AN ADAPTIVE PERFECTLY MATCHED LAYER TECHNIQUE FOR 3-D TIME-HARMONIC ELECTROMAGNETIC SCATTERING PROBLEMS

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Abstract. An adaptive perfectly matched layer (PML) technique for solving the time harmonic electromagnetic scattering problems is developed. The PML parameters such as the thickness of the layer and the fictitious medium property are determined through sharp a posteriori error estimates. Combined with the adaptive finite element method, the adaptive PML technique provides a complete numerical strategy to solve the scattering problem in the framework of FEM which produces automatically a coarse mesh size away from the fixed domain and thus makes the total computational costs insensitive to the thickness of the PML absorbing layer. Numerical experiments are included to illustrate the competitive behavior of the proposed adaptive method.

1. Introduction

We propose and study an adaptive perfectly matched layer (PML) technique for solving the time harmonic electromagnetic scattering problem with the perfectly conducting boundary condition

$$\nabla \times \nabla \times \mathbf{E} - k^2\mathbf{E} = 0 \quad \text{in } \mathbb{R}^3 \backslash \bar{D}, \tag{1.1}$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{g} \quad \text{on } \Gamma_D, \tag{1.2}$$

$$|\mathbf{x}|\Big[(\nabla \times \mathbf{E}) \times \hat{\mathbf{x}} - \mathbf{i}k\mathbf{E}\Big] \to 0 \quad \text{as } |\mathbf{x}| \to \infty. \tag{1.3}$$

Here $D \subset \mathbb{R}^3$ is a bounded domain with Lipschitz polyhedral boundary Γ_D, $\mathbf{E}$ is the electric field, $\mathbf{g}$ is determined by the incoming wave, $\hat{\mathbf{x}} = \mathbf{x}/|\mathbf{x}|$, 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 Neumann or the impedance boundary condition on Γ_D, or to solve the electromagentic wave propagation through inhomogeneous media with a variable wave number $k^2(\mathbf{x})$ inside some bounded domain.

Since the work of Bérénger [5] which proposed a PML technique for solving 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 [24], Teixeira and Chew [23] 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

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designed model medium that would either slow down or attenuate all the waves that propagate from inside the computational domain.

The convergence of the PML method is studied in Lassas and Somersalo [16], Hohage, Schmidt and Zschiedrich [15] for the acoustic scattering problems and in Bao and Wu [3], Bramble and Pasciak [7] for the electromagnetic scattering problems. It is proved in [16, 15, 7] that the PML solution converges exponentially to the solution of the original scattering problem as the thickness of the PML layer tends to infinite. We remark that in practical applications involving PML techniques, one cannot afford to use a very thick PML layer if uniform 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.

The adaptive PML technique was first proposed in Chen and Wu [10] for a scattering problem by periodic structures (the grating problem) and in Chen and Liu [8] for the acoustic scattering problem in which one uses the a posteriori error estimate to determine the PML parameters. Combined with the adaptive finite element method, the adaptive PML technique provides a complete numerical strategy to solve the scattering problems in the framework of finite element which produces automatically a coarse mesh size away from the fixed domain and thus makes the total computational costs insensitive to the thickness of the PML absorbing 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. The adaptive finite element method based on a posteriori error estimates provides a systematic way to achieve the optimal computational complexity by refining the mesh according to the local a posteriori error estimator on the elements. A posteriori error estimates for the Nédélec $\mathbf{H}(\mathbf{curl})$-conforming edge elements are obtained in Monk [17] for Maxwell scattering problems, in Beck, Hiptmair, Hoppe and Wohlmuth [4] for eddy current problems, and in Chen, Wang and Zheng [9] for Maxwell cavity problems. The restriction in [17, 4] that the domain should be convex or have smooth boundary in order to ensure the regularity of the function in the Helmholtz decomposition is removed in [9] by using the Birman-Solomyak decomposition [6].

In this paper we extend the idea of using a posteriori error estimates to determine the PML parameters for solving the electromagnetic scattering problem (1.1)-(1.3). Our technique to prove the PML convergence is different from the methods used in [7, 3]. The key ingredient in our analysis is the following uniform estimate for the Hankel function $H_\nu^{(1)}(z)$ in [8]

$$|H_\nu^{(1)}(z)| \le e^{-\mathrm{Im}(z)(1-\frac{\Theta^2}{|z|^2})^{1/2}} |H_\nu^{(1)}(\Theta)|$$

for any $z \in \mathbb{C}$ such that $\mathrm{Im}(z) \ge 0, \mathrm{Re}(z) \ge 0$ and $\Theta \in \mathbb{R}$ satisfying $0 < \Theta < |z|$. This estimate, together with a uniform estimate of $\delta_n(z) = 1 + z\frac{h_n^{(1)'}(z)}{h_n^{(1)}(z)}$ for $z > 0$ due to Nédeléc [20], leads to the following crucial exponentially decaying property of the PML extension $\mathbb{E}(\lambda)$ (see (2.9) below for the definition)

$$\| \hat{\mathbf{x}} \times \mathbb{E}(\lambda) \|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)} \le C(1+kR) e^{-\mathrm{Im}(k\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}} \| \lambda \|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}.$$

Based on this estimate and the stability estimates for the PML equation in the PML layer, the following error estimate between the solution $\mathbf{E}$ of the scattering problem and the solution $\hat{\mathbf{E}}$ of the PML problem is proved (see Theorem 3.1 below)

$$\|\mathbf{E}-\hat{\mathbf{E}}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)} \leq C\hat{C}^{-1}(1+kR)^3|\alpha_0|^3 e^{-\mathrm{Im}(k\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}} \|\, \hat{\mathbf{x}}\times\hat{\mathbf{E}}\,\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}.$$

Let $\mathbf{E}_h$ be the finite element solution of the PML problem. The following a posteriori error estimate which is the basis of our adaptive PML method is derived (see Theorem 4.1 below)

$$\begin{aligned} &\|\mathbf{E}-\mathbf{E}_h\|_{\mathbf{H}(\mathbf{curl};\Omega_R)} \\ \leq\;& C\|\,\mathbf{g}-\mathbf{g}_h\,\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{D}})} + C\hat{C}^{-1}|\alpha_0|^3(1+kR)^3R^{1/2}\Big(\sum_{K\in\mathcal{M}_h}\eta_K^2\Big)^{1/2} \\ &+C\hat{C}^{-1}|\alpha_0|^3(1+kR)^3 e^{-\mathrm{Im}(k\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}}\|\,\hat{\mathbf{x}}\times\mathbf{E}_h\,\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}. \end{aligned}$$

Here $\mathbf{g}_h$ is the finite element approximation of the boundary value $\mathbf{g}$ and η_K is the a posteriori error indicator on the element K of residual type.

The layout of the paper is as follows. In section 2 we recall the PML formulation for (1.1)-(1.3). In section 3 we study the existence, uniqueness and convergence of the PML formulation. In section 4 we introduce the finite element discretization. In section 5 we derive the sharp a posteriori error estimate which lays down the basis of the combined adaptive PML and finite element methods. In section 6 we discuss the implementation of the adaptive method and present several numerical examples to illustrate the competitive behavior of the method.

2. The PML equation

Let D be contained in the interior of the ball $B_R=\{\mathbf{x}\in\mathbb{R}^3, |\mathbf{x}|<R\}$ with boundary Γ_R. We first recall the series solution of the scattering problem (1.1)-(1.3) outside the ball B_R by following the development in Monk [18]. Let $Y_n^m(\hat{\mathbf{x}})$, $m=-n,\ldots,n$, $n=1,2,\ldots$, be the *spherical harmonics* which satisfies

$$\Delta_{\partial B_1}Y_n^m(\hat{\mathbf{x}})+n(n+1)Y_n^m(\hat{\mathbf{x}})=0 \quad \text{on } \partial B_1, \tag{2.1}$$

where $\Delta_{\partial B_1}=\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta})+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$ is the Laplace-Beltrami operator for the surface of the unit sphere ∂B_1. The set of all spherical harmonics $\{Y_n^m(\hat{\mathbf{x}}): m=-n,\ldots,n,n=1,2,\ldots\}$ forms a complete orthonormal basis of $L^2(\partial B_1)$.

Denote the *vector spherical harmonics*

$$\mathbf{U}_n^m=\frac{1}{\sqrt{n(n+1)}}\nabla_{\partial B_1}Y_n^m, \qquad \mathbf{V}_n^m=\hat{\mathbf{x}}\times\mathbf{U}_n^m, \tag{2.2}$$

where $\nabla_{\partial B_1}Y_n^m=\frac{\partial Y_n^m}{\partial\theta}\mathbf{e}_\theta+\frac{1}{\sin\theta}\frac{\partial Y_n^m}{\partial\phi}\mathbf{e}_\phi$, and $\{\mathbf{e}_r,\mathbf{e}_\theta,\mathbf{e}_\phi\}$ are the unit vectors of the spherical coordinates. The set of all vector spherical harmonics $\{\mathbf{U}_n^m,\mathbf{V}_n^m: m=-n,\ldots,n,n=1,2,\ldots\}$ forms a complete orthonormal basis of $\mathbf{L}_t^2(\partial B_1)=\{\mathbf{u}\in L^2(\partial B_1)^3:\mathbf{u}\cdot\hat{\mathbf{x}}=0 \text{ on } \partial B_1\}$.

For any $\boldsymbol{\Phi}\in\mathbf{H}(\mathbf{curl},B_R)$, $\hat{\mathbf{x}}\times\boldsymbol{\Phi}|_{\Gamma_R}$ is in the trace space $\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})$, whose norm, for any $\lambda=\sum_{n=1}^\infty\sum_{m=-n}^n a_{nm}\mathbf{U}_n^m+b_{nm}\mathbf{V}_n^m$, is defined by

$$\|\,\lambda\,\|^2_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}=\sum_{n=1}^\infty\sum_{m=-n}^n\sqrt{n(n+1)}|a_{nm}|^2+\frac{1}{\sqrt{n(n+1)}}|b_{nm}|^2. \tag{2.3}$$

It is also known that for $\mathbf{\Phi} \in \mathbf{H}(\mathbf{curl}; B_R)$, the tangential component $(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}|_{\Gamma_R}$ belongs to $\mathbf{H}^{-1/2}(\mathrm{Curl};\Gamma_\mathrm{R})$ which is the dual space of $\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\mathrm{R})$ with respect to the scalar product in $\mathbf{L}_t^2(\Gamma_R)$ [20, Theorem 5.4.2, Lemma 5.3.1]. In the following we will always denote by $\langle\cdot,\cdot\rangle_{\Gamma_R}$ the duality pairing between $\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\mathrm{R})$ and $\mathbf{H}^{-1/2}(\mathrm{Curl};\Gamma_\mathrm{R})$.

Let $h_n^{(1)}(z)$ be the spherical Hankel function of the first kind of order n. We introduce the *vector wave functions*

$$\mathbf{M}_n^m(r,\hat{\mathbf{x}}) = \nabla\times\{\mathbf{x}h_n^{(1)}(kr)Y_n^m(\hat{\mathbf{x}})\}, \qquad \mathbf{N}_n^m(r,\hat{\mathbf{x}}) = \frac{1}{\mathbf{i}k}\nabla\times\mathbf{M}_n^m(r,\hat{\mathbf{x}}),$$

which are the radiation solutions of the Maxwell equation (1.1) in $\mathbb{R}^3\backslash\{0\}$. In the domain $\mathbb{R}^3\backslash\bar{B}_R$, the solution $\mathbf{E}$ of (1.1)-(1.3) can be written as

$$\mathbf{E}(r,\hat{\mathbf{x}}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{a_{nm}\mathbf{M}_n^m(r,\hat{\mathbf{x}})}{h_n^{(1)}(kR)\sqrt{n(n+1)}} + \frac{\mathbf{i}kRb_{nm}\mathbf{N}_n^m(r,\hat{\mathbf{x}})}{z_n^{(1)}(kR)\sqrt{n(n+1)}}, \tag{2.4}$$

where $z_n^{(1)}(kR) = h_n^{(1)}(kR) + kRh_n^{(1)\prime}(kR)$, and a_{nm}, b_{nm} are determined by the trace of $\mathbf{E}$ on Γ_R through $\hat{\mathbf{x}}\times\mathbf{E}|_{\Gamma_R} = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} a_{nm}\mathbf{U}_n^m + b_{nm}\mathbf{V}_n^m$. The series in (2.4) converges uniformly of $r > R$.

