Cartesian PML approximation to resonances in open systems in $\mathbb{R}^2$

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Abstract

In this paper, we consider a Cartesian PML approximation to resonance values of time-harmonic problems posed on unbounded domains in $\mathbb{R}^2$. A PML is a fictitious layer designed to find solutions arising from wave propagation and scattering problems supplemented with an outgoing radiation condition at infinity. Solutions obtained by a PML coincide with original solutions near wave sources or scatterers while they decay exponentially as they propagate into the layer. Due to rapid decay of solutions, it is natural to truncate unbounded domains to finite regions of computational interest. In this analysis, we introduce a PML in Cartesian geometry to transform a resonance problem (characterized as an eigenvalue problem with improper eigenfunctions) on an unbounded domain to a standard eigenvalue problem on a finite computational region. Truncating unbounded domains gives rise to perturbation of resonance values, however we show that eigenvalues obtained by the truncated problem converge to resonance values as the size of computational domain increases. In addition, our analysis shows that this technique is free of spurious resonance values provided truncated domains are sufficiently large. Finally, we present the results of numerical experiments with simple model problems.

Key words: Helmholtz equation, perfectly matched layer, Cartesian PML, acoustic resonance, photonic resonance, spectral theory
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1. Introduction

In this paper we will analyze perfectly matched layer (PML) approximation based on Cartesian geometry to resonance values of problems on unbounded domains in $\mathbb{R}^2$. Research on resonances in open systems has been extensively developed because of their many potential applications. For example, applications of acoustic resonance include designing musical instruments such as violins and guitars [13, 23] and determining frequencies of acoustic noise arising from an airplane wing and its slat and flap (see [21] and reference therein). The other example is photonic resonances and they take place in special structures of dielectric materials. It is known that periodic dielectric structures (photonic crystals) can prohibit waves of frequencies in a particular range (called a photonic band gap or PBG) from propagating in the structures [25, 30, 34]. While the ideal photonic crystals have an infinite periodic pattern, in a practical application dielectric materials are arranged in a periodic pattern to a finite extent [15, 35]. If a defect is introduced in the structures, then they may produce localized resonance modes of frequencies in PBG. This unique properties of photonic crystals allow many applications including lasers, waveguides, optical filters and optical communications.

In this paper, for acoustic models we consider a problem to find complex wavenumbers k for which there exists a nonzero solution u satisfying

$$\begin{aligned} \Delta u + k^2 u = 0 \text{ in } \bar{\Omega}^c, \\ u = 0 \text{ on } \Gamma \end{aligned} \tag{1.1}$$

with an *outgoing radiation condition* at infinity, which will be discussed below. Here Ω is a bounded scatterer with a Lipschitz boundary Γ and we denote the complement of the closure of Ω in $\mathbb{R}^2$ by $\bar{\Omega}^c := \mathbb{R}^2 \setminus \bar{\Omega}$.

For photonic resonance models, we consider two basic polarizations of electromagnetic equations with dielectric materials contained in a bounded region of $\mathbb{R}^2$. In case of the TE polarization, magnetic fields satisfy the scalar Helmholtz equation

$$\begin{aligned} \nabla \cdot \frac{1}{\varepsilon} \nabla u + k^2 u = 0 \text{ in } \mathbb{R}^2 \setminus \partial G, \\ u^- - u^+ = 0 \text{ on } \partial G, \\ \frac{1}{\varepsilon^-}\frac{\partial u^-}{\partial n} - \frac{1}{\varepsilon^+}\frac{\partial u^+}{\partial n} = 0 \text{ on } \partial G, \end{aligned} \tag{1.2}$$

where G is a finite-sized periodic dielectric material and ε is a dielectric constant of the photonic structure such that $\varepsilon = \varepsilon^+ = 1$ on the background material and $\varepsilon = \varepsilon^-$ on G. Also, u^+ and u^- represent the restriction of the function u to $\mathbb{R}^2 \setminus \bar{G}$ and G respectively, and in the transmission conditions on ∂G, $u^\pm$ and $\partial u^\pm / \partial n$ are understood as their traces on ∂G with n the outward unit normal vector on the boundary of G.

For the TM polarization, electric fields satisfy

$$\begin{aligned} \Delta u + k^2 \varepsilon u = 0 \text{ in } \mathbb{R}^2 \setminus \partial G, \\ u^- - u^+ = 0 \text{ on } \partial G, \\ \frac{\partial u^-}{\partial n} - \frac{\partial u^+}{\partial n} = 0 \text{ on } \partial G. \end{aligned} \tag{1.3}$$

As in the acoustic model problem (1.1), the model problems (1.2) and (1.3) require an outgoing radiation condition at infinity. In this paper, for $|\arg(k)| < \pi$ a solution $u \in H^1_{loc}(\bar{\Omega}^c)$ to the Helmholtz equation is said to be an *outgoing* solution if u has a series representation in terms of Hankel functions of the first kind

$$u(x) = \sum_{n=-\infty}^{\infty} a_n H_n^1(k|x|) e^{in\theta_x} \text{ for } |x| > r_0 \tag{1.4}$$

for some $r_0 > 0$, where $\theta_x = \arg(x)$ and H_n^1 are Hankel functions of the first kind of order n [1, 32]. Now, we are interested in k for which the model problems have nonzero solutions and such a k is called a *resonance*.

In the acoustic scattering theory, it is known that for k with $\mathrm{Im}(k) \geq 0$, the outgoing radiation condition given by a series (1.4) is equivalent to the Sommerfeld radiation condition

$$\lim_{r\to\infty} \sqrt{r} \left(\frac{\partial u}{\partial r} - iku \right) = 0 \tag{1.5}$$

with $r = |x|$ (see e.g, [10]). Furthermore, by using variational arguments one can show that the Helmholtz equation with $\mathrm{Im}(k) \geq 0$ supplemented with the Sommerfeld radiation condition (1.5) has a unique solution [11]. Therefore resonance values have necessarily a negative imaginary part. Due to this fact and the outgoing radiation condition (1.4) together with an asymptotic behavior of Hankel functions of the first kind (3.8), one can show that resonance functions are not square integrable. Hence they can be thought of as *improper* eigenfunctions.

A PML is an artificial absorbing layer surrounding the area of computational interest. This fictitious layer can be introduced by a certain complex coordinate stretching in a way that solutions obtained by the method are preserved outside of PML and decay exponentially in the layer. So it is natural to truncate unbounded domains to a finite region, which allows one to apply standard computational techniques, e.g., finite element methods. Since Bérenger proposed a PML method to study electromagnetic waves [4, 5] in time domain, many accurate and efficient variants of PML were applied to many different areas such as acoustics [6, 31], elastics [8, 19, 18] and electromagnetics [6, 7, 9] in time domain and frequency domain.

Also, PML methods have successfully employed for computing acoustic resonances [21, 20] and photonic resonances [17, 24]. A PML technique deforms the original resonance problem to a standard eigenvalue problem posed on a bounded domain in the following steps

(i) resonance problem (problem with improper eigenfunctions),

(ii) eigenvalue problem posed in an unbounded domain (infinite PML problem),

(iii) eigenvalue problem posed in a bounded domain (truncated PML problem).

Applying a coordinate stretching associated with PML transforms the original resonance problem (i) to an eigenvalue problem in an unbounded domain (ii). Truncating the unbounded domain of the problem (ii) results in an eigenvalue problem in a bounded domain (iii). In converting the problem (i) to the problem (ii), resonance values in a region of interest turn out to be eigenvalues of the infinite PML problem. The domain truncation however perturbs eigenvalues of the infinite PML problem. Most literature mentioned above demonstrated computationally that the perturbation resulting from domain truncation can be as small as we wish by increasing the domain size. In this paper we will provide a theoretical convergence analysis of approximate resonance values obtained by Cartesian PML. We remark that there is an analysis for convergence of approximate resonance values in a spherical PML framework in [27].

The analysis in this paper proceeds based on the ideas used in [27]. However, there are difficulties in carrying out the ideas directly in Cartesian PML. In case of spherical PML [27], we observe that a Laplace operator deformed by spherical PML used in [27] is reduced to a Laplace operator multiplied by a complex constant coefficient outside of a compact set. This property plays an important role for deriving stability estimates of solutions to spherical PML Helmholtz equation. In contrast, since Cartesian PML uses direction dependent coordinate stretching functions, Cartesian PML Laplace operators do not have the same property. To overcome this difficulty, we use the spectral structure of a Cartesian PML Laplace operator investigated in [29] and develop the same stability analysis for Cartesian PML Helmholtz equation.

Solutions to spherical PML Helmholtz equations have a series representation resembling (1.4) in terms of Hankel functions, which is a main ingredient for establishing a one-to-one correspondence between resonance values and eigenvalues of infinite spherical PML problems. However, solutions to Cartesian PML problems do not have a series representation. In this analysis, alternatively we derive an integral representation of solutions to Cartesian PML Helmholtz equations by using Green's theorem and the fundamental solution to the Cartesian Helmholtz equation. The integral representation will be used to find a connection between resonance values and eigenvalues of infinite Cartesian PML problems.

As mentioned in [27], a convergence analysis of approximate resonance values of PML methods needs to be done in a non-standard way unlike classical perturbation theory, e.g., [26]. Indeed, in classical perturbation theory, it can be shown that eigenvalue convergence is a result of norm convergence of approximate operators. In our case, inverse operators of truncated PML operators are compact but those for infinite PML operators are not, which implies that truncated PML operators can not converge to infinite PML operators. Thus, our analysis of eigenvalue convergence is developed based on the property of eigenfunctions, that is exponential decay of eigenfunctions.

The remainder of this paper is organized as follows. In Section 2, we reformulate model problems by applying a Cartesian PML. Section 3 provides a fundamental solution to the Cartesian PML Helmholtz equation and its exponential decay. Integral representations of solutions to the Helmholtz equation satisfying an outgoing radiation condition and the Cartesian PML Helmholtz equation are given in Section 3. We use the integral representations to derive a one-to-one correspondence between resonance values in a region of interest and eigenvalues of the reformulated problems in Section 4. Section 5 verifies inf-sup conditions of Cartesian PML problems on both infinite domains and truncated domains. A convergence analysis for eigenvalues of the truncated Cartesian PML Helmholtz equation is given in Section 6. Numerical experiments in Section 7 illustrate a behavior of eigenvalues obtained by Cartesian PML methods.

2. Cartesian PML reformulation

From here on, we will give the detail only of the acoustic model (1.1) for simple presentation. In order to define a Cartesian PML, we shall use a sequence of strictly increasing square domains $\Omega_0 \subset \Omega_1 \subset \Omega_2 \subset \Omega_\delta$, where $\Omega_j = (-a_j, a_j)^2$ for $j = 0, 1, 2$ and $\Omega_\delta = (-\delta, \delta)^2$. We assume that $\Omega \subset \Omega_0$. Also, Γ_j denotes the boundary of Ω_j for $j = 0, 1, 2$ and δ. A Cartesian PML can be introduced in terms of a formal complex coordinate shift in Cartesian coordinates via an even function $\tilde{\sigma} \in C^2(\mathbb{R})$ satisfying

$$\begin{aligned} &\tilde{\sigma}(t) = 0 \text{ for } |t| \le a_1, \\ &\tilde{\sigma}(t): \text{ increasing } \text{ for } a_1 < t < a_2, \\ &\tilde{\sigma}(t) = \sigma_0 \text{ for } |t| \ge a_2. \end{aligned} \tag{2.1}$$

Here σ_0 is a positive constant that represents a PML strength. The smoothness of $\tilde{\sigma}$ is required for results of a spectral structure of the Cartesian PML Laplace operator in [29] but this restriction does not cause any problem in numerical computations. A Cartesian PML is defined by the coordinate stretching $(\tilde{x}_1, \tilde{x}_2)$ for $(x_1, x_2) \in \mathbb{R}^2$, where

$$\tilde{x}(t) \equiv t(1 + i\tilde{\sigma}(t)) \text{ for } t \in \mathbb{R} \;\text{ and }\; \tilde{x}_j \equiv \tilde{x}(x_j) \text{ for } j = 1, 2.$$

The following functions and constants will be used throughout the paper.

$$\begin{aligned} \sigma(t) &\equiv (t\tilde{\sigma}(t))' \text{ for } t \in \mathbb{R}, \\ d(t) &\equiv (\tilde{x}(t))' = 1 + i\sigma(t) \text{ for } t \in \mathbb{R}, \\ d_0 &\equiv 1 + i\sigma_0, \end{aligned}$$

where $'$ represents the derivative with respect to t. We note that the coordinate stretching function can be written in the equivalent form used elsewhere

$$\tilde{x}(x) = x + i \int_0^x \sigma(t)\, \mathrm{dt}.$$

We see here that the coordinate stretching takes real variables $(x_1, x_2) \in \mathbb{R}^2$ to complex variables $(\tilde{x}_1, \tilde{x}_2) = (\tilde{x}(x_1), \tilde{x}(x_2)) \in \mathbb{C}^2$. Specifically, the imaginary part $x_j\tilde{\sigma}(x_j)$ of each component becomes nonzero for $|x_j| > a_1$ and it plays a crucial role for PML solutions to decay exponentially in the perfectly matched layer.

Remark 2.1. For an application where a scatterer Ω has a large aspect ratio, it is more efficient in terms of computational costs to choose a sequence of rectangles fitting Ω and use direction dependent coordinate stretchings. For example, we use the functions $\tilde{\sigma}_k$ for $k = 1, 2$ satisfying

$$
\begin{aligned}
&\tilde{\sigma}_k(t) = 0 \text{ for } b_{k,1} \le t \le a_{k,1}, \\
&\tilde{\sigma}_k(t) : \text{ increasing } \text{ for } a_{k,1} < t < a_{k,2}, \\
&\tilde{\sigma}_k(t) : \text{ decreasing } \text{ for } b_{k,2} < t < b_{k,1}, \\
&\tilde{\sigma}_k(t) = \sigma_{k,0}^{\text{right}} \text{ for } t \ge a_{k,2}, \\
&\tilde{\sigma}_k(t) = \sigma_{k,0}^{\text{left}} \text{ for } t \le b_{k,2},
\end{aligned}
$$

for some $b_{k,2} < b_{k,1} < 0 < a_{k,1} < a_{k,2}$ and $\sigma_{k,0}^{\text{left}}, \sigma_{k,0}^{\text{right}} > 0$. However since the analysis for the simple case can be carried out in general settings without essential changes, the analysis in this presentation is restricted to the simple case.

