CONVERGENCE OF THE PML SOLUTION FOR ELASTIC WAVE SCATTERING BY BIPERIODIC STRUCTURES*

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Abstract. This paper is concerned with the analysis of elastic wave scattering of a time-harmonic plane wave by a biperiodic rigid surface, where the wave propagation is governed by the three-dimensional Navier equation. An exact transparent boundary condition is developed to reduce the scattering problem equivalently into a boundary value problem in a bounded domain. The Perfectly Matched Layer (PML) technique is adopted to truncate the unbounded physical domain into a bounded computational domain. The well-posedness and exponential convergence of the solution are established for the truncated PML problem by developing a PML equivalent transparent boundary condition. The proofs rely on a careful study of the error between the two transparent boundary operators. The work significantly extends the results from one-dimensional periodic structures to two-dimensional biperiodic structures. Numerical experiments are included to demonstrate the competitive behavior of the proposed method.

Keywords. Elastic wave equation; perfectly matched layer; biperiodic structures; transparent boundary condition.

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

1. Introduction

Scattering theory in periodic structures has many important applications in diffractive optics [7,8], where the periodic structures are often named as gratings. The scattering problems have been studied extensively in periodic structures by many researchers for all the commonly encountered waves including the acoustic, electromagnetic, and elastic waves [1,2,4,5,15,22–24,30,34]. The governing equations of these waves are known as the Helmholtz equation, the Maxwell equations, and the Navier equation, respectively. In this paper, we consider the scattering of a time-harmonic elastic plane wave by a biperiodic rigid surface, which is also called a two-dimensional or crossed grating. The elastic wave scattering problems have received ever-increasing attention in both engineering and mathematical communities for their important applications in geophysics and seismology. The elastic wave motion is governed by the three-dimensional Navier equation. A fundamental challenge of this problem is to truncate the unbounded physical domain into a bounded computational domain. An appropriate boundary condition

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is needed on the boundary of the truncated domain to avoid artificial wave reflection. We adopt the perfectly matched layer (PML) technique to handle this issue.

The research on the PML technique has undergone a tremendous development since Berenger proposed a PML for solving the time-dependent Maxwell equations [11]. The basic idea of the PML technique is to surround the domain of interest by a layer of finite thickness fictitious material which absorbs all the waves coming from inside the computational domain. When the waves reach the outer boundary of the PML region, their values are so small that the homogeneous Dirichlet boundary conditions can be imposed. Various constructions of PML absorbing layers have been proposed and investigated for the acoustic and electromagnetic wave scattering problems [10, 12, 19–21, 26, 28, 33]. In particular, combined with the PML technique, an effective adaptive finite element method was proposed in [6, 16] to solve the two-dimensional diffraction grating problem where the one-dimensional grating was considered. Due to the competitive numerical performance, the method was quickly adopted to solve many other scattering problems including the obstacle scattering problems [14, 17] and the three-dimensional diffraction grating problem [9]. However, the PML technique is much less studied for the elastic wave scattering problems [25], especially for the rigorous convergence analysis. We refer to [13, 18] for recent study on convergence analysis of the elastic obstacle scattering problems.

Recently, we have proposed an adaptive finite element method combining with the PML technique to solve the elastic scattering problem in one-dimensional periodic structures [27]. Using the quasi-periodicity of the solution, we develop a transparent boundary condition and formulate the scattering problem equivalently into a boundary value problem in a bounded domain. Following the complex coordinate stretching, we study the truncated PML problem and show that it has a unique weak solution which converges exponentially to the solution of the original scattering problem.

This paper's goal is to extend our previous work on one-dimensional periodic structures in [27] to two-dimensional biperiodic structures. We point out that the extension is nontrivial because the more complicated three-dimensional Navier equation needs to be considered. The analysis is mathematically more sophisticated and the numerical implementation is computationally more intense. This work presents an important application of the PML method for the scattering problem of elastic waves.

The elastic wave equation is complicated due to the coexistence of compressional and shear waves that have different wavenumbers. To take into account this feature, we introduce two potential functions, one scalar and one vector, to split the wave field into its compressional and shear parts via the Helmholtz decomposition. As a consequence, the scalar potential function satisfies the Helmholtz equation while the vector potential function satisfies the Maxwell equation. Using these two potential functions, we develop an exact transparent boundary condition to reduce the scattering problem from an open domain into a boundary value problem in a bounded domain. The energy conservation is proved for the propagating wave modes of the model problem and is used for verification of our numerical results. The well-posedness and exponential convergence of the solution are established for the truncated PML problem by developing a PML equivalent transparent boundary condition. The proofs rely on a careful study of the error between the two transparent boundary operators. Two numerical examples are also included to demonstrate the competitive behavior of the proposed method.

The paper is organized as follows. In Section 2, we introduce the model problem of the elastic wave scattering by a biperiodic surface and formulate it into a boundary value problem by using a transparent boundary condition. In Section 3, we introduce

the PML formulation and prove the well-posedness and convergence of the truncated PML problem. In Section 4, we discuss the numerical implementation of our numerical algorithm and present some numerical experiments to illustrate the performance of the proposed method. The paper is concluded with some general remarks in Section 5.

2. Problem formulation

In this section, we introduce the model problem and present an exact transparent boundary condition to reduce the problem into a boundary value problem in a bounded domain. The energy distribution is studied for the diffracted propagating waves of the scattering problem.

2.1. Navier equation.   Let $\boldsymbol{r} = (x_1, x_2)^\top$ and $\boldsymbol{x} = (x_1, x_2, x_3)^\top$. Consider the elastic scattering of a time-harmonic plane wave by a biperiodic surface $\Gamma_f = \{\boldsymbol{x} \in \mathbb{R}^3 : x_3 = f(\boldsymbol{r})\}$, where f is a Lipschitz continuous and biperiodic function with period (Λ_1, Λ_2) in (x_1, x_2). Denote by $\Omega_f = \{\boldsymbol{x} \in \mathbb{R}^3 : x_3 > f(\boldsymbol{r})\}$ the open space above Γ_f which is assumed to be filled with a homogeneous isotropic linear elastic medium. Let h be a constant satisfying $h > \max_{\boldsymbol{r} \in \mathbb{R}^2} f(\boldsymbol{r})$. Denote $\Omega = \{\boldsymbol{x} \in \mathbb{R}^3 : 0 < x_1 < \Lambda_1, 0 < x_2 < \Lambda_2, f(\boldsymbol{r}) < x_3 < h\}$ and $\Gamma_h = \{\boldsymbol{x} \in \mathbb{R}^3 : 0 < x_1 < \Lambda_1, 0 < x_2 < \Lambda_2, x_3 = h\}$. Let $\Omega_h = \{\boldsymbol{x} \in \mathbb{R}^3 : 0 < x_1 < \Lambda_1, 0 < x_2 < \Lambda_2, x_3 > h\}$ be the open space above Γ_h. The problem geometry is shown in Figure 2.1.
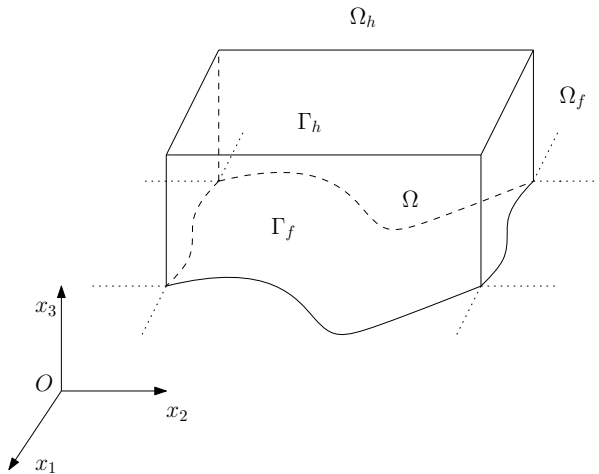

Fig. 2.1. *The problem geometry.*

The propagation of a time-harmonic elastic wave is governed by the Navier equation:

$$\mu \Delta \boldsymbol{u} + (\lambda + \mu) \nabla \nabla \cdot \boldsymbol{u} + \omega^2 \boldsymbol{u} = 0 \quad \text{in } \Omega_f, \tag{2.1}$$

where $\boldsymbol{u} = (u_1, u_2, u_3)^\top$ is the displacement vector of the total elastic wave field, $\omega > 0$ is the angular frequency, μ and λ are the Lamé constants satisfying $\mu > 0$ and $\lambda + \mu > 0$. Assuming that the surface Γ_f is elastically rigid, we have

$$\boldsymbol{u} = 0 \quad \text{on } \Gamma_f. \tag{2.2}$$

Define

$$\kappa_1 = \frac{\omega}{(\lambda + 2\mu)^{1/2}} \quad \text{and} \quad \kappa_2 = \frac{\omega}{\mu^{1/2}},$$

which are the compressional wavenumber and the shear wavenumber, respectively.

Let the scattering surface Γ_f be illuminated from above by a time-harmonic compressional plane wave:

$$\boldsymbol{u}^{\mathrm{inc}}(\boldsymbol{x}) = \boldsymbol{q}e^{\mathrm{i}\kappa_1 \boldsymbol{x} \cdot \boldsymbol{q}},$$

where $\boldsymbol{q} = (\sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2, -\cos\theta_1)^\top$ is the propagation direction vector, and θ_1, θ_2 are called the latitudinal and longitudinal incident angles satisfying $\theta_1 \in [0, \pi/2), \theta_2 \in [0, 2\pi]$. It can be verified that the incident wave also satisfies the Navier equation:

$$\mu\Delta\boldsymbol{u}^{\mathrm{inc}} + (\lambda+\mu)\nabla\nabla\cdot\boldsymbol{u}^{\mathrm{inc}} + \omega^2\boldsymbol{u}^{\mathrm{inc}} = 0 \quad \text{in } \Omega_f. \tag{2.3}$$

REMARK 2.1.   The scattering surface may be also illuminated by a time-harmonic shear plane wave:

$$\boldsymbol{u}^{\mathrm{inc}} = \boldsymbol{p}e^{\mathrm{i}\kappa_2 \boldsymbol{x} \cdot \boldsymbol{q}},$$

where $\boldsymbol{p}$ is the polarization vector satisfying $\boldsymbol{p}\cdot\boldsymbol{q} = 0$. More generally, the scattering surface can be illuminated by any linear combination of the time-harmonic compressional and shear plane waves. For clarity, we take the time-harmonic compressional plane wave as an example since the results and analysis are the same for other forms of the incident wave.

Motivated by uniqueness, we are interested in a quasi-periodic solution of $\boldsymbol{u}$, i.e., $\boldsymbol{u}(\boldsymbol{x})e^{-\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{r}}$ is biperiodic in x_1 and x_2 with periods Λ_1 and Λ_2, respectively. Here $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)^\top$ with $\alpha_1 = \kappa_1\sin\theta_1\cos\theta_2, \alpha_2 = \kappa_1\sin\theta_1\sin\theta_2$. In addition, the following radiation condition is imposed: the total displacement $\boldsymbol{u}$ consists of bounded outgoing waves plus the incident wave in Ω_h.

We introduce some notation and Sobolev spaces. Let $\boldsymbol{u} = (u_1, u_2, u_3)^\top$ be a vector function. Define the Jacobian matrix of $\boldsymbol{u}$:

$$\nabla\boldsymbol{u} = \begin{bmatrix} \partial_{x_1}u_1 & \partial_{x_2}u_1 & \partial_{x_3}u_1 \\ \partial_{x_1}u_2 & \partial_{x_2}u_2 & \partial_{x_3}u_2 \\ \partial_{x_1}u_3 & \partial_{x_2}u_3 & \partial_{x_3}u_3 \end{bmatrix}.$$

Define a quasi-biperiodic functional space

$$H^1_{\mathrm{qp}}(\Omega) = \{u \in H^1(\Omega) : u(x_1 + n_1\Lambda_1, x_2 + n_2\Lambda_2, x_3)$$
$$= u(x_1, x_2, x_3)e^{\mathrm{i}(n_1\alpha_1\Lambda_1 + n_2\alpha_2\Lambda_2)}, n = (n_1, n_2)^\top \in \mathbb{Z}^2\},$$

which is a subspace of $H^1(\Omega)$ with the norm $\|\cdot\|_{H^1(\Omega)}$. For any quasi-biperiodic function u defined on Γ_h, it admits the Fourier series expansion:

$$u(\boldsymbol{r}, h) = \sum_{n\in\mathbb{Z}^2} u^{(n)}(h)e^{\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r}},$$

where $\boldsymbol{\alpha}^{(n)} = (\alpha_1^{(n)}, \alpha_2^{(n)})^\top, \alpha_1^{(n)} = \alpha_1 + 2\pi n_1/\Lambda_1, \alpha_2^{(n)} = \alpha_2 + 2\pi n_2/\Lambda_2$, and

$$u^{(n)}(h) = \frac{1}{\Lambda_1\Lambda_2}\int_0^{\Lambda_1}\int_0^{\Lambda_2} u(\boldsymbol{r}, h)e^{-\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{r}.$$

We define a trace functional space $H^s(\Gamma_h)$ with the norm given by

$$\|u\|_{H^s(\Gamma_h)} = \left(\Lambda_1 \Lambda_2 \sum_{n \in \mathbb{Z}^2} (1 + |\boldsymbol{\alpha}^{(n)}|^2)^s |u^{(n)}(h)|^2\right)^{1/2}.$$

Let $H^1_{\mathrm{qp}}(\Omega)^3$ and $H^s(\Gamma_h)^3$ be the Cartesian product spaces equipped with the corresponding 2-norms of $H^1_{\mathrm{qp}}(\Omega)$ and $H^s(\Gamma_h)$, respectively. It is known that $H^{-s}(\Gamma_h)^3$ is the dual space of $H^s(\Gamma_h)^3$ with respect to the $L^2(\Gamma_h)^3$ inner product

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\Gamma_h} = \int_{\Gamma_h} \boldsymbol{u} \cdot \bar{\boldsymbol{v}} \, \mathrm{d}\boldsymbol{r},$$

where the bar denotes the complex conjugate.

2.2. Boundary value problem.   We wish to reduce the problem equivalently into a boundary value problem in Ω by introducing an exact transparent boundary condition on Γ_h.

The total field $\boldsymbol{u}$ consists of the incident field $\boldsymbol{u}^{\mathrm{inc}}$ and the diffracted field $\boldsymbol{v}$, i.e.,

$$\boldsymbol{u} = \boldsymbol{u}^{\mathrm{inc}} + \boldsymbol{v}. \tag{2.4}$$

Subtracting (2.3) from (2.1) and noting (2.4), we obtain the Navier equation for the diffracted field $\boldsymbol{v}$:

$$\mu \Delta \boldsymbol{v} + (\lambda + \mu) \nabla \nabla \cdot \boldsymbol{v} + \omega^2 \boldsymbol{v} = 0 \quad \text{in } \Omega_h. \tag{2.5}$$

For any solution $\boldsymbol{v}$ of (2.5), we introduce the Helmholtz decomposition to split it into the compressional and shear parts:

$$\boldsymbol{v} = \nabla \phi + \nabla \times \boldsymbol{\psi}, \quad \nabla \cdot \boldsymbol{\psi} = 0, \tag{2.6}$$

where ϕ is a scalar potential function and $\boldsymbol{\psi}$ is a vector potential function. Substituting (2.6) into (2.5) gives

$$(\lambda + 2\mu) \nabla \left(\Delta \phi + \kappa_1^2 \phi\right) + \mu \nabla \times (\Delta \boldsymbol{\psi} + \kappa_2^2 \boldsymbol{\psi}) = 0,$$

which is fulfilled if ϕ and $\boldsymbol{\psi}$ satisfy the Helmholtz equation:

$$\Delta \phi + \kappa_1^2 \phi = 0, \quad \Delta \boldsymbol{\psi} + \kappa_2^2 \boldsymbol{\psi} = 0. \tag{2.7}$$

It follows from $\nabla \cdot \boldsymbol{\psi} = 0$ and (2.7) that the vector potential function $\boldsymbol{\psi}$ satisfies the Maxwell equation:

$$\nabla \times (\nabla \times \boldsymbol{\psi}) - \kappa_2^2 \boldsymbol{\psi} = 0.$$

By (2.4) and (2.6), we have

$$\boldsymbol{v} = \nabla \phi + \nabla \times \boldsymbol{\psi} = -\boldsymbol{u}^{\mathrm{inc}} \quad \text{on } \Gamma_f.$$

Taking the dot product and cross product of the above equation with the unit normal vector $\boldsymbol{\nu}$ on Γ_f, respectively, we get

$$\partial_{\boldsymbol{\nu}} \phi + (\nabla \times \boldsymbol{\psi}) \cdot \boldsymbol{\nu} = -\boldsymbol{u}^{\mathrm{inc}} \cdot \boldsymbol{\nu}, \quad (\nabla \times \boldsymbol{\psi}) \times \boldsymbol{\nu} + \nabla \phi \times \boldsymbol{\nu} = -\boldsymbol{u}^{\mathrm{inc}} \times \boldsymbol{\nu},$$

which are the boundary conditions of ϕ and $\boldsymbol{\psi}$ on Γ_f. The Helmholtz decomposition and corresponding boundary conditions for the potential functions can also be found in [29, 31] for the elastic obstacle scattering problems.