Now we turn to the introduction of the absorbing PML layer. We surround the domain $\Omega_R = B_R\backslash\bar{D}$ with a PML layer $\Omega^{\mathrm{PML}} = \{\mathbf{x}\in\mathbb{R}^3 : R < |\mathbf{x}| < \rho\}$. Throughout the paper we assume $\rho \le CR$ for some generic constant $C > 0$. Let $\alpha(r) = 1 + \mathbf{i}\sigma(r)$ be the model medium property which satisfies

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

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

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

It is easy to check that the vector wave functions satisfy

$$\mathbf{M}_n^m(r,\hat{\mathbf{x}}) = h_n^{(1)}(kr)\nabla_{\partial B_1}Y_n^m(\hat{\mathbf{x}})\times\hat{\mathbf{x}}, \tag{2.5}$$

$$\begin{aligned}\mathbf{N}_n^m(r,\hat{\mathbf{x}}) &= \frac{1}{\mathbf{i}k}\nabla\times\mathbf{M}_n^m\\ &= \frac{\sqrt{n(n+1)}}{\mathbf{i}kr}z_n^{(1)}(kr)\mathbf{U}_n^m(\hat{\mathbf{x}}) + \frac{n(n+1)}{\mathbf{i}kr}h_n^{(1)}(kr)Y_n^m(\hat{\mathbf{x}})\hat{\mathbf{x}}.\end{aligned} \tag{2.6}$$

We introduce

$$\tilde{\mathbf{M}}_n^m(\tilde{r},\hat{\mathbf{x}}) = h_n^{(1)}(k\tilde{r})\nabla_{\partial B_1}Y_n^m(\hat{\mathbf{x}})\times\hat{\mathbf{x}}, \tag{2.7}$$

$$\begin{aligned}\tilde{\mathbf{N}}_n^m(\tilde{r},\hat{\mathbf{x}}) &= \frac{1}{\mathbf{i}k}\tilde{\nabla}\times\tilde{\mathbf{M}}_n^m\\ &= \frac{\sqrt{n(n+1)}}{\mathbf{i}k\tilde{r}}z_n^{(1)}(k\tilde{r})\mathbf{U}_n^m(\hat{\mathbf{x}}) + \frac{n(n+1)}{\mathbf{i}k\tilde{r}}h_n^{(1)}(k\tilde{r})Y_n^m(\hat{\mathbf{x}})\hat{\mathbf{x}},\end{aligned} \tag{2.8}$$

where $\tilde{\nabla}\times$ is the curl operator with respect to the complex spherical variables $(\tilde{r},\theta,\phi)$, that is, for $\mathbf{\Phi}=\mathbf{\Phi}_r\mathbf{e}_r+\mathbf{\Phi}_\theta\mathbf{e}_\theta+\mathbf{\Phi}_\phi\mathbf{e}_\phi$,

$$\begin{aligned}\tilde{\nabla}\times\mathbf{\Phi} &= \frac{1}{\tilde{r}\sin\theta}\left(\frac{\partial}{\partial\theta}(\sin\theta\mathbf{\Phi}_\phi)-\frac{\partial\mathbf{\Phi}_\theta}{\partial\phi}\right)\mathbf{e}_r\\ &\quad+\frac{1}{\tilde{r}}\left(\frac{1}{\sin\theta}\frac{\partial\mathbf{\Phi}_r}{\partial\phi}-\frac{\partial(\tilde{r}\mathbf{\Phi}_\phi)}{\partial\tilde{r}}\right)\mathbf{e}_\theta\\ &\quad+\frac{1}{\tilde{r}}\left(\frac{\partial(\tilde{r}\mathbf{\Phi}_\theta)}{\partial\tilde{r}}-\frac{\partial\mathbf{\Phi}_\phi}{\partial\theta}\right)\mathbf{e}_\phi.\end{aligned}$$

It is easy to check that $\tilde{\nabla}\times\mathbf{\Phi}=A\nabla\times B\mathbf{\Phi}$, where $A=\mathrm{diag}(\beta^{-2},\alpha^{-1}\beta^{-1},\alpha^{-1}\beta^{-1})$ and $B=\mathrm{diag}(\alpha,\beta,\beta)$ are 3×3 diagonal matrices.

We follow [18] to derive the PML equation. For any $\lambda=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}a_{nm}\mathbf{U}_n^m+b_{nm}\mathbf{V}_n^m\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\mathrm{R})$, let $\mathbb{E}(\lambda)(\tilde{r},\hat{\mathbf{x}})$ be the PML extension given by

$$\mathbb{E}(\lambda)(\tilde{r},\hat{\mathbf{x}})=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{a_{nm}\tilde{\mathbf{M}}_n^m(\tilde{r},\hat{\mathbf{x}})}{h_n^{(1)}(kR)\sqrt{n(n+1)}}+\frac{\mathbf{i}kRb_{nm}\tilde{\mathbf{N}}_n^m(\tilde{r},\hat{\mathbf{x}})}{z_n^{(1)}(kR)\sqrt{n(n+1)}},\quad r>R. \tag{2.9}$$

For the solution $\mathbf{E}$ of the scattering problem (1.1)-(1.3), let $\tilde{\mathbf{E}}=\mathbb{E}(\hat{\mathbf{x}}\times\mathbf{E}|_{\Gamma_R})$ be the PML extension of $\hat{\mathbf{x}}\times\mathbf{E}|_{\Gamma_R}$. Since $\tilde{r}=r$ on Γ_R, we know that $\hat{\mathbf{x}}\times\tilde{\mathbf{E}}=\hat{\mathbf{x}}\times\mathbf{E}$ on Γ_R. On the other hand, since $h_n^{(1)}(z)\sim\frac{1}{z}e^{\mathbf{i}(z-\frac{1}{2}n\pi-\frac{1}{2}\pi)}$ asymptotically as $|z|\to\infty$, heuristically $\tilde{\mathbf{E}}(\tilde{r},\hat{\mathbf{x}})$ will decay exponentially for large $r>R$. It is obvious that $\tilde{\mathbf{E}}$ satisfies

$$\tilde{\nabla}\times\tilde{\nabla}\times\tilde{\mathbf{E}}-k^2\tilde{\mathbf{E}}=0\quad\text{in}\quad\mathbb{R}^3\backslash\bar{B}_R,$$

which gives the desired PML equation in the spherical coordinates

$$\nabla\times B(A\nabla\times B\tilde{\mathbf{E}})-k^2A^{-1}\tilde{\mathbf{E}}=0\quad\text{in}\quad\mathbb{R}^3\backslash\bar{B}_R.$$

The PML problem is then to find $\hat{\mathbf{E}}$, which approximates $\mathbf{E}$ in Ω_R and $B\tilde{\mathbf{E}}$ in $\Omega^{\mathrm{PML}}=B_\rho\backslash\bar{B}_R$, as the solution of the following system

$$\nabla\times BA(\nabla\times\hat{\mathbf{E}})-k^2(BA)^{-1}\hat{\mathbf{E}}=0\ \text{ in }\Omega_\rho=B_\rho\backslash\bar{D}, \tag{2.10}$$

$$\mathbf{n}\times\hat{\mathbf{E}}=\mathbf{g}\ \text{ on }\Gamma_D,\qquad\hat{\mathbf{x}}\times\hat{\mathbf{E}}=0\ \text{ on }\Gamma_\rho. \tag{2.11}$$

The well-posedness of the PML problem (2.10)-(2.11) and the convergence of its solution to the solution of the original problem (1.1)-(1.3) will be studied in the next section.

In the remainder of this section we introduce the equivalent variational form of the scattering problem (1.1)-(1.3) and the PML problem (2.10)-(2.11) on the bounded domain $\Omega_R=B_R\backslash\bar{D}$ using the Calderon operators.

Given a tangential vector λ on Γ_R, the Calderon operator $G_e:\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\mathrm{R})\to\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\mathrm{R})$ is the Dirichlet to Neumann operator defined by

$$G_e(\lambda)=\frac{1}{\mathbf{i}k}\hat{\mathbf{x}}\times(\nabla\times\mathbf{E}^s),$$

where $\mathbf{E}^s$ satisfies

$$\begin{aligned}&\nabla\times\nabla\times\mathbf{E}^s-k^2\mathbf{E}^s=0\quad\text{in }\mathbb{R}^3\backslash\bar{B}_R,\\ &\hat{\mathbf{x}}\times\mathbf{E}^s=\lambda\quad\text{on }\Gamma_R,\\ &|\mathbf{x}|\Big[(\nabla\times\mathbf{E}^s)\times\hat{\mathbf{x}}-\mathbf{i}k\mathbf{E}^s\Big]\to0\ \text{ as }|\mathbf{x}|\to\infty.\end{aligned}$$

Let $\lambda=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}a_{nm}\mathbf{U}_n^m+b_{nm}\mathbf{V}_n^m$, the function $\mathbf{E}^s$ is given as in (2.4)

$$\mathbf{E}^s(r,\hat{\mathbf{x}})=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{a_{nm}\mathbf{M}_n^m(r,\hat{\mathbf{x}})}{h_n^{(1)}(kR)\sqrt{n(n+1)}}+\frac{\mathbf{i}kRb_{nm}\mathbf{N}_n^m(r,\hat{\mathbf{x}})}{z_n^{(1)}(kR)\sqrt{n(n+1)}},\quad r>R.$$

Since $\frac{1}{\mathbf{i}k}\nabla\times\mathbf{M}_n^m=\mathbf{N}_m^n$, $-\frac{1}{\mathbf{i}k}\nabla\times\mathbf{N}_n^m=\mathbf{M}_n^m$, we have

$$\frac{1}{\mathbf{i}k}\nabla\times\mathbf{E}^s\;=\;\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{a_{mn}\mathbf{N}_n^m}{h_n^{(1)}(kR)\sqrt{n(n+1)}}-\frac{\mathbf{i}kRb_{mn}\mathbf{M}_n^m}{z_n^{(1)}(kR)\sqrt{n(n+1)}}.$$

Thus, by (2.5)-(2.6),

$$G_e(\lambda)=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{-\mathbf{i}kRb_{nm}h_n^{(1)}(kR)}{z_n^{(1)}(kR)}\mathbf{U}_n^m(\hat{\mathbf{x}})+\frac{a_{nm}z_n^{(1)}(kR)}{\mathbf{i}kRh_n^{(1)}(kR)}\mathbf{V}_n^m(\hat{\mathbf{x}}).\tag{2.12}$$

Let $a:\mathbf{H}(\mathbf{curl},\Omega_R)\times\mathbf{H}(\mathbf{curl},\Omega_R)\to\mathbb{C}$ be the sesquilinear form

$$a(\mathbf{E},\mathbf{\Phi})=\int_{\Omega_R}(\nabla\times\mathbf{E}\cdot\nabla\times\bar{\mathbf{\Phi}}-k^2\mathbf{E}\cdot\bar{\mathbf{\Phi}})d\mathbf{x}+\mathbf{i}k\langle G_e(\hat{\mathbf{x}}\times\mathbf{E}),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.$$

The scattering problem (1.1)-(1.3) is equivalent to the following weak formulation: Given $\mathbf{g}\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{D}})$, find $\mathbf{E}\in\mathbf{H}(\mathbf{curl};\Omega_R)$ such that $\mathbf{n}\times\mathbf{E}=\mathbf{g}$ on Γ_D, and

$$a(\mathbf{E},\mathbf{\Phi})=0,\quad\forall\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R),\tag{2.13}$$

where $\mathbf{H}_D(\mathbf{curl};\Omega_R)=\{\mathbf{v}\in\mathbf{H}(\mathbf{curl};\Omega_R):\mathbf{n}\times\mathbf{v}=0\ \text{ on }\Gamma_D\}$.

The existence of a unique solution of the variational problem (2.13) is known [18, 20]. Then the general theory in Babuška and Aziz [1] implies that there exists a constant $\mu>0$ such that the following inf-sup condition holds

$$\sup_{\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R)}\frac{|a(\mathbf{\Psi},\mathbf{\Phi})|}{\|\mathbf{\Phi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}}\geq\mu\|\mathbf{\Psi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)},\quad\forall\mathbf{\Psi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R).\tag{2.14}$$

To study the convergence of the PML problem (2.10)-(2.11), we need to reformulate it in the bounded domain Ω_R by imposing the boundary condition

$$\hat{\mathbf{x}}\times(\nabla\times\hat{\mathbf{E}})|_{\Gamma_R}=\mathbf{i}k\hat{G}_e(\hat{\mathbf{x}}\times\hat{\mathbf{E}}|_{\Gamma_R}),$$

where the approximate Calderon operator $\hat{G}_e:\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})\to\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})$ is defined as

$$\hat{G}_e(\lambda):=\frac{1}{\mathbf{i}k}\hat{\mathbf{x}}\times(\nabla\times\mathbf{\Psi}),\tag{2.15}$$

with $\mathbf{\Psi}$ satisfying

$$\nabla\times BA(\nabla\times\mathbf{\Psi})-k^2(BA)^{-1}\mathbf{\Psi}=0\quad\text{in }\Omega^{\mathrm{PML}},\tag{2.16}$$

$$\hat{\mathbf{x}}\times\mathbf{\Psi}=\lambda\text{ on }\Gamma_R,\qquad\hat{\mathbf{x}}\times\mathbf{\Psi}=0\text{ on }\Gamma_\rho.\tag{2.17}$$

That the approximate Calderon operator $\hat{G}_e$ is well-defined will be studied in the next section. Based on the operator $\hat{G}_e$, let $\hat{a}:\mathbf{H}(\mathbf{curl};\Omega_R)\times\mathbf{H}(\mathbf{curl};\Omega_R)\to\mathbb{C}$ be the sesquilinear form

$$\hat{a}(\hat{\mathbf{E}},\mathbf{\Phi})=\int_{\Omega_R}(\nabla\times\hat{\mathbf{E}}\cdot\nabla\times\bar{\mathbf{\Phi}}-k^2\hat{\mathbf{E}}\cdot\bar{\mathbf{\Phi}})d\mathbf{x}+\mathbf{i}k\langle\hat{G}_e(\hat{\mathbf{x}}\times\hat{\mathbf{E}}),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.$$

Then the weak formulation of (2.10)-(2.11) on the bounded domain Ω_R is: Given $\mathbf{g}\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{D}})$, find $\hat{\mathbf{E}}\in\mathbf{H}(\mathbf{curl};\Omega_R)$, such that $\mathbf{n}\times\hat{\mathbf{E}}=\mathbf{g}$ on Γ_D, and

$$\hat{a}(\hat{\mathbf{E}},\mathbf{\Phi})=0,\qquad\forall\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R).\tag{2.18}$$

3. Convergence of the PML problem

We start by considering the Dirichlet problem of the PML equation in the layer

$$\nabla\times BA\nabla\times\mathbf{v}-k^2(BA)^{-1}\mathbf{v}=0\ \text{ in }\Omega^{\rm PML},\tag{3.1}$$

$$\hat{\mathbf{x}}\times\mathbf{v}=0\text{ on }\Gamma_R,\quad \hat{\mathbf{x}}\times\mathbf{v}=\mathbf{q}\text{ on }\Gamma_\rho,\tag{3.2}$$

where $\mathbf{q}\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)$. Introduce the sesquilinear form $c:\mathbf{H}(\mathbf{curl};\Omega^{\rm PML})\times\mathbf{H}(\mathbf{curl};\Omega^{\rm PML})\to\mathbb{C}$ as

$$c(\mathbf{v},\mathbf{\Phi})=\int_{\Omega^{\rm PML}}(BA\nabla\times\mathbf{v}\cdot\nabla\times\bar{\mathbf{\Phi}}-k^2(BA)^{-1}\mathbf{v}\cdot\bar{\mathbf{\Phi}})d\mathbf{x}.$$

Then the weak formulation for (3.1)-(3.2) is: Given $\mathbf{q}\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)$, find $\mathbf{v}\in\mathbf{H}(\mathbf{curl};\Omega^{\rm PML})$ such that $\hat{\mathbf{x}}\times\mathbf{v}=0$ on Γ_R, $\hat{\mathbf{x}}\times\mathbf{v}=\mathbf{q}$ on Γ_ρ, and

$$c(\mathbf{v},\mathbf{\Phi})=0,\quad\forall\mathbf{\Phi}\in\mathbf{H}_0(\mathbf{curl};\Omega^{\rm PML}).\tag{3.3}$$

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

(H1) $\sigma=\sigma_0\left(\frac{r-R}{\rho-R}\right)^m$ for some constant $\sigma_0>0$ and some integer $m\geq1$.

