\|T_\delta - T_\delta^h\|_{L^2(\Omega_\delta)} \le Ch^s \|T\|_{H^1(\Omega_\delta)}.$$

Thus there is a one-parameter family of compact operators $T_\delta^h : H^1(\mathbb{R}^3) \to S_h \subset H^1(\mathbb{R}^3)$ converging to T_δ as $h \to 0$. An eigenvalue convergence result for T_δ and T_δ^h is standard and it is presented in the following lemma [12].

Lemma VI.4. *Let λ be a non-zero eigenvalue of T_δ with algebraic multiplicity m and let Γ be a circle centered at λ which lies in $\rho(T_\delta)$ and contains no other points of $\sigma(T_\delta)$. If $\|T_\delta - T_\delta^h\|_{L^2(\Omega_\delta)} \to 0$ as $h \to 0$, then there is an h_0 such that, for $0 < h \le h_0$, there are exactly m eigenvalues (counting algebraic multiplicities) of T_δ^h lying inside Γ and all points of $\sigma(T_\delta^h)$ are bounded away from Γ.*

B. Numerical results

In this section, we will give simple one and two dimensional resonance problems illustrating the behavior of finite element approximations of the PML eigenvalue problem. Although some experiments appear to have spurious numerical eigenvalues, we shall see that they can be controlled by keeping the transition layer close to the non-homogeneous phenomena, i.e. the region where the operator differs from the Laplacian.

We start with a one dimensional problem, i.e.,

$$-a\Delta u = k^2 u \quad \text{in} \quad \mathbb{R}$$

with the outgoing wave condition. Here a is a piecewise constant function defined by

$$a = \begin{cases} 1/4 & \text{if } |x| < 1, \\ 1 & \text{otherwise.} \end{cases}$$

We impose the continuity of u and au' at $x = \pm 1$. The analytic resonances corresponding to this problem are given by

$$k = \frac{n\pi}{4} - \frac{\ln 3}{4} i$$

for $n \in \mathbb{Z}$ and $n > 0$.

For the first experiment, we choose the PML parameters $r_0 = 2$, $r_1 = 4$, $\delta = 8$, $\sigma_0 = 1$ and discretize the system with a mesh size $h = 1/50$. Figure 3 shows the resulting eigenvalues. Note that the eigenvalues labeled "true resonances" are very close to the analytic resonances given above. In Figure 4, we report the error observed when approximating the resonance of smallest magnitude as a function of δ for fixed values of h. The PML parameters were $r_0 = 1$, $r_1 = 2$ and $\sigma_0 = 1$. As expected, increasing δ for a fixed value of h improves the accuracy to the point where the mesh size errors dominate.

The remaining eigenvalues in Figure 3 either correspond to those clearly approximating the essential spectrum or spurious eigenvalues. Those far away from the true resonances and those to the left of the essential spectrum are easily ignored. However

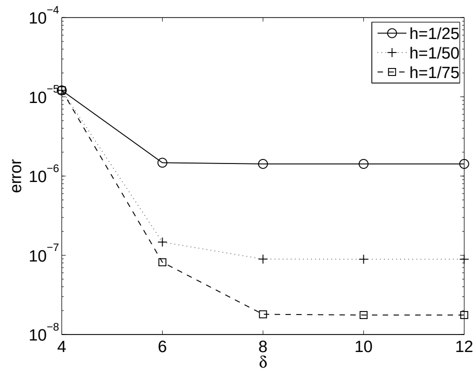


Fig. 4. Eigenvalue error for the resonance of smallest magnitude

the group of spurious eigenvalues running below and parallel to the true resonances are somewhat disturbing, especially so since they do not move much when either the mesh size is decreased (at least, within reasonable parameters) or the computational region is increased. This will be discussed in the next section in detail.

We next consider a model problem on $\mathbb{R}^2$. Let Ω_0 be the open unit disk in $\mathbb{R}^2$ and consider

$$-a\Delta u = k^2 u \quad \text{in} \quad \mathbb{R}^2$$

with the outgoing wave condition and the transmission conditions of the continuity of u and $a\nabla u$ at the interface, where

$$a = \begin{cases} 1/4 & \text{if } (x,y) \in \Omega_0, \\ 1 & \text{otherwise.} \end{cases}$$

An outgoing solution bounded in Ω_0 is of the form (in polar coordinates)

$$u(x,y) = \begin{cases} \displaystyle\sum_{n=-\infty}^{\infty} a_n J_n(2kr) e^{in\theta} & \text{for} \quad (x,y) \in \Omega_0, \\ \displaystyle\sum_{n=-\infty}^{\infty} b_n H_n^1(kr) e^{in\theta} & \text{for} \quad (x,y) \in \Omega_0^c, \end{cases}$$

where J_n are Bessel functions of the first kind of order n and H_n^1 are Hankel functions of the first kind of order n. The continuity conditions at the interface lead to

$$a_n J_n(2k) = b_n H_n^1(k) \quad \text{and} \quad \frac{1}{2} a_n J_n'(2k) = b_n (H_n^1(k))'.$$

Non-zero solutions exist when k satisfies

$$J_n'(2k) H_n^1(k) - 2 J_n(2k) (H_n^1(k))' = 0. \tag{VI.13}$$

This equation can be solved by iteration and its solutions are used as a reference. It is easy to see that each solution k to the problem (VI.13) for $n > 0$ is of multiplicity 2.

For the one dimensional case, we simply computed all eigenvalues using MatLab. This approach fails for the two dimensional problem as the problem size is much too large. We clearly have to be more selective. Our goal is to focus on computing the eigenvalues corresponding to resonances which are close to the origin. We are able to do this by defining a related eigenvalue problem which transforms the eigenvalues of interest into the eigenvalues of greatest magnitude. These eigenvalues can then be selectively computed using a general eigensolver software. Specifically, we use the software package SLEPc [37], which is a general purpose eigensolver built on top of PETSc [4].

The computational eigenvalue problem (after introducing PML, truncating the domain and applying finite elements) can be written

$$Su = k^2 N u$$

for appropriate complex valued matrices S and N. The idea is to use linear fractional transformations. We consider $\zeta_2 \circ \zeta_1$ where

$$\zeta_1(z) = \frac{1}{z} \quad \text{and} \quad \zeta_2(z) = \frac{d_0 + iz}{d_0 - iz}.$$

Table 1. Numerical results for the first ten resonances of the two dimensional problem

Approximate PML Resonances		Resonances	Multiplicity	n
$h = 1/100$	$h = 1/120$			
$1.1169 - 0.2393i$	$1.1165 - 0.2392i$	$1.1155 - 0.2396i$	1	0
$2.7211 - 0.2667i$	$2.7200 - 0.2665i$	$2.7167 - 0.2665i$	1	0
$1.8264 - 0.2916i$ $1.8264 - 0.2916i$	$1.8256 - 0.2914i$ $1.8256 - 0.2914i$	$1.8238 - 0.2921i$	2	1
$2.4021 - 0.3759i$ $2.4026 - 0.3761i$	$2.4009 - 0.3755i$ $2.4012 - 0.3757i$	$2.3981 - 0.3781i$	2	2
$2.8249 - 0.3182i$ $2.8249 - 0.3182i$	$2.8242 - 0.3173i$ $2.8242 - 0.3173i$	$2.8161 - 0.3161i$	2	3
$3.4066 - 0.1881i$ $3.4068 - 0.1885i$	$3.4058 - 0.1877i$ $3.4059 - 0.1880i$	$3.3993 - 0.1851i$	2	4

The first transformation maps points near the origin to points of large absolute value. Under this transformation, the sector $2\arg(1/d_0) \leq \arg(z) \leq 0$ maps to the sector $0 \leq \arg(z) \leq 2\arg(d_0)$. The second transformation gets rid of the "essential spectrum" (which was mapped to $\arg(z) = 2\arg(d_0)$) by mapping $\arg(z) = 2\arg(d_0)$ to the interior of the unit disk and anything in the sector $0 \leq \arg(z) < \arg(d_0)$ to the exterior of the unit disk. Thus, we look for the eigenvalues of largest magnitude for the operator

$$(d_0 S + iN)u = \mu(d_0 S - iN)u$$

and recover k^2 from the formula

$$k^2 = \frac{(\mu+1)i}{(\mu-1)d_0}.$$

We consider computing on a square domain of side length 2δ. Table 1 gives the values of the first ten numerical and analytical resonances for the above problem as a function of h. The truncated domain corresponded to $\delta = 5$ and the PML parameters were $\sigma_0 = 1$, $r_0 = 1$ and $r_1 = 4$. Note that errors of less than one percent were obtained and improved results were observed when the mesh size was decreased. These are relatively large problems, indeed, the case of $h = 1/120$ corresponds to almost a million and a half complex unknowns.

C. Spurious resonances

Spurious eigenvalues appearing in PML approximations to resonance problems have been discussed elsewhere in the literature. In particular, Zworski [56] explains this phenomenon in terms of the pseudo-spectra concept (cf. [55]). While the set of the pseudo-spectrum of selfadjoint operators H

$$\Lambda_\epsilon(H) = \{z \in \mathbb{C} \ : \ \|(H - zI)^{-1}\| \leq \epsilon^{-1}\}$$

is exactly the same as the ϵ-neighborhood of the spectrum of H, we can not expect this result for non-selfadjoint operators, and $\Lambda_\epsilon(H)$ may be larger than that. In other words, the norms of the resolvent of a non-selfadjoint operator can be quite large for points located far away from the spectrum. We shall demonstrate that this is an important issue for the PML eigenvalue problem. Note that the central theorems (Theorem V.2 and Theorem VI.2) require that δ is large enough that

$$C(\|R_z(T)\|)e^{-\alpha\delta} < 1 \qquad \text{(VI.14)}$$

(See the inequalities (V.9) and (V.8) with $A_1(\cdot,\cdot)$ replaced with $\widetilde{A}_z(\cdot,\cdot)$). The situation at the discrete level is worse. To guarantee eigenvalue convergence without spurious eigenvalues from the discretization, the problem $(T_\delta^h - z)u_h = f_h$, or equivalently $\widetilde{A}_z(u_h,\phi_h) = A_1(f_h,\phi_h)$ for $f_h \in S_h$ and $z \in \rho(T_\delta)$ needs to be uniquely solvable. For this, assume that $f_h = 0$. Let χ be the solution to the adjoint problem

$$\widetilde{A}_z(\phi,\chi) = A_1(e_h,\phi) \ \text{ for all } \ \phi \in H_0^1(\Omega_\delta)$$

with the error $e_h = u_h$. Since $A_1(\cdot,\cdot)$ is coercive for sufficiently small h from (VI.11),

$$\|e_h\|^2_{H^1(\Omega_\delta)} \le C|A_1(e_h,e_h)| = C|\widetilde{A}_z(e_h,\chi)| = C|\widetilde{A}_z(e_h,\chi - v_h)| \tag{VI.15}$$

for any $v_h \in S_h$. Applying an interpolation estimate $\|\chi - v_h\|_{H^1(\Omega_\delta)} \le Ch\|\chi\|_{H^2(\Omega_\delta)}$ for some $v_h \in S_h$ and the regularity $\|\chi\|_{H^2(\Omega_\delta)} \le C(\|R_z(T_\delta)\|)\|e_h\|_{H^1(\Omega_\delta)}$ to (VI.15), it follows that

$$\|e_h\|^2_{H^1(\Omega_\delta)} \le C(\|R_z(T_\delta)\|)h\|e_h\|^2_{H^1(\Omega_\delta)}.$$

To achieve a unique solution $u_h = 0$, one needs to have that $h \le h_0$ with h_0 satisfying

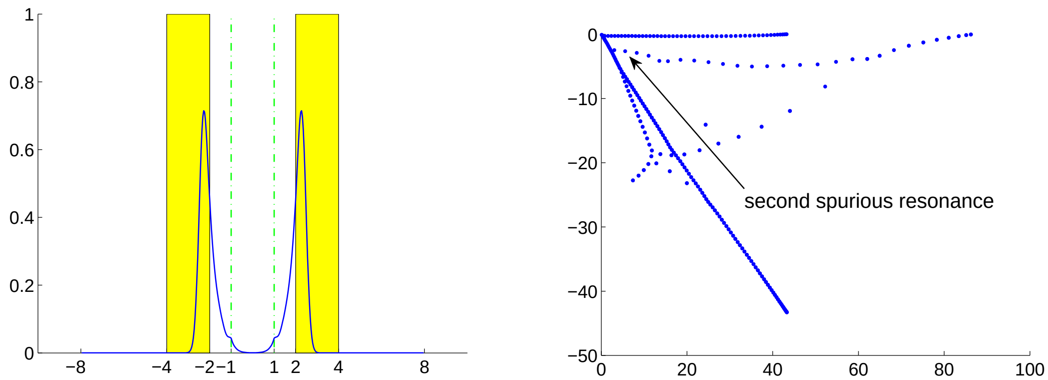
$$C(\|R_z(T_\delta)\|)h_0 < 1. \tag{VI.16}$$

Thus, in cases where the norm of the resolvent is large, to get rid of the spurious eigenvalues, it appears to be necessary to make h too small to be practical.

To shed some light on the behavior of the resolvent, we consider the above one dimensional problem. Let k be a complex number with $\text{Im}(k) < 0$, $\text{Im}(d_0 k) > 0$ and k not a resonance. The function $f(x) = e^{ik\tilde{d}|x|}$ satisfies the PML equation

$$(\widetilde{L} - k^2)f \equiv -\frac{1}{d}\left(\frac{1}{d}f'\right)' - k^2 f = 0 \ \text{ for } \ |x| > 1. \tag{VI.17}$$

Note that with $r_0 > 1$, f increases exponentially from $|x| = 1$ to $|x| = r_0$ while



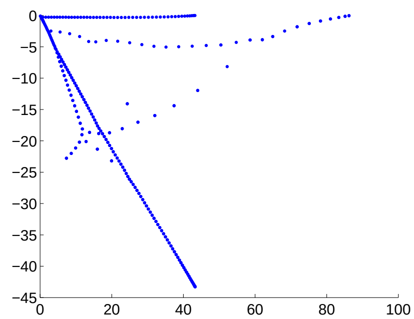
(a) Magnitude of second spurious eigenfunction

(b) Spectrum of the one dimensional problem

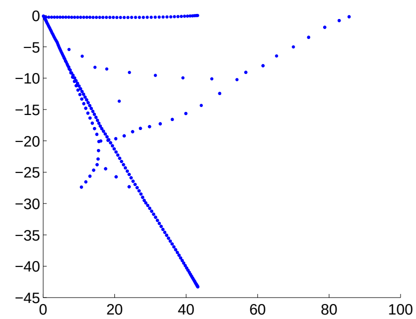
Fig. 5. Spurious eigenfunction

decreasing exponentially outside of the transition region. Figure 5 shows magnitude of the second spurious eigenfunction. Because f is relatively small for $|x| \le 1$ and satisfies (VI.17), $\|(\widetilde{L}-k^2)f\|$ is much smaller than $\|f\|$. This implies that the constant in the inf-sup condition (V.9) is large. This constant is directly proportional to the norm of the resolvent $R_z(T)$ (see the proof of Theorem V.2 for details). Accordingly, to keep the norm of $R_z(T)$ manageable, we need to avoid a large region allowing exponential increase. This can be attained by keeping the start of the transitional region as close as possible to the region of inhomogeneity, i.e., $|x| = 1$. The analysis for problems of dimension greater than one is similar.

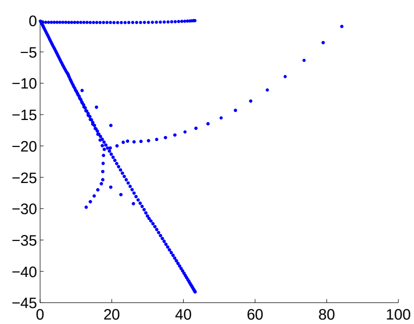
The behavior of the spurious resonances as a function of the location of the transitional layer is illustrated in Figure 6. Notice that the spurious eigenvalues can be moved away from the true resonances simply by placing the transition region closer to one. In fact, the best results are obtained by starting the transition region on the interface. This also illustrates the fact that there does not need to be any area extending outside of Ω where the original equation is retained.



