AN ADAPTIVE PERFECTLY MATCHED LAYER TECHNIQUE FOR TIME-HARMONIC SCATTERING PROBLEMS

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Abstract. We develop an adaptive perfectly matched layer (PML) technique for solving the time harmonic scattering problems. The PML parameters such as the thickness of the layer and the fictitious medium property are determined through sharp a posteriori error estimates. The derived finite element a posteriori estimate for adapting meshes has the nice feature that it decays exponentially away from the boundary of the fixed domain where the PML layer is placed. This property makes the total computational costs insensitive to the thickness of the PML absorbing layers. Numerical experiments are included to illustrate the competitive behavior of the proposed adaptive method.

Key words. Adaptivity, perfectly matched layer, a posteriori error analysis, scattering problems.

AMS subject classifications. 65N30, 78A45, 35Q60

1. Introduction.

We propose and study an adaptive perfectly matched layer (PML) technique for solving Helmholtz-type scattering problems with perfectly conducting boundary:

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}^2 \backslash \bar{D}, \tag{1.1a}$$

$$\frac{\partial u}{\partial \mathbf{n}} = -g \quad \text{on } \Gamma_D, \tag{1.1b}$$

$$\sqrt{r}\left(\frac{\partial u}{\partial r} - \mathbf{i}ku\right) \to 0 \quad \text{as } r = |x| \to \infty. \tag{1.1c}$$

Here $D \subset \mathbb{R}^2$ is a bounded domain with Lipschitz boundary Γ_D, $g \in H^{-1/2}(\Gamma_D)$ is determined by the incoming wave, and $\mathbf{n}$ is the unit outer normal to Γ_D. We assume the wave number $k \in \mathbb{R}$ is a constant. We remark that the results in this paper can be easily extended to solve the scattering problems with other boundary conditions such as Dirichlet or the impedance boundary condition on Γ_D, or to solve the acoustic wave propagation through inhomogeneous media with a variable wave number $k^2(x)$ inside some bounded domain.

Since the work of Berenger [3] which proposed a PML technique for solving with the time dependent Maxwell equations, various constructions of PML absorbing layers have been proposed and studied in the literature (cf. e.g. Turkel and Yefet [20], Teixeira and Chew [19] for the reviews). Under the assumption that the exterior solution is composed of outgoing waves only, the basic idea of the PML technique is to surround the computational domain by a layer of finite thickness with specially designed model medium that would either slow down or attenuate all the waves that propagate from inside the computational domain. The PML equation for the time-harmonic scattering problem (1.1a) is derived in Collino and Monk [10] by a complex

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extension of the solution u in the exterior domain. It is proved in Lassas and Somersalo [13], Hohage, Schmidt and Zschiedrich [12] that the resultant PML solution converges exponentially to the solution of the original scattering problem as the thickness of the PML layer tends to infinity. We remark that in practical applications involving PML techniques, one cannot afford to use a very thick PML layer if uniform finite element meshes are used because it requires excessive grid points and hence more computer time and more storage. On the other hand, a thin PML layer requires a rapid variation of the artificial material property which deteriorates the accuracy if too coarse mesh is used in the PML layer.

A posteriori error estimates are computable quantities in terms of the discrete solution and data that measure the actual discrete errors without the knowledge of exact solutions. They are essential in designing algorithms for mesh modification which equi-distribute the computational effort and optimize the computation. Ever since the pioneering work of Babuška and Rheinboldt [2], the adaptive finite element methods based on a posteriori error estimates have become a central theme in scientific and engineering computations. The ability of error control and the asymptotically optimal approximation property (see e.g. Morin, Nochetto and Siebert [17], Chen and Dai [5]) make the adaptive finite element method attractive for complicated physical and industrial processes (cf. e.g. Chen and Dai [4], Chen, Nochetto and Schmidt [7]). For the efforts to solve scattering problems using adaptive methods based on a posterior error estimate, we refer to the recent work Monk [15], Monk and Süli [16].

It is proposed in Chen and Wu [8] for scattering problem by periodic structures (the grating problem) that one can use the a posteriori error estimate to determine the PML parameters. Moreover, the derived a posteriori error estimate in [8] has the nice feature of exponential decay in terms of the distance to the boundary of the fixed domain where the PML layer is placed. This property leads to coarse mesh size away from the fixed domain and thus makes the total computational costs insensitive to the thickness of the PML absorbing layer.

In this paper we extend the idea of using a posteriori error estimates to determine the PML parameters and propose an adaptive PML technique for solving the scattering problem (1.1a)-(1.1c). The main difficulty of the analysis is that in contrast to the grating problems in which there are only finite number of outgoing modes [8], now there are infinite number of outgoing modes expressed in terms of Hankel functions. We overcome this difficulty by exploiting the following uniform estimate for the Hankel functions H^1_ν, $\nu \in \mathbb{R}$,:

$$|H^{(1)}_\nu(z)| \le e^{-\mathrm{Im}\,(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}} |H^{(1)}_\nu(\Theta)|, \tag{1.2}$$

for any $z \in \mathbb{C}_{++}, \Theta \in \mathbb{R}$ such that $0 < \Theta \le |z|$, where $\mathbb{C}_{++} = \{z \in \mathbb{C} : \mathrm{Im}\,(z) \ge 0, \mathrm{Re}\,(z) \ge 0\}$. To our knowledge this sharp estimate is new and allows us to prove the exponentially decaying property of the PML solution without resorting to the integral equation technique in [13] or the representation formula in [12]. We remark that in [13], [12], it is required that the fictitious absorbing coefficient must be linear after certain distance away from the boundary where the PML layer is placed. The estimate (1.2) is proved in Lemma 2.2 which depends on the Macdonald formula for the modified Bessel functions. We also remark that since (1.2) is valid for all real order ν, the results of this paper can be extended directly to study three dimensional Helmholtz-type scattering problems. We will report progress in this direction as well as the study of the electromagnetic scattering problems elsewhere in future.

Let $\Omega^{\rm PML} = B_\rho \backslash \bar{B}_R$, where $0 < R < \rho$ and B_a denotes the circle of radius $a > 0$. Let $\alpha(r) = 1 + \mathbf{i}\sigma(r)$ be the fictitious medium property. In practical applications, σ is usually taken as power functions:

$$\sigma = \sigma(r) = \sigma_0 \left(\frac{r-R}{\rho-R}\right)^m \quad \text{for some constant } \sigma_0 > 0 \text{ and integer } m \geq 1.$$

Under the assumption that the Dirichlet problem of the PML equation in the PML layer is uniquely solvable, we prove the following key estimate between the Dirichlet-to-Neumann mapping for the original scattering problem $T : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$ and the PML problem $\hat{T}$ (cf. Lemma 2.5), where $\Gamma_R = \partial B_R$,

$$\| T - \hat{T} \|_{L(H^{1/2}(\Gamma_R), H^{-1/2}(\Gamma_R))} \leq C(1+kR)^2 |\alpha_0|^2 e^{-k{\rm Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}},$$

where $\alpha_0 = 1 + \mathbf{i}\sigma_0$, and $\tilde{\rho} = \int_0^\rho \alpha(t)dt$ is the complex radius corresponding to ρ. We remark that the assumption of the unique solvability of the PML Dirichlet problem in the PML layer is rather mild in practical applications because standard Fredholm alternative theory implies that the PML Dirichlet problem in the PML layer is uniquely solvable for all but a discrete number of real k. Moreover, in the appendix of this paper, we show that for any given ρ, R, the Dirichlet PML problem in the PML layer is uniquely solvable for sufficiently large $\sigma_0 > 0$.

The layout of the paper is as follows. In section 2 we recall the PML formulation for (1.1a)-(1.1c), derive the key estimates for Hankel functions, and study the properties of the PML equation in the PML layer. Existence, uniqueness and convergence of the PML formulation are considered. In section 3 we introduce the finite element discretization. In section 4 we derive the sharp a posteriori error estimate which lays down the basis of the combined adaptive PML and finite element methods. In section 5 we discuss the implementation of the adaptive method and present several numerical examples to illustrate the competitive behavior of the method. Finally in the appendix we show the unique solvability of the Dirichlet PML problem in the PML layer for sufficiently large σ_0.

2. The PML formulation. Let D be contained in the interior of the circle $B_R = \{x \in \mathbb{R}^2 : |x| < R\}$. We start by introducing an equivalent variational formulation of (1.1a)-(1.1c) in the bounded domain $\Omega_R = B_R \backslash \bar{D}$. In the domain $\mathbb{R}^2 \backslash \bar{B}_R$, the solution u of (1.1a)-(1.1c) can be written under the polar coordinates as follows:

$$u(r,\theta) = \sum_{n\in\mathbb{Z}} \frac{H_n^{(1)}(kr)}{H_n^{(1)}(kR)} \hat{u}_n e^{\mathbf{i}n\theta}, \qquad \hat{u}_n = \frac{1}{2\pi}\int_0^{2\pi} u(R,\theta) e^{-\mathbf{i}n\theta} d\theta. \tag{2.1}$$

where $H_n^{(1)}$ is the Hankel function of the first kind and order n. The series in (2.1) converges uniformly for $r > R$ (cf. e.g. Colten and Kress [11]). Let $T : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$, where $\Gamma_R = \partial B_R$, be the Dirichlet-to-Neumann operator defined as follows: for any $f \in H^{1/2}(\Gamma_R)$,

$$Tf = \sum_{n\in\mathbb{Z}} k \frac{H_n^{(1)\prime}(kR)}{H_n^{(1)}(kR)} \hat{f}_n e^{\mathbf{i}n\theta}, \qquad \hat{f}_n = \frac{1}{2\pi}\int_0^{2\pi} f e^{-\mathbf{i}n\theta} d\theta. \tag{2.2}$$

It is known that T is well-defined and the solution u written as in (2.1) satisfies

$$\left.\frac{\partial u}{\partial \mathbf{n}}\right|_{\Gamma_R} = Tu.$$

Let $a : H^1(\Omega_R) \times H^1(\Omega_R) \to \mathbb{C}$ be the sesquilinear form:

$$a(\varphi, \psi) = \int_{\Omega_R} \left(\nabla\varphi \cdot \nabla\bar{\psi} - k^2 \varphi\bar{\psi} \right) dx - \langle T\varphi, \psi \rangle_{\Gamma_R}, \tag{2.3}$$

where $\langle \cdot, \cdot \rangle_{\Gamma_R}$ stands for the inner product on $L^2(\Gamma_R)$ or the duality pairing between $H^{-1/2}(\Gamma_R)$ and $H^{1/2}(\Gamma_R)$. Similar notation applies for $\langle \cdot, \cdot \rangle_{\Gamma_D}$, $\langle \cdot, \cdot \rangle_{\Gamma_\rho}$. The scattering problem (1.1a)-(1.1c) is equivalent to the following weak formulation (cf. e.g. [11]): Given $g \in H^{-1/2}(\Gamma_D)$, find $u \in H^1(\Omega_R)$ such that

$$a(u, \psi) = \langle g, \psi \rangle_{\Gamma_D} \qquad \forall \psi \in H^1(\Omega_R). \tag{2.4}$$

The existence of a unique solution of the variational problem (2.4) is known (cf. e.g. [11], McLean [14]). Then the general theory in Babuška and Aziz [1, Chapter 5] implies that there exists a constant $\mu > 0$ such that the following inf-sup condition holds:

$$\sup_{0 \neq \psi \in H^1(\Omega_R)} \frac{|a(\varphi, \psi)|}{\| \psi \|_{H^1(\Omega_R)}} \geq \mu \| \varphi \|_{H^1(\Omega_R)} \qquad \forall \varphi \in H^1(\Omega_R). \tag{2.5}$$

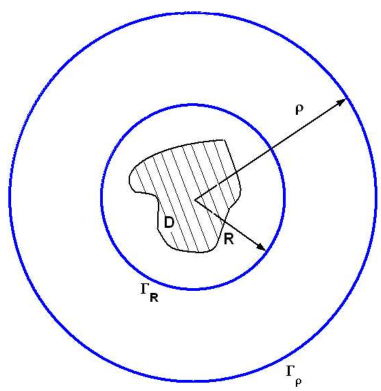

FIG. 2.1. *Setting of the scattering problem with the PML layer.*

Now we turn to the introduction of the absorbing PML layer. We surround the domain Ω_R with a PML layer $\Omega^{\mathrm{PML}} = \{x \in \mathbb{R}^2 : R < |x| < \rho\}$. The specially designed model medium in the PML layer should basically be so chosen that either the wave never reaches its external boundary or the amplitude of the reflected wave is so small that it does not essentially contaminate the solution in Ω_R. Throughout the paper we assume $\rho \leq CR$ for some generic fixed constant $C > 0$.