From (**H**1) 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 $\hat\sigma\leq\sigma$ for all $r\geq R$. Notice that $BA=\mathrm{diag}(\alpha\beta^{-2},\alpha^{-1},\alpha^{-1})$, we have

$$\begin{aligned}&\mathrm{Re}\Big[c(\mathbf{\Phi},\mathbf{\Phi})\Big]\\ =&\int_{\Omega^{\rm PML}}\Big\{\frac{1-\hat\sigma^2+2\sigma\hat\sigma}{(1+\hat\sigma^2)^2}|(\nabla\times\mathbf{\Phi})_r|^2+\frac{1}{|\alpha|^2}|(\nabla\times\mathbf{\Phi})_\theta|^2+\frac{1}{|\alpha|^2}|(\nabla\times\mathbf{\Phi})_\phi|^2\Big\}d\mathbf{x}\\ &-k^2\int_{\Omega^{\rm PML}}\Big\{\frac{1-\hat\sigma^2+2\hat\sigma\sigma}{1+\sigma^2}|\mathbf{\Phi}_r|^2+|\mathbf{\Phi}_\theta|^2+|\mathbf{\Phi}_\phi|^2\Big\}d\mathbf{x}.\end{aligned}$$

Since

$$\frac{1-\hat\sigma^2+2\sigma\hat\sigma}{(1+\hat\sigma^2)^2}\geq\frac{1+\sigma\hat\sigma}{(1+\hat\sigma^2)^2}\geq\frac{1}{1+\sigma_0^2},\quad\frac{1-\hat\sigma^2+2\hat\sigma\sigma}{1+\sigma^2}\geq\frac{1}{1+\sigma_0^2},$$

we know by using the spectral theory of compact operators that (3.3) has a unique solution for every real k except possibly for a discrete set of values of k (see [12, Theorem 2] for a similar discussion on the PML equation for acoustic scattering problems). In this paper we will not elaborate on this issue and simply make the following assumption

(H2) The Dirichlet PML problem in the layer (3.3) has a unique solution.

The uniqueness and existence of the Dirichlet PML problem for the acoustic scattering problem is proved in [8] for sufficiently large $\sigma_0>0$. How to extend the analysis in [8] to the electromagnetic PML problem in the layer is an interesting open problem.

For any $\mathbf{\Phi}\in\mathbf{H}(\mathbf{curl};\Omega^{\rm PML})$, we define

$$\|\mathbf{\Phi}\|^2_{*,\Omega^{\rm PML}} = \int_{\Omega^{\rm PML}}\Big[\frac{1+\sigma\hat\sigma}{(1+\hat\sigma)^2}|(\nabla\times\mathbf{\Phi})_r|^2+\frac{1}{1+\sigma^2}|(\nabla\times\mathbf{\Phi})_\theta|^2 +\frac{1}{1+\sigma^2}|(\nabla\times\mathbf{\Phi})_\phi|^2+k^2\Big(\frac{1+\hat\sigma\sigma}{1+\sigma^2}|\mathbf{\Phi}_r|^2+|\mathbf{\Phi}_\theta|^2+|\mathbf{\Phi}_\phi|^2\Big)\Big]\,d\mathbf{x}.$$

It is clear that $\|\mathbf{\Phi}\|_{*,\Omega^{\rm PML}}$ is an equivalent norm of $\mathbf{H}(\mathbf{curl};\Omega^{\rm PML})$. Thus by (H2), there exists a constant $\hat C>0$ such that

$$\sup_{\mathbf{\Psi}\in\mathbf{H}_0(\mathbf{curl};\Omega^{\rm PML})}\frac{|c(\mathbf{\Phi},\mathbf{\Phi})|}{\|\mathbf{\Phi}\|_{*,\Omega^{\rm PML}}}\ge\hat C\|\mathbf{\Psi}\|_{*,\Omega^{\rm PML}},\quad\forall\mathbf{\Psi}\in\mathbf{H}_0(\mathbf{curl};\Omega^{\rm PML}).\tag{3.4}$$

Without loss of generality we assume $\hat C\le 1$. The following theorem is the main result of this section.

Theorem 3.1. *Let* ($\mathbf{H}$1)-($\mathbf{H}$2) *be satisfied. Then for sufficiently large* $\sigma_0>0$, *the PML problem* (2.10)-(2.11) *has a unique solution* $\hat{\mathbf{E}}\in\mathbf{H}(\mathbf{curl};\Omega_\rho)$. *Moreover, we have the following estimate*

$$\|\mathbf{E}-\hat{\mathbf{E}}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}\le C\hat C^{-1}(1+kR)^3|\alpha_0|^3e^{-{\rm Im}(k\tilde\rho)(1-\frac{R^2}{|\tilde\rho|^2})^{1/2}}\|\,\hat{\mathbf{x}}\times\hat{\mathbf{E}}\,\|_{\mathbf{H}^{-1/2}({\rm Div};\Gamma_{\rm R})},$$

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

The proof of this theorem will be given in Section 3.3 which depends on the exponential decay estimates for the PML extension and the stability estimates of the Dirichlet problem of the PML equation in the layer.

3.1. **Estimates for the PML extension.** We first recall some estimates for the Hankel functions. The following estimate which is proved in [8] based on the Macdonald formula will play an important role in our analysis.

Lemma 3.2. *For any* $\nu\in\mathbb{R},z\in\mathbb{C}_{++}=\{z\in\mathbb{C}:{\rm Im}(z)\ge0,{\rm Re}(z)\ge0\}$ *and* $\Theta\in\mathbb{R}$ *such that* $0<\Theta<|z|$, *we have*

$$|H^{(1)}_\nu(z)|\le e^{-{\rm Im}(z)(1-\frac{\Theta^2}{|z|^2})^{1/2}}|H^{(1)}_\nu(\Theta)|.$$

We also need the following important estimate of the spherical Hankel functions [20, p.195].

Lemma 3.3. *For any* $\Theta>0$, $\delta_n(\Theta)=\frac{z^{(1)}_n(\Theta)}{h^{(1)}_n(\Theta)}$ *satisfies* $|\delta_n(\Theta)|\ge\frac{n(n+1)}{2\Theta^2+n+1}$.

Lemma 3.4. *For any* $\lambda=\sum_{n=1}^\infty\sum_{m=-n}^n a_{nm}\mathbf{U}^m_n+b_{nm}\mathbf{V}^m_n\in\mathbf{H}^{-1/2}({\rm Div};\Gamma_{\rm R})$, *let* $\mathbb{E}(\lambda)(\tilde r,\hat{\mathbf{x}})$ *be the PML extension in* (2.9). *Then we have*

$$\begin{aligned}\frac{1}{\mathbf{i}k}\tilde\nabla\times\mathbb{E}(\lambda) &= \sum_{n=1}^\infty\sum_{m=-n}^n\frac{a_{mn}\tilde{\mathbf{N}}^m_n}{h^{(1)}_n(kR)\sqrt{n(n+1)}}-\frac{\mathbf{i}kRb_{mn}\tilde{\mathbf{M}}^m_n}{z^{(1)}_n(kR)\sqrt{n(n+1)}},\\ \hat{\mathbf{x}}\times\mathbb{E}(\lambda) &= \sum_{n=1}^\infty\sum_{m=-n}^n\frac{h^{(1)}_n(k\tilde r)}{h^{(1)}_n(kR)}a_{nm}\mathbf{U}^m_n+\frac{R}{\tilde r}\frac{z^{(1)}_n(k\tilde r)}{z^{(1)}_n(kR)}b_{nm}\mathbf{V}^m_n,\\ \frac{1}{\mathbf{i}k}\hat{\mathbf{x}}\times(\tilde\nabla\times\mathbb{E}(\lambda)) &= \sum_{n=1}^\infty\sum_{m=-n}^n\frac{-\mathbf{i}kRb_{mn}h^{(1)}_n(k\tilde r)}{z^{(1)}_n(kR)}\mathbf{U}^m_n+\frac{a_{mn}z^{(1)}_n(k\tilde r)}{\mathbf{i}k\tilde r h^{(1)}_n(kR)}\mathbf{V}^m_n.\end{aligned}$$

Proof. The first equality follows since $\frac{1}{\mathbf{i}k}\tilde{\nabla}\times\tilde{\mathbf{M}}_n^m = \tilde{\mathbf{N}}_n^m$ and $-\frac{1}{\mathbf{i}k}\tilde{\nabla}\times\tilde{\mathbf{N}}_n^m = \tilde{\mathbf{M}}_n^m$. From the definition of the vector spherical harmonics in (2.2), we derive from (2.7) and (2.8) that

$$\hat{\mathbf{x}}\times\tilde{\mathbf{M}}_n^m = \sqrt{n(n+1)}h_n^{(1)}(k\tilde{r})\mathbf{U}_n^m, \tag{3.5}$$

$$\hat{\mathbf{x}}\times\tilde{\mathbf{N}}_n^m = \sqrt{n(n+1)}\frac{1}{\mathbf{i}k\tilde{r}}z_n^{(1)}(k\tilde{r})\mathbf{V}_n^m. \tag{3.6}$$

This proves the second and third equalities. □

The following exponential decay estimate of the PML extension provides the first hint of the convergence of the PML problem (2.10)-(2.11).

Lemma 3.5. *For any* $\lambda\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})$*, let* $\mathbb{E}(\lambda)$ *be the PML extension in* (2.9)*. Then, for any* $r>R$*, we have*

$$\|\,\hat{\mathbf{x}}\times\mathbb{E}(\lambda)\,\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{r}})} \le C(1+kR)e^{-\mathrm{Im}(k\tilde{r})(1-\frac{R^2}{|\tilde{r}|^2})^{1/2}}\|\,\lambda\,\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}.$$

Proof. By Lemma 3.2 and using the relation $h_n^{(1)}(z)=\sqrt{\frac{\pi}{2z}}H_{n+1/2}^{(1)}(z)$, we obtain

$$\Big|\frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big| \le \Big|\frac{R}{\tilde{r}}\Big|^{1/2}e^{-\mathrm{Im}(k\tilde{r})(1-\frac{R^2}{|\tilde{r}|^2})^{1/2}} \le e^{-\mathrm{Im}(k\tilde{r})(1-\frac{R^2}{|\tilde{r}|^2})^{1/2}}. \tag{3.7}$$

Since $h_n^{(1)}(z) = -\frac{n+1}{z}h_n^{(1)}(z)+h_{n-1}^{(1)}(z)$, we have

$$\begin{aligned}
\Big|\frac{R}{\tilde{r}}\frac{z_n^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)}\Big| &= \Big|\frac{R}{\tilde{r}}\frac{h_n^{(1)}(k\tilde{r})+k\tilde{r}h_n^{(1)\prime}(k\tilde{r})}{z_n^{(1)}(kR)}\Big| \\
&= \Big|\frac{R}{\tilde{r}}\frac{-nh_n^{(1)}(\tilde{r})+k\tilde{r}h_{n-1}^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)}\Big| \\
&\le \left(n\Big|\frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big| + kR\Big|\frac{h_{n-1}^{(1)}(k\tilde{r})}{h_{n-1}^{(1)}(kR)}\frac{h_{n-1}^{(1)}(kR)}{h_n^{(1)}(kR)}\Big|\right)\Big|\frac{h_n^{(1)}(kR)}{z_n^{(1)}(kR)}\Big| \\
&\le (n+kR)|\delta_n(kR)|^{-1}e^{-\mathrm{Im}(k\tilde{r})\left(1-\frac{R^2}{|\tilde{r}|^2}\right)^{1/2}},
\end{aligned} \tag{3.8}$$

where we use the inequality that $|h_{n-1}^{(1)}(kR)|\le|h_n^{(1)}(kR)|$ which is a consequence of the Nicholson integral (see [8, (2.18)]).

It remains to estimate $|\delta_n(\Theta)|$ for $\Theta>0$. Since $h_n^{(1)\prime}(z)=\frac{n}{z}h_n^{(1)}(z)-h_{n+1}^{(1)}(z)$, we have

$$\delta_n(\Theta)=\frac{z_n^{(1)}(\Theta)}{h_n^{(1)}(\Theta)} = n+1-\Theta\frac{h_{n+1}^{(1)}(\Theta)}{h_n^{(1)}(\Theta)},$$

which implies, for $\Theta\ge 2n+1$, $|\delta_n(\Theta)|\ge\Theta-(n+1)\ge n$ and thus $|\delta_n(\Theta)|^{-1}\le n^{-1}$. For $\Theta\le(2n+1)$, we resort to the estimate of Nédeléc in Lemma 3.3 to get

$$|\delta_n(\Theta)|^{-1}\le\frac{1}{n}(1+4\Theta),\quad \Theta\le 2n+1.$$

Hence

$$(n+kR)|\delta_n(kR)|^{-1}\le 3(1+4kR). \tag{3.9}$$

Substitute it into (3.8), we conclude that

$$\Big|\frac{R}{\tilde r}\frac{z_n^{(1)}(k\tilde r)}{z_n^{(1)}(kR)}\Big| \le C(1+kR)e^{-\mathrm{Im}(k\tilde r)(1-\frac{R^2}{|\tilde r|^2})^{1/2}}. \tag{3.10}$$

The lemma now follows from the second equality in Lemma 3.4 by using the estimates (3.7), (3.10) and the definition (2.3). □

3.2. **The PML equation in the layer.** In this subsection we derive the stability estimates for the Dirichlet problem of the PML equation in the layer. We need the following weighted norm of $\mathbf{H}(\mathbf{curl};\Omega^{\rm PML})$

$$\|\mathbf{\Phi}\|_{\mathbf{curl};\Omega^{\rm PML}} = (\|\nabla\times\mathbf{\Phi}\|^2_{\mathbf{L}^2(\Omega^{\rm PML})} + R^{-2}\|\mathbf{\Phi}\|^2_{\mathbf{L}^2(\Omega^{\rm PML})})^{1/2}.$$