Since $\boldsymbol{v}$ is a quasi-biperiodic function, we have from (2.6)–(2.7) that ϕ and $\boldsymbol{\psi} = (\psi_1, \psi_2, \psi_3)^\top$ are also quasi-biperiodic functions. They have the Fourier series expansions:

$$\phi(\boldsymbol{x}) = \sum_{n \in \mathbb{Z}^2} \phi^{(n)}(x_3) e^{i\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}}, \quad \boldsymbol{\psi}^{(n)}(\boldsymbol{x}) = \sum_{n \in \mathbb{Z}^2} \boldsymbol{\psi}^{(n)}(x_3) e^{i\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}}.$$

Plugging the above Fourier series into (2.7) yields

$$\frac{\mathrm{d}^2 \phi^{(n)}(x_3)}{\mathrm{d}x_3^2} + \left(\beta_1^{(n)}\right)^2 \phi^{(n)}(x_3) = 0, \quad \frac{\mathrm{d}^2 \boldsymbol{\psi}^{(n)}(x_3)}{\mathrm{d}x_3^2} + \left(\beta_2^{(n)}\right)^2 \boldsymbol{\psi}^{(n)}(x_3) = 0,$$

where

$$\beta_j^{(n)} = \begin{cases} \left(\kappa_j^2 - |\boldsymbol{\alpha}^{(n)}|^2\right)^{1/2}, & |\boldsymbol{\alpha}^{(n)}| < \kappa_j, \\ i\left(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_j^2\right)^{1/2}, & |\boldsymbol{\alpha}^{(n)}| > \kappa_j, \end{cases} \tag{2.8}$$

j=1,2. Note that $\beta_1^{(0)} = \beta = \kappa_1 \cos\theta_1$. We assume that $\kappa_j \neq |\boldsymbol{\alpha}_n|$ for all $n \in \mathbb{Z}^2$ to exclude all possible resonances. Noting (2.8) and using the bounded outgoing radiation condition, we obtain

$$\phi^{(n)}(x_3) = \phi^{(n)}(h) e^{i\beta_1^{(n)}(x_3 - h)}, \quad \boldsymbol{\psi}^{(n)}(x_3) = \boldsymbol{\psi}^{(n)}(h) e^{i\beta_2^{(n)}(x_3 - h)}.$$

Hence we deduce Rayleigh's expansions of ϕ and $\boldsymbol{\psi}$ for $x_3 > h$:

$$\phi(\boldsymbol{x}) = \sum_{n \in \mathbb{Z}^2} \phi^{(n)}(h) e^{i\left(\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} + \beta_1^{(n)}(x_3 - h)\right)},$$

$$\boldsymbol{\psi}(\boldsymbol{x}) = \sum_{n \in \mathbb{Z}^2} \boldsymbol{\psi}^{(n)}(h) e^{i\left(\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} + \beta_2^{(n)}(x_3 - h)\right)}.$$

Combining the above expansions and the Helmholtz decomposition (2.6) yields

$$\boldsymbol{v}(\boldsymbol{x}) = i \sum_{n \in \mathbb{Z}^2} \begin{bmatrix} \alpha_1^{(n)} \\ \alpha_2^{(n)} \\ \beta_1^{(n)} \end{bmatrix} \phi^{(n)}(h) e^{i\left(\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} + \beta_1^{(n)}(x_3 - h)\right)}$$

$$+ \begin{bmatrix} \alpha_2^{(n)} \psi_3^{(n)}(h) - \beta_2^{(n)} \psi_2^{(n)}(h) \\ \beta_2^{(n)} \psi_1^{(n)}(h) - \alpha_1^{(n)} \psi_3^{(n)}(h) \\ \alpha_1^{(n)} \psi_2^{(n)}(h) - \alpha_2^{(n)} \psi_1^{(n)}(h) \end{bmatrix} e^{i\left(\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} + \beta_2^{(n)}(x_3 - h)\right)}. \tag{2.9}$$

On the other hand, as a quasi-biperiodic function, the diffracted field $\boldsymbol{v}$ has the Fourier series expansion:

$$\boldsymbol{v}(\boldsymbol{r}, h) = \sum_{n \in \mathbb{Z}^2} \boldsymbol{v}^{(n)}(h) e^{i\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}}. \tag{2.10}$$

It follows from (2.9)–(2.10) and $\nabla \cdot \boldsymbol{\psi} = 0$ that we obtain a linear system of algebraic equations for $\phi^{(n)}(h)$ and $\psi_k^{(n)}(h)$:

$$
\mathrm{i}
\begin{bmatrix}
\alpha_1^{(n)} & 0 & -\beta_2^{(n)} & \alpha_2^{(n)} \\
\alpha_2^{(n)} & \beta_2^{(n)} & 0 & -\alpha_1^{(n)} \\
\beta_1^{(n)} & -\alpha_2^{(n)} & \alpha_1^{(n)} & 0 \\
0 & \alpha_1^{(n)} & \alpha_2^{(n)} & \beta_2^{(n)}
\end{bmatrix}
\begin{bmatrix}
\phi^{(n)}(h) \\
\psi_1^{(n)}(h) \\
\psi_2^{(n)}(h) \\
\psi_3^{(n)}(h)
\end{bmatrix}
=
\begin{bmatrix}
v_1^{(n)}(h) \\
v_2^{(n)}(h) \\
v_3^{(n)}(h) \\
0
\end{bmatrix}. \tag{2.11}
$$

Solving the above linear system directly via Cramer's rule gives

$$
\phi^{(n)}(h) = -\frac{\mathrm{i}}{\chi^{(n)}} \big(\alpha_1^{(n)} v_1^{(n)}(h) + \alpha_2^{(n)} v_2^{(n)}(h) + \beta_2^{(n)} v_3^{(n)}(h) \big)
$$

$$
\psi_1^{(n)}(h) = -\frac{\mathrm{i}}{\chi^{(n)}} \big(\alpha_1^{(n)} \alpha_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) v_1^{(n)}(h)/\kappa_2^2
$$
$$
+ [(\alpha_1^{(n)})^2 \beta_2^{(n)} + (\alpha_2^{(n)})^2 \beta_1^{(n)} + \beta_1^{(n)} (\beta_2^{(n)})^2] v_2^{(n)}(h)/\kappa_2^2 - \alpha_2^{(n)} v_3^{(n)}(h) \big)
$$

$$
\psi_2^{(n)}(h) = -\frac{\mathrm{i}}{\chi^{(n)}} \big(- [(\alpha_1^{(n)})^2 \beta_1^{(n)} + (\alpha_2^{(n)})^2 \beta_2^{(n)} + \beta_1^{(n)} (\beta_2^{(n)})^2] v_1^{(n)}(h)/\kappa_2^2
$$
$$
- \alpha_1^{(n)} \alpha_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) v_2^{(n)}(h)/\kappa_2^2 + \alpha_1^{(n)} v_3^{(n)}(h) \big)
$$

$$
\psi_3^{(n)}(h) = -\frac{\mathrm{i}}{\kappa_2^2} \big(\alpha_2^{(n)} v_1^{(n)}(h) - \alpha_1^{(n)} v_2^{(n)}(h) \big),
$$

where

$$
\chi^{(n)} = |\boldsymbol{\alpha}^{(n)}|^2 + \beta_1^{(n)} \beta_2^{(n)}. \tag{2.12}
$$

It is shown in Proposition A.1 that $\chi^{(n)} \neq 0$ for $n \in \mathbb{Z}^2$.

Given a vector field $\boldsymbol{v} = (v_1, v_2, v_3)^\top$, we define a differential operator $\mathscr{D}$ on Γ_h:

$$
\mathscr{D}\boldsymbol{v} = \mu \partial_{x_3} \boldsymbol{v} + (\lambda + \mu)(\nabla \cdot \boldsymbol{v}) \boldsymbol{e}_3, \tag{2.13}
$$

where $\boldsymbol{e}_3 = (0,0,1)^\top$. Substituting the Helmholtz decomposition (2.6) into (2.13) and using (2.7), we get

$$
\mathscr{D}\boldsymbol{v} = \mu \partial_{x_3} (\nabla \phi + \nabla \times \boldsymbol{\psi}) - (\lambda + \mu) \kappa_1^2 \phi \boldsymbol{e}_3.
$$

It follows from (2.9) that

$$
(\mathscr{D}\boldsymbol{v})^{(n)} = -\mu
\begin{bmatrix}
\alpha_1^{(n)} \beta_1^{(n)} & 0 & -(\beta_2^{(n)})^2 & \alpha_2^{(n)} \beta_2^{(n)} \\
\alpha_2^{(n)} \beta_1^{(n)} & (\beta_2^{(n)})^2 & 0 & -\alpha_1^{(n)} \beta_2^{(n)} \\
(\beta_2^{(n)})^2 & -\alpha_2^{(n)} \beta_2^{(n)} & \alpha_1^{(n)} \beta_2^{(n)} & 0
\end{bmatrix}
\begin{bmatrix}
\phi^{(n)}(h) \\
\psi_1^{(n)}(h) \\
\psi_2^{(n)}(h) \\
\psi_3^{(n)}(h)
\end{bmatrix}. \tag{2.14}
$$

By (2.11) and (2.14), we deduce the transparent boundary conditions for the diffracted field:

$$
\mathscr{D}\boldsymbol{v} = \mathscr{T}\boldsymbol{v} := \sum_{n \in \mathbb{Z}^2} M^{(n)} \boldsymbol{v}^{(n)}(h) e^{\mathrm{i}\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}} \quad \text{on } \Gamma_h,
$$

where the matrix

$$M^{(n)} = \frac{\mathrm{i}\mu}{\chi^{(n)}}$$

$$\begin{bmatrix} (\alpha_1^{(n)})^2(\beta_1^{(n)}-\beta_2^{(n)})+\beta_2^{(n)}\chi^{(n)} & \alpha_1^{(n)}\alpha_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)}) & \alpha_1^{(n)}\beta_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)}) \\ \alpha_1^{(n)}\alpha_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)}) & (\alpha_2^{(n)})^2(\beta_1^{(n)}-\beta_2^{(n)})+\beta_2^{(n)}\chi^{(n)} & \alpha_2^{(n)}\beta_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)}) \\ -\alpha_1^{(n)}\beta_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)}) & -\alpha_2^{(n)}\beta_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)}) & \kappa_2^2\beta_2^{(n)} \end{bmatrix}.$$

Equivalently, we have the transparent boundary condition for the total field $\boldsymbol{u}$:

$$\mathscr{D}\boldsymbol{u} = \mathscr{T}\boldsymbol{u} + \boldsymbol{g} \quad \text{on} \ \ \Gamma_h,$$

where

$$\boldsymbol{g} = \mathscr{D}\boldsymbol{u}_{\mathrm{inc}} - \mathscr{T}\boldsymbol{u}^{\mathrm{inc}} = -\frac{2\mathrm{i}\omega^2\beta_1^{(0)}}{\kappa_1\chi^{(0)}}(\alpha_1,\alpha_2,-\beta_2^{(0)})^\top e^{\mathrm{i}(\alpha_1 x_1 + \alpha_2 x_2 - \beta_1^{(0)} h)}.$$

The scattering problem can be reduced to the following boundary value problem:

$$\begin{cases} \mu\Delta\boldsymbol{u} + (\lambda+\mu)\nabla\nabla\cdot\boldsymbol{u} + \omega^2\boldsymbol{u} = 0 & \text{in } \Omega, \\ \mathscr{D}\boldsymbol{u} = \mathscr{T}\boldsymbol{u} + \boldsymbol{g} & \text{on } \Gamma_h, \\ \boldsymbol{u} = 0 & \text{on } \Gamma_f. \end{cases} \tag{2.15}$$

The weak formulation of (2.15) reads as follows: to find $\boldsymbol{u} \in H_{\mathrm{qp}}^1(\Omega)^3$ such that

$$a(\boldsymbol{u},\boldsymbol{v}) = \langle\boldsymbol{g},\boldsymbol{v}\rangle_{\Gamma_h}, \quad \forall\boldsymbol{v} \in H_{\mathrm{qp}}^1(\Omega)^3, \tag{2.16}$$

where the sesquilinear form $a: H_{\mathrm{qp}}^1(\Omega)^3 \times H_{\mathrm{qp}}^1(\Omega)^3 \to \mathbb{C}$ is defined by

$$a(\boldsymbol{u},\boldsymbol{v}) = \mu\int_\Omega \nabla\boldsymbol{u}:\nabla\bar{\boldsymbol{v}}\,\mathrm{d}\boldsymbol{x} + (\lambda+\mu)\int_\Omega (\nabla\cdot\boldsymbol{u})(\nabla\cdot\bar{\boldsymbol{v}})\,\mathrm{d}\boldsymbol{x}$$

$$-\omega^2\int_\Omega \boldsymbol{u}\cdot\bar{\boldsymbol{v}}\,\mathrm{d}\boldsymbol{x} - \langle\mathscr{T}\boldsymbol{u},\boldsymbol{v}\rangle_{\Gamma_h}. \tag{2.17}$$

Here $A:B = \mathrm{tr}(AB^\top)$ is the Frobenius inner product of square matrices A and B.

In this paper we assume that the variational problem (2.16) admits a unique solution. It follows from the general theory in [3] that there exists a constant $\gamma_1 > 0$ such that the following inf-sup condition holds:

$$\sup_{0\neq\boldsymbol{v}\in H_{\mathrm{qp}}^1(\Omega)^3} \frac{|a(\boldsymbol{u},\boldsymbol{v})|}{\|\boldsymbol{v}\|_{H^1(\Omega)^3}} \geq \gamma_1\|\boldsymbol{u}\|_{H^1(\Omega)^3}, \quad \forall\boldsymbol{u}\in H_{\mathrm{qp}}^1(\Omega)^3. \tag{2.18}$$

2.3. Energy distribution.   We study the energy distribution for the scattering problem. The result can be used to verify the accuracy of our numerical method for examples where the analytical solutions are not available. In general, the energy is distributed away from the scattering surface through propagating wave modes.

Consider the Helmholtz decomposition for the total field:

$$\boldsymbol{u} = \nabla\phi^{\mathrm{t}} + \nabla\times\boldsymbol{\psi}^{\mathrm{t}}, \quad \nabla\cdot\boldsymbol{\psi}^{\mathrm{t}} = 0. \tag{2.19}$$

Substituting (2.19) into (2.1), we can similarly verify that the scalar potential function ϕ^{t} and the vector potential function $\boldsymbol{\psi}^{\mathrm{t}}$ satisfy

$$\Delta\phi^{\mathrm{t}} + \kappa_1^2\phi^{\mathrm{t}} = 0, \quad \nabla\times(\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) - \kappa_2^2\boldsymbol{\psi}^{\mathrm{t}} = 0 \quad \text{in } \Omega_f.$$

We also introduce the Helmholtz decomposition for the incident field:

$$\boldsymbol{u}^{\mathrm{inc}} = \nabla\phi^{\mathrm{inc}} + \nabla\times\boldsymbol{\psi}^{\mathrm{inc}}, \quad \nabla\cdot\boldsymbol{\psi}^{\mathrm{inc}} = 0,$$

which gives explicitly that

$$\phi^{\mathrm{inc}} = -\frac{1}{\kappa_1^2}\nabla\cdot\boldsymbol{u}^{\mathrm{inc}} = -\frac{\mathrm{i}}{\kappa_1}e^{\mathrm{i}(\boldsymbol{\alpha}\cdot\boldsymbol{r}-\beta x_3)}, \quad \boldsymbol{\psi}^{\mathrm{inc}} = \frac{1}{\kappa_2^2}\nabla\times\boldsymbol{u}^{\mathrm{inc}} = 0.$$

Hence we have

$$\phi^{\mathrm{t}} = \phi^{\mathrm{inc}} + \phi, \quad \boldsymbol{\psi}^{\mathrm{t}} = \boldsymbol{\psi}.$$

Using the Rayleigh expansions, we get

$$\phi^{\mathrm{t}}(\boldsymbol{x}) = a_0 e^{\mathrm{i}(\boldsymbol{\alpha}\cdot\boldsymbol{r}-\beta x_3)} + \sum_{n\in\mathbb{Z}^2} a_1^{(n)} e^{\mathrm{i}\left(\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r}+\beta_1^{(n)}x_3\right)} \tag{2.20}$$

$$\boldsymbol{\psi}^{\mathrm{t}}(\boldsymbol{x}) = \sum_{n\in\mathbb{Z}^2} \boldsymbol{b}^{(n)} e^{\mathrm{i}\left(\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r}+\beta_2^{(n)}x_3\right)}, \tag{2.21}$$

where

$$a_0 = -\frac{\mathrm{i}}{\kappa_1}, \quad a_1^{(n)} = \phi^{(n)}(h)e^{-\mathrm{i}\beta_1^{(n)}h}, \quad \boldsymbol{b}^{(n)} = \boldsymbol{\psi}^{(n)}(h)e^{-\mathrm{i}\beta_2^{(n)}h}.$$

The grating efficiency is defined by

$$e_1^{(n)} = \frac{\beta_1^{(n)}|a_1^{(n)}|^2}{\beta|a_0|^2}, \quad e_2^{(n)} = \frac{\beta_2^{(n)}|\boldsymbol{b}^{(n)}|^2}{\beta|a_0|^2}, \tag{2.22}$$

where $e_1^{(n)}$ and $e_2^{(n)}$ are the efficiency of the n-th order reflected modes for the compressional wave and the shear wave, respectively. In practice, the grating efficiency (2.22) can be computed from (2.11) once the scattering problem is solved and the diffracted field $\boldsymbol{v}$ is available on Γ_h.