Now, the Cartesian PML Laplace operator is defined by

$$
\widetilde{\Delta} \equiv \frac{1}{d(x_1)} \frac{\partial}{\partial x_1} \left(\frac{1}{d(x_1)} \frac{\partial}{\partial x_1} \right) + \frac{1}{d(x_2)} \frac{\partial}{\partial x_2} \left(\frac{1}{d(x_2)} \frac{\partial}{\partial x_2} \right) = \frac{1}{J} \nabla \cdot H \nabla,
$$

where

$$
\begin{aligned}
J(x) &\equiv d(x_1) d(x_2), \\
H(x) &\equiv \begin{bmatrix} d(x_2)/d(x_1) & 0 \\ 0 & d(x_1)/d(x_2) \end{bmatrix}.
\end{aligned}
$$

As a weak form of $-\widetilde{\Delta}$, we introduce an 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 $u \in H_0^1(\bar{\Omega}^c)$ by $\widetilde{L} u = f$, where $f \in H^{-1}(\bar{\Omega}^c)$ is given by

$$
< f, \bar{J} \phi >= A(u, \phi) \text{ for all } \phi \in H_0^1(\bar{\Omega}^c). \tag{2.2}
$$

Here $< \cdot, \cdot >$ is the duality pairing and

$$
A(u, v) = \int_{\bar{\Omega}^c} H \nabla u \cdot \nabla \bar{v} \, \mathrm{d}x \text{ for all } u, v \in H_0^1(\bar{\Omega}^c). \tag{2.3}
$$

By the definition of $\tilde{\sigma}$, we observe that $0 \leq \sigma(t) \leq \sigma_M$ for some σ_M and it then follows that $d(t)$ is in the set $\{z \in \mathbb{C} \ : \ \mathrm{Re}(z) = 1, 0 \leq \mathrm{Im}(z) \leq \sigma_M\}$. Setting $\theta_M = \arg(1 + i\sigma_M)$, it is easy to show that

$$\mathrm{Re}(d(t)/d(s)) \geq c_0 \ \text{ and } \ \mathrm{Re}(e^{-i\theta_M} d(t)d(s)) \geq c_0 \ \text{ for all } t, s \in \mathbb{R}$$

for $c_0 = 1/(1+\sigma_M^2)$. This implies that for $z_0 = -e^{-i\theta_M}$ and for all $u \in H^1(\bar{\Omega}^c)$

$$\begin{aligned} c_0 \|\nabla u\|^2_{L^2(\bar{\Omega}^c)} &\leq |A(u,u)|, \\ c_0 \|u\|^2_{H^1(\bar{\Omega}^c)} &\leq |A(u,u) - z_0 (Ju, u)_{\bar{\Omega}^c}| \,, \end{aligned} \tag{2.4}$$

where $(\cdot, \cdot)_D$ denotes the L^2-inner product on the domain D.

The spectrum (the complement of the resolvent set of $\widetilde{L}$) of the operator $\widetilde{L}$, especially essential spectrum, is investigated in [29]. Among other notions of essential spectrum (see e.g., [12]), the definition of essential spectrum of $\widetilde{L}$ is given by the set of points in the spectrum excluding those in discrete eigenvalues of $\widetilde{L}$ (isolated points of spectrum with finite algebraic multiplicity). The main result (Theorem 4.6) of [29] is that if we denote

$$E = \{z \in \mathbb{C} \ : \ \arg(z) = -2\arg(1 + i\sigma_0)\}, \tag{2.5}$$

then the essential spectrum of $\widetilde{L}$ is contained in E. Discrete eigenvalues of $\widetilde{L}$ are k^2 such that there exists a nonzero solution $u \in H^1_0(\bar{\Omega}^c)$ satisfying

$$(\widetilde{L} - k^2 I)u = 0. \tag{2.6}$$

The following sections will reveal that resonance values in the sector S between E and the positive real axis,

$$S \equiv \{z \in \mathbb{C} \ : \ -2\arg(1 + i\sigma_0) < \arg(z) < 0\}. \tag{2.7}$$

are in fact eigenvalues of $\widetilde{L}$, from which we observe that the resonance problem becomes an eigenvalue problem (2.6) of the operator $\widetilde{L}$ on $H^{-1}(\bar{\Omega}^c)$.

3. Fundamental solution to the Cartesian PML Helmholtz equation

In this section, we find the fundamental solution to the Cartesian PML Helmholtz equation in terms of the fundamental solution to the Helmholtz equation and a certain *complexified distance* $\tilde{r}(x,y)$. Also, we study exponential decay of the fundamental solution for $k^2 \in S$ with $\mathrm{Im}(k) < 0$. Let $\Phi(r) = \frac{i}{4}H_0^1(kr)$ be the fundamental solution to the Helmholtz equation. With $\tilde{y}_j = \tilde{x}(y_j)$ for $y = (y_1, y_2) \in \mathbb{R}^2$, the complexified distance $\tilde{r}(x,y)$ between $\tilde{x} = (\tilde{x}_1, \tilde{x}_2)$ and $\tilde{y} = (\tilde{y}_1, \tilde{y}_2)$ is defined by

$$\tilde{r}(x,y) \equiv \sqrt{(\tilde{x}_1 - \tilde{y}_1)^2 + (\tilde{x}_2 - \tilde{y}_2)^2}. \tag{3.1}$$

Here we take the negative real axis for the branch cut of the square root. The well-definedness and an important property of the complexified distance $\tilde{r}$ are given in the following lemma.

Lemma 3.1. *(See [28, Lemma 3.1, Lemma 3.3]) Let $x, y \in \mathbb{R}^2$ with $x \neq y$. Then, there exists a small constant $\varepsilon > 0$ such that*

$$0 \leq \arg((\tilde{x}_1 - \tilde{y}_1)^2 + (\tilde{x}_2 - \tilde{y}_2)^2) < \pi - \varepsilon. \tag{3.2}$$

Therefore, $\tilde{r}(x,y)$ is well-defined. In addition, there exists positive constants C_{r1} and C_{r2} such that

$$C_{r1}|x - y| \leq |\tilde{r}(x,y)| \leq C_{r2}|x - y|.$$

Then the fundamental solution to the Cartesian Helmholtz equation is defined by

$$\widetilde{\Phi}(x,y) = J(y)\Phi(\tilde{r}(x,y))$$

and its proof is given in [28].

Theorem 3.2. *(See [28, Theorem 3.4, Remark 3.8, Lemma 3.9]) The function $\widetilde{\Phi}(x,y)$ satisfies*

$$u(x) = -\int_{\mathbb{R}^2} ((\widetilde{\Delta}_y + k^2 I)u(y))\widetilde{\Phi}(x,y)\,\mathrm{d}y \tag{3.3}$$

for all $u \in H^2(\mathbb{R}^2)$. In addition, for $x \neq y$, $\Phi(\tilde{r}(x,y))$ solves the Cartesian PML Helmholtz equation,

$$(\widetilde{\Delta}_y + k^2 I)\Phi(\tilde{r}(x,y)) = 0.$$

To study exponential decay of $\widetilde{\Phi}$ for $k^2 \in S$ with $\mathrm{Im}(k) < 0$, we need one more property of $\tilde{r}(x,y)$ regarding convergence of $\arg(\tilde{r})$ as $\|x - y\|_\infty \to \infty$.

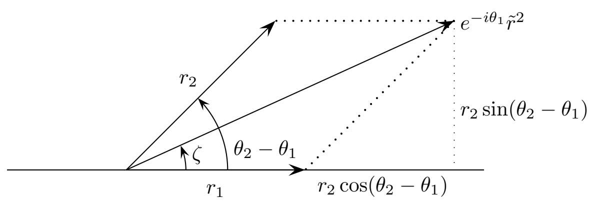


Figure 1: Geometry of three complex numbers after rotating by $-\theta_1$

Lemma 3.3. *For any $\varepsilon > 0$ there exists a positive constant M_{arg} such that if $\|x-y\|_\infty > M_{arg}$, then*

$$|\arg(\tilde{r}) - \arg(d_0)| < \varepsilon. \tag{3.4}$$

Proof. We first claim that for $\varepsilon > 0$ there exists a positive constant M_1 such that if $t - s > M_1$ for $t, s \in \mathbb{R}$, then

$$|\arg(\tilde{x}(t) - \tilde{x}(s)) - \arg(d_0)| < \varepsilon. \tag{3.5}$$

To prove the convergence of $\arg(\tilde{x}(t) - \tilde{x}(s))$, we note that

$$\arg(\tilde{x}(t) - \tilde{x}(s)) = \tan^{-1}\left(\frac{t\tilde{\sigma}(t) - s\tilde{\sigma}(s)}{t-s}\right) \text{ and } \arg(d_0) = \tan^{-1}(\sigma_0).$$

By the continuity of $\tan^{-1}$, it suffices to show that for $\varepsilon > 0$ there exists a positive constant M_2 such that if $t - s > M_2$, then

$$\left|\frac{t\tilde{\sigma}(t) - s\tilde{\sigma}(s)}{t-s} - \sigma_0\right| < \varepsilon. \tag{3.6}$$

For t and s with $|t|, |s| \geq a_2$, clearly we have (3.6) with the vanishing left hand side. Therefore, we need to consider only the case that $|s| < a_2$ and t is a positive large number. For such s, since $|s|$ and $|s\tilde{\sigma}(s)|$ are bounded, we can choose $M_2 > 0$ such that the inequality (3.6) holds for $t > M_2 - a_2$. Then (3.6) holds if $t - s > M_2$.

Now, let $\theta_j = \arg((\tilde{x}_j - \tilde{y}_j)^2)$ and $r_j = |(\tilde{x}_j - \tilde{y}_j)^2|$ for $j = 1, 2$. Suppose that $|x_2 - y_2| < M_1$. A simple computation (see Figure 1) shows

$$\arg(\tilde{r}^2) = \zeta + \theta_1,$$

where

$$\zeta = \tan^{-1}\left(\frac{r_2\sin(\theta_2 - \theta_1)}{r_1 + r_2\cos(\theta_2 - \theta_1)}\right).$$

Here ζ is an angle between $-\pi/2$ and $\pi/2$ for large r_1. Since r_2 is bounded for $|x_2 - y_2| < M_1$, we observe that $\zeta \to 0$ and $\theta_1 \to \arg(d_0^2)$ as $|x_1 - y_1|$ approaches infinity. Thus, we can choose a large $M_{arg} > M_1$ such that

$$|\arg(\tilde{r}^2) - \arg(d_0^2)| < 2\varepsilon \tag{3.7}$$

for $|x_1 - y_1| > M_{arg}$ and $|x_2 - y_2| < M_1$. By the same argument as above, the inequality (3.7) holds for the other case, $|x_2 - y_2| > M_{arg}$ and $|x_1 - y_1| < M_1$.

Finally, to prove (3.4), suppose that $\|x - y\|_\infty > M_{arg}$. If both $|x_j - y_j|$ for $j = 1, 2$ are larger than M_1, then from (3.5) it follows that $|\theta_j - \arg(d_0^2)| < 2\varepsilon$ for $j = 1, 2$. Since the set $\{z \in \mathbb{C} \ : \ |\arg(z) - \arg(d_0^2)| < 2\varepsilon\}$ is closed under addition, (3.4) immediately follows. On the other hand, if one of $|x_j - y_j|$ is less than M_1, then since the other is larger than M_{arg}, the inequality (3.7) holds and so does (3.4), which completes the proof.

□

For exponential decay of $\widetilde{\Phi}$, the following asymptotic behavior of Hankel function of the first kind of the zeroth order at infinity is required. For large $|z|$, one can show that

$$\begin{aligned} H_0^1(z) &= \left(\frac{2}{\pi z}\right)^{1/2} e^{i(z-\pi/4)} \left(1 + O\left(\frac{1}{z}\right)\right) \quad \text{for} \quad |\arg(z)| \le \pi - \varepsilon, \\ H_0^{1\prime}(z) &= \left(\frac{2}{\pi z}\right)^{1/2} e^{i(z+\pi/4)} \left(1 + O\left(\frac{1}{z}\right)\right) \quad \text{for} \quad |\arg(z)| \le \pi - \varepsilon \end{aligned} \tag{3.8}$$

with arbitrary small $\varepsilon > 0$ [1, 32].

Lemma 3.4. *Assume that $k^2 \in S$ and $\mathrm{Im}(k) < 0$. Then there exist positive constants α, C and M_f such that*

$$|\Phi(\tilde{r})| \ \ \textit{and} \ \ |\partial\Phi(\tilde{r})/\partial y_j| < Ce^{-\alpha|x-y|} \ \ \textit{for } j = 1, 2, \tag{3.9}$$

for $\|x - y\|_\infty > M_f$, where $\tilde{r} = \tilde{r}(x, y)$.

Proof. By (3.8) and Lemma 3.1, there exists a constant M_d such that

$$|H_0^1(k\tilde{r})| \ \text{ and } \ |H_0^{1\prime}(k\tilde{r})| \le Ce^{-\mathrm{Im}(k\tilde{r})} \text{ for } \|x - y\|_\infty > M_d. \tag{3.10}$$

For $\varepsilon = \frac{1}{2}\arg(kd_0) > 0$, by Lemma 3.3 there exists a positive M_{arg} such that if $\|x - y\|_\infty > M_{arg}$, then

$$\arg(d_0) - \varepsilon < \arg(\tilde{r}) < \arg(d_0) + \varepsilon$$

so that

$$\varepsilon = \tfrac{1}{2}\arg(kd_0) < \arg(k\tilde{r}) < \tfrac{3}{2}\arg(kd_0) < \tfrac{3\pi}{4}$$

As a consequence, using Lemma 3.1 for $\|x-y\|_\infty > M_{arg}$

$$e^{-\mathrm{Im}(k\tilde{r})} = e^{-|k\tilde{r}|\sin(\arg(k\tilde{r}))} \leq e^{-\alpha|x-y|} \tag{3.11}$$

for a positive $\alpha = C_{r1}|k|\min\{\sin(\varepsilon), \sin(\frac{3\pi}{4})\}$. Finally, applying (3.11) to (3.10) shows that

$$|H_0^1(k\tilde{r})| \ \text{ and } \ |H_0^{1\prime}(k\tilde{r})| \leq Ce^{-\alpha|x-y|} \tag{3.12}$$

for $\|x-y\|_\infty > M_f \equiv \max\{M_d, M_{arg}\}$. In addition, by Lemma 3.1 and (3.12)

$$\left|\frac{\partial H_0^1(\tilde{r})}{\partial y_j}\right| = \left|H_0^{1\prime}(\tilde{r})\frac{(\tilde{x}_j - \tilde{y}_j)(-d(y_j))}{\tilde{r}}\right| \leq Ce^{-\alpha|x-y|} \tag{3.13}$$

for $\|x-y\|_\infty > M_f$, which completes the proof. □

4. Integral representation

In this section, we study integral representations of solutions to the Helmholtz equation satisfying the outgoing radiation condition and the Cartesian PML Helmholtz equation.

4.1. Helmholtz equation with the outgoing radiation condition

Theorem 4.1. *Assume that k is a complex number with $|\arg(k)| < \pi$. Let $u \in H^1_{loc}(\bar{\Omega}^c)$ be a solution to the Helmholtz equation $\Delta u + k^2 u = 0$ on $\bar{\Omega}^c$. Then u satisfies the outgoing radiation condition* (1.4) *if and only if u has the integral representation*

$$u(x) = \int_{\Gamma_0}\left[u(y)\frac{\partial\Phi(|x-y|)}{\partial n_y} - \Phi(|x-y|)\frac{\partial u(y)}{\partial n_y}\right]\mathrm{d}S_y \tag{4.1}$$

for $x \in \bar{\Omega}_0^c$. Here n_y is the outward unit normal vector on the boundary of Ω_0.

To find a series expression of functions defined by (4.1), the Graf's addition theorem is needed (see e.g., [1, 33]).

Theorem 4.2. *Assume that k is a complex number with $|\arg(k)| < \pi$. Let $\theta_x = \arg(x)$ and $\theta_y = \arg(y)$. Then the following holds:*

$$H_0^1(k|x-y|) = \sum_{n=-\infty}^{\infty} J_n(k|y|) H_n^1(k|x|) e^{in(\theta_x - \theta_y)}. \tag{4.2}$$

for $x, y \in \mathbb{R}^2$ with $|y| < |x|$. The series and its first order derivatives as a function of y converge uniformly on compact subsets of $|y| < |x|$.