Lemma 3.6. *Let* $(\mathbf{H}1)$-$(\mathbf{H}2)$ *be satisfied. There exists a constant* $C>0$ *independent of* k, R, ρ *and* σ_0 *such that the following estimates are satisfied*

$$\|\mathbf{v}\|_{\mathbf{curl};\Omega^{\rm PML}} \le C\hat C^{-1}|\alpha_0|^2\|\mathbf{q}\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)}, \tag{3.11}$$

$$\|\hat{\mathbf{x}}\times(\nabla\times\mathbf{v})\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\rm R})} \le C\hat C^{-1}(1+kR)^2|\alpha_0|^2\|\mathbf{q}\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)}, \tag{3.12}$$

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

Proof. From the definition of the sesquilinear form c it is easy to see that

$$\begin{aligned} |c(\mathbf{v},\mathbf{\Phi})| \le& \int_{\Omega^{\rm PML}}\Big\{|\alpha\beta^{-2}||(\nabla\times\mathbf{v})_r||(\nabla\times\mathbf{\Phi})_r| \\ &+|\alpha|^{-1}|(\nabla\times\mathbf{v})_\theta||(\nabla\times\mathbf{\Phi})_\theta| + |\alpha|^{-1}|(\nabla\times\mathbf{v})_\phi||(\nabla\times\mathbf{\Phi})_\phi| \\ &+k^2(|\alpha^{-1}\beta^2||\mathbf{v}_r\mathbf{\Phi}_r| + |\alpha||\mathbf{v}_\theta\mathbf{\Phi}_\theta| + |\alpha||\mathbf{v}_\phi\mathbf{\Phi}_\phi|)\Big\}d\mathbf{x} \\ \le& C(1+kR)|\alpha_0|\|\mathbf{v}\|_{*,\Omega^{\rm PML}}\|\mathbf{\Phi}\|_{\mathbf{curl};\Omega^{\rm PML}}. \end{aligned} \tag{3.13}$$

To show (3.11), let $\mathbf{\Psi}\in\mathbf{H}(\mathbf{curl};\Omega^{\rm PML})$ be such that $\hat{\mathbf{x}}\times\mathbf{\Psi}=0$ on Γ_R and $\hat{\mathbf{x}}\times\mathbf{\Psi}=\mathbf{q}$ on Γ_ρ, then $\mathbf{\Phi}=\mathbf{v}-\mathbf{\Psi}\in\mathbf{H}_0(\mathbf{curl};\Omega^{\rm PML})$. Thus $c(\mathbf{v},\mathbf{v}-\mathbf{\Psi})=0$ by (3.3), and consequently

$$|c(\mathbf{v},\mathbf{v})| = |c(\mathbf{v},\mathbf{\Psi})| \le C(1+kR)|\alpha_0|\|\mathbf{v}\|_{*,\Omega^{\rm PML}}\|\mathbf{\Psi}\|_{\mathbf{curl};\Omega^{\rm PML}}.$$

Thus by (3.4),

$$\|\mathbf{v}\|_{*,\Omega^{\rm PML}} \le C\hat C^{-1}(1+kR)|\alpha_0|\|\mathbf{\Psi}\|_{\mathbf{curl};\Omega^{\rm PML}},$$

for any $\mathbf{\Psi}$ such that $\hat{\mathbf{x}}\times\mathbf{\Psi}=0$ on Γ_R and $\hat{\mathbf{x}}\times\mathbf{\Psi}=\mathbf{q}$ on Γ_ρ. By the trace theorem, we obtain

$$\|\mathbf{v}\|_{*,\Omega^{\rm PML}} \le C\hat C^{-1}(1+kR)|\alpha_0|\|\mathbf{q}\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)}. \tag{3.14}$$

This proves (3.11) since

$$\begin{aligned} \|\mathbf{v}\|^2_{*,\Omega^{\rm PML}} \ge& |\alpha_0|^{-2}\|\nabla\times\mathbf{v}\|_{L^2(\Omega^{\rm PML})} + k^2|\alpha_0|^{-2}\|\mathbf{v}\|_{L^2(\Omega^{\rm PML})} \\ \ge& |\alpha_0|^{-2}(1+k^2R^2)\|\mathbf{v}\|^2_{\mathbf{curl};\Omega^{\rm PML}}. \end{aligned}$$

To show (3.12), noticing that $\mathbf{v}$ satisfies the differential equation (3.1), we integrate by parts to get, for any $\mathbf{\Phi}\in\mathbf{H}(\mathbf{curl};\Omega^{\rm PML})$ such that $\hat{\mathbf{x}}\times\mathbf{\Phi}=0$ on Γ_ρ,

$$c(\mathbf{v},\mathbf{\Phi}) = -\langle\hat{\mathbf{x}}\times(\nabla\times\mathbf{v}), (\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.$$

Thus, by (3.13) and (3.14),

$$\begin{aligned}\|\hat{\mathbf{x}}\times(\nabla\times\mathbf{v})\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})} &\le \sup_{\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega^{\mathrm{PML}})}\frac{|c(\mathbf{v},\mathbf{\Phi})|}{\|\mathbf{\Phi}\|_{\mathbf{curl};\Omega^{\mathrm{PML}}}}\\ &\le C(1+kR)|\alpha_0|\|\mathbf{v}\|_{*,\Omega^{\mathrm{PML}}}\\ &\le C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2\|\mathbf{q}\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)}.\end{aligned}$$

This concludes the proof. □

3.3. **Convergence of the PML problem.** We start by introducing the propagation operator $\mathbb{P}:\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})\to\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)$. For any $\lambda\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})$, we define $\mathbb{P}(\lambda)=\hat{\mathbf{x}}\times\mathbb{E}(\lambda)(\tilde{\rho},\hat{\mathbf{x}})$, where $\mathbb{E}(\lambda)$ is the PML extension of λ in (2.9). By Lemma 3.5, we know that

$$\|\mathbb{P}(\lambda)\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)}\le C(1+kR)e^{-\mathrm{Im}(k\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}}\|\lambda\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}. \tag{3.15}$$

Lemma 3.7. *Let* (**H**1)-(**H**2) *be satisfied. We have*

$$\begin{aligned}&\|\mathbf{i}k(\hat{G}_e-G_e)(\lambda)\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}\\ \le\ &C\hat{C}^{-1}(1+kR)^3|\alpha_0|^3e^{-\mathrm{Im}(k\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}}\|\lambda\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}.\end{aligned}$$

Proof. For any $\lambda\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})$, by (2.12) and the third equality in Lemma 3.4, we know that

$$G_e(\lambda)=\frac{1}{\mathbf{i}k}\hat{\mathbf{x}}\times(\tilde{\nabla}\times\mathbb{E}(\lambda))|_{\Gamma_R}.$$

Since $\tilde{\nabla}\times\mathbb{E}(\lambda)=A\nabla\times B\mathbb{E}(\lambda)$ and $A=\mathrm{diag}\{1,1,1\}$ on Γ_R, we have

$$G_e(\lambda)=\frac{1}{\mathbf{i}k}\hat{\mathbf{x}}\times(\nabla\times B\mathbb{E}(\lambda))|_{\Gamma_R}.$$

Now by (2.16)-(2.17), we know that $(G_e-\hat{G}_e)(\lambda)=\frac{1}{\mathbf{i}k}\hat{\mathbf{x}}\times(\nabla\times\mathbf{w})$, where $\mathbf{w}$ satisfies

$$\begin{aligned}&\nabla\times BA(\nabla\times\mathbf{w})-k^2(BA)^{-1}\mathbf{w}=0\ \text{ in }\Omega^{\mathrm{PML}},\\ &\hat{\mathbf{x}}\times\mathbf{w}=0\text{ on }\Gamma_R,\quad \hat{\mathbf{x}}\times\mathbf{w}=B\mathbb{P}(\lambda)\text{ on }\Gamma_\rho.\end{aligned}$$

By Lemma 3.6 and (3.15), we have

$$\begin{aligned}&\|\hat{\mathbf{x}}\times(\nabla\times B\mathbf{w})\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}\\ \le\ &C\hat{C}^{-1}(1+kR)^2|\alpha_0|^2\|B\mathbb{P}(\lambda)\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\rho)}\\ \le\ &C\hat{C}^{-1}(1+kR)^3|\alpha_0|^3e^{-\mathrm{Im}(k\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}}\|\lambda\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}.\end{aligned}$$

This completes the proof. □

Now we are ready to prove the main theorem of this section.

Proof of Theorem 3.1. The existence of a unique solution for (2.18) follows from Lemma 3.7 by using the small perturbation argument the same as that in [10, Theorem 2.4]. Next, by (2.13) and (2.18) we have, for any $\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R)$,

$$a(\mathbf{E}-\hat{\mathbf{E}},\mathbf{\Phi})=\hat{a}(\hat{\mathbf{E}},\mathbf{\Phi})-a(\hat{\mathbf{E}},\mathbf{\Phi})=\mathbf{i}k\langle(\hat{G}_e-G_e)(\hat{\mathbf{x}}\times\hat{\mathbf{E}}),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.$$

This yields the desired estimate upon using Lemma 3.7 and (2.14). □

4. Finite element discretization

We start by introducing the weak formulation of the PML problem (2.10)-(2.11). Let

$$b(\mathbf{\Psi},\mathbf{\Phi}) = \int_{\Omega_\rho} (BA\nabla\times\mathbf{\Psi}\cdot\nabla\times\bar{\mathbf{\Phi}} - k^2(BA)^{-1}\mathbf{\Psi}\cdot\bar{\mathbf{\Phi}})d\mathbf{x}. \tag{4.1}$$

Then the weak formulation of (2.10)-(2.11) is: Given $\mathbf{g}\in\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{D}})$, find $\hat{\mathbf{E}}\in\mathbf{H}(\mathbf{curl},\Omega_\rho)$, such that $\mathbf{n}\times\hat{\mathbf{E}}=\mathbf{g}$ on Γ_D, $\hat{\mathbf{x}}\times\hat{\mathbf{E}}=0$ on Γ_ρ, and

$$b(\hat{\mathbf{E}},\mathbf{\Phi}) = 0,\quad \forall\mathbf{\Phi}\in\mathbf{H}_0(\mathbf{curl};\Omega_\rho). \tag{4.2}$$

Let Γ_ρ^h, which consists of piecewise triangles 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 will use the lowest order Nédeléc edge element [19] for which the finite element space $\mathbf{U}_h$ over $\mathcal{M}_h$ is defined by

$$\mathbf{U}_h = \{\mathbf{u}\in\mathbf{H}(\mathbf{curl};\Omega_\rho^h) : \mathbf{u}|_K = \mathbf{a}_K + \mathbf{b}_K\times\mathbf{x}, \forall\mathbf{a}_K,\mathbf{b}_K\in\mathbb{R}^3, \forall K\in\mathcal{M}_h\}.$$

Degrees of freedom of functions $\mathbf{u}\in\mathbf{U}_h$ on every $K\in\mathcal{M}_h$ are $\int_{e_i}\mathbf{u}\cdot\mathbf{dl}, i=1,\ldots,6$, where $e_1,\ldots,e_6$ are the six edges of K. Denote by $\mathring{\mathbf{U}}_h = \mathbf{U}_h\cap\mathbf{H}_0(\mathbf{curl};\Omega_\rho^h)$. In the following, we will always assume that the functions in $\mathring{\mathbf{U}}_h$ are extended to the domain Ω_ρ by zero so that any function $\mathbf{u}\in\mathring{\mathbf{U}}_h$ is also a function in $\mathbf{H}_0(\mathbf{curl};\Omega_\rho)$. The finite element approximation to (4.2) reads as follows: Find $\mathbf{E}_h\subset\mathbf{U}_h$ such that $\mathbf{n}\times\mathbf{E}_h=\mathbf{g}_h$ on Γ_D, $\mathbf{n}\times\mathbf{E}_h=0$ on Γ_ρ^h, and

$$b(\mathbf{E}_h,\mathbf{\Phi}_h) = 0,\qquad \forall\mathbf{\Phi}_h\in\mathring{\mathbf{U}}_h. \tag{4.3}$$

Here $\mathbf{g}_h$ is some edge element approximation of $\mathbf{g}$ on Γ_D. Notice that the integral in $b(\mathbf{E}_h,\mathbf{\Phi}_h)$ is actually over Ω_ρ^h since $\mathbf{\Phi}_h=0$ in $\Omega_\rho\backslash\Omega_\rho^h$ by our convention. The existence and uniqueness of the discrete problem (4.3) is a difficult problem due to the non-coerciveness of the sesquilinear form $b:\mathbf{H}(\mathbf{curl};\Omega_\rho)\times\mathbf{H}(\mathbf{curl};\Omega_\rho)\to\mathbb{C}$. Based on a general argument in Schatz [21], the unique existence of (4.3) for sufficiently small mesh size $h<h^*$ can be proved by using the unique existence of the continuous problem (4.2). In this paper we are interested in a posteriori error estimates and the associated adaptive algorithm. Thus in the following, we simply assume the discrete problem (4.3) has a unique solution $\mathbf{E}_h$.

For any $K\in\mathcal{M}_h$, we denote by h_K its diameter. Let $\mathcal{F}_h$ be the set of all faces of the mesh $\mathcal{M}_h$ that do not lie on Γ_D and Γ_ρ^h. For any $F\in\mathcal{F}_h$, h_F stands for its diameter. For any interior face F which is a common face of K_1 and K_2 in $\mathcal{M}_h$, we define the following jump residuals across F

$$[\![\mathbf{n}\times(BA\nabla\times\mathbf{E}_h)]\!] = \mathbf{n}_F\times(BA\nabla\times(\mathbf{E}_h|_{K_1}-\mathbf{E}_h|_{K_2})),$$
$$[\![k^2(BA)^{-1}\mathbf{E}_h\cdot\mathbf{n}]\!] = k^2(BA)^{-1}(\mathbf{E}_h|_{K_1}-\mathbf{E}_h|_{K_2})\cdot\mathbf{n}_F,$$

using the convention that the unit norm vector $\mathbf{n}_F$ to F points from K_2 to K_1. The local error indicator η_K for any $K \in \mathcal{M}_h$ is defined as

$$\begin{aligned}\eta_K^2 = \quad & h_K^2 \| \, k^2(BA)^{-1}\mathbf{E}_h - \nabla \times (BA\nabla \times \mathbf{E}_h) \, \|^2_{\mathbf{L}^2(K)} \\ + \quad & h_K^2 \| \, \mathrm{div}(k^2(BA)^{-1}\mathbf{E}_h) \, \|^2_{L^2(K)} \\ + \quad & h_K \| \, [\![\mathbf{n} \times (BA\nabla \times \mathbf{E}_h)]\!] \, \|^2_{\mathbf{L}^2(\partial K)} + h_K \| \, [\![k^2(BA)^{-1}\mathbf{E}_h \cdot \mathbf{n}]\!] \, \|^2_{L^2(\partial K)}.\end{aligned}$$

The following theorem is the main result of this paper.