THEOREM 2.1. *The total energy is conserved, i.e.,*

$$\sum_{n\in U_1} e_1^{(n)} + \sum_{n\in U_2} e_2^{(n)} = 1,$$

where $U_j = \{n\in\mathbb{Z}^2 : |\boldsymbol{\alpha}^{(n)}| \leq \kappa_j\}$, $j\in\{1,2\}$.

Proof. It follows from the boundary condition (2.2) and the Helmholtz decomposition (2.19) that

$$\nabla\phi^{\mathrm{t}} + \nabla\times\boldsymbol{\psi}^{\mathrm{t}} = 0 \quad \text{on } \Gamma_f,$$

which gives

$$\boldsymbol{\nu}\cdot\nabla\phi^{\mathrm{t}} + \boldsymbol{\nu}\cdot(\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) = 0, \quad \boldsymbol{\nu}\times\nabla\phi^{\mathrm{t}} + \boldsymbol{\nu}\times(\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) = 0.$$

Here $\boldsymbol{\nu}$ is the unit normal vector on Γ_f.

Consider the following coupled problem:

$$\begin{cases} \Delta\phi^{\mathrm{t}} + \kappa_1^2\phi^{\mathrm{t}} = 0, \quad \nabla\times(\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) - \kappa_2^2\boldsymbol{\psi}^{\mathrm{t}} = 0 & \text{in } \Omega, \\ \boldsymbol{\nu}\cdot\nabla\phi^{\mathrm{t}} + \boldsymbol{\nu}\cdot(\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) = 0, \quad \boldsymbol{\nu}\times\nabla\phi^{\mathrm{t}} + \boldsymbol{\nu}\times(\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) = 0 & \text{on } \Gamma_f. \end{cases} \tag{2.23}$$

Note that $(\bar{\phi}^{\mathrm{t}}, \bar{\boldsymbol{\psi}}^{\mathrm{t}})$ also satisfies the problem (2.23) since the wavenumbers κ_j are real. Using Green's theorem and quasi-periodicity of the solution, we get

$$\begin{aligned} 0 &= \int_\Omega (\bar{\phi}^{\mathrm{t}}\Delta\phi^{\mathrm{t}} - \phi^{\mathrm{t}}\Delta\bar{\phi}^{\mathrm{t}})\mathrm{d}\boldsymbol{x} - \int_\Omega (\bar{\boldsymbol{\psi}}^{\mathrm{t}}\cdot\nabla\times(\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) - \boldsymbol{\psi}^{\mathrm{t}}\cdot\nabla\times(\nabla\times\bar{\boldsymbol{\psi}}^{\mathrm{t}}))\mathrm{d}\boldsymbol{x} \\ &= \int_{\Gamma_f} (\bar{\phi}^{\mathrm{t}}\partial_{\boldsymbol{\nu}}\phi^{\mathrm{t}} - \phi^{\mathrm{t}}\partial_{\boldsymbol{\nu}}\bar{\phi}^{\mathrm{t}})\mathrm{d}\gamma - \int_{\Gamma_f} (\bar{\boldsymbol{\psi}}^{\mathrm{t}}\cdot(\boldsymbol{\nu}\times\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) - \boldsymbol{\psi}^{\mathrm{t}}\cdot(\boldsymbol{\nu}\times\nabla\times\bar{\boldsymbol{\psi}}^{\mathrm{t}}))\mathrm{d}\gamma \\ &\quad + \int_{\Gamma_h} (\bar{\phi}^{\mathrm{t}}\partial_{x_3}\phi^{\mathrm{t}} - \phi^{\mathrm{t}}\partial_{x_3}\bar{\phi}^{\mathrm{t}})\mathrm{d}\boldsymbol{r} \\ &\quad - \int_{\Gamma_h} (\bar{\boldsymbol{\psi}}^{\mathrm{t}}\cdot(\boldsymbol{e}_3\times\nabla\times\boldsymbol{\psi}^{\mathrm{t}}) - \boldsymbol{\psi}^{\mathrm{t}}\cdot(\boldsymbol{e}_3\times\nabla\times\bar{\boldsymbol{\psi}}^{\mathrm{t}}))\mathrm{d}\boldsymbol{r}. \end{aligned} \tag{2.24}$$

It follows from the integration by parts and the boundary conditions in (2.23) that

$$\begin{aligned} \int_{\Gamma_f} \partial_{\boldsymbol{\nu}}\phi^{\mathrm{t}}\bar{\phi}^{\mathrm{t}}\mathrm{d}\gamma &= -\int_{\Gamma_f} \boldsymbol{\nu}\cdot(\nabla\times\boldsymbol{\psi}^{\mathrm{t}})\bar{\phi}^{\mathrm{t}}\mathrm{d}\gamma \\ &= \int_{\Gamma_f} \boldsymbol{\psi}^{\mathrm{t}}\cdot(\boldsymbol{\nu}\times\nabla\bar{\phi}^{\mathrm{t}})\mathrm{d}\gamma = -\int_{\Gamma_f} \boldsymbol{\psi}^{\mathrm{t}}\cdot(\boldsymbol{\nu}\times(\nabla\times\bar{\boldsymbol{\psi}}^{\mathrm{t}}))\mathrm{d}\gamma, \end{aligned}$$

which gives, after taking the imaginary part of (2.24), that

$$\operatorname{Im}\int_{\Gamma_h} (\bar{\phi}^{\mathrm{t}}\partial_{x_3}\phi^{\mathrm{t}} - \bar{\boldsymbol{\psi}}^{\mathrm{t}}\cdot(\boldsymbol{e}_3\times\nabla\times\boldsymbol{\psi}^{\mathrm{t}}))\mathrm{d}\boldsymbol{r} = 0. \tag{2.25}$$

Let $\Delta_j^{(n)} = |\kappa_j^2 - |\boldsymbol{\alpha}^{(n)}|^2|^{1/2}$. Note that $\beta_j^{(n)} = \Delta_j^{(n)}$ for $n \in U_j$ and $\beta_j^{(n)} = \mathrm{i}\Delta_j^{(n)}$ for $n \notin U_j$. It follows from (2.20) and (2.21) that we have

$$\phi^{\mathrm{t}}(\boldsymbol{r}, h) = a_0 e^{\mathrm{i}(\boldsymbol{\alpha}\cdot\boldsymbol{r} - \beta h)} + \sum_{n\in U_1} a_1^{(n)} e^{\left(\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r} + \mathrm{i}\Delta_1^{(n)}h\right)} + \sum_{n\notin U_1} a_1^{(n)} e^{\left(\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r} - \Delta_1^{(n)}h\right)},$$

$$\boldsymbol{\psi}^{\mathrm{t}}(\boldsymbol{r}, h) = \sum_{n\in U_2} \boldsymbol{b}^{(n)} e^{\left(\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r} + \mathrm{i}\Delta_2^{(n)}h\right)} + \sum_{n\notin U_2} \boldsymbol{b}^{(n)} e^{\left(\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r} - \Delta_2^{(n)}h\right)},$$

and

$$\partial_{x_3}\phi^{\mathrm{t}}(\boldsymbol{r}, h) = -\mathrm{i}\beta a_0 e^{\mathrm{i}(\boldsymbol{\alpha}\cdot\boldsymbol{r} - \beta h)} + \sum_{n\in U_1} \mathrm{i}\Delta_1^{(n)} a_1^{(n)} e^{\left(\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r} + \mathrm{i}\Delta_1^{(n)}h\right)}$$
$$- \sum_{n\notin U_1} \Delta_1^{(n)} a_1^{(n)} e^{\left(\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r} - \Delta_1^{(n)}h\right)},$$

$$\boldsymbol{e}_3\times(\nabla\times\boldsymbol{\psi}^{\mathrm{t}}(\boldsymbol{r}, h)) = \sum_{n\in U_2} \begin{bmatrix} \mathrm{i}\alpha_1^{(n)}b_3^{(n)} - \mathrm{i}\Delta_2^{(n)}b_1^{(n)} \\ \mathrm{i}\alpha_2^{(n)}b_3^{(n)} - \mathrm{i}\Delta_2^{(n)}b_2^{(n)} \\ 0 \end{bmatrix} e^{\left(\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r} + \mathrm{i}\Delta_2^{(n)}h\right)}$$

$$+ \sum_{n \notin U_2} \begin{bmatrix} i\alpha_1^{(n)} b_3^{(n)} + \Delta_2^{(n)} b_1^{(n)} \\ i\alpha_2^{(n)} b_3^{(n)} + \Delta_2^{(n)} b_2^{(n)} \\ 0 \end{bmatrix} e^{\left(i\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} - \Delta_2^{(n)} h \right)},$$

where $\boldsymbol{b}^{(n)} = (b_1^{(n)}, b_2^{(n)}, b_3^{(n)})^\top$. Substituting the above four functions into (2.25), using the orthogonality of the Fourier series and the divergence free condition, we obtain

$$\beta |a_0|^2 = \sum_{n \in U_1} \Delta_1^{(n)} |a_1^{(n)}|^2 + \sum_{n \in U_2} \Delta_2^{(n)} |\boldsymbol{b}^{(n)}|^2,$$

which completes the proof. □

3. The PML problem

In this section, we introduce the PML formulation for the scattering problem and establish the well-posedness of the PML problem. An error estimate will be shown for the solutions between the original scattering problem and the PML problem.

3.1. PML formulation.

Now we turn to the introduction of an absorbing PML layer. The domain Ω is covered by a PML layer of thickness δ in Ω_h. Let $\rho(\tau) = \rho_1(\tau) + i\rho_2(\tau)$ be the PML function which is continuous and satisfies

$$\rho_1 = 1, \quad \rho_2 = 0 \quad \text{for } \tau < h \quad \text{and} \quad \rho_1 \geq 1, \quad \rho_2 > 0 \quad \text{otherwise.}$$

We introduce the PML by complex coordinate stretching:

$$\hat{x}_3 = \int_0^{x_3} \rho(\tau) d\tau. \tag{3.1}$$

Let $\hat{\boldsymbol{x}} = (\boldsymbol{r}, \hat{x}_3)$. Introduce the new field

$$\hat{\boldsymbol{u}}(\boldsymbol{x}) = \begin{cases} \boldsymbol{u}^{\text{inc}}(\boldsymbol{x}) + (\boldsymbol{u}(\hat{\boldsymbol{x}}) - \boldsymbol{u}^{\text{inc}}(\hat{\boldsymbol{x}})), & \boldsymbol{x} \in \Omega_h, \\ \boldsymbol{u}(\hat{\boldsymbol{x}}), & \boldsymbol{x} \in \Omega. \end{cases} \tag{3.2}$$

It is clear to note that $\hat{\boldsymbol{u}}(\boldsymbol{x}) = \boldsymbol{u}(\boldsymbol{x})$ in Ω since $\hat{\boldsymbol{x}} = \boldsymbol{x}$ in Ω. It can be verified from (2.1) and (3.1) that $\hat{\boldsymbol{u}}$ satisfies

$$\mathscr{L}(\hat{\boldsymbol{u}} - \boldsymbol{u}^{\text{inc}}) = 0 \quad \text{in } \Omega_f.$$

Here the PML differential operator

$$\mathscr{L}\boldsymbol{u} = (w_1, w_2, w_3)^\top,$$

where

$$\begin{aligned} w_1 &= (\lambda + 2\mu)\partial_{x_1 x_1}^2 u_1 + \mu(\partial_{x_2 x_2}^2 u_1 + \rho^{-1}(x_3)\partial_{x_3}(\rho^{-1}(x_3)\partial_{x_3} u_1)) \\ &\quad + (\lambda + \mu)(\partial_{x_1 x_2}^2 u_2 + \rho^{-1}(x_3)\partial_{x_1 x_3}^2 u_3) + \omega^2 u_1, \\ w_2 &= (\lambda + 2\mu)\partial_{x_2 x_2}^2 u_2 + \mu(\partial_{x_1 x_1}^2 u_2 + \rho^{-1}(x_3)\partial_{x_3}(\rho^{-1}(x_3)\partial_{x_3} u_2)) \\ &\quad + (\lambda + \mu)(\partial_{x_1 x_2}^2 u_1 + \rho^{-1}(x_3)\partial_{x_2 x_3}^2 u_3) + \omega^2 u_2 \\ w_3 &= (\lambda + 2\mu)\rho^{-1}(x_3)\partial_{x_3}(\rho^{-1}(x_3)\partial_{x_3} u_3) + \mu(\partial_{x_1 x_1}^2 u_3 + \partial_{x_2 x_2}^2 u_3)) \\ &\quad + (\lambda + \mu)\rho^{-1}(x_3)(\partial_{x_1 x_3}^2 u_1 + \partial_{x_2 x_3}^2 u_2) + \omega^2 u_3. \end{aligned}$$

Define the PML regions

$$\Omega^{\mathrm{PML}} = \{\boldsymbol{x} \in \mathbb{R}^3 : 0 < x_1 < \Lambda_1, 0 < x_2 < \Lambda_2, h < x_3 < h + \delta\}.$$

It is clear to note from (3.2) that the outgoing wave $\hat{\boldsymbol{u}}(\boldsymbol{x}) - \boldsymbol{u}^{\mathrm{inc}}(\boldsymbol{x})$ in Ω_h decay exponentially as $x_3 \to +\infty$. Therefore, the homogeneous Dirichlet boundary condition can be imposed on

$$\Gamma^{\mathrm{PML}} = \{\boldsymbol{x} \in \mathbb{R}^3 : 0 < x_1 < \Lambda_1, 0 < x_2 < \Lambda_2, x_3 = h + \delta\}$$

to truncate the PML problem. Define the computational domain for the PML problem $D = \Omega \cup \Omega^{\mathrm{PML}}$. We arrive at the following truncated PML problem: to find a quasi-periodic solution $\hat{\boldsymbol{u}}$ such that

$$\begin{cases} \mathscr{L}\hat{\boldsymbol{u}} = \boldsymbol{g} & \text{in } D, \\ \hat{\boldsymbol{u}} = \boldsymbol{u}^{\mathrm{inc}} & \text{on } \Gamma^{\mathrm{PML}}, \\ \hat{\boldsymbol{u}} = 0 & \text{on } \Gamma_f, \end{cases} \tag{3.3}$$

where

$$\boldsymbol{g} = \begin{cases} \mathscr{L}\boldsymbol{u}^{\mathrm{inc}} & \text{in } \Omega^{\mathrm{PML}}, \\ 0 & \text{in } \Omega. \end{cases}$$

Define $H^1_{0,\mathrm{qp}}(D) = \{u \in H^1_{\mathrm{qp}}(D) : u = 0 \text{ on } \Gamma^{\mathrm{PML}} \cup \Gamma_f\}$. The weak formulation of the PML problem (3.3) reads as follows: to find $\hat{\boldsymbol{u}} \in H^1_{\mathrm{qp}}(D)^3$ such that $\hat{\boldsymbol{u}} = \boldsymbol{u}^{\mathrm{inc}}$ on Γ^{PML} and

$$b_D(\hat{\boldsymbol{u}}, \boldsymbol{v}) = -\int_D \boldsymbol{g} \cdot \bar{\boldsymbol{v}} \mathrm{d}\boldsymbol{x}, \quad \forall \boldsymbol{v} \in H^1_{0,\mathrm{qp}}(D)^3. \tag{3.4}$$

Here for any domain $G \subset \mathbb{R}^3$, the sesquilinear form $b_G : H^1_{\mathrm{qp}}(G)^3 \times H^1_{\mathrm{qp}}(G)^3 \to \mathbb{C}$ is defined by

$$\begin{aligned} b_G(\boldsymbol{u}, \boldsymbol{v}) = \int_G &(\lambda + 2\mu)(\partial_{x_1} u_1 \partial_{x_1} \bar{v}_1 + \partial_{x_2} u_2 \partial_{x_2} \bar{v}_2 + (\rho^{-1})^2 \partial_{x_3} u_3 \partial_{x_3} \bar{v}_3) \\ &+ \mu(\partial_{x_2} u_1 \partial_{x_2} \bar{v}_1 + \partial_{x_1} u_2 \partial_{x_1} \bar{v}_2 + \partial_{x_1} u_3 \partial_{x_1} \bar{v}_3 + \partial_{x_2} u_3 \partial_{x_2} \bar{v}_3) \\ &+ \mu(\rho^{-1})^2 (\partial_{x_3} u_1 \partial_{x_3} \bar{v}_1 + \partial_{x_3} u_2 \partial_{x_3} \bar{v}_2) + (\lambda + \mu)(\partial_{x_2} u_2 \partial_{x_1} \bar{v}_1 + \partial_{x_1} u_1 \partial_{x_2} \bar{v}_2) \\ &+ (\lambda + \mu)\rho^{-1}(\partial_{x_3} u_3 \partial_{x_1} \bar{v}_1 + \partial_{x_3} u_3 \partial_{x_2} \bar{v}_2 + \partial_{x_1} u_1 \partial_{x_3} \bar{v}_3 + \partial_{x_2} u_2 \partial_{x_3} \bar{v}_3) \\ &- \omega^2 (u_1 \bar{v}_1 + u_2 \bar{v}_2 + u_3 \bar{v}_3) \mathrm{d}\boldsymbol{x}. \end{aligned}$$

We will reformulate the variational problem (3.4) in the domain D into an equivalent variational formulation in the domain Ω, and discuss the existence and uniqueness of the weak solution to the equivalent weak formulation. To do so, we need to introduce the transparent boundary condition for the truncated PML problem.