Proof of Theorem 4.1. For large $r > r_0$ (given in (1.4)), let B_r be a ball centered at the origin and of radius r, which contains Ω_0. If u is a solution to the Helmholtz equation, then by the Green's identity it satisfies

$$\begin{aligned} u(x) = &\int_{\Gamma_0} \left[u(y) \frac{\partial \Phi(|x-y|)}{\partial n_y} - \Phi(|x-y|) \frac{\partial u(y)}{\partial n_y} \right] \mathrm{d}S_y \\ &- \int_{|y|=r} \left[u(y) \frac{\partial \Phi(|x-y|)}{\partial n_y} - \Phi(|x-y|) \frac{\partial u(y)}{\partial n_y} \right] \mathrm{d}S_y \end{aligned} \tag{4.3}$$

for $x \in \bar{\Omega}_0^c \cap B_r$, where n_y is the outward unit normal vector on the boundaries of Ω_0 and B_r. To obtain the integral formula (4.1), it suffices to show that the outer boundary integral vanishes.

To do this, we first show that for $|x| < r$

$$\int_{|y|=r} \left[H_n^1(kr) \frac{\partial H_0^1(k|x-y|)}{\partial n_y} - H_0^1(k|x-y|) \frac{\partial H_n^1(kr)}{\partial n_y} \right] e^{in\theta_y} \, \mathrm{d}S_y = 0. \tag{4.4}$$

Then uniform convergence of (1.4) on any compact subset outside of B_{r_0} proves that the integral on $|y| = r$ vanishes. To prove (4.4), let $F(k)$ denote the integral of the left hand side of (4.4). $F(k)$ is clearly an analytic function defined on the region of $|\arg(k)| < \pi$. Since $H_n^1(k|x|)e^{in\theta_x}$ for real $k > 0$ is a solution to the Helmholtz equation satisfying the Sommerfeld radiation condition (1.5), it follows that $F(k) = 0$ for real $k > 0$. Therefore the analyticity of $F(k)$ shows (4.4) for any k with $|\arg k| < \pi$.

Conversely, assume that u has the integral expression (4.1). Then, by the definition of the fundamental solution to the Helmholtz equation, we have

$$u(x) = \frac{i}{4} \int_{\Gamma_0} \left[u(y) \frac{\partial H_0^1(k|x-y|)}{\partial n_y} - H_0^1(k|x-y|) \frac{\partial u(y)}{\partial n_y} \right] \mathrm{d}S_y \tag{4.5}$$

for $x \in \bar{\Omega}_0^c$. Now, we choose $r_0 > 0$ such that $\bar{\Omega}_0$ is strictly contained in B_{r_0}. For $|x| > r_0$ and $y \in \Gamma_0$, substituting (4.2) in (4.5) leads to

$$u(x) = \sum_{n=-\infty}^{\infty} a_n H_n^1(k|x|)e^{in\theta_x} \text{ for } |x| > r_0,$$

where

$$a_n = \frac{i}{4}\int_{\Gamma_0} \left[u(y)\left(kJ_n'(k|y|)\frac{\partial |y|}{\partial n_y} - in\frac{\partial \theta_y}{\partial n_y}\right) - J_n(k|y|)\frac{\partial u(y)}{\partial n_y}\right] e^{-in\theta_y}\, \mathrm{d}S_y,$$

which completes the proof.

□

4.2. Cartesian PML Helmholtz equation

Using exponential decay of the fundamental solution to the Cartesian PML Helmholtz equation, the analogous integral representation for solutions to the Cartesian PML Helmholtz equation is obtained.

Lemma 4.3. *Assume that $k^2 \in S$ and $\mathrm{Im}(k) < 0$. If $u \in H^1(\bar{\Omega}^c)$ satisfies $\widetilde{\Delta}u + k^2u = 0$ in $\bar{\Omega}^c$, then u has the following integral representation: for $x \in \bar{\Omega}_0^c$,*

$$u(x) = \int_{\Gamma_0} \left[u(y)\frac{\partial \Phi(\tilde{r})}{\partial n_y} - \Phi(\tilde{r})\frac{\partial u(y)}{\partial n_y}\right] \mathrm{d}S_y, \tag{4.6}$$

where n_y is the outward unit normal vector on the boundary of Ω_0.

Proof. For fixed $x \in \bar{\Omega}_0^c$, we denote $\Omega_R = (-R, R)^2$ for $R > |x|$ and let Γ_R be the boundary of Ω_R. We can choose an open set $\tilde{D}$ strictly containing $D = \Omega_R \setminus \bar{\Omega}_0$. Since u is in $H^2_{loc}(\bar{\Omega}^c)$ by an interior regularity (see e.g., [16, Theorem 8.8]), we observe that $u \in H^2(\tilde{D})$. By using a cutoff function χ which is one on D and zero outside $\tilde{D}$, we can find an extension $\tilde{u} = \chi u$ in $H^2(\mathbb{R}^2)$ of u defined on D. Now, noting that H is the identity matrix and $J = 1$ on Ω_0, from Theorem 3.2 and integration by parts, it follows that

$$\begin{aligned}
u(x) &= -\int_{\mathbb{R}^2} ((\widetilde{\Delta}_y + k^2I)\tilde{u}(y))\widetilde{\Phi}(x,y)\,\mathrm{d}y \\
&= -\int_{\Omega_0} ((\Delta_y + k^2I)\tilde{u}(y))\widetilde{\Phi}(x,y)\,\mathrm{d}y - \int_{\mathbb{R}^2\setminus\bar{\Omega}_R} ((\widetilde{\Delta}_y + k^2I)\tilde{u}(y))\widetilde{\Phi}(x,y)\,\mathrm{d}y \\
&= \int_{\Gamma_0} \left[u(y)\frac{\partial \Phi(\tilde{r})}{\partial n_y} - \Phi(\tilde{r})\frac{\partial u(y)}{\partial n_y}\right] \mathrm{d}S_y - \int_{\Gamma_R} \left[u(y)n_y^t H\nabla\Phi(\tilde{r}) - \Phi(\tilde{r})n_y^t H\nabla u(y)\right] \mathrm{d}S_y,
\end{aligned}$$

where n_y is the outward unit normal vector on the boundaries of Ω_0 and Ω_R.

Therefore, it suffices to show that the integral on Γ_R vanishes. Since $d(y_j)$ and $1/d(y_j)$ are bounded for $j = 1, 2$, a Schwarz inequality leads to

$$\begin{aligned} I &\equiv \left| \int_{\Gamma_R} \left[u(y) n_y^t H \nabla \Phi(\tilde{r}) - \Phi(\tilde{r}) n_y^t H \nabla u(y) \right] \, \mathrm{d}S_y \right| \\ &\leq C(\|u\|_{L^2(\Gamma_R)} \|\nabla \Phi(\tilde{r})\|_{L^2(\Gamma_R)} + \|\Phi(\tilde{r})\|_{L^2(\Gamma_R)} \|\nabla u\|_{L^2(\Gamma_R)}) \end{aligned}$$

If $R > M_f + \|x\|_\infty$, then $\|x - y\|_\infty > M_f$ for $y \in \Gamma_R$ and hence Lemma 3.4 shows that

$$\int_{\Gamma_R} |\Phi(\tilde{r})|^2 \, \mathrm{d}S_y \leq \int_{\Gamma_R} C e^{-2\alpha R + 2\alpha |x|} \, \mathrm{d}S_y \leq C e^{2\alpha |x|} R e^{-2\alpha R}. \tag{4.7}$$

By the same argument as above, we have

$$\int_{\Gamma_R} \left| \frac{\partial \Phi(\tilde{r})}{\partial y_j} \right|^2 \, \mathrm{d}S_y \leq C e^{2\alpha |x|} R e^{-2\alpha R}. \tag{4.8}$$

It is obvious that by a trace theorem

$$\|u\|_{L^2(\Gamma_R)} \leq C \|u\|_{H^1(\bar{\Omega}^c)}. \tag{4.9}$$

For estimating ∇u in $L^2(\Gamma_R)$, let S_γ be a γ-neighborhood of Γ_R for a small $\gamma > 0$ independent of R. Since u solves the equation

$$A(u, \phi) - k^2 (Ju, \phi)_{S_{2\gamma}} = 0 \text{ for all } \phi \in H_0^1(S_{2\gamma}),$$

by an interior regularity (see e.g., [16, Theorem 8.8]) we have

$$\|u\|_{H^2(S_\gamma)} \leq C \|u\|_{L^2(S_{2\gamma})}, \tag{4.10}$$

where the constant C depends only on k, γ and σ. Then a trace inequality and (4.10) shows that

$$\|\nabla u\|_{L^2(\Gamma_R)} \leq C \|u\|_{H^2(S_\gamma)} \leq C \|u\|_{L^2(\bar{\Omega}^c)}. \tag{4.11}$$

Combining (4.7), (4.8), (4.9) and (4.11) yields that

$$I \leq C e^{\alpha |x|} \sqrt{R} e^{-\alpha R} \|u\|_{H^1(\bar{\Omega}^c)},$$

which means that I can be arbitrarily small as R approaches infinity. Consequently, it can be concluded that $I = 0$, which completes the proof.

□

Conversely, we have the following lemma.

Lemma 4.4. *Assume that* $k^2 \in S$ *with* $\mathrm{Im}(k) < 0$. *If* $u \in H^1(\Omega_0) \cap H^2_{loc}(\bar{\Omega}^c)$ *is defined by* (4.6) *for* $x \in \bar{\Omega}_0^c$, *then* u *satisfies* $\widetilde{\Delta} u + k^2 u = 0$ *in* $\bar{\Omega}_0^c$ *and* $u \in H^1(\bar{\Omega}^c)$.

Proof. By Theorem 3.2, we know that $\Phi(\tilde{r})$ solves the Cartesian PML Helmholtz equation with respect to $x \in \bar{\Omega}_0^c$ for $y \in \Gamma_0$, which immediately implies that

$$\widetilde{\Delta} u + k^2 u = 0 \text{ in } \bar{\Omega}_0^c. \tag{4.12}$$

To verify that u is in $H^1(\bar{\Omega}^c)$, we first show that u decays exponentially. By a Schwarz inequality

$$\begin{aligned} |u(x)| &= \left| \int_{\Gamma_0} \left[u(y) \frac{\partial \Phi(\tilde{r})}{\partial n_y} - \Phi(\tilde{r}) \frac{\partial u(y)}{\partial n_y} \right] \mathrm{d}S_y \right| \\ &\leq \|u\|_{L^2(\Gamma_0)} \|\nabla \Phi(\tilde{r})\|_{L^2(\Gamma_0)} + \|\Phi(\tilde{r})\|_{L^2(\Gamma_0)} \|\nabla u\|_{L^2(\Gamma_0)}. \end{aligned}$$

If $\|x\|_\infty > M_f + a_0$, then $\|x - y\|_\infty > M_f$ for $y \in \Gamma_0$ and hence Lemma 3.4 leads to

$$\int_{\Gamma_0} |\Phi(\tilde{r})|^2 \, \mathrm{d}S_y \leq \int_{\Gamma_0} C e^{-2\alpha|x| + 2\alpha|y|} \, \mathrm{d}S_y \leq C e^{-2\alpha|x|}.$$

By Lemma 3.4 the analogous inequality for $\nabla \Phi(\tilde{r})$ holds and therefore

$$|u(x)| \leq C e^{-\alpha|x|} (\|u\|_{L^2(\Gamma_0)} + \|\nabla u\|_{L^2(\Gamma_0)}) \quad \text{for } \|x\|_\infty > M_f + a_0,$$

which implies that u is in $L^2(\bar{\Omega}^c)$.

Now, to prove that ∇u is in $L^2(\bar{\Omega}^c)$, let Ω_R and Γ_R be defined as in the proof of Lemma 4.3. Since u solves (4.12), by the argument similar to (2.4) and integration by parts we observe that

$$\begin{aligned} c_0 \|\nabla u\|^2_{L^2(\Omega_R \setminus \bar{\Omega}_0)} &\leq |(H \nabla u, \nabla u)_{\Omega_R \setminus \bar{\Omega}_0}| \\ &= \left| \int_{\Gamma_R} (n^t H \nabla u) \bar{u} \, \mathrm{d}S - \int_{\Gamma_0} \frac{\partial u}{\partial n} \bar{u} \, \mathrm{d}S + k^2 \int_{\Omega_R \setminus \bar{\Omega}_0} J |u|^2 \, \mathrm{d}x \right|, \end{aligned}$$

where n is the outward normal vector on the boundaries of Ω_R and Ω_0. Since $u \in H^2_{loc}(\bar{\Omega}^c)$ and $u \in L^2(\bar{\Omega}^c)$, (4.11) holds and hence Schwarz inequalities yield the boundedness of the right hand side independent of R, which implies that ∇u is in $L^2(\bar{\Omega}_0^c)$. Finally, from the fact that $u \in H^1(\Omega_0)$, it follows that ∇u is in $L^2(\bar{\Omega}^c)$, which completes the proof.

□

5. Correspondence between infinite Cartesian PML eigenvalues and resonances

In this section, we establish a one-to-one correspondence between eigenvalues of the infinite Cartesian PML Helmholtz equation and resonance values in the sector S defined in (2.7). The analysis proceeds by using the integral representations studied in the previous section. We use them to construct an eigenfunction of the Cartesian PML Helmholtz equation from a resonance function of the Helmholtz equation and vice versa.

We define for $z \in \mathbb{C}$

$$A_z(\cdot,\cdot) \equiv A(\cdot,\cdot) - zB(\cdot,\cdot),$$

where

$$B(u,v) \equiv (Ju,v)_{\bar{\Omega}^c} \text{ for all } u,v \in L^2(\bar{\Omega}^c).$$

We first review important results of a Cartesian PML approximation to acoustic scattering problems in [28].

Lemma 5.1. *(See [28, Lemma 4.6, Lemma 5.2]) Let z be a positive real number. An inf-sup condition for the Cartesian PML Helmholtz equation on the unbounded domain holds: for $u \in H^1(\bar{\Omega}^c)$,*

$$\|u\|_{H^1(\bar{\Omega}^c)} \le C \sup_{\phi \in H_0^1(\bar{\Omega}^c)} \frac{|A_z(u,\phi)|}{\|\phi\|_{H^1(\bar{\Omega}^c)}}.$$

In addition, there exists $\delta_0 > 0$ such that for $\delta > \delta_0$ an inf-sup condition for the Cartesian PML Helmholtz equation on the truncated domain holds: for $u \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$

$$\|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \le C \sup_{\phi \in H_0^1(\Omega_\delta \setminus \bar{\Omega})} \frac{|A_z(u,\phi)|}{\|\phi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}},$$

where C is independent of δ.

Remark 5.2. Since $A_z(\cdot,\cdot)$ is symmetric (but not Hermitian), that is $A_z(u,\phi) = A_z(\bar{\phi},\bar{u})$, the inf-sup conditions imply inf-sup conditions for the adjoint problems.