Let $\alpha(r) = 1 + \mathbf{i}\sigma(r)$ be the model medium property which satisfies

$$\sigma \in C(\mathbb{R}), \qquad \sigma \geq 0, \qquad \text{and } \sigma = 0 \ \text{ for } r \leq R.$$

Denote by $\tilde{r}$ the complex radius defined by

$$\tilde{r} = \tilde{r}(r) = \begin{cases} r & \text{if } r \leq R, \\ \int_0^r \alpha(t) dt = r\beta(r) & \text{if } r \geq R. \end{cases} \tag{2.6}$$

Following [10], we introduce the PML equation

$$\nabla \cdot (A\nabla w) + \alpha\beta k^2 w = 0 \quad \text{in } \Omega^{\mathrm{PML}}, \tag{2.7}$$

where $A = A(x)$ is a matrix which satisfies, in polar coordinates,

$$\nabla \cdot (A\nabla) = \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{\beta r}{\alpha}\frac{\partial}{\partial r}\right) + \frac{\alpha}{\beta r^2}\frac{\partial^2}{\partial \theta^2}. \tag{2.8}$$

The PML solution $\hat{u}$ in $\Omega_\rho = B_\rho \backslash \bar{D}$ is defined as the solution of the following system

$$\nabla \cdot (A\nabla \hat{u}) + \alpha\beta k^2 \hat{u} = 0 \quad \text{in } \Omega_\rho, \tag{2.9a}$$

$$\frac{\partial \hat{u}}{\partial \mathbf{n}} = -g \quad \text{on } \Gamma_D, \qquad \hat{u} = 0 \quad \text{on } \Gamma_\rho. \tag{2.9b}$$

This problem can be reformulated in the bounded domain Ω_R by imposing the boundary condition

$$\frac{\partial \hat{u}}{\partial \mathbf{n}}\Big|_{\Gamma_R} = \hat{T}\hat{u},$$

where the operator $\hat{T} : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$ is defined as follows: Given $f \in H^{1/2}(\Gamma_R)$,

$$\hat{T}f = \frac{\partial \zeta}{\partial \mathbf{n}}\Big|_{\Gamma_R},$$

where $\zeta \in H^1(\Omega^{\mathrm{PML}})$ satisfies

$$\nabla \cdot (A\nabla \zeta) + \alpha\beta k^2 \zeta = 0 \quad \text{in } \Omega^{\mathrm{PML}}, \tag{2.10a}$$

$$\zeta = f \quad \text{on } \Gamma_R, \qquad \zeta = 0 \quad \text{on } \Gamma_\rho. \tag{2.10b}$$

The existence and uniqueness of the solutions of the PML problem (2.10a)-(2.10b) will be studied in the subsection 2.2 below.

Based on the operator $\hat{T}$, we introduce the sesquilinear form $\hat{a} : H^1(\Omega_R) \times H^1(\Omega_R) \to \mathbb{C}$ by

$$\hat{a}(\varphi, \psi) = \int_{\Omega_R} \left(A\nabla\varphi \cdot \nabla\bar{\psi} - k^2\alpha\beta\varphi\bar{\psi}\right) dx - \langle \hat{T}\varphi, \psi \rangle_{\Gamma_R}. \tag{2.11}$$

Then the weak formulation for (2.9a)-(2.9b) is: Given $g \in H^{-1/2}(\Gamma_D)$, find $\hat{u} \in H^1(\Omega_R)$ such that

$$\hat{a}(\hat{u}, \psi) = \langle g, \psi \rangle_{\Gamma_D} \quad \forall \psi \in H^1(\Omega_R). \tag{2.12}$$

The well-posedness of the PML problem (2.12) and the convergence of its solution to the solution of the original scattering problem (2.4) will be studied in the subsection 2.3. In the following we first derive some basic estimates for the Hankel function $H_n^{(1)}$ which play a key role in the analysis in this paper.

2.1. Hankel functions. For $\nu \in \mathbb{C}$, the two Hankel functions $H_\nu^{(1)}(z), H_\nu^{(2)}(z)$, where $z \in \mathbb{C}$, are two fundamental solutions of the Bessel equation for functions of order ν:

$$z^2 \frac{d^2 y}{dz^2} + z\frac{dy}{dz} + (z^2 - \nu^2) y = 0, \tag{2.13}$$

which satisfy the following asymptotic behaviors as $|z| \to \infty$:

$$H_\nu^{(1)}(z) \sim \left(\frac{2}{\pi z}\right)^{1/2} e^{\mathbf{i}\left(z - \frac{1}{2}\nu\pi - \frac{1}{4}\pi\right)}, \quad H_\nu^{(2)}(z) \sim \left(\frac{2}{\pi z}\right)^{1/2} e^{-\mathbf{i}\left(z - \frac{1}{2}\nu\pi - \frac{1}{4}\pi\right)}. \tag{2.14}$$

We also need the Bessel functions of purely imaginary argument $K_\nu(z)$, also called the modified Bessel functions, which is the solution of the differential equation

$$z^2 \frac{d^2 y}{dz^2} + z\frac{dy}{dz} - (z^2 + \nu^2) y = 0. \tag{2.15}$$

It is connected with $H_\nu^{(1)}(z)$ through the relation

$$K_\nu(z) = \frac{1}{2}\pi \mathbf{i} e^{\frac{1}{2}\nu\pi\mathbf{i}} H_\nu^{(1)}(\mathbf{i}z). \tag{2.16}$$

The importance of the function $K_\nu(z)$ in mathematical physics lies in the fact that it is a solution of (2.15) which tends to zero exponentially as $z \to \infty$ through positive values. We refer to the treatise Watson [21] for extensive studies on the functions $H_\nu^{(1)}(z), H_\nu^{(2)}(z)$ and $K_\nu(z)$.

The following lemma is proved in [21, P.439].

LEMMA 2.1 (Macdonald formula). *For any $\nu \in \mathbb{C}$ and $z_1, z_2 \in \mathbb{C}$ satisfying*

$$|\arg z_1| < \pi, \quad |\arg z_2| < \pi \quad \text{and } |\arg(z_1 + z_2)| < \frac{1}{4}\pi,$$

we have

$$K_\nu(z_1)K_\nu(z_2) = \frac{1}{2}\int_0^\infty e^{-\frac{v}{2} - \frac{z_1^2 + z_2^2}{2v}} K_\nu\left(\frac{z_1 z_2}{v}\right) \frac{dv}{v}.$$

An important consequence of this lemma is that for real ν, $K_\nu(z)$ has no zeros if $|\arg z| \le \frac{1}{2}\pi$ [21, P.511], which, by (2.16), implies that $H_\nu^{(1)}(z)$ has no zeros when $\mathrm{Im}\,(z) \le 0$. In particular, we have $H_n^{(1)}(kR) \neq 0$ for any $n \in \mathbb{Z}, R > 0$. This justifies the writing of $H_n^{(1)}(kR)$ in the denominator in (2.1), (2.2).

LEMMA 2.2. *For any $\nu \in \mathbb{R}, z \in \mathbb{C}_{++} = \{z \in \mathbb{C} : \mathrm{Im}\,(z) \ge 0, \mathrm{Re}\,(z) \ge 0\}$, and $\Theta \in \mathbb{R}$ such that $0 < \Theta \le |z|$, we have*

$$|H_\nu^{(1)}(z)| \le e^{-\mathrm{Im}\,(z)\left(1 - \frac{\Theta^2}{|z|^2}\right)^{1/2}} |H_\nu^{(1)}(\Theta)|. \tag{2.17}$$

This estimate, which to our knowledge is new, will play an important role in the analysis of this paper. The importance of the estimate (2.17) lies in the fact that it is uniform with respect to ν. We remark that the large argument asymptotic expansions such as (2.14) in the literature usually depend on ν and thus are insufficient for our purpose.

Proof. By (2.16) we know that

$$|H_\nu^{(1)}(z)|^2 = H_\nu^{(1)}(z)\overline{H_\nu^{(1)}(z)} = \frac{4}{\pi^2}K_\nu(-\mathbf{i}z)\overline{K_\nu(-\mathbf{i}z)} = \frac{4}{\pi^2}K_\nu(-\mathbf{i}z)K_\nu(\mathbf{i}\bar{z}),$$

where we have used the formula $K_\nu(\bar{z}) = \overline{K_\nu(z)}$ for real ν. Since $z \in \mathbb{C}_{++}$, we know that $|\arg(-\mathbf{i}z)| < \pi$, $|\arg(\mathbf{i}\bar{z})| < \pi$ and $|\arg(-\mathbf{i}z + \mathbf{i}\bar{z})| = 0 < \frac{\pi}{4}$. Thus by Lemma 2.1 we obtain

$$|H_\nu^{(1)}(z)|^2 = \frac{2}{\pi^2}\int_0^\infty e^{-\frac{v}{2}-\frac{-z^2-\bar{z}^2}{2v}}K_\nu\left(\frac{|z|^2}{v}\right)\frac{dv}{v}.$$

After the change of variable $w = |z|^2/v$, we get

$$|H_\nu^{(1)}(z)|^2 = \frac{2}{\pi^2}\int_0^\infty e^{-\frac{|z|^2}{2w}+\frac{z^2+\bar{z}^2}{2|z|^2}w}K_\nu(w)\frac{dw}{w},$$

which, for any $\Theta > 0$, we rewrite as

$$|H_\nu^{(1)}(z)|^2 = \frac{2}{\pi^2}\int_0^\infty e^{-\frac{|z|^2-\Theta^2}{2w}-\frac{2|z|^2-z^2-\bar{z}^2}{2|z|^2}w}\cdot e^{-\frac{\Theta^2}{2w}+w}K_\nu(w)\frac{dw}{w}.$$

Now for $0 < \Theta \le |z|$, by Cauchy-Schwarz inequality, we deduce that

$$e^{-\frac{|z|^2-\Theta^2}{2w}-\frac{2|z|^2-z^2-\bar{z}^2}{2|z|^2}w} = e^{-\frac{|z|^2-\Theta^2}{2w}-\frac{2\mathrm{Im}\,(z)^2}{|z|^2}w} \le e^{-2\mathrm{Im}\,(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}}.$$

Therefore

$$\begin{aligned}|H_\nu^{(1)}(z)|^2 &\le e^{-2\mathrm{Im}\,(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}}\frac{2}{\pi^2}\int_0^\infty e^{-\frac{\Theta^2}{2w}+w}K_\nu(w)\frac{dw}{w}\\ &= e^{-2\mathrm{Im}\,(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}}|H_\nu^{(1)}(\Theta)|^2.\end{aligned}$$

This completes the proof. □

To proceed further, we recall the following Nicholson integral [21, P.441]:

$$J_\nu^2(z) + Y_\nu^2(z) = \frac{8}{\pi^2}\int_0^\infty K_0(2z\sinh t)\cosh(2\nu t)dt \quad \text{for } z \in \mathbb{C}, \mathrm{Re}\,(z) > 0.$$

Here $K_0(z)$ is the modified Bessel function of order zero in (2.16). Since $\cosh(t) = (e^t + e^{-t})/2$ is an increasing function in $\mathbb{R}^+$, we have, for $\Theta > 0$, $n \ge 1$ that

$$\begin{aligned}J_{n-1}^2(\Theta) + Y_{n-1}^2(\Theta) &= \frac{8}{\pi^2}\int_0^\infty K_0(2\Theta\sinh t)\cosh(2(n-1)t)dt\\ &\le \frac{8}{\pi^2}\int_0^\infty K_0(2\Theta\sinh t)\cosh(2nt)dt\\ &= J_n^2(\Theta) + Y_n^2(\Theta).\end{aligned}$$

Thus

$$|H_{n-1}^{(1)}(\Theta)| \le |H_n^{(1)}(\Theta)| \quad \text{for any } \Theta > 0, n \ge 1. \tag{2.18}$$

LEMMA 2.3. *For any $z \in \mathbb{C}_{++}$ and $\Theta \in \mathbb{R}$ such that $0 < \Theta \le |z|$, we have*

$$|H_n^{(1)\prime}(z)| \le e^{-\mathrm{Im}\,(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}} \left(1+\frac{|n|}{|z|}\right) |H_n^{(1)}(\Theta)| \quad \text{for } n \in \mathbb{Z}, |n| \ge 1, \tag{2.19}$$

$$|H_0^{(1)\prime}(z)| \le e^{-\mathrm{Im}\,(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}} |H_0^{(1)\prime}(\Theta)|. \tag{2.20}$$