3.2. Transparent boundary condition of the PML problem. Let $\hat{\boldsymbol{v}}(\boldsymbol{x}) = \boldsymbol{v}(\hat{\boldsymbol{x}}) = \boldsymbol{u}(\hat{\boldsymbol{x}}) - \boldsymbol{u}_{\mathrm{inc}}(\hat{\boldsymbol{x}})$ in Ω^{PML}. It is clear to note that $\hat{\boldsymbol{v}}$ satisfies the Navier equation in the complex coordinate:

$$\mu \Delta_{\hat{\boldsymbol{x}}} \hat{\boldsymbol{v}} + (\lambda + \mu) \nabla_{\hat{\boldsymbol{x}}} \nabla_{\hat{\boldsymbol{x}}} \cdot \hat{\boldsymbol{v}} + \omega^2 \hat{\boldsymbol{v}} = 0 \quad \text{in } \Omega^{\mathrm{PML}}, \tag{3.5}$$

where $\nabla_{\hat{\boldsymbol{x}}} = (\partial_{x_1}, \partial_{x_2}, \partial_{\hat{x}_3})^\top$ with $\partial_{\hat{x}_3} = \rho^{-1}(x_3)\partial_{x_3}$.

We introduce the Helmholtz decomposition for the solution of (3.5):

$$\hat{\boldsymbol{v}} = \nabla_{\hat{\boldsymbol{x}}} \hat{\phi} + \nabla_{\hat{\boldsymbol{x}}} \times \hat{\boldsymbol{\psi}}, \quad \nabla_{\hat{\boldsymbol{x}}} \cdot \hat{\boldsymbol{\psi}} = 0, \tag{3.6}$$

Plugging (3.6) into (3.5) gives

$$\Delta_{\hat{\boldsymbol{x}}} \hat{\phi} + \kappa_1^2 \hat{\phi} = 0, \quad \Delta_{\hat{\boldsymbol{x}}} \hat{\boldsymbol{\psi}} + \kappa_2^2 \hat{\boldsymbol{\psi}} = 0. \tag{3.7}$$

Due to the quasi-periodicity of the solution, we have the Fourier series expansions

$$\hat{\phi}(\boldsymbol{x}) = \sum_{n \in \mathbb{Z}^2} \hat{\phi}^{(n)}(x_3) e^{\mathrm{i}\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}},$$

and

$$\hat{\boldsymbol{\psi}}(\boldsymbol{x}) = \sum_{n \in \mathbb{Z}^2} \left(\hat{\psi}_1^{(n)}(x_3), \hat{\psi}_2^{(n)}(x_3), \hat{\psi}_3^{(n)}(x_3) \right)^\top e^{\mathrm{i}\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}}.$$

Substituting the above Fourier series expansions into (3.7) yields

$$\rho^{-1} \frac{\mathrm{d}}{\mathrm{d}x_3} \left(\rho^{-1} \frac{\mathrm{d}}{\mathrm{d}x_3} \hat{\phi}^{(n)}(x_3) \right) + (\beta_1^{(n)})^2 \hat{\phi}^{(n)}(x_3) = 0$$

and

$$\rho^{-1} \frac{\mathrm{d}}{\mathrm{d}x_3} \left(\rho^{-1} \frac{\mathrm{d}}{\mathrm{d}x_3} \hat{\psi}_k^{(n)}(x_3) \right) + (\beta_2^{(n)})^2 \hat{\psi}_k^{(n)}(x_3) = 0, \quad k = 1, 2, 3.$$

The general solutions of the above equations are

$$\begin{cases} \hat{\phi}^{(n)}(x_3) = A^{(n)} e^{\mathrm{i}\beta_1^{(n)} \int_h^{x_3} \rho(\tau)\mathrm{d}\tau} + B^{(n)} e^{-\mathrm{i}\beta_1^{(n)} \int_h^{x_3} \rho(\tau)\mathrm{d}\tau}, \\ \hat{\psi}_k^{(n)}(x_3) = C_k^{(n)} e^{\mathrm{i}\beta_2^{(n)} \int_h^{x_3} \rho(\tau)\mathrm{d}\tau} + D_k^{(n)} e^{-\mathrm{i}\beta_2^{(n)} \int_h^{x_3} \rho(\tau)\mathrm{d}\tau}. \end{cases} \tag{3.8}$$

Define

$$\zeta = \int_h^{h+\delta} \rho(\tau)\mathrm{d}\tau, \quad \zeta(x_3) = \int_h^{x_3} \rho(\tau)\mathrm{d}\tau. \tag{3.9}$$

The coefficients $A^{(n)}$, $B^{(n)}$, $C_k^{(n)}$, $D_k^{(n)}$ can be uniquely determined by solving the following linear system:

$$\mathbf{A}^{(n)} \mathbf{X}^{(n)} = \mathbf{V}^{(n)}, \tag{3.10}$$

where

$$\mathbf{X}^{(n)} = \left(A^{(n)}, B^{(n)}, C_1^{(n)}, D_1^{(n)}, C_2^{(n)}, D_2^{(n)}, C_3^{(n)}, D_3^{(n)} \right)^\top,$$
$$\mathbf{V}^{(n)} = -\mathrm{i} \left(v_1^{(n)}(h), v_2^{(n)}(h), v_3^{(n)}(h), 0, 0, 0, 0, 0 \right)^\top,$$

and

$$\mathbf{A}^{(n)} = \begin{bmatrix} A_{11}^{(n)} & A_{12}^{(n)} \\ A_{21}^{(n)} & A_{22}^{(n)} \end{bmatrix}.$$

Here the block matrices are

$$
A_{11}^{(n)} = \begin{bmatrix}
\alpha_1^{(n)} & \alpha_1^{(n)} & 0 & 0 \\
\alpha_2^{(n)} & \alpha_2^{(n)} & \beta_2^{(n)} & -\beta_2^{(n)} \\
\beta_1^{(n)} & -\beta_1^{(n)} & -\alpha_2^{(n)} & -\alpha_2^{(n)} \\
\alpha_1^{(n)} e^{i\beta_1^{(n)}\zeta} & \alpha_1^{(n)} e^{-i\beta_1^{(n)}\zeta} & 0 & 0
\end{bmatrix},
$$

$$
A_{12}^{(n)} = \begin{bmatrix}
-\beta_2^{(n)} & \beta_2^{(n)} & \alpha_2^{(n)} & \alpha_2^{(n)} \\
0 & 0 & -\alpha_1^{(n)} & -\alpha_1^{(n)} \\
\alpha_1^{(n)} & \alpha_1^{(n)} & 0 & 0 \\
-\beta_2^{(n)} e^{i\beta_2^{(n)}\zeta} & \beta_2^{(n)} e^{-i\beta_2^{(n)}\zeta} & \alpha_2^{(n)} e^{i\beta_2^{(n)}\zeta} & \alpha_2^{(n)} e^{-i\beta_2^{(n)}\zeta}
\end{bmatrix},
$$

$$
A_{21}^{(n)} = \begin{bmatrix}
\alpha_2^{(n)} e^{i\beta_1^{(n)}\zeta} & \alpha_2^{(n)} e^{-i\beta_1^{(n)}\zeta} & \beta_2^{(n)} e^{i\beta_2^{(n)}\zeta} & -\beta_2^{(n)} e^{-i\beta_2^{(n)}\zeta} \\
\beta_1^{(n)} e^{i\beta_1^{(n)}\zeta} & -\beta_1^{(n)} e^{-i\beta_1^{(n)}\zeta} & -\alpha_2 e^{i\beta_2^{(n)}\zeta} & -\alpha_2 e^{-i\beta_2^{(n)}\zeta} \\
0 & 0 & \alpha_1^{(n)} & \alpha_1^{(n)} \\
0 & 0 & \alpha_1^{(n)} e^{i\beta_2^{(n)}\zeta} & \alpha_1^{(n)} e^{-i\beta_2^{(n)}\zeta}
\end{bmatrix},
$$

$$
A_{22}^{(n)} = \begin{bmatrix}
0 & 0 & -\alpha_1^{(n)} e^{i\beta_2^{(n)}\zeta} & -\alpha_1^{(n)} e^{-i\beta_2^{(n)}\zeta} \\
\alpha_1^{(n)} e^{i\beta_2^{(n)}\zeta} & \alpha_1^{(n)} e^{-i\beta_2^{(n)}\zeta} & 0 & 0 \\
\alpha_2^{(n)} & \alpha_2^{(n)} & \beta_2^{(n)} & -\beta_2^{(n)} \\
\alpha_2^{(n)} e^{i\beta_2^{(n)}\zeta} & \alpha_2^{(n)} e^{-i\beta_2^{(n)}\zeta} & \beta_2^{(n)} e^{i\beta_2^{(n)}\zeta} & -\beta_2^{(n)} e^{-i\beta_2^{(n)}\zeta}
\end{bmatrix}.
$$

To obtain the above linear system (3.10), we have used the Helmholtz decomposition (3.6) and the homogeneous Dirichlet boundary condition

$$
\hat{\boldsymbol{v}}(\boldsymbol{r}, h+\delta) = 0 \quad \text{on } \Gamma^{\text{PML}}
$$

due to the PML absorbing layer.

Using the Helmholtz decomposition (3.6) and (3.8), we get

$$
\hat{\boldsymbol{v}}(\boldsymbol{x}) = i \sum_{n \in \mathbb{Z}^2} \begin{bmatrix} \alpha_1^{(n)} \\ \alpha_2^{(n)} \\ \beta_1^{(n)} \end{bmatrix} A^{(n)} e^{i\left(\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} + \beta_1^{(n)} \int_h^{x_3} \rho(\tau) d\tau\right)}
$$

$$
+ \begin{bmatrix} \alpha_1^{(n)} \\ \alpha_2^{(n)} \\ -\beta_1^{(n)} \end{bmatrix} B^{(n)} e^{i\left(\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} - \beta_1^{(n)} \int_h^{x_3} \rho(\tau) d\tau\right)}
$$

$$
+ \begin{bmatrix} \alpha_2^{(n)} C_3^{(n)} - \beta_2^{(n)} C_2^{(n)} \\ \beta_2^{(n)} C_1^{(n)} - \alpha_1^{(n)} C_3^{(n)} \\ \alpha_1^{(n)} C_2^{(n)} - \alpha_2^{(n)} C_1^{(n)} \end{bmatrix} e^{\mathrm{i}\left(\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} + \beta_2^{(n)} \int_h^{x_3} \rho(\tau) \mathrm{d}\tau\right)}
$$

$$
+ \begin{bmatrix} \alpha_2^{(n)} D_3^{(n)} + \beta_2^{(n)} D_2^{(n)} \\ -\beta_2^{(n)} D_1^{(n)} - \alpha_1^{(n)} D_3^{(n)} \\ \alpha_1^{(n)} D_2^{(n)} - \alpha_2^{(n)} D_1^{(n)} \end{bmatrix} e^{\mathrm{i}\left(\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r} - \beta_2^{(n)} \int_h^{x_3} \rho(\tau) \mathrm{d}\tau\right)}. \tag{3.11}
$$

It follows from (3.11) that we have

$$
\mathscr{D}\hat{\boldsymbol{v}} = \mu \partial_{x_3} \hat{\boldsymbol{v}} + (\lambda + \mu)(\nabla \cdot \hat{\boldsymbol{v}}) \boldsymbol{e}_3 = \sum_{n \in \mathbb{Z}^2} \mu \mathbf{P}^{(n)} \mathbf{X}^{(n)} e^{\mathrm{i}\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{x}} \quad \text{on } \Gamma_h,
$$

where

$$
\mathbf{P}^{(n)} =
$$
$$
\begin{bmatrix} -\alpha_1^{(n)}\beta_1^{(n)} & \alpha_1^{(n)}\beta_1^{(n)} & 0 & 0 & (\beta_2^{(n)})^2 & (\beta_2^{(n)})^2 & -\alpha_2^{(n)}\beta_2^{(n)} & \alpha_2^{(n)}\beta_2^{(n)} \\ -\alpha_2^{(n)}\beta_1^{(n)} & \alpha_2^{(n)}\beta_1^{(n)} & -(\beta_2^{(n)})^2 & -(\beta_2^{(n)})^2 & 0 & 0 & \alpha_1^{(n)}\beta_2^{(n)} & -\alpha_1^{(n)}\beta_2^{(n)} \\ -(\beta_2^{(n)})^2 & -(\beta_2^{(n)})^2 & \alpha_2^{(n)}\beta_2^{(n)} & -\alpha_2^{(n)}\beta_2^{(n)} & -\alpha_1^{(n)}\beta_2^{(n)} & \alpha_1^{(n)}\beta_2^{(n)} & 0 & 0 \end{bmatrix}.
$$

Combining (3.11) and (3.10), we derive the transparent boundary condition for the PML problem:

$$
\mathscr{D}\hat{\boldsymbol{v}} = \mathscr{T}^{\mathrm{PML}}\hat{\boldsymbol{v}} := \sum_{n \in \mathbb{Z}^2} \hat{\mathbf{M}}^{(n)} \hat{\boldsymbol{v}}^{(n)}(h) e^{\mathrm{i}\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}} \quad \text{on } \Gamma_h,
$$

where the matrix

$$
\hat{\mathbf{M}}^{(n)} = \begin{bmatrix} \hat{m}_{11}^{(n)} & \hat{m}_{12}^{(n)} & \hat{m}_{13}^{(n)} \\ \hat{m}_{21}^{(n)} & \hat{m}_{22}^{(n)} & \hat{m}_{23}^{(n)} \\ \hat{m}_{31}^{(n)} & \hat{m}_{32}^{(n)} & \hat{m}_{33}^{(n)} \end{bmatrix}.
$$

Here the entries of $\hat{\mathbf{M}}^{(n)}$ are

$$
\hat{m}_{11}^{(n)} = \frac{\mathrm{i}\mu}{\chi^{(n)}\hat{\chi}^{(n)}} \Big[\chi^{(n)}\big((\alpha_1^{(n)})^2(\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)}\chi^{(n)}\big)(\varepsilon^{(n)} + 1)
$$
$$
+ 4(\alpha_2^{(n)})^2\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)} + 1) - 2(\alpha_1^{(n)})^2\beta_1^{(n)}\kappa_2^2\eta^{(n)} \Big],
$$

$$
\hat{m}_{12}^{(n)} = \hat{m}_{21}^{(n)} = \frac{\mathrm{i}\mu\alpha_1^{(n)}\alpha_2^{(n)}}{\chi^{(n)}\hat{\chi}^{(n)}} \Big[\chi^{(n)}(\beta_1^{(n)} - \beta_2^{(n)})(\varepsilon^{(n)} + 1) - 2\chi^{(n)}\beta_1^{(n)}\eta^{(n)}
$$
$$
- 4\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)} + 1) - 2\beta_1^{(n)}\beta_2^{(n)}(\beta_1^{(n)} - \beta_2^{(n)})\gamma^{(n)} \Big],
$$

$$
\hat{m}_{13}^{(n)} = -\hat{m}_{31}^{(n)} = \frac{\mathrm{i}\mu\alpha_1^{(n)}\beta_2^{(n)}}{\chi^{(n)}\hat{\chi}^{(n)}} \Big[\chi^{(n)}(\beta_1^{(n)} - \beta_2^{(n)}) + 2\beta_1^{(n)}(\kappa_2^2 - 2(\beta_2^{(n)})^2)\theta^{(n)} \Big],
$$

$$
\hat{m}_{22}^{(n)} = \frac{\mathrm{i}\mu}{\chi^{(n)}\hat{\chi}_n^{(n)}} \Big[\chi^{(n)}[(\alpha_2^{(n)})^2(\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)}\chi^{(n)}](\varepsilon^{(n)} + 1)
$$

$$+4(\alpha_1^{(n)})^2\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)}+1)-2(\alpha_2^{(n)})^2\beta_1^{(n)}\kappa_2^2\eta^{(n)}\Big],$$

$$\hat{m}_{23}^{(n)}=-\hat{m}_{32}^{(n)}=\frac{\mathrm{i}\mu\alpha_2^{(n)}\beta_2^{(n)}}{\chi^{(n)}\hat{\chi}^{(n)}}\Big[\chi^{(n)}(\beta_1^{(n)}-\beta_2^{(n)})+2\beta_1^{(n)}(\kappa_2^2-2(\beta_2^{(n)})^2)\theta^{(n)}\Big],$$

$$\hat{m}_{33}^{(n)}=\frac{\mathrm{i}\mu\beta_2^{(n)}\kappa_2^2}{\chi^{(n)}\hat{\chi}^{(n)}}\Big[\chi^{(n)}(\varepsilon^{(n)}+1)-2\beta_1^{(n)}\beta_2^{(n)}\eta^{(n)}\Big],$$

where

$$\varepsilon^{(n)}=2e^{\mathrm{i}\beta_2^{(n)}\zeta}/(e^{-\mathrm{i}\beta_2^{(n)}\zeta}-e^{\mathrm{i}\beta_2^{(n)}\zeta}),$$

$$\theta^{(n)}=(e^{\mathrm{i}\beta_2^{(n)}\zeta}-e^{\mathrm{i}\beta_1^{(n)}\zeta})^2/((1-e^{2\mathrm{i}\beta_1^{(n)}\zeta})(1-e^{2\mathrm{i}\beta_2^{(n)}\zeta})),$$

$$\eta^{(n)}=(e^{2\mathrm{i}\beta_2^{(n)}\zeta}-e^{2\mathrm{i}\beta_1^{(n)}\zeta})/((1-e^{2\mathrm{i}\beta_1^{(n)}\zeta})(1-e^{2\mathrm{i}\beta_2^{(n)}\zeta})),$$

$$\gamma^{(n)}=(e^{2\mathrm{i}\beta_1^{(n)}\zeta}+e^{4\mathrm{i}\beta_2^{(n)}\zeta})^2/((1-e^{2\mathrm{i}\beta_1^{(n)}\zeta})(1-e^{2\mathrm{i}\beta_2^{(n)}\zeta})^2),$$

$$\hat{\chi}^{(n)}=\chi^{(n)}+4\big((\alpha_1^{(n)})^2+(\alpha_2^{(n)})^2\big)\beta_1^{(n)}\beta_2^{(n)}\theta_n/\chi^{(n)}.$$