Lemma 5.1 and Remark 5.2 imply that for $z = 1$ there exists a solution operator $T : H_0^1(\bar{\Omega}^c) \to H_0^1(\bar{\Omega}^c)$ defined by $Tf = u$ for $f \in H_0^1(\bar{\Omega}^c)$, where u is the unique solution in $H_0^1(\bar{\Omega}^c)$ to the problem

$$A_1(u, \phi) = B(f, \phi) \text{ for all } \phi \in H_0^1(\bar{\Omega}^c). \tag{5.1}$$

Now, the main result about the connection between Cartesian PML eigenvalues and resonance values is given in the following theorem.

Theorem 5.3. *There is a one-to-one correspondence between eigenvalues λ of T and resonance values k of* (1.1) *with $k^2 \in S$ and* $\mathrm{Im}(k) < 0$ *by the formula $\lambda = 1/(k^2 - 1)$.*

Proof. First, suppose that k is a resonance value of (1.1) satisfying $k^2 \in S$ with $\mathrm{Im}(k) < 0$ and u is a resonance function associated with the resonance value k. Now, let $\tilde{u}$ be defined by

$$\tilde{u}(x) = \begin{cases} u(x) & \text{for } x \in \bar{\Omega}_0 \setminus \bar{\Omega}, \\ \displaystyle\int_{\Gamma_0} \left[u(y) \frac{\partial \Phi(\tilde{r})}{\partial n_y} - \Phi(\tilde{r}) \frac{\partial u(y)}{\partial n_y} \right] \mathrm{d}S_y & \text{for } x \in \bar{\Omega}_0^c. \end{cases}$$

We note that the transition around Γ_0 is smooth since on $\Omega_1 \setminus \bar{\Omega}$ (a neighborhood of Γ_0)

$$\begin{aligned} \tilde{u}(x) &= \int_{\Gamma_0} \left[u(y) \frac{\partial \Phi(\tilde{r})}{\partial n_y} - \Phi(\tilde{r}) \frac{\partial u(y)}{\partial n_y} \right] \mathrm{d}S_y \\ &= \int_{\Gamma_0} \left[u(y) \frac{\partial \Phi(|x-y|)}{\partial n_y} - \Phi(|x-y|) \frac{\partial u(y)}{\partial n_y} \right] \mathrm{d}S_y = u(x), \end{aligned} \tag{5.2}$$

where we used Lemma 4.1 in the last equality. Then $\tilde{u}$ is an eigenfunction in $H_0^1(\bar{\Omega}^c)$ of T associated with the eigenvalue λ. Indeed, by Lemma 4.4 $\tilde{u}$ is in $H_0^1(\bar{\Omega}^c)$ and satisfies $\widetilde{\Delta}\tilde{u} + k^2\tilde{u} = 0$ in $\bar{\Omega}^c$. A simple computation shows that

$$A_1(\tilde{u}, \phi) = (k^2 - 1) B(\tilde{u}, \phi) = (k^2 - 1) A_1(T\tilde{u}, \phi) \text{ for all } \phi \in H_0^1(\bar{\Omega}^c), \tag{5.3}$$

which implies that $\tilde{u}$ is an eigenfunction of T associated with $\lambda = 1/(k^2 - 1)$.

Conversely, if $\tilde{u}$ is an eigenfunction of T associated with an eigenvalue λ, then the same computation as (5.3) shows that $\tilde{u}$ solves the equation $\widetilde{\Delta}\tilde{u} + k^2\tilde{u} = 0$ in $\bar{\Omega}^c$. It follows that u defined by

$$u(x) = \begin{cases} \tilde{u}(x) & \text{for } x \in \bar{\Omega}_0 \setminus \bar{\Omega}, \\ \displaystyle\int_{\Gamma_0} \left[\tilde{u}(y) \frac{\partial \Phi(|x-y|)}{\partial n_y} - \Phi(|x-y|) \frac{\partial \tilde{u}(y)}{\partial n_y} \right] \mathrm{d}S_y & \text{for } x \in \bar{\Omega}_0^c. \end{cases}$$

satisfies $\Delta u + k^2 u = 0$ (the transition on Γ_0 is smooth by the argument similar to that used in (5.2)) and the outgoing radiation condition by Lemma 4.1. Thus, u is a resonance function associated with the resonance value $k = \sqrt{1 + 1/\lambda}$. $\square$

6. Inf-sup conditions

We recall that $\widetilde{L}$ is the weakly defined Cartesian PML Laplace operator defined in $H^{-1}(\bar{\Omega}^c)$ with domain $H^1_0(\bar{\Omega}^c)$. Now, $\rho(\widetilde{L})$ denotes the resolvent set of $\widetilde{L}$. In this section, we study inf-sup conditions of $A_z(\cdot, \cdot)$ with $z \in \rho(\widetilde{L})$ on three different domains as depicted in Figure 2.

It is clear that $(\widetilde{L} - zI)^{-1}$ for $z \in \rho(\widetilde{L})$ is bounded in $H^{-1}(\bar{\Omega}^c)$. However, for the analysis of eigenvalue convergence a stability of solutions in $H^1_0(\bar{\Omega}^c)$ is required. Noting that $\widetilde{L}$ is defined in terms of the sesquilinear form $A_z(\cdot, \cdot)$ as in (2.2), in Lemma 6.1 we first verify an inf-sup condition associated with $A_z(\cdot, \cdot)$ with $z \in \rho(\widetilde{L})$ on the infinite domain (see Figure 2(a)), which provides the stability of solutions in $H^1_0(\bar{\Omega}^c)$. Next, an inf-sup condition on the square domain Ω_δ (see Figure 2(b)) for large δ is introduced in Lemma 6.3, which will be used to establish an inf-sup condition of the truncated PML operator. Finally, we investigate an inf-sup condition on the truncated domain $\Omega_\delta \setminus \bar{\Omega}$ for large δ (see Figure 2(c)) in Theorem 6.4. Once the inf-sup condition with $z \in \rho(\widetilde{L})$ is established for large δ, it can be shown that z still belongs to the resolvent set of the truncated PML operator. The inf-sup condition on the truncated domain is a main ingredient for showing that Cartesian PML does not produce spurious resonance values, which will be studied in the next section.

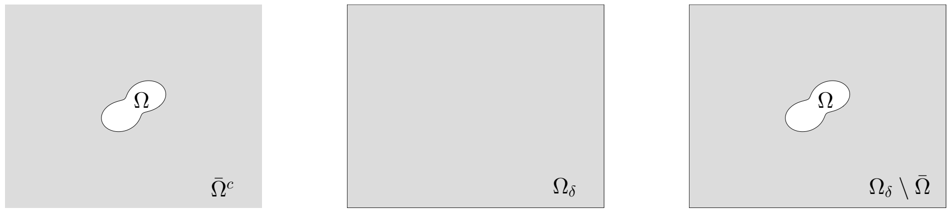
We start with an inf-sup condition for the infinite Cartesian PML Laplace operator.

Lemma 6.1. *For any compact subset $K \subset \rho(\widetilde{L}) \cap S$, there exists a positive constant C independent of $z \in K$ such that for all $u \in H^1_0(\bar{\Omega}^c)$*

$$\|u\|_{H^1(\bar{\Omega}^c)} \le C \sup_{\phi \in H^1_0(\bar{\Omega}^c)} \frac{|A_z(u, \phi)|}{\|\phi\|_{H^1(\bar{\Omega}^c)}}.$$

Proof. Since the resolvent operator $(\widetilde{L} - zI)^{-1}$ is a holomorphic function on $\rho(\widetilde{L})$, there exists $C > 0$ such that

$$\|(\widetilde{L} - zI)^{-1}\|_{H^{-1}(\bar{\Omega}^c)} \le C \text{ for all } z \in K. \tag{6.1}$$



(a) infinite domain $\bar{\Omega}^c$ (b) square domain Ω_δ (c) truncated domain $\Omega_\delta \setminus \bar{\Omega}$

Figure 2: Three domains on which inf-sup conditions of $A_z(\cdot,\cdot)$ for $z \in \rho(\widetilde{L})$ are verified

For $z_0 = -e^{-i\theta_M}$ given above (2.4), we note that $A_{z_0}(\cdot,\cdot)$ is coercive on $H_0^1(\bar{\Omega}^c)$ by (2.4). Let u be in $C_0^\infty(\bar{\Omega}^c)$ and $v \in H_0^1(\bar{\Omega}^c)$ be the unique solution to

$$A_{z_0}(v,\phi) = A_z(u,\phi) \text{ for all } \phi \in H_0^1(\bar{\Omega}^c). \tag{6.2}$$

Now, if we show that

$$\|u - v\|_{H^1(\bar{\Omega}^c)} \le C\|v\|_{H^1(\bar{\Omega}^c)}, \tag{6.3}$$

then

$$\begin{aligned}\|u\|_{H^1(\bar{\Omega}^c)} &\le \|v\|_{H^1(\bar{\Omega}^c)} + \|u-v\|_{H^1(\bar{\Omega}^c)} \le C\|v\|_{H^1(\bar{\Omega}^c)} \\ &\le C \sup_{\phi\in H_0^1(\bar{\Omega}^c)} \frac{|A_{z_0}(v,\phi)|}{\|\phi\|_{H^1(\bar{\Omega}^c)}} = C \sup_{\phi\in H_0^1(\bar{\Omega}^c)} \frac{|A_z(u,\phi)|}{\|\phi\|_{H^1(\bar{\Omega}^c)}},\end{aligned}$$

which completes the proof.

To prove (6.3), a simple computation from (6.2) leads to

$$A_z(u-v,\phi) = (z-z_0)B(v,\phi) \text{ for all } \phi \in H_0^1(\bar{\Omega}^c),$$

equivalently, $(\widetilde{L} - zI)(u-v) = (z-z_0)v$. Since $z - z_0$ is bounded for $z \in K$, it follows from (6.1) that

$$\|u - v\|_{H^{-1}(\bar{\Omega}^c)} \le C\|v\|_{H^{-1}(\bar{\Omega}^c)}. \tag{6.4}$$

Again, from (6.2) we see that

$$A_{z_0}(u-v,\phi) = (z-z_0)B(u,\phi) \text{ for all } \phi \in H_0^1(\bar{\Omega}^c).$$

Thus, by the coercivity (2.4) and (6.4)

$$\|u-v\|_{H^1(\bar{\Omega}^c)} \le C\|u\|_{H^{-1}(\bar{\Omega}^c)} \le C(\|v\|_{H^{-1}(\bar{\Omega}^c)} + \|u-v\|_{H^{-1}(\bar{\Omega}^c)}) \le C\|v\|_{H^{-1}(\bar{\Omega}^c)},$$

which leads to (6.3) and completes the proof. □

The inf-sup condition above and Remark 5.2 imply that for $z \in \rho(\widetilde{L})$ and $g \in H^{1/2}(\Gamma)$, the adjoint exterior problem

$$\begin{aligned} A_z(\theta, \phi) = 0 \text{ for all } \theta \in H_0^1(\bar{\Omega}^c), \\ \phi = g \text{ on } \Gamma \end{aligned} \tag{6.5}$$

is well-posed. Furthermore, solutions to (6.5) decay exponentially in the sense of the following lemma. Exponential decay of solutions to the exterior problem is an essential part in proving the inf-sup condition for the truncated Cartesian PML Helmholtz equation. The proof will be provided in the appendix.

Lemma 6.2. *For any compact subset $K \subset \rho(\widetilde{L}) \cap S$, there exist positive constants α, C and M independent of $z \in K$ and $\delta \geq M$ such that solutions ϕ to the problem* (6.5) *satisfy*

$$\|\phi\|_{H^{1/2}(\Gamma_\delta)} \leq Ce^{-\alpha\delta}\|\phi\|_{H^1(\bar{\Omega}^c)} \tag{6.6}$$

for $\delta \geq M$.

Next, we examine an inf-sup condition for the Cartesian PML Helmholtz equation on the square domain Ω_δ. We define $-\widetilde{\Delta}$ by an operator defined in $L^2(\mathbb{R}^2)$ with domain $H^2(\mathbb{R}^2)$ and $-\widetilde{\Delta}_\delta$ by a realization of $-\widetilde{\Delta}$ on $L^2(\Omega_\delta)$ with domain $H^2(\Omega_\delta) \cap H_0^1(\Omega_\delta)$. The spectrum of $-\widetilde{\Delta}$ is studied in [29, Theorem 4.5] and is the set E defined as in (2.5). Therefore $\rho(\widetilde{L}) \cap S$ is contained in $\rho(-\widetilde{\Delta})$.

Lemma 6.3. *For any compact subset $K \subset \rho(\widetilde{L}) \cap S$, there exist positive constants δ_0 and C independent of $z \in K$ such that*

$$\|u\|_{H^1(\Omega_\delta)} \leq C \sup_{\phi \in H_0^1(\Omega_\delta)} \frac{|A_z(u, \phi)|}{\|\phi\|_{H^1(\Omega_\delta)}} \tag{6.7}$$

for all $\delta > \delta_0$ and $u \in H_0^1(\Omega_\delta)$. Here C does not depend on $\delta > \delta_0$.

Proof. In the proof of [29, Theorem 4.8], we observe that for each $z \in \rho(-\widetilde{\Delta})$ there exist positive constants δ_z and C_z such that

$$\|(-\widetilde{\Delta}_\delta - zI)^{-1}\|_{L^2(\Omega_\delta)} \leq C_z \quad \text{for} \quad \delta > \delta_z. \tag{6.8}$$

Once we prove that the constants δ_z and C_z in (6.8) can be taken independently of $z \in K$, the same arguments used in the proof of Lemma 6.1 can be carried out with $H_0^1(\bar{\Omega}^c)$ and $H^{-1}(\bar{\Omega}^c)$ replaced by $H^2(\Omega_\delta) \cap H_0^1(\Omega_\delta)$ and $L^2(\Omega_\delta)$, respectively.

We first show that for each $z \in K$ there exists an open ball $B(z, \varepsilon)$ centered at z of radius ε such that $B(z, \varepsilon) \subset \rho(-\widetilde{\Delta}_\delta)$ for all $\delta > \delta_z$. To the contrary, suppose that there exist sequences $\delta_j > \delta_z$ and $\lambda_j \in \mathbb{C}$ such that λ_j is an eigenvalue of $-\widetilde{\Delta}_{\delta_j}$ and

$$\delta_j \to \infty \quad \text{and} \quad \lambda_j \to z \quad \text{as } j \to \infty.$$

Then there exists a sequence of $u_j \in H^2(\Omega_{\delta_j}) \cap H_0^1(\Omega_{\delta_j})$ satisfying

$$\|u_j\|_{L^2(\Omega_{\delta_j})} = 1 \ \text{ and } \ (-\widetilde{\Delta}_{\delta_j} - \lambda_j I) u_j = 0.$$

We are led to

$$\|(-\widetilde{\Delta}_{\delta_j} - zI) u_j\|_{L^2(\Omega_{\delta_j})} = \|(\lambda_j - z) u_j\|_{L^2(\Omega_{\delta_j})} \to 0 \text{ as } j \to \infty,$$

which contradicts to the uniform boundedness (6.8) for $\delta > \delta_z$.