Theorem 4.1. *Let* $(\mathbf{H}1)$-$(\mathbf{H}2)$ *be satisfied. There exists a constant* C *depending only on the minimum angle of the mesh* $\mathcal{M}_h$ *such that the following a posteriori error estimate is valid*

$$\begin{aligned} & \|\mathbf{E} - \mathbf{E}_h\|_{\mathbf{H}(\mathbf{curl};\Omega_R)} \\ \le \quad & C\| \, \mathbf{g} - \mathbf{g}_h \, \|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\mathrm{D})} + C\hat{C}^{-1}|\alpha_0|^3(1+kR)^3R^{1/2}\Big(\sum_{K\in\mathcal{M}_h}\eta_K^2\Big)^{1/2} \\ & + C\hat{C}^{-1}|\alpha_0|^3(1+kR)^3 e^{-\mathrm{Im}(k\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}} \| \, \hat{\mathbf{x}} \times \mathbf{E}_h \, \|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\mathrm{R})}.\end{aligned}$$

The proof of this theorem will be given in Section 5.3. One of the key ingredients of the a posteriori error analysis is the Birman-Solomyak decomposition theorem in Lipschitz domains [6, 14, 9]. More precisely, the following result whose proof can be found in [14, 9] will be used.

Lemma 4.2. *For any* $\mathbf{u} \in \mathbf{H}_0(\mathbf{curl}, \Omega_\rho)$, *there exists a* $\mathbf{\Phi} \in \mathbf{H}_0(\mathbf{curl}, \Omega_\rho) \cap H^1(\Omega_\rho)^3$ *and a* $\varphi \in H_0^1(\Omega_\rho)$ *such that* $\mathbf{u} = \mathbf{\Phi} + \nabla\varphi$ *in* Ω_ρ, *and*

$$\| \, \varphi \, \|_{H^1(\Omega_\rho)} + \| \, \mathbf{\Phi} \, \|_{\mathbf{H}^1(\Omega_\rho)} \le C\|\mathbf{u}\|_{\mathbf{H}(\mathbf{curl};\Omega_\rho)}.$$

Let V_h be the standard H^1-conforming piecewise linear finite element space over $\mathcal{M}_h$ and $\overset{\circ}{V}_h = H_0^1(\Omega_\rho^h) \cap V_h$. In the following, we will also assume that the functions in $\overset{\circ}{V}_h$ are extended to the domain Ω_ρ by zero so that any function in $\overset{\circ}{V}_h$ is also a function in $H_0^1(\Omega_\rho)$. In §5.3, we will use the Clément operator $r_h : H_0^1(\Omega_\rho) \to \overset{\circ}{V}_h$ [11] and the Beck-Hiptmair-Hoppe-Wohlmuth interpolation operator $\pi_h : H^1(\Omega_\rho)^3 \cap \mathbf{H}_0(\mathbf{curl}; \Omega_\rho) \to \overset{\circ}{\mathbf{U}}_h$ [4] which satisfy the following estimates

$$\| \, \varphi - r_h\varphi \, \|_{L^2(K)} \le Ch_K \| \, \nabla\varphi \, \|_{\mathbf{L}^2(\tilde{K})}, \| \, \varphi - r_h\varphi \, \|_{L^2(F)} \le Ch_F^{1/2} \| \, \nabla\varphi \, \|_{\mathbf{L}^2(\tilde{F})}, \tag{4.4}$$

$$\| \, \mathbf{\Phi} - \pi_h\mathbf{\Phi} \, \|_{\mathbf{L}^2(K)} \le Ch_K \| \, \nabla\mathbf{\Phi} \, \|_{\mathbf{L}^2(\tilde{K})}, \| \, \mathbf{\Phi} - \pi_h\mathbf{\Phi} \, \|_{\mathbf{L}^2(F)} \le Ch_F^{1/2} \| \, \nabla\mathbf{\Phi} \, \|_{\mathbf{L}^2(\tilde{F})}, \tag{4.5}$$

where $\tilde{A}$ is the union of elements on $\mathcal{M}_h$ with non-empty intersection with A, $A = K \in \mathcal{M}_h$ or $F \in \mathcal{F}_h$.

5. A posteriori error analysis

In this section, we prove the a posteriori error estimates in Theorem 4.1. To begin with, let $\mathbf{\Psi} \in \mathbf{H}(\mathbf{curl}; \Omega_R)$ such that $\mathbf{n} \times \mathbf{\Psi} = \mathbf{g} - \mathbf{g}_h$ on Γ_D, then $\mathbf{E} - \mathbf{E}_h - \mathbf{\Psi} \in \mathbf{H}_D(\mathbf{curl}; \Omega_R)$. Thus by (2.14) we have

$$\|\mathbf{E} - \mathbf{E}_h - \mathbf{\Psi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)} \le C \sup_{\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R)} \frac{|a(\mathbf{E} - \mathbf{E}_h - \mathbf{\Psi}, \mathbf{\Phi})|}{\|\mathbf{\Phi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}}.$$

Since $|a(\mathbf{\Psi},\mathbf{\Phi})|\le C\|\mathbf{\Psi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}\|\mathbf{\Phi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}$, we obtain

$$\|\mathbf{E}-\mathbf{E}_h\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}\le C\|\mathbf{\Psi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}+C\sup_{\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R)}\frac{|a(\mathbf{E}-\mathbf{E}_h,\mathbf{\Phi})|}{\|\mathbf{\Phi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}}.$$

The above estimate is valid for any $\mathbf{\Psi}\in\mathbf{H}(\mathbf{curl};\Omega_R)$ such that $\mathbf{n}\times\mathbf{\Psi}=\mathbf{g}-\mathbf{g}_h$ on Γ_D, we get by the trace theorem

$$\begin{aligned}\|\mathbf{E}-\mathbf{E}_h\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}\le\ & C\|\,\mathbf{g}-\mathbf{g}_h\,\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_D)}\\ &+\ C\sup_{\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R)}\frac{|a(\mathbf{E}-\mathbf{E}_h,\mathbf{\Phi})|}{\|\mathbf{\Phi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}}.\end{aligned}\tag{5.1}$$

5.1. **Error representation formula.** For any $\mathbf{\Phi}\in\mathbf{H}_D(\mathbf{curl};\Omega_R)$ which satisfies $\mathbf{n}\times\mathbf{\Phi}=0$ on Γ_D, we extend $\mathbf{\Phi}$ to Ω^{PML}, denoted by $\hat{\mathbf{\Phi}}$, through the following conditions

$$\nabla\times\overline{BA}\nabla\times\hat{\mathbf{\Phi}}-k^2(\overline{BA})^{-1}\hat{\mathbf{\Phi}}=0\quad\text{in }\Omega^{\mathrm{PML}},\tag{5.2}$$

$$\hat{\mathbf{x}}\times\hat{\mathbf{\Phi}}=\hat{\mathbf{x}}\times\mathbf{\Phi}\quad\text{on }\Gamma_R,\qquad\hat{\mathbf{x}}\times\hat{\mathbf{\Phi}}=0\quad\text{on }\Gamma_\rho.\tag{5.3}$$

By $(\mathbf{H}2)$ we know that $\hat{\mathbf{\Phi}}$ is well-defined.

Lemma 5.1. *Let* $(\mathbf{H}2)$ *be satisfied. For any* $\mathbf{\Phi},\mathbf{\Psi}\in\mathbf{H}(\mathbf{curl};\Omega_R)$*, we have*

$$\langle\hat{G}_e(\hat{\mathbf{x}}\times\mathbf{\Phi}),(\hat{\mathbf{x}}\times\mathbf{\Psi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}=\langle\hat{G}_e(\hat{\mathbf{x}}\times\bar{\mathbf{\Psi}}),(\hat{\mathbf{x}}\times\bar{\mathbf{\Phi}})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.$$

Proof. By the definition of the approximate Calderon operator $\hat{G}_e$ in (2.16)-(2.17) we know that

$$\hat{G}_e(\hat{\mathbf{x}}\times\mathbf{\Phi}|_{\Gamma_R})=\frac{1}{\mathbf{i}k}\hat{\mathbf{x}}\times(\nabla\times\mathbf{w})|_{\Gamma_R},$$

where $\mathbf{w}$ satisfies

$$\nabla\times BA\nabla\times\mathbf{w}-k^2(BA)^{-1}\mathbf{w}=0\quad\text{in }\Omega^{\mathrm{PML}},\tag{5.4}$$

$$\hat{\mathbf{x}}\times\mathbf{w}=\hat{\mathbf{x}}\times\mathbf{\Phi}\text{ on }\Gamma_R,\qquad\hat{\mathbf{x}}\times\mathbf{w}=0\text{ on }\Gamma_\rho.\tag{5.5}$$

The solution of (5.4)-(5.5) can be represented as

$$\mathbf{w}=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\alpha_{nm}\mathbf{M}_n^m(\tilde{r},\hat{\mathbf{x}})+\beta_{nm}\mathbf{N}_n^m(\tilde{r},\hat{\mathbf{x}})+\alpha'_{nm}\hat{\mathbf{M}}_n^m(\tilde{r},\hat{\mathbf{x}})+\beta'_{nm}\hat{\mathbf{N}}_n^m(\tilde{r},\hat{\mathbf{x}}),$$

where, corresponding to $\mathbf{M}_n^m,\mathbf{N}_n^m$ for $h_n^{(1)}(k\tilde{r})$ in (2.7)-(2.8),

$$\begin{aligned}\hat{\mathbf{M}}_n^m(\tilde{r},\hat{\mathbf{x}})&=h_n^{(2)}(k\tilde{r})\nabla_{\partial B_1}Y_n^m(\hat{\mathbf{x}})\times\hat{\mathbf{x}},\\ \hat{\mathbf{N}}_n^m(\tilde{r},\hat{\mathbf{x}})&=\frac{1}{\mathbf{i}k}\tilde{\nabla}\times\hat{\mathbf{M}}_n^m(\tilde{r},\hat{\mathbf{x}})\\ &=\frac{\sqrt{n(n+1)}}{\mathbf{i}k\tilde{r}}z_n^{(2)}(k\tilde{r})\mathbf{U}_n^m(\hat{\mathbf{x}})+\frac{n(n+1)}{\mathbf{i}k\tilde{r}}h_n^{(2)}(k\tilde{r})Y_n^m(\hat{\mathbf{x}})\hat{\mathbf{x}}.\end{aligned}$$

Here $z_n^{(2)}(k\tilde{r})=h_n^{(2)}(k\tilde{r})+k\tilde{r}h_n^{(2)\prime}(k\tilde{r})$ and $h_n^{(2)}(z)$ is the spherical Hankel function of the second kind of order n. The constants $\alpha_{nm},\beta_{nm},\alpha'_{nm},\beta'_{nm}$ are determined by the boundary conditions (5.3). By (3.5)-(3.6) and similar identities for $\hat{\mathbf{M}}_n^m, \hat{\mathbf{N}}_n^m$, we know that

$$\hat{\mathbf{x}} \times \mathbf{w} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \sqrt{n(n+1)}\Big(\alpha_{nm} h_n^{(1)}(k\tilde{r}) + \alpha'_{nm} h_n^{(2)}(k\tilde{r})\Big)\mathbf{U}_n^m(\hat{\mathbf{x}}) + \sqrt{n(n+1)}\frac{1}{\tilde{r}}\Big(\beta_{nm} z_n^{(1)}(k\tilde{r}) + \beta'_{nm} z_n^{(2)}(k\tilde{r})\Big)\mathbf{V}_n^m(\hat{\mathbf{x}}).$$

If $\hat{\mathbf{x}} \times \mathbf{\Phi}|_{\Gamma_R} = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} a_{nm}\mathbf{U}_n^m + b_{nm}\mathbf{V}_n^m$, then (5.3) implies

$$\alpha_{nm} h_n^{(1)}(kR) + \alpha'_{nm} h_n^{(2)}(kR) = \frac{a_{nm}}{\sqrt{n(n+1)}}, \quad \alpha_{nm} h_n^{(1)}(k\tilde{\rho}) + \alpha'_{nm} h_n^{(2)}(k\tilde{\rho}) = 0,$$

$$\beta_{nm} z_n^{(1)}(kR) + \beta'_{nm} z_n^{(2)}(kR) = \frac{Rb_{nm}}{\sqrt{n(n+1)}}, \quad \beta_{nm} z_n^{(1)}(k\tilde{\rho}) + \beta'_{nm} z_n^{(2)}(k\tilde{\rho}) = 0.$$

By (**H**2), the problem (5.2)-(5.3) has a unique solution and consequently the above linear system of equations for $\alpha_{mn}, \alpha'_{mn}, \beta_{mn}, \beta'_{mn}$ has a unique solution. Denote by

$$H_n = h_n^{(1)}(kR)h_n^{(2)}(k\tilde{\rho}) - h_n^{(2)}(kR)h_n^{(1)}(k\tilde{\rho}),$$
$$I_n = z_n^{(1)}(kR)z_n^{(2)}(k\tilde{\rho}) - z_n^{(2)}(kR)z_n^{(1)}(k\tilde{\rho}),$$

then $H_n \neq 0, I_n \neq 0$, and

$$\alpha_{nm} = \frac{h_n^{(2)}(k\tilde{\rho})}{H_n\sqrt{n(n+1)}}a_{nm}, \quad \alpha'_{nm} = -\frac{h_n^{(1)}(k\tilde{\rho})}{H_n\sqrt{n(n+1)}}a_{nm},$$

$$\beta_{nm} = \frac{z_n^{(2)}(k\tilde{\rho})R}{I_n\sqrt{n(n+1)}}b_{nm}, \quad \beta'_{nm} = -\frac{z_n^{(1)}(k\tilde{\rho})R}{I_n\sqrt{n(n+1)}}b_{nm}.$$