Equivalently, we have the transparent boundary condition for the total field $\hat{\boldsymbol{u}}$:

$$\mathscr{D}\hat{\boldsymbol{u}}=\mathscr{T}^{\mathrm{PML}}\hat{\boldsymbol{u}}+\boldsymbol{g}^{\mathrm{PML}}\quad\text{on }\Gamma_h,$$

where $\boldsymbol{g}^{\mathrm{PML}}=\mathscr{D}\hat{\boldsymbol{u}}_{\mathrm{inc}}-\mathscr{T}^{\mathrm{PML}}\hat{\boldsymbol{u}}_{\mathrm{inc}}$.

The PML problem can be reduced to the following boundary value problem:

$$\begin{cases}\mu\Delta\boldsymbol{u}^{\mathrm{PML}}+(\lambda+\mu)\nabla\nabla\cdot\boldsymbol{u}^{\mathrm{PML}}+\omega^2\boldsymbol{u}^{\mathrm{PML}}=0 & \text{in }\Omega,\\ \mathscr{D}\boldsymbol{u}^{\mathrm{PML}}=\mathscr{T}^{\mathrm{PML}}\boldsymbol{u}^{\mathrm{PML}}+\boldsymbol{g}^{\mathrm{PML}} & \text{on }\Gamma_h,\\ \boldsymbol{u}^{\mathrm{PML}}=0 & \text{on }\Gamma_f.\end{cases}\tag{3.12}$$

The weak formulation of (3.12) is to find $\boldsymbol{u}^{\mathrm{PML}}\in H_{\mathrm{qp}}^1(\Omega)^3$ such that

$$a^{\mathrm{PML}}(\boldsymbol{u}^{\mathrm{PML}},\boldsymbol{v})=\langle\boldsymbol{g}^{\mathrm{PML}},\boldsymbol{v}\rangle_{\Gamma_h}\quad\forall\boldsymbol{v}\in H_{\mathrm{qp}}^1(\Omega)^3,\tag{3.13}$$

where the sesquilinear form $a^{\mathrm{PML}}:H_{\mathrm{qp}}^1(\Omega)^3\times H_{\mathrm{qp}}^1(\Omega)^3\to\mathbb{C}$ is defined by

$$a^{\mathrm{PML}}(\boldsymbol{u},\boldsymbol{v})=\mu\int_\Omega\nabla\boldsymbol{u}:\nabla\bar{\boldsymbol{v}}\mathrm{d}\boldsymbol{x}+(\lambda+\mu)\int_\Omega(\nabla\cdot\boldsymbol{u})(\nabla\cdot\bar{\boldsymbol{v}})\mathrm{d}\boldsymbol{x}$$
$$-\omega^2\int_\Omega\boldsymbol{u}\cdot\bar{\boldsymbol{v}}\mathrm{d}\boldsymbol{x}-\langle\mathscr{T}^{\mathrm{PML}}\boldsymbol{u},\boldsymbol{v}\rangle_{\Gamma_h}.\tag{3.14}$$

The following lemma establishes the relationship between the variational problem (3.13) and the weak formulation (3.4). The proof is straightforward based on our constructions of the transparent boundary conditions for the PML problem. The details of the proof are omitted for simplicity.

LEMMA 3.1. *Any solution $\hat{\boldsymbol{u}}$ of the variational problem (3.4) restricted to Ω is a solution of the variational (3.13); conversely, any solution $\boldsymbol{u}^{\mathrm{PML}}$ of the variational problem (3.13) can be uniquely extended to the whole domain to be a solution $\hat{\boldsymbol{u}}$ of the variational problem (3.4) in D.*

3.3. Convergence of the PML solution. Now we turn our attention to estimate the error between $\boldsymbol{u}^{\mathrm{PML}}$ and $\boldsymbol{u}$. The key is to estimate the error of the boundary operators $\mathscr{T}^{\mathrm{PML}}$ and $\mathscr{T}$.

Let

$$\Delta_j^- = \min\{\Delta_j^{(n)} : n \in U_j\}, \quad \Delta_j^+ = \min\{\Delta_j^{(n)} : n \notin U_j\},$$

where

$$\Delta_j^{(n)} = |\kappa_j^2 - |\boldsymbol{\alpha}^{(n)}|^2|^{1/2}, \quad U_j = \{n : |\boldsymbol{\alpha}^{(n)}| < \kappa_j\}.$$

Denote

$$K = \frac{48(49 + \kappa_2^2)^{7/2}}{\kappa_1^2} \times \max\left\{ \frac{1}{e^{\Delta_1^- \mathrm{Im}\zeta} - 1}, \frac{1}{(e^{\frac{1}{2}\Delta_1^- \mathrm{Im}\zeta} - 1)^2}, \frac{1}{(e^{\frac{1}{3}\Delta_1^- \mathrm{Im}\zeta} - 1)^3}, \right.$$
$$\frac{1}{e^{\Delta_2^+ \mathrm{Re}\zeta} - 1}, \frac{1}{(e^{\frac{1}{2}\Delta_2^+ \mathrm{Re}\zeta} - 1)^2}, \frac{1}{(e^{\frac{1}{3}\Delta_2^+ \mathrm{Re}\zeta} - 1)^3},$$
$$\left. \frac{1}{e^{\Delta_2^- \mathrm{Im}\zeta} - 1}, \frac{(e^{-\Delta_1^+ \mathrm{Re}\zeta} + e^{-\Delta_2^- \mathrm{Im}\zeta})^2}{(1 - e^{-2\Delta_1^+ \mathrm{Im}\zeta})(1 - e^{-2\Delta_2^- \mathrm{Re}\zeta})^2}, \right\}.$$

The constant K can be used to control the modeling error between the PML problem and the original scattering problem. Once the incoming plane wave $\boldsymbol{u}^{\mathrm{inc}}$ is fixed, the quantities Δ_j^-, Δ_j^+ are fixed. Thus the constant K approaches to zero exponentially as the PML parameters $\mathrm{Re}\zeta$ and $\mathrm{Im}\zeta$ tend to infinity. Recalling the definition of ζ in (3.9), we know that $\mathrm{Re}\zeta$ and $\mathrm{Im}\zeta$ can be calculated by the medium property $\rho(x_3)$, which is usually taken as a power function:

$$\rho(x_3) = 1 + \sigma\left(\frac{x_3 - h}{\delta}\right)^m \quad \text{if } x_3 \geq h, \quad m \geq 1.$$

Thus we have

$$\mathrm{Re}\zeta = \left(1 + \frac{\mathrm{Re}\sigma}{m+1}\right)\delta, \quad \mathrm{Im}\zeta = \left(\frac{\mathrm{Im}\sigma}{m+1}\right)\delta.$$

In practice, we may pick some appropriate PML parameters σ and δ such that $\mathrm{Re}\zeta \geq 1$.

LEMMA 3.2. *For any $\boldsymbol{u}, \boldsymbol{v} \in H_{\mathrm{qp}}^1(\Omega)^3$, we have*

$$|\langle(\mathscr{T}^{\mathrm{PML}} - \mathscr{T})\boldsymbol{u}, \boldsymbol{v}\rangle_{\Gamma_h}| \leq \hat{K}\|\boldsymbol{u}\|_{L^2(\Gamma_h)^3}\|\boldsymbol{v}\|_{L^2(\Gamma_h)^3},$$

where $\hat{K} = 11\mu^2 K / \kappa_1^4$.

Proof. For any $\boldsymbol{u}, \boldsymbol{v} \in H_{\mathrm{qp}}^1(\Omega)^3$, we have the following Fourier series expansions:

$$\boldsymbol{u}(\boldsymbol{r}, h) = \sum_{n \in \mathbb{Z}^2} \boldsymbol{u}^{(n)}(h) e^{\mathrm{i}\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}}, \quad \boldsymbol{v}(\boldsymbol{r}, h) = \sum_{n \in \mathbb{Z}^2} \boldsymbol{v}^{(n)}(h) e^{\mathrm{i}\boldsymbol{\alpha}^{(n)} \cdot \boldsymbol{r}},$$

which gives

$$\|\boldsymbol{u}\|_{L^2(\Gamma_h)^3}^2 = \Lambda_1 \Lambda_2 \sum_{n \in \mathbb{Z}^2} |\boldsymbol{u}^{(n)}(h)|^2, \quad \|\boldsymbol{v}\|_{L^2(\Gamma_h)^3}^2 = \Lambda_1 \Lambda_2 \sum_{n \in \mathbb{Z}^2} |\boldsymbol{v}^{(n)}(h)|^2.$$

It follows from the orthogonality of Fourier series, the Cauchy–Schwarz inequality, and Proposition A.3 that we have

$$|\langle(\mathscr{T}^{\mathrm{PML}}-\mathscr{T})\boldsymbol{u},\boldsymbol{v}\rangle_{\Gamma_h}|=\left|\Lambda_1\Lambda_2\sum_{n\in\mathbb{Z}^2}\left((M^{(n)}-\hat{M}^{(n)})\boldsymbol{u}^{(n)}(h)\right)\cdot\bar{\boldsymbol{v}}^{(n)}(h)\right|$$

$$\leq\left(\Lambda_1\Lambda_2\sum_{n\in\mathbb{Z}^2}\|M^{(n)}-\hat{M}^{(n)}\|_F^2|\boldsymbol{u}^{(n)}(h)|^2\right)^{1/2}\left(\Lambda_1\Lambda_2\sum_{n\in\mathbb{Z}^2}|\boldsymbol{v}^{(n)}(h)|^2\right)^{1/2}$$

$$\leq\hat{K}\|\boldsymbol{u}\|_{L^2(\Gamma_h)^3}\|\boldsymbol{v}\|_{L^2(\Gamma_h)^3},$$

which completes the proof. □

Let $a=\min\{f(\boldsymbol{x}):\boldsymbol{x}\in\Gamma_f\}$.   Denote $\tilde{\Omega}=\{\boldsymbol{x}\in\mathbb{R}^3:0<x_1<\Lambda_1,0<x_2<\Lambda_2,a<x_3<h\}$.

LEMMA 3.3.   *For any* $\boldsymbol{u}\in H^1_{\mathrm{qp}}(\Omega)^3$, *we have*

$$\|\boldsymbol{u}\|_{L^2(\Gamma_h)^3}\leq\|\boldsymbol{u}\|_{H^{1/2}(\Gamma_h)^3}\leq\gamma_2\|\boldsymbol{u}\|_{H^1(\Omega)^3},$$

where $\gamma_2=(1+(h-a)^{-1})^{1/2}$.

Proof.   A simple calculation yields

$$(h-a)|u(h)|^2=\int_a^h|u(x_3)|^2\mathrm{d}x_3+\int_a^h\int_{x_3}^h\frac{\mathrm{d}}{\mathrm{d}t}|u(t)|^2\mathrm{d}t\mathrm{d}x_3$$

$$\leq\int_a^h|u(x_3)|^2\mathrm{d}x_3+(h-a)\int_a^h2|u(t)||u'(t)|\mathrm{d}t,$$

which gives by applying the Young's inequality that

$$(1+|\boldsymbol{\alpha}^{(n)}|^2)^{1/2}|u(h)|^2\leq\gamma_2^2(1+|\boldsymbol{\alpha}^{(n)}|^2)\int_a^h|u(t)|^2\mathrm{d}t+\int_a^h|u'(t)|^2\mathrm{d}t.$$

Given $\boldsymbol{u}\in H^1_{\mathrm{qp}}(\Omega)^3$, we consider the zero extension

$$\tilde{\boldsymbol{u}}=\begin{cases}\boldsymbol{u} & \text{in }\Omega,\\0 & \text{in }\tilde{\Omega}\backslash\bar{\Omega},\end{cases}$$

which has the Fourier series expansion

$$\tilde{\boldsymbol{u}}(\boldsymbol{x})=\sum_{n\in\mathbb{Z}^2}\tilde{\boldsymbol{u}}^{(n)}(x_3)e^{\mathrm{i}\boldsymbol{\alpha}^{(n)}\cdot\boldsymbol{r}}\quad\text{in }\tilde{\Omega}.$$

By definition, we have

$$\|\tilde{\boldsymbol{u}}\|^2_{H^{1/2}(\Gamma_h)^3}=\Lambda_1\Lambda_2\sum_{n\in\mathbb{Z}^2}(1+|\boldsymbol{\alpha}^{(n)}|^2)^{1/2}|\tilde{\boldsymbol{u}}^{(n)}(h)|^2$$

and

$$\|\tilde{\boldsymbol{u}}\|^2_{H^1(\Omega)^3}=\Lambda_1\Lambda_2\sum_{n\in\mathbb{Z}^2}\int_a^h(1+|\boldsymbol{\alpha}^{(n)}|^2)|\tilde{\boldsymbol{u}}^{(n)}(x_3)|^2+|\boldsymbol{u}^{(n)'}(x_3)|^2\mathrm{d}x_3.$$

The proof is completed by combining the above estimates and noting $\|\boldsymbol{u}\|^2_{H^{1/2}(\Gamma_h)^3} = \|\tilde{\boldsymbol{u}}\|^2_{H^{1/2}(\Gamma_h)^3}$ and $\|\boldsymbol{u}\|^2_{H^1(\Omega)^3} = \|\tilde{\boldsymbol{u}}\|^2_{H^1(\tilde{\Omega})^3}$. $\qquad\square$

THEOREM 3.1. *Let γ_1 and γ_2 be the constants in the inf-sup condition* (2.18) *and in Lemma 3.3, respectively. If $\hat{K}\gamma_2^2 < \gamma_1$, then the PML variational problem* (3.13) *has a unique weak solution $\boldsymbol{u}^{\mathrm{PML}}$, which satisfies the error estimate*

$$\|\boldsymbol{u} - \boldsymbol{u}^{\mathrm{PML}}\|_\Omega := \sup_{0 \neq \boldsymbol{v} \in H^1_{\mathrm{qp}}(\Omega)^3} \frac{|a(\boldsymbol{u} - \boldsymbol{u}^{\mathrm{PML}}, \boldsymbol{v})|}{\|\boldsymbol{v}\|_{H^1(\Omega)^3}} \leq \gamma_2 \hat{K} \|\boldsymbol{u}^{\mathrm{PML}} - \boldsymbol{u}^{\mathrm{inc}}\|_{L^2(\Gamma_h)^3}, \qquad (3.15)$$

where $\boldsymbol{u}$ is the unique weak solution of the variational problem (2.16).