Proof. Since $H_{-n}^{(1)} = e^{\mathbf{i}n\pi} H_n^{(1)}(z)$, we only need to prove (2.19) for $n \in \mathbb{Z}$, $n \ge 1$. By the formula

$$z\frac{dH_n^{(1)}(z)}{dz} + nH_n^{(1)}(z) = zH_{n-1}^{(1)}(z),$$

Lemma 2.2, and (2.18), we know that

$$\begin{aligned}
|H_n^{(1)\prime}(z)| &\le |H_{n-1}^{(1)}(z)| + \frac{n}{|z|}|H_n^{(1)}(z)| \\
&\le e^{-\mathrm{Im}\,(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}} \left(|H_{n-1}^{(1)}(\Theta)| + \frac{n}{|z|}|H_n^{(1)}(\Theta)|\right) \\
&\le e^{-\mathrm{Im}\,(z)\left(1-\frac{\Theta^2}{|z|^2}\right)^{1/2}} \left(1+\frac{n}{|z|}\right) |H_n^{(1)}(\Theta)|.
\end{aligned}$$

This proves (2.19). The estimate (2.20) can be proved similarly by using the formula $dH_0^{(1)}(z)/dz = -H_1^{(1)}(z)$. This completes the proof. ∎

2.2. The PML equation in the layer. In this subsection we consider the Dirichlet problem of the PML equation in the layer Ω^{PML}:

$$\nabla\cdot(A\nabla w) + \alpha\beta k^2 w = 0 \quad \text{in } \Omega^{\mathrm{PML}}, \tag{2.21a}$$

$$w = 0 \;\text{ on } \Gamma_R, \qquad w = q \;\text{ on } \Gamma_\rho. \tag{2.21b}$$

where $q \in H^{1/2}(\Gamma_\rho)$. Let $\hat{b} : H^1(\Omega^{\mathrm{PML}}) \times H^1(\Omega^{\mathrm{PML}}) \to \mathbb{C}$ be the sesquilinear form:

$$\hat{b}(\varphi,\psi) = \int_R^\rho \int_0^{2\pi} \left(\frac{\beta r}{\alpha}\frac{\partial\varphi}{\partial r}\frac{\partial\bar{\psi}}{\partial r} + \frac{\alpha}{\beta r}\frac{\partial\varphi}{\partial\theta}\frac{\partial\bar{\psi}}{\partial\theta} - \alpha\beta k^2 r\varphi\bar{\psi}\right) dr\,d\theta. \tag{2.22}$$

Then from (2.8) we know that the weak formulation for (2.21a)-(2.21b) is: Given $q \in H^{1/2}(\Gamma_\rho)$, find $w \in H^1(\Omega^{\mathrm{PML}})$ such that $w = 0$ on Γ_R, $w = q$ on Γ_ρ, and

$$\hat{b}(w,\varphi) = 0 \quad \forall \varphi \in H_0^1(\Omega^{\mathrm{PML}}). \tag{2.23}$$

We make the following assumption on the fictitious medium property σ, which is rather mild in the practical application of the PML techniques:

(H1) $\sigma = \sigma_0 \left(\dfrac{r-R}{\rho-R}\right)^m$ for some constant $\sigma_0 > 0$ and some integer $m \ge 1$.

From (H1) we know that $\beta(r) = 1 + \mathbf{i}\hat{\sigma}(r)$, where

$$\hat{\sigma}(r) = \frac{1}{r}\int_R^r \sigma(t)dt = \frac{\sigma_0}{m+1}\frac{r-R}{r}\left(\frac{r-R}{\rho-R}\right)^m.$$

Thus $\hat\sigma \le \sigma$ for all $r \ge R$. Notice that for $\alpha = 1 + \mathbf{i}\sigma$, $\beta = 1 + \mathbf{i}\hat\sigma$, we have

$$\operatorname{Re}\left(\frac{\beta}{\alpha}\right) = \frac{1+\sigma\hat\sigma}{1+\sigma^2}, \quad \operatorname{Re}\left(\frac{\alpha}{\beta}\right) = \frac{1+\sigma\hat\sigma}{1+\hat\sigma^2}, \quad \operatorname{Re}(\alpha\beta) = 1 - \sigma\hat\sigma,$$

and, consequently,

$$\operatorname{Re}[\hat b(v,v)] = \int_R^\rho \int_0^{2\pi} \left[\frac{1+\sigma\hat\sigma}{1+\sigma^2} r \left|\frac{\partial v}{\partial r}\right|^2 + \frac{1+\sigma\hat\sigma}{1+\hat\sigma^2}\frac{1}{r}\left|\frac{\partial v}{\partial \theta}\right|^2 + (\sigma\hat\sigma - 1)k^2 r|v|^2\right] dr\, d\theta.$$

Since

$$\frac{1+\sigma\hat\sigma}{1+\sigma^2} \ge \frac{1}{1+\sigma^2} \ge |\alpha_0|^{-2}, \quad \frac{1+\sigma\hat\sigma}{1+\hat\sigma^2} \ge 1 \ge |\alpha_0|^{-2}, \tag{2.24}$$

where $\alpha_0 = 1 + \mathbf{i}\sigma_0$, by using the analytic Fredholm alternative theorem we know that the PML problem in the layer (2.23) exists a unique solution for every real k except possibly for a discrete set of values of k (cf. e.g. the argument in [10, Theorem 2]). In this paper we will not elaborate on this issue and simply make the following assumption:

(H2) There exists a unique solution to the Dirichlet PML problem (2.23) in the layer.

For any $\varphi \in H^1(\Omega^{\rm PML})$, define

$$\|\,\varphi\,\|_{*,\Omega^{\rm PML}} = \left[\int_R^\rho \int_0^{2\pi} \left(\frac{1+\sigma\hat\sigma}{1+\sigma^2} r \left|\frac{\partial \varphi}{\partial r}\right|^2 + \frac{1+\sigma\hat\sigma}{1+\hat\sigma^2}\frac{1}{r}\left|\frac{\partial \varphi}{\partial \theta}\right|^2 + (1+\sigma\hat\sigma)k^2 r|\varphi|^2\right)\right]^{1/2}.$$

It is easy to see that $\|\cdot\|_{*,\Omega^{\rm PML}}$ is an equivalent norm on $H^1(\Omega^{\rm PML})$. By using the general theory in [1, Chapter 5], (H2) implies that there exists a constant $\hat C > 0$ such that

$$\sup_{0\ne\psi\in H_0^1(\Omega^{\rm PML})} \frac{|\hat b(\varphi,\psi)|}{\|\,\psi\,\|_{*,\Omega^{\rm PML}}} \ge \hat C \|\,\varphi\,\|_{*,\Omega^{\rm PML}} \quad \forall \varphi \in H_0^1(\Omega^{\rm PML}). \tag{2.25}$$

The constant $\hat C$ depends in general on the domain $\Omega^{\rm PML}$ and the wave number k. In the appendix of the paper, however, we will show that for sufficiently large σ_0, (H2) can be proved and $\hat C$ can be chosen as independent of $\Omega^{\rm PML}$ and k. Without loss of generality we assume $\hat C \le 1$.

To proceed, we introduce the following notation. For any function ξ defined on a circle $\Gamma_a = \{x \in \mathbb{R}^2 : |x| = a\}$ having the Fourier expansion:

$$\xi = \sum_{n\in\mathbb{Z}} \hat\xi_n e^{\mathbf{i}n\theta}, \quad \hat\xi_n = \frac{1}{2\pi}\int_0^{2\pi} \xi e^{-\mathbf{i}n\theta} d\theta,$$

we define

$$\|\,\xi\,\|^2_{H^{1/2}(\Gamma_a)} = 2\pi \sum_{n\in\mathbb{Z}} (1+n^2)^{1/2}|\hat\xi_n|^2, \quad \|\,\xi\,\|^2_{H^{-1/2}(\Gamma_a)} = 2\pi \sum_{n\in\mathbb{Z}} (1+n^2)^{-1/2}|\hat\xi_n|^2.$$

The following theorem is the main objective of this subsection.

THEOREM 2.4. *Let* (H1)-(H2) *be satisfied. There exists a constant* $C > 0$ *independent of* $k, R, \rho,$ *and* σ_0 *such that the following estimates are satisfied*

$$\| \, |\alpha|^{-1} \nabla w \, \|_{L^2(\Omega^{\rm PML})} \le C\hat{C}^{-1}(1+kR)|\alpha_0| \| \, q \, \|_{H^{1/2}(\Gamma_\rho)}, \tag{2.26}$$

$$\left\| \frac{\partial w}{\partial \mathbf{n}} \right\|_{H^{-1/2}(\Gamma_R)} \le C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2 \| \, q \, \|_{H^{1/2}(\Gamma_\rho)}, \tag{2.27}$$

where $\alpha_0 = 1 + \mathbf{i}\sigma_0$.

Proof. We first show that there exists a constant C independent of k, ρ, R and σ_0 such that

$$|\hat{b}(\varphi, \psi)| \le C(1+kR)|\alpha_0| \| \, \psi \, \|_{*,\Omega^{\rm PML}} |||\varphi|||_{H^1(\Omega^{\rm PML})}, \tag{2.28}$$

where $|||\varphi|||_{H^1(\Omega^{\rm PML})} = (\| \, \nabla\varphi \, \|^2_{L^2(\Omega^{\rm PML})} + R^{-2} \| \, \varphi \, \|^2_{L^2(\Omega^{\rm PML})})^{1/2}$ is the weighted H^1-norm. In fact, since $\hat{\sigma} \le \sigma \le \sigma_0$, we have

$$\begin{aligned}
&\left| \int_R^\rho \int_0^{2\pi} \left(\frac{\beta}{\alpha} r \frac{\partial \varphi}{\partial r} \frac{\partial \bar{\psi}}{\partial r} + \frac{\alpha}{\beta r} \frac{\partial \varphi}{\partial \theta} \frac{\partial \bar{\psi}}{\partial \theta} - \alpha\beta k^2 r \varphi \bar{\psi} \right) dr \, d\theta \right| \\
\le& \left(\int_R^\rho \int_0^{2\pi} \frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left| \frac{\partial \psi}{\partial r} \right|^2 \right)^{1/2} \left(\int_R^\rho \int_0^{2\pi} \frac{1+\hat{\sigma}^2}{1+\sigma\hat{\sigma}} r \left| \frac{\partial \varphi}{\partial r} \right|^2 \right)^{1/2} \\
&+ \left(\int_R^\rho \int_0^{2\pi} \frac{1+\sigma\hat{\sigma}}{1+\hat{\sigma}^2} \frac{1}{r} \left| \frac{\partial \psi}{\partial \theta} \right|^2 \right)^{1/2} \left(\int_R^\rho \int_0^{2\pi} \frac{1+\sigma^2}{1+\sigma\hat{\sigma}} \frac{1}{r} \left| \frac{\partial \varphi}{\partial \theta} \right|^2 \right)^{1/2} \\
&+ \left(\int_R^\rho \int_0^{2\pi} k^2(1+\sigma\hat{\sigma}) r |\psi|^2 \right)^{1/2} \left(\int_R^\rho \int_0^{2\pi} k^2 r \frac{|\alpha\beta|^2}{1+\sigma\hat{\sigma}} |\varphi|^2 \right)^{1/2} \\
\le& \, C(1+kR)|\alpha_0| \| \, \psi \, \|_{*,\Omega^{\rm PML}} |||\varphi|||_{H^1(\Omega^{\rm PML})}.
\end{aligned}$$

This implies the estimate (2.28).

Now we turn to the proof the estimate (2.26). Let $\psi \in H^1(\Omega^{\rm PML})$ such that $\psi = 0$ on Γ_R and $\psi = q$ on Γ_ρ. By taking $\varphi = w - \psi \in H_0^1(\Omega^{\rm PML})$ in (2.23), we know from (2.28) that

$$|\hat{b}(\varphi, \varphi)| = |\hat{b}(w - \psi, \varphi)| = |\hat{b}(\psi, \varphi)| \le C(1+kR)|\alpha_0| \| \, \varphi \, \|_{*,\Omega^{\rm PML}} |||\psi|||_{H^1(\Omega^{\rm PML})},$$

which implies by (2.25) that

$$\| \, \varphi \, \|_{*,\Omega^{\rm PML}} \le C\hat{C}^{-1}(1+kR)|\alpha_0| |||\psi|||_{H^1(\Omega^{\rm PML})}.$$

Notice that

$$\| \, \psi \, \|_{*,\Omega^{\rm PML}} \le C(1+kR)|\alpha_0| |||\psi|||_{H^1(\Omega^{\rm PML})},$$

we get

$$\| \, w \, \|_{*,\Omega^{\rm PML}} = \| \, \varphi + \psi \, \|_{*,\Omega^{\rm PML}} \le C\hat{C}^{-1}(1+kR)|\alpha_0| |||\psi|||_{H^1(\Omega^{\rm PML})}.$$

Since the above estimate is valid for any $\psi \in H^1(\Omega^{\rm PML})$ such that $\psi = 0$ on Γ_R, $\psi = q$ on Γ_ρ, we deduce by standard scaling argument using the assumption $\rho \le CR$ that

$$\| \, w \, \|_{*,\Omega^{\rm PML}} \le C\hat{C}^{-1}(1+kR)|\alpha_0| \| \, q \, \|_{H^{1/2}(\Gamma_\rho)}. \tag{2.29}$$

This shows the estimate (2.26) upon using (2.24).