Since $\tilde{\mathbf{N}}_n^m = \frac{1}{\mathbf{i}k}\tilde{\nabla}\times\mathbf{M}_n^m, \hat{\mathbf{N}}_n^m = \frac{1}{\mathbf{i}k}\tilde{\nabla}\times\hat{\mathbf{M}}_n^m$, $\tilde{\mathbf{M}}_n^m = -\frac{1}{\mathbf{i}k}\nabla\times\tilde{\mathbf{N}}_n^m, \hat{\mathbf{M}}_n^m = -\frac{1}{\mathbf{i}k}\nabla\times\hat{\mathbf{N}}_n^m$, we have

$$\begin{aligned} & \hat{G}_e(\hat{\mathbf{x}} \times \mathbf{\Phi}|_{\Gamma_R}) \\ = \quad & \frac{1}{\mathbf{i}k}\hat{\mathbf{x}} \times (\nabla \times \mathbf{w})|_{\Gamma_R} \\ = \quad & \hat{\mathbf{x}} \times \sum_{n=1}^{\infty}\sum_{m=-n}^{n} \Big(\alpha_{nm}\tilde{\mathbf{N}}_n^m - \beta_{nm}\tilde{\mathbf{M}}_n^m + \alpha'_{nm}\hat{\mathbf{N}}_n^m - \beta'_{nm}\hat{\mathbf{M}}_n^m\Big)\Big|_{\Gamma_R}. \end{aligned}$$

By (3.5)-(3.6) and similar identities for $\hat{\mathbf{M}}_n^m, \hat{\mathbf{N}}_n^m$, we then get

$$\begin{aligned} & \hat{G}_e(\hat{\mathbf{x}} \times \mathbf{\Phi}|_{\Gamma_R}) \\ = \quad & \sum_{n=1}^{\infty}\sum_{m=-n}^{n} \frac{1}{\mathbf{i}kR}\sqrt{n(n+1)}\Big(\alpha_{nm} z_n^{(1)}(kR) + \alpha'_{nm} z_n^{(2)}(kR)\Big)\mathbf{V}_n^m \\ & \qquad + \sqrt{n(n+1)}\Big(-\beta_{nm} h_n^{(1)}(kR) - \beta'_{nm} h_n^{(2)}(kR)\Big)\mathbf{U}_n^m \\ = \quad & \sum_{n=1}^{\infty}\sum_{m=-n}^{n} \frac{1}{\mathbf{i}kR}\gamma_n a_{nm}\mathbf{V}_n^m - R\eta_n b_{nm}\mathbf{U}_n^m, \end{aligned}$$

where $\gamma_n = (h_n^{(2)}(k\tilde{\rho})z_n^{(1)}(kR) - h_n^{(1)}(k\tilde{\rho})z_n^{(2)}(kR))/H_n$ and $\eta_n = (z_n^{(2)}(k\tilde{\rho})h_n^{(1)}(kR) - z_n^{(1)}(k\tilde{\rho})h_n^{(2)}(kR))/I_n$.

Now suppose that $\hat{\mathbf{x}}\times\mathbf{\Psi}|_{\Gamma_R}=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}a'_{nm}\mathbf{U}_n^m+b'_{nm}\mathbf{V}_n^m$, then

$$\begin{aligned}(\hat{\mathbf{x}}\times\mathbf{\Psi})\times\hat{\mathbf{x}}|_{\Gamma_R} &= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}a'_{nm}\mathbf{U}_n^m\times\hat{\mathbf{x}}+b'_{nm}\mathbf{V}_n^m\times\hat{\mathbf{x}}\\ &= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}-a'_{nm}\mathbf{V}_n^m-b'_{nm}\mathbf{U}_n^m.\end{aligned}$$

Therefore

$$\begin{aligned}\langle\hat{G}_e(\hat{\mathbf{x}}\times\mathbf{\Phi}),(\hat{\mathbf{x}}\times\mathbf{\Psi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R} &= \langle\hat{G}_e(\hat{\mathbf{x}}\times\mathbf{\Phi}),\hat{\mathbf{x}}\times\mathbf{\Psi}\times\hat{\mathbf{x}}\rangle_{\Gamma_R}\\ &= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}-\frac{1}{\mathbf{i}kR}\gamma_n a_{nm}\bar{a}'_{nm}+R\eta_n b_{nm}\bar{b}'_{nm}.\end{aligned}$$

This completes the proof. □

Lemma 5.2 (Error representational formula)**.** *For any* $\mathbf{\Phi}\in\mathbf{H}(\mathbf{curl};\Omega_R)$*, which is extended to be a function* $\hat{\mathbf{\Phi}}$ *in* $\mathbf{H}(\mathbf{curl};\Omega_\rho)$ *according to* (5.2)-(5.3)*, and* $\mathbf{\Phi}_h\in\mathring{\mathbf{U}}_h$*, we have*

$$a(\mathbf{E}-\mathbf{E}_h,\mathbf{\Phi})=-b(\mathbf{E}_h,\hat{\mathbf{\Phi}}-\mathbf{\Phi}_h)+\mathbf{i}k\langle(\hat{G}_e-G_e)(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.$$

Proof. By (2.13) and the definition of the sesquilinear forms $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$, we have

$$\begin{aligned}a(\mathbf{E}-\mathbf{E}_h,\mathbf{\Phi}) &= -\int_{\Omega_R}(\nabla\times\mathbf{E}_h\cdot\nabla\times\bar{\mathbf{\Phi}}-k^2\mathbf{E}_h\cdot\bar{\mathbf{\Phi}})d\mathbf{x}\\ &\quad -\mathbf{i}k\langle G_e(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}\\ &= -b(\mathbf{E}_h,\hat{\mathbf{\Phi}})+\int_{\Omega^{\rm PML}}(BA\nabla\times\mathbf{E}_h\cdot\nabla\times\bar{\hat{\mathbf{\Phi}}}-k^2(BA)^{-1}\mathbf{E}_h\cdot\bar{\hat{\mathbf{\Phi}}})\\ &\quad -\mathbf{i}k\langle G_e(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.\end{aligned}$$

Integrate by parts and use (5.2) to obtain $\nabla\times BA\nabla\times\bar{\hat{\mathbf{\Phi}}}-k^2(BA)^{-1}\bar{\hat{\mathbf{\Phi}}}=0$ in $\Omega^{\rm PML}$, we have

$$\begin{aligned}a(\mathbf{E}-\mathbf{E}_h,\mathbf{\Phi}) &= -b(\mathbf{E}_h,\hat{\mathbf{\Phi}})+\langle\mathbf{n}\times\mathbf{E}_h,\mathbf{n}\times(\overline{BA}\nabla\times\hat{\mathbf{\Phi}})\times\mathbf{n}\rangle_{\Gamma_R\bigcup\Gamma_\rho}\\ &\quad -\mathbf{i}k\langle G_e(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.\end{aligned}$$

Since $\mathbf{n}\times\mathbf{E}_h=0$ on Γ_ρ and $\mathbf{n}=-\hat{\mathbf{x}}$ on Γ_R for the domain $\Omega^{\rm PML}$, we get

$$\begin{aligned}&a(\mathbf{E}-\mathbf{E}_h,\mathbf{\Phi})\\ =\ & -b(\mathbf{E}_h,\hat{\mathbf{\Phi}})-\langle\hat{\mathbf{x}}\times\mathbf{E}_h,\hat{\mathbf{x}}\times(\nabla\times\hat{\mathbf{\Phi}})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}-\mathbf{i}k\langle G_e(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}.\end{aligned}$$

By (2.15) and (5.2)-(5.3), we know that $\hat{G}_e(\hat{\mathbf{x}}\times\bar{\mathbf{\Phi}})=\frac{1}{\mathbf{i}k}\hat{\mathbf{x}}\times(\nabla\times\bar{\hat{\mathbf{\Phi}}})$. Thus

$$\begin{aligned}&a(\mathbf{E}-\mathbf{E}_h,\mathbf{\Phi})\\ =\ & -b(\mathbf{E}_h,\hat{\mathbf{\Phi}})+\mathbf{i}k\langle\hat{\mathbf{x}}\times\mathbf{E}_h,\hat{G}_e(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}-\mathbf{i}k\langle G_e(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}\\ =\ & -b(\mathbf{E}_h,\hat{\mathbf{\Phi}})+\mathbf{i}k\langle\hat{G}_e(\hat{\mathbf{x}}\times\bar{\hat{\mathbf{\Phi}}}),(\hat{\mathbf{x}}\times\bar{\mathbf{E}}_h)\times\hat{\mathbf{x}}\rangle_{\Gamma_R}-\mathbf{i}k\langle G_e(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}\\ =\ & -b(\mathbf{E}_h,\hat{\mathbf{\Phi}})+\mathbf{i}k\langle(\hat{G}_e-G_e)(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R},\end{aligned}$$

where in the last equality we have used Lemma 5.1. This completes the proof by using (4.3). □

5.2. **Stability estimates for the extension.** We start by proving two estimates for the PML extension in (2.9).

Lemma 5.3. *There exists a constant $C > 0$ independent of k, R, ρ and σ_0 such that for any $\lambda \in \mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})$,*

$$\|\,\nabla \times B\mathbb{E}(\lambda)\,\|_{\mathbf{L}^2(\Omega^{\mathrm{PML}})} \le CR^{1/2}|\alpha_0|^2(1+kR)^3\|\,\lambda\,\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_{\mathrm{R}})}.$$

Proof. Let $\lambda = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} a_{mn}\mathbf{U}_n^m + b_{mn}\mathbf{V}_n^m$ and denote by $\tilde{\mathbf{\Phi}} = \mathbb{E}(\lambda)$. By Lemma 3.4 and (2.7)-(2.8), we obtain

$$\begin{aligned}\frac{1}{\mathbf{i}k}\tilde{\nabla}\times\tilde{\mathbf{\Phi}} &= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\Bigg(\frac{a_{nm}}{\mathbf{i}k\tilde{r}}\frac{z_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\mathbf{U}_n^m + \mathbf{i}kRb_{mn}\frac{h_n^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)}\mathbf{V}_n^m \\ &\qquad + \frac{a_{nm}}{\mathbf{i}k\tilde{r}}\frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\sqrt{n(n+1)}Y_n^m\hat{\mathbf{x}}\Bigg),\end{aligned}$$

which yields

$$\begin{aligned}(5.6)\qquad &\int_{\Omega^{\mathrm{PML}}}\frac{1}{k^2r^2}|\tilde{\nabla}\times\tilde{\mathbf{\Phi}}|^2d\mathbf{x} \\ &= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\int_R^{\rho}\frac{|a_{nm}|^2}{k^2|\tilde{r}|^2}\left(\Big|\frac{z_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2 + n(n+1)\Big|\frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2\right)dr \\ &\quad + \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\int_R^{\rho}k^2R^2\Big|\frac{h_n^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)}\Big|^2|b_{nm}|^2dr.\end{aligned}$$

By the identity $h_n^{(1)\prime}(z) = -\frac{n+1}{z}h_n^{(1)}(z) + h_{n-1}^{(1)}(z)$, we get

$$\begin{aligned}\int_R^{\rho}\frac{1}{k^2|\tilde{r}|^2}\Big|\frac{z_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2dr &= \int_R^{\rho}\frac{1}{k^2|\tilde{r}|^2}\Big|\frac{-nh_n^{(1)}(k\tilde{r}) + k\tilde{r}h_{n-1}^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2dr \\ &\le \frac{n^2}{k^2R^2}\int_R^{\infty}\Big|\frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2dr + \int_R^{\rho}\Big|\frac{h_{n-1}^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2dr.\end{aligned}$$

To proceed, we recall the following estimate due to Nédeléc [20, (2.6.59)]

$$\int_1^{\infty}\Big|\frac{h_n^{(1)}(kr)}{h_n^{(1)}(k)}\Big|^2dr \le \frac{6k^2+n+1}{6k^2+(2n+1)(n+1)},\quad \forall n\ge 1.$$

Thus

$$\begin{aligned}(5.7)\qquad \int_R^{\infty}\Big|\frac{h_n^{(1)}(kr)}{h_n^{(1)}(kR)}\Big|^2dr &= R\int_1^{\infty}\Big|\frac{h_n^{(1)}(kRr)}{h_n^{(1)}(kR)}\Big|^2dr \\ &\le R\cdot\frac{6k^2R^2+n+1}{6k^2R^2+(2n+1)(n+1)} \\ &\le \frac{R}{2n+1}\Big(1+\frac{6k^2R^2}{n+1}\Big).\end{aligned}$$

Therefore

$$\begin{aligned}\int_R^\rho \frac{1}{k^2|\tilde r|^2}\Big|\frac{z_n^{(1)}(k\tilde r)}{h_n^{(1)}(kR)}\Big|^2 dr &\le \frac{n^2}{k^2R^2}\cdot\frac{R}{2n+1}\Big(1+\frac{6k^2R^2}{n+1}\Big)+(\rho-R)\\ &\le CR\sqrt{n(n+1)}\Big(1+\frac{1}{k^2R^2}\Big),\end{aligned}$$

where we have used (5.7), (3.7) and the inequality $|h_{n-1}^{(1)}(\Theta)|\le|h_n^{(1)}(\Theta)|$ for any $\Theta>0$ to conclude that $|h_{n-1}^{(1)}(k\tilde r)|\le|h_n^{(1)}(kR)|$. Similarly

$$n(n+1)\int_R^\rho \frac{1}{k^2|\tilde r|^2}\Big|\frac{h_n^{(1)}(k\tilde r)}{h_n^{(1)}(kR)}\Big|^2 dr \le CR\sqrt{n(n+1)}\Big(1+\frac{1}{k^2R^2}\Big). \tag{5.8}$$

By (3.9) we have $|\delta_n(kR)|^{-1}\le C$, thus

$$\begin{aligned}\int_R^\rho k^2R^2\Big|\frac{h_n^{(1)}(k\tilde r)}{z_n^{(1)}(kR)}\Big|^2 dr &= k^2R^2|\delta_n(kR)|^{-2}\int_R^\rho\Big|\frac{h_n^{(1)}(k\tilde r)}{h_n^{(1)}(kR)}\Big|^2 dr\\ &\le Ck^2R^2\int_R^\rho\Big|\frac{h_n^{(1)}(k\tilde r)}{h_n^{(1)}(kR)}\Big|^2 dr\\ &\le Ck^2R^2\cdot\frac{R}{2n+1}\Big(1+\frac{6k^2R^2}{n+1}\Big)\\ &\le Ck^2R^2(1+k^2R^2)\frac{R}{\sqrt{n(n+1)}}.\end{aligned} \tag{5.9}$$