Proof. It suffices to show the coercivity of the sesquilinear form a^{PML} defined in (3.14) in order to prove the unique solvability of the weak problem (3.13). Using Lemmas 3.2, 3.3 and the assumption $\hat{K}\gamma_2^2 < \gamma_1$, we get for any $\boldsymbol{u}, \boldsymbol{v}$ in $H^1_{\mathrm{qp}}(\Omega)^3$ that

$$\begin{aligned}
|a^{\mathrm{PML}}(\boldsymbol{u}, \boldsymbol{v})| &\geq |a(\boldsymbol{u}, \boldsymbol{v})| - |\langle(\mathscr{T}^{\mathrm{PML}} - \mathscr{T})\boldsymbol{u}, \boldsymbol{v}\rangle_{\Gamma_h}| \\
&\geq |a(\boldsymbol{u}, \boldsymbol{v})| - \hat{K}\gamma_2^2 \|\boldsymbol{u}\|_{H^1(\Omega)^3} \|\boldsymbol{v}\|_{H^1(\Omega)^3} \\
&\geq (\gamma_1 - \hat{K}\gamma_2^2) \|\boldsymbol{u}\|_{H^1(\Omega)^3} \|\boldsymbol{v}\|_{H^1(\Omega)^3}.
\end{aligned}$$

It remains to show the error estimate (3.15). It follows from (2.16)–(2.17) and (3.13)–(3.14) that

$$\begin{aligned}
a(\boldsymbol{u} - \boldsymbol{u}^{\mathrm{PML}}, \boldsymbol{v}) &= a(\boldsymbol{u}, \boldsymbol{v}) - a(\boldsymbol{u}^{\mathrm{PML}}, \boldsymbol{v}) \\
&= \langle \boldsymbol{f}, \boldsymbol{v}\rangle_{\Gamma_h} - \langle \boldsymbol{f}^{\mathrm{PML}}, \boldsymbol{v}\rangle_{\Gamma_h} + a^{\mathrm{PML}}(\boldsymbol{u}^{\mathrm{PML}}, \boldsymbol{v}) - a(\boldsymbol{u}^{\mathrm{PML}}, \boldsymbol{v}) \\
&= \langle(\mathscr{T}^{\mathrm{PML}} - \mathscr{T})\boldsymbol{u}^{\mathrm{inc}}, \boldsymbol{v}\rangle_{\Gamma_h} - \langle(\mathscr{T}^{\mathrm{PML}} - \mathscr{T})\boldsymbol{u}^{\mathrm{PML}}, \boldsymbol{v}\rangle_{\Gamma_h} \\
&= \langle(\mathscr{T} - \mathscr{T}^{\mathrm{PML}})(\boldsymbol{u}^{\mathrm{PML}} - \boldsymbol{u}^{\mathrm{inc}}), \boldsymbol{v}\rangle_{\Gamma_h},
\end{aligned}$$

which completes the proof after using Lemmas 3.2 and 3.3. $\qquad\square$

We remark that the PML approximation error can be reduced exponentially by either enlarging the thickness δ of the PML layers or enlarging the medium parameters $\mathrm{Re}\,\sigma$ and $\mathrm{Im}\,\sigma$.

4. Numerical experiments

In this section, we present two examples to demonstrate the numerical performance of the PML solution. The first-order linear element is used to solve the problem. Our implementation is based on parallel hierarchical grid (PHG) [32], which is a toolbox for developing parallel adaptive finite element programs on unstructured tetrahedral meshes. The linear system resulted from finite element discretization is solved by the Supernodal LU (SuperLU) direct solver, which is a general purpose library for the direct solution of large, sparse, nonsymmetric systems of linear equations.

Example 1. We consider the simplest periodic structure, a straight line, where the exact solution is available. We assume that a plane compressional plane wave $\boldsymbol{u}^{\mathrm{inc}} = \boldsymbol{q} e^{i(\boldsymbol{\alpha}\cdot\boldsymbol{r} - \beta x_3)}$ is incident on the straight line $x_3 = 0$, where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)^\top, \alpha_1 = \kappa_1 \sin\theta_1 \cos\theta_2, \alpha_2 = \kappa_1 \sin\theta_1 \sin\theta_2, \beta = \kappa_1 \cos\theta_1, \boldsymbol{q} = (q_1, q_2, q_3), q_1 = \sin\theta_1 \cos\theta_2, q_2 = \sin\theta_1 \sin\theta_2, q_3 = -\cos\theta_1, \theta_1 \in [0, \pi/2), \theta_2 \in [0, 2\pi]$ are incident angles. It follows from the Navier equation and the Helmholtz decomposition that we obtain the
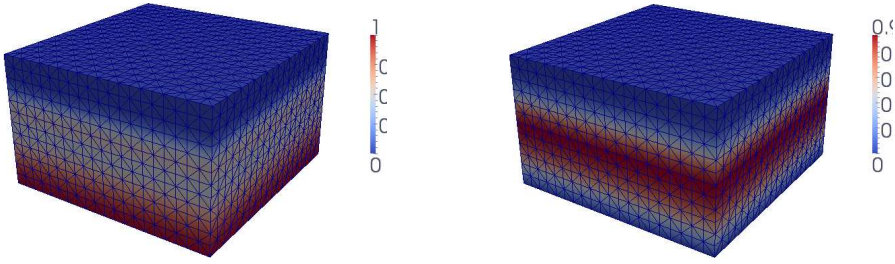
FIG. 4.1. *The mesh and surface plots of the amplitude of the associated solution for the scattered field* $\boldsymbol{v}_h^{\mathrm{PML}}$ *for Example 1: (left) the amplitude of the real part of the solution* $|\mathrm{Re}\boldsymbol{v}_h^{\mathrm{PML}}|$; *(right) the amplitude of the imaginary part of the solution* $|\mathrm{Im}\boldsymbol{v}_h^{\mathrm{PML}}|$.
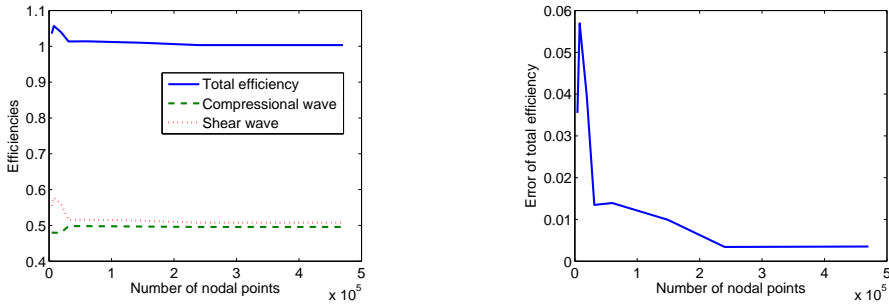
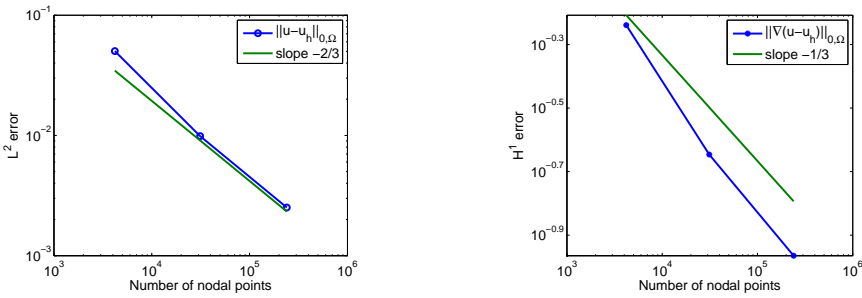FIG. 4.2. *Grating efficiencies and robustness of grating efficiency for Example 1.*
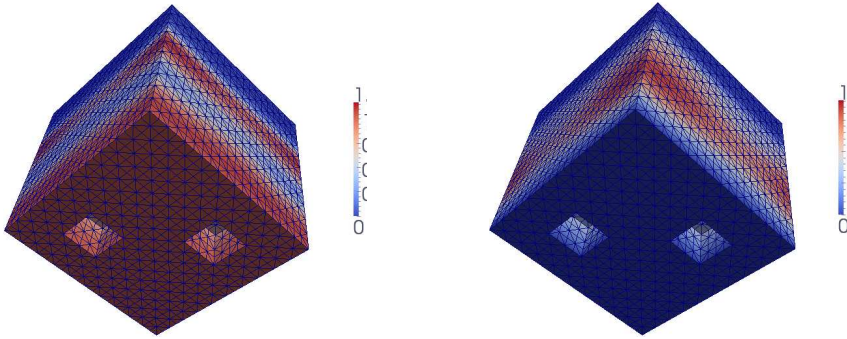

FIG. 4.3. *Quasi-optimality of* L^2- *and* H^1- *error estimates for Example 1.*
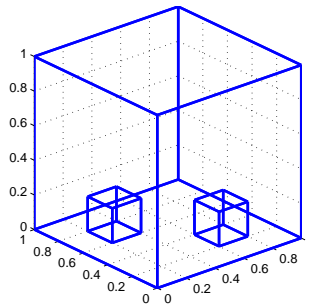
FIG. 4.4. *Geometry of the domain for Example 2.*
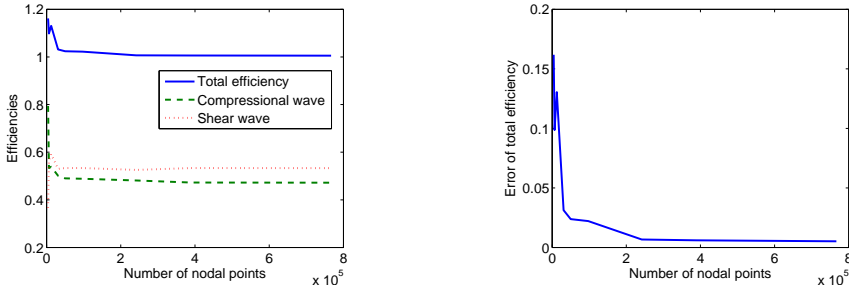
FIG. 4.5. *Grating efficiencies and robustness of grating efficiency for Example 2.*

FIG. 4.6. *The mesh and surface plots of the amplitude of the associated solution for the scattered field $\boldsymbol{v}_h^{\mathrm{PML}}$ for Example 2: (left) the amplitude of the real part of the solution $|\mathrm{Re}\boldsymbol{v}_h^{\mathrm{PML}}|$; (right) the amplitude of the imaginary part of the solution $|\mathrm{Im}\boldsymbol{v}_h^{\mathrm{PML}}|$.*

exact solution:

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{u}^{\mathrm{inc}}(\boldsymbol{x}) + \mathrm{i} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \beta \end{bmatrix} a e^{\mathrm{i}(\boldsymbol{\alpha} \cdot \boldsymbol{r} + \beta x_3)} + \mathrm{i} \begin{bmatrix} \alpha_2 b_3 - \beta_2^{(0)} b_2 \\ \beta_2^{(0)} b_1 - \alpha_1 b_3 \\ \alpha_1 b_2 - \alpha_2 b_1 \end{bmatrix} e^{\mathrm{i}(\boldsymbol{\alpha} \cdot \boldsymbol{r} + \beta_2^{(0)} x_3)},$$

where (a, b_1, b_2, b_3) is the solution of the following linear system:

$$\mathrm{i} \begin{bmatrix} \alpha_1 & 0 & -\beta_2^{(0)} & \alpha_2 \\ \alpha_2 & \beta_2^{(0)} & 0 & -\alpha_1 \\ \beta & -\alpha_2 & \alpha_1 & 0 \\ 0 & \alpha_1 & \alpha_2 & \beta_2^{(0)} \end{bmatrix} \begin{bmatrix} a \\ b_1 \\ b_2 \\ b_3 \end{bmatrix} = - \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ 0 \end{bmatrix}.$$

Solving the above equations via Cramer's rule gives

$$a = \frac{\mathrm{i}}{\chi} \left(\alpha_1 q_1 + \alpha_2 q_2 + \beta_2^{(0)} q_3 \right)$$

$$b_1 = \frac{\mathrm{i}}{\chi} \left(\alpha_1 \alpha_2 (\beta - \beta_2^{(0)}) q_1 / \kappa_2^2 + \left[(\alpha_1)^2 \beta_2^{(0)} + (\alpha_2)^2 \beta + \beta (\beta_2^{(0)})^2 \right] q_2 / \kappa_2^2 - \alpha_2 q_3 \right)$$

$$b_2 = \frac{\mathrm{i}}{\chi} \left(- \left[(\alpha_1)^2 \beta + (\alpha_2)^2 \beta_2^{(0)} + \beta (\beta_2^{(0)})^2 \right] q_1 / \kappa_2^2 - \alpha_1 \alpha_2 (\beta - \beta_2^{(0)}) q_2 / \kappa_2^2 + \alpha_1 q_3 \right)$$

$$b_3 = \frac{i}{\kappa_2^2}\big(\alpha_2 q_1 - \alpha_1 q_2\big),$$

where

$$\chi = (|\boldsymbol{\alpha}|^2 + \beta\beta_2^{(0)}).$$

In our experiment, the parameters are chosen as $\lambda = 1, \mu = 2, \theta_1 = \theta_2 = \pi/6, \omega = 2\pi$. The computational domain $\Omega = (0,1) \times (0,1) \times (0,0.6)$ and the PML domain is $\Omega^{\mathrm{PML}} = (0,1) \times (0,1) \times (0.3,0.6)$, i.e., the thickness of the PML layer is 0.3. We choose $\sigma = 25.39$ and $m = 2$ for the medium property to ensure the constant K is so small that the PML error is negligible compared to the finite element error. The mesh and surface plots of the amplitude of the field $\boldsymbol{v}_h^{\mathrm{PML}}$ are shown in Figure 4.1. The mesh has 57600 tetrahedrons and the total number of degrees of freedom (DoFs) on the mesh is 60000. The grating efficiencies are displayed in Figure 4.2, which verifies the conservation of the energy in Theorem 2.1. Figure 4.3 shows the curves of N_k versus $\|\boldsymbol{u} - \boldsymbol{u}_k\|_{0,\Omega}$, i.e., L^2-error, and $\|\nabla(\boldsymbol{u} - \boldsymbol{u}_k)\|_{0,\Omega}$, i.e., H^1-error, where N_k is the total number of DoFs of the mesh. It indicates that the meshes and the associated numerical complexity are quasi-optimal: $\|\boldsymbol{u} - \boldsymbol{u}_k\|_{0,\Omega} = O(N_k^{-2/3})$ and $\|\nabla(\boldsymbol{u} - \boldsymbol{u}_k)\|_{0,\Omega} = O(N_k^{-1/3})$ are valid asymptotically.

Example 2. This example concerns the scattering of the time-harmonic compressional plane wave $\boldsymbol{u}^{\mathrm{inc}}$ on a flat grating surface with two square bumps, as seen in Figure 4.4. The parameters are chosen as $\lambda = 1, \mu = 2, \theta_1 = \theta_2 = \pi/6$, $\omega = 2\pi$. The computational domain is $\Omega = (0,1) \times (0,1) \times (0,1)$ and the PML domain is $\Omega^{\mathrm{PML}} = (0,1) \times (0,1) \times (0.5,1.0)$, i.e., the thickness of the PML layer is 0.5. Again, we choose $\sigma = 28.57$ and $m = 2$ for the medium property to ensure that the PML error is negligible compared to the finite element error. Since there is no analytical solution for this example, we plot the grating efficiencies against the DoFs in Figure 4.5 to verify the conservation of the energy. Figure 4.6 shows the mesh and the amplitude of the associated solution for the scattered field $\boldsymbol{v}_h^{\mathrm{PML}}$ when the mesh has 49968 nodes.

5. Concluding remarks

We have studied a variational formulation for the elastic wave scattering problem in a biperiodic structure and adopted the PML to truncate the physical domain. The scattering problem is reduced to a boundary value problem by using transparent boundary conditions. We prove that the truncated PML problem has a unique weak solution which converges exponentially to the solution of the original problem by increasing the PML parameters. Numerical results show that the proposed method is effective to solve the scattering problem of elastic waves in biperiodic structures. Although the paper presents the results for the rigid boundary condition, the method is applicable to other boundary conditions or the transmission problem where the structures are penetrable. This work considers only the uniform mesh refinement. We plan to incorporate the adaptive mesh refinement with a posteriori error estimate for the finite element method to handle the problems where the solutions may have singularities. The progress will be reported elsewhere in a future work.

Appendix A. Technical estimates. In this section, we present the proofs for some technical estimates which are used in our analysis for the error estimate between the solutions of the PML problem and the original scattering problem.

PROPOSITION A.1. *For any $n \in \mathbb{Z}^2$, we have $\kappa_1^2 < |\chi^{(n)}| < \kappa_2^2$.*

Proof. Recalling (2.12) and (2.8), we consider three cases:

(i) For $n \in U_1$, $\beta_1^{(n)} = (\kappa_1^2 - |\boldsymbol{\alpha}^{(n)}|^2)^{1/2}$ and $\beta_2^{(n)} = (\kappa_2^2 - |\boldsymbol{\alpha}^{(n)}|^2)^{1/2}$. We have

$$\chi^{(n)} = |\boldsymbol{\alpha}^{(n)}|^2 + \beta_1^{(n)}\beta_2^{(n)} = |\boldsymbol{\alpha}^{(n)}|^2 + (\kappa_1^2 - |\boldsymbol{\alpha}^{(n)}|^2)^{1/2}(\kappa_2^2 - |\boldsymbol{\alpha}^{(n)}|^2)^{1/2}.$$

Noting that $\kappa_1 < \kappa_2$, one can get $\kappa_1^2 < \chi^{(n)} < \kappa_2^2$.