To show (2.27) we multiply the equation (2.21a) by any function $\varphi \in H^1(\Omega^{\rm PML})$ such that $\varphi = 0$ on Γ_ρ and integrate over $\Omega^{\rm PML}$ to obtain

$$-\int_{\Omega^{\rm PML}} A\nabla w \cdot \nabla\varphi dx - \int_{\Gamma_R} \frac{\partial w}{\partial r}\varphi ds + \int_{\Omega^{\rm PML}} \alpha\beta k^2 w\varphi dx = 0.$$

Thus

$$\left|\int_{\Gamma_R} \frac{\partial w}{\partial r}\varphi ds\right| = |\hat{b}(w,\bar{\varphi})| \le C(1+kR)|\alpha_0| \| w \|_{*,\Omega^{\rm PML}} |||\varphi|||_{H^1(\Omega^{\rm PML})},$$

for any $\varphi \in H^1(\Omega^{\rm PML})$ such that $\varphi = 0$ on Γ_ρ. This implies by (2.29) that

$$\left|\int_{\Gamma_R} \frac{\partial w}{\partial r}\varphi ds\right| \le C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2 \| q \|_{H^{1/2}(\Gamma_\rho)} \|\varphi\|_{H^{1/2}(\Gamma_R)} \quad \forall \varphi \in H^{1/2}(\Gamma_R).$$

This completes the proof of the theorem. ☐

2.3. Convergence of the PML problem. In this subsection we consider the convergence of the PML problem (2.12) to the original scattering problem (2.4). Following an idea in [13], for any function $f \in H^{1/2}(\Gamma_R)$, we introduce the propagation operator $P : H^{1/2}(\Gamma_R) \to H^{1/2}(\Gamma_\rho)$:

$$P(f) = \sum_{n\in\mathbb{Z}} \frac{H_n^{(1)}(k\tilde{\rho})}{H_n^{(1)}(kR)}\hat{f}_n e^{\mathbf{i}n\theta}, \qquad \hat{f}_n = \frac{1}{2\pi}\int_0^{2\pi} f e^{-\mathbf{i}n\theta} d\theta. \tag{2.30}$$

By Lemma 2.2, it is easy to see that $P : H^{1/2}(\Gamma_R) \to H^{1/2}(\Gamma_\rho)$ is well-defined, and

$$\| P(f) \|_{H^{1/2}(\Gamma_\rho)} \le e^{-k{\rm Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \| f \|_{H^{1/2}(\Gamma_R)} \quad \forall r \ge R. \tag{2.31}$$

Moreover, by Theorem 2.4, under the assumptions (H1)-(H2), the operator $\hat{T} : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$, which is defined through the Dirichlet problem of the PML equation in the layer, is also well-defined. Furthermore, we have the following estimate.

Lemma 2.5. *Let* (H1)-(H2) *be satisfied. We have*

$$\| Tf - \hat{T}f \|_{H^{-1/2}(\Gamma_R)} \le C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2 e^{-k{\rm Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \| f \|_{H^{1/2}(\Gamma_R)}.$$

Proof. For any $f \in H^{1/2}(\Gamma_R)$, we know that

$$Tf - \hat{T}f = \frac{\partial w}{\partial \mathbf{n}}\Big|_{\Gamma_R},$$

where $w \in H^1(\Omega^{\rm PML})$ satisfies

$$\nabla\cdot(A\nabla w) + \alpha\beta k^2 w = 0 \quad \text{in } \Omega^{\rm PML},$$
$$w = 0 \ \text{ on } \Gamma_R, \qquad w = P(f) \ \text{ on } \Gamma_\rho.$$

By (2.27) and (2.31) we then have

$$\left\| \frac{\partial w}{\partial \mathbf{n}} \right\|_{H^{-1/2}(\Gamma_R)} \le C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2 \| P(f) \|_{H^{1/2}(\Gamma_\rho)}$$
$$\le C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2 e^{-k\mathrm{Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \| f \|_{H^{1/2}(\Gamma_R)}.$$

This completes the proof. $\square$

The following theorem is the main results of this section.

THEOREM 2.6. *Let (H1)-(H2) be satisfied. Then for sufficiently large $\sigma_0 > 0$, the PML problem* (2.12) *has a unique solution $\hat{u} \in H^1(\Omega_\rho)$. Moreover, we have the following estimate*

$$\| u - \hat{u} \|_{H^1(\Omega_R)} \le C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2 e^{-k\mathrm{Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \| \hat{u} \|_{H^{1/2}(\Gamma_R)}. \quad (2.32)$$

Proof. The existence of a unique solution for (2.12) follows from Lemma 2.5 by using the same argument as in [8, Theorem 2.4]. Next, by (2.4) and (2.12), we have

$$a(u-\hat{u},\varphi) = \hat{a}(\hat{u},\varphi) - a(\hat{u},\varphi) = \langle T\hat{u} - \hat{T}\hat{u}, \varphi\rangle_{\Gamma_R} \quad \forall \varphi \in H^1(\Omega^{\mathrm{PML}}).$$

This implies the desired estimate (2.32) upon using Lemma 2.5 and (2.5). $\square$

3. Finite element approximations. In this section we introduce the finite element approximations of the PML problems (2.9a)-(2.9b). From now on we assume $g \in L^2(\Gamma_D)$. Let $b : H^1(\Omega_\rho) \times H^1(\Omega_\rho) \to \mathbb{C}$ be the sesquilinear form given by

$$b(\varphi,\psi) = \int_{\Omega_\rho} \left(A\nabla\varphi \cdot \nabla\bar{\psi} - \alpha\beta k^2 \varphi\bar{\psi} \right) dx. \quad (3.1)$$

Denote by $H^1_{(0)}(\Omega_\rho) = \{v \in H^1(\Omega_\rho) : v = 0 \text{ on } \Gamma_\rho\}$. Then the weak formulation of (2.9a)-(2.9b) is: Given $g \in L^2(\Gamma_D)$, find $\hat{u} \in H^1_{(0)}(\Omega_\rho)$ such that

$$b(\hat{u},\psi) = \int_{\Gamma_D} g\bar{\psi} ds \quad \forall \psi \in H^1_{(0)}(\Omega_\rho). \quad (3.2)$$

Let Γ_ρ^h, which consists of piecewise segments whose vertices lie on Γ_ρ, be an approximation of Γ_ρ. Let Ω_ρ^h be the subdomain of Ω_ρ bounded by Γ_D and Γ_ρ^h. Let $\mathcal{M}_h$ be a regular triangulation of the domain Ω_ρ^h. We assume the elements $K \in \mathcal{M}_h$ may have one curved edge align with Γ_D so that $\Omega_\rho^h = \cup_{K\in\mathcal{M}_h} K$.

Let $V_h \subset H^1(\Omega_\rho^h)$ be the conforming linear finite element space over Ω_ρ^h, and $\overset{\circ}{V}_h = \{v_h \in V_h : v_h = 0 \text{ on } \Gamma_\rho^h\}$. In the following we will always assume that the functions in $\overset{\circ}{V}_h$ are extended to the domain Ω_ρ by zero so that any function $v_h \in \overset{\circ}{V}_h$ is also a function in $H^1_{(0)}(\Omega_\rho)$. The finite element approximation to the PML problem (2.9a)-(2.9b) reads as follows: Find $u_h \in \overset{\circ}{V}_h$ such that

$$b(u_h,\psi_h) = \int_{\Gamma_D} g\bar{\psi}_h ds \quad \forall\, \psi_h \in \overset{\circ}{V}_h. \quad (3.3)$$

Following the general theory in [1, Chap. 5], the existence of unique solution of the discrete problem (3.3) and the finite element convergence analysis depend on the following discrete inf-sup condition

$$\sup_{0\neq\psi_h\in\overset{\circ}{V}_h}\frac{|b(\varphi_h,\psi_h)|}{\|\,\psi_h\,\|_{H^1(\Omega_\rho)}}\geq\hat{\mu}\;\|\,\varphi_h\,\|_{H^1(\Omega_\rho)}\quad\forall\;\varphi_h\in\overset{\circ}{V}_h,\tag{3.4}$$

where the constant $\hat{\mu}>0$ is independent of the finite element mesh size. Since the continuous problem (3.2) has a unique solution by Theorem 2.6, the sesquilinear form $b\,:\,H^1_{(0)}(\Omega_\rho)\times H^1_{(0)}(\Omega_\rho)\to\mathbb{C}$ satisfies the continuous inf-sup condition. Then a general argument of Schatz [18] implies (3.4) is valid for sufficiently small mesh size $h<h^*$. Based on (3.4), appropriate a priori error estimate can also be derived which depends on the regularity of the PML solution $\hat{u}$. In this paper, we are interested in a posterior error estimates and the associated adaptive algorithm. Thus in the following we simply assume the discrete problem (3.3) has a unique solution $u_h\in\overset{\circ}{V}_h$.

For any $K\in\mathcal{M}_h$, we denote by h_K its diameter. Let $\mathcal{B}_h$ denote the set of all sides that do not lie on Γ_D and Γ^h_ρ. For any $e\in\mathcal{B}_h$, h_e stands for its length. For any $K\in\mathcal{M}_h$, we introduce the residual:

$$R_h:=\nabla\cdot(A\nabla u_h|_K)+\alpha\beta k^2u_h|_K.\tag{3.5}$$

For any interior side $e\in\mathcal{B}_h$ which is the common side of K_1 and $K_2\in\mathcal{M}_h$, we define the jump residual across e:

$$J_e:=(A\nabla u_h|_{K_1}-A\nabla u_h|_{K_2})\cdot\nu_e,\tag{3.6}$$

using the convention that the unit normal vector ν_e to e points from K_2 to K_1. If $e=\Gamma_D\cap\partial K$ for some element $K\in\mathcal{M}_h$, then we define the jump residual

$$J_e:=2(\nabla u_h|_K\cdot\mathbf{n}+g)\tag{3.7}$$

For any $K\in\mathcal{M}_h$, denote by η_K the local error estimator which is defined by

$$\eta_K=\max_{x\in\tilde{K}}\omega(x)\cdot\left(\|h_KR_h\|^2_{L^2(K)}+\frac{1}{2}\sum_{e\subset\partial K}h_e\|\,J_e\,\|^2_{L^2(e)}\right)^{1/2},\tag{3.8}$$

where $\tilde{K}$ is the union of all elements having nonempty intersection with K, and

$$\omega(x)=\begin{cases}1 & \text{if } x\in\overline{\Omega_R},\\ |\alpha_0\alpha|e^{-k\mathrm{Im}\,(\tilde{r})\left(1-\frac{r^2}{|\tilde{r}|^2}\right)^{1/2}} & \text{if } x\in\Omega^{\mathrm{PML}},\end{cases}$$

The following theorem is the main result of this paper.

THEOREM 3.1. *There exists a constant C depending only on the minimum angle of the mesh $\mathcal{M}_h$ such that the following a posterior error estimate is valid*

$$\|\,u-u_h\,\|_{H^1(\Omega_R)}\leq C\hat{C}^{-1}\Lambda(kR)^{1/2}(1+kR)\left(\sum_{K\in\mathcal{M}_h}\eta^2_K\right)^{1/2}$$
$$+C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2e^{-k\mathrm{Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}}\|\,u_h\,\|_{H^{1/2}(\Gamma_R)}.\tag{3.9}$$

Here $\Lambda(kR)$ is defined in Lemma 4.3 below.

The proof of this theorem will be given in §4. The important exponentially decaying factor $e^{-k\mathrm{Im}\,(\tilde{r})\left(1-\frac{r^2}{|\tilde{r}|^2}\right)^{1/2}}$ in the PML region Ω^{PML} allows us to take thicker PML layers without introducing unnecessary fine meshes away from the fixed domain Ω_R. Recall that thicker PML layers allow smaller PML medium property, which enhances numerical stability.