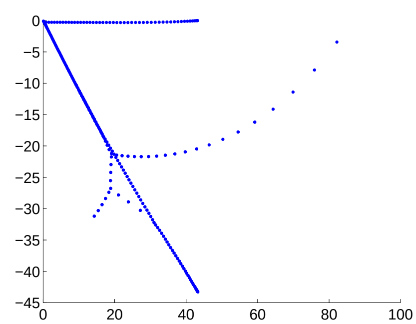
(a) $r_0 = 2$



(b) $r_0 = 1.5$



(c) $r_0 = 1.2$



(d) $r_0 = 1$

Fig. 6. Eigenvalues from different PML's (r_0 is the radius of the inside boundary of PML)

CHAPTER VII

APPLICATION OF CARTESIAN PML TO ACOUSTIC SCATTERING PROBLEMS

From this chapter on we study an application of Cartesian PML to acoustic scattering problems. When PML is introduced in a Cartesian geometry, each coordinate is stretched independently. The analysis of Cartesian PML problems requires a significantly different approach from that of spherical PML problems. This chapter provides preliminaries for the analysis in the subsequent chapters. We start with reformulating acoustic scattering problems in the Cartesian PML framework and introduce a complexified distance between two complex stretched points. We also discuss the fundamental solution to the Cartesian PML Helmholtz equation.

A. Cartesian PML reformulation

We consider the exterior Helmholtz problem with Sommerfeld radiation condition,

$$\begin{aligned} -\Delta u - k^2 u = 0 \ \text{ in } \ \bar{\Omega}^c, \\ u = g \ \text{ on } \ \partial\Omega, \\ \lim_{r\to\infty} r^{1/2}\left|\frac{\partial u}{\partial r} - iku\right| = 0. \end{aligned} \tag{VII.1}$$

Here k is real and positive and Ω is a bounded domain with a Lipschitz continuous boundary contained in the square[†] $[-a, a]^2$ for some positive a.

The simplest example of a Cartesian PML approximation involves an even func-

[†]We consider a domain in $\mathbb{R}^2$ for convenience. The extension to domains in $\mathbb{R}^3$ is completely analogous.

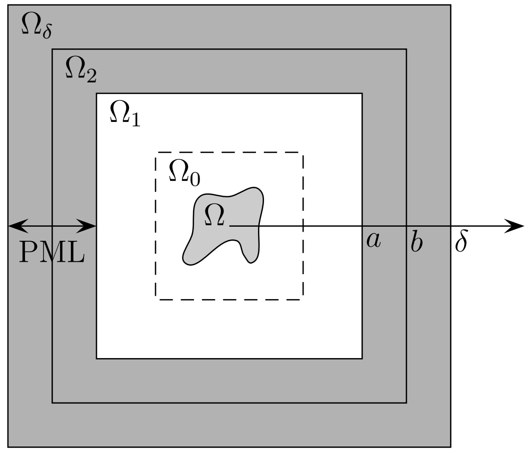


Fig. 7. Cartesian perfectly matched layer in $\mathbb{R}^2$

tion $\tilde{\sigma} \in C^2$ satisfying

$$\begin{aligned}
&\tilde{\sigma}(x) = 0 \quad \text{for} \quad |x| \le a, \\
&\tilde{\sigma}(x) : \ \text{increasing} \quad \text{for} \quad a < x < b, \qquad \text{(VII.2)} \\
&\tilde{\sigma}(x) = \sigma_0 \quad \text{for} \quad |x| \ge b.
\end{aligned}$$

Here $0 < a < b$ and $\sigma_0 > 0$ is a parameter that represents the PML strength.

We shall use the sequence of the strictly increasing square domains, $\Omega_1 = (-a, a)^2$, $\Omega_2 = (-b, b)^2$ (a and b are defined as above) and $\Omega_\delta = (-\delta, \delta)^2$ such that $\Omega \subset \Omega_0 \subset \Omega_1 \subset \Omega_2 \subset \Omega_\delta$ (see Figure 7). Here Ω_0 is an auxiliary square domain between Ω and Ω_1. Let Γ_j denote the boundary of Ω_j for $j = 0, 1, 2$ and δ. In particular, as we shall see, the infinite domain PML model preserves the solution of (VII.1) in Ω_1 and $\Omega_\delta \setminus \bar{\Omega}$ is the domain of numerical computation. Here we assume that the origin is inside the scatterer Ω and the sides of square domains are parallel to the coordinate axes.

We shall use the following notations: for $j = 1, 2$

$$\begin{aligned} \tilde{x}_j(x_j) &\equiv x_j(1 + i\tilde{\sigma}(x_j)), \\ \sigma(x_j) &\equiv (x_j\tilde{\sigma}(x_j))', \\ d(x_j) &\equiv (\tilde{x}_j)' = 1 + i\sigma(x_j), \\ J(x) &\equiv d(x_1)d(x_2), \\ H(x) &\equiv \begin{bmatrix} d(x_2)/d(x_1) & 0 \\ 0 & d(x_1)/d(x_2) \end{bmatrix}. \end{aligned} \tag{VII.3}$$

Then, the Cartesian PML Laplacian is defined by

$$\begin{aligned} \widetilde{\Delta} &= \frac{1}{d(x_1)}\frac{\partial}{\partial x_1}\left(\frac{1}{d(x_1)}\frac{\partial}{\partial x_1}\right) + \frac{1}{d(x_2)}\frac{\partial}{\partial x_2}\left(\frac{1}{d(x_2)}\frac{\partial}{\partial x_2}\right) \\ &= \frac{1}{J(x)}\nabla \cdot H(x)\nabla. \end{aligned} \tag{VII.4}$$

Sometimes we shall use $\widetilde{\Delta}_x$ for $\widetilde{\Delta}$ in order to indicate that the operator acts on functions of x.

The PML reformulation leads to the study of a source problem: for $f \in L^2(\bar{\Omega}^c)$, find $\hat{u} \in H_0^1(\bar{\Omega}^c)$ satisfying

$$A(\hat{u}, \phi) - k^2(d(x_1)d(x_2)\hat{u}, \phi) = (d(x_1)d(x_2)f, \phi) \quad \text{for all} \quad \phi \in H_0^1(\bar{\Omega}^c). \tag{VII.5}$$

Here

$$\begin{aligned} A(u, v) &= \int_{\Omega^c}\left[\frac{d(x_2)}{d(x_1)}\frac{\partial u}{\partial x_1}\frac{\partial \bar{v}}{\partial x_1} + \frac{d(x_1)}{d(x_2)}\frac{\partial u}{\partial x_2}\frac{\partial \bar{v}}{\partial x_2}\right]\mathrm{d}x, \\ (f, g) &= \int_{\Omega^c} f\bar{g}\,\mathrm{d}x. \end{aligned} \tag{VII.6}$$

In [13], an analysis of the source problem on the infinite domain with spherical PML was given by first showing that the resulting form was coercive up to a lower order perturbation on a bounded domain. A standard argument by compact perturbation [47, 54] then shows stability of the source problem once uniqueness has been established. Unfortunately, this perturbation approach fails for Cartesian PML. The problem is, e.g., that the coefficient of the x_1 derivatives in the form on the left hand side of (VII.5) equals $-k^{-2}$ times that of the zeroth order term when $x_1 \in (-a, a)$, i.e., when $d(x_1) = 1$. As $\bar{\Omega}^c \cap ((-a, a) \times \mathbb{R})$ is an unbounded domain, we cannot restore coercivity by a zeroth order perturbation on a BOUNDED domain.

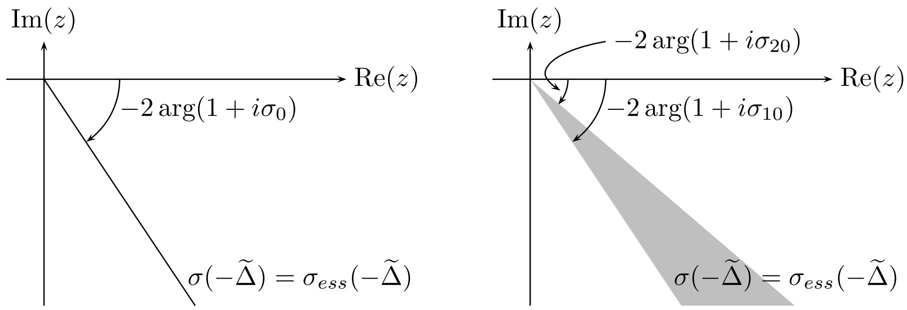
We need to circumvent the compact perturbation approach. We do this by analyzing the essential spectrum of the unbounded operator $\widetilde{L} : H^{-1}(\bar{\Omega}^c) \to H^{-1}(\bar{\Omega}^c)$ with domain $H_0^1(\bar{\Omega}^c)$ defined for $v \in H_0^1(\bar{\Omega}^c)$ by $\widetilde{L}v = f$, where $f \in H^{-1}(\bar{\Omega}^c)$ is given by

$$< f, \bar{d}(x_1)\, \bar{d}(x_2)\phi >= A(v, \phi) \quad \text{for all} \quad \phi \in H_0^1(\bar{\Omega}^c). \tag{VII.7}$$

Here $< \cdot, \cdot >$ denotes the duality pairing. As usual, if $f \in L^2(\bar{\Omega}^c)$, then the duality pairing coincides with the L^2-inner product. We shall see that $\widetilde{L}$ is a (well-defined) closed unbounded operator on $H^{-1}(\bar{\Omega}^c)$ with domain $H_0^1(\bar{\Omega}^c)$ provided that $\tilde{\sigma}$ is smooth enough. Note that $\widetilde{L}$ is a weak form of the operator $-\widetilde{\Delta}$ given by (VII.4).

We take the definition of essential spectrum $\sigma_{ess}(\widetilde{L})$ to be the set of points in the spectrum (the complement of the resolvent $\rho(\widetilde{L})$) excluding those in the discrete spectrum $\sigma_d(\widetilde{L})$ (isolated points of the spectrum with finite algebraic multiplicity). There are other notions of essential spectrum, some of which are discussed in [24].

We will identify the essential spectrum $\sigma_{ess}(\widetilde{L})$ (see Figure 8) and conclude that $\sigma_{ess}(\widetilde{L})$ intersects the real axis only at the origin (in Chapter VIII). This means that the only way that k^2 (for real k with $k \neq 0$) can fail to be in the resolvent set for $\widetilde{L}$ is that there is an eigenvector of $\widetilde{L}$ associated with k^2. Thus by showing uniqueness of solutions for k^2 (in Chapter IX), we conclude that k^2 is in the resolvent set of $\widetilde{L}$ for any real nonzero k. This conclusion implies the "inf-sup" conditions for the variational problem (VII.5) and leads to existence, uniqueness and stability of its



(a) The case of $\sigma_{10} = \sigma_{20} = \sigma_0$. (b) The case when $\sigma_{10} \neq \sigma_{20}$.

Fig. 8. The essential spectrum of $-\widetilde{\Delta}$ on $L^2(\mathbb{R}^2)$ (which coincides with that of $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$)

solution (for suitable f).

Remark VII.1. In the above, we consider a simple PML example where the same stretching function is used in each direction. In an application where the domain more naturally fits into a rectangle $[-a_1, a_1] \times [-a_2, a_2]$, it is more reasonable (and computationally efficient) to use direction dependent PML stretching functions. For example, we use even functions $\tilde{\sigma}_j$ for $j = 1, 2$ satisfying (VII.2) with a, b and σ_0 replaced by a_j, b_j and σ_{j0}, respectively. The only changes in (VII.5) and (VII.7) involve replacement of $d(x_j)$ by $d_j(x_j) \equiv 1 + i(x_j\tilde{\sigma}_j(x_j))'$. As the analysis presented below is identical for direction dependent PML stretching, for convenience of notation, from here on, we shall revert back to the case of $\tilde{\sigma}_1 = \tilde{\sigma}_2 = \tilde{\sigma}$.

B. Complexified distance

In this section we present some technical lemmas that will be used in the following sections. We first shall generalize the complex stretching functions. Let σ_M denote the maximum of σ, $\sigma_M \equiv \max_{t\in\mathbb{R}}\{\sigma(t)\}$, and

$$U \equiv \{z \in \mathbb{C} \ : \ \ \mathrm{Re}(z) > -1/(2\sigma_M)\}.$$

For $z \in U$, we define $\tilde{x}_j^z \equiv x_j(1 + z\tilde{\sigma}(x_j))$ and $\tilde{d}^z, \sigma^z, d^z, J^z$ in (VII.3) with z in place of i in (VII.3). We also introduce a "stretched" differential operator $\widetilde{\Delta}^z$ given by

$$\widetilde{\Delta}^z = \frac{1}{d^z(x_1)}\frac{\partial}{\partial x_1}\left(\frac{1}{d^z(x_1)}\frac{\partial}{\partial x_1}\right) + \frac{1}{d^z(x_2)}\frac{\partial}{\partial x_2}\left(\frac{1}{d^z(x_2)}\frac{\partial}{\partial x_2}\right).$$

Finally, we define a complexified distance between $\tilde{x}^z \equiv (\tilde{x}_1^z, \tilde{x}_2^z)$ and $\tilde{y}^z \equiv (\tilde{y}_1^z, \tilde{y}_2^z)$ by

$$\tilde{r}^z \equiv \sqrt{(\tilde{x}_1^z - \tilde{y}_1^z)^2 + (\tilde{x}_2^z - \tilde{y}_2^z)^2}.$$

The properties of $\tilde{r}^z$ are presented in the following lemmas. In case of $z = i$, we will use $\tilde{x}$ and $\tilde{r}$ without z dependency.

Lemma VII.2. *For $z \in U$ there exists $\varepsilon > 0$ such that for $x \neq y$,*

$$-\pi + \varepsilon \leq \arg((\tilde{x}_1^z - \tilde{y}_1^z)^2 + (\tilde{x}_2^z - \tilde{y}_2^z)^2) \leq \pi - \varepsilon.$$

The constant ε appearing above depends on $|\mathrm{Im}(z)|$ and hence holds uniformly on subsets

$$U_\beta \equiv \{z \in U \ : \ |\mathrm{Im}(z)| \leq \beta\},$$

i.e., $\varepsilon = \varepsilon(\beta)$ on U_β.

Proof. We first consider the case of $\mathrm{Im}(z) \geq 0$. Let $x \neq y$. By the mean value theorem,

$$x_j\tilde{\sigma}(x_j) - y_j\tilde{\sigma}(y_j) = \sigma(\xi_j)(x_j - y_j)$$

for some ξ_j between x_j and y_j and hence

$$\begin{aligned} \mathrm{Re}(\tilde{x}_j - \tilde{y}_j) &= (1 + \mathrm{Re}(z)\sigma(\xi_j))(x_j - y_j), \\ \mathrm{Im}(\tilde{x}_j - \tilde{y}_j) &= \mathrm{Im}(z)\sigma(\xi_j)(x_j - y_j). \end{aligned} \tag{VII.8}$$

Since $\mathrm{Re}(z) > -1/(2\sigma_M)$,

$$(1 + \mathrm{Re}(z)\sigma(\xi_j)) \geq 1/2 \tag{VII.9}$$

and so for $\tilde{x}_j - \tilde{y}_j \geq 0$

$$0 \leq \arg(\tilde{x}_j - \tilde{y}_j) = \tan^{-1}\frac{\mathrm{Im}(z)\sigma(\xi_j)}{1 + \mathrm{Re}(z)\sigma(\xi_j)} \leq \tan^{-1}(2\sigma_M \mathrm{Im}(z)) \leq \frac{\pi}{2} - \varepsilon/2 \tag{VII.10}$$

for some $\varepsilon > 0$. Therefore, it follows immediately that

$$0 \leq \arg((\tilde{x}_j - \tilde{y}_j)^2) \leq \pi - \varepsilon.$$

It also holds for the case of $\tilde{x}_j - \tilde{y}_j < 0$.

Now the sector $S_{0,\pi-\varepsilon} = \{\eta \in \mathbb{C} \ : 0 \leq \arg(\eta) \leq \pi - \varepsilon\}$ is closed under addition so it follows that

$$0 \leq \arg((\tilde{x}_1 - \tilde{y}_1)^2 + (\tilde{x}_2 - \tilde{y}_2)^2) \leq \pi - \varepsilon.$$

When $\mathrm{Im}(z) \leq 0$, the argument is the same except both terms end up in the sector $S_{-\pi+\varepsilon,0}$.

□

The following lemma shows that $|\tilde{r}|$ is equivalent to the Euclidean distance between x and y.

Lemma VII.3. *For $z \in U$ and $x, y \in \mathbb{R}^2$, there exist positive constants C_1 and C_2 depending on z such that*

$$C_1|x - y| \leq |\tilde{r}^z| \leq C_2|x - y|. \tag{VII.11}$$

Moreover, the constants $C_1 = C_1(\alpha)$ *and* $C_2 = C_2(\alpha)$ *can be chosen independent of* $z \in U$ *provided that* $|z| \leq \alpha$.

Proof. The upper inequality is immediate from (VII.8) as $|1 + z\sigma(\xi_j)|$ is uniformly bounded when z is uniformly bounded, $|z| < \alpha$.