(ii) For $n \in U_2 \setminus U_1$, $\beta_1^{(n)} = i(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_1^2)^{1/2}, \beta_2^{(n)} = (\kappa_2^2 - |\boldsymbol{\alpha}^{(n)}|^2)^{1/2}$. We have

$$\chi^{(n)} = |\boldsymbol{\alpha}^{(n)}|^2 + i(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_1^2)^{1/2}(\kappa_2^2 - |\boldsymbol{\alpha}^{(n)}|^2)^{1/2}$$

and

$$|\chi^{(n)}|^2 = (\kappa_1^2 + \kappa_2^2)|\boldsymbol{\alpha}^{(n)}|^2 - (\kappa_1\kappa_2)^2,$$

which gives $\kappa_1^2 < |\chi^{(n)}| < \kappa_2^2$.

(iii) For $n \notin U_2$, $\beta_1^{(n)} = i(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_1^2)^{1/2}, \beta_2^{(n)} = i(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}$. We have

$$\chi^{(n)} = |\boldsymbol{\alpha}^{(n)}|^2 - (|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_1^2)^{1/2}(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}.$$

Again using the fact $\kappa_1 < \kappa_2$ yields $\kappa_1^2 < \chi^{(n)} < \kappa_2^2$.
Combining the above estimates, we get $\kappa_1^2 < |\chi^{(n)}| < \kappa_2^2$ for any $n \in \mathbb{Z}^2$. □

PROPOSITION A.2. *The function $g_1(t) = t^k / e^{(t^2 - s^2)^{1/2}}$ satisfies $g_1(t) \leq (s^2 + k^2)^{k/2}$ for any $t > s > 0$, $k \in \mathbb{R}^1$.*

Proof. Using the change of variables $\tau = (t^2 - s^2)^{1/2}$, we have

$$\hat{g}_1(\tau) = \frac{(\tau^2 + s^2)^{k/2}}{e^\tau}.$$

Taking the derivative of $\hat{g}_1$ gives

$$\hat{g}_1'(\tau) = -\frac{(\tau^2 - k\tau + s^2)(\tau^2 + s^2)^{\frac{k}{2} - 1}}{e^\tau}.$$

(i) If $s \geq k/2$, then $\hat{g}_1' \leq 0$ for $\tau > 0$. The function $\hat{g}_1$ is decreasing and reaches its maximum at $\tau = 0$, i.e.,

$$g_1(t) \leq \hat{g}_1(0) = s^k.$$

(ii) If $s < k/2$, then $\hat{g}_1' < 0$ for $\tau \in (0, (k - (k^2 - 4s^2)^{1/2})/2) \cup ((k + (k^2 - 4s^2)^{1/2})/2, \infty)$ and $\hat{g}_1 > 0$ for $\tau \in ((k - (k^2 - 4s^2)^{1/2})/2, (k + (k^2 - 4s^2)^{1/2})/2)$. Thus $\hat{g}_1$ reaches its maximum at either $\tau_1 = 0$ or $\tau_2 = (k + (k^2 - 4s^2)^{1/2})/2$. Thus we have

$$g_1(t) = \hat{g}_1(\tau) \leq \max\{\hat{g}_1(\tau_1), \hat{g}_1(\tau_2)\} \leq (s^2 + k^2)^{k/2}.$$

The proof is completed by combining the above estimates. □

PROPOSITION A.3. *For any $n \in \mathbb{Z}^2$, we have $\|M^{(n)} - \hat{M}^{(n)}\|_F \leq \hat{K}$, where $\hat{K} = 11\mu K/\kappa_1^4$.*

Proof. We consider the three cases:

(i) For $n \in U_1$, we have $|\boldsymbol{\alpha}^{(n)}| < \kappa_1, \beta_1^{(n)} = \Delta_1^{(n)} < \kappa_1, \beta_2^{(n)} = \Delta_2^{(n)} < \kappa_2$, and $\Delta_1^{(n)} < \Delta_2^{(n)}$. Using the facts that $\kappa_1 < \kappa_2$, $\Delta_i^{(n)} \geq \Delta_i^-$ for $n \in U_1$, we obtain from (2.12) and Proposition A.1 and A.2 that

$$|\varepsilon^{(n)}| \leq \frac{2e^{-\Delta_2^{(n)}\mathrm{Im}\zeta}}{e^{\Delta_2^{(n)}\mathrm{Im}\zeta} - e^{-\Delta_2^{(n)}\mathrm{Im}\zeta}} \leq \frac{2}{e^{2\Delta_2^{(n)}\mathrm{Im}\zeta} - 1} \leq \frac{2}{e^{\Delta_1^{(n)}\mathrm{Im}\zeta} - 1} \leq \frac{2}{e^{\Delta_1^-\mathrm{Im}\zeta} - 1},$$

$$|\theta^{(n)}| \leq \frac{(e^{-\Delta_2^{(n)}\mathrm{Im}\zeta} + e^{-\Delta_1^{(n)}\mathrm{Im}\zeta})^2}{(1 - e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta})(1 - e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta})} \leq \frac{4e^{-2\Delta_1^-\mathrm{Im}\zeta}}{(1 - e^{-2\Delta_1^-\mathrm{Im}\zeta})^2} \leq \frac{4}{(e^{\frac{1}{2}\Delta_1^-\mathrm{Im}\zeta} - 1)^2},$$

$$|\eta^{(n)}| \leq \frac{e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta} + e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta}}{(1 - e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta})(1 - e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta})} \leq \frac{2e^{-2\Delta_1^-\mathrm{Im}\zeta}}{(1 - e^{-2\Delta_1^-\mathrm{Im}\zeta})^2} \leq \frac{2}{(e^{\frac{1}{2}\Delta_1^-\mathrm{Im}\zeta} - 1)^2},$$

$$|\gamma^{(n)}| \leq \frac{e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta} + e^{-4\Delta_2^{(n)}\mathrm{Im}\zeta}}{(1 - e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta})(1 - e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta})^2} \leq \frac{2e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta}}{(1 - e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta})^3} \leq \frac{2}{(e^{\frac{1}{3}\Delta_1^-\mathrm{Im}\zeta} - 1)^3},$$

$$|\theta^{(n)}(\varepsilon^{(n)} + 1)| \leq \frac{4e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta}}{(1 - e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta})^2} \frac{e^{\Delta_2^{(n)}\mathrm{Im}\zeta} + e^{-\Delta_2^{(n)}\mathrm{Im}\zeta}}{e^{\Delta_2^{(n)}\mathrm{Im}\zeta} - e^{-\Delta_2^{(n)}\mathrm{Im}\zeta}}$$

$$\leq \frac{4e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta}}{(1 - e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta})^2} \frac{2}{1 - e^{-2\Delta_1^{(n)}\mathrm{Im}\zeta}} \leq \frac{8}{(e^{\frac{1}{3}\Delta_1^-\mathrm{Im}\zeta} - 1)^3},$$

$$|\hat{\chi}^{(n)} - \chi^{(n)}| \leq 4\kappa_2^2|\theta^{(n)}| \leq F,$$

$$\max\left\{ |((\alpha_1^{(n)})^2(\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)}\chi^{(n)})\chi^{(n)}\varepsilon^{(n)}|, \right.$$
$$|\alpha_1^{(n)}\alpha_2^{(n)}(\beta_1^{(n)} - \beta_2^{(n)})\chi^{(n)}\varepsilon^{(n)}|,$$
$$|((\alpha_2^{(n)})^2(\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)}\chi^{(n)})\chi^{(n)}\varepsilon^{(n)}|,$$
$$\left. |\beta_2^{(n)}\kappa_2^2\chi^{(n)}\varepsilon^{(n)}| \right\}$$
$$\leq 3\kappa_2^5|\varepsilon^{(n)}| \leq F,$$

$$\max\left\{ |((\alpha_1^{(n)})^2(\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)}\chi^{(n)})(\hat{\chi}^{(n)} - \chi^{(n)})|, \right.$$
$$|\alpha_1^{(n)}\alpha_2^{(n)}(\beta_1^{(n)} - \beta_2^{(n)})(\hat{\chi}^{(n)} - \chi^{(n)})|,$$
$$|((\alpha_2^{(n)})^2(\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)}\chi^{(n)})(\hat{\chi}^{(n)} - \chi^{(n)})|,$$
$$|\alpha_1^{(n)}\beta_2^{(n)}(\beta_1^{(n)} - \beta_2^{(n)})(\hat{\chi}^{(n)} - \chi^{(n)})|,$$
$$\left. |\alpha_2^{(n)}\beta_2^{(n)}(\beta_1^{(n)} - \beta_2^{(n)})(\hat{\chi}^{(n)} - \chi^{(n)})|, |\beta_2^{(n)}\kappa_2^2(\hat{\chi}^{(n)} - \chi^{(n)})| \right\}$$
$$\leq 12\kappa_2^5|\theta^{(n)}| \leq F,$$

$$\max\left\{ |4(\alpha_2^{(n)})^2\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)} + 1)|, |4\alpha_1^{(n)}\alpha_2^{(n)}\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)} + 1)|, \right.$$

$$\left.|4(\alpha_1^{(n)})^2\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)}+1)|\right\} \le 4\kappa_2^5|\theta^{(n)}(\varepsilon^{(n)}+1)| \le F,$$

$$\max\left\{|2(\alpha_1^{(n)})^2\beta_1^{(n)}\kappa_2^2\eta^{(n)}|,|2\alpha_1^{(n)}\alpha_2^{(n)}\beta_1^{(n)}\chi^{(n)}\eta^{(n)}|,\right.$$
$$\left.2(\alpha_2^{(n)})^2\beta_1^{(n)}\kappa_2^2\eta^{(n)}|,|2\beta_1^{(n)}(\beta_2^{(n)})^2\kappa_2^2\eta^{(n)}|\right\} \le 2\kappa_2^5|\eta^{(n)}| \le F,$$

$$|2\alpha_1^{(n)}\alpha_1^{(n)}\beta_1^{(n)}\beta_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)})\gamma^{(n)}| \le 4\kappa_2^5|\gamma^{(n)}| \le F,$$

$$\max\left\{|2\alpha_1^{(n)}\beta_1^{(n)}\beta_2^{(n)}(\kappa_2^2-2(\beta_2^{(n)})^2)\theta^{(n)}|,\right.$$
$$\left.|2\alpha_2^{(n)}\beta_1^{(n)}\beta_2^{(n)}(\kappa_2^2-2(\beta_2^{(n)})^2)\theta^{(n)}|\right\} \le 6\kappa_2^5|\theta^{(n)}| \le F,$$

(ii) For $n\in U_2\setminus U_1$, we have $|\boldsymbol{\alpha}^{(n)}|<\kappa_2,\beta_1^{(n)}=\mathrm{i}\Delta_1^{(n)},\beta_2^{(n)}=\Delta_2^{(n)}<\kappa_2,\Delta_1^{(n)}<(\kappa_2^2-\kappa_1^2)^{1/2}<\kappa_2$. Using the facts that $\Delta_1^{(n)}\ge\Delta_1^+,\Delta_2^{(n)}\ge\Delta_2^-$ for $n\in U_2\setminus U_1$, we get from Proposition A.1 and A.2 that

$$|\varepsilon^{(n)}|=\frac{2e^{-\Delta_2^{(n)}\mathrm{Im}\zeta}}{e^{\Delta_2^{(n)}\mathrm{Im}\zeta}-e^{-\Delta_2^{(n)}\mathrm{Im}\zeta}}\le\frac{2}{e^{2\Delta_2^{(n)}\mathrm{Im}\zeta}-1}\le\frac{2}{e^{2\Delta_2^-\mathrm{Im}\zeta}-1}\le\frac{2}{e^{\Delta_2^-\mathrm{Im}\zeta}-1},$$

$$|\theta^{(n)}|\le\frac{(e^{-\Delta_2^{(n)}\mathrm{Im}\zeta}+e^{-\Delta_1^{(n)}\mathrm{Re}\zeta})^2}{(1-e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta})(1-e^{-2\Delta_{2,j}^{(n)}\mathrm{Im}\zeta})}\le\frac{(e^{-\Delta_2^-\mathrm{Im}\zeta}+e^{-\Delta_1^+\mathrm{Re}\zeta})^2}{(1-e^{-2\Delta_1^+\mathrm{Re}\zeta})(1-e^{-2\Delta_2^-\mathrm{Im}\zeta})},$$

$$|\eta^{(n)}|\le\frac{e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta}+e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta}}{(1-e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta})(1-e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta})}\le\frac{e^{-2\Delta_2^-\mathrm{Im}\zeta}+e^{-2\Delta_1^+\mathrm{Re}\zeta}}{(1-e^{-2\Delta_1^+\mathrm{Re}\zeta})(1-e^{-2\Delta_2^-\mathrm{Im}\zeta})}$$
$$\le\frac{(e^{-\Delta_2^-\mathrm{Im}\zeta}+e^{-\Delta_1^+\mathrm{Re}\zeta})^2}{(1-e^{-2\Delta_1^+\mathrm{Re}\zeta})(1-e^{-2\Delta_2^-\mathrm{Im}\zeta})},$$

$$|\gamma^{(n)}|\le\frac{e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta}+e^{-4\Delta_2^{(n)}\mathrm{Im}\zeta}}{(1-e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta})(1-e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta})^2}\le\frac{e^{-2\Delta_1^+\mathrm{Re}\zeta}+e^{-4\Delta_2^-\mathrm{Im}\zeta}}{(1-e^{-2\Delta_1^+\mathrm{Re}\zeta})(1-e^{-2\Delta_2^-\mathrm{Im}\zeta})^2}$$
$$\le\frac{(e^{-\Delta_2^-\mathrm{Im}\zeta}+e^{-\Delta_1^+\mathrm{Re}\zeta})^2}{(1-e^{-2\Delta_1^+\mathrm{Re}\zeta})(1-e^{-2\Delta_2^-\mathrm{Im}\zeta})},$$

$$|\theta^{(n)}(\varepsilon^{(n)}+1)|\le\frac{(e^{-\Delta_2^{(n)}\mathrm{Im}\zeta}+e^{-\Delta_1^{(n)}\mathrm{Re}\zeta})^2}{(1-e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta})(1-e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta})}\frac{2}{1-e^{-2\Delta_2^{(n)}\mathrm{Im}\zeta}}$$
$$\le\frac{2(e^{-\Delta_2^-\mathrm{Im}\zeta}+e^{-\Delta_1^+\mathrm{Re}\zeta})^2}{(1-e^{-2\Delta_1^+\mathrm{Re}\zeta})(1-e^{-2\Delta_2^-\mathrm{Im}\zeta})^2},$$

$$|\hat\chi^{(n)}-\chi^{(n)}|\le\frac{4\kappa_2^4}{\kappa_1^2}|\theta^{(n)}|\le F,$$

$$\max\left\{|((\alpha_1^{(n)})^2(\beta_1^{(n)}-\beta_2^{(n)})+\beta_2^{(n)}\chi^{(n)})\chi^{(n)}\varepsilon^{(n)}|,\right.$$
$$|\alpha_1^{(n)}\alpha_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)})\chi^{(n)}\varepsilon^{(n)}|,$$

$$\big|\big((\alpha_2^{(n)})^2(\beta_1^{(n)}-\beta_2^{(n)})+\beta_2^{(n)}\chi^{(n)}\big)\chi^{(n)}\varepsilon^{(n)}\big|,\big|\beta_2^{(n)}\kappa_2^2\chi^{(n)}\varepsilon^{(n)}\big|\Big\}$$
$$\leq 3\kappa_2^5|\varepsilon^{(n)}|\leq F,$$

$$\max\Big\{\big|\big((\alpha_1^{(n)})^2(\beta_1^{(n)}-\beta_2^{(n)})+\beta_2^{(n)}\chi^{(n)}\big)(\hat{\chi}^{(n)}-\chi^{(n)})\big|,$$
$$\big|\alpha_1^{(n)}\alpha_2^{(n)}(\beta_1^{(n)}-\beta_{2,j}^{(n)})(\hat{\chi}^{(n)}-\chi^{(n)})\big|,$$
$$\big|\big((\alpha_2^{(n)})^2(\beta_1^{(n)}-\beta_2^{(n)})+\beta_2^{(n)}\chi^{(n)}\big)(\hat{\chi}^{(n)}-\chi^{(n)})\big|,$$
$$\big|\alpha_1^{(n)}\beta_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)})(\hat{\chi}^{(n)}-\chi^{(n)})\big|,$$
$$\big|\alpha_2^{(n)}\beta_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)})(\hat{\chi}^{(n)}-\chi^{(n)})\big|,\big|\beta_2^{(n)}\kappa_2^2(\hat{\chi}^{(n)}-\chi^{(n)})\big|\Big\}$$
$$\leq\frac{12\kappa_2^7}{\kappa_1^2}|\theta^{(n)}|\leq F,$$

$$\max\Big\{\big|4(\alpha_2^{(n)})^2\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)}+1)\big|,\big|4\alpha_1^{(n)}\alpha_2^{(n)}\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)}+1)\big|,$$
$$\big|4(\alpha_1^{(n)})^2\beta_1^{(n)}(\beta_2^{(n)})^2\theta^{(n)}(\varepsilon^{(n)}+1)\big|\Big\}\leq 4\kappa_2^5|\theta^{(n)}(\varepsilon^{(n)}+1)|$$
$$\leq F,$$

$$\max\Big\{\big|2(\alpha_1^{(n)})^2\beta_1^{(n)}\kappa_2^2\eta^{(n)}\big|,\big|2\alpha_1^{(n)}\alpha_2^{(n)}\beta_1^{(n)}\chi^{(n)}\eta^{(n)}\big|,$$
$$\big|2(\alpha_2^{(n)})^2\beta_1^{(n)}\kappa_2^2\eta^{(n)}\big|,\big|2\beta_1^{(n)}(\beta_2^{(n)})^2\kappa_2^2\eta^{(n)}\big|\Big\}$$
$$\leq 2\kappa_2^5|\eta^{(n)}|\leq F,$$

$$\big|2\alpha_1^{(n)}\alpha_2^{(n)}\beta_1^{(n)}\beta_2^{(n)}(\beta_1^{(n)}-\beta_2^{(n)})\gamma^{(n)}\big|\leq 4\kappa_2^5|\gamma^{(n)}|\leq F,$$

$$\max\Big\{\big|2\alpha_1^{(n)}\beta_1^{(n)}\beta_2^{(n)}(\kappa_2^2-2(\beta_2^{(n)})^2)\theta^{(n)}\big|,\big|2\alpha_2^{(n)}\beta_1^{(n)}\beta_2^{(n)}(\kappa_2^2-2(\beta_2^{(n)})^2)\theta^{(n)}\big|\Big\}$$
$$\leq 6\kappa_2^5|\theta^{(n)}|\leq F.$$