4. A posteriori error estimates. In this section we prove the a posteriori error estimates in Theorem 3.1.

4.1. Error representation formula. For any $\varphi \in H^1(\Omega_R)$, let $\tilde{\varphi}$ be its extension in Ω^{PML} such that

$$\nabla\cdot(\bar{A}\nabla\tilde{\varphi}) + \overline{\alpha\beta}k^2\tilde{\varphi} = 0 \quad \text{in } \Omega^{\mathrm{PML}}, \tag{4.1a}$$

$$\tilde{\varphi} = \varphi \ \text{ on } \Gamma_R, \quad \tilde{\varphi} = 0 \ \text{ on } \Gamma_\rho. \tag{4.1b}$$

LEMMA 4.1. *Let* (H2) *be satisfied. For any $\varphi, \psi \in H^1(\Omega^{\mathrm{PML}})$, we have*

$$\langle \hat{T}\varphi, \psi\rangle_{\Gamma_R} = \langle \hat{T}\bar{\psi}, \bar{\varphi}\rangle_{\Gamma_R}.$$

Proof. By definition, $\hat{T}\varphi = \partial w/\partial \mathbf{n}$ on Γ_R, where w satisfies

$$\nabla\cdot(A\nabla w) + \alpha\beta k^2 w = 0 \quad \text{in } \Omega^{\mathrm{PML}},$$
$$w = \varphi \ \text{ on } \Gamma_R, \quad w = 0 \ \text{ on } \Gamma_\rho.$$

Thus

$$w(x) = \sum_{n\in\mathbb{Z}} \left(a_n H_n^{(1)}(k\tilde{r}) + b_n H_n^{(2)}(k\tilde{r})\right) e^{\mathbf{i}n\theta}$$

with the coefficients a_n, b_n being determined by the boundary conditions in (4.1b)

$$a_n H_n^{(1)}(kR) + b_n H_n^{(2)}(kR) = \hat{\varphi}_n, \quad a_n H_n^{(1)}(k\tilde{\rho}) + b_n H_n^{(2)}(k\tilde{\rho}) = 0,$$

where $\hat{\varphi}_n = \frac{1}{2\pi}\int_0^{2\pi}\varphi(R,\theta)e^{-\mathbf{i}n\theta}d\theta$ is the n-th Fourier coefficient of $\varphi|_{\Gamma_R}$. Denote by

$$H_n(k\tilde{r}) = H_n^{(1)}(k\tilde{r})H_n^{(2)}(k\tilde{\rho}) - H_n^{(2)}(k\tilde{r})H_n^{(1)}(k\tilde{\rho}).$$

Then since by (H2) the Dirichlet PML problem in the layer has a unique solution, we get $H_n(kR) \neq 0$, and

$$a_n = \frac{H_n^{(2)}(k\tilde{\rho})}{H_n(kR)}\hat{\varphi}_n, \quad b_n = -\frac{H_n^{(1)}(k\tilde{\rho})}{H_n(kR)}\hat{\varphi}_n.$$

Thus

$$w = w(r,\theta) = \sum_{n\in\mathbb{Z}} \frac{H_n(k\tilde{r})}{H_n(kR)}\hat{\varphi}_n e^{\mathbf{i}n\theta},$$

which, since $\tilde{r}'(R) = \alpha(R) = 1$ and $\tilde{R} = R$, implies

$$\hat{T}\varphi|_{\Gamma_R} = \sum_{n\in\mathbb{Z}} k\frac{H_n'(kR)}{H_n(kR)}\hat{\varphi}_n e^{\mathbf{i}n\theta}.$$

Therefore

$$\langle \hat{T}\varphi, \psi\rangle_{\Gamma_R} = \sum_{n\in\mathbb{Z}} k\frac{H_n'(kR)}{H_n(kR)}\hat{\varphi}_n\bar{\hat{\psi}}_n \quad \forall \varphi, \psi \in H^1(\Omega^{\mathrm{PML}}).$$

This completes the proof. ◻

Whenever no confusion of the notation incurred, we shall write in the following $\tilde{\varphi}$ as φ in Ω^{PML}.

LEMMA 4.2 (Error representational formula). *For any $\varphi \in H^1(\Omega_R)$, which is extended to be a function in $H^1(\Omega_\rho)$ according to* (4.1a)-(4.1b), *and $\varphi_h \in \overset{\circ}{V}_h$, we have*

$$a(u-u_h, \varphi) = \int_{\Gamma_D} g(\overline{\varphi - \varphi_h}) - b(u_h, \varphi - \varphi_h) + \langle Tu_h - \hat{T}u_h, \varphi\rangle_{\Gamma_R}. \tag{4.2}$$

Proof. By (2.4) and the definitions (2.3) and (3.1),

$$\begin{aligned} & a(u-u_h,\varphi) \\ &= \int_{\Gamma_D} g\bar{\varphi} - \int_{\Omega_R} (A\nabla u_h \cdot \nabla\bar{\varphi} - \alpha\beta k^2 u_h\bar{\varphi}) + \langle Tu_h, \varphi\rangle_{\Gamma_R} \\ &= \int_{\Gamma_D} g\bar{\varphi} - b(u_h,\varphi) + \int_{\Omega^{\mathrm{PML}}} (A\nabla u_h \cdot \nabla\bar{\tilde{\varphi}} - \alpha\beta k^2 u_h\bar{\tilde{\varphi}}) + \langle Tu_h, \varphi\rangle_{\Gamma_R}. \end{aligned} \tag{4.3}$$

On the other hand, by multiplying (4.1a) by $\bar{u}_h$, integrating by parts, and recalling that $\mathbf{n}$ is the unit outer normal to Γ_R which points outside Ω_R, we deduce that

$$-\int_{\Omega^{\mathrm{PML}}} (\bar{A}\nabla\tilde{\varphi} \cdot \nabla\bar{u}_h - \overline{\alpha\beta}k^2\tilde{\varphi}\bar{u}_h) - \left\langle \frac{\partial\tilde{\varphi}}{\partial\mathbf{n}}, u_h \right\rangle_{\Gamma_R} = 0,$$

which is equivalent to

$$\int_{\Omega^{\mathrm{PML}}} (A\nabla u_h \cdot \nabla\bar{\tilde{\varphi}} - \alpha\beta k^2 u_h\bar{\tilde{\varphi}}) = -\left\langle \frac{\partial\bar{\tilde{\varphi}}}{\partial\mathbf{n}}, \bar{u}_h \right\rangle_{\Gamma_R}. \tag{4.4}$$

Since by the definition of $\hat{T} : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$,

$$\frac{\partial\bar{\tilde{\varphi}}}{\partial\mathbf{n}}\Big|_{\Gamma_R} = \hat{T}\bar{\varphi},$$

we obtain by substituting (4.4) into (4.3) that

$$a(u-u_h,\varphi) = \int_{\Gamma_D} g\bar{\varphi} - b(u_h,\varphi) + \langle Tu_h, \varphi\rangle - \langle \hat{T}\bar{\varphi}, \bar{u}_h\rangle.$$

This completes the proof upon using Lemma 4.1 and (3.3). ◻

4.2. Estimates for the extension. For any $\varphi \in H^1(\Omega_R)$, we define, for $r \ge R$,

$$\phi = \phi(r,\theta) = \sum_{n\in\mathbb{Z}} \frac{H_n^{(1)}(k\tilde{r})}{H_n^{(1)}(kR)}\bar{\hat{\varphi}}_n e^{\mathbf{i}n\theta}, \quad \hat{\varphi}_n = \frac{1}{2\pi}\int_0^{2\pi} \varphi(R,\theta)e^{-\mathbf{i}n\theta}d\theta. \tag{4.5}$$

The function ϕ satisfies

$$\nabla \cdot (A\nabla\phi) + \alpha\beta k^2\phi = 0 \quad \text{in } \mathbb{R}^2\backslash \bar{B}_R, \tag{4.6a}$$

$$\phi = \bar{\varphi} \quad \text{on } \Gamma_R, \tag{4.6b}$$

$$|\phi| \text{ is uniformly bounded as } r = |x| \to \infty. \tag{4.6c}$$

By Lemma 2.2, it is easy to see that

$$\|\,\phi\,\|_{H^{1/2}(\Gamma_\rho)} \le e^{-k\mathrm{Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \|\,\varphi\,\|_{H^{1/2}(\Gamma_R)}. \tag{4.7}$$

Set

$$\gamma(r) = e^{k\mathrm{Im}\,(\tilde{r})\left(1-\frac{r^2}{|\tilde{r}|^2}\right)^{1/2}}.$$

Since $\tilde{r} = r(1 + \mathbf{i}\hat{\sigma})$, we obatin by simple calculation that

$$\gamma'(r) = \gamma(r) \cdot k\left(\frac{\sigma\hat{\sigma}}{(1+\hat{\sigma}^2)^{1/2}} + \frac{r\hat{\sigma}\hat{\sigma}'}{(1+\hat{\sigma}^2)^{3/2}}\right),$$

which, together with $r\hat{\sigma}' = \sigma - \hat{\sigma} \le \sigma$, implies

$$0 \le \gamma'(r) \le 2\sigma k\gamma(r) \quad \forall r \ge R. \tag{4.8}$$

Lemma 4.3. *Let* $\Lambda(kR) = max\left(1, \frac{|H_0^{(1)\prime}(kR)|}{|H_0^{(1)}(kR)|}\right)$. *Then there exists a constant* $C > 0$ *independent of* $k, R, \rho,$ *and* σ_0 *such that*

$$\|\,|\alpha|^{-1}\gamma\nabla\phi\,\|_{L^2(\Omega^{\mathrm{PML}})} \le C\Lambda(kR)^{1/2}(1 + kR)|\alpha_0|\|\,\varphi\,\|_{H^{1/2}(\Gamma_R)}.$$

Proof. We multiply (4.6a) by $\gamma^2\bar{\phi}$ and integrate over Ω^{PML} to obtain

$$\begin{aligned}
&\int_R^\rho \int_0^{2\pi} \gamma^2\left(\frac{\beta r}{\alpha}\left|\frac{\partial\phi}{\partial r}\right|^2 + \frac{\alpha}{\beta r}\left|\frac{\partial\phi}{\partial\theta}\right|^2\right) dr\,d\theta \\
&= -\int_R^\rho \int_0^{2\pi} \left(\frac{\beta r}{\alpha}\frac{\partial\phi}{\partial r}(\gamma^2)'\bar{\phi} - \alpha\beta k^2 r\gamma^2|\phi|^2\right) dr\,d\theta \\
&\quad + \int_0^{2\pi}\left[\frac{\beta r}{\alpha}\gamma^2\frac{\partial\phi}{\partial r}\bar{\phi}\right](\rho)d\theta - \int_0^{2\pi}\left[\frac{\beta r}{\alpha}\gamma^2\frac{\partial\phi}{\partial r}\bar{\phi}\right](R)d\theta.
\end{aligned}$$

Taking the real part of the equation we get

$$\begin{aligned}
&\int_R^\rho \int_0^{2\pi} \gamma^2\left(\frac{1+\sigma\hat{\sigma}}{1+\sigma^2}r\left|\frac{\partial\phi}{\partial r}\right|^2 + \frac{1+\sigma\hat{\sigma}}{1+\hat{\sigma}^2}\frac{1}{r}\left|\frac{\partial\phi}{\partial\theta}\right|^2\right) dr\,d\theta \\
&\le \int_R^\rho \int_0^{2\pi} \left|\frac{\beta r}{\alpha}\frac{\partial\phi}{\partial r}2\gamma\gamma'\bar{\phi}\right| dr\,d\theta + \int_R^\rho \int_0^{2\pi} |\alpha\beta|k^2 r\gamma^2|\phi|^2 dr\,d\theta \\
&\quad + \int_0^{2\pi}\left|\left[\frac{\beta r}{\alpha}\gamma^2\frac{\partial\phi}{\partial r}\bar{\phi}\right](\rho)\right| d\theta + \int_0^{2\pi}\left|\left[\frac{\beta r}{\alpha}\gamma^2\frac{\partial\phi}{\partial r}\bar{\phi}\right](R)\right| d\theta. \\
&:= \mathrm{I}_1 + \cdots + \mathrm{I}_4.
\end{aligned} \tag{4.9}$$

Since $\gamma' \le 2k\sigma\gamma$ by (4.8), we obtain by Cauchy-Schwarz inequality and the fact $\hat{\sigma} \le \sigma$ that

$$\begin{aligned}
\mathrm{I}_1 &\le \left(\int_R^\rho \int_0^{2\pi} \gamma^2 \frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left| \frac{\partial \phi}{\partial r} \right|^2 \right)^{1/2} \left(\int_R^\rho \int_0^{2\pi} 16k^2\sigma^2\gamma^2 \left| \frac{\beta}{\alpha} \right|^2 \frac{1+\sigma^2}{1+\sigma\hat{\sigma}}\ r|\phi|^2 \right)^{1/2} \\
&\le 4 \left(\int_R^\rho \int_0^{2\pi} \gamma^2 \frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left| \frac{\partial \phi}{\partial r} \right|^2 dr\, d\theta \right)^{1/2} \left(\int_R^\rho \int_0^{2\pi} k^2\sigma^2\gamma^2 r|\phi|^2 dr\, d\theta \right)^{1/2}.
\end{aligned}$$