For the lower, we again consider the case of $\mathrm{Im}(z) \geq 0$ and the other case is verified in the same way. We observe that

$$\begin{aligned} |\tilde{r}^2|^2 &= \left|(\tilde{x}_1 - \tilde{y}_1)^2 + (\tilde{x}_2 - \tilde{y}_2)^2\right|^2 \\ &= |\tilde{x}_1 - \tilde{y}_1|^4 + |\tilde{x}_2 - \tilde{y}_2|^4 - 2|\tilde{x}_1 - \tilde{y}_1|^2|\tilde{x}_2 - \tilde{y}_2|^2 \cos(\pi - \theta), \end{aligned}$$

where θ is the positive angle between $(\tilde{x}_1 - \tilde{y}_1)^2$ and $(\tilde{x}_2 - \tilde{y}_2)^2$ (See Figure 9). Since the angle θ is in $[0, \pi - \varepsilon]$ (from the previous proof), there exists a constant $C_c = C_c(\alpha)$ such that

$$-1 \leq \cos(\pi - \theta) < C_c < 1. \tag{VII.12}$$

Then by a Schwarz inequality

$$\begin{aligned} |\tilde{r}^2|^2 &\geq |\tilde{x}_1 - \tilde{y}_1|^4 + |\tilde{x}_2 - \tilde{y}_2|^4 - C_c(|\tilde{x}_1 - \tilde{y}_1|^4 + |\tilde{x}_2 - \tilde{y}_2|^4) \\ &= (1 - C_c)(|\tilde{x}_1 - \tilde{y}_1|^4 + |\tilde{x}_2 - \tilde{y}_2|^4) \\ &\geq \frac{(1 - C_c)}{2^5}(|x_1 - y_1|^2 + |x_1 - y_1|^2)^2. \end{aligned}$$

For the last inequality above, we used the arithmetic-geometric mean inequality, (VII.8) and (VII.9). This completes the proof of the lemma. □

Lemma VII.4. *There is a constant* $\alpha > 0$ *such that for* $y \in [-a, a]^2$ *and* $\|x\|_\infty \geq b$,

$$\mathrm{Im}(\tilde{r}) \geq \alpha|x|. \tag{VII.13}$$

In addition, (VII.13) *holds also if* $y \in [-m, m]^2$, $\|x\|_\infty = R \geq 2m$ *and* $m \geq b$.

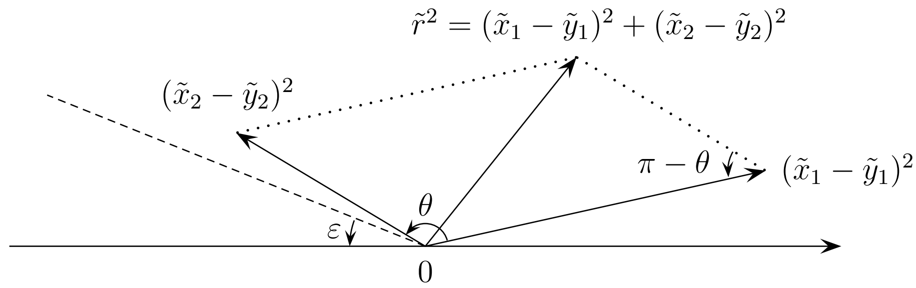


Fig. 9. $\tilde{r}^2$ in the complex plane $\mathbb{C}$

Proof. Let y be in $[-a,a]^2$ and $\|x\|_\infty \geq b$. Assume without loss of generality that $|x_1| = \|x\|_\infty$. Then

$$\begin{aligned}\tilde{r}^2 &= (x_1 - y_1)^2 - (\sigma_0 x_1)^2 + 2(x_1 - y_1)\sigma_0 x_1 i \\ &\quad + (x_2 - y_2)^2 - (\tilde{\sigma}(x_2)x_2)^2 + 2(x_2 - y_2)\tilde{\sigma}(x_2)x_2 i \\ &\equiv R_1 + I_1 i + R_2 + I_2 i \equiv R_3 + I_3 i.\end{aligned} \tag{VII.14}$$

Now $I_1 > 0$ and $I_2 \geq 0$ and there is a positive constant c_1 satisfying

$$2\mathrm{Re}(\tilde{r})\mathrm{Im}(\tilde{r}) = I_3 \geq I_1 \geq c_1\|x\|_\infty^2. \tag{VII.15}$$

Moreover, the proof of Lemma VII.2 shows that the real part of $\tilde{r}$ is non-negative, and using Lemma VII.3

$$\mathrm{Re}(\tilde{r}) \leq |\tilde{r}| \leq c_2\|x\|_\infty. \tag{VII.16}$$

An elementary calculation using (VII.15) and (VII.16) gives

$$\mathrm{Im}(\tilde{r}) \geq \frac{c_1}{2c_2}\|x\|_\infty \geq \frac{c_1}{2\sqrt{2}c_2}|x|.$$

For the second case, we start with (for $j = 1,2$)

$$\tilde{x}_j - \tilde{y}_j = (x_j - y_j) + (\tilde{\sigma}(x_j)x_j - \tilde{\sigma}(y_j)y_j)i.$$

Now,

$$\tilde{\sigma}(x_j)x_j - \tilde{\sigma}(y_j)y_j = \int_{y_j}^{x_j} \sigma(s)\,\mathrm{d}s = \sigma(\zeta_j)(x_j - y_j) \tag{VII.17}$$

for some ζ_j between x_j and y_j. Assume without loss of generality that $|x_1| = \|x\|_\infty$. We expand $\tilde{r}^2$ analogous to (VII.14), i.e.,

$$\tilde{r}^2 \equiv R_1 + I_1 i + R_2 + I_2 i \equiv R_3 + I_3 i.$$

Now, (VII.17) and the fact that $\sigma \geq 0$ implies that $I_2 \geq 0$. Moreover, the integral representation of the difference in (VII.17) implies that if $x_1 \geq 2m$, then

$$\int_{y_1}^{x_1} \sigma(s)\,\mathrm{d}s \geq \sigma_0(x_1 - b) \geq \frac{\sigma_0}{3}(x_1 - y_1) > 0.$$

Thus

$$I_1 \geq \frac{2\sigma_0}{3}(x_1 - y_1)^2 \geq \frac{\sigma_0}{3}\|x\|_\infty^2.$$

The same argument implies the above inequality when $x_1 < 0$. Thus, (VII.15) and (VII.16) follow for this case as well, and the conclusion of the lemma immediately follows as above. □

C. Fundamental solution to the Cartesian PML Helmholtz equation

In this section we will find the fundamental solution to the Cartesian PML Helmholtz equation in $\mathbb{R}^2$. The fundamental solution to the Helmholtz equation in $\mathbb{R}^2$ satisfying the Sommerfeld radiation condition at infinity with k real and positive is $\Phi(r) = \frac{i}{4}H_0^1(kr)$. We have

$$\int_{\mathbb{R}^2} (-(\Delta_y + k^2)u(y))\Phi(|x-y|)\,\mathrm{d}y = u(x) \quad \text{for} \quad u \in C_0^\infty(\mathbb{R}^2). \tag{VII.18}$$

Here $H_0^1 = J_0 + iY_0$ is the Hankel function of the first kind of zero order and J_0 and Y_0 are the Bessel functions of the first and second kind, respectively. We have

$$J_0(z) = \sum_{k=0}^{\infty} \frac{(-1)^k (z/2)^{2k}}{(k!)^2},$$

and for $z \in \mathbb{C} \setminus (-\infty, 0]$

$$Y_0(z) = \frac{2}{\pi} J_0(z) \ln \frac{z}{2} + W_0(z)$$

for an entire function $W_0(z)$ with $\lim_{z\to 0} W_0(z) = 2\gamma/\pi$, where $\gamma = 0.57721566\cdots$ is Euler's constant (See, e.g., [45]). Thus

$$\begin{aligned} H_0^1(z) &= \frac{2i}{\pi} J_0(z) \ln \frac{z}{2} + E(z), \\ H_0^{1\prime}(z) &= \frac{2i}{\pi} \left(J_0'(z) \ln \frac{z}{2} + J_0(z) \frac{1}{z} \right) + E'(z) \end{aligned}$$

for an entire function $E(z)$ with $\lim_{z\to 0} E(z) = 1 + 2\gamma i/\pi$. It follows that there exist $C_b > 0$ and $r_b > 0$ such that

$$\begin{aligned} |\Phi(z)| &\le C_b |\ln |z||, \\ |\Phi'(z)| &\le \frac{C_b}{|z|} \end{aligned} \tag{VII.19}$$

on $B(0, r_b) \setminus ((-r_b, 0] \times 0)$. Here $B(0, r_b) \subset \mathbb{C}$ is a ball of radius r_b centered at $z = 0$. On the other hand, for large $|z|$, we have

$$\begin{aligned} H_0^1(z) &= \left(\frac{2}{\pi z} \right)^{1/2} e^{i(z-\pi/4)} \left(1 + O\left(\frac{1}{z} \right) \right) \quad \text{for} \quad |\arg(z)| \le \pi - \varepsilon, \\ H_0^{1\prime}(z) &= \left(\frac{2}{\pi z} \right)^{1/2} e^{i(z+\pi/4)} \left(1 + O\left(\frac{1}{z} \right) \right) \quad \text{for} \quad |\arg(z)| \le \pi - \varepsilon \end{aligned} \tag{VII.20}$$

with arbitrary small ε [1, 45].

Theorem VII.5. *Assume that* $z \in U$. *Then* $\widetilde{\Phi}^z(x,y) \equiv J^z(y)\Phi(\tilde{r}^z)$ *satisfies*

$$u(x) = \int_{\mathbb{R}^2} (-(\widetilde{\Delta}_y^z + k^2)u(y))\widetilde{\Phi}^z(x,y)\,\mathrm{d}y \tag{VII.21}$$

for all $u \in C_0^\infty(\mathbb{R}^2)$. *Moreover, for* $z \in U$ *with* $\mathrm{Im}(z) > 0$ *and any compact set* $K \subset \mathbb{R}^2$, $\widetilde{\Phi}^z(x,y)$ *decays exponentially uniformly for* $x \in K$ *as* $|y| \to \infty$.

To prove (VII.21), for $u \in C_0^\infty(\mathbb{R}^2)$ and $x \in \mathbb{R}^2$, we define

$$F(z) \equiv \int_{\mathbb{R}^2} (-(\widetilde{\Delta}_y^z + k^2)u(y))\widetilde{\Phi}^z(x,y)\,\mathrm{d}y = \int_{\mathbb{R}^2} J^z(y)(-(\widetilde{\Delta}_y^z + k^2)u(y))\Phi(\tilde{r}^z)\,\mathrm{d}y$$

and we shall show that $F(z)$ is analytic on U. This will be treated in the following lemmas.

First, we need to justify that the integral in (VII.21) is well-defined. To this end, fix $x \in \mathbb{R}^2$, set $P(y,z) \equiv J^z(y)(\widetilde{\Delta}_y^z + k^2)u(y)$ and $G(y,z) \equiv P(y,z)\Phi(\tilde{r}^z)$. For any $z_0 \in U$ there exists $\epsilon > 0$ such that $\bar{B}(z_0,\epsilon) \subset U$.

Lemma VII.6. *Let* z_0, ϵ *and* $G(y,z)$ *be defined as above. Then,* $G(\cdot,z)$ *and* $\frac{\partial}{\partial z}G(\cdot,z)$ *are integrable for each* $z \in B(z_0,\epsilon)$. *In addition, there exists an integrable function* $\mathcal{G}(y)$ *such that*

$$\left|\frac{\partial}{\partial z}G(y,z)\right| \leq \mathcal{G}(y) \quad \textit{for all} \quad z \in B(z_0,\epsilon) \quad \textit{and} \quad y \neq x. \tag{VII.22}$$

Proof. Note that $\Phi(\tilde{r}^z)$ is a continuous function of y except at $y = x$. By Lemma VII.3, there exists $0 < s$ such that $|\tilde{r}^z| < r_b$ for $(y,z) \in B(x,s) \times B(z_0,\epsilon)$. It follows from (VII.19) and Lemma VII.3 that there exists a constant $C_{sing} > 0$ such that

$$\begin{aligned} |\Phi(\tilde{r}^z)| &\leq C_b\,|\ln|\tilde{r}^z|| \leq C_{sing}\,|\ln|x-y||\,, \\ |\Phi'(\tilde{r}^z)| &\leq \frac{C_b}{|\tilde{r}^z|} \leq \frac{C_{sing}}{|x-y|} \end{aligned} \tag{VII.23}$$

for $(y,z) \in \tilde{B}(x,s) \times B(z_0,\epsilon)$. Here $\tilde{B}(x,s)$ denotes $B(x,s) \setminus \{x\}$.

Moreover,

$$|P(y,z)|, \left|\frac{\partial}{\partial z}P(y,z)\right| \leq C_p(|\Delta u(y)| + |\nabla u(y)| + |u(y)|) \text{ for all } y \in \mathbb{R}^2 \quad \text{(VII.24)}$$

with C_p independent of $z \in B(z_0, \epsilon)$.

By (VII.23)-(VII.24), $G(\cdot, z)$ is integrable on the neighborhood $B(x,s)$ for all $z \in B(z_0, \epsilon)$. Its integrability outside of $B(x,s)$ follows from (VII.24) and the fact that u is compactly supported (since $\Phi(\tilde{r}^z)$ is bounded on $\mathrm{supp}(u) \setminus B(x,s)$).

For the derivative

$$\begin{aligned} \frac{\partial}{\partial z}G(y,z) &= \left(\frac{\partial}{\partial z}P(y,z)\right)\Phi(\tilde{r}^z) + P(y,z)\frac{\partial}{\partial z}\Phi(\tilde{r}^z) \\ &= \left(\frac{\partial}{\partial z}P(y,z)\right)\Phi(\tilde{r}^z) + P(y,z)\Phi'(\tilde{r}^z)\frac{\partial \tilde{r}^z}{\partial z}. \end{aligned} \quad \text{(VII.25)}$$

Except for the derivative of $\tilde{r}^z$ with respect to z, the functions in (VII.25) are estimated as above.

For $\partial\tilde{r}^z/\partial z$, we observe $x_j\tilde{\sigma}(x_j) - y_j\tilde{\sigma}(y_j) = \sigma(\xi_j)(x_j - y_j)$ for ξ_j between x_j and y_j. Thus for $z \in B(z_0, \epsilon)$,

$$\begin{aligned} \left|\frac{\partial \tilde{r}^z}{\partial z}\right| &= \left|\frac{\sum_{j=1,2}(\tilde{x}_j - \tilde{y}_j)(x_j\tilde{\sigma}(x_j) - y_j\tilde{\sigma}(y_j))}{\tilde{r}^z}\right| \\ &= \left|\frac{\sum_{j=1,2}(x_j - y_j)^2(1 + z\sigma(\xi_j))\sigma(\xi_j)}{\tilde{r}^z}\right| \leq C_r|x-y|, \end{aligned} \quad \text{(VII.26)}$$

where we used Lemma VII.3.