(iii) For $n\notin U_2$, we have $\kappa_2<|\boldsymbol{\alpha}^{(n)}|,\beta_1^{(n)}=\mathrm{i}\Delta_1^{(n)},\beta_2^{(n)}=\mathrm{i}\Delta_2^{(n)}$, and $\Delta_2^{(n)}<\Delta_1^{(n)}<|\boldsymbol{\alpha}^{(n)}|$. Noting $\mathrm{Re}\zeta\geq 1$, we obtain from Proposition A.2 that

$$|\varepsilon^{(n)}|\leq\frac{2e^{-\Delta_2^{(n)}\mathrm{Re}\zeta}}{e^{\Delta_2^{(n)}\mathrm{Re}\zeta}-e^{-\Delta_2^{(n)}\mathrm{Re}\zeta}}\leq\frac{2}{e^{\Delta_2^{(n)}\mathrm{Re}\zeta}}\frac{1}{e^{\Delta_2^{(n)}\mathrm{Re}\zeta}-1}$$
$$\leq\frac{2}{e^{(|\boldsymbol{\alpha}^{(n)}|^2-\kappa_2^2)^{1/2}}}\frac{1}{e^{\Delta_2^+\mathrm{Re}\zeta}-1},$$

$$|\theta^{(n)}|\leq\frac{(e^{-\Delta_2^{(n)}\mathrm{Re}\zeta}+e^{-\Delta_1^{(n)}\mathrm{Re}\zeta})^2}{(1-e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta})(1-e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})}\leq\frac{4e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1-e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^2}$$
$$\leq\frac{4}{e^{\Delta_2^{(n)}\mathrm{Re}\zeta}}\frac{e^{-\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1-e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^2}\leq\frac{4}{e^{\Delta_2^{(n)}\mathrm{Re}\zeta}}\frac{1}{(e^{\frac{1}{2}\Delta_2^{(n)}\mathrm{Re}\zeta}-1)^2}$$

$$\le \frac{4}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{1}{(e^{\frac{1}{2}\Delta_2^+ \mathrm{Re}\zeta} - 1)^2},$$

$$|\eta^{(n)}| \le \frac{e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta} + e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta}}{(1 - e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta})(1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})} \le \frac{2e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^2}$$

$$\le \frac{2}{e^{\Delta_2^{(n)}\mathrm{Re}\zeta}} \frac{e^{-\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^2} \le \frac{2}{e^{\Delta_2^{(n)}}} \frac{1}{(e^{\frac{1}{2}\Delta_2^{(n)}\mathrm{Re}\zeta} - 1)^2}$$

$$\le \frac{2}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{1}{(e^{\frac{1}{2}\Delta_2^+ \mathrm{Re}\zeta} - 1)^2},$$

$$|\gamma^{(n)}| \le \frac{e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta} + e^{-4\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1 - e^{-2\Delta_1^{(n)}\mathrm{Re}\zeta})(1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^2} \le \frac{2e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^3}$$

$$\le \frac{2}{e^{\Delta_2^{(n)}\mathrm{Re}\zeta}} \frac{e^{-\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^3} \le \frac{2}{e^{\Delta_2^{(n)}}} \frac{1}{(e^{\frac{1}{3}\Delta_2^{(n)}\mathrm{Re}\zeta} - 1)^3}$$

$$\le \frac{2}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{1}{(e^{\frac{1}{3}\Delta_2^+ \mathrm{Re}\zeta} - 1)^3},$$

$$|\theta^{(n)}(\varepsilon^{(n)} + 1)| \le \frac{4e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^2} \frac{2}{1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta}} \le \frac{8}{e^{\Delta_2^{(n)}\mathrm{Re}\zeta}} \frac{e^{-\Delta_2^{(n)}\mathrm{Re}\zeta}}{(1 - e^{-2\Delta_2^{(n)}\mathrm{Re}\zeta})^3}$$

$$\le \frac{8}{e^{\Delta_2^{(n)}}} \frac{1}{(e^{\frac{1}{3}\Delta_2^{(n)}\mathrm{Re}\zeta} - 1)^3} \le \frac{8}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{1}{(e^{\frac{1}{3}\Delta_2^+ \mathrm{Re}\zeta} - 1)^3},$$

$$|\hat{\chi}^{(n)} - \chi^{(n)}| \le \frac{4|\boldsymbol{\alpha}^{(n)}|^4 |\theta^{(n)}|}{\kappa_1^2} \le \frac{16}{\kappa_1^2} \frac{|\boldsymbol{\alpha}^{(n)}|^4}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{1}{(e^{\frac{1}{2}\Delta_2^+ \mathrm{Re}\zeta} - 1)^2}$$

$$\le \frac{16(\kappa_2^2 + 16)^2}{\kappa_1^2 (e^{\frac{1}{2}\Delta_2^+ \mathrm{Re}\zeta} - 1)^2} \le F,$$

$$\max \Big\{ |\big((\alpha_1^{(n)})^2 (\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)} \chi^{(n)}\big) \chi^{(n)} \varepsilon^{(n)}|,$$

$$|\alpha_1^{(n)} \alpha_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) \chi^{(n)} \varepsilon^{(n)}|,$$

$$|\big((\alpha_2^{(n)})^2 (\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)} \chi^{(n)}\big) \chi^{(n)} \varepsilon^{(n)}|, |\beta_2^{(n)} \kappa_2^2 \chi^{(n)} \varepsilon^{(n)}| \Big\}$$

$$\le 3\kappa_2^2 |\boldsymbol{\alpha}^{(n)}|^3 |\varepsilon^{(n)}| \le \frac{|\boldsymbol{\alpha}^{(n)}|^3}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{6\kappa_2^2}{e^{\Delta_2^+ \mathrm{Re}\zeta} - 1} \le \frac{6\kappa_2^2 (\kappa_2^2 + 9)^{3/2}}{e^{\Delta_2^+ \mathrm{Re}\zeta} - 1} \le F,$$

$$\max \Big\{ |\big((\alpha_1^{(n)})^2 (\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)} \chi^{(n)}\big) (\hat{\chi}^{(n)} - \chi^{(n)})|,$$

$$|\alpha_1^{(n)} \alpha_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) (\hat{\chi}^{(n)} - \chi^{(n)})|,$$

$$|\big((\alpha_2^{(n)})^2 (\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)} \chi^{(n)}\big) (\hat{\chi}^{(n)} - \chi^{(n)})|,$$

$$|\alpha_1^{(n)} \beta_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) (\hat{\chi}^{(n)} - \chi^{(n)})|,$$

$$|\alpha_2^{(n)} \beta_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) (\hat{\chi}^{(n)} - \chi^{(n)})|, |\beta_2^{(n)} \kappa_2^2 (\hat{\chi}^{(n)} - \chi^{(n)})| \Big\}$$

$$\le \frac{12|\boldsymbol{\alpha}^{(n)}|^7 |\theta^{(n)}|}{\kappa_1^2} \le \frac{48}{\kappa_1^2} \frac{|\boldsymbol{\alpha}^{(n)}|^7}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{1}{(e^{\frac{1}{2}\Delta_2^+ \mathrm{Re}\zeta} - 1)^2}$$

$$\leq \frac{48(\kappa_2^2 + 49)^{7/2}}{\kappa_1^2 (e^{\frac{1}{2}\Delta_2^+ \operatorname{Re}\zeta} - 1)^2} \leq F,$$

$$\max\left\{ |4(\alpha_2^{(n)})^2 \beta_1^{(n)} (\beta_2^{(n)})^2 \theta^{(n)} (\varepsilon^{(n)} + 1)|, |4\alpha_1^{(n)} \alpha_2^{(n)} \beta_1^{(n)} (\beta_2^{(n)})^2 \theta^{(n)} (\varepsilon^{(n)} + 1)|, \right.$$
$$\left. |4(\alpha_1^{(n)})^2 \beta_1^{(n)} (\beta_2^{(n)})^2 \theta^{(n)} (\varepsilon^{(n)} + 1)| \right\}$$

$$\leq 4|\boldsymbol{\alpha}^{(n)}|^5 |\theta^{(n)} (\varepsilon^{(n)} + 1)| \leq \frac{32|\boldsymbol{\alpha}^{(n)}|^5}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - (\kappa_2^2)^{1/2})}} \frac{1}{(e^{\frac{1}{3}\Delta_2^+ \operatorname{Re}\zeta} - 1)^3}$$

$$\leq \frac{32(\kappa_2^2 + 25)^{5/2}}{(e^{\frac{1}{3}\Delta_2^+ \operatorname{Re}\zeta} - 1)^3} \leq F,$$

$$\max\left\{ |2(\alpha_1^{(n)})^2 \beta_1^{(n)} \kappa_2^2 \eta^{(n)}|, |2\alpha_1^{(n)} \alpha_2^{(n)} \beta_1^{(n)} \chi^{(n)} \eta^{(n)}|, \right.$$
$$\left. |2(\alpha_2^{(n)})^2 \beta_1^{(n)} \kappa_2^2 \eta^{(n)}|, |2\beta_1^{(n)} (\beta_2^{(n)})^2 \kappa_2^2 \eta^{(n)}| \right\}$$

$$\leq 2\kappa_2^2 |\boldsymbol{\alpha}^{(n)}|^3 |\eta^{(n)}| \leq 4\kappa_2^2 \frac{|\boldsymbol{\alpha}^{(n)}|^3}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{1}{(e^{\frac{1}{2}\Delta_2^+ \operatorname{Re}\zeta} - 1)^2}$$

$$\leq \frac{4\kappa_2^2 (\kappa_2^2 + 9)^{3/2}}{(e^{\frac{1}{2}\Delta_2^+ \operatorname{Re}\zeta} - 1)^2} \leq F,$$

$$|2\alpha_1^{(n)} \alpha_2^{(n)} \beta_1^{(n)} \beta_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) \gamma^{(n)}| \leq 4|\boldsymbol{\alpha}^{(n)}|^5 |\gamma^{(n)}|$$

$$\leq \frac{8|\boldsymbol{\alpha}^{(n)}|^5}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{1}{(e^{\frac{1}{3}\Delta_2^+ \operatorname{Re}\zeta} - 1)^3} \leq \frac{8(\kappa_2^2 + 25)^{5/2}}{(e^{\frac{1}{3}\Delta_2^+ \operatorname{Re}\zeta} - 1)^3} \leq F,$$

$$\max\left\{ |2\alpha_1^{(n)} \beta_1^{(n)} \beta_2^{(n)} (\kappa_2^2 - 2(\beta_2^{(n)})^2) \theta^{(n)}|, |2\alpha_2^{(n)} \beta_1^{(n)} \beta_2^{(n)} (\kappa_2^2 - 2(\beta_2^{(n)})^2) \theta^{(n)}| \right\}$$

$$\leq 6|\boldsymbol{\alpha}^{(n)}|^5 |\theta^{(n)}| \leq \frac{|\boldsymbol{\alpha}^{(n)}|^5}{e^{(|\boldsymbol{\alpha}^{(n)}|^2 - \kappa_2^2)^{1/2}}} \frac{24}{(e^{\frac{1}{2}\Delta_2^+ \operatorname{Re}\zeta} - 1)^2} \leq \frac{24((\kappa_2)^2 + 25)^{\frac{5}{2}}}{(e^{\frac{1}{2}\Delta_2^+ \operatorname{Re}\zeta} - 1)^2} \leq F,$$

where we have used the estimate for g_3 and the facts that $\Delta_i^{(n)} \geq \Delta_i^+$ for $n \notin U_2$.

It follows from Proposition A.1 and the estimate $|\hat{\chi}^{(n)} - \chi^{(n)}| \leq K$ that $\kappa_1^2 - K \leq |\hat{\chi}^{(n)}| \leq \kappa_2^2 + K$. Again, we may choose some proper PML parameters σ and δ such that $K \leq \kappa_1^2/2$, which gives $|\hat{\chi}^{(n)}| \geq \kappa_1^2/2$. Using the matrix Frobenius norm and combining all the above estimates, we get

$$\|M^{(n)} - \hat{M}^{(n)}\|_F^2 \leq \frac{4\mu^2}{\kappa_1^8} \left(|((\alpha_1^{(n)})^2 (\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)} \chi^{(n)}) \chi^{(n)} \varepsilon^{(n)}|^2 + |2(\alpha_1^{(n)})^2 \beta_1^{(n)} \kappa_2^2 \eta^{(n)}|^2 \right.$$

$$+ |((\alpha_1^{(n)})^2 (\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)} \chi^{(n)}) (\hat{\chi}^{(n)} - \chi^{(n)})|^2 + |4(\alpha_2^{(n)})^2 \beta_1^{(n)} (\beta_2^{(n)})^2 \theta^{(n)} (\varepsilon^{(n)} + 1)|^2$$

$$+ 2|\alpha_1^{(n)} \alpha_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) \chi^{(n)} \varepsilon^{(n)}|^2 + 2|\alpha_1^{(n)} \alpha_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) (\hat{\chi}^{(n)} - \chi^{(n)})|^2$$

$$+ 2|2\alpha_1^{(n)} \alpha_2^{(n)} \beta_1^{(n)} \chi^{(n)} \eta^{(n)}|^2 + 2|4\alpha_1^{(n)} \alpha_2^{(n)} \beta_1^{(n)} (\beta_2^{(n)})^2 \theta^{(n)} (\varepsilon^{(n)} + 1)|^2 + |2(\alpha_2^{(n)})^2 \beta_1^{(n)} \kappa_2^2 \eta^{(n)}|^2$$

$$+ 2|2\alpha_1^{(n)} \alpha_2^{(n)} \beta_1^{(n)} \beta_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) \gamma^{(n)}|^2 + 2|\alpha_1^{(n)} \beta_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) (\hat{\chi}^{(n)} - \chi^{(n)})|^2$$

$$+ 2|2\alpha_1^{(n)} \beta_1^{(n)} \beta_2^{(n)} (\kappa_2^2 - 2(\beta_2^{(n)})^2) \theta^{(n)}|^2 + |((\alpha_2^{(n)})^2 (\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)} \chi^{(n)}) \chi^{(n)} \varepsilon^{(n)}|^2$$

$$+ |((\alpha_2^{(n)})^2 (\beta_1^{(n)} - \beta_2^{(n)}) + \beta_2^{(n)} \chi^{(n)}) (\hat{\chi}^{(n)} - \chi^{(n)})|^2 + |4(\alpha_1^{(n)})^2 \beta_1^{(n)} (\beta_2^{(n)})^2 \theta^{(n)} (\varepsilon^{(n)} + 1)|^2$$

$$+ 2|\alpha_2^{(n)} \beta_2^{(n)} (\beta_1^{(n)} - \beta_2^{(n)}) (\hat{\chi}^{(n)} - \chi^{(n)})|^2 + 2|2\alpha_2^{(n)} \beta_1^{(n)} \beta_2^{(n)} (\kappa_2^2 - 2(\beta_2^{(n)})^2) \theta^{(n)}|^2$$

$$+|\beta_2^{(n)2}\kappa_2^2\chi^{(n)}\varepsilon^{(n)}|^2+|\beta_2^{(n)2}\kappa_2^2(\hat{\chi}^{(n)}-\chi^{(n)})|^2+|2\beta_1^{(n)}(\beta_2^{(n)})^2\kappa_2^2\eta^{(n)}|^2\big) \leq \frac{116\mu^2}{\kappa_1^8}K^2,$$

which completes the proof. □

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