Substitute (5.8)-(5.9) into (5.6) we get

$$\begin{aligned}&\int_{\Omega^{\rm PML}}\frac{1}{r^2}|\tilde\nabla\times\tilde{\mathbf\Phi}|^2 d\mathbf x\\ \le\ & CR\Big(1+\frac{1}{k^2R^2}+k^4R^4\Big)\sum_{n=1}^\infty\sum_{m=-n}^n\sqrt{n(n+1)}|a_{nm}|^2+\frac{1}{\sqrt{n(n+1)}}|b_{nm}|^2\\ =\ & CR\Big(1+\frac{1}{k^2R^2}+k^4R^4\Big)\|\lambda\|^2_{\mathbf H^{-1/2}({\rm Div};\Gamma_{\rm R})}.\end{aligned}$$

Hence

$$\|\tilde\nabla\times\tilde{\mathbf\Phi}\|_{\mathbf L^2(\Omega^{\rm PML})}\le CR^{1/2}(1+kR)^3\|\lambda\|_{\mathbf H^{-1/2}({\rm Div};\Gamma_{\rm R})}.$$

This completes the proof since $\tilde\nabla\times\tilde{\mathbf\Phi}=A\nabla\times B\tilde{\mathbf\Phi}$, $A={\rm diag}(\beta^{-2},\alpha^{-1}\beta^{-1},\alpha^{-1}\beta^{-1})$, and $|\beta^{-2}|\ge|\alpha_0|^{-2}$, $|\alpha^{-1}\beta^{-1}|\ge|\alpha_0|^{-2}$. □

Lemma 5.4. *There exists a constant $C>0$ independent of k,R,ρ, and σ_0 such that for any $\lambda\in\mathbf H^{-1/2}({\rm Div};\Gamma_{\rm R})$,*

$$\|B\mathbb E(\lambda)\|_{\mathbf L^2(\Omega^{\rm PML})}\le CR^{3/2}|\alpha_0|(1+kR)^2\|\lambda\|_{\mathbf H^{-1/2}({\rm Div};\Gamma_{\rm R})}.$$

Proof. Let $\lambda=\sum_{n=1}^\infty\sum_{m=-n}^n a_{mn}\mathbf U_n^m+b_{mn}\mathbf V_n^m$ and denote by $\tilde{\mathbf\Phi}=\mathbb E(\lambda)$. From (2.9) and (2.7)-(2.8), we have

$$\begin{aligned}\tilde{\mathbf\Phi}=\sum_{n=1}^\infty\sum_{m=-n}^n\Bigg(&\frac{R}{\tilde r}\frac{z_n^{(1)}(k\tilde r)}{z_n^{(1)}(kR)}b_{nm}\mathbf U_n^m-\frac{h_n^{(1)}(k\tilde r)}{h_n^{(1)}(kR)}a_{nm}\mathbf V_n^m\\ &+\frac{R}{\tilde r}\sqrt{n(n+1)}\frac{h_n^{(1)}(k\tilde r)}{z_n^{(1)}(kR)}b_{mn}Y_n^m\hat{\mathbf x}\Bigg).\end{aligned}$$

Thus

$$\begin{aligned}\int_{\Omega^{\rm PML}} \frac{1}{r^2}|\tilde{\mathbf{\Phi}}|^2 d\mathbf{x} &= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\int_R^\rho \Big|\frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2|a_{nm}|^2dr \\ &\quad + \int_R^\rho \Big|\frac{R}{\tilde{r}}\Big|^2\left(\Big|\frac{z_n^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)}\Big|^2 + n(n+1)\Big|\frac{h_n^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)}\Big|^2\right)|b_{nm}|^2dr.\end{aligned}$$

Since $|h_n^{(1)}(k\tilde{r})| \le |h_n^{(1)}(kR)|$ by Lemma 3.2, we have

$$\int_R^\rho \Big|\frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2 dr \le \rho - R \le CR. \tag{5.10}$$

By (3.9) we have $|\delta_n(kR)|^{-1} \le Cn^{-1}(1+kR)$. Thus by (5.8), we have

$$\begin{aligned}&\int_R^\rho \Big|\frac{R}{\tilde{r}}\Big|^2\Big|\frac{z_n^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)}\Big|^2 dr \\ &= k^2R^2\int_R^\rho \frac{1}{k^2|\tilde{r}|^2}\Big|\frac{z_n^{(1)}(k\tilde{r})}{h_n^{(1)}kR}\Big|^2 dr\cdot|\delta_n(kR)|^{-2} \\ &\le k^2R^2\cdot CR\sqrt{n(n+1)}\Big(1+\frac{1}{k^2R^2}\Big)\cdot C\frac{(1+kR)^2}{n^2} \\ &\le CR\frac{1}{\sqrt{n(n+1)}}(1+kR)^4.\end{aligned} \tag{5.11}$$

Finally, by (5.8) we get

$$\begin{aligned}&n(n+1)\int_R^\rho \frac{R^2}{|\tilde{r}|^2}\Big|\frac{h_n^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)}\Big|^2 dr \\ &= k^2R^2\cdot n(n+1)\cdot\int_R^\rho \frac{1}{k^2|\tilde{r}|^2}\Big|\frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)}\Big|^2 dr\cdot|\delta_n(kR)|^{-2} \\ &\le k^2R^2\cdot CR\sqrt{n(n+1)}\Big(1+\frac{1}{k^2R^2}\Big)\cdot C\frac{(1+kR)^2}{n^2} \\ &\le CR\frac{1}{\sqrt{n(n+1)}}(1+kR)^4.\end{aligned} \tag{5.12}$$

Substitute (5.10)-(5.12) into (5.10), we obtain

$$\begin{aligned}\int_{\Omega^{\rm PML}} \frac{1}{r^2}|\tilde{\mathbf{\Phi}}|^2 d\mathbf{x} &\le CR(1+kR)^4\sum_{n=1}^{\infty}\sum_{m=-n}^{n}|a_{nm}|^2 + \frac{1}{\sqrt{n(n+1)}}|b_{nm}|^2 \\ &\le CR(1+kR)^4\|\,\lambda\,\|^2_{\mathbf{H}^{-1/2}({\rm Div};\Gamma_{\rm R})},\end{aligned}$$

which implies

$$\|\,\tilde{\mathbf{\Phi}}\,\|_{\mathbf{L}^2(\Omega^{\rm PML})} \le CR^{3/2}(1+kR)^2\|\,\lambda\,\|_{\mathbf{H}^{-1/2}({\rm Div};\Gamma_{\rm R})}.$$

This completes the proof by using the fact that $B = \mathrm{diag}(\alpha,\beta,\beta)$ and $|\alpha| \le |\alpha_0|, |\beta| \le |\alpha_0|$. □

The following result on the extension $\hat{\mathbf{\Phi}}$ is the main objective of this subsection.

Lemma 5.5. *Let* $\hat{\mathbf{\Phi}}$ *be the extension of* $\mathbf{\Phi} \in \mathbf{H}(\mathbf{curl};\Omega_R)$ *according to* (5.2)-(5.3). *Then we have*

$$\|\hat{\mathbf{\Phi}}\|_{\mathbf{curl};\Omega^{\rm PML}} \le C\hat{C}^{-1}|\alpha_0|^3 R^{1/2}(1+kR)^3 \|\,\hat{\mathbf{x}}\times\mathbf{\Phi}\,\|_{\mathbf{H}^{-1/2}({\rm Div};\Gamma_{\rm R})}.$$

Proof. Let $\tilde{\mathbf{\Phi}} = \mathbb{E}(\hat{\mathbf{x}}\times\bar{\mathbf{\Phi}}|_{\Gamma_R})$ be the PML extension of $\hat{\mathbf{x}}\times\bar{\mathbf{\Phi}}|_{\Gamma_R}$. Then $\tilde{\mathbf{\Phi}}$ satisfies

$$\begin{aligned}\nabla\times BA\nabla\times\tilde{\mathbf{\Phi}} - k^2(BA)^{-1}\tilde{\mathbf{\Phi}} &= 0 \quad \text{in } \mathbb{R}^3\backslash\bar{B}_R,\\ \hat{\mathbf{x}}\times\tilde{\mathbf{\Phi}} &= \hat{\mathbf{x}}\times\bar{\mathbf{\Phi}} \quad \text{on } \Gamma_R.\end{aligned}$$

Let $\mathbf{w} = \hat{\mathbf{\Phi}} - B\bar{\tilde{\mathbf{\Phi}}}$, then $\mathbf{w}$ satisfies

$$\begin{aligned}&\nabla\times BA\nabla\times\mathbf{w} - k^2(BA)^{-1}\mathbf{w} = 0 \quad \text{in } \Omega^{\rm PML},\\ &\hat{\mathbf{x}}\times\mathbf{w} = 0 \text{ on } \Gamma_R, \qquad \hat{\mathbf{x}}\times\mathbf{w} = -B\mathbb{P}(\hat{\mathbf{x}}\times\bar{\mathbf{\Phi}}|_{\Gamma_R}) \text{ on } \Gamma_\rho.\end{aligned}$$

By Lemma 3.6 and (3.15)

$$\begin{aligned}\|\mathbf{w}\|_{\mathbf{curl};\Omega^{\rm PML}} &\le C\hat{C}^{-1}|\alpha_0|^2\|\,B\mathbb{P}(\hat{\mathbf{x}}\times\bar{\mathbf{\Phi}}|_{\Gamma_R})\,\|_{\mathbf{H}^{-1/2}({\rm Div};\Gamma_\rho)}\\ &\le C\hat{C}^{-1}(1+kR)|\alpha_0|^3\|\,\hat{\mathbf{x}}\times\mathbf{\Phi}\,\|_{\mathbf{H}^{-1/2}({\rm Div};\Gamma_{\rm R})}.\end{aligned}$$

By Lemmas 5.3-5.5, we have

$$\|B\tilde{\mathbf{\Phi}}\|_{\mathbf{curl};\Omega^{\rm PML}} \le CR^{1/2}(1+kR)^3|\alpha_0|^3\|\,\hat{\mathbf{x}}\times\mathbf{\Phi}\,\|_{\mathbf{H}^{-1/2}({\rm Div};\Gamma_{\rm R})}.$$

This completes the proof by using the triangle inequality. □

5.3. **Proof of Theorem 4.1.** Our starting point is (5.1). To estimate the second term in (5.1), for any $\mathbf{\Phi} \in \mathbf{H}(\mathbf{curl};\Omega_R)$ such that $\mathbf{n}\times\mathbf{\Phi} = 0$ on Γ_D, we denote by $\hat{\mathbf{\Phi}}$ its extension to $\Omega^{\rm PML}$ according to (5.2)-(5.3). Thus $\hat{\mathbf{\Phi}} \in \mathbf{H}_0(\mathbf{curl};\Omega_\rho)$. By Lemma 4.2, there exists $\mathbf{\Psi} \in \mathbf{H}_0(\mathbf{curl};\Omega_\rho)\bigcap H^1(\Omega_\rho)^3$ and $\varphi \in H_0^1(\Omega_\rho)$ such that $\hat{\mathbf{\Phi}} = \mathbf{\Psi} + \nabla\varphi$, and

$$\|\varphi\|_{H^1(\Omega_\rho)} + \|\mathbf{\Psi}\|_{\mathbf{H}^1(\Omega_\rho)} \le C\|\hat{\mathbf{\Phi}}\|_{\mathbf{H}(\mathbf{curl};\Omega_\rho)}.$$

By Lemma 5.5 and the trace inequality for $\mathbf{H}(\mathbf{curl};\Omega_R)$, we have then

$$\|\varphi\|_{H^1(\Omega_\rho)} + \|\mathbf{\Psi}\|_{\mathbf{H}^1(\Omega_\rho)} \le C\hat{C}^{-1}R^{1/2}|\alpha_0|^3(1+kR)^3\|\mathbf{\Phi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}. \tag{5.13}$$

Let $\mathbf{\Phi}_h = \nabla r_h\varphi + \pi_h\mathbf{\Psi}$, where $r_h : H_0^1(\Omega_\rho) \to \mathring{V}_h$ and $\pi_h : H^1(\Omega_\rho)^3\bigcap\mathbf{H}_0(\mathbf{curl};\Omega_\rho) \to \mathring{\mathbf{U}}_h$ are the interpolation operators defined at the end of §4. By the error representation formula in Lemma 5.2, we have

$$\begin{aligned}&a(\mathbf{E}-\mathbf{E}_h,\mathbf{\Phi})\\ =\;& -b(\mathbf{E}_h,\mathbf{\Psi}+\nabla\varphi-(\pi_h\mathbf{\Psi}+\nabla r_h\varphi)) + \mathbf{i}k\langle(\hat{G}_e-G_e)(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}\\ =\;& -\int_{\Omega_\rho}\Big(BA\nabla\times\mathbf{E}_h\cdot\nabla\times(\bar{\mathbf{\Psi}}-\pi_h\bar{\mathbf{\Psi}}) - k^2(BA)^{-1}\mathbf{E}_h\cdot(\bar{\mathbf{\Psi}}-\pi_h\bar{\mathbf{\Psi}})\Big)d\mathbf{x}\\ &+\int_{\Omega_\rho}k^2(BA)^{-1}\mathbf{E}_h\cdot\nabla(\bar{\varphi}-r_h\bar{\varphi})d\mathbf{x}\\ &+\mathbf{i}k\langle(\hat{G}_e-G_e)(\hat{\mathbf{x}}\times\mathbf{E}_h),(\hat{\mathbf{x}}\times\mathbf{\Phi})\times\hat{\mathbf{x}}\rangle_{\Gamma_R}\\ :=\;& \mathrm{I}+\mathrm{II}+\mathrm{III}.\end{aligned}$$

By using integration by parts, the estimates (4.4)-(4.5), and standard argument in the a posteriori error analysis, we obtain

$$\begin{aligned}|\mathrm{I}+\mathrm{II}| &\leq C\Big(\sum_{K\in\mathcal{M}_h}\eta_K^2\Big)^{1/2}(\|\varphi\|_{H^1(\Omega_\rho)}+\|\mathbf{\Psi}\|_{\mathbf{H}^1(\Omega_\rho)})\\ &\leq C\hat{C}^{-1}R^{1/2}|\alpha_0|^3(1+kR)^3\Big(\sum_{K\in\mathcal{M}_h}\eta_K^2\Big)^{1/2}\|\mathbf{\Phi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)},\end{aligned}$$

where we have used (5.13) in the last inequality. By Lemma 3.7 and trace inequality for $\mathbf{H}(\mathbf{curl};\Omega_R)$, we have

$$|\mathrm{III}|\leq C\hat{C}^{-1}(1+kR)^3|\alpha_0|^3e^{-\mathrm{Im}(k\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}}\|\,\hat{\mathbf{x}}\times\mathbf{E}_h\,\|_{\mathbf{H}^{-1/2}(\mathrm{Div};\Gamma_\mathrm{R})}\|\mathbf{\Phi}\|_{\mathbf{H}(\mathbf{curl};\Omega_R)}.$$

This completes the proof by (5.1). □

6. Numerical examples

The implementation of the adaptive algorithm in this section is based on the adaptive finite element package ALBERT [22] and its adaptation to the edge element by Dr. Long Wang. The computation is carried out on a Origin 3800. We use the a posteriori error estimate in Theorem 4.1 to determine the PML parameters. According to the discussion in §3, 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 4.1 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:

$$e^{-k\mathrm{Im}(\tilde{\rho})(1-\frac{R^2}{|\tilde{\rho}|^2})^{1/2}}\leq 10^{-8}, \tag{6.1}$$

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 (cf. e.g. [8]).