Let $h(y)$ be defined by

$$h(y) = \begin{cases} \dfrac{C_{sing}}{|x-y|} & \text{for } y \in \tilde{B}(x,s), \\ C_{sup} & \text{for } y \in \mathbb{R}^2 \setminus B(x,s), \end{cases}$$

where C_{sup} is the supremum of $|\Phi(\tilde{r}^z)|$ and $|\Phi'(\tilde{r}^z)|$ for $y \in \mathrm{supp}(u) \setminus B(x,s)$ and

$z \in B(z_0, \epsilon)$. Since $|\ln|x-y|| \le 1/|x-y|$ for $|x-y| < s < 1$,

$$|\Phi(\tilde{r}^z)|, |\Phi'(\tilde{r}^z)| \le h(y) \quad \text{on} \quad \mathrm{supp}(u).$$

Then applying (VII.23), (VII.24) and (VII.26) to (VII.25) gives

$$\left|\frac{\partial}{\partial z} G(y,z)\right| \le C_p(|\Delta u(y)| + |\nabla u(y)| + |u(y)|)h(y)(1 + C_r|x-y|)$$

and (VII.22) follows. This completes the proof. □

Lemma VII.7. *For $u \in C_0^\infty(\mathbb{R}^2)$ and $x \in \mathbb{R}^2$, $F(z)$ defined as above is analytic on U.*

Proof. For $z_0 \in U$ choose ϵ as in Lemma VII.6. It suffices to show that the limit of $(F(z+h) - F(z))/h$ as $h \to 0$ exists for $z \in B(z_0, \epsilon)$. This, in turn, will follow by dominated convergence once we show that there exists an integrable function $\tilde{\mathcal{G}}(y)$ such that

$$\left|\frac{G(y, z+h) - G(y,z)}{h}\right| \le \tilde{\mathcal{G}}(y).$$

Then,

$$\begin{aligned} \frac{\mathrm{d}F}{\mathrm{d}z} &= \int_{\mathbb{R}^2} \lim_{h\to 0} \frac{G(y,z+h) - G(y,z)}{h}\, \mathrm{d}y \\ &= \int_{\mathbb{R}^2} \frac{\partial}{\partial z} G(y,z)\, \mathrm{d}y. \end{aligned}$$

By applying the mean value theorem and the Cauchy-Riemann equations, it is easy to show that for an analytic function w,

$$|w(z_1) - w(z_2)| \le 2|z_1 - z_2| \max_{\alpha \in (0,1)} \left|\frac{\mathrm{d}w}{\mathrm{d}z}(\alpha z_1 + (1-\alpha) z_2)\right|.$$

Thus, by (VII.22),

$$\left|\frac{G(y, z+h) - G(y,z)}{h}\right| < 2\mathcal{G}(y) \quad \text{for} \quad z \in B(z_0, \epsilon),$$

which completes the proof. $\square$

Proof of Theorem VII.5. First, we will prove (VII.21) for real $z \in U$. In this case the mapping $y \mapsto \tilde{y}^z$ is a diffeomorphism of $\mathbb{R}^2$ with the Jacobian $J^z(y)$ and $\tilde{r}^z$ is $|\tilde{x}^z - \tilde{y}^z|$, l^2-norm of $\tilde{x}^z - \tilde{y}^z$ in $\mathbb{R}^2$. Let $u \in C_0^\infty(\mathbb{R}^2)$ and define $v(\tilde{y}^z) \equiv u(y)$. By change of variables and (VII.18),

$$\begin{aligned} F(z) &= \int_{\mathbb{R}^2} J^z(y)(-(\widetilde{\Delta}_y^z + k^2)u(y))\Phi(|\tilde{x}^z - \tilde{y}^z|)\, \mathrm{d}y \\ &= \int_{\mathbb{R}^2} (-(\Delta_{\tilde{y}^z} + k^2)v(\tilde{y}^z))\Phi(|\tilde{x}^z - \tilde{y}^z|)\, \mathrm{d}\tilde{y}^z \\ &= v(\tilde{x}^z) = u(x), \end{aligned}$$

which means that $F(z)$ is constant on $U \cap \mathbb{R}$. Since $F(z)$ is analytic on U by Lemma VII.7 and constant on $U \cap \mathbb{R}$, $F(z)$ must be constant. Therefore $F(z) = u(x)$ for all $z \in U$.

$\square$

Remark VII.8. The formula (VII.21) can be extended to $u \in H^2(\mathbb{R}^2)$ with compact support.

For each $x \in \mathbb{R}^2$, the function $\Phi(\tilde{r}^z)$ (as a function of y) satisfies the Cartesian PML Helmholtz equation as noted in the following lemma.

Lemma VII.9. *Assume that $y \neq x$ in $\mathbb{R}^2$ and $z \in U$. Then*

$$(\widetilde{\Delta}_y^z + k^2)\Phi(\tilde{r}^z) = 0.$$

Proof. Let x, y, z be as above. We note that

$$\widetilde{F}(z) \equiv (\widetilde{\Delta}_y^z + k^2)\Phi(\tilde{r}^z) = \Phi''(\tilde{r}^z) + \frac{1}{\tilde{r}^z}\Phi'(\tilde{r}^z) + k^2\Phi(\tilde{r}^z). \qquad \text{(VII.27)}$$

As $\widetilde{F}(z)$ is analytic on U and vanishes for real $z \in U$, $\widetilde{F}(z)$ vanishes identically. $\square$

CHAPTER VIII

THE SPECTRUM OF A CARTESIAN PML LAPLACE OPERATOR

In this chapter we study the spectrum of a Cartesian PML Laplace operator on an unbounded domain. It is important to understand the structure of the spectrum of the Cartesian PML Laplace operator because the solvability of the problem (VII.5) is intimately related to the spectrum of the operator.

The outline of this chapter is as follows. In Section A, we give some preliminaries and state some tools for identifying the boundary of the essential spectrum of operators from their behavior at infinity. In Section B, we study the spectrum of the one dimensional PML operator. These results are used in Section C to identify the essential spectrum of the operator $-\widetilde{\Delta}$ defined on $L^2(\mathbb{R}^2)$ and subsequently that of $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$.

A. Preliminary tools

We give some preliminary results and tools for the analysis of the spectrum of operators in this section.

Remark VIII.1. We assumed that the PML function $\tilde{\sigma}$ is in $C^2(\mathbb{R})$. This will be sufficient to guarantee that the unbounded operators discussed in the previous chapter are well-defined and closed.

We next show that $\widetilde{L}$ is well-defined. Indeed, for $v \in H_0^1(\bar{\Omega}^c)$,

$$|A(v,\phi)| \leq C^{\ddagger} \|v\|_{H^1(\bar{\Omega}^c)} \|\phi\|_{H^1(\bar{\Omega}^c)} \quad \text{for all} \quad \phi \in H_0^1(\bar{\Omega}^c).$$

‡Here and in the remainder of the dissertation, C denotes a generic positive constant which may take on different values in different places often depending on the spectral parameter (z or z_0).

As multiplication by a bounded C^1 function whose absolute value is bounded away from zero gives an isomorphism of $H_0^1(\bar{\Omega}^c)$ onto $H_0^1(\bar{\Omega}^c)$, it follows that

$$|A(v, (\bar{d}(x_1)\bar{d}(x_2))^{-1}\phi)| \leq C\|v\|_{H^1(\bar{\Omega}^c)}\|\phi\|_{H^1(\bar{\Omega}^c)}$$

so there is a unique $f \in H^{-1}(\bar{\Omega}^c)$ satisfying (VII.7) and $\widetilde{L}$ is well-defined. Moreover,

$$\|\widetilde{L}v\|_{H^{-1}(\bar{\Omega}^c)} \leq C\|v\|_{H^1(\bar{\Omega}^c)} \text{ for all } v \in H_0^1(\bar{\Omega}^c). \tag{VIII.1}$$

Examining the properties of $\tilde{\sigma}(x)$, it follows that there are real numbers $\alpha > 0$ and $0 < \theta < \pi/2$ satisfying

$$\mathrm{Re}(d(x)/d(y)) \geq \alpha \text{ and } \mathrm{Re}(e^{-i\theta}d(x)d(y)) \geq \alpha \text{ for all } x, y \in \mathbb{R}.$$

This implies that for $z_0 = -e^{-i\theta}$,

$$|A(u, u) - z_0(d(x_1)d(x_2)u, u)| \geq \alpha\|u\|^2_{H^1(\bar{\Omega}^c)} \text{ for all } u \in H_0^1(\bar{\Omega}^c). \tag{VIII.2}$$

This, and the discussion above, implies that given $f \in H^{-1}(\bar{\Omega}^c)$, there is a unique $u \in H_0^1(\bar{\Omega}^c)$ satisfying

$$A(u, \phi) - z_0(d(x_1)d(x_2)u, \phi) =< f, \bar{d}(x_1)\,\bar{d}(x_2)\phi > \quad \text{for all } \phi \in H_0^1(\bar{\Omega}^c). \tag{VIII.3}$$

Moreover,

$$\|u\|_{H^1(\bar{\Omega}^c)} \leq C\|f\|_{H^{-1}(\bar{\Omega}^c)}. \tag{VIII.4}$$

It is immediate that $(\widetilde{L} - z_0 I)u = f$ and so z_0 is in the the resolvent set $\rho(\widetilde{L})$. This implies that the operator $\widetilde{L}$ is closed, its resolvent set is non-empty and its spectrum is well-defined.

Now, we define an extended operator (still denoted by $\widetilde{L}$) defined for $v \in H^1(\mathbb{R}^2)$

by $\widetilde{L}v = f$, where $f \in H^{-1}(\mathbb{R}^2)$ is defined by

$$< f, \bar{d}(x_1)\bar{d}(x_2)\phi >= A(v, \phi) \text{ for all } \phi \in H^1(\mathbb{R}^2). \tag{VIII.5}$$

Clearly, $d(x)$ is well-defined for all $x \in \mathbb{R}$ and (VIII.5) makes sense. For $f \in L^2(\mathbb{R}^2)$ the duality pairing is the integral $(\cdot, \cdot)_{\mathbb{R}^2}$.

The argument above shows that $z_0 \in \rho(\widetilde{L})$ for the extended operator and so $\widetilde{L}$ is closed, its resolvent set is non-empty, and its spectrum is well-defined.

To develop the same properties for $-\widetilde{\Delta}$ as an operator on $L^2(\mathbb{R}^2)$ with domain $H^2(\mathbb{R}^2)$, elliptic regularity comes into play. Specifically since $\tilde{\sigma}$ is $C^2(\mathbb{R})$, classical arguments involving difference quotients (see, also, [13, 49]) can be used to show that when $f \in L^2(\mathbb{R}^2)$, the solution u of the extended version of (VIII.3) is in $H^2(\mathbb{R}^2)$ and satisfies

$$\|u\|_{H^2(\mathbb{R}^2)} \leq C\|f\|_{L^2(\mathbb{R}^2)}. \tag{VIII.6}$$

This means that u is in the domain of $-\widetilde{\Delta}$ and satisfies

$$(-\widetilde{\Delta} - z_0 I)u = f,$$

i.e., $z_0 \in \rho(-\widetilde{\Delta})$. This immediately gives the desired results as above.

In this chapter, we describe the essential spectrum of $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$ by studying the spectrum of $-\widetilde{\Delta}$ on $L^2(\mathbb{R}^2)$ and $\widetilde{L}$ on $H^{-1}(\mathbb{R}^2)$. As a first step, we have the following theorem.

Theorem VIII.2. *The spectrum of $\widetilde{L}$ as an unbounded operator on $H^{-1}(\mathbb{R}^2)$ (with domain $H^1(\mathbb{R}^2)$) is the same as the spectrum of $-\widetilde{\Delta}$ on $L^2(\mathbb{R}^2)$ (with domain $H^2(\mathbb{R}^2)$).*

Before proving the theorem, we observe the following lemma.

Lemma VIII.3. *The point z is in $\rho(\widetilde{L})$ (as an operator on $H^{-1}(\mathbb{R}^2)$) if and only if* *the following two inf-sup conditions hold: For all* u *in* $H^1(\mathbb{R}^2)$,

$$\|u\|_{H^1(\mathbb{R}^2)} \leq C \sup_{\phi \in H^1(\mathbb{R}^2)} \frac{|A_z(u,\phi)|}{\|\phi\|_{H^1(\mathbb{R}^2)}} \tag{VIII.7}$$

and

$$\|u\|_{H^1(\mathbb{R}^2)} \leq C \sup_{\phi \in H^1(\mathbb{R}^2)} \frac{|A_z(\phi,u)|}{\|\phi\|_{H^1(\mathbb{R}^2)}}, \tag{VIII.8}$$

where $A_z(\cdot,\cdot) \equiv A(\cdot,\cdot) - z(d(x_1)d(x_2)\cdot,\cdot)_{\mathbb{R}^2}$.

Proof. The inf-sup conditions immediately imply that the map $\widetilde{L} - zI : H^1(\mathbb{R}^2) \to H^{-1}(\mathbb{R}^2)$ is an isomorphism. This means that if the inf-sup conditions hold for z, then z is in the resolvent set $\rho(\widetilde{L})$.

We already know from (VIII.2) that the inf-sup conditions hold for z_0. It suffices to prove the first inf-sup condition as the second follows from it since the coefficients of $A_z(\cdot,\cdot)$ are complex symmetric (but not Hermitian).

Suppose that z is in $\rho(\widetilde{L})$. To prove (VIII.7), let u be in $C_0^\infty(\mathbb{R}^2)$ and $v \in H^1(\mathbb{R}^2)$ be the unique function satisfying (cf., (VIII.2))

$$A_{z_0}(v,\phi) = A_z(u,\phi) \quad \text{for all} \quad \phi \in H^1(\mathbb{R}^2).$$

Setting $u_0 = u - v$, a simple computation gives

$$A_z(u_0,\phi) = (z - z_0)(d(x_1)d(x_2)v,\phi)_{\mathbb{R}^2} \quad \text{for all} \quad \phi \in H^1(\mathbb{R}^2)$$

or

$$(\widetilde{L} - zI)u_0 = (z - z_0)v. \tag{VIII.9}$$

Since $z \in \rho(\widetilde{L})$,

$$\|u_0\|_{H^{-1}(\mathbb{R}^2)} \leq C\|v\|_{H^{-1}(\mathbb{R}^2)}. \tag{VIII.10}$$

Also,

$$A_{z_0}(u_0,\phi) = (z - z_0)(d(x_1)d(x_2)[v + u_0], \phi)_{\mathbb{R}^2} \quad \text{for all} \quad \phi \in H^1(\mathbb{R}^2)$$

and hence by (VIII.4) and (VIII.10)

$$\|u_0\|_{H^1(\mathbb{R}^2)} \le C\|v\|_{H^{-1}(\mathbb{R}^2)}.$$

Thus, using (VIII.2) gives

$$\begin{aligned} \|u\|_{H^1(\mathbb{R}^2)} &\le \|v\|_{H^1(\mathbb{R}^2)} + \|u_0\|_{H^1(\mathbb{R}^2)} \le C\|v\|_{H^1(\mathbb{R}^2)} \\ &\le C \sup_{\phi\in H^1(\mathbb{R}^2)} \frac{|A_{z_0}(v,\phi)|}{\|\phi\|_{H^1(\mathbb{R}^2)}} = C \sup_{\phi\in H^1(\mathbb{R}^2)} \frac{|A_z(u,\phi)|}{\|\phi\|_{H^1(\mathbb{R}^2)}}. \end{aligned}$$

This proves (VIII.7) and completes the proof of the lemma. □

Remark VIII.4. The lemma holds for $\widetilde{L}$ defined on $H^{-1}(\bar{\Omega}^c)$ with the inf-sup conditions involving the supremum over $H^1_0(\bar{\Omega}^c)$. The proof is identical.

Corollary VIII.5. *If z in $\rho(-\widetilde{\Delta})$ (as an operator on $L^2(\mathbb{R}^2)$), then* (VIII.7) *and* (VIII.8) *hold for z and hence $z \in \rho(\widetilde{L})$ on $H^{-1}(\mathbb{R}^2)$.*

Proof. The proof that $z \in \rho(-\widetilde{\Delta})$ implies (VIII.7) and (VIII.8) is essentially identical to that of the lemma except that (VIII.10) is replaced by

$$\|u_0\|_{L^2(\mathbb{R}^2)} \le C\|v\|_{L^2(\mathbb{R}^2)}. \tag{VIII.11}$$

□

Remark VIII.6. Let Ω_δ denote the square domain $[-\delta,\delta]^2$ with $\delta \ge b$. We fix $z \in \rho(-\widetilde{\Delta})$ (as an operator on $L^2(\mathbb{R}^2)$). For the analysis of the truncated PML problem in Chapter IX, we shall require that the inf-sup conditions of Lemma VIII.3 still hold with $H^1(\mathbb{R}^2)$ replaced by $H^1_0(\Omega_\delta)$ uniformly for $\delta > \delta_0 = \delta_0(z)$. Examining the proof of the above lemma, we see that for this to hold it suffices to show that for $\delta > \delta_0$, $z \in \rho(\widetilde{\Delta}_\delta)$ (as an operator on $L^2(\Omega_\delta)$ with domain $H^2(\Omega_\delta) \cap H_0^1(\Omega_\delta)$) and there is a constant C depending only on δ_0 and z satisfying

$$\|(-\widetilde{\Delta}_\delta - zI)^{-1}\|_{L^2(\Omega_\delta)} \leq C \tag{VIII.12}$$

for all $\delta > \delta_0$. The existence of δ_0 and C will be verified in the proof of Theorem VIII.22.

Proof of Theorem VIII.2. That $\rho(-\widetilde{\Delta})$ is contained in $\rho(\widetilde{L})$ is given by the above corollary. The other direction, $\rho(\widetilde{L}) \subseteq \rho(-\widetilde{\Delta})$, follows from Lemma VIII.3, the two inf-sup conditions and elliptic regularity (the argument is identical that used earlier in this section to show $z_0 \in \rho(-\widetilde{\Delta})$). □

To connect the spectrum of the extended operators to that of $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$, we require the concepts of local compactness of operators, the Weyl spectrum and the Zhislin spectrum. Let $\mathcal{U}$ be $\bar{\Omega}^c$ or $\mathbb{R}^m$ for $m = 1, 2$.

Definition VIII.7. For $B \subset \mathcal{U}$, let χ_B denote the characteristic function on B. If a closed operator T with $\rho(T) \neq \emptyset$ satisfies the condition that $\chi_B(T - \lambda I)^{-1}$ is compact for any bounded open set $B \subset \mathcal{U}$ and for some $\lambda \in \rho(T)$ (and so any $\lambda \in \rho(T)$), then T is called *locally compact*.