On the other hand, by (4.5) and Lemma 2.2, we know that

$$\begin{aligned}
\int_R^\rho \int_0^{2\pi} k^2\sigma^2\gamma^2 r|\phi|^2 dr\, d\theta &= 2\pi \sum_{n\in\mathbb{Z}} \int_R^\rho k^2\sigma^2\gamma^2 r \left| \frac{H_n^{(1)}(k\tilde{r})}{H_n^{(1)}(kR)} \right|^2 dr \cdot |\hat{\phi}_n|^2 \\
&\le 2\pi \sum_{n\in\mathbb{Z}} \int_R^\rho k^2\sigma^2 r dr \cdot |\hat{\phi}_n|^2 \\
&\le C(1+kR)^2 |\alpha_0|^2 \| \phi \|^2_{L^2(\Gamma_R)}. \qquad (4.10)
\end{aligned}$$

Hence

$$\mathrm{I}_1 \le \frac{1}{2} \int_R^\rho \int_0^{2\pi} \gamma^2 \frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left| \frac{\partial \phi}{\partial r} \right|^2 dr\, d\theta + C(1+kR)^2 |\alpha_0|^2 \| \phi \|^2_{L^2(\Gamma_R)}.$$

By (4.10) we also have

$$\mathrm{I}_2 \le C(1+kR)^2 |\alpha_0|^2 \| \phi \|^2_{L^2(\Gamma_R)}.$$

Next, since $\tilde{r}'(r) = \alpha(r)$, by (4.5) and Lemma 2.3, we have

$$\begin{aligned}
\mathrm{I}_3 &\le 2\pi \sum_{n\in\mathbb{Z}} \left| k\rho\beta(\rho)\gamma(\rho)^2 \frac{H_n^{(1)\prime}(k\tilde{\rho})}{H_n^{(1)}(kR)} \frac{H_n^{(1)}(k\tilde{\rho})}{H_n^{(1)}(kR)} \right| \cdot |\hat{\phi}_n|^2 \\
&\le 2\pi|\alpha_0| \sum_{n\ne 0} k\rho \left(1 + \frac{|n|}{|k\tilde{\rho}|} \right) |\hat{\phi}_n|^2 + 2\pi|\alpha_0| k\rho \left| \frac{H_0^{(1)\prime}(kR)}{H_0^{(1)}(kR)} \right| \cdot |\hat{\phi}_0|^2 \\
&\le 2\pi|\alpha_0| \sum_{n\ne 0} (k\rho + |n|) |\hat{\phi}_n|^2 + 2\pi|\alpha_0| k\rho\Lambda(kR) |\hat{\phi}_0|^2,
\end{aligned}$$

where in the last inequality we have used the relation $\rho \le |\tilde{\rho}|$. Since $k\rho + |n| \le (1+k\rho)(1+n^2)^{1/2}$, we deduce finally

$$\mathrm{I}_3 \le C\Lambda(kR)(1+k\rho)|\alpha_0| \| \phi \|^2_{H^{1/2}(\Gamma_R)} \le C\Lambda(kR)(1+kR)|\alpha_0| \| \phi \|^2_{H^{1/2}(\Gamma_R)}.$$

Similarly, we can prove

$$\mathrm{I}_4 \le C\Lambda(kR)(1+kR) \| \phi \|^2_{H^{1/2}(\Gamma_R)}.$$

Substituting the estimates for $\mathrm{I}_1, \cdots, \mathrm{I}_4$ into (4.9), we conclude that

$$\begin{aligned}
&\int_R^\rho \int_0^{2\pi} \gamma^2 \left(\frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left| \frac{\partial \phi}{\partial r} \right|^2 + \frac{1+\sigma\hat{\sigma}}{1+\hat{\sigma}^2} \frac{1}{r} \left| \frac{\partial \phi}{\partial \theta} \right|^2 \right) dr\, d\theta \\
&\le C\Lambda(kR)(1+kR)^2 |\alpha_0|^2 \| \phi \|^2_{H^{1/2}(\Gamma_R)}.
\end{aligned}$$

This completes the proof. □

The following lemma is the main objective of this subsection.

LEMMA 4.4. *For any $\varphi \in H^1(\Omega_R)$, which is extended to be a function $\tilde{\varphi} \in H^1(\Omega^{\rm PML})$ according to* (4.1a)-(4.1b)*, we have the following estimate*

$$\| \, |\alpha|^{-1}\gamma\nabla\tilde{\varphi} \,\|_{L^2(\Omega^{\rm PML})} \le C\hat{C}^{-1}\Lambda(kR)^{1/2}(1+kR)|\alpha_0| \| \, \varphi \, \|_{H^{1/2}(\Gamma_R)}.$$

Proof. Let $w = \tilde{\varphi} - \bar{\phi}$, then from (4.1a)-(4.1b) and (4.6a)-(4.6b) we know that w satisfies

$$\nabla\cdot(A\nabla w) + \alpha\beta k^2 w = 0 \quad \text{in } \Omega^{\rm PML},$$
$$w = 0 \ \text{ on } \Gamma_R, \qquad w = -\bar{\phi} \ \text{ on } \Gamma_\rho.$$

By Theorem 2.4 and (4.7) we have

$$\begin{aligned}\| \, |\alpha|^{-1}\nabla w \,\|_{L^2(\Omega^{\rm PML})} &\le C\hat{C}^{-1}(1+kR)|\alpha_0| \| \, w \,\|_{H^{1/2}(\Gamma_\rho)} \\ &= C\hat{C}^{-1}(1+kR)|\alpha_0| \| \, \phi \,\|_{H^{1/2}(\Gamma_\rho)} \\ &\le C\hat{C}^{-1}(1+kR)|\alpha_0| e^{-k{\rm Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \| \, \varphi \,\|_{H^{1/2}(\Gamma_R)}.\end{aligned}$$

By (4.8), γ is a increasing function, we know that, for $r \le \rho$,

$$\gamma(r) e^{-k{\rm Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \le \gamma(\rho) e^{-k{\rm Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \le 1.$$

Hence

$$\| \, |\alpha|^{-1}\gamma\nabla w \,\|_{L^2(\Omega^{\rm PML})} \le C\hat{C}^{-1}(1+kR)|\alpha_0| \| \, \varphi \,\|_{H^{1/2}(\Gamma_R)}.$$

This completes the proof upon using Lemma 4.3. □

To conclude this subsection we remark that a direct consequence of this lemma is that

$$\| \, \omega^{-1}\nabla\varphi \,\|_{L^2(\Omega^{\rm PML})} \le C\hat{C}^{-1}\Lambda(kR)^{1/2}(1+kR) \| \, \varphi \,\|_{H^{1/2}(\Gamma_R)}. \tag{4.11}$$

4.3. Proof of Theorem 3.1. Since we are going to interpolate nonsmooth functions, we resort to an interpolation operator $\Pi_h : H^1_{(0)}(\Omega_\rho) \to \overset{\circ}{V}_h$ of Clement type [9], where $H^1_{(0)}(\Omega_\rho) = \{v \in H^1(\Omega_\rho) : v = 0 \ \text{ on } \Gamma_\rho\}$. Let $\mathcal{N}_h = \{a_i\}_{i=1}^N$ be the set of the nodes of $\mathcal{M}_h$ which is interior to Ω_ρ^h or on the boundary Γ_D, and $\{\phi_i\}_{i=1}^N$ be the corresponding nodal basis of V_h. Define $\Delta_i = {\rm supp}\,\phi_i \cap \Omega_\rho$. Then the interpolation operator $\Pi_h : H^1_{(0)}(\Omega_\rho) \to V_h$ is defined by

$$\Pi_h v(x) = \sum_{i=1}^N \left(\frac{1}{|\Delta_i|} \int_{\Delta_i} v(x)dx \right) \phi_i(x).$$

Since the nodes on Γ_ρ^h are not included in the definition of Π_h, we know that $\Pi_h v \in \overset{\circ}{V}_h$. Moreover, by slightly modifying the argument in [6, Lemma 3.1 and Lemma 3.2], one can show that the operator Π_h enjoys the following interpolation estimates, for any $v \in H^1_{(0)}(\Omega_\rho)$,

$$\| \, v - \Pi_h v \,\|_{L^2(K)} \le C h_K \| \, \nabla v \,\|_{L^2(\tilde{K})}, \| \, v - \Pi_h v \,\|_{L^2(e)} \le C h_e^{1/2} \| \, \nabla v \,\|_{L^2(\tilde{e})}, \tag{4.12}$$

where $\tilde{K}$ and $\tilde{e}$ are the union of all elements in $\mathcal{M}_h$ having non-empty intersection with $K \in \mathcal{M}_h$ and the side e, respectively.

Now we take $\varphi_h = \Pi_h \varphi \in \overset{\circ}{V}_h$ in the error representation formular (4.2) to get

$$\begin{aligned} a(u-u_h,\varphi) &= \int_{\Gamma_D} g(\overline{\varphi - \Pi_h\varphi}) - b(u_h, \varphi - \Pi_h\varphi) + \langle Tu_h - \hat{T}u_h, \varphi\rangle_{\Gamma_R} \\ &:= \mathrm{II}_1 + \mathrm{II}_2 + \mathrm{II}_3. \end{aligned} \tag{4.13}$$

We observe that, by integration by parts and using (3.5)-(3.7),

$$\mathrm{II}_1 + \mathrm{II}_2 = \sum_{K\in\mathcal{M}_h} \left(\int_K R_h(\overline{\varphi - \Pi_h\varphi})dx + \sum_{e\subset\partial K} \frac{1}{2}\int_e J_e(\overline{\varphi - \Pi_h\varphi})ds \right).$$

Standard argument in the a posteriori error analysis using (4.12) and (4.11) implies

$$\begin{aligned} |\mathrm{II}_1 + \mathrm{II}_2| &\le C \sum_{K\in\mathcal{M}_h} \left(\| h_K R_h \|^2_{L^2(K)} + \frac{1}{2}\sum_{e\subset\partial K} \| h_e^{1/2} J_e \|^2_{L^2(e)} \right)^{1/2} \| \nabla\varphi \|_{L^2(\tilde{K})} \\ &\le C \sum_{K\in\mathcal{M}_h} \eta_K \| \omega^{-1}\nabla\varphi \|_{L^2(\tilde{K})} \\ &\le C\hat{C}^{-1}\Lambda(kR)^{1/2}(1+kR) \left(\sum_{K\in\mathcal{M}_h} \eta_K^2 \right)^{1/2} \| \varphi \|_{H^{1/2}(\Gamma_R)}. \end{aligned}$$

By Lemma 2.5, we obtain

$$|\mathrm{II}_3| \le C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2 e^{-k\mathrm{Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \| u_h \|_{H^{1/2}(\Gamma_R)} \| \varphi \|_{H^{1/2}(\Gamma_R)}.$$

Therefore, by the inf-sup condition (2.5), we finally get

$$\begin{aligned} \| u - u_h \|_{H^1(\Omega_R)} &\le C \sup_{0\ne\varphi\in H^1(\Omega_R)} \frac{|a(u-u_h,\varphi)|}{\| \varphi \|_{H^1(\Omega_R)}} \\ &\le C\hat{C}^{-1}\Lambda(kR)^{1/2}(1+kR) \left(\sum_{K\in\mathcal{M}_h} \eta_K^2 \right)^{1/2} \\ &\quad + C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2 e^{-k\mathrm{Im}\,(\tilde{\rho})\left(1-\frac{R^2}{|\tilde{\rho}|^2}\right)^{1/2}} \| u_h \|_{H^{1/2}(\Gamma_R)}. \end{aligned}$$

This completes the proof. □

5. Implementation and numerical examples. The implementation of the adaptive algorithm in this section is based on the PDE toolbox of MATLAB. We use the a posteriori error estimate in Theorem 3.1 to determine the PML parameters. According to the discussion in §2, we choose the PML medium property as the power function and thus we need only to specify the thickness $\rho - R$ of the layer and the medium parameter σ_0. Recall from Theorem 3.1 that the a posteriori error estimate consists of two parts: the PML error and the finite element discretization error. In our implementation we first choose ρ and σ_0 such that the exponentially decaying factor:

$$\hat{\omega} = e^{-k\mathrm{Im}\,(\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}} \le 10^{-8}, \tag{5.1}$$

which makes the PML error negligible compared with the finite element discretization errors. Once the PML region and the medium property are fixed, we use the standard finite element adaptive strategy to modify the mesh according to the a posteriori error estimate. Now we describe the adaptive algorithm we used in the paper.

Algorithm 5.1. Given tolerance TOL > 0. Let $m = 2$.