In the following we report two numerical examples to demonstrate the competitive behavior of the proposed algorithm.

Example 1. Let the scatterer D be the unit ball and $k=1$. We consider the scattering problem whose exact solution is known

$$\mathbf{E}=\mathbf{M}_1^0(|\mathbf{x}|,\hat{\mathbf{x}})=\nabla\times\{\mathbf{x}h_1^{(1)}(|\mathbf{x}|)Y_1^0(\hat{\mathbf{x}})\}$$

Figure 6.1 shows the $\log N_k$-$\log\|\,\nabla\times(\mathbf{E}-\mathbf{E}_k)\,\|_{\mathbf{L}^2(\Omega_R)}$ curves, where N_k is the number of edges of the mesh $\mathcal{M}_k$ and $\mathbf{E}_k$ is the finite element solution of (4.3) over the mesh $\mathcal{M}_k$. It indicates that the meshes and the associated numerical complexity are quasi-optimal: $\|\,\nabla\times(\mathbf{E}-\mathbf{E}_k)\,\|_{\mathbf{L}^2(\Omega_R)}\approx CN_k^{-1/3}$ is valid asymptotically.

One of the important quantities in the scattering problem is the far field

$$\mathbf{E}_\infty(\hat{\mathbf{x}})=\frac{\mathbf{i}k}{4\pi}\hat{\mathbf{x}}\times\int_{\Gamma_D}((\mathbf{n}\times\mathbf{E})(\mathbf{y})+(\mathbf{n}\times\frac{1}{\mathbf{i}k}\nabla\times\mathbf{E})(\mathbf{y})\times\hat{\mathbf{x}})e^{-\mathbf{i}k\hat{\mathbf{x}}\cdot\mathbf{y}}dS_{\mathbf{y}}.$$

Figures 6.2 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

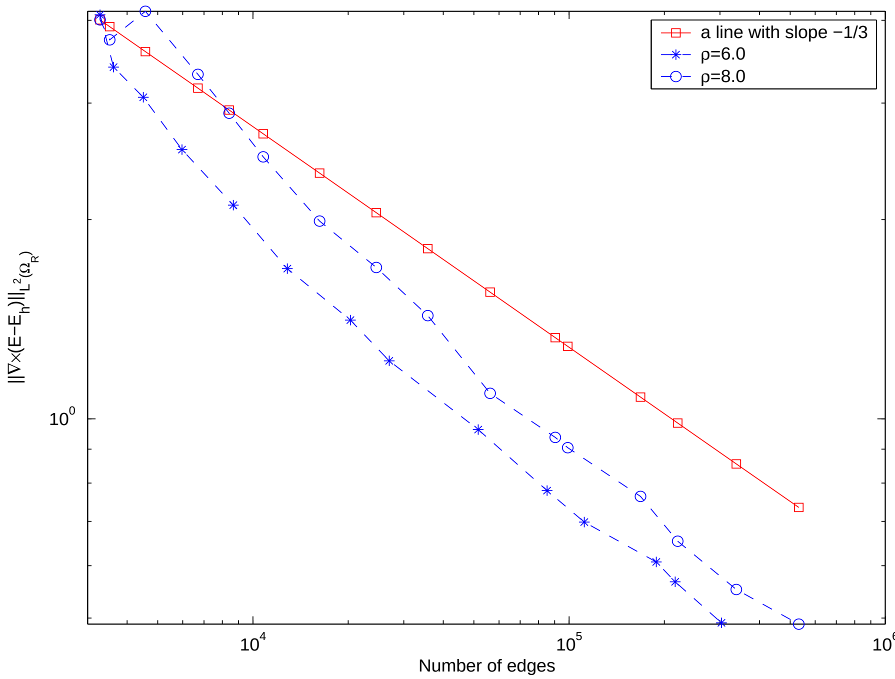

FIGURE 6.1. The quasi-optimality of the adaptive mesh refinements of the error $\| \nabla \times (\mathbf{E} - \mathbf{E}_k) \|_{\mathbf{L}^2(\Omega_R)}$ for Example 1.

thickness of PML layer: the far fields of the scattering solutions are insensitive to the choices of the PML parameters.

Example 2. This example concerns the scattering of the plane wave $\mathbf{E}^i = e^{\mathbf{i}x_3}\mathbf{e}_1$ from a perfectly conducting metal. The scatterer D is shown in Figure 6.3.

In Figure 6.4 we show the mesh after 18 adaptive iterations when $\rho = 2R = 6$ with 817078 edges. Figure 6.5 shows the $\log N_k$-$\log \mathcal{E}_k$ curves, where $\mathcal{E}_k = (\sum_{K\in\mathcal{M}_k} \eta_K^2)^{1/2}$ is the associated a posteriori error estimate. It indicates that the meshes and the associated numerical complexity are quasi-optimal: $\mathcal{E}_k \approx C N_k^{-1/3}$ is valid asymptotically.

Figure 6.6 shows the far fields in the direction $(1, 0, 0)$ for different choices of the PML parameters. Again we observe that the far fields are insensitive to the choices of the PML parameters.

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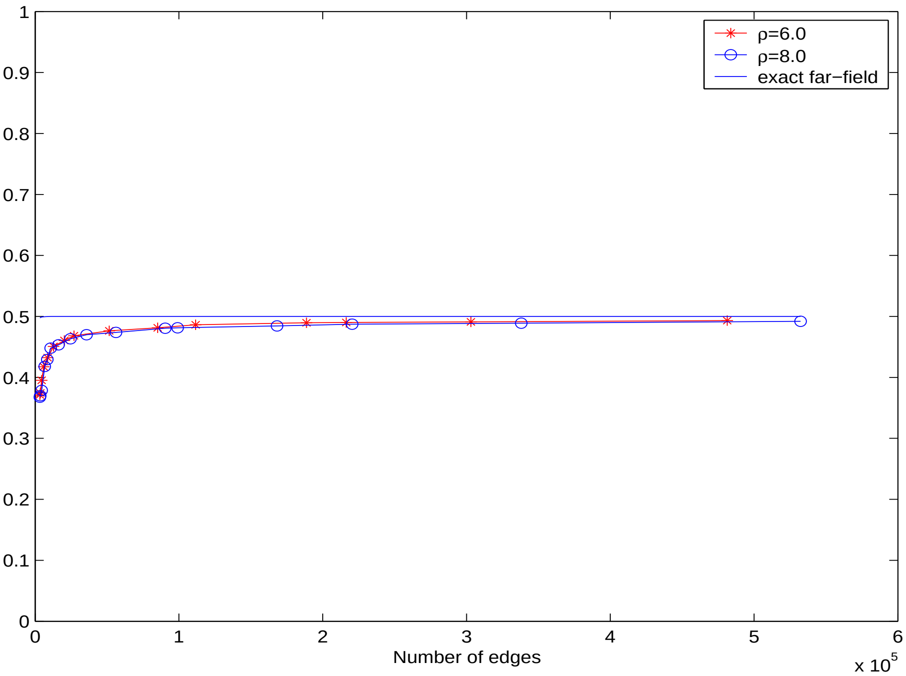

FIGURE 6.2. The module of the real part of the far fields in the direction $(1, 0, 0)$ for Example 1.

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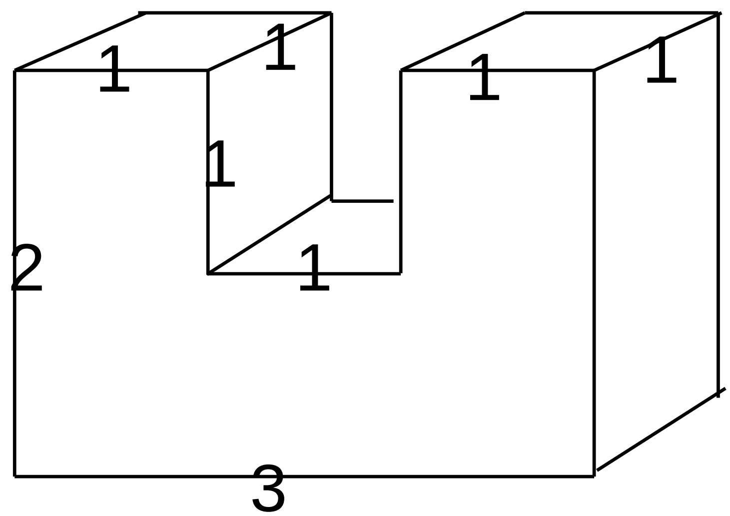

FIGURE 6.3. The U-shape scatterer for Example 2.

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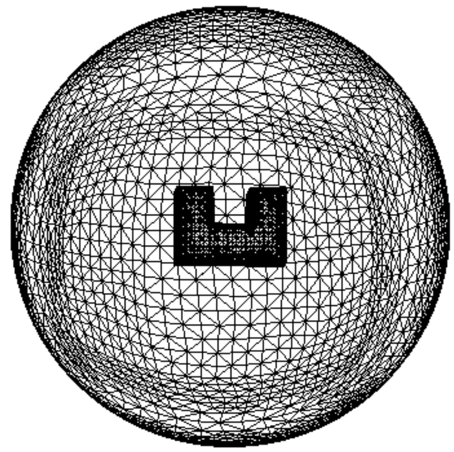

FIGURE 6.4. The mesh of 817078 edges after 18 adaptive refinements, $\rho = 2R = 6$ for Example 2.

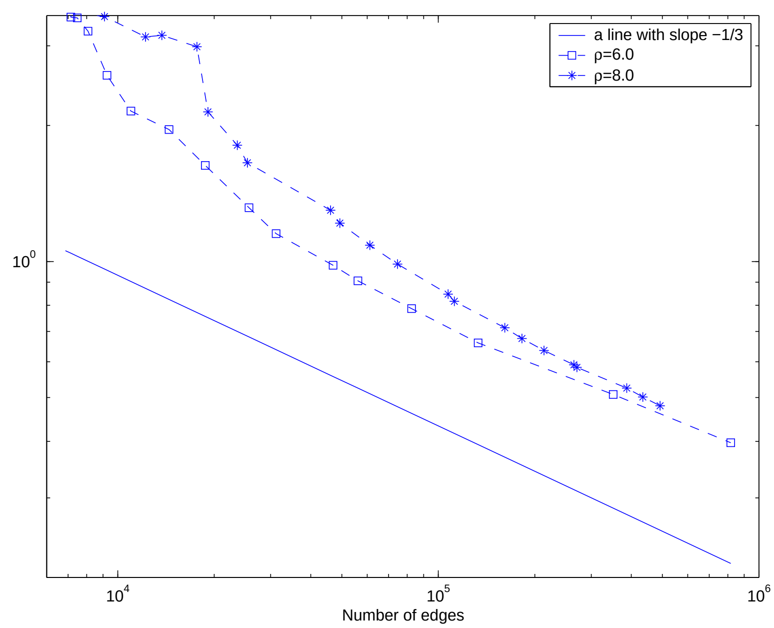

FIGURE 6.5. The quasi-optimality of the adaptive mesh refinements of the a posteriori error estimator for Example 2.

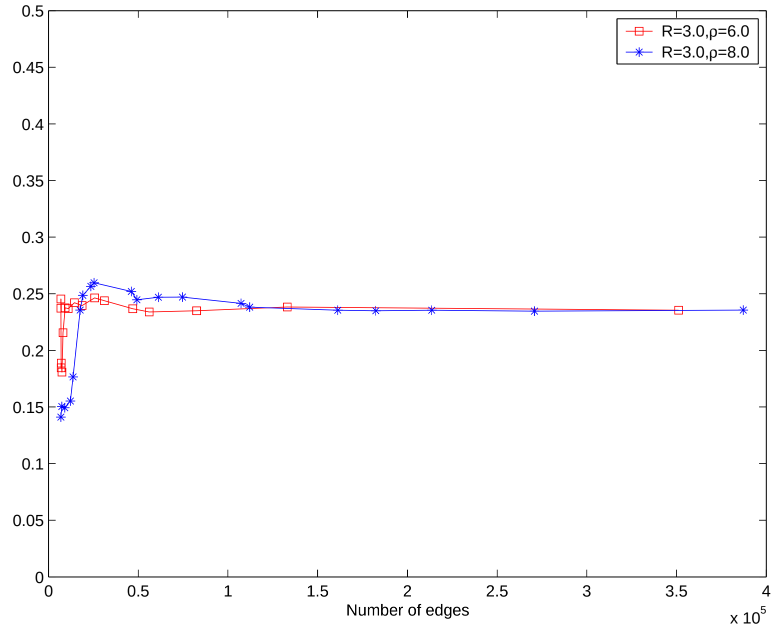

FIGURE 6.6. The module of the real part of the far fields in the direction $(1, 0, 0)$ for Example 2.

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