Definition VIII.8. Let T be a closed operator on a Hilbert space $\mathcal{H}$. A *Weyl sequence* $\{u_n\}$ for T and $\lambda \in \mathbb{C}$ is a sequence such that $\|u_n\|_{\mathcal{H}} = 1$, $u_n \to 0$ weakly and $\|(T - \lambda I)u_n\|_{\mathcal{H}} \to 0$. The set of all λ such that a Weyl sequence exists for T and λ is called the *Weyl spectrum* $W(T)$ of T.

The Weyl spectrum $W(T)$ of a closed operator T is related to the essential spectrum $\sigma_{ess}(T)$ of T as follows.

Theorem VIII.9. *[23, Theorem 3.1] Let T be a closed operator on a Hilbert space $\mathcal{H}$ with $\rho(T) \neq \emptyset$. Then $W(T) \subset \sigma_{ess}(T)$ and the boundary of $\sigma_{ess}(T)$ is contained in $W(T)$. Finally, $W(T) = \sigma_{ess}(T)$ if and only if each connected component of the complement of $W(T)$ contains a point of $\rho(T)$.*

Definition VIII.10. Let T be a closed operator on $\mathcal{H} \equiv H^{-1}(\mathcal{U})$ or $L^2(\mathbb{R}^m)$ for $m = 1, 2$. A *Zhislin sequence* u_n for T and $\lambda \in \mathbb{C}$ is a sequence such that $\|u_n\|_{\mathcal{H}} = 1$, $\text{supp}(u_n) \cap K = \emptyset$ for each compact set $K \subset \mathcal{U}$ and for all n large, and such that $\|(T - \lambda I)u_n\|_{\mathcal{H}} \to 0$ as $n \to \infty$. The set of all λ such that a Zhislin sequence exists for T and λ is called the *Zhislin spectrum* $Z(T)$ of T.

Since every Zhislin sequence converges to zero weakly, it is obvious that $Z(T) \subset W(T)$. In general, these two sets are not necessarily equal but sometimes they coincide as shown in the following theorems.

Theorem VIII.11. *Let T be a locally compact, closed operator on $L^2(\mathbb{R}^m)$ such that $\rho(T) \neq \emptyset$ and $C_0^\infty(\mathbb{R}^m)$ is a core. Let $\chi \in C_0^\infty(\mathbb{R}^m)$ be such that $\chi|_{B(0,r)} = 1$ for some $r > 0$, where $B(0, r)$ is a ball centered at the origin and of radius r. We define $\chi_n(x) \equiv \chi(x/n)$. Suppose that there exists $\varepsilon(n)$ such that $\varepsilon(n) \to 0$ as $n \to \infty$, and that for all $u \in C_0^\infty(\mathbb{R}^m)$*

$$\|[T, \chi_n]u\|_{L^2(\mathbb{R}^m)} \leq \varepsilon(n)(\|Tu\|_{L^2(\mathbb{R}^m)} + \|u\|_{L^2(\mathbb{R}^m)}). \tag{VIII.13}$$

Here $[T, \chi_n]$ is the commutator of T and χ_n: $[T, \chi_n]u = T(\chi_n u) - \chi_n Tu$ for $u \in C_0^\infty(\mathbb{R}^m)$. Then $Z(T) = W(T)$.

This result for operators on $L^2(\mathbb{R}^m)$ is given in [23, Theorem 3.2]. We note that $C_0^\infty(\bar{\Omega}^c)$ is still a core of $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$ and we have a similar theorem. Its proof is essentially the same as that of Theorem VIII.11 in [23].

Theorem VIII.12. *Let T be a locally compact, closed operator on $H^{-1}(\mathcal{U})$ with domain $H_0^1(\mathcal{U})$ such that $\rho(T) \neq \emptyset$. Let χ_n be as in the previous theorem. Suppose that there exists $\varepsilon(n)$ such that $\varepsilon(n) \to 0$ as $n \to \infty$, and that for all $u \in H_0^1(\mathcal{U})$*

$$\|[T, \chi_n]u\|_{H^{-1}(\mathcal{U})} \leq \varepsilon(n)(\|Tu\|_{H^{-1}(\mathcal{U})} + \|u\|_{H^{-1}(\mathcal{U})}). \tag{VIII.14}$$

Then $Z(T) = W(T)$.

B. Spectrum of the one dimensional PML operator on $L^2(\mathbb{R})$

In this section, we consider the spectrum of the one dimensional stretched operator on $L^2(\mathbb{R})$ with domain $H^2(\mathbb{R})$ defined by

$$\widetilde{\mathcal{D}} = -\frac{1}{d(x)}\frac{\partial}{\partial x}\left(\frac{1}{d(x)}\frac{\partial}{\partial x}\right).$$

A weak form corresponding to $\widetilde{\mathcal{D}}u = f$ for $f \in L^2(\mathbb{R})$ is given by: find $u \in H^1(\mathbb{R})$ satisfying

$$a(u, v) = (d(x)f, v)_{\mathbb{R}} \quad \text{for all} \quad v \in H^1(\mathbb{R}),$$

where

$$a(u, v) = \left(\frac{1}{d(x)}u', v'\right)_{\mathbb{R}} \quad \text{for all} \quad u, v \in H^1(\mathbb{R}).$$

The arguments showing that $\widetilde{\mathcal{D}}$ is well-defined as an operator on $L^2(\mathbb{R})$ with domain $H^2(\mathbb{R})$ are identical to those given in Section 2 for $-\widetilde{\Delta}$. In fact, z_0 is in $\rho(\widetilde{\mathcal{D}})$. Additional properties are given in the following lemma.

Lemma VIII.13. *The operator $\widetilde{\mathcal{D}}$ on $L^2(\mathbb{R})$ is locally compact and satisfies* (VIII.13).

Proof. The local compactness of $\widetilde{\mathcal{D}}$ immediately follows from the compact embedding of $H^2(B)$ as a subset of $L^2(B)$ for bounded B (we take $\lambda = z_0 \in \rho(\widetilde{\mathcal{D}})$).

It remains to show that $\widetilde{\mathcal{D}}$ satisfies (VIII.13). As in Section 2, for $u \in C_0^\infty(\mathbb{R})$,

$$\|u'\|^2_{L^2(\mathbb{R})} \leq \alpha^{-1}\mathrm{Re}(d(x)^{-1}u', u')_{\mathbb{R}} = \alpha^{-1}\mathrm{Re}(\widetilde{\mathcal{D}}u, \bar{d}(x)u)_{\mathbb{R}}.$$

Thus,

$$\|u'\|_{L^2(\mathbb{R})} \leq C(\|\widetilde{\mathcal{D}}u\|_{L^2(\mathbb{R})} + \|u\|_{L^2(\mathbb{R})}). \tag{VIII.15}$$

Expanding $[\widetilde{\mathcal{D}}, \chi_n]u$ and noting that all terms cancel except those involving differentiation of χ_n gives

$$\|[\widetilde{\mathcal{D}}, \chi_n]u\|_{L^2(\mathbb{R})} \leq C(\|\chi_n''u\|_{L^2(\mathbb{R})} + \|\chi_n'u'\|_{L^2(\mathbb{R})} + \|\chi_n'u\|_{L^2(\mathbb{R})}).$$

Since $\|\chi_n'\|_\infty, \|\chi_n''\|_\infty \leq C/n$ for large n, by (VIII.15),

$$\begin{aligned}\|[\widetilde{\mathcal{D}}, \chi_n]u\|_{L^2(\mathbb{R})} &\leq \frac{C}{n}(\|u'\|_{L^2(\mathbb{R})} + \|u\|_{L^2(\mathbb{R})}) \\ &\leq \frac{C}{n}(\|\widetilde{\mathcal{D}}u\|_{L^2(\mathbb{R})} + \|u\|_{L^2(\mathbb{R})}),\end{aligned}$$

which completes the proof. □

Proposition VIII.14. *Let $\widetilde{\mathcal{D}}$ be as above. Then*

$$\sigma(\widetilde{\mathcal{D}}) = \sigma_{ess}(\widetilde{\mathcal{D}}) = \{z \in \mathbb{C} \ : \ \arg(z) = -2\arg(1 + i\sigma_0)\}.$$

Proof. Let $S \equiv -(1 + i\sigma_0)^{-2}\partial^2/\partial x^2$ be defined on $L^2(\mathbb{R})$ with domain $H^2(\mathbb{R})$. Note that S coincides with $\widetilde{\mathcal{D}}$ for $x \notin [-b, b]$. Lemma VIII.13 holds for S so

$$W(S) = Z(S) = Z(\widetilde{\mathcal{D}}) = W(\widetilde{\mathcal{D}}) \tag{VIII.16}$$

by Theorem VIII.11. Moreover,

$$\sigma(S) = \sigma_{ess}(S) = \{z \in \mathbb{C} \ : \ \arg(z) = -2\arg(1 + i\sigma_0)\} = W(S), \tag{VIII.17}$$

where the last equality followed from Theorem VIII.9. Applying Theorem VIII.9 to

$\widetilde{\mathcal{D}}$ and using (VIII.16) shows that $\sigma_{ess}(\widetilde{\mathcal{D}})$ is also given by (VIII.17).

To complete the proof, we will show that the discrete spectrum of $\widetilde{\mathcal{D}}$ is empty. Indeed, if λ is in the discrete spectrum of $\widetilde{\mathcal{D}}$, then there is an eigenvector $u \in H^2(\mathbb{R})$ such that $\widetilde{\mathcal{D}}u = \lambda u$. It is easy to see that

$$u(x) = C_1 e^{i\sqrt{\lambda}x(1+i\tilde{\sigma}(x))} + C_2 e^{-i\sqrt{\lambda}x(1+i\tilde{\sigma}(x))}. \tag{VIII.18}$$

For $x \notin [-b, b]$,

$$u(x) = C_1 e^{i\sqrt{\lambda}x(1+i\sigma_0)} + C_2 e^{-i\sqrt{\lambda}x(1+i\sigma_0)}.$$

Examining this expression, it is clear that the only way that u can be in $L^2(\mathbb{R})$ is that $C_1 = C_2 = 0$, i.e., $u = 0$. This completes the proof of the lemma. □

C. The spectrum of $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$

We prove the main theorem concerning the essential spectrum of $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$ in this section. We start by examining the spectrum of $-\widetilde{\Delta}$ on $L^2(\mathbb{R}^2)$. We first consider the tensor product operator associated with components coming from the one dimensional operator $\widetilde{\mathcal{D}}$, specifically

$$\widetilde{\mathcal{T}} = \widetilde{\mathcal{D}} \otimes I + I \otimes \widetilde{\mathcal{D}}. \tag{VIII.19}$$

This operator is defined on $L^2(\mathbb{R}) \otimes L^2(\mathbb{R}) = L^2(\mathbb{R}^2)$ with domain $H^2(\mathbb{R}) \otimes H^2(\mathbb{R})$. We note that $H^2(\mathbb{R}) \otimes H^2(\mathbb{R})$ is dense in $H^2(\mathbb{R}^2)$ and that $\widetilde{\mathcal{T}}$ coincides with $-\widetilde{\Delta}$ on $H^2(\mathbb{R}) \otimes H^2(\mathbb{R})$. This means that $-\widetilde{\Delta}$ is the closure of $\widetilde{\mathcal{T}}$.

To characterize the spectrum of $-\widetilde{\Delta}$, we introduce the following theorem on tensor product operators.

Theorem VIII.15. *[48, Theorem XIII.35] Let $\mathcal{A}$ and $\mathcal{B}$ be the generators of bounded holomorphic semigroups on a Hilbert space $\mathcal{H}$. Let dom($\mathcal{A}$) and dom($\mathcal{B}$) be the domains of $\mathcal{A}$ and $\mathcal{B}$ in $\mathcal{H}$, respectively. If $\mathcal{C}$ is the closure of the operator $\mathcal{A} \otimes I + I \otimes \mathcal{B}$*

defined on $dom(\mathcal{A}) \otimes dom(\mathcal{B})$*, then* $\mathcal{C}$ *generates a bounded holomorphic semigroup and*

$$\sigma(\mathcal{C}) = \sigma(\mathcal{A}) + \sigma(\mathcal{B}).$$

The next theorem provides a criterion for an operator to be a generator of a holomorphic semigroup. First, the following definition is required.

Definition VIII.16. Let T be a closed operator on a Hilbert space $\mathcal{H}$. T is called m-sectorial with a vertex at $z = 0$ and a semi-angle $\delta \in [0, \pi/2)$ if the numerical range of T, $\mathcal{N}(T) = \{(Tu, u) \in \mathbb{C} \ : \ u \in dom(T) \text{ with } \|u\|_{\mathcal{H}} = 1\}$, is contained in a sector $S_\delta = \{z \in \mathbb{C} \ : \ |\arg(z)| \leq \delta\}$ and $(\mathbb{C} \setminus S_\delta) \cap \rho(T) \neq \emptyset$.

Theorem VIII.17. *[41, IX Theorem 1.24] Let* T *be an* m*-sectorial operator on a Hilbert space* $\mathcal{H}$*. Then* T *generates a bounded holomorphic semigroup.*

Lemma VIII.18. *There exist a real and positive constant* β *and a complex constant* η *such that* $T \equiv \eta\widetilde{\mathcal{D}} + \beta I$ *is* m*-sectorial.*

Proof. The spectrum of T is a line from β to infinity and hence $(\mathbb{C} \setminus S_\delta) \cap \rho(T) \neq \emptyset$ for any $\delta \in [0, \pi/2)$.

Let $\eta = 1 + i\sigma_M$, where $\sigma_M = \max_{t\in\mathbb{R}}\{\sigma(t)\}$. It suffices to show that for a positive β, there exists a positive constant C such that $\mathrm{Re}(Tu, u)_{\mathbb{R}} \geq C|\mathrm{Im}(Tu, u)_{\mathbb{R}}|$ for all $u \in H^2(\mathbb{R})$ with $\|u\|_{L^2(\mathbb{R})} = 1$ since this implies that the numerical range $\mathcal{N}(T)$ of T is contained in the sector S_δ with a vertex at $z = 0$ and a semi-angle $\delta = \tan^{-1}(1/C)$. Now, for $u \in C_0^\infty(\mathbb{R})$ with $\|u\|_{L^2(\mathbb{R})} = 1$

$$\begin{aligned}(Tu, u)_{\mathbb{R}} &= -\int_{\mathbb{R}} \frac{\eta}{d(x)} \frac{\partial}{\partial x} \left(\frac{1}{d(x)} \frac{\partial u}{\partial x} \right) \bar{u} \, \mathrm{d}x + \beta \|u\|^2_{L^2(\mathbb{R})} \\ &= \int_{\mathbb{R}} \frac{\eta}{d(x)^2} \left| \frac{\partial u}{\partial x} \right|^2 \mathrm{d}x + \int_{\mathbb{R}} \frac{\eta}{d(x)} \left(\frac{1}{d(x)} \right)' \frac{\partial u}{\partial x} \bar{u} \, \mathrm{d}x + \beta \|u\|^2_{L^2(\mathbb{R})}.\end{aligned} \quad \text{(VIII.20)}$$

Note that there exist positive constants c_1 and c_2 such that

$$\operatorname{Re}\left(\frac{\eta}{d(x)^2}\right) \geq c_1 \qquad \text{and} \qquad \left|\frac{\eta}{d(x)}\left(\frac{1}{d(x)}\right)'\right| \leq c_2. \tag{VIII.21}$$

Using (VIII.21), applying the Schwarz inequality and the arithmetic-geometric mean inequality gives that for any positive γ,

$$\begin{aligned}\operatorname{Re}(Tu,u)_{\mathbb{R}} &\geq c_1\|u'\|^2_{L^2(\mathbb{R})} + \beta\|u\|^2_{L^2(\mathbb{R})} - \frac{c_2}{2}(\gamma\|u'\|^2_{L^2(\mathbb{R})} + 1/\gamma\|u\|^2_{L^2(\mathbb{R})}) \\ &= (c_1 - \gamma c_2/2)\|u'\|^2_{L^2(\mathbb{R})} + (\beta - c_2/(2\gamma))\|u\|^2_{L^2(\mathbb{R})}.\end{aligned} \tag{VIII.22}$$

Choosing γ small enough and β large enough implies

$$\operatorname{Re}(Tu,u)_{\mathbb{R}} \geq C_R\|u\|^2_{H^1(\mathbb{R})}.$$

On the other hand, it easily follows that

$$|\operatorname{Im}(Tu,u)_{\mathbb{R}}| \leq C_I\|u\|^2_{H^1(\mathbb{R})}. \tag{VIII.23}$$

Combining these results and noting that $C_0^\infty(\mathbb{R})$ is dense in $H^2(\mathbb{R})$ finishes the proof of the lemma. □

Combining the above results gives the following theorem concerning the spectrum of $-\widetilde{\Delta}$, which we state for the more general PML formulation discussed in Remark VII.1. Let

$$\mathcal{S} \equiv \{z \in \mathbb{C} \ : \ -2\arg(1+i\sigma_{20}) \leq \arg(z) \leq -2\arg(1+i\sigma_{10})\}$$

when $\sigma_{10} \leq \sigma_{20}$ and

$$\mathcal{S} \equiv \{z \in \mathbb{C} \ : \ -2\arg(1+i\sigma_{10}) \leq \arg(z) \leq -2\arg(1+i\sigma_{20})\}$$

when $\sigma_{10} > \sigma_{20}$.