Now, by compactness of K, there are finitely many open coverings $B(z_j, \varepsilon_j)$ of K and constants C_{z_j}, $\delta_{z_j} > 0$ for $j = 1, \ldots, N$ such that for all $\delta > \delta_{z_j}$

$$B(z_j, \varepsilon_j) \subset \rho(-\widetilde{\Delta}_\delta), \qquad \|(-\widetilde{\Delta}_\delta - z_j I)^{-1}\|_{L^2(\Omega_\delta)} \leq C_{z_j}$$

and $\varepsilon_j < 1/(2C_{z_j})$. Let $\delta_0 = \max\{\delta_{z_j}\}_{j=1}^N$ and $C = \max\{C_{z_j}\}_{j=1}^N$. For $z \in B(z_j, \varepsilon_j)$ and $\delta > \delta_0$, estimating the Neumann series for $(-\widetilde{\Delta}_\delta - zI)^{-1} = (-\widetilde{\Delta}_\delta - z_j I)^{-1}(I - (z - z_j)(-\widetilde{\Delta}_\delta - z_j I)^{-1})^{-1}$ yields

$$\|(-\widetilde{\Delta}_\delta - zI)^{-1}\|_{L^2(\Omega_\delta)} \leq \sum_{n=0}^{\infty} |z - z_j|^n \|(-\widetilde{\Delta}_\delta - z_j I)^{-1}\|_{L^2(\Omega_\delta)}^{n+1} \leq 2C_{z_j} \leq 2C,$$

which shows uniform boundedness of resolvent operators independent of $z \in K$ and $\delta > \delta_0$.

□

An inf-sup condition for the truncated Cartesian PML Helmholtz equation on $\Omega_\delta \setminus \bar{\Omega}$ is given in the next theorem.

Theorem 6.4. *For any compact subset $K \subset \rho(\widetilde{L}) \cap S$, there exist positive constants $\tilde{\delta}_0$ and C independent of $z \in K$ such that*

$$\|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \leq C \sup_{\phi \in H_0^1(\Omega_\delta \setminus \bar{\Omega})} \frac{|A_z(u, \phi)|}{\|\phi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}}, \tag{6.9}$$

for all $\delta > \tilde{\delta}_0$ and $u \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$. Here C does not depend on $\delta > \tilde{\delta}_0$.

Proof. We will construct a function $\phi \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$ which solves the adjoint problem

$$A_z(\theta, \phi) = (\theta, u)_{H^1(\Omega_\delta \setminus \bar{\Omega})} \text{ for all } \theta \in H_0^1(\Omega_\delta \setminus \bar{\Omega}) \tag{6.10}$$

and satisfies

$$\|\phi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \leq C \|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}.$$

Here $(\cdot, \cdot)_{H^1(D)}$ is the H^1-inner product on a domain D. Then the theorem follows since

$$\|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} = \frac{A_z(u, \phi)}{\|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}} \leq C \frac{|A_z(u, \phi)|}{\|\phi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}}.$$

To find such ϕ, we start with the unique solution $\tilde{\phi} \in H^1(\bar{\Omega}^c)$ to the exterior problem

$$A_z(\theta, \tilde{\phi}) = (\theta, \tilde{u})_{H^1(\bar{\Omega}^c)} \text{ for all } \theta \in H_0^1(\bar{\Omega}^c)$$

by Lemma 6.1 and Remark 5.2, where $\tilde{u}$ is the zero extension of u to the outside of Ω_δ. Also, by stability $\tilde{\phi}$ satisfies

$$\|\tilde{\phi}\|_{H^1(\bar{\Omega}^c)} \leq C \|u\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}.$$

Now, if we can construct another function $\tilde{\psi} \in H^1(\Omega_\delta \setminus \bar{\Omega})$ such that

$$\begin{gathered} A_z(\theta, \tilde{\psi}) = 0 \text{ for all } \theta \in H_0^1(\Omega_\delta \setminus \bar{\Omega}), \\ \tilde{\psi} = 0 \text{ on } \Gamma \text{ and } \tilde{\psi} = \tilde{\phi} \text{ on } \Gamma_\delta, \\ \|\tilde{\psi}\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \leq C \|\tilde{\phi}\|_{H^1(\bar{\Omega}^c)}, \end{gathered} \tag{6.11}$$

then $\tilde{\phi} - \tilde{\psi}$ on $\Omega_\delta \setminus \bar{\Omega}$ is the desired function ϕ.

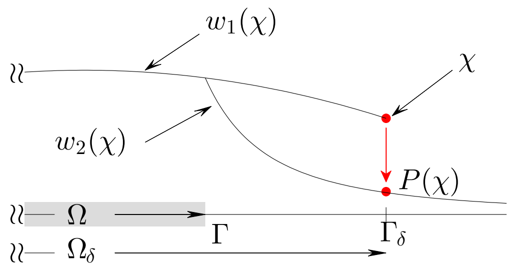


Figure 3: Geometric interpretation of the operator $P : H^{1/2}(\Gamma_\delta) \to H^{1/2}(\Gamma_\delta)$

For the construction of $\tilde{\psi}$, we define an operator $P : H^{1/2}(\Gamma_\delta) \to H^{1/2}(\Gamma_\delta)$ given by solving the following two problems: for a given $\chi \in H^{1/2}(\Gamma_\delta)$ we define $w_1 = w_1(\chi) \in H^1(\Omega_\delta)$ solving

$$\begin{aligned} A_z(\theta, w_1) = 0 \text{ for all } \theta \in H_0^1(\Omega_\delta), \\ w_1 = \chi \text{ on } \Gamma_\delta, \end{aligned} \tag{6.12}$$

and $w_2 = w_2(\chi) \in H^1(\bar{\Omega}^c)$ solving

$$\begin{aligned} A_z(\theta, w_2) = 0 \quad \text{for all } \theta \in H_0^1(\bar{\Omega}^c), \\ w_2 = w_1 \text{ on } \Gamma. \end{aligned} \tag{6.13}$$

Then $P(\chi)$ is defined by the trace of w_2 on Γ_δ (see Figure 3). Here by Lemma 6.1, Lemma 6.3 and Remark 5.2, w_1 and w_2 are well-defined and they satisfy

$$\begin{aligned} \|w_1\|_{H^1(\Omega_\delta)} \leq C\|\chi\|_{H^{1/2}(\Gamma_\delta)}, \\ \|w_2\|_{H^1(\bar{\Omega}^c)} \leq C\|w_1\|_{H^{1/2}(\Gamma)}. \end{aligned} \tag{6.14}$$

Furthermore, for δ large enough, $\|P\|_{H^{1/2}(\Gamma_\delta)} < \gamma < 1$ for a positive constant γ. Indeed, by Lemma 6.2, a trace theorem and (6.14),

$$\|P(\chi)\|_{H^{1/2}(\Gamma_\delta)} \leq Ce^{-\alpha\delta}\|w_2\|_{H^1(\bar{\Omega}^c)} \leq Ce^{-\alpha\delta}\|w_1\|_{H^1(\Omega_\delta)} \leq Ce^{-\alpha\delta}\|\chi\|_{H^{1/2}(\Gamma_\delta)}.$$

We choose $\tilde{\delta}_0$ large enough so that $\gamma = Ce^{-\alpha\delta} < 1$ for all $\delta > \tilde{\delta}_0$. Thus, $\mathcal{P} = \sum_{j=0}^{\infty} P^j$ is well-defined.

Finally, for $\chi = \mathcal{P}(\tilde{\phi})$ where $\tilde{\phi}$ is the trace of $\tilde{\phi}$ on Γ_δ by abuse of notation, we can find $\tilde{\psi} = w_1(\chi) - w_2(\chi)$ by solving (6.12) and (6.13). Then $\tilde{\psi}$ satisfies all conditions in (6.11) because

$$\tilde{\psi} = \chi - P(\chi) = (1-P)\sum_{j=0}^{\infty} P^j \tilde{\phi} = \tilde{\phi} \quad \text{on } \Gamma_\delta,$$

$$\|\tilde{\psi}\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \leq C(\|w_1\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} + \|w_2\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}) \leq C\|\tilde{\phi}\|_{H^1(\Omega_\delta \setminus \bar{\Omega})}$$

by (6.14) and a trace theorem. We note here that all constants C involved in the analysis are independent of $z \in K$ and $\delta > \tilde{\delta}_0$. □

7. Eigenvalue convergence

In this section, we study convergence of eigenvalues of the truncated Cartesian PML problem. Opposed to the solution operator T for the infinite Cartesian PML problem defined in Section 5, we define a solution operator $T_\delta : H_0^1(\bar{\Omega}^c) \to H_0^1(\Omega_\delta \setminus \bar{\Omega}) \subset H_0^1(\bar{\Omega}^c)$ for the truncated Cartesian PML problem: for $f \in H_0^1(\bar{\Omega}^c)$, $T_\delta(f) = u \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$ is the unique solution to

$$A_1(u, \phi) = B(f, \phi) \text{ for all } \phi \in H_0^1(\Omega_\delta \setminus \bar{\Omega}). \tag{7.1}$$

Clearly, T_δ is well-defined by Lemma 5.1 and Remark 5.2.

Now, the aim of this section is to present the main results:

- the PML technique is free of spurious resonances (in Theorem 7.1) and
- eigenvalues of T_δ converge to those of T (in Theorem 7.3)

as computational domains increase. Our analysis is based on the ideas used in [27].

The first result is that any compact subset of the resolvent set $\rho(T)$ of T of the infinite Cartesian PML problem (which is mapped into a compact subset in the sector S via the relation studied in Theorem 5.3) is still contained in the resolvent set $\rho(T_\delta)$ of T_δ of the truncated Cartesian PML problem provided δ is large enough, which leads to that the Cartesian PML technique is free of spurious eigenvalues for large δ.

Theorem 7.1. *Let U be a subset of $\rho(T)$ which is an image of a compact subset $K \subset \rho(\widetilde{L}) \cap S$ by the mapping $\lambda = 1/(k^2 - 1)$ defined in Theorem 5.3. Then there exists $\tilde{\delta}_0 > 0$ such that $U \subset \rho(T_\delta)$ for $\delta > \tilde{\delta}_0$.*

Proof. It suffices to show that there exists $\tilde{\delta}_0 > 0$ such that for $\delta > \tilde{\delta}_0$, $\lambda \in U$ and $w \in H_0^1(\bar{\Omega}^c)$, the problem $(T_\delta - \lambda I)v = w$ has a unique solution $v \in H_0^1(\bar{\Omega}^c)$ satisfying

$$\|v\|_{H^1(\bar{\Omega}^c)} \leq C\|w\|_{H^1(\bar{\Omega}^c)}. \tag{7.2}$$

By the fact that $T_\delta(v) = 0$ in $\bar{\Omega}_\delta^c$ and the definition of T_δ, the solution v needs to be a function satisfying $v = -\frac{1}{\lambda}w$ in $\bar{\Omega}_\delta^c$ and

$$\begin{aligned} B(v,\phi) - \lambda A_1(v,\phi) = A_1(w,\phi) \text{ for all } \phi \in H_0^1(\Omega_\delta \setminus \bar{\Omega}), \\ v = 0 \text{ on } \Gamma, \quad v = -\tfrac{1}{\lambda}w \text{ on } \Gamma_\delta. \end{aligned} \tag{7.3}$$

Noting that $A_{k^2}(\cdot,\cdot) = A_1(\cdot,\cdot) - 1/\lambda B(\cdot,\cdot)$ and $1/\lambda$ for $\lambda \in U$ is bounded, Theorem 6.4 shows that there exists $\tilde{\delta}_0 > 0$ such that for $u \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$

$$\begin{aligned} \|u\|_{H^1(\Omega_\delta\setminus\bar{\Omega})} &\leq C \sup_{\phi\in H_0^1(\Omega_\delta\setminus\bar{\Omega})} \frac{|A_{k^2}(u,\phi)|}{\|\phi\|_{H^1(\Omega_\delta\setminus\bar{\Omega})}} \\ &\leq C \sup_{\phi\in H_0^1(\Omega_\delta\setminus\bar{\Omega})} \frac{|B(u,\phi) - \lambda A_1(u,\phi)|}{\|\phi\|_{H^1(\Omega_\delta\setminus\bar{\Omega})}} \end{aligned}$$

holds uniformly for $\delta > \tilde{\delta}_0$ and $\lambda \in U$. It then follows that the problem (7.3) has a unique solution $v_1 \in H^1(\Omega_\delta \setminus \bar{\Omega})$ such that

$$\|v_1\|_{H^1(\Omega_\delta\setminus\bar{\Omega})} \leq C\|w\|_{H^1(\Omega_\delta\setminus\bar{\Omega})}.$$

Now, we define v by v_1 in $\Omega_\delta \setminus \bar{\Omega}$ and by $-\frac{1}{\lambda}w$ in $\bar{\Omega}_\delta^c$. Since v has the same trace from the both sides of Γ_δ, clearly v is in $H_0^1(\bar{\Omega}^c)$ and satisfies (7.2), which completes the proof.

□

Let λ be an isolated eigenvalue of T, whose image under the map $\lambda \mapsto \sqrt{1 + 1/\lambda} \equiv k(\lambda)$ satisfies $k^2 \in \rho(\widetilde{L}) \cap S$ and let Υ_ε denote a circle centered at λ and of radius $\varepsilon > 0$. Since λ is an isolated eigenvalue of T, we can choose ε small enough so that Υ_ε is contained in $\rho(T)$ and excludes all other eigenvalues except λ inside it. Let V be the generalized eigenspace spanned by generalized eigenfunctions that are associated with the eigenvalue λ.

By Theorem 7.1, it is clear that Υ_ε is contained in $\rho(T_\delta)$ for δ large enough. Let V_δ be the generalized eigenspace spanned by generalized eigenfunctions associated with the eigenvalues of T_δ inside Υ_ε. Then, V and V_δ are identified as the ranges of the Riesz projections

$$P_{\Upsilon_\varepsilon}(u) \equiv \frac{1}{2\pi i}\int_{\Upsilon_\varepsilon} (T - zI)^{-1} u \,\mathrm{d}z,$$
$$P^\delta_{\Upsilon_\varepsilon}(u) \equiv \frac{1}{2\pi i}\int_{\Upsilon_\varepsilon} (T_\delta - zI)^{-1} u \,\mathrm{d}z,$$

respectively.

As T_δ is compact, there are only finitely many eigenvalues λ_i^δ for $i = 1, \dots, k$ of T_δ inside Υ_ε. Furthermore, noting the Jordan form of T_δ in the finite dimensional space V_δ, it has a basis of the form $\psi_{i,j}$, $i = 1, \dots, k$, $j = 1, \dots, m(i)$, which satisfy

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

Although *a priori* a bound on the dimension of V_δ is not known when δ varies, we can consider subspaces $\widetilde{V}_\delta$ of dimension at most $\dim(V) + 1$. Specifically, we can choose a subspace $\widetilde{V}_\delta$ spanned by $\{\psi_{i,j}\}$ for $i = 1, \dots, k$, $j = 1, \dots, \tilde{m}(i)$ with $\tilde{m} = \sum_i \tilde{m}(i) \leq \dim(V) + 1$. It is important to note that the space $\widetilde{V}_\delta$ is invariant under T_δ and $P^\delta_{\Upsilon_\varepsilon}$.

Exponential decay of generalized eigenfunctions of T and T_δ is provided in the following lemma and its proof will be given in the appendix.