- Choose ρ and σ_0 such that the exponentially decaying factor $\hat{\omega} \leq 10^{-8}$;
- Set the computational domain $\Omega_\rho = B_\rho \backslash \bar{\Gamma}_D$ and generate an initial mesh $\mathcal{M}_h$ over Ω_ρ;
- While $\mathcal{E}_{FEM} = \left(\sum_{K\in\mathcal{M}_h} \eta_K^2\right)^{1/2} > \mathrm{TOL}$ do
  - refine the mesh $\mathcal{M}_h$ according to the strategy:

    if $\eta_K > \frac{1}{2}\max_{K\in\mathcal{M}_h} \eta_K$, refine the element $K \in \mathcal{M}_h$

  - solve the discrete problem (3.3) on $\mathcal{M}_h$
  - compute error estimators on $\mathcal{M}_h$

  end while

In the following we report two numerical examples to demonstrate the competitive behavior of the proposed algorithm. In the computations we first prescribe ρ and then determine σ_0 according to (5.1). We scale the error estimator for determining finite element meshes by a factor 0.15 as in the PDE toolbox of MATLAB.

Example 1. Let the scatter D be unit circle. We consider the scattering problem whose exact solution is known: $u = H_0^{(1)}(kr)$, where $r = |x|$. We take $R = 2$, and $k = 1$. Table 5.1 shows the different choices of the PML parameters ρ and σ_0 determined by the relation (5.1).

TABLE 5.1
The PML parameters for Example 1 and Example 2.

Example 1		Example 2	
ρ	σ_0	ρ	σ_0
2R	30	2R	4
3R	15	3R	2
4R	10	4R	1
8R	5		

Figure 5.1 shows the $\log N_k$-$\log \| \nabla(u-u_k) \|_{L^2(\Omega_R)}$ curves, where N_k is the number of nodes of the mesh $\mathcal{M}_k$ and u_k is the finite element solution of (3.3) over the mesh $\mathcal{M}_k$. It indicates that the meshes and the associated numerical complexity are quasi-optimal: $\| \nabla(u-u_k) \|_{L^2(\Omega_R)} = CN_k^{-1/2}$ is valid asymptotically.

One of the important quantities in the scattering problems is the far field pattern:

$$u_\infty(\hat{x}) = \frac{e^{i\frac{\pi}{4}}}{\sqrt{8\pi k}} \int_{\partial D} \left(u(y)\frac{\partial e^{-ik\hat{x}\cdot y}}{\partial \upsilon(y)} - \frac{\partial u(y)}{\partial \upsilon(y)} e^{-ik\hat{x}\cdot y} \right) ds(y), \qquad \hat{x} = \frac{x}{|x|}.$$

We compute the far field $u_\infty(\hat{x})$, $\hat{x} = (\cos(\theta), \sin(\theta))^T$ in the observation direction $\theta = \pi/4$. Figures 5.2 shows the far fields for different choices of PML parameters ρ

and σ_0. We observe that our adaptive algorithm is robust with respect to the choice of the thickness of PML layer: the far fields of the scattering solutions are insensitive to the choices of the PML parameters.

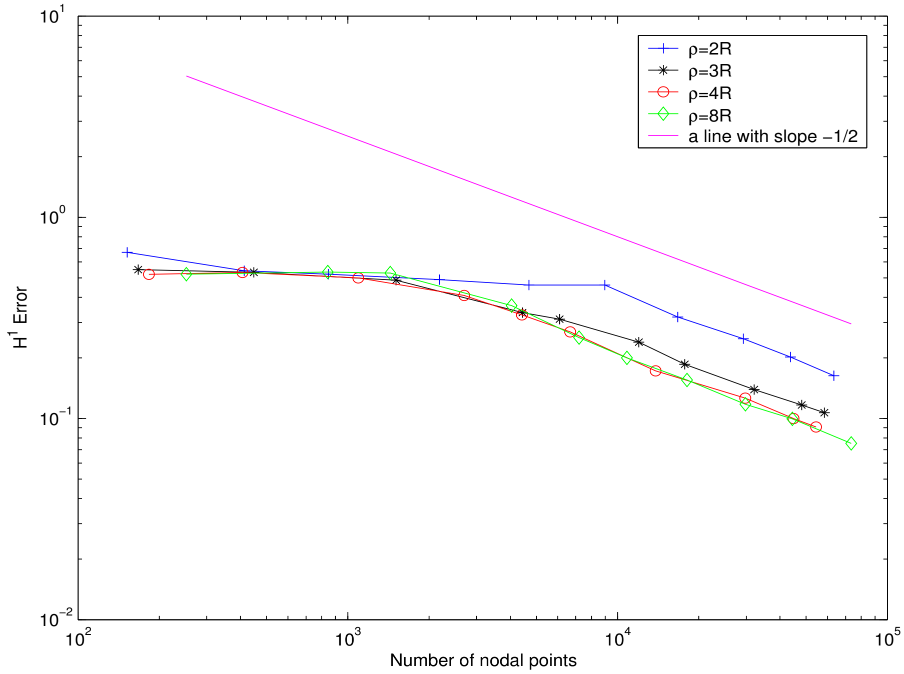

FIG. 5.1. *Quasi-optimality of the adaptive mesh refinements of the error* $\| \nabla(u - u_h \|_{L^2(\Omega_R)}$ *for Example 1.*

Example 2. This example is taken from [10] which concerns the scattering of the plane wave $u_I = e^{\mathbf{i}kx_1}$ from a perfectly conducting metal. The scatter D is contained in the box $\{x \in \mathbb{R} : -2 < x_1 < 2.2, -0.7 < x_2 < 0.7\}$ as plotted in Figure 5.3. W take $R = 3$ and $k = 2\pi$. The different choices of PML parameters ρ and σ_0 determined by the relation (5.1) are shown in Table 5.1.

Figure 5.4 shows the $\log N_k$-$\log \mathcal{E}_k$ curves, where N_k is the number of nodes of the mesh $\mathcal{M}_k$ and the $\mathcal{E}_k = (\sum_{K\in\mathcal{M}_k} \eta_K^2)^{1/2}$ is the associated a posteriori error estimate. It indicates that the meshes and the associated numerical complexity are quasi-optimal: $\mathcal{E}_k = CN_k^{-1/2}$ is valid asymptotically.

Figures 5.5 and 5.6 show the far fields in the incident direction $\theta = 0$ and the reflective direction $\theta = \pi$. Again we observe that the far fields are insensitive to the choices of PML parameters.

In Figure 5.7 we show the mesh after 13 adaptive iterations when $\rho = 3R$. We observe that the mesh near the boundary Γ_ρ is rather coarse, as a consequence of the exponentially decaying factor in our finite element a posteriori error estimator.

Appendix: The PML equation in the layer for large σ_0. The purpose of the appendix is to show that for sufficiently large σ_0, the PML problem in the layer (2.23) has a unique solution w. Moreover, the constant $\hat{C}$ in (2.25) can be chosen independent of Ω^{PML} and k.

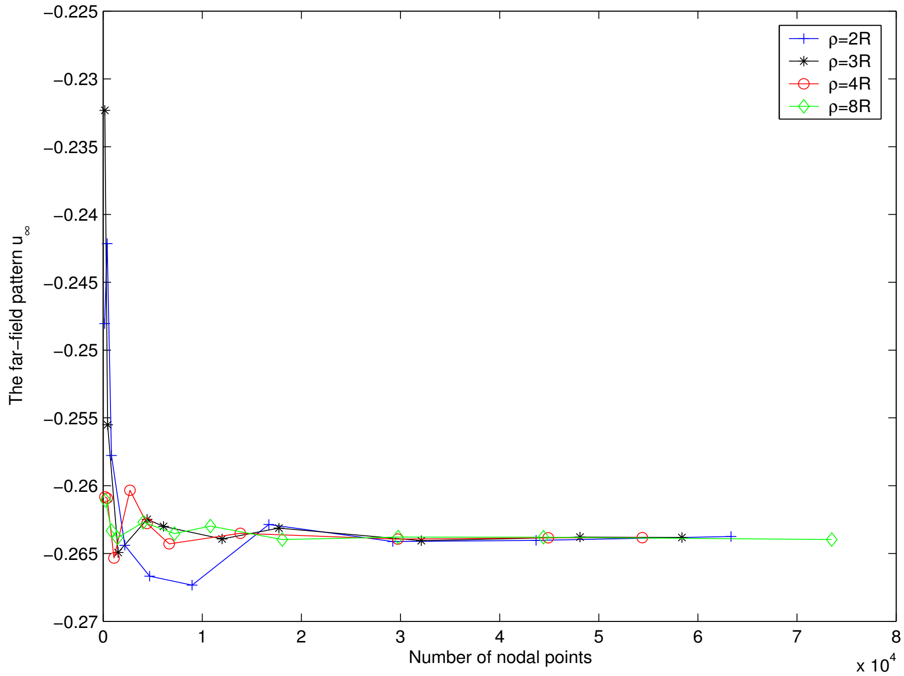

FIG. 5.2. *The real part of the far fields when the observing angle $\theta = \pi/4$ for Example 1.*

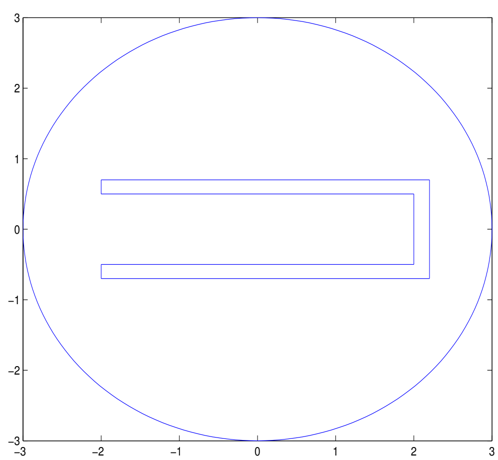

FIG. 5.3. *The geometry of the scatter for Example 2.*

From (H1) we know that $\beta(r) = 1 + \mathbf{i}\hat{\sigma}(r)$, where

$$\hat{\sigma}(r) = \frac{1}{r}\int_R^r \sigma(t)dt = \frac{\sigma_0}{m+1}\frac{r-R}{r}\left(\frac{r-R}{\rho-R}\right)^m.$$

Define

$$\zeta(r) := \frac{2\sigma_0^2}{\sigma\hat{\sigma}(r)} = \frac{2(m+1)r(\rho-R)^{2m}}{(r-R)^{2m+1}}, \qquad \forall r > R.$$

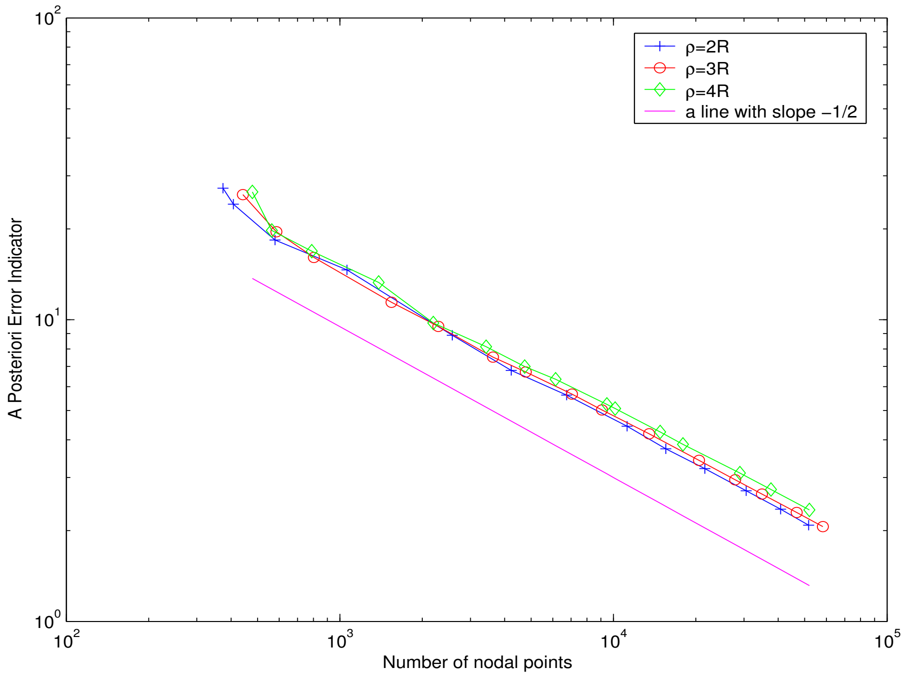

FIG. 5.4. *Quasi-optimality of the adaptive mesh refinements of the a posteriori error estimator for Example 2.*