Theorem VIII.19. *The spectrum of* $-\widetilde{\Delta}$ *on* $L^2(\mathbb{R}^2)$ *with domain* $H^2(\mathbb{R}^2)$ *is given by*

$$\sigma(-\widetilde{\Delta}) = \sigma_{ess}(-\widetilde{\Delta}) = \mathcal{S} \tag{VIII.24}$$

(see Figure 8.).

Proof. We first consider the case when $\sigma_{10} = \sigma_{20} = \sigma_0$. Since $\eta\widetilde{\mathcal{D}} + \beta I$ is m-sectorial, it follows from Theorem VIII.17 that $\eta\widetilde{\mathcal{D}} + \beta I$ generates a bounded holomorphic semigroup. By Theorem VIII.15

$$\sigma(-\eta\widetilde{\Delta} + 2\beta I) = \sigma(\eta\widetilde{\mathcal{D}} + \beta I) + \sigma(\eta\widetilde{\mathcal{D}} + \beta I) = \sigma(\eta\widetilde{\mathcal{D}} + 2\beta I).$$

Translating by -2β and multiplying by $1/\eta$ gives

$$\sigma(-\widetilde{\Delta}) = \sigma(\widetilde{\mathcal{D}}).$$

In the case when $\sigma_{10} \neq \sigma_{20}$, $\widetilde{\mathcal{D}}_1, \widetilde{\mathcal{D}}_2$ are $\widetilde{\mathcal{D}}$ defined with $\tilde{\sigma}_1$, $\tilde{\sigma}_2$, respectively for each component. As above, we have

$$\sigma(-\widetilde{\Delta}) = \sigma(\widetilde{\mathcal{D}}_1) + \sigma(\widetilde{\mathcal{D}}_2) = \mathcal{S}.$$

This completes the proof of the theorem. □

We are now in a position to state and prove the main result of this chapter.

Theorem VIII.20. *The essential spectrum of* $\widetilde{L}$ *on* $H^{-1}(\bar{\Omega}^c)$ *with domain* $H_0^1(\bar{\Omega}^c)$ *is contained in* $\mathcal{S}$*.*

Proof. The spectrum of $-\widetilde{\Delta}$ on $L^2(\mathbb{R}^2)$ is the same as $\widetilde{L}$ on $H^{-1}(\mathbb{R}^2)$ by Theorem VIII.2. Clearly, both $\widetilde{L}$ on $H^{-1}(\mathbb{R}^2)$ and $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$ are locally compact. To finish the proof of the theorem, it suffices to show that they satisfy (VIII.14).

Indeed, in that case, we apply Theorem VIII.12 to conclude that

$$\begin{aligned}\mathcal{S} \supseteq W(\widetilde{L})(\text{on } H^{-1}(\mathbb{R}^2)) &= Z(\widetilde{L})(\text{on } H^{-1}(\mathbb{R}^2)) \\ &= Z(\widetilde{L})(\text{on } H^{-1}(\bar{\Omega}^c)) = W(\widetilde{L})(\text{on } H^{-1}(\bar{\Omega}^c)).\end{aligned}$$

The theorem follows from Theorem VIII.9 since $W(\widetilde{L})(\text{on } H^{-1}(\bar{\Omega}^c))$ contains the boundary of $\sigma_{ess}(\widetilde{L})$ (on $H^{-1}(\bar{\Omega}^c)$).

We verify (VIII.14) in the case of $H^{-1}(\bar{\Omega}^c)$. The other case is essentially identical. For χ_n defined in Theorem VIII.12 and $u \in H_0^1(\bar{\Omega}^c)$, a simple computation shows that for $\phi \in C_0^\infty(\bar{\Omega}^c)$,

$$\begin{aligned}< [\widetilde{L}, \chi_n]u, \bar{d}(x_1)\, \bar{d}(x_2)\phi > &= A(\chi_n u, \phi) - A(u, \bar{\chi}_n \phi) \\ &= \left(\frac{d(x_2)}{d(x_1)} \frac{\partial \chi_n}{\partial x_1} u, \frac{\partial \phi}{\partial x_1}\right) + \left(\frac{d(x_1)}{d(x_2)} \frac{\partial \chi_n}{\partial x_2} u, \frac{\partial \phi}{\partial x_2}\right) \\ &\quad - \left(\frac{d(x_2)}{d(x_1)} \frac{\partial \chi_n}{\partial x_1} \frac{\partial u}{\partial x_1}, \phi\right) - \left(\frac{d(x_1)}{d(x_2)} \frac{\partial \chi_n}{\partial x_2} \frac{\partial u}{\partial x_2}, \phi\right).\end{aligned}$$

Using the fact that the first derivatives of χ_n can be bounded by C/n gives

$$| < [\widetilde{L}, \chi_n]u, \bar{d}(x_1)\, \bar{d}(x_2)\phi > | \leq \frac{C}{n} \|u\|_{H^1(\bar{\Omega}^c)} \|\phi\|_{H^1(\bar{\Omega}^c)}.$$

Now

$$\|u\|_{H^1(\bar{\Omega}^c)} \leq C\|(\widetilde{L} - z_0 I)u\|_{H^{-1}(\bar{\Omega}^c)} \leq C(\|\widetilde{L}u\|_{H^{-1}(\bar{\Omega}^c)} + \|u\|_{H^{-1}(\bar{\Omega}^c)}). \tag{VIII.25}$$

Combining the above results shows that

$$| < [\widetilde{L}, \chi_n]u, \bar{d}(x_1)\, \bar{d}(x_2)\phi > | \leq \frac{C}{n} (\|\widetilde{L}u\|_{H^{-1}(\bar{\Omega}^c)} + \|u\|_{H^{-1}(\bar{\Omega}^c)}) \|\phi\|_{H^1(\bar{\Omega}^c)}.$$

The desired result (VIII.14) follows as in the proof of (VIII.1). This completes the proof of the theorem. $\square$

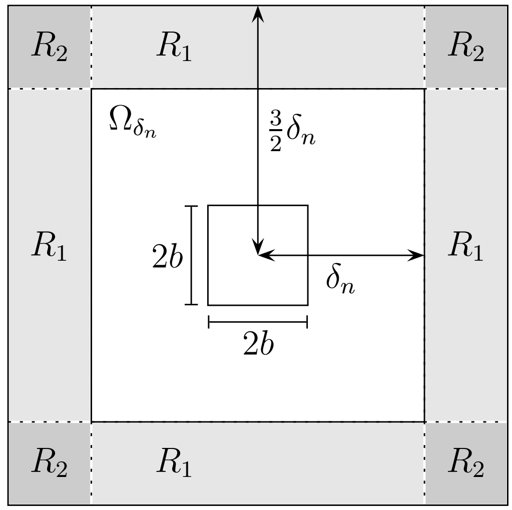


Fig. 10. The reflection subdomains

Remark VIII.21. By cutting down functions of the form

$$f(x,y) = e^{i[\gamma x/(1+i\sigma_{10})+\beta y/(1+i\sigma_{20})]}$$

with γ and β positive, it is possible to show that

$$\gamma^2/(1+i\sigma_{10})^2 + \beta^2/(1+i\sigma_{20})^2 \in Z(\widetilde{L}).$$

As any point of $\mathcal{S}$ can be obtained this way, $\sigma_{ess}(\widetilde{L})$ (on $H^{-1}(\bar{\Omega}^c)$) equals $\mathcal{S}$.

The following result provides uniform inf-sup conditions for the truncated problem.

Theorem VIII.22. *Let z be in $\rho(-\widetilde{\Delta})$. Then there is a δ_0 such that for all $\delta > \delta_0$ and u in $H_0^1(\Omega_\delta)$,*

$$\|u\|_{H_0^1(\Omega_\delta)} \le C \sup_{\phi \in H_0^1(\Omega_\delta)} \frac{|A_z(u,\phi)|}{\|\phi\|_{H_0^1(\Omega_\delta)}} \tag{VIII.26}$$

and

$$\|u\|_{H_0^1(\Omega_\delta)} \le C \sup_{\phi \in H_0^1(\Omega_\delta)} \frac{|A_z(\phi,u)|}{\|\phi\|_{H_0^1(\Omega_\delta)}}. \tag{VIII.27}$$

Proof. Let z be in $\rho(-\widetilde{\Delta})$. As observed in Remark VIII.6, it suffices to verify (VIII.12). If the constants in (VIII.12) are not uniformly bounded as δ goes to infinity, then there is a sequence $\{(\delta_n, u_n)\}$ satisfying

$$u_n \in H^2(\Omega_{\delta_n}) \cap H_0^1(\Omega_{\delta_n}), \qquad \delta_n \to \infty \quad \text{as } n \to \infty,$$
$$\|(-\widetilde{\Delta} - zI)u_n\|_{L^2(\Omega_{\delta_n})} \le \frac{1}{n}, \qquad \|u_n\|_{L^2(\Omega_{\delta_n})} = 1.$$

We assume that $\delta_n \ge 2b$. We next extend u_n to $\Omega_{3\delta_n/2}$ by odd reflection. Specifically, we define the extended function $\tilde{u}_n$ by first doing an odd reflection across $\partial\Omega_{\delta_n}$ into the regions labeled R_1 in Figure 10. Next, we do another odd reflection (across the boundary between R_1 and R_2) from the regions labeled R_1 into those labeled R_2. The values obtained in a R_2 region are independent of the choice of component of R_1 used in the reflection. It is easy to see that the resulting function $\tilde{u}_n$ is in $H^2(\Omega_{3\delta_n/2})$. Moreover, $(-\widetilde{\Delta} - zI)\tilde{u}_n(\tilde{x})$ for any $\tilde{x} \in \Omega_{3\delta_n/2} \setminus \Omega_{\delta_n}$ coincides with $\pm(-\widetilde{\Delta} - zI)u_n(x)$ where x is the point in Ω_{δ_n} which reflects into $\tilde{x}$. Accordingly,

$$\|(-\widetilde{\Delta} - zI)\tilde{u}_n\|_{L^2(\Omega_{3\delta_n/2})} \le 2\|(-\widetilde{\Delta} - zI)u_n\|_{L^2(\Omega_{\delta_n})} \le \frac{2}{n}.$$

Let χ be a smooth function on $\mathbb{R}^2$ with values in $[0,1]$ satisfying $\chi(x) = 1$ on $[-1,1]^2$ and $\chi(x) = 0$ outside of $(-3/2, 3/2)^2$. Define $\chi^n(x) = \chi(x/\delta_n)$. We shall show that

$$\|[\widetilde{\Delta}, \chi^n]\tilde{u}_n\|_{L^2(\Omega_{3\delta_n/2})} \le \frac{C}{n}. \tag{VIII.28}$$

Note that if (VIII.28) holds, then $w_n = \chi_n \tilde{u}_n$ is in $H^2(\mathbb{R})$ and satisfies:

$$\|w_n\|_{L^2(\mathbb{R})} \ge \|u_n\|_{L^2(\Omega_{\delta_n})} = 1$$

and

$$\|(-\widetilde{\Delta} - zI)w_n\|_{L^2(\mathbb{R})} \le \|[\widetilde{\Delta}, \chi^n]\tilde{u}_n\|_{L^2(\Omega_{3\delta_n/2})} + \|\chi^n(-\widetilde{\Delta} - zI)\tilde{u}_n\|_{L^2(\Omega_{3\delta_n/2})} \le \frac{C}{n}.$$

This contradicts the fact that $z \in \rho(-\widetilde{\Delta})$ ($-\widetilde{\Delta}$ as an operator on $L^2(\mathbb{R}^2)$).

To verify (VIII.28), we first note that by (VIII.2),

$$\|u_n\|^2_{H^1(\Omega_{\delta_n})} \leq C(\|u_n\|^2_{L^2(\Omega_{\delta_n})} + |A(u_n, u_n)|).$$

Now, u_n is in $H^2(\Omega_{\delta_n}) \cap H^1_0(\Omega_{\delta_n})$ and integration by parts gives

$$|A(u_n, u_n)| = (-\widetilde{\Delta} u_n, \bar{d}(x_1)\,\bar{d}(x_2)u_n)_{\Omega_{\delta_n}} \leq C\|\widetilde{\Delta} u_n\|_{L^2(\Omega_{\delta_n})}\|u_n\|_{L^2(\Omega_{\delta_n})},$$

from which it follows that

$$\|u_n\|_{H^1(\Omega_{\delta_n})} \leq C(\|u_n\|_{L^2(\Omega_{\delta_n})} + \|(-\widetilde{\Delta} - zI)u_n\|_{L^2(\Omega_{\delta_n})}).$$

Because of the reflection construction, this inequality extends to

$$\|\tilde{u}_n\|_{H^1(\Omega_{3\delta_n/2})} \leq 2C(\|u_n\|_{L^2(\Omega_{\delta_n})} + \|(-\widetilde{\Delta} - zI)u_n\|_{L^2(\Omega_{\delta_n})}) \leq C. \tag{VIII.29}$$

Expanding $[\widetilde{\Delta}, \chi^n]$ gives

$$\begin{aligned}[\widetilde{\Delta}, \chi^n]\tilde{u}_n = {} & \frac{1}{d(x)}\frac{\partial}{\partial x}\left(\frac{1}{d(x)}\chi^n_x \tilde{u}\right) + \frac{1}{d(x)^2}\chi^n_x \tilde{u}_x \\ & + \frac{1}{d(y)}\frac{\partial}{\partial y}\left(\frac{1}{d(y)}\chi^n_y \tilde{u}\right) + \frac{1}{d(y)^2}\chi^n_y \tilde{u}_y.\end{aligned} \tag{VIII.30}$$

We note that $d^{-1}(x)$ and $d'(x)$ are uniformly bounded and $\|\chi^n_x\|_{L^\infty(\mathbb{R}^2)}$, $\|\chi^n_{xx}\|_{L^\infty(\mathbb{R}^2)}$, $\|\chi^n_y\|_{L^\infty(\mathbb{R}^2)}$ and $\|\chi^n_{yy}\|_{L^\infty(\mathbb{R}^2)}$ are all bounded by C/n. Thus (VIII.28) follows from integrating (VIII.30), using the above estimates, (VIII.29) and the triangle inequality. This completes the proof of the theorem. $\square$

CHAPTER IX

CARTESIAN PML APPROXIMATION TO ACOUSTIC SCATTERING PROBLEMS

In this chapter we study the solvability of a Cartesian PML approximation to acoustic problems on infinite and truncated domains in $\mathbb{R}^2$. We first show uniqueness of solutions to the infinite domain problem using the Green's integral formula of Chapter VII. Once uniqueness of solutions is established, the spectral structure of the Cartesian PML operator given in Chapter VIII will be used to show the well-posedness of the infinite domain problem. We also show that truncated problems are well-posed provided that computational domains are large enough and their solutions converge exponentially to that of the infinite domain problem as the thickness of PML increases. Analysis of finite element approximations on the truncated domains is then classical. Numerical experiments illustrating the results of the Cartesian PML approach will be given.

A. Solvability of the PML problem in the infinite domain

From this section on, we take $z = i$ and z-dependency in notations will be omitted for simplicity. Also, C and α represent generic constants which do not depend on δ. We first derive an integral formula of solutions to $(\widetilde{\Delta} + k^2)u = 0$ on $\bar{\Omega}^c$.

Theorem IX.1. *Assume that $u \in H^1(\bar{\Omega}^c)$ satisfies $(\widetilde{\Delta} + k^2)u = 0$ on $\bar{\Omega}^c$. Then, for $x \in \mathbb{R}^2 \setminus \bar{\Omega}_0$,*

$$u(x) = \int_{\Gamma_0} \left[u(y) \frac{\partial \Phi(\tilde{r})}{\partial n_y} - \Phi(\tilde{r}) \frac{\partial u}{\partial n}(y) \right] \mathrm{d}S_y, \tag{IX.1}$$

where n is the outward unit normal vector on Γ_0.