Lemma 7.2. *Let V and $\widetilde{V}_\delta$ be defined as above.*

1. *There exist positive constants α, C and M such that for $\psi \in V$*

$$|\psi(x)| \leq C e^{-\alpha|x|} \|\psi\|_{H^1(\bar{\Omega}^c)} \text{ for } |x| > M. \tag{7.4}$$

2. *There exists $\delta_0 > 0$ such that for $\delta > \delta_0$ and $\psi_\delta \in \widetilde{V}_\delta$*

$$|\psi_\delta(x)| \leq C e^{-\alpha|x|} \|\psi_\delta\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \text{ for } |x| > M \tag{7.5}$$

   for positive constant α, C and M independent of δ.

3. *There exists $\delta_0 > 0$ such that for $\delta > \delta_0$ and for ψ in V or $\widetilde{V}_\delta$ (as a zero extension to $\bar{\Omega}_\delta^c$)*

$$\|(T - T_\delta)\psi\|_{H^1(\bar{\Omega}^c)} \leq C e^{-\alpha\delta} \|\psi\|_{H^1(\bar{\Omega}^c)}. \tag{7.6}$$

   for positive constant α and C independent of δ.

Now, we are in the position to give the main theorem for eigenvalue convergence of the truncated Cartesian PML Helmholtz equation. To this end, we will show that the dimension of the space V coincides with that of the space V_δ for δ large enough. It is equivalent to say that the same number of eigenvalues counting algebraic multiplicities of T and T_δ are inside the small circle Υ_ε centered at λ of radius ε provided that δ is large enough, i.e., if $\dim(V) = n$ is the multiplicity of the isolated eigenvalue λ of T, then for any small ε, there exists $\delta_1 > 0$ and the eigenvalues of λ_i^δ of T_δ for $j = 1, 2, \ldots, n$ counting their multiplicities such that $|\lambda_i^\delta - \lambda| < \varepsilon$ for all $\delta > \delta_1$.

Theorem 7.3. *Let $\lambda, \Upsilon_\varepsilon$, V and V_δ be defined as above. For any sufficiently small ε, there exists $\delta_1 > 0$ such that*

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

for $\delta > \delta_1$. That is, there are the same number of eigenvalues of T_δ counting algebraic multiplicities inside Υ_ε as the multiplicity of the isolated eigenvalue λ of T for $\delta > \delta_1$.

Proof. Let $R_z(T)$ and $R_z(T_\delta)$ be the resolvent operators of T and T_δ for $\delta > \tilde{\delta}_0$ in Theorem 7.1,

$$R_z(T) = (T - zI)^{-1} \quad \text{and} \quad R_z(T_\delta) = (T_\delta - zI)^{-1}.$$

Since they are holomorphic on the compact set Υ_ε, we have that for $z \in \Upsilon_\varepsilon$,

$$\|R_z(T)\|_{H^1(\bar{\Omega}^c)} \leq C \quad \text{and} \quad \|R_z(T_\delta)\|_{H^1(\bar{\Omega}^c)} \leq C \tag{7.7}$$

with C independent of δ, from which it follows that P_{Υ_ε} and $P_{\Upsilon_\varepsilon}^\delta$ are bounded operators in $H_0^1(\bar{\Omega}^c)$.

We first show that $\dim(V) \leq \dim(V_\delta)$. We do this by showing that $P_{\Upsilon_\varepsilon}^\delta$ maps V injectively into V_δ. It suffices to show that for $\psi \in V$

$$\|(I - P_{\Upsilon_\varepsilon}^\delta)\psi\|_{H^1(\bar{\Omega}^c)} \leq c\|\psi\|_{H^1(\bar{\Omega}^c)} \tag{7.8}$$

for a positive constant $c < 1$. That is because (7.8) leads to

$$\|P_{\Upsilon_\varepsilon}^\delta \psi\|_{H^1(\bar{\Omega}^c)} \geq (1 - c)\|\psi\|_{H^1(\bar{\Omega}^c)}.$$

Let ψ be in V. Then we see that since $P_{\Upsilon_\varepsilon}\psi = \psi$,

$$(I - P_{\Upsilon_\varepsilon}^\delta)\psi = (I - P_{\Upsilon_\varepsilon}^\delta)P_{\Upsilon_\varepsilon}\psi = (P_{\Upsilon_\varepsilon} - P_{\Upsilon_\varepsilon}^\delta)\psi.$$

Therefore, a straightforward computation shows that

$$\begin{aligned}\|(I - P^{\delta}_{\Upsilon_\varepsilon})\psi\|_{H^1(\bar{\Omega}^c)} &= \frac{1}{2\pi}\left\|\int_{\Upsilon_\varepsilon} (R_z(T) - R_z(T_\delta))\psi \,\mathrm{d}z\right\|_{H^1(\bar{\Omega}^c)} \\ &= \frac{1}{2\pi}\left\|\int_{\Upsilon_\varepsilon} R_z(T_\delta)(T - T_\delta)R_z(T)\psi \,\mathrm{d}z\right\|_{H^1(\bar{\Omega}^c)} \\ &\leq \frac{1}{2\pi}\int_{\Upsilon_\varepsilon} \|R_z(T_\delta)\|_{H^1(\bar{\Omega}^c)}\|(T - T_\delta)R_z(T)\psi\|_{H^1(\bar{\Omega}^c)} \,\mathrm{d}z \end{aligned} \tag{7.9}$$

Since V is invariant under the action of $R_z(T)$, by Lemma 7.2, there exists δ_0 such that for $\delta > \delta_0$

$$\|(T - T_\delta)R_z(T)\psi\|_{H^1(\bar{\Omega}^c)} \leq Ce^{-\alpha\delta}\|\psi\|_{H^1(\bar{\Omega}^c)}. \tag{7.10}$$

It then follows from (7.7), (7.9) and (7.10) that

$$\|(I - P^{\delta}_{\Upsilon_\varepsilon})\psi\|_{H^1(\bar{\Omega}^c)} \leq Ce^{-\alpha\delta}\|\psi\|_{H^1(\bar{\Omega}^c)}.$$

Thus, we choose $\delta_1 \geq \delta_0$ so that $Ce^{-\alpha\delta_1}$ is less than one, which yields (7.8).

For the opposite inequality, let ψ be in $\widetilde{V}_\delta$ with $\widetilde{V}_\delta$ defined as above. Noting the invariance of $\widetilde{V}_\delta$ under T_δ and $P^{\delta}_{\Upsilon_\varepsilon}$, an argument similar to that used above shows

$$\|(I - P_{\Upsilon_\varepsilon})\psi\|_{H^1(\bar{\Omega}^c)} \leq Ce^{-\alpha\delta}\|\psi\|_{H^1(\bar{\Omega}^c)}.$$

Again, choosing $\delta_1 \geq \delta_0$ so that $Ce^{-\alpha\delta_1} < 1$ 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 $\dim(V)$ for $\delta > \delta_1$, i.e., $\dim(V_\delta) = \dim(V)$. $\square$

8. Numerical experiments

We consider a simple photonic resonance problem (1.2) for TE polarization with G a unit disc. The dielectric constant is defined as

$$\varepsilon = \begin{cases} 4 \text{ on } G, \\ 1 \text{ otherwise.} \end{cases}$$

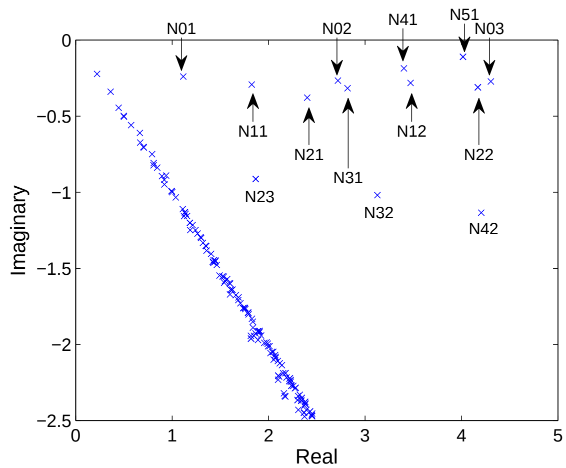


Figure 4: Plot of resonance values computed by Cartesian PML

We find k such that the problem (1.2) has a non-zero solution

$$u(x) = \begin{cases} \displaystyle\sum_{n=-\infty}^{\infty} c_n J_n(2k|x|) e^{in\theta_x} \text{ for } x \in G, \\ \displaystyle\sum_{n=-\infty}^{\infty} d_n H_n^1(k|x|) e^{in\theta_x} \text{ for } x \in \mathbb{R}^2 \setminus \bar{G}, \end{cases}$$

where J_n is Bessel functions of the first kind of order n. It is easy to see that by the transmission conditions on the interface ∂G, resonance values k's are the solution satisfying

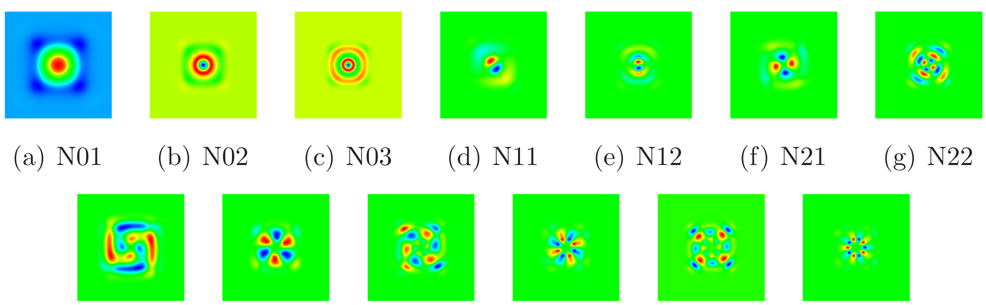
$$J_n'(2k) H_n^1(k) - 2J_n(2k)(H_n^1(k))' = 0 \tag{8.1}$$

for $n \geq 0$.

The computational result obtained by Cartesian PML with the parameters $a_0 = 1, a_1 = 4, \sigma_0 = 1$ on the finite computational domain Ω_δ with $\delta = 5$ is given in Figure 4. As analyzed in [29], the eigenvalues forming the line of slope -1 (determined by $\sigma_0 = 1$) in the figure are those that correspond to essential spectrum of the infinite PML Laplace operator, the set E defined by (2.5). The labeled eigenvalues are those that approximate the exact resonance values in Table 1, which are obtained by solving (8.1) by iteration and displayed with only the four significant digits. In addition, we see that there is no spurious resonance observed in the eigenvalue plot of the truncated

n	Label	Resonance
0	N01	$1.1155 - 0.2396i$
	N02	$2.7167 - 0.2665i$
	N03	$4.2985 - 0.2711i$
1	N11	$1.8238 - 0.2921i$
	N12	$3.4679 - 0.2813i$
2	N21	$2.3981 - 0.3781i$
	N22	$4.1637 - 0.3100i$
	N23	$1.8658 - 0.9125i$
3	N31	$2.8161 - 0.3161i$
	N32	$3.1265 - 1.0190i$
4	N41	$3.3993 - 0.1851i$
	N42	$4.2026 - 1.1329i$
5	N51	$4.0104 - 0.1096i$

Table 1: Exact resonance values with only four significant digits displayed



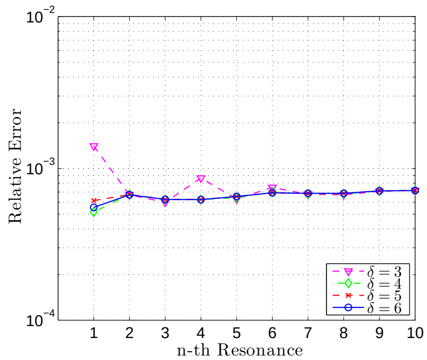
(a) N01 (b) N02 (c) N03 (d) N11 (e) N12 (f) N21 (g) N22

(h) N23 (i) N31 (j) N32 (k) N41 (l) N42 (m) N51

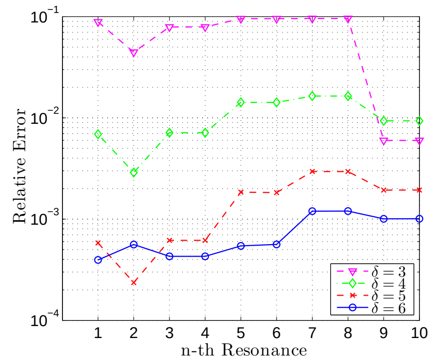
Figure 5: Real parts of the resonance functions

δ	a_0	a_1	σ_0	h	# of DOFs
3	1	2	1	0.01	360,270
4	1	3	1	0.01	641,997
5	1	4	1	0.01	1,002,235
6	1	5	1	0.01	1,442,535

Table 2: PML parameters and the number of DOFs of the discrete problems



(a) Relative errors in the Cartesian PML approximations



(b) Relative errors in Cylindrical PML approximations

Figure 6: Relative errors of the first ten resonance values of smallest magnitude obtained by Cartesian PML and Cylindrical PML

problem, which confirms Theorem 7.1. The localized resonance functions are illustrated in Figure 5.

In order to see convergence of approximate resonance values as δ increases, we take $\delta = 3, 4, 5, 6$ and choose the PML parameters a_0, a_1 and σ_0 as in Table 2

for the both x- and y-directions. In this computation, a bilinear finite element approximation is applied with the mesh size $h = 0.01$ by using the finite element library `deal.ii` [2, 3] and the eigenvalue solver library SLEPc [22]. Here we also compare the performance of Cartesian PML with that of cylindrical PML employing the same PML parameters as above. The relative errors in the first ten approximate resonance values (N01, N02 of multiplicity 1 and N11, N21, N31, N41 of multiplicity 2) are plotted in Figure 6. It is observed that the cylindrical PML approximations are improved when δ increases as expected from the theory in [27]. In case of the Cartesian PML

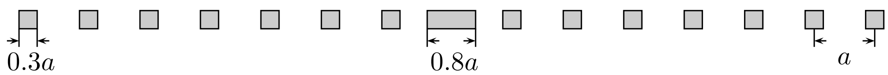


Figure 7: The structure of dielectric materials

h	# of DOFs	PML resonance approximations k	frequency $\omega = \mathrm{Re}(k)/(2\pi)$
1/10	7,421	$1.89769 - 0.00137i$	0.30203
1/20	29,241	$2.02031 - 0.00036i$	0.32154
1/40	116,081	$2.01491 - 0.00018i$	0.32068
1/80	462,561	$2.01358 - 0.00014i$	0.32047
1/160	1,846,721	$2.01325 - 0.00013i$	0.32042

Table 3: PML resonance approximations of the most localized resonance mode

application, it appears that the approximations on an even small domain with $\delta = 3$ or 4 are accurate up to mesh size errors. In particular, the Cartesian PML method only with 360,270 DOFs achieves the approximations with the relative errors less than 0.1 percent while the spherical PML method requires 1,442,535 DOFs to have the similar result. It suggests that overall, Cartesian PML has a better performance than cylindrical PML for this particular example.

The next example is a one-dimensional array of dielectric square materials of length $0.3a$ for a waveguide of TM modes. See the structure in Figure 7. Here a is a lattice constant and is set to be one in this example. A defect is introduced at the center of the array by increasing a width of a dielectric square to $0.8a$. The dielectric constant ε of the squares is set to be 13 in contrast to a unit for that of the free space. We consider a structure composed of seven dielectric materials on each side of the defect.