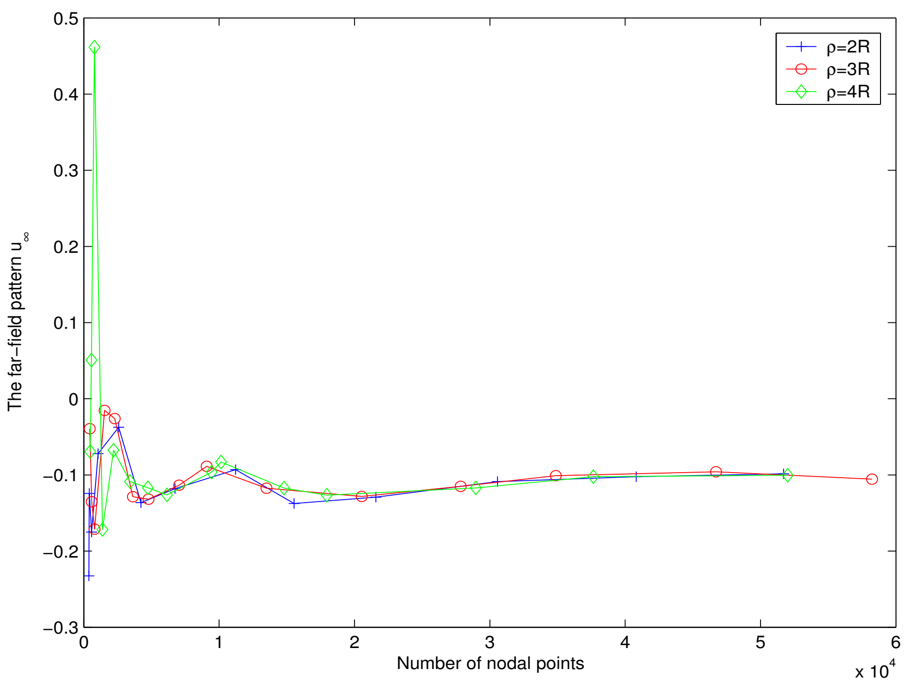

FIG. 5.5. *The real part of the far fields in the incident direction for Example 2.*

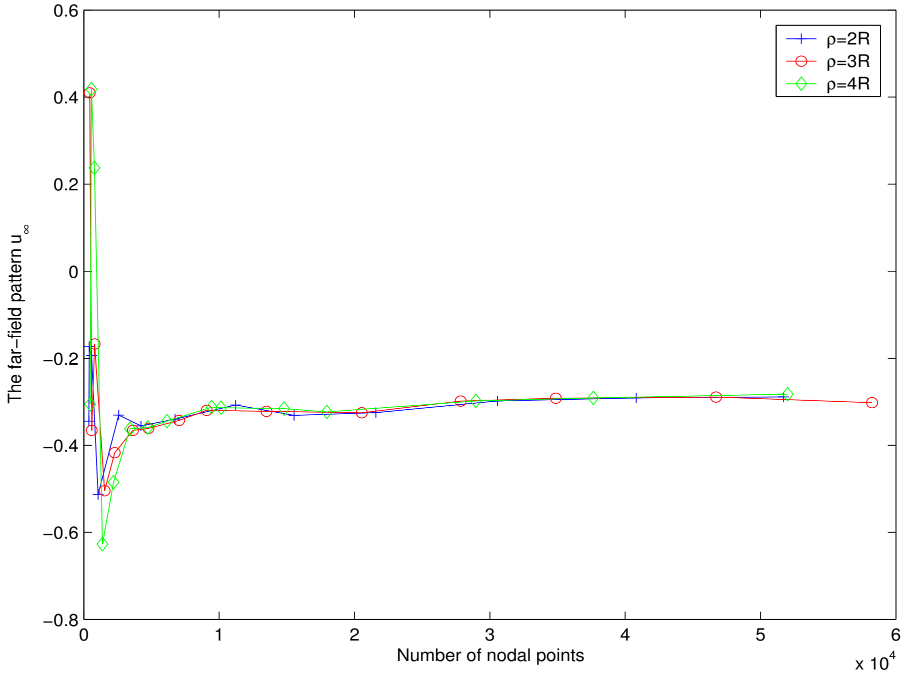

FIG. 5.6. *The real part of the far fields in the reflective direction for Example 2.*

It is clear that $\zeta : (R,\infty) \to \mathbb{R}$ is strictly monotone decreasing and $\zeta(r) \to \infty$ as $r \to R$, $\zeta(r) \to 0$ as $r \to \infty$. Thus, for any $\sigma_0 > 0$, there exists a unique $\hat{R} = \hat{R}(\sigma_0) > R$ such that

$$\sigma_0^2 = \zeta(\hat{R}) = \frac{2(m+1)\hat{R}(\rho - R)^{2m}}{(\hat{R} - R)^{2m+1}}. \tag{5.1}$$

Hence, since $\sigma\hat{\sigma} : (R,\infty) \to \mathbb{R}$ is increasing, we have

$$\sigma\hat{\sigma}(r) \geq \sigma\hat{\sigma}(\hat{R}) = \frac{2\sigma_0^2}{\zeta(\hat{R})} = 2 \quad \text{for } r \geq \hat{R}. \tag{5.2}$$

In this appendix we make the following assumption on the choice of σ_0:

(H3) $\sigma_0^2 \geq \zeta(\hat{R}_{\max})$, where $\hat{R}_{\max} := \max\{r \in (R,\rho) : \theta(r) \leq 1\}$ with

$$\theta(r) = k^2R^2\left[\left(\frac{r^2}{R^2} - 1\right)\ln\frac{r}{R} + \frac{2r^2(r-R)}{(2m+1)R^3}\right] \qquad \forall r \geq R.$$

Since the function $\theta : (R,\rho) \to \mathbb{R}$ is strictly monotone increasing and $\theta(R) = 0$, $\hat{R}_{\max}$ is well-defined.

LEMMA 5.1. *Let* (H1) *and* (H3) *be satisfied. Then*

$$\int_R^{\hat{R}} k^2 r\left(\int_R^r \frac{1+\sigma^2(t)}{t}dt\right)dr \leq \frac{1}{2}.$$

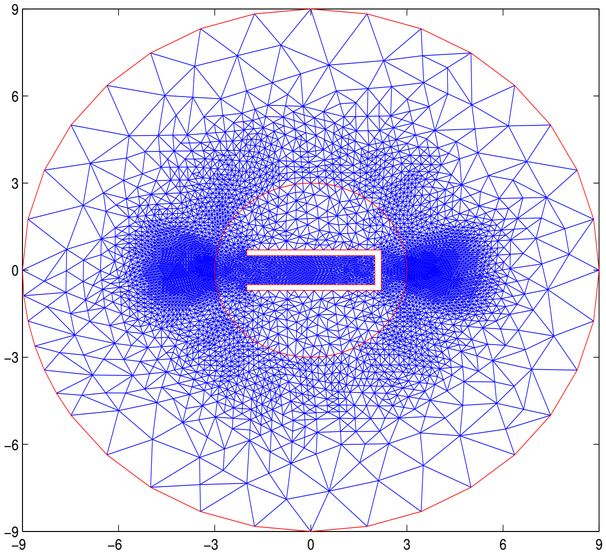

FIG. 5.7. *The mesh of* 7048 *nodes after 13 adaptive iterations when* $\rho = 3R$ *for Example 2.*

Proof. First we have

$$\int_R^{\hat{R}} r \left(\int_R^r \frac{1}{t} dt \right) dr = \int_R^{\hat{R}} r \ln \frac{r}{R} dr \leq \frac{1}{2} (\hat{R}^2 - R^2) \ln \frac{\hat{R}}{R}.$$

Next by (H1) and (5.1) we know that

$$\begin{aligned} \int_R^{\hat{R}} r \left(\int_R^r \frac{\sigma^2}{t} dt \right) dr &\leq \frac{\hat{R}}{R} \int_R^{\hat{R}} \left(\int_R^r \sigma^2(t) dt \right) dr \\ &= \frac{\hat{R}}{R} \int_R^{\hat{R}} \frac{\sigma_0^2}{2m+1} \frac{(r-R)^{2m+1}}{(\rho - R)^{2m}} dr \\ &= \frac{\hat{R}}{R} \frac{\sigma_0^2}{(2m+1)(2m+2)} \frac{(\hat{R}-R)^{2m+2}}{(\rho-R)^{2m}} \\ &= \frac{\hat{R}^2(\hat{R}-R)}{(2m+1)R}. \end{aligned}$$

Thus

$$\begin{aligned} \int_R^{\hat{R}} k^2 r \left(\int_R^r \frac{1+\sigma^2(t)}{t} dt \right) dr &\leq \frac{1}{2} k^2 R^2 \left[\left(\frac{\hat{R}^2}{R^2} - 1 \right) \ln \frac{\hat{R}}{R} + \frac{2\hat{R}^2(\hat{R}-R)}{(2m+1)R^3} \right] \\ &= \frac{1}{2} \theta(\hat{R}). \end{aligned}$$

Now if $\sigma_0^2 \geq \zeta(\hat{R}_{\max})$, we know from the monotonicity of ζ that $\hat{R} = \hat{R}(\sigma_0) \leq \hat{R}_{\max}$. Thus $\theta(\hat{R}) \leq \theta(\hat{R}_{\max}) \leq 1$ by (H3). This completes the proof. ∎

Now we are ready to prove the main result of this appendix.

THEOREM 5.2. *Under the assumptions* (H1) *and* (H3) *there exists a constant* $C > 0$ *independent of* $k, R, \rho,$ *and* σ_0 *such that*

$$\mathrm{Re}\,[\hat{b}(v,v)] \geq C \| v \|^2_{*,\Omega^{\mathrm{PML}}} \qquad \forall v \in H_0^1(\Omega^{\mathrm{PML}}).$$

Proof. For any $v \in H_0^1(\Omega^{\rm PML})$, we have

$$\mathrm{Re}\,[\hat{b}(v,v)] = \int_R^\rho \int_0^{2\pi} \left[\frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left|\frac{\partial v}{\partial r}\right|^2 + \frac{1+\sigma\hat{\sigma}}{1+\hat{\sigma}^2}\frac{1}{r}\left|\frac{\partial v}{\partial \theta}\right|^2 + (\sigma\hat{\sigma}-1)k^2 r|v|^2 \right].$$

By (5.2) we know that

$$\begin{aligned}
&\int_R^\rho \int_0^{2\pi} (\sigma\hat{\sigma}-1)k^2 r|v|^2 dr\,d\theta \\
&= \int_R^{\hat{R}} \int_0^{2\pi} (\sigma\hat{\sigma}-1)k^2 r|v|^2 dr\,d\theta + \int_{\hat{R}}^\rho \int_0^{2\pi} (\sigma\hat{\sigma}-1)k^2 r|v|^2 dr\,d\theta \\
&\ge -\frac{3}{2}\int_R^{\hat{R}} \int_0^{2\pi} k^2 r|v|^2 dr\,d\theta + \frac{1}{4}\int_R^\rho \int_0^{2\pi} (1+\sigma\hat{\sigma})k^2 r|v|^2 dr\,d\theta.
\end{aligned}$$

Notice that since $v=0$ on Γ_R,

$$|v(r)| = \left|\int_R^r \frac{\partial v}{\partial r} dr\right| \le \left(\int_R^r \frac{1+\sigma\hat{\sigma}}{1+\sigma^2} t \left|\frac{\partial v}{\partial r}\right|^2 dt\right)^{1/2} \left(\int_R^r \frac{1}{t}\frac{1+\sigma^2}{1+\sigma\hat{\sigma}} dt\right)^{1/2},$$

which, by Lemma 5.1, yields

$$\begin{aligned}
\int_R^{\hat{R}} \int_0^{2\pi} k^2 r|v|^2 dr &\le \left(\int_R^{\hat{R}} \int_0^{2\pi} \frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left|\frac{\partial v}{\partial r}\right|^2\right) \cdot \int_R^{\hat{R}} k^2 r \left(\int_R^r \frac{1}{t}\frac{1+\sigma^2}{1+\sigma\hat{\sigma}} dt\right) \\
&\le \frac{1}{2}\int_R^{\hat{R}} \int_0^{2\pi} \frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left|\frac{\partial v}{\partial r}\right|^2.
\end{aligned}$$

Thus

$$\mathrm{Re}\,[\hat{b}(v,v)] \ge \frac{1}{4}\int_R^\rho \int_0^{2\pi} \left[\frac{1+\sigma\hat{\sigma}}{1+\sigma^2} r \left|\frac{\partial v}{\partial r}\right|^2 + \frac{1+\sigma\hat{\sigma}}{1+\hat{\sigma}^2}\frac{1}{r}\left|\frac{\partial v}{\partial \theta}\right|^2 + (1+\sigma\hat{\sigma})k^2 r|v|^2 \right].$$

This completes the proof. ◻

Acknowledgments. The authors wish to thank Peter Monk for several inspiring discussions and the referees for constructive comments.

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