Proof. We verify the theorem for $x \in [-m, m]^2$ with $m \geq b$. Let Ω_R be a square domain $(-R,R)^2$ with $R \geq 2m$ and Γ_R its boundary. Let $D = \Omega_R \setminus \bar{\Omega}_0$. Since u is in $H^2_{loc}(\bar{\Omega}^c)$, u is in H^2 on a neighborhood $\widetilde{D}$ of D. Using a cutoff function, which is one on D and supported on $\widetilde{D}$, we can define a compactly supported extension $\tilde{u}$ in $H^2(\mathbb{R}^2)$ of u defined on D. For $x \in D$ it follows from Theorem VII.5 and Remark VII.8 that

$$\begin{aligned}
-u(x) &= \int_{\mathbb{R}^2} ((\widetilde{\Delta}_y + k^2)\tilde{u}(y))\widetilde{\Phi}(x,y)\,\mathrm{d}y \\
&= \int_{\Omega_0} ((\widetilde{\Delta}_y + k^2)\tilde{u}(y))\widetilde{\Phi}(x,y)\,\mathrm{d}y + \int_{\Omega_R^c} ((\widetilde{\Delta}_y + k^2)\tilde{u}(y))\widetilde{\Phi}(x,y)\,\mathrm{d}y.
\end{aligned}$$

By integration by parts and Lemma VII.9

$$\begin{aligned}
u(x) = &-\int_{\Gamma_0} \left[\Phi(\tilde{r})n^t H\nabla u(y) - u(y)n^t H\nabla\Phi(\tilde{r})\right]\,\mathrm{d}S_y \\
&+ \int_{\Gamma_R} \left[\Phi(\tilde{r})n^t H\nabla u(y) - u(y)n^t H\nabla\Phi(\tilde{r})\right]\,\mathrm{d}S_y,
\end{aligned}$$

where n is the outward unit normal vector on the boundaries of Ω_0 and Ω_R.

Since $|d(y_j)|$ for $j = 1,2$ is bounded above and below away from zero, by a Schwarz inequality

$$\begin{aligned}
I \equiv &\left|\int_{\Gamma_R} \left[\Phi(\tilde{r})n^t H\nabla u(y) - u(y)n^t H\nabla\Phi(\tilde{r})\right]\,\mathrm{d}S_y\right| \\
&\leq C\left(\|\Phi(\tilde{r})\|_{L^2(\Gamma_R)}\|\nabla u\|_{L^2(\Gamma_R)} + \|u\|_{L^2(\Gamma_R)}\|\nabla\Phi(\tilde{r})\|_{L^2(\Gamma_R)}\right).
\end{aligned}$$

Set $S_\gamma = \{x \in \mathbb{R}^2 \;:\; \mathrm{dist}(x,\Gamma_R) < \gamma\}$ with γ independent of R and small enough so that $S_\gamma \subset \bar{\Omega}_0^c$. Using a trace inequality and an interior regularity result,

$$\begin{gathered}
\|u\|_{L^2(\Gamma_R)} \leq C\|u\|_{H^1(\mathbb{R}^2)} \quad \text{and} \\
\|\nabla u\|_{L^2(\Gamma_R)} \leq C\|u\|_{H^2(S_\gamma)} \leq C\|u\|_{H^1(\mathbb{R}^2)}.
\end{gathered} \tag{IX.2}$$

It follows from (VII.20) and Lemma VII.4 that

$$|\Phi(\tilde{r}^z)| \leq Ce^{-k\mathrm{Im}(\tilde{r}^z)} \leq Ce^{-\alpha k|y|}. \tag{IX.3}$$

This implies

$$\left(\int_{\Gamma_R} |\Phi(\tilde{r})|^2 \,\mathrm{d}S_y\right)^{1/2} \leq C\left(\int_{\Gamma_R} e^{-2\alpha kR} \,\mathrm{d}S_y\right)^{1/2} \leq Ce^{-\alpha_1 kR} \tag{IX.4}$$

for some $0 < \alpha_1 < \alpha$. To estimate the derivatives of $\Phi(\tilde{r})$, using Lemma VII.3, (VII.20) and the above lemma, we see that

$$\left|\frac{\partial\Phi(\tilde{r})}{\partial y_j}\right| = \left|\Phi'(\tilde{r})\frac{(\tilde{x}_j - \tilde{y}_j)(-d(y_j))}{\tilde{r}}\right| \leq C\,|\Phi'(\tilde{r})| \leq Ce^{-\alpha k|y|}. \tag{IX.5}$$

A simple computation as in (IX.4) shows that

$$\|\nabla\Phi(\tilde{r})\|_{L^2(\Gamma_R)} \leq Ce^{-\alpha_1 kR} \tag{IX.6}$$

for some positive α_1. Combining (IX.2), (IX.4), and (IX.6) gives

$$I \leq Ce^{-\alpha_1 kR}\|u\|_{H^1(\mathbb{R}^2)}.$$

Since I converges to zero as R tends towards infinity, there is no contribution of the outer boundary Γ_R. Finally, we obtain (IX.1) since H is the identity on Γ_0.

□

The following proposition shows the uniqueness of solutions to the Cartesian PML problem in the infinite domain (VII.5).

Proposition IX.2. *The Cartesian PML problem* (VII.5) *with* $f = 0$ *has only a trivial solution in* $H_0^1(\bar{\Omega}^c)$.

Proof. Let $\tilde{u}$ be a solution to (VII.5) with $f = 0$ in $H_0^1(\bar{\Omega}^c)$. By Theorem IX.1, $\tilde{u}$ can be expressed in the integral formula

$$\tilde{u}(x) = \int_{\Gamma_0} \left[\tilde{u}(y) \frac{\partial \Phi(\tilde{r})}{\partial n_y} - \Phi(\tilde{r}) \frac{\partial \tilde{u}}{\partial n}(y) \right] \mathrm{d}S_y \tag{IX.7}$$

for $x \in \mathbb{R}^2 \setminus \bar{\Omega}_0$.

Define

$$u(x) = \begin{cases} \tilde{u}(x) & \text{for } \; x \in \bar{\Omega}_0 \setminus \bar{\Omega}, \\ \displaystyle\int_{\Gamma_0} \left[\tilde{u}(y) \frac{\partial \Phi(|x-y|)}{\partial n_y} - \Phi(|x-y|) \frac{\partial \tilde{u}}{\partial n}(y) \right] \mathrm{d}S_y & \text{for } \; x \in \mathbb{R}^2 \setminus \bar{\Omega}_0. \end{cases} \tag{IX.8}$$

Note that the transition at Ω_0 is smooth since $\Phi(|x-y|)$ coincides with $\Phi(\tilde{r})$ near Ω_0. It follows that u satisfies (VII.1) with $g = 0$. As (VII.1) has unique solutions, u and, hence, $\tilde{u}$ must vanish identically. □

We combine the sesquilinear forms in (VII.5) and define

$$A_{k^2}(\cdot, \cdot) = A(\cdot, \cdot) - k^2 (J \;\cdot, \cdot).$$

We then have the following lemma which provides stability of the PML problem on $\bar{\Omega}^c$.

Lemma IX.3. *For any real $k \neq 0$, the following two inf-sup conditions hold: For u in $H^1(\bar{\Omega}^c)$,*

$$\|u\|_{H^1(\bar{\Omega}^c)} \leq C \sup_{\phi \in H_0^1(\bar{\Omega}^c)} \frac{|A_{k^2}(u, \phi)|}{\|\phi\|_{H^1(\bar{\Omega}^c)}},$$

and

$$\|u\|_{H^1(\bar{\Omega}^c)} \leq C \sup_{\phi \in H_0^1(\bar{\Omega}^c)} \frac{|A_{k^2}(\phi, u)|}{\|\phi\|_{H^1(\bar{\Omega}^c)}}.$$

Proof. It follows from Lemma VIII.3 and Theorem VIII.20, that for any real $k \neq 0$, either the above two inf-sup conditions hold or there is an eigenvector corresponding to k^2, i.e., a non-zero function $w \in H_0^1(\bar{\Omega}^c)$ satisfying

$$A_{k^2}(w, \phi) = 0 \text{ for all } \phi \in H_0^1(\bar{\Omega}^c).$$

The lemma follows since Proposition IX.2 prohibits such a w. $\square$

We have now the first main result of solvability of the infinite domain problem (VII.5).

Theorem IX.4. *Let k be real and positive, and $g \in H^{1/2}(\Gamma)$. Then there exists a unique solution $\tilde{u} \in H^1(\bar{\Omega}^c)$ to the problem*

$$A_{k^2}(\tilde{u}, \phi) = 0 \quad \textit{for all} \quad \phi \in H_0^1(\bar{\Omega}^c) \tag{IX.9}$$

with $\tilde{u} = g$ satisfying $\|\tilde{u}\|_{H^1(\bar{\Omega}^c)} \leq C\|g\|_{H^{1/2}(\Gamma)}$. In addition, the solution $\tilde{u}$ decays exponentially, i.e., there exist $C > 0$ and $\alpha > 0$ independent of x and δ such that for $\|x\|_\infty \geq b$ and $\delta \geq b$,

$$|\tilde{u}(x)| \leq Ce^{-\alpha k|x|}\|g\|_{H^{1/2}(\Gamma)} \quad \textit{and} \quad \|\tilde{u}\|_{H^{1/2}(\Gamma_\delta)} \leq Ce^{-\alpha k\delta}\|g\|_{H^{1/2}(\Gamma)}. \tag{IX.10}$$

Proof. The solvability of (IX.9) easily follows from Lemma IX.3 and we conclude that the problem (IX.9) has a unique weak solution $\tilde{u} \in H^1(\bar{\Omega}^c)$ satisfying

$$\|\tilde{u}\|_{H^1(\bar{\Omega}^c)} \leq C\|g\|_{H^{1/2}(\Gamma)}.$$

Because of interior regularity estimates, $\tilde{u}$ is in $H^2((-3b/2, 3b/2)^2 \setminus [-b, b]^2)$ and hence it suffices to prove (IX.10) for $\|x\|_\infty \geq 3b/2$ and $\delta \geq 3b/2$. This will follow from the integral formula (IX.1), Lemma VII.4, and exponential decay of the fundamental solution (IX.3) and (IX.5). Indeed, by a Schwarz inequality and an interior regularity as in (IX.2)

$$
\begin{aligned}
|\tilde{u}(x)|^2 &= \left| \int_{\Gamma_0} \tilde{u}(y) \frac{\partial \Phi(\tilde{r})}{\partial n_y} - \Phi(\tilde{r}) \frac{\partial \tilde{u}}{\partial n}(y)\, \mathrm{d}S_y \right|^2 \\
&\leq Ce^{-2\alpha k|x|} (\|\tilde{u}\|^2_{L^2(\Gamma_0)} + \|\nabla \tilde{u}\|^2_{L^2(\Gamma_0)}) \leq Ce^{-2\alpha k|x|} \|\tilde{u}\|^2_{H^1(\bar{\Omega}^c)}.
\end{aligned}
\tag{IX.11}
$$

For $\gamma = b/8$ let S_γ be a γ-neighborhood of Γ_δ and set $\gamma' = b/4$. Clearly $S_\gamma \subset S_{\gamma'}$ and both are contained in the complement of $[-b, b]^2$. Applying an interior regularity on $S_\gamma \subset S_{\gamma'}$ and integrating (IX.11) over $S_{\gamma'}$ gives

$$
\begin{aligned}
\|\tilde{u}\|_{H^{1/2}(\Gamma_\delta)} &\leq C\|\tilde{u}\|_{H^2(S_\gamma)} \leq C\|\tilde{u}\|_{L^2(S_{\gamma'})} \\
&\leq C\delta e^{-\alpha k \delta} \|\tilde{u}\|_{H^1(\bar{\Omega}^c)} \leq Ce^{-\alpha_1 k \delta} \|\tilde{u}\|_{H^1(\bar{\Omega}^c)}.
\end{aligned}
$$

The factor of δ is absorbed by choosing a slightly smaller $\alpha_1 < \alpha$.

□

Remark IX.5. Theorem IX.4 holds for the adjoint problem as well.

B. Solvability of the truncated Cartesian PML problem

Our goal is to study the truncated Cartesian PML problem on $\Omega_\delta \setminus \bar{\Omega}$. The analysis involves an iteration involving the solution of the exterior problem (on $\bar{\Omega}^c$) and a full truncated problem (on $\Omega_\delta = (-\delta, \delta)^2$).

We start by considering the full truncated variational problem: Find $u \in H^1_0(\Omega_\delta)$ satisfying

$$
a_{k^2}(u, \theta) = < F, \theta > \quad \text{for all} \;\; \theta \in H^1_0(\Omega_\delta). \tag{IX.12}
$$

Here F is a bounded linear functional on $H^1_0(\Omega_\delta)$, $< \cdot, \cdot >$ denotes the duality pairing and

$$
a_{k^2}(u, v) = \int_{\Omega_\delta} \left[\frac{d(x_2)}{d(x_1)} \frac{\partial u}{\partial x_1} \frac{\partial \bar{v}}{\partial x_1} + \frac{d(x_1)}{d(x_2)} \frac{\partial u}{\partial x_2} \frac{\partial \bar{v}}{\partial x_2} - k^2 J(x) u \bar{v} \right] \mathrm{d}x.
$$

It was shown in Chapter VIII that there is a positive constant δ_0 (cf. Remark VIII.6 and Theorem VIII.22) such that the solution of (IX.12) exists and is unique provided that $\delta > \delta_0$. Moreover, there is a constant C independent of δ satisfying

$$\|u\|_{H^1_0(\Omega_\delta)} \le C\|F\|_{(H^1_0(\Omega_\delta))^*}.$$

These results hold for the adjoint problem as well. The following proposition is an immediate consequence.

Proposition IX.6. *Let g be in $H^{1/2}(\Gamma_\delta)$ with $\delta > \delta_0$. Then the problem*

$$a_{k^2}(u,\phi) = 0 \quad \textit{for all} \quad \phi \in H^1_0(\Omega_\delta) \tag{IX.13}$$

with $u = g$ on Γ_δ has a unique solution satisfying

$$\|u\|_{H^1(\Omega_\delta)} \le C\|g\|_{H^{1/2}(\Gamma_\delta)}. \tag{IX.14}$$

The same result holds for the adjoint solution, i.e., (IX.13) *replaced by*

$$a_{k^2}(\phi,u) = 0 \quad \textit{for all} \quad \phi \in H^1_0(\Omega_\delta).$$

Here C is independent of δ.

The next proposition provides an inf-sup condition for the truncated PML problem (on $\Omega_\delta \setminus \bar{\Omega}$).

Proposition IX.7. *There is a constant $\tilde{\delta}_0$ and $C = C(\tilde{\delta}_0)$ such that if $\delta > \tilde{\delta}_0$,*

$$\|u\|_{H^1(\Omega_\delta\setminus\bar{\Omega})} \le C \sup_{\phi\in H^1_0(\Omega_\delta\setminus\bar{\Omega})} \frac{|a_{k^2}(u,\phi)|}{\|\phi\|_{H^1(\Omega_\delta\setminus\bar{\Omega})}} \quad \textit{for all} \quad u \in H^1_0(\Omega_\delta\setminus\bar{\Omega}). \tag{IX.15}$$

In the above inequality, we have extended u and ϕ by zero to all of Ω_δ (in $a_{k^2}(u,\phi)$).

Proof. Let u be in $H^1_0(\Omega_\delta\setminus\bar{\Omega})$. To prove (IX.15), we construct a solution $\phi \in H^1_0(\Omega_\delta \setminus$

$\bar{\Omega}$) of the adjoint equation

$$a_{k^2}(\theta, \phi) = (\theta, u)_{H^1(\Omega_\delta \setminus \bar{\Omega})} \text{ for all } \theta \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$$

satisfying

$$\|\phi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \le C \|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}.$$

The proposition then follows since

$$\|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} = \frac{a_{k^2}(u, \phi)}{\|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}} \le C \frac{|a_{k^2}(u, \phi)|}{\|\phi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}}.$$

To construct ϕ, we start by letting $\tilde{\phi} \in H_0^1(\bar{\Omega}^c)$ solve the exterior problem

$$A_{k^2}(\theta, \tilde{\phi}) = (\theta, u)_{H^1(\bar{\Omega}^c)} \text{ for all } \theta \in H_0^1(\bar{\Omega}^c),$$

where we extend u by zero outside of $\Omega_\delta \setminus \bar{\Omega}$. By Lemma IX.3, $\tilde{\phi}$ is well-defined and

$$\|\tilde{\phi}\|_{H^1(\bar{\Omega}^c)} \le C \|u\|_{H^1(\bar{\Omega}^c)}.$$

Thus, we need only to construct a function χ satisfying:

$$\begin{aligned} \chi = \tilde{\phi} \text{ on } \Gamma_\delta \text{ and } \chi = 0 \text{ on } \Gamma, \\ a_{k^2}(\theta, \chi) = 0 \text{ for all } \theta \in H_0^1(\Omega_\delta \setminus \bar{\Omega}), \\ \|\chi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \le C \|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}. \end{aligned} \tag{IX.16}$$

Indeed, then $\phi = \tilde{\phi} - \chi$ has the desired properties.

We construct χ by iteration on Γ_δ. To start, we set $\chi_0 = \tilde{\phi}$ on Γ_δ. Clearly, $\chi_0 \in H^{1/2}(\Gamma_\delta)$. We set up a sequence $\{\chi_j\} \subset H^{1/2}(\Gamma_\delta)$ by induction. Given χ_j, we first define $w_j^1 \in H^1(\Omega_\delta)$ for $\delta > \delta_0$ in Proposition IX.6 to be the unique solution of

$$a_{k^2}(\theta, w_j^1) = 0 \text{ for all } \theta \in H_0^1(\Omega_\delta)$$

with $w_j^1 = \chi_j$ on Γ_δ. Next we define $w_j^2 \in H^1(\bar{\Omega}^c)$ by

$$A_{k^2}(\theta, w_j^2) = 0 \text{ for all } \theta \in H_0^1(\bar{\Omega}^c)$$

and $w_j^2 = w_j^1$ on Γ. We finally set $\chi_{j+1} = w_j^2$ on Γ_δ.

Now, by Proposition IX.6 and Theorem IX.4,

$$\|w_j^1\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \leq C\|\chi_j\|_{H^{1/2}(\Gamma_\delta)}$$

and

$$\begin{aligned} \|\chi_{j+1}\|_{H^{1/2}(\Gamma_\delta)} = \|w_j^2\|_{H^{1/2}(\Gamma_\delta)} &\leq Ce^{-\alpha k\delta}\|w_j^1\|_{H^{1/2}(\Gamma)} \\ &\leq Ce^{-\alpha k\delta}\|\chi_j\|_{H^{1/2}(\Gamma_\delta)}. \end{aligned} \tag{IX.17}$$

We set $\tilde{\delta}_0$ by $\gamma = Ce^{-\alpha k\tilde{\delta}_0} < 1$ for C in (IX.17) so that

$$\|\chi_j\|_{H^{1/2}(\Gamma_\delta)} \leq \gamma^j\|\chi_0\|_{H^{1/2}(\Gamma_\delta)}.$$

Because of this, the telescoping sequence

$$\chi_0 = \sum_{j=0}^{\infty}(\chi_j - \chi_{j+1})$$

converges in $H^{1/2}(\Gamma_\delta)$ and the corresponding sequence

$$\sum_{j=0}^{\infty}(w_j^1 - w_j^2) \tag{IX.18}$$

converges in $H^1(\Omega_\delta \setminus \bar{\Omega})$. By construction, the limit (which we denote by χ) equals $\tilde{\phi}$ on Γ_δ. By the definitions of w_j^1 and w_j^2, it is also clear that each term in (IX.18) vanishes on Γ and satisfies the homogeneous equation

$$a_{k^2}(\theta, w_j^1 - w_j^2) = 0 \text{ for all } \theta \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$$

and so these properties hold for χ as well. Finally, by Theorem IX.4 and Proposition IX.6

$$\begin{aligned} \|\chi\|_{H^1(\Omega_\delta\setminus\bar\Omega)} &\leq \sum_{j=0}^{\infty} \|w_j^1 - w_j^2\|_{H^1(\Omega_\delta\setminus\bar\Omega)} \\ &\leq C\sum_{j=0}^{\infty} \|\chi_j\|_{H^{1/2}(\Gamma_\delta)} \leq C\|\chi_0\|_{H^{1/2}(\Gamma_\delta)} \leq C\|u\|_{H^1(\Omega_\delta\setminus\bar\Omega)}. \end{aligned}$$

Thus, χ satisfies all of the conditions of (IX.16) and the proof is completed. □

Remark IX.8. The inf-sup condition for the adjoint problem follows immediately from (IX.15) and the fact that the coefficients in the forms are symmetric.

The following theorem shows exponential convergence of solutions of the truncated problems.

Theorem IX.9. *For $\delta > \tilde\delta_0$, there exists a unique solution $\tilde u_t \in H^1(\Omega_\delta \setminus \bar\Omega)$ to the problem*

$$A_{k^2}(\tilde u_t, \phi) = 0 \quad \textit{for all} \quad \phi \in H_0^1(\Omega_\delta \setminus \bar\Omega) \tag{IX.19}$$

with $\tilde u_t = g$ on Γ and $\tilde u_t = 0$ on Γ_δ satisfying

$$\|\tilde u_t\|_{H^1(\Omega_\delta\setminus\bar\Omega)} \leq C\|g\|_{H^{1/2}(\Gamma)}. \tag{IX.20}$$

Here C is independent of δ. In addition, if $\tilde u$ is the solution to the infinite PML problem (IX.9), *then*

$$\|\tilde u - \tilde u_t\|_{H^1(\Omega_\delta\setminus\bar\Omega)} \leq Ce^{-\alpha k\delta}\|g\|_{H^{1/2}(\Gamma)}. \tag{IX.21}$$

Proof. The existence and uniqueness of $\tilde u_t$ and (IX.20) are an immediate consequence of Proposition IX.7 and Remark IX.8.

Note that $\tilde u - \tilde u_t$ satisfies

$$\begin{aligned} A_{k^2}(\tilde u - \tilde u_t, \phi) = 0 \quad &\text{for all} \quad \phi \in H_0^1(\Omega_\delta \setminus \bar\Omega), \\ \tilde u - \tilde u_t = 0 \quad \text{on} \quad \Gamma \quad &\text{and} \quad \tilde u - \tilde u_t = \tilde u \quad \text{on} \quad \Gamma_\delta. \end{aligned}$$

Proposition IX.7 and Remark IX.8 then implies that

$$\|\tilde{u} - \tilde{u}_t\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \le C \|\tilde{u}\|_{H^{1/2}(\Gamma_\delta)}$$

and (IX.21) follows from Theorem IX.4. □

C. Finite element analysis

In this section, we discuss properties of the finite element approximation of the solution $\tilde{u}_t$ of the variational problem (IX.19). As this analysis is standard, we only give a brief sketch of the arguments. For simplicity, we assume that Γ is polygonal as the errors which result from the finite element method associated with boundary approximation are well understood.

Let $\mathcal{T}_h$ denote a partition of shape-regular triangular (or quadrilateral) meshes of $\Omega_\delta \setminus \bar{\Omega}$, and h represents the diameters of elements, e.g., $h = \max_{K \in \mathcal{T}_h} \operatorname{diam}(K)$. Let S_h denote a subspace of $H^1(\Omega_\delta \setminus \bar{\Omega})$ consisting of piecewise polynomial finite element functions and S_h^0 denote the subset of functions in S_h which vanish on $\Gamma \cup \Gamma_\delta$. We assume that g is the trace of a function in our approximation space as the additional errors associated with boundary quadrature in the finite element method are well understood. Let $\tilde{S}_h$ be the set of functions in S_h which coincide with g on Γ and vanish on Γ_δ. In this case, the finite element approximation to $\tilde{u}_t$ is the function in $\tilde{u}_h \in \tilde{S}_h$ satisfying

$$a_{k^2}(\tilde{u}_h, \theta) = 0 \quad \text{for all} \quad \theta \in S_h^0.$$

The unique solvability of $\tilde{u}_h$ is a consequence of an argument of Schatz [50]. Since the real parts of the elements of H are uniformly bounded from below by a positive constant and J is bounded, the sesquilinear form $a_{k^2}(\cdot, \cdot)$ satisfies a Gärding inequality.

Given $g \in L^2(\Omega_\delta \setminus \bar{\Omega})$, let $\phi \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$ be the solution to the adjoint problem:

$$a_{k^2}(\theta, \phi) = (\theta, g) \quad \text{for all} \quad \theta \in H_0^1(\Omega_\delta \setminus \bar{\Omega}).$$

As the coefficients defining $\tilde{\sigma}$ are C^2, the elliptic regularity for the adjoint problem is determined by its behavior near Γ, i.e., $\phi \in H^{1+s}(\Omega_\delta \setminus \bar{\Omega})$ for some $s > 1/2$.

Under these conditions, the technique of [50] (see, also, [51]) gives that there is a positive number h_0 such that for $h < h_0$, $\tilde{u}_h$ is uniquely defined and satisfies

$$\|\tilde{u}_t - \tilde{u}_h\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \leq C \inf_{\phi_h \in \tilde{S}_h} \|\tilde{u}_t - \phi_h\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}.$$

Remark IX.10. In contrast to earlier sections, the analysis suggested in this section leads to constants (i.e., h_0 and C above) which may depend on δ.

D. Numerical experiments

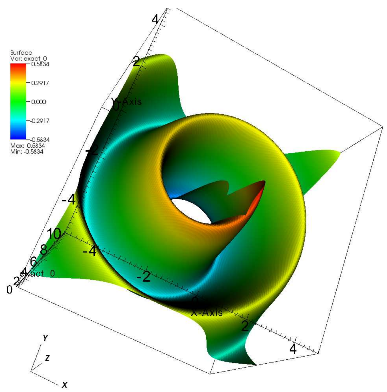
As a numerical example, we consider a scattering problem (VII.1) with a square scatterer $\Omega = (-1,1)^2$ in $\mathbb{R}^2$ with the wave number $k = 2$. The boundary condition is given by $g = e^{i\theta} H_1^1(kr)$ on Γ, where (r, θ) is the polar coordinate of x. Clearly, $u(x) = e^{i\theta} H_1^1(kr)$ satisfies (VII.1).

A Cartesian PML with the parameters

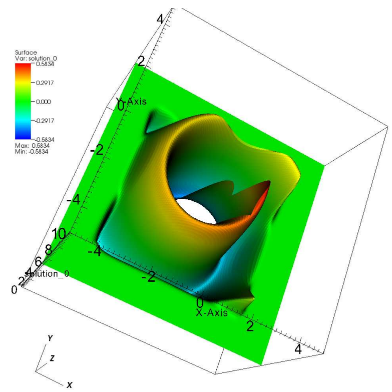
$$a = 3, b = 4, \sigma_0 = 1$$

is applied to (VII.1) and we will observe that finite element PML solutions converges to the exact one on the region of computational interest $[-3,3]^2 \setminus [-1,1]^2$. For numerical computation, the infinite domain is truncated to a finite domain $[-5,5]^2 \setminus [-1,1]^2$ with $\delta = 5$.

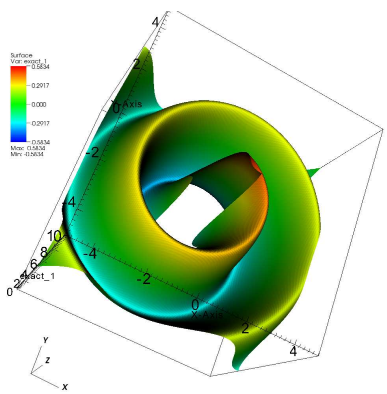
The numerical results obtained using the finite element library deal.II [6, 7] are



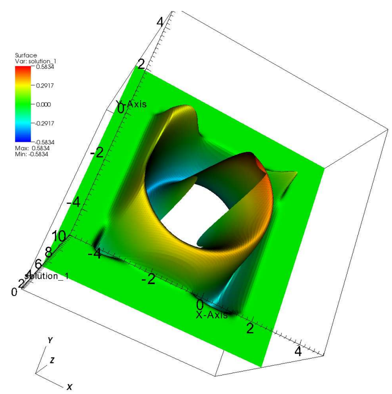
(a) Real part of the exact solution



(b) Real part of the finite element PML solution



(c) Imaginary part of the exact solution

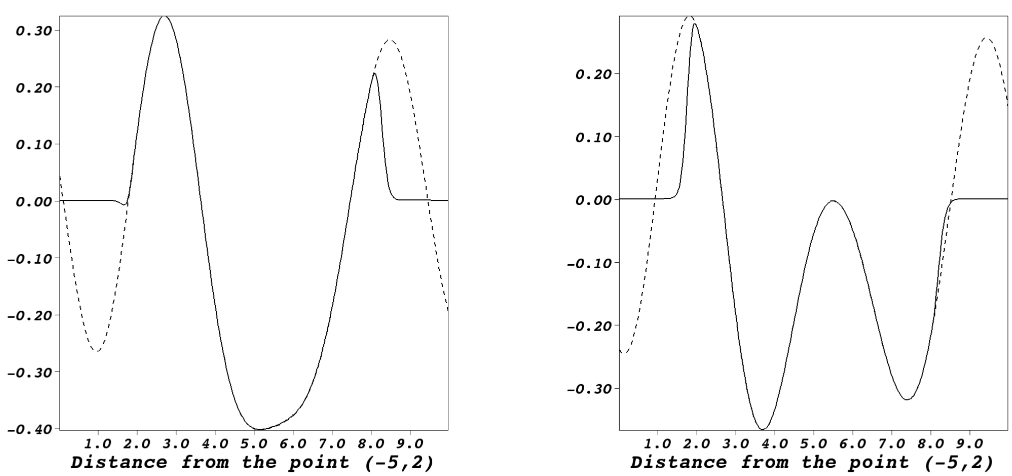


(d) Imaginary part of the finite element PML solution

Fig. 11. Exact solution and its finite element PML approximation

Table 2. Convergence of the real part of the finite element PML approximate solutions

h	# dofs	real H^1-error		real L^2-error	
1	240	1.678e+00	ratio	5.621e-01	ratio
1/2	864	9.791e-01	1.71	2.955e-01	1.90
1/4	3264	5.642e-01	1.74	1.949e-01	1.90
1/8	12672	2.104e-01	2.68	3.957e-02	4.93
1/16	49920	9.913e-02	2.12	1.042e-02	3.80
1/32	198144	4.866e-02	2.04	2.646e-03	3.94
1/64	789504	2.421e-02	2.01	6.643e-04	3.98



(a) Real part at $x_2 = 2$ (b) Imaginary part at $x_2 = 2$

Fig. 12. Graphs of real and imaginary parts of the exact solution (dashed curves) and the finite element PML approximation (solid curves for $h = 1/32$) at $x_2 = 2$ as functions of x_1 in $[-5, 5]$

given in Figure 11 and Table 2. As shown in Figure 11, the finite element PML solution is very close to the exact solution in $[-3,3]^2 \setminus [-1,1]^2$, and decays rapidly outside. This is also illustrated in Figure 12. Figure 12 shows the graphs of the real and imaginary parts of the exact solution and the finite element PML approximation at $x_2 = 2$ as functions of x_1 with $-5 \leq x_1 \leq 5$.

To further illustrate convergence of the finite element PML solutions, the errors between the interpolant of the exact solution u and finite element PML solution $\tilde{u}_h$ are reported in Table 2 on the region $[-3,3]^2 \setminus [-1,1]^2$ for different h. Note that the finite element PML solution $\tilde{u}_h$ approximates the truncated PML solution $\tilde{u}_t$, which is not available analytically. The table suggests the first order convergence in $H^1(\Omega_\delta \setminus \bar{\Omega})$ and second order convergence in $L^2(\Omega_\delta \setminus \bar{\Omega})$. This is not surprising because the truncated solution $\tilde{u}_t$ is exponentially close to u in $[-3,3]^2 \setminus [-1,1]^2$ by Theorem IX.7.

CHAPTER X

CONCLUSIONS

We have studied a domain truncation method for an artificial boundary condition based on perfectly matched layer (PML) approach. This technique was applied to resonance problems in open systems and acoustic scattering problems.

In the first part of this dissertation, from Chapter II through Chapter VI, we discussed application of spherical PML to resonance problems posed on unbounded domains. We observed that application of PML converted the resonance problems to an eigenvalue problem (on the infinite domain) and its eigenfunctions decayed exponentially. This exponential decay made it possible to truncate the infinite domain eigenvalue problem to one on a finite domain with a convenient boundary condition, e.g., a homogeneous Dirichlet boundary condition. We proved that the domain truncation does not produce spurious eigenvalues provided that computational domains are large enough. Moreover, the corresponding eigenvalues converge to those of the infinite domain problem counted with their algebraic multiplicity as the size of computational domains increases. The numerical experiments presented confirmed these results.

In the second part, from Chapter VII through Chapter IX, we investigated a Cartesian PML approximation to acoustic scattering problems. We examined the essential spectrum of the Cartesian PML operator associated with the scattering problem with a real and positive wave number and established uniqueness of solutions. We verified the well-posedness of the Cartesian PML scattering problem on the infinite domain and exponential decay of its solutions. These results played an important role in the proof that truncated problems are well-posed provided that the computational domain is large enough. Moreover, the solution to the truncated domain problem is exponentially close to that of the infinite domain problem on the region of computational interest. The numerical experiments illustrated these results.

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APPENDIX

NOTATION INDEX

VITA

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