The infinite periodic case with a defect was investigated in [14] by using the supercell method with the supercell shown in Figure 7. There, the most localized eigenmode was found to have frequency $\omega = 0.3130$. Now, we use the PML method to compute the localized resonance mode. Obviously, as the structure has a large aspect ratio, Cartesian PML has an advantage over cylindrical PML in terms of computational costs (the approximate frequency 0.321 was obtained by using cylindrical PML with the number of DOFs = 221,201 [17]). The PML parameters for the coordinate shift of the x-direction

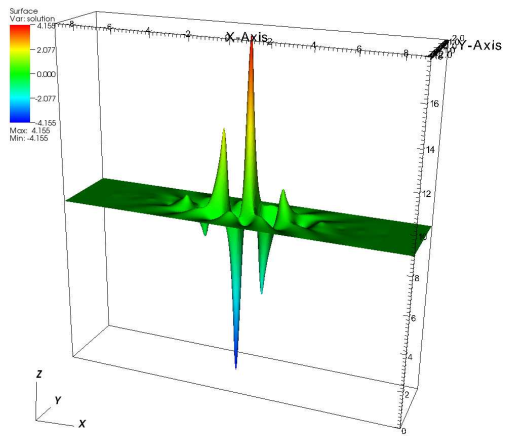


Figure 8: Localized resonance mode

are set as

$$a_1 = 7.15, a_2 = 8, \delta = 9,$$

and those of the y-direction are chosen as

$$a_1 = 0.15, a_2 = 1, \delta = 2$$

with the same $\sigma_0 = 1$. The approximate resonance values, whose mode is highly localized, are reported in Table 3 as a function of the mesh size. Here we observe the difference between the frequency $\omega = 0.3130$ in [14] and the approximate frequency $\omega = 0.3204$ by the Cartesian PML. This difference may be explained in terms of the boundary conditions of two methods. In the PML application, the size of the dielectric structure of the model problem is finite and the system is embedded in the unbounded free space. Thus, the resonance function satisfies the radiation condition at infinity, that is replaced with a perfectly matched layer in the numerical scheme. In contrast, the assumption of the supercell method is that the dielectric structure is infinitely periodic. In the application of the practical supercell method, it is expected that if the size of supercells is large enough, then interaction between neighboring supercells is negligible and hence approximate eigenvalues on a supercell with a periodic boundary condition converge to those of the ideal defected infinitely periodic photonic crystals.

Finally, the localized mode associated with the resonance is shown in Figure 8 and is qualitatively similar to the localized eigenmode of the defected infinite periodic structure in [14].

9. Acknowledgments

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10. Appendix

This appendix is devoted to showing exponential decay of generalized eigenfunctions to the Cartesian PML Helmholtz equation and providing proofs of lemmas given in earlier sections without proof.

First, we shall derive an equation for functions in $\widetilde{V}_\delta$ defined in Section 7. Let λ_i for $i = 1, \ldots, \tilde{m}$ be eigenvalues of T_δ inside Υ_ε after renumbering the eigenvalues λ_i^δ. It is clear that for any nonzero $\psi^\delta \in \widetilde{V}_\delta$,

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

and hence there is a positive integer $n \le \tilde{m}$ such that

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

Starting with $\psi_n^\delta = \psi^\delta$, we define ψ_j^δ recursively by $\psi_j^\delta \equiv (T_\delta - \lambda_{n-j} I)\psi_{j+1}^\delta$ for $j = 0, \cdots, n-1$. Here we note that ψ_1^δ is an eigenfunction of T_δ associated with the eigenvalue λ_n and hence observe that $\psi_0^\delta \equiv 0$. By using the definition of T_δ, we have

$$\widetilde{\Delta}\psi_{j+1}^\delta + (k(\lambda_{n-j}))^2\psi_{j+1}^\delta = -\tfrac{1}{\lambda_{n-j}}(\widetilde{\Delta}\psi_j^\delta + \psi_j^\delta) \text{ in } \Omega_\delta \setminus \bar{\Omega}, \tag{10.1}$$

where $(k(\lambda_{n-j}))^2 = 1 + 1/\lambda_{n-j}$. In particular, ψ_1^δ solves

$$\widetilde{\Delta}\psi_1^\delta + (k(\lambda_n))^2\psi_1^\delta = 0 \text{ in } \Omega_\delta \setminus \bar{\Omega} \tag{10.2}$$

and by an induction argument applied to (10.1), $\psi^\delta = \psi_n^\delta$ satisfies

$$\widetilde{\Delta}\psi^\delta + (k(\lambda_1))^2\,\psi^\delta = \sum_{j=1}^{n-1}\frac{(-1)^{j+1}}{\Pi_{l=1}^{j+1}\lambda_l}\psi_{n-j}^\delta \text{ in } \Omega_\delta \setminus \bar{\Omega}. \tag{10.3}$$

For V, the situation is much simpler since there is only one eigenvalue λ inside Υ_ε. In this case, let m be the algebraic multiplicity of λ. Since $(T-\lambda I)^m\psi = 0$ for any non-zero $\psi \in V$, there exists a positive integer $n \le m$ such that

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

Setting $\psi_n = \psi$ and $\psi_j = (T-\lambda I)\psi_{j+1}$ for $j = 0, \cdots, n-1$, the same computation as above shows that ψ_1 solves

$$\widetilde{\Delta}\psi_1 + (k(\lambda))^2\psi_1 = 0 \text{ in } \bar{\Omega}^c \tag{10.4}$$

and $\psi = \psi_n$ satisfies

$$\widetilde{\Delta}\psi + (k(\lambda))^2\psi = \sum_{j=1}^{n-1} \frac{(-1)^{j+1}}{\lambda^{j+1}}\psi_{n-j} \text{ in } \bar{\Omega}^c. \tag{10.5}$$

Exponential decay of generalized eigenfunctions of T and T_δ which satisfy the equations (10.3) or (10.5), respectively, will be proved inductively based on the following two lemmas.

Lemma 10.1. *Assume that $k^2 \in S$ and $\mathrm{Im}(k) < 0$. Suppose that $u \in H_0^1(\bar{\Omega}^c)$ satisfies*

$$\widetilde{\Delta}u + k^2u = f \ \text{ in } \bar{\Omega}^c \tag{10.6}$$

for $f \in H_0^1(\bar{\Omega}^c)$. If f decays exponentially, i.e., there exist positive constants β and M such that $|f(x)| \le Ce^{-\beta|x|}\|f\|_{H^1(\bar{\Omega}^c)}$ for $|x| > M$, then there exist positive constants α_1, C_1 and $M_1 > M$ such that

$$|u(x)| \le C_1e^{-\alpha_1|x|}\left(\|u\|_{H^1(\bar{\Omega}^c)} + \|f\|_{H^1(\bar{\Omega}^c)}\right) \tag{10.7}$$

and

$$\|u\|_{H^{1/2}(\Gamma_\delta)} \le C_1e^{-\alpha_1\delta}\left(\|u\|_{H^1(\bar{\Omega}^c)} + \|f\|_{H^1(\bar{\Omega}^c)}\right) \tag{10.8}$$

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

Lemma 10.2. *Assume that $k^2 \in S$ and $\mathrm{Im}(k) < 0$. There exists a positive constant $\tilde{\delta}_0$ for which the following holds. For $\delta > \tilde{\delta}_0$, suppose that $u_\delta \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$ satisfies*

$$\widetilde{\Delta}u_\delta + k^2u_\delta = f \ \text{ in } \Omega_\delta \setminus \bar{\Omega}$$

for $f \in H_0^1(\Omega_\delta \setminus \bar{\Omega})$. If f decays exponentially, i.e., there exist positive constants β, C and M such that $|f(x)| \le Ce^{-\beta|x|}\|f\|_{H^1(\Omega_\delta\setminus\bar{\Omega})}$ for $|x| > M$, then there exist positive constants α_1, C_1 and $M_1 > M$ such that

$$|u_\delta(x)| \le C_1 e^{-\alpha_1|x|}\left(\|u_\delta\|_{H^1(\Omega_\delta\setminus\bar{\Omega})} + \|f\|_{H^1(\Omega_\delta\setminus\bar{\Omega})}\right) \tag{10.9}$$

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

Proof of Lemma 10.1. Let M_f be the constant in Lemma 3.4 and let $\tilde{M}_1 = M + \sqrt{2}M_f$. For $|x| > \tilde{M}_1$, B_M and B_R denote the open balls centered at the origin and of radius M and $2|x|$ with the boundaries Γ_M and Γ_R, respectively. By an argument similar to that used in Theorem 4.3, we have that for $|x| > \tilde{M}_1$,

$$u(x) = \int_{\Gamma_M\cup\Gamma_R}\left[\Phi(\tilde{r})n_y^t H\nabla u(y) - u(y)n_y^t H\nabla\Phi(\tilde{r})\right]\mathrm{d}S_y - \int_D f(y)J(y)\Phi(\tilde{r})\,\mathrm{d}y, \tag{10.10}$$

where n_y is the outward unit normal vector on the boundaries of $D = B_R \setminus \bar{B}_M$.

For the integral on the inner boundary Γ_M, we note that $\|x-y\|_\infty > M_f$ for $y \in \Gamma_M$ and $|x| > \tilde{M}_1$. By Lemma 3.4 we are led to

$$\int_{\Gamma_M}|\Phi(\tilde{r})|^2\,\mathrm{d}S_y \le \int_{\Gamma_M} Ce^{-2\alpha|x-y|}\,\mathrm{d}S_y \le \int_{\Gamma_M} Ce^{-2\alpha|x|+2\alpha|y|}\,\mathrm{d}S_y \le Ce^{-2\alpha|x|}.$$

The similar inequality for $\nabla\Phi(\tilde{r})$ holds and hence by a Schwarz inequality and an interior regularity similar to (4.11), we obtain that for $|x| > \tilde{M}_1$

$$\begin{aligned}&\left|\int_{\Gamma_M}\left[\Phi(\tilde{r})n_y^t H\nabla u(y) - u(y)n_y^t H\nabla\Phi(\tilde{r})\right]\mathrm{d}S_y\right|^2 \\ &\qquad \le Ce^{-2\alpha|x|}\left(\|\nabla u\|^2_{L^2(\Gamma_M)} + \|u\|^2_{L^2(\Gamma_M)}\right) \le Ce^{-2\alpha|x|}(\|u\|^2_{H^1(\bar{\Omega}^c)} + \|f\|^2_{H^1(\bar{\Omega}^c)}).\end{aligned}$$

For the integral on the outer boundary Γ_R, we have that $\|x-y\|_\infty > M_f$ for $y \in \Gamma_R$ and $|x| > \tilde{M}_1$. It follows from Lemma 3.4 that

$$\int_{\Gamma_R}|\Phi(\tilde{r})|^2\,\mathrm{d}S_y \le \int_{\Gamma_R} Ce^{-2\alpha|x-y|}\,\mathrm{d}S_y \le \int_{\Gamma_R} Ce^{-2\alpha|x|}\,\mathrm{d}S_y \le C|x|e^{-2\alpha|x|}.$$

Therefore, the same technique used as above shows the analogous inequality bounding the integral on Γ_R and hence we have

$$\begin{aligned}\left| \int_{\Gamma_M \cup \Gamma_R} \left[\Phi(\tilde{r}) n_y^t H \nabla u(y) - u(y) n_y^t H \nabla \Phi(\tilde{r}) \right] \mathrm{d}S_y \right|^2 \\ \leq C(|x|+1) e^{-2\alpha|x|} (\|u\|^2_{H^1(\bar{\Omega}^c)} + \|f\|^2_{H^1(\bar{\Omega}^c)}).\end{aligned} \tag{10.11}$$

For the volume integral in (10.10), we separate the domain D into two subregions according to the distance from x with respect to $\|\cdot\|_\infty$. Let $D_x = \{y \in \mathbb{R}^2 \ : \ \|x-y\|_\infty \leq M_f\}$. For $y \in D_x$, it is obvious that

$$|y| \geq \|y\|_\infty \geq \|x\|_\infty - M_f \geq \tfrac{1}{\sqrt{2}}|x| - M_f.$$

Using boundedness of J and the above inequality,

$$\begin{aligned}\left| \int_{D \cap D_x} f(y) J(y) \Phi(\tilde{r}) \,\mathrm{d}y \right| &\leq C \|f\|_{H^1(\bar{\Omega}^c)} \int_{D \cap D_x} e^{-\beta|y|} |\Phi(\tilde{r})| \,\mathrm{d}y \\ &\leq C \|f\|_{H^1(\bar{\Omega}^c)} \int_{D \cap D_x} e^{-\frac{\beta}{\sqrt{2}}|x|} |\Phi(\tilde{r})| \,\mathrm{d}y \leq C e^{-\frac{\beta}{\sqrt{2}}|x|} \|f\|_{H^1(\bar{\Omega}^c)}.\end{aligned} \tag{10.12}$$

Here in the last inequality, we used the fact that $\Phi(|x-y|)$ has an integrable singularity at $y = x$ and $C_1|x-y| \leq |\tilde{r}|$ in Lemma 3.1 and so the integral of $|\Phi(\tilde{r})|$ on $D \cap D_x$ depends only on M_f.

For the integral on the other subregion, let $\tilde{\alpha} = \min\{\alpha, \frac{1}{\sqrt{2}}\beta\}$. By Lemma 3.4 we are led to

$$\begin{aligned}\left| \int_{D \setminus D_x} f(y) J(y) \Phi(\tilde{r}) \,\mathrm{d}y \right| &\leq C \|f\|_{H^1(\bar{\Omega}^c)} \int_{D \setminus D_x} e^{-\beta|y|} e^{-\alpha|x-y|} \,\mathrm{d}y \\ &\leq C \|f\|_{H^1(\bar{\Omega}^c)} \int_{D \setminus D_x} e^{-\tilde{\alpha}|x|} \,\mathrm{d}y \leq C|x|^2 e^{-\tilde{\alpha}|x|} \|f\|_{H^1(\bar{\Omega}^c)}.\end{aligned} \tag{10.13}$$

Therefore, combining (10.12) and (10.13), the volume integral satisfies

$$\left| \int_D f(y) \Phi(x,y) \,\mathrm{d}y \right| \leq C(|x|^2+1) e^{-\tilde{\alpha}|x|} \|f\|_{H^1(\bar{\Omega}^c)} \tag{10.14}$$

for $|x| > \tilde{M}_1$.

The polynomial growth in (10.11) and (10.14) can be absorbed in generic constants C by taking a slightly smaller $\alpha_1 < \tilde{\alpha}$ and a larger $M_1 > \tilde{M}_1$.

Finally, (10.11) and (10.14) imply that

$$|u(x)| \le Ce^{-\alpha_1|x|}(\|u\|_{H^1(\bar{\Omega}^c)} + \|f\|_{H^1(\bar{\Omega}^c)})$$

for $|x| > M_1$.

For the second inequality (10.8), let S_γ be a γ-neighborhood of Γ_δ with γ independent of δ. Using a trace theorem and an interior regularity estimate, we see that

$$\|u\|_{H^{1/2}(\Gamma_\delta)} \le C\|u\|_{H^2(S_\gamma)} \le C(\|u\|_{L^2(S_{2\gamma})} + \|f\|_{L^2(S_{2\gamma})}) \tag{10.15}$$

Finally, it follows from (10.15) that integrating (10.7) and the similar inequality for f on $S_{2\gamma}$ gives

$$\|u\|_{H^{1/2}(\Gamma_\delta)} \le Ce^{-\alpha_1\delta}\left(\|u\|_{H^1(\bar{\Omega}^c)} + \|f\|_{H^1(\bar{\Omega}^c)}\right). \tag{10.16}$$

□

Remark 10.3. The above lemma deals with exponential decay of solutions to the Cartesian PML Helmholtz equation with wavenumber located only in the region $-\arg(d_0) < \arg(k) < 0$, where resonance values appear. However, it holds for k with $|\arg(k)| < \arg(d_0)$ as well. Indeed, since $\mathrm{Im}(k\tilde{r}) > 0$ for $|\arg(k)| < \arg(d_0)$ provided $|x-y|$ is large enough, the fundamental solution $\widetilde{\Phi}$ of the Cartesian PML Helmholtz equation decays exponentially as in Lemma 3.4 and the above analysis can be carried over to this case.

Proof of Lemma 10.2. To prove exponential decay of u_δ, the function u_δ is decomposed into $u_\delta = u + w$ by solving two problems: $u \in H^1(\bar{\Omega}^c)$ is a solution to the exterior problem

$$\begin{aligned} \widetilde{\Delta}u + k^2u &= \tilde{f} \ \text{ in } \bar{\Omega}^c, \\ u &= u_\delta \text{ on } \Gamma, \end{aligned} \tag{10.17}$$

where $\tilde{f}$ is the zero extension of f to $\bar{\Omega}^c_\delta$, and $w \in H^1(\Omega_\delta \setminus \bar{\Omega})$ is a solution to the truncated problem

$$\begin{aligned} \widetilde{\Delta}w + k^2w &= 0 \quad \text{in } \Omega_\delta \setminus \bar{\Omega}, \\ w &= 0 \quad \text{on } \Gamma, \\ w &= -u \ \text{ on } \Gamma_\delta. \end{aligned} \tag{10.18}$$

Here we note that the exterior problem (10.17) and the truncated problem (10.18) for $\delta > \tilde{\delta}_0$ both are well-posed by Lemma 6.1 and Theorem 6.4, respectively.

First, exponential decay of the solution u follows from Lemma 10.1 and hence by using the stability of the problem (10.17) and a trace theorem we infer that

$$|u(x)| \leq C_1 e^{-\alpha_1 |x|} \left(\|u_\delta\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} + \|f\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \right) \tag{10.19}$$

for all $|x| > M_1$ with the constants α_1, C_1 and M_1 given in Lemma 10.1.

Second, in order to show exponential decay of w, we introduce a slightly larger smooth domain $\mathcal{D}_1$ independent of δ such that $\Omega_\delta \setminus \bar{\mathcal{D}}_1$. We shall show that

$$\|w\|_{H^2(\Omega_\delta \setminus \bar{\mathcal{D}}_1)} \leq C_\delta \|u\|_{H^2(S_\gamma \cap \Omega_\delta)} \tag{10.20}$$

for some C_δ which may grow only polynomially as a function of δ. Here S_γ is a γ-neighborhood of Γ_δ for $\gamma > 0$ independent of δ. Once we have the estimation (10.20), by a Sobolev embedding theorem and an interior regularity (see e.g., [16, Theorem 8.8]) we obtain that for $x \in \Omega_\delta \setminus \bar{\mathcal{D}}_1$

$$|w(x)| \leq C \|w\|_{H^2(\Omega_\delta \setminus \bar{\mathcal{D}}_1)} \leq C_\delta \|u\|_{H^2(S_\gamma \cap \Omega_\delta)} \leq C_\delta (\|u\|_{L^2(S_{2\gamma})} + \|\tilde{f}\|_{L^2(S_{2\gamma})}).$$

Then, integrating the exponentially decaying function u and $\tilde{f}$ on $S_{2\gamma}$ as in (10.16) and absorbing the polynomial growth in C_δ by taking a smaller α_1, we are led to

$$|w(x)| \leq C_1 e^{-\alpha_1 |x|} (\|u_\delta\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} + \|f\|_{L^2(\Omega_\delta \setminus \bar{\Omega})}).$$

for all $|x| > M_1$.

To verify (10.20), let χ_1 be a cutoff function defined on $\Omega_\delta \setminus \bar{\mathcal{D}}_1$ which is one on a neighborhood of Γ_δ and zero outside of $S_\gamma \cap (\Omega_\delta \setminus \bar{\mathcal{D}}_1)$. We decompose $w = w_1 + w_2$, where $w_1 = -\chi_1 u$ and w_2 is a unique solution to

$$\begin{aligned} \widetilde{\Delta} w_2 + k^2 w_2 &= g \quad \text{in } \Omega_\delta \setminus \bar{\mathcal{D}}_1, \\ w_2 &= 0 \quad \text{on } \partial \mathcal{D}_1 \cup \Gamma_\delta, \end{aligned} \tag{10.21}$$

where $g = -(\widetilde{\Delta} w_1 + k^2 w_1)$ and we note that

$$\|w_2\|_{H^1(\Omega_\delta \setminus \bar{\mathcal{D}}_1)} \leq C \|g\|_{L^2(\Omega_\delta \setminus \bar{\mathcal{D}}_1)} \quad \text{and} \quad \|g\|_{L^2(\Omega_\delta \setminus \bar{\mathcal{D}}_1)} \leq C \|u\|_{H^2(S_\gamma \cap \Omega_\delta)}. \tag{10.22}$$

Therefore, we only have to show

$$\|w_j\|_{H^2(\Omega_\delta \setminus \bar{\mathcal{D}}_1)} \leq C_\delta \|u\|_{H^2(S_\gamma \cap \Omega_\delta)} \text{ for } j = 1, 2 \tag{10.23}$$

with C_δ growing only polynomially as a function of δ.

For $j = 1$, obviously we have $\|w_1\|_{H^2(\Omega_\delta\setminus\bar{\mathcal{D}}_1)} \leq C\|u\|_{H^2(S_\gamma\cap\Omega_\delta)}$. For $j = 2$, let $\mathcal{D}_2$ be a smooth domain independent of δ between $\mathcal{D}_1$ and Ω_δ such that $\bar{\mathcal{D}}_1 \subset \mathcal{D}_2$ and $\bar{\mathcal{D}}_2 \subset \Omega_\delta$. We introduce another cutoff function χ_2 with domain $\Omega_\delta\setminus\bar{\mathcal{D}}_1$, which is one on $\Omega_\delta\setminus\bar{\mathcal{D}}_2$ and vanishes near $\partial\mathcal{D}_1$. Then $\chi_2 w_2$ (considered as an extension by zero in $\mathcal{D}_1$) and $(1-\chi_2)w_2$ satisfy the equations similar to (10.21) on domains Ω_δ and $\mathcal{D}_2\setminus\bar{\mathcal{D}}_1$, respectively, with the right hand sides which involve g and at most first derivative of w_2. Therefore, by a regularity on the smooth domain $\mathcal{D}_2\setminus\bar{\mathcal{D}}_1$,

$$\|(1-\chi_2)w_2\|_{H^2(\Omega_\delta\setminus\bar{\mathcal{D}}_1)} = \|(1-\chi_2)w_2\|_{H^2(\mathcal{D}_2\setminus\bar{\mathcal{D}}_1)} \leq C(\|g\|_{L^2(\Omega_\delta\setminus\bar{\mathcal{D}}_1)}+\|w_2\|_{H^1(\Omega_\delta\setminus\bar{\mathcal{D}}_1)}). \tag{10.24}$$

Finally, using dilation of a fixed square domain and a regularity of solutions on the reference domain, we have

$$\|\chi_2 w_2\|_{H^2(\Omega_\delta\setminus\bar{\mathcal{D}}_1)} = \|\chi_2 w_2\|_{H^2(\Omega_\delta)} \leq C_\delta(\|g\|_{L^2(\Omega_\delta\setminus\bar{\mathcal{D}}_1)} + \|w_2\|_{H^1(\Omega_\delta\setminus\bar{\mathcal{D}}_1)}). \tag{10.25}$$

By combining (10.24), (10.25) together with (10.22), the inequality (10.23) for $j = 2$ immediately follows. □

Proof of Lemma 6.2. Since the symmetry of the sesquilinear form $A_z(\cdot,\cdot)$, the adjoint problem is equivalent to the problem to find ϕ such that

$$\begin{aligned} A_{\bar{z}}(\phi,\theta) &= 0 \text{ for all } \theta \in H_0^1(\bar{\Omega}^c), \\ \phi &= \bar{g} \text{ on } \Gamma. \end{aligned}$$

Then since $0 < \arg(\sqrt{\bar{z}}) < \arg(d_0)$, Lemma 10.1 and Remark 10.3 show exponential decay of the solution to the above problem. □

Proof of Lemma 7.2. For the first exponential decay estimation (7.4), we begin with noting that the equations (10.4) and (10.5) hold for ψ in V. Applying Lemma (10.1) to (10.4) shows the exponential decay of ψ_1, there exist α_1 and $M_1 > 0$ such that

$$|\psi_1(x)| \leq Ce^{-\alpha_1 x}\|\psi_1\|_{H^1(\bar{\Omega}^c)}$$

for $|x| > M_1$. The repeated use of Lemma 10.1 for the recursively defined ψ_j for $j = 0,\ldots,n$ shows that there exist α, C and M such that $\psi = \psi_n$ satisfies

$$|\psi_n(x)| \leq Ce^{-\alpha|x|}\sum_{j=1}^{n}\|\psi_j\|_{H^1(\bar{\Omega}^c)}$$

for all $|x| > M$, where α, C and M may depend on λ and n but not on δ. The continuity of $T - \lambda I$ in $H^1(\bar{\Omega}^c)$ and the recursive relation for ψ_j imply that there exists a positive constant C such that

$$\|\psi_j\|_{H^1(\bar{\Omega}^c)} \leq C\|\psi_n\|_{H^1(\bar{\Omega}^c)} \text{ for } j = 1, \ldots, n,$$

from which it follows that

$$|\psi_n(x)| \leq Ce^{-\alpha|x|}\|\psi_n\|_{H^1(\bar{\Omega}^c)}.$$

The second inequality (7.5) can be proved in the same way as above with Lemma 10.2 applied to the equations (10.2) and (10.3) for functions in $\widetilde{V}_\delta$.

For the last estimation (7.6), it suffices to prove (7.6) for ψ satisfying (7.4) since functions in $\widetilde{V}_\delta$ also fulfill the decaying condition (7.4). We prove it by estimating

$$\|(T - T_\delta)\psi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \leq C_1 e^{-\alpha_1 \delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)}), \tag{10.26}$$

$$\|(T - T_\delta)\psi\|_{H^1(\bar{\Omega}_\delta^c)} \leq C_1 e^{-\alpha_1 \delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)}). \tag{10.27}$$

for some constants α_1 and C_1, which leads to (7.6). We note that $T\psi$ solves the equation

$$\widetilde{\Delta} T\psi + T\psi = -\psi \text{ in } \bar{\Omega}^c \tag{10.28}$$

by the definition of T and hence it follows from Lemma 10.1 and Remark 10.3 that $T\psi$ satisfies

$$|T\psi(x)| \leq C_1 e^{-\alpha_1|x|}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)}) \text{ for } |x| > M_1 \tag{10.29}$$

$$\|T\psi\|_{H^{1/2}(\Gamma_\delta)} \leq C_1 e^{-\alpha_1 \delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)}) \text{ for } \delta > M_1. \tag{10.30}$$

For (10.26), we observe that $(T - T_\delta)\psi$ on $\Omega_\delta \setminus \bar{\Omega}$ is a unique solution to the truncated problem

$$A_1((T - T_\delta)\psi, \theta) = 0 \quad \text{for all } \theta \in H_0^1(\Omega_\delta \setminus \bar{\Omega}),$$
$$(T - T_\delta)\psi = T\psi \text{ on } \Gamma_\delta \;\text{ and }\; (T - T_\delta)\psi = 0 \text{ on } \Gamma$$

for $\delta > \delta_0$ (given in Lemma 5.1 and $\delta_0 > M_1$). By the stability of the above problem and (10.30), we have (10.26),

$$\|(T - T_\delta)\psi\|_{H^1(\Omega_\delta \setminus \bar{\Omega})} \leq C\|T\psi\|_{H^{1/2}(\Gamma_\delta)} \leq C_1 e^{-\alpha_1 \delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)}).$$

For (10.27), we shall estimate $T\psi$ in $\bar{\Omega}^c_\delta$ since $(T - T_\delta)\psi = T\psi$ on $\bar{\Omega}^c_\delta$. Integrating (10.29) on $\bar{\Omega}^c_\delta$ implies that

$$\|T\psi\|_{L^2(\bar{\Omega}^c_\delta)} \le C_\delta e^{-\alpha_1\delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)}), \tag{10.31}$$

where C_δ grows polynomially. For H^1-seminorm of $T\psi$ on $\bar{\Omega}^c_\delta$, applying the L^2 inner product against $\bar{J}T\psi$ to (10.28) and integrating it by parts shows that

$$(H\nabla T\psi, \nabla T\psi)_{\bar{\Omega}^c_\delta} = \int_{\Gamma_\delta} (n^t H\nabla T\psi)(\overline{T\psi})\,\mathrm{d}S + (JT\psi, T\psi)_{\bar{\Omega}^c_\delta} + (J\psi, T\psi)_{\bar{\Omega}^c_\delta}. \tag{10.32}$$

In the first term of the right hand side, the same argument as that used in (10.15) and (10.16) (with u and f replaced by $T\psi$ and ψ, respectively) yields

$$\|T\psi\|_{L^2(\Gamma_\delta)}, \|\nabla T\psi\|_{L^2(\Gamma_\delta)} \le Ce^{-\alpha_1\delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)})$$

and hence Schwarz inequality yields

$$\left|\int_{\Gamma_\delta} n^t H\nabla T\psi\overline{T\psi}\,\mathrm{d}S\right| \le Ce^{-2\alpha_1\delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)})^2. \tag{10.33}$$

In the last two terms, by Schwarz inequalities and integrating (7.4) and (10.29) on $\bar{\Omega}^c_\delta$, we are led to

$$\begin{aligned} |(JT\psi, T\psi)_{\bar{\Omega}^c_\delta}| &\le C\|T\psi\|^2_{L^2(\bar{\Omega}^c_\delta)} \le C_\delta e^{-2\alpha_1\delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)})^2 \\ |(J\psi, T\psi)_{\bar{\Omega}^c_\delta}| &\le C\|\psi\|_{L^2(\bar{\Omega}^c_\delta)}\|T\psi\|_{L^2(\bar{\Omega}^c_\delta)} \le C_\delta e^{-2\alpha_1\delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)})^2. \end{aligned} \tag{10.34}$$

By applying the coercivity (2.4) to (10.32), it follows from (10.33) and (10.34) that

$$\|\nabla T\psi\|_{L^2(\bar{\Omega}^c_\delta)} \le C_\delta e^{-\alpha_1\delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)}). \tag{10.35}$$

Finally, the H-norm estimate

$$\|T\psi\|_{H^1(\bar{\Omega}^c_\delta)} \le Ce^{-\alpha_1\delta}(\|T\psi\|_{H^1(\bar{\Omega}^c)} + \|\psi\|_{H^1(\bar{\Omega}^c)})$$

is obtained by combining (10.31) and (10.35). Here we choose a smaller α_1 to remove the polynomial dependence of δ.

$\